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IB DIPLOMA CHEMISTRY · FIRST ASSESSMENT 2025

Reactivity 2.1 Limiting Reactant, Yield and Atom Economy

Booklet 2 · Understandings 2.1.3 – 2.1.5

Which reactant runs out first, how much product you should get, how much you actually get, and how much of what you start with ends up as waste

Complete revision notes, 16 worked examples, model answers & 38 practice questions · Standard Level & Higher Level

How the level tags work in this booklet

SL + HL Every understanding in Reactivity 2.1 is common to both levels, so the whole booklet is core material.

HL Reactivity 2.1 has no HL-only content. The ideal gas equation (Structure 1.5) appears in one question and is an SL + HL skill. ★ marks harder, multi-step examples and questions. All the calculation skills of Booklet 1 are assumed.

Inside this booklet

1. What the syllabus actually asks of you
2. 2.1.3 — Limiting and excess reactants
3. 2.1.3 — Theoretical yield
4. 2.1.4 — Percentage yield
5. 2.1.5 — Atom economy
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1 What the syllabus actually asks of you

Booklet 1 assumed that every reactant was present in exactly the right amount and that every reaction went to completion. Real reactions do neither. One reactant usually runs out first and limits how much product can form; some product is always lost; and even a perfect reaction may turn much of its starting material into unwanted by-products. Understandings 2.1.3 to 2.1.5 give you three ways to measure this: the **limiting reactant**, the **percentage yield** and the **atom economy**. They are tested as calculations in Paper 1A and 1B and as multi-step problems with "explain" and "evaluate" parts in Paper 2, often set in an industrial or Green Chemistry context.

Understanding	What it says	What you must be able to do	Level
2.1.3 Limiting reactant	The limiting reactant determines the theoretical yield.	Identify the limiting and excess reactants from given data. Distinguish between the theoretical yield and the experimental yield.	SL+HL
2.1.4 Percentage yield	The percentage yield is calculated from the ratio of experimental yield to theoretical yield.	Solve problems involving reacting quantities, limiting and excess reactants, theoretical, experimental and percentage yields.	SL+HL
2.1.5 Atom economy	The atom economy is a measure of efficiency in Green Chemistry.	Calculate the atom economy from the stoichiometry of a reaction. **Include discussion of the inverse relationship between atom economy and wastage in industrial processes.** The equation for the atom economy is given in the data booklet.	SL+HL

Understandings 2.1.1 (chemical equations) and 2.1.2 (reacting masses, volumes and concentrations) are covered in Booklet 1.

Linking questions and connections for 2.1.3 – 2.1.5

- **Tool 1, Inquiry 1, 2, 3:** what errors may cause the experimental yield to be (i) higher and (ii) lower than the theoretical yield? → section 3.2
- **Structure 2.4, Reactivity 2.2:** the atom economy and the percentage yield both give important information about the "efficiency" of a chemical process. What other factors should be considered in this assessment? → section 5.4
- **Reactivity 2.3:** reversible reactions reach equilibrium, so they can never give a 100 % yield → sections 3.2 and 4
- **Reactivity 1.3:** bioethanol by fermentation versus ethanol by hydration of ethene → worked example 14
- **Booklet 1:** every calculation here starts with moles from m/M, V/V_m or cV.

What the data booklet does and does not give you

It gives you: the atom economy equation, relative atomic masses to two decimal places, the molar volume at STP and the gas constant.

It does not give you: the percentage yield equation; any method for finding the limiting reactant; or which product in an equation is the "desired" one. Learn the yield equation, and always read the question to see which product is wanted.

2 Reactivity 2.1.3 — Limiting and excess reactants SL + HL

2.1 Which reactant runs out first?

A sandwich needs two slices of bread and one slice of cheese. With ten slices of bread and three slices of cheese you can make only three sandwiches. The cheese runs out first and *limits* the number you can make; four slices of bread are left over, in *excess*. Reactions behave in exactly the same way, except that the "recipe" is the mole ratio in the balanced equation.

Definitions to learn

The **limiting reactant** is the reactant that is completely used up first. It determines the maximum amount of product that can form.

A reactant **in excess** is present in more than the amount needed to react with the limiting reactant, so some of it is left over at the end.

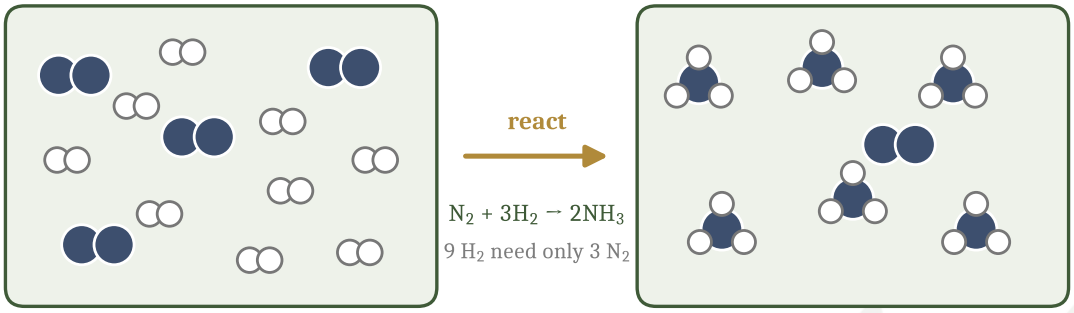


Figure 1 — Hydrogen is the limiting reactant. Nine H_2 molecules can react with only three N_2 molecules, giving six NH_3. One N_2 molecule is in excess and is left over.

The limiting reactant depends on the **mole ratio**, not on which reactant has the smaller mass or the smaller number of moles. Always convert to moles first.

Method — three ways to find the limiting reactant

1. **Divide by the coefficient.** For each reactant, calculate $n \div$ (its coefficient in the equation). The reactant with the **smallest** value is limiting. This is usually the quickest method.
2. **Compare with what is needed.** Use the mole ratio to calculate how much of reactant B is needed to react with all of A. If less B is available than that, B is limiting; if more, A is limiting.
3. **Product test.** Calculate the amount of product that each reactant could make on its own. The reactant that gives the **smaller** amount of product is limiting, and that smaller amount is the theoretical yield.

Then always calculate the product from the limiting reactant, never from the excess one.

Worked example 1 — the limiting reactant from amounts in moles

Q. 0.50 mol of nitrogen is mixed with 1.20 mol of hydrogen: $N_2(g) + 3H_2(g) \rightarrow 2NH_3(g)$. Identify the limiting reactant, and calculate the maximum amount of ammonia and the amount of the excess reactant left over.

Divide by the coefficient: N_2: 0.50 / 1 = 0.50 · H_2: 1.20 / 3 = 0.40 → the smaller value is H_2: **H_2 is limiting**

Check by comparison: 0.50 mol N_2 would need 3 × 0.50 = 1.50 mol H_2, but only 1.20 mol is available.

$n(NH_3)$ = 1.20 × 2/3 = **0.800 mol**; N_2 used = 1.20/3 = 0.400 mol, so N_2 left = 0.50 − 0.40 = **0.10 mol**

There are fewer moles of N_2 than of H_2, yet N_2 is in excess. A smaller number of moles does not mean limiting.

Worked example 2 — the limiting reactant from masses

Q. 5.40 g of aluminium is heated in 14.2 g of chlorine: $2Al(s) + 3Cl_2(g) \rightarrow 2AlCl_3(s)$. Calculate the mass of aluminium chloride formed and the mass of the excess reactant left over.

$n(Al)$ = 5.40 / 26.98 = 0.2001 mol; $n(Cl_2)$ = 14.2 / 70.90 = 0.2003 mol

÷ coefficient: Al 0.2001/2 = 0.1001; Cl_2 0.2003/3 = 0.0668 → **Cl_2 is limiting**

$n(AlCl_3)$ = 0.2003 × 2/3 = 0.1335 mol; $M(AlCl_3)$ = 133.33 g mol^{-1}; m = 0.1335 × 133.33 = **17.8 g**

Al used = 0.1335 mol; Al left = 0.2001 − 0.1335 = 0.0666 mol × 26.98 = **1.80 g**

Check with conservation of mass: 5.40 + 14.2 = 19.6 g at the start, and 17.8 + 1.80 = 19.6 g at the end.

Worked example 3 — the product test

Q. 10.0 g of ammonia is passed over 50.0 g of heated copper(II) oxide: $2NH_3(g) + 3CuO(s) \rightarrow N_2(g) + 3Cu(s) + 3H_2O(g)$. Calculate the maximum mass of copper produced.

$n(NH_3)$ = 10.0 / 17.04 = 0.5869 mol; $n(CuO)$ = 50.0 / 79.55 = 0.6285 mol

Cu that NH_3 could make: 0.5869 × 3/2 = 0.8803 mol; Cu that CuO could make: 0.6285 × 3/3 = 0.6285 mol

CuO gives less product, so **CuO is limiting**: $m(Cu)$ = 0.6285 × 63.55 = **39.9 g**

Worked example 4 — limiting reactants with gas volumes

Q. All volumes are measured at the same temperature and pressure, with water as a liquid. (a) 60 cm^3 of hydrogen is exploded with 40 cm^3 of oxygen. (b) 30 cm^3 of carbon monoxide is burned in 20 cm^3 of oxygen. Find the limiting reactant and the final volume of gas in each case.

(a) $2H_2(g) + O_2(g) \rightarrow 2H_2O(l)$: 60 cm^3 H_2 needs 30 cm^3 O_2, and 40 cm^3 is available → **H_2 is limiting**; 10 cm^3 of O_2 is left; water is liquid, so the final volume = **10 cm^3**

(b) $2CO(g) + O_2(g) \rightarrow 2CO_2(g)$: 30 cm^3 CO needs 15 cm^3 O_2 → **CO is limiting**; final gas = 30 cm^3 CO_2 + 5 cm^3 O_2 = **35 cm^3**

By Avogadro's law, volume ratios are mole ratios for gases, so no conversion to moles is needed.

Worked example 5 — limiting reactants in solution

Q. (a) 2.00 g of magnesium is added to 50.0 cm^3 of 2.00 mol dm^{-3} hydrochloric acid. Calculate the volume of hydrogen formed at STP and the mass of magnesium left over. (b) 25.0 cm^3 of 0.200 mol dm^{-3} $AgNO_3(aq)$ is mixed with 20.0 cm^3 of 0.150 mol dm^{-3} $CaCl_2(aq)$. Calculate the mass of silver chloride precipitated.

(a) $Mg(s) + 2HCl(aq) \rightarrow MgCl_2(aq) + H_2(g)$ · $n(Mg) = 2.00/24.31 = 0.08227$ mol; $n(HCl) = 2.00 \times 0.0500 = 0.100$ mol

0.08227 mol Mg would need 0.1645 mol HCl, but only 0.100 mol is present → **HCl is limiting**

$n(H_2) = 0.100/2 = 0.0500$ mol; $V = 0.0500 \times 22.7 =$ **1.14 dm^3**; Mg left = 0.08227 − 0.0500 = 0.03227 mol × 24.31 = **0.784 g**

(b) $Ag^+(aq) + Cl^-(aq) \rightarrow AgCl(s)$ · $n(Ag^+) = 0.200 \times 0.0250 = 5.00 \times 10^{-3}$ mol; $n(Cl^-) = 2 \times 0.150 \times 0.0200 = 6.00 \times 10^{-3}$ mol

1 : 1 ratio, so **Ag^+ is limiting**: $m(AgCl) = 5.00 \times 10^{-3} \times 143.32 =$ **0.717 g**

In (b), each $CaCl_2$ supplies two Cl^- ions. Write the ionic equation and count the ions that actually react.

2.2 Using an excess on purpose

Chemists often add one reactant in deliberate excess. This makes the other reactant limiting, so that all of it reacts. It is done when one reactant is expensive or toxic, when it must be removed completely, or simply to drive a reaction further towards products.

Worked example 6 — removing lead ions from water ★

Q. 5000 dm^3 of contaminated water contains 2.00×10^{-4} mol dm^{-3} of Pb^{2+} ions. Sodium carbonate precipitates lead(II) carbonate: $Pb^{2+}(aq) + CO_3^{2-}(aq) \rightarrow PbCO_3(s)$. Calculate the minimum mass of sodium carbonate needed, and the mass used if a 50 % excess is added.

$n(Pb^{2+}) = 2.00 \times 10^{-4} \times 5000 = 1.00$ mol, so 1.00 mol of Na_2CO_3 is needed (1 : 1)

minimum mass = 1.00 × 105.99 = **106 g**; with a 50 % excess: 1.50 × 105.99 = **159 g**

Model answer: "Explain why sodium carbonate is added in excess." (2 marks)

The excess makes the Pb^{2+} ions the limiting reactant [1], so all of the toxic lead ions are precipitated and removed from the water; sodium carbonate is cheap and the excess is harmless [1].

Examiner traps in finding the limiting reactant

- Choosing the reactant with the smaller mass, or the smaller number of moles, without using the mole ratio.
- Calculating the product from the reactant in excess. The theoretical yield always comes from the limiting reactant.
- Forgetting that the amount of excess reactant *left over* is the amount present minus the amount that reacted.
- In solutions, using the concentration of a salt instead of the ions it supplies ($CaCl_2$ gives two Cl^-).
- Counting liquid water as a gas when finding the final volume of a gas mixture.

3 Reactivity 2.1.3 — Theoretical and experimental yield SL + HL

3.1 Two different yields

Definitions to learn

The **theoretical yield** is the maximum amount of product that could form, calculated from the balanced equation by assuming that all of the limiting reactant is converted into product. It is usually given in grams or moles.

The **experimental yield** (actual yield) is the amount of product actually obtained in the experiment, measured after it has been separated and purified.

The theoretical yield is a calculation; the experimental yield is a measurement. Every calculation in Booklet 1 found a theoretical yield. In practice the two are almost never the same.

3.2 Why the experimental yield is different

Experimental yield lower than theoretical	Experimental yield higher than theoretical
◆ **side reactions** form other products from the same reactants ◆ the reaction is **reversible** and reaches equilibrium (Reactivity 2.3), or is **incomplete** because it is slow ◆ product is **lost** during transfer, filtration, recrystallisation or distillation; some stays dissolved in the solvent ◆ reactants or products **decompose** or evaporate ◆ the reactants are **impure**, so there is less limiting reactant than you think	◆ the product is **not fully dried**: water or solvent adds to the mass ◆ the product contains **impurities**, such as unreacted starting material or by-products ◆ the product has reacted with something in the air, e.g. absorbed CO_2 or water ◆ a **weighing or measurement error** A percentage yield above 100 % is a sign that something extra is in the product. It is never "extra product".

Model answer: "A student made crystals of a salt. Suggest two reasons why the experimental yield was lower than the theoretical yield, and one reason why another student obtained a yield above 100 %." (3 marks)

Some of the product remained dissolved in the solution after crystallisation (or was left on the filter paper or glassware) [1]. The reaction did not go to completion, or side reactions used up some of the reactants [1]. A yield above 100 % means the crystals were not fully dried, so the water still present added to their mass (or the product was impure) [1].

4 Reactivity 2.1.4 — Percentage yield SL + HL

4.1 The percentage yield equation

Definition to learn (not in the data booklet)

$$\textbf{percentage yield} = (\text{experimental yield} \div \text{theoretical yield}) \times 100$$

Both yields must be in the same units: both in grams, or both in moles.

The percentage yield measures how efficiently reactants are converted into the product that is actually collected. It matters in research and above all in industry, where a few per cent of yield on a pharmaceutical synthesis can be worth millions. Reducing losses and increasing yield is one of the aims of Green Chemistry.

Method — percentage yield problems

1. Write the balanced equation and find the limiting reactant if more than one amount is given.
2. Calculate the theoretical yield from the limiting reactant.
3. **Forward:** percentage yield = experimental ÷ theoretical × 100.
4. **Backward:** to find the mass you will actually get, experimental = theoretical × (yield ÷ 100). To find how much you must *start with*, first divide the target by (yield ÷ 100) to get the theoretical yield you need, then work back to the reactant.

Worked example 7 — a simple percentage yield

Q. 25.0 g of calcium carbonate was heated and 12.6 g of calcium oxide was obtained: $CaCO_3(s) \rightarrow CaO(s) + CO_2(g)$. Calculate the percentage yield.

theoretical yield = (25.0 / 100.09) × 56.08 = 0.2498 mol × 56.08 = 14.01 g CaO

percentage yield = 12.6 / 14.01 × 100 = **90.0 %**

Worked example 8 — percentage yield with a limiting reactant

Q. 6.00 g of ethanoic acid was heated with 6.00 g of ethanol and a little concentrated sulfuric acid. 5.28 g of ethyl ethanoate was obtained. Calculate the percentage yield. $CH_3COOH(l) + C_2H_5OH(l) \rightleftharpoons CH_3COOC_2H_5(l) + H_2O(l)$

$n(CH_3COOH)$ = 6.00 / 60.06 = 0.09990 mol; $n(C_2H_5OH)$ = 6.00 / 46.08 = 0.1302 mol

1 : 1 ratio, so **ethanoic acid is limiting** and ethanol is in excess

theoretical yield = 0.09990 × 88.12 = 8.803 g; percentage yield = 5.28 / 8.803 × 100 = **60.0 %**

The yield is well below 100 % mainly because esterification is reversible: the mixture reaches equilibrium. Using excess ethanol pushes the equilibrium to the right and makes the more expensive acid limiting (Reactivity 2.3).

Worked example 9 — the mass you will actually get

Q. Aspirin, $C_9H_8O_4$, is made from salicylic acid, $C_7H_6O_3$: $C_7H_6O_3 + C_4H_6O_3 \rightarrow C_9H_8O_4 + CH_3COOH$. Ethanoic anhydride, $C_4H_6O_3$, is used in excess. Calculate the mass of aspirin obtained from 3.00 g of salicylic acid if the yield is 72.0 %.

$M(C_7H_6O_3)$ = 138.13; $M(C_9H_8O_4)$ = 180.17 g mol^{-1}

theoretical yield = (3.00 / 138.13) × 180.17 = 0.02172 mol × 180.17 = 3.913 g

experimental yield = 3.913 × 0.720 = **2.82 g**

Worked example 10 — how much must you start with?

Q. A student needs 25.0 g of bromoethane, C_2H_5Br, made by $C_2H_5OH + HBr \rightarrow C_2H_5Br + H_2O$, which has a yield of 75.0 %. Calculate the minimum mass of ethanol needed.

theoretical yield needed = 25.0 / 0.750 = 33.33 g of C_2H_5Br (more than 25.0 g, because some will be lost)

$M(C_2H_5Br)$ = 108.97 g mol^{-1}; n = 33.33 / 108.97 = 0.3059 mol, so 0.3059 mol of ethanol is needed

$m(C_2H_5OH)$ = 0.3059 × 46.08 = **14.1 g**

A quick check: when you work backwards from a yield, the amount you start with must be *larger* than for a 100 % yield. Multiplying by 0.750 instead of dividing would give too little.

4.2 Multi-step syntheses

Most medicines are made in several steps. The product of one step is the starting material for the next, so the losses multiply: the **overall yield** is the product of the yields of the individual steps (as decimals). Even good yields at each step soon give a low overall yield, which is why chemists look for shorter routes.

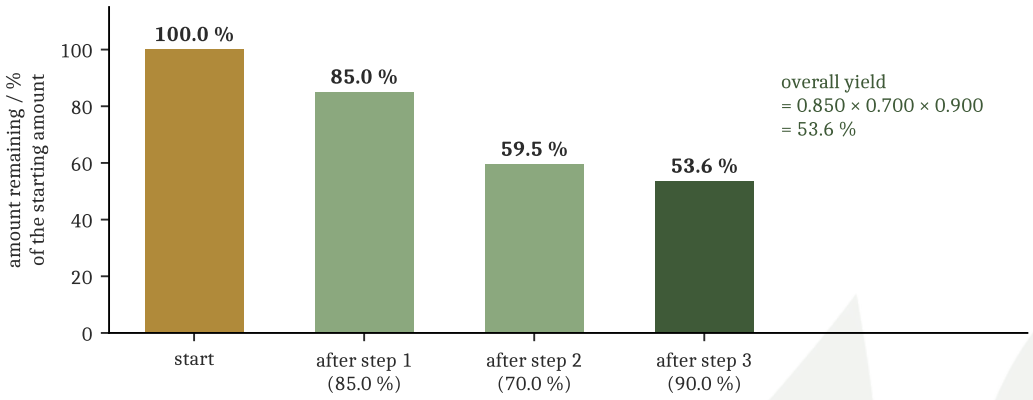


Figure 2 — Worked example 11. Three steps with yields of 85.0 %, 70.0 % and 90.0 % leave only 53.6 % of the starting material as final product.

Worked example 11 — overall yield of a three-step synthesis ★

Q. Paracetamol (M = 151.18 g mol^{-1}) is made from a starting material in three steps, each with a 1 : 1 mole ratio, with yields of 85.0 %, 70.0 % and 90.0 %. Calculate the overall yield and the mass of paracetamol made from 0.200 mol of the starting material.

overall yield = 0.850 × 0.700 × 0.900 = 0.5355 = **53.6 %**

n(paracetamol) = 0.200 × 0.5355 = 0.1071 mol; m = 0.1071 × 151.18 = **16.2 g**

Averaging the three yields (81.7 %) would be wrong: each step works only on what the previous step produced.

Worked example 12 — yield and purity together ★

Q. Haematite ore contains 72.0 % Fe_2O_3 by mass. In the blast furnace, $Fe_2O_3 + 3CO \rightarrow 2Fe + 3CO_2$ with an overall yield of 92.0 %. Calculate the mass of ore needed to produce 1.00 tonne of iron.

theoretical yield of Fe needed = 1.00 / 0.920 = 1.087 t

mass ratio: 159.70 t of Fe_2O_3 gives 2 × 55.85 = 111.70 t of Fe, so Fe_2O_3 needed = 1.087 × 159.70 / 111.70 = 1.554 t

mass of ore = 1.554 / 0.720 = **2.16 t**

Both the yield and the purity make the mass needed larger, so both are *divisions*. Mass ratios work directly in tonnes.

Examiner traps with percentage yield

- Calculating the theoretical yield from the reactant in excess.
- Dividing a mass by an amount in moles: both yields must be in the same units.
- Working backwards by multiplying by the yield instead of dividing, so the starting mass comes out too small.
- Averaging step yields instead of multiplying them for a multi-step synthesis.
- Explaining a yield above 100 % as "more product formed". It means the product is wet or impure.

5 Reactivity 2.1.5 — Atom economy and Green Chemistry SL + HL

5.1 Green Chemistry

Green Chemistry is the sustainable design of chemical products and processes, to reduce or eliminate the use and generation of substances that are hazardous to human health and the environment. A reaction with a 100 % yield can still be wasteful if most of the atoms in the reactants end up in by-products that nobody wants. The second principle of Green Chemistry is that syntheses should be designed to **maximize atom economy**: to build as many of the reactant atoms as possible into the desired product.

Definition to learn (the equation is in the data booklet)

% atom economy = (molar mass of desired product ÷ molar mass of all reactants) × 100

Use the coefficients in the balanced equation: multiply each molar mass by its coefficient. Atom economy is calculated from the equation alone, assuming a 100 % yield and exactly stoichiometric amounts.

5.2 The inverse relationship with waste

By conservation of mass, everything in the reactants that does not become the desired product becomes a by-product. So, for a reaction run to completion,

percentage of the reactant mass wasted = 100 − % atom economy

mass of by-products per tonne of product = (100 ÷ % atom economy) − 1 tonnes

The higher the atom economy, the less waste is produced and the fewer raw materials are used. An **addition reaction**, including addition polymerization, has an atom economy of 100 % because it has only one product. **Substitution** and **elimination** reactions always have lower atom economies because they make a second product, such as HCl, H_2O or CO_2.

Worked example 13 — atom economy of extracting iron

Q. Calculate the atom economy for the production of iron by (a) $Fe_2O_3 + 3CO \rightarrow 2Fe + 3CO_2$ and (b) $2Fe_2O_3 + 3C \rightarrow 4Fe + 3CO_2$.

(a) desired: 2 × 55.85 = 111.70; reactants: 159.70 + 3(28.01) = 243.73; 111.70 / 243.73 × 100 = **45.8 %**

(b) desired: 4 × 55.85 = 223.40; reactants: 2(159.70) + 3(12.01) = 355.43; 223.40 / 355.43 × 100 = **62.9 %**

The coefficients matter. In (a), using 55.85 for one Fe instead of 111.70 would halve the answer.

Worked example 14 — two routes to ethanol (link to Reactivity 1.3)

Q. Compare the atom economies of making ethanol by (a) hydration of ethene, $C_2H_4 + H_2O \rightarrow C_2H_5OH$, and (b) fermentation, $C_6H_{12}O_6 \rightarrow 2C_2H_5OH + 2CO_2$. Calculate the mass of by-product made per tonne of ethanol in (b).

(a) one product only: **100 %** atom economy

(b) desired: 2 × 46.08 = 92.16; reactant: 180.18; 92.16 / 180.18 × 100 = **51.1 %**

by-product per tonne of ethanol = (100 / 51.15) − 1 = **0.955 t of CO_2**

On atom economy alone hydration wins. But ethene comes from crude oil, which is non-renewable, and the hydration needs a high temperature and pressure; fermentation uses a renewable crop, runs at about 35 °C, and the CO_2 it releases was recently absorbed by photosynthesis. Atom economy is only one measure of how “green” a process is.

Worked example 15 — when a by-product is useful ★

Q. Calculate the atom economy for hydrogen made by (a) steam reforming, $CH_4 + H_2O \rightarrow CO + 3H_2$, and (b) electrolysis of water, $2H_2O \rightarrow 2H_2 + O_2$.

(a) 3 × 2.02 = 6.06; reactants 16.05 + 18.02 = 34.07; 6.06 / 34.07 × 100 = **17.8 %** (4.62 t of CO per tonne of H_2)

(b) 2 × 2.02 = 4.04; reactants 2 × 18.02 = 36.04; 4.04 / 36.04 × 100 = **11.2 %**

Hydrogen is so light that both atom economies are very low. Neither by-product is necessarily waste, though: the CO is used to make methanol and other chemicals, and pure oxygen can be sold. Electrolysis using renewable electricity releases no CO_2 at all. If a by-product is sold or used, the effective waste is much smaller than the atom economy suggests.

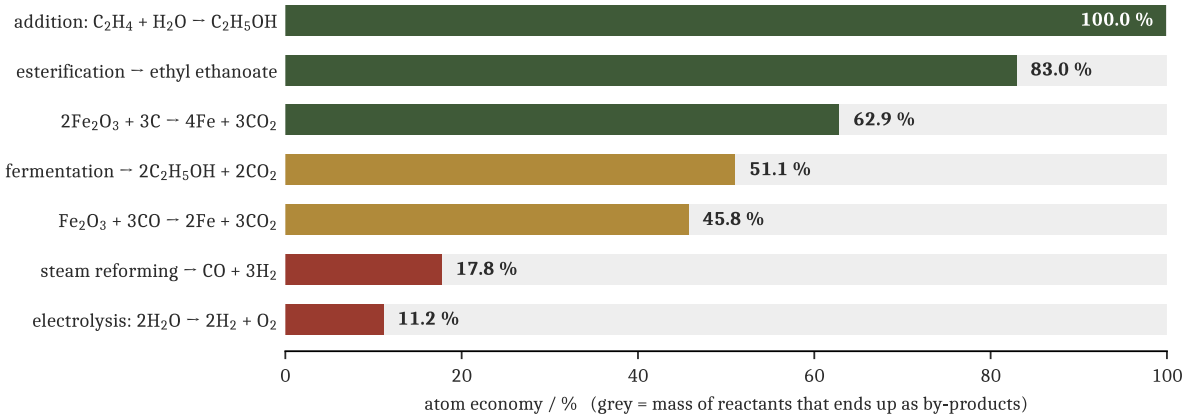


Figure 3 — Atom economies calculated in this booklet. Addition reactions waste nothing; reactions that release a light, desired product such as hydrogen, or a heavy by-product such as CO_2, have low atom economies.

5.3 Atom economy and percentage yield are different

	Percentage yield	Atom economy
measures	how much of the possible product is actually collected	how much of the mass of the reactants could end up in the desired product
found from	an experiment: needs the experimental yield	the balanced equation alone: no experiment needed
improved by	better conditions, purer reactants, less loss in purification	choosing a different reaction (route), or finding a use for the by-products
ignores	the by-products and the excess reagents	losses, excess reagents, solvents, catalysts and energy

Worked example 16 — combining the two measures ★

Q. For the esterification in worked example 8, calculate the atom economy, and the percentage of the total mass of the reactants that ends up in the collected ester if the reactants are mixed in exactly a 1 : 1 mole ratio and the yield is 60.0 %.

atom economy = 88.12 / (60.06 + 46.08) × 100 = 88.12 / 106.14 × 100 = **83.0 %**

mass of reactants in collected product = 0.830 × 0.600 = 0.498 → **49.8 %**

A high atom economy with a modest yield still wastes about half of the starting material. In worked example 8 the excess ethanol makes the real figure even lower.

Model answer: “Distinguish between percentage yield and atom economy, and explain why a high atom economy is important in industry.” (3 marks)

Percentage yield compares the amount of product actually obtained with the maximum possible, so it needs experimental data [1]. Atom economy compares the molar mass of the desired product with the molar mass of all the reactants, from the balanced equation alone [1]. A high atom economy means a smaller mass of by-products (less waste) and fewer raw materials used per tonne of product, so the process is more sustainable and cheaper [1].

5.4 Other factors in judging efficiency

The syllabus asks what else should be considered beyond atom economy and yield (Structure 2.4, Reactivity 2.2). A full assessment also looks at the **rate** of reaction (a slow process ties up plant and energy); the **energy** used for heating, pressure and separation; the **solvents and catalysts**, which are not in the equation but may be hazardous or need recovery; whether the raw materials are **renewable**; the **toxicity** of reagents and by-products; whether by-products can be **sold or recycled**; and the overall **cost**.

Examiner traps with atom economy

- Forgetting the coefficients: use 2 × M(Fe) for 2Fe, and include every reactant with its coefficient.
- Putting the molar mass of all the *products* on the bottom. The denominator is the reactants (by conservation of mass the totals are equal, but only if every product is counted).
- Including a catalyst or a reactant in excess. Atom economy uses the balanced equation only.
- Thinking a 100 % yield means 100 % atom economy, or the reverse.
- Calling every by-product "waste": a by-product that is sold or used reduces the real waste.

6 Key points to memorise

Everything below is either wording that examiners look for or knowledge you must carry into the exam yourself.

A Definitions

- **Limiting reactant:** the reactant completely used up first; it determines the amount of product. **Excess reactant:** some is left over.
- **Theoretical yield:** the maximum amount of product, assuming complete conversion of the limiting reactant.
- **Experimental yield:** the amount of product actually obtained.
- **Green Chemistry:** designing products and processes that reduce or eliminate the use and generation of hazardous substances.
- **Atom economy:** the percentage of the mass of the reactants that ends up in the desired product, from the balanced equation.

B Equations

- Limiting reactant: the smallest value of n ÷ coefficient. Excess left = amount present − amount that reacted.
- Percentage yield = experimental yield / theoretical yield × 100 (same units). **Not in the data booklet.**
- Working back: theoretical yield needed = target ÷ (yield/100); impure starting material: mass needed = pure mass ÷ (purity/100).
- Overall yield of a multi-step synthesis = product of the step yields (as decimals).
- % atom economy = M(desired product) / M(all reactants) × 100, using coefficients. % waste = 100 − % atom economy.

C Explanations you will be asked for

- The limiting reactant depends on the mole ratio, not on the masses or the numbers of moles alone.
- An excess of a cheap reactant makes the expensive or toxic one limiting, so all of it reacts.
- Yield below theoretical: side reactions, reversible or incomplete reaction, losses in transfer and purification, impure reactants.
- Yield above 100 %: product not dry, or impure.
- Addition reactions have 100 % atom economy; substitution and elimination produce by-products, so they have less.
- High atom economy → less waste, fewer raw materials, more sustainable. Atom economy ignores yield, energy, solvents and the value of by-products.

7 Check yourself

Use A_r values from the data booklet (H 1.01, C 12.01, N 14.01, O 16.00, Na 22.99, Mg 24.31, Al 26.98, S 32.07, Cl 35.45, Ca 40.08, Ti 47.87, Fe 55.85, Cu 63.55, Zn 65.38, Br 79.90, Ag 107.87, I 126.90, Pb 207.20), V_m = 22.7 dm^3 mol^{-1} at STP and R = 8.31 J K^{-1} mol^{-1}. Marks are shown in brackets; allow about 1.2 minutes per mark. Full answers are in section 8.

Part A — Multiple choice SL + HL

1. 0.40 mol of magnesium is added to 0.30 mol of hydrochloric acid: $Mg + 2HCl \rightarrow MgCl_2 + H_2$. Which is correct?

A Mg is limiting; 0.40 mol H_2
B HCl is limiting; 0.30 mol H_2
C HCl is limiting; 0.15 mol H_2
D Mg is limiting; 0.15 mol H_2

2. 10 cm^3 of nitrogen reacts with 24 cm^3 of hydrogen at constant temperature and pressure: $N_2 + 3H_2 \rightarrow 2NH_3$. What is the maximum volume of ammonia?

A 10 cm^3 **B** 16 cm^3 **C** 20 cm^3 **D** 24 cm^3

3. In which mixture is NaOH the limiting reactant? $H_2SO_4 + 2NaOH \rightarrow Na_2SO_4 + 2H_2O$

A 0.10 mol NaOH + 0.04 mol H_2SO_4
B 0.10 mol NaOH + 0.06 mol H_2SO_4
C 0.20 mol NaOH + 0.10 mol H_2SO_4
D 0.30 mol NaOH + 0.10 mol H_2SO_4

4. 4.0 mol of methane is burned in 6.0 mol of oxygen: $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$. What amount of methane remains?

A 0 mol **B** 1.0 mol **C** 2.0 mol **D** 3.0 mol

5. What is the theoretical yield of a reaction?

A the maximum amount of product, assuming complete conversion of the limiting reactant
B the amount of product actually collected
C the amount of the excess reactant left over
D the mass of all the products divided by the mass of all the reactants

6. Which could cause a percentage yield above 100 %?

A the product was not fully dried
B a side reaction occurred
C product was lost during filtration
D the reaction is reversible

7. 8.0 g of ethene produces 9.2 g of ethanol: $C_2H_4 + H_2O \rightarrow C_2H_5OH$. What is the percentage yield?

A 57 % **B** 70 % **C** 87 % **D** 115 %

8. A 1 : 1 reaction has an 80 % yield. What minimum amount of reactant is needed to obtain 4.0 mol of product?

A 3.2 mol **B** 4.0 mol **C** 4.8 mol **D** 5.0 mol

9. A two-step synthesis has yields of 80 % and 50 %. What is the overall yield?

A 30 % **B** 40 % **C** 65 % **D** 130 %

10. Which reaction has an atom economy of 100 %?

A $C_2H_4 + Br_2 \rightarrow C_2H_4Br_2$ **B** $CH_4 + Cl_2 \rightarrow CH_3Cl + HCl$

C $C_2H_5OH \rightarrow C_2H_4 + H_2O$ **D** $CaCO_3 \rightarrow CaO + CO_2$

11. What is the atom economy for making calcium oxide by $CaCO_3 \rightarrow CaO + CO_2$?

A 44.0 % **B** 56.0 % **C** 78.5 % **D** 100 %

12. A reaction with an atom economy of 40 % goes to completion. What percentage of the mass of the reactants becomes by-products?

A 40 % **B** 60 % **C** 100 % **D** 140 %

13. Which statement is correct?

A Atom economy can be calculated from the balanced equation alone, but percentage yield needs experimental data.

B Both atom economy and percentage yield need experimental data.

C A reaction with a 100 % yield must have a 100 % atom economy.

D Atom economy takes account of reactants used in excess.

14. Why is a cheap reactant often used in excess?

A to make sure that the more expensive reactant is limiting and fully used up

B to increase the atom economy

C to reduce the mass of by-products

D to make the cheap reactant the limiting reactant

15. 2.00 g of hydrogen is exploded with 32.0 g of oxygen: $2H_2 + O_2 \rightarrow 2H_2O$. What mass of the excess reactant remains?

A 0 g **B** 8.0 g of O_2 **C** 16.2 g of O_2 **D** 1.0 g of H_2

16. 6.0 mol of carbon monoxide is burned in 4.0 mol of oxygen: $2CO + O_2 \rightarrow 2CO_2$. What is the total amount of gas at the end?

A 6.0 mol **B** 7.0 mol **C** 8.0 mol **D** 10.0 mol

17. What is the atom economy for making hydrogen by $Zn + 2HCl \rightarrow ZnCl_2 + H_2$?

A 1.46 % **B** 2.92 % **C** 50.0 % **D** 98.5 %

Part B — Structured questions SL + HL

18. 0.600 mol of iron is heated with 0.750 mol of chlorine: $2Fe(s) + 3Cl_2(g) \rightarrow 2FeCl_3(s)$.

(a) Identify the limiting reactant, showing your working. [1]

(b) Calculate the amount and the mass of $FeCl_3$ formed. [2]

(c) Calculate the amount of the excess reactant left over. [1]

19. 10.0 g of hydrogen is mixed with 50.0 g of nitrogen: $N_2(g) + 3H_2(g) \rightarrow 2NH_3(g)$.

(a) Determine the limiting reactant. [2]

(b) Calculate the theoretical yield of ammonia. [2]

(c) Calculate the mass of the excess reactant left over, and show that mass is conserved. [1]

20. 7.00 g of ethene reacts with 30.0 g of bromine: $C_2H_4(g) + Br_2(l) \rightarrow C_2H_4Br_2(l)$.

(a) Determine the limiting reactant. [2]

(b) Calculate the theoretical yield of 1,2-dibromoethane. [1]

(c) State the atom economy of the reaction and explain your answer. [1]

21. 50 cm^3 of methane is burned in 80 cm^3 of oxygen and the products are cooled to room temperature: $CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(l)$. Identify the limiting reactant, and deduce the final volume and composition of the gas mixture (same temperature and pressure). [3]

22. 1.00 g of calcium carbonate is added to 20.0 cm^3 of 0.800 mol dm^{-3} hydrochloric acid.

(a) Write the equation, with state symbols. [1]

(b) Determine the limiting reactant. [2]

(c) Calculate the volume of carbon dioxide formed at STP. [1]

(d) Calculate the mass of calcium carbonate left unreacted. [1]

23. 30.0 cm^3 of 0.100 mol dm^{-3} $Pb(NO_3)_2(aq)$ is mixed with 25.0 cm^3 of 0.200 mol dm^{-3} KI(aq). A yellow precipitate of lead(II) iodide forms.

(a) Write the ionic equation, with state symbols. [1]

(b) Identify the limiting reactant. [1]

(c) Calculate the theoretical yield of PbI_2. [1]

(d) The dried precipitate had a mass of 0.968 g. Calculate the percentage yield. [1]

24. A student makes a solid product, filters it and dries it in an oven.

(a) Suggest two reasons why the experimental yield is lower than the theoretical yield. [2]

(b) Suggest why the student weighs the product, heats it again and reweighs it before calculating the yield. [1]

25. In a trial of the Haber process, 28.0 kg of nitrogen reacted with excess hydrogen and 5.10 kg of ammonia was collected.

(a) Calculate the theoretical yield of ammonia. [2]

(b) Calculate the percentage yield. [1]

(c) Suggest the main reason why the yield is so low. [1]

26. Copper(II) sulfate crystals are made by warming 4.00 g of copper(II) oxide with 40.0 cm^3 of 1.00 mol dm^{-3} sulfuric acid, filtering, and crystallising $CuSO_4 \cdot 5H_2O$. $CuO(s) + H_2SO_4(aq) \rightarrow CuSO_4(aq) + H_2O(l)$

(a) Determine the limiting reactant. [2]

(b) Calculate the theoretical yield of $CuSO_4 \cdot 5H_2O$. [1]

(c) 7.42 g of crystals were obtained. Calculate the percentage yield. [1]

(d) Explain why the copper(II) oxide is used in excess, and how the excess is removed. [1]

27. 1-bromobutane is made from butan-1-ol: $C_4H_9OH + HBr \rightarrow C_4H_9Br + H_2O$, with a yield of 65.0 %. Calculate the minimum mass of butan-1-ol needed to make 10.0 g of 1-bromobutane. [3]

28. In the first step of nitric acid manufacture, $4NH_3 + 5O_2 \rightarrow 4NO + 6H_2O$, with a yield of 96.0 %. Calculate the mass of NO produced from 1.00 kg of ammonia. [2]

29. ★ A drug (M = 206.28 g mol^{-1}) is made from a starting material (M = 120.15 g mol^{-1}) in four steps, each with a 1 : 1 mole ratio. The step yields are 92 %, 75 %, 88 % and 60 %.

(a) Calculate the overall yield. [1]

(b) Calculate the mass of starting material needed to make 50.0 g of the drug. [2]

(c) Suggest why chemists try to find routes with fewer steps. [1]

30. ★ Bauxite ore contains 55.0 % Al_2O_3 by mass. Aluminium is produced by electrolysis, $2Al_2O_3 \rightarrow 4Al + 3O_2$, with an overall yield of 90.0 %. Calculate the mass of bauxite needed to produce 1.00 tonne of aluminium. [4]

31. Magnesium sulfate can be made by two reactions: Route 1, $MgCO_3 + H_2SO_4 \rightarrow MgSO_4 + H_2O + CO_2$; Route 2, $MgO + H_2SO_4 \rightarrow MgSO_4 + H_2O$.

(a) Calculate the atom economy of route 1. [1]

(b) Calculate the atom economy of route 2. [1]

(c) Identify the greener route on this basis, and state one other factor that should be considered. [2]

32. Ethene can be made by cracking decane, $C_{10}H_{22} \rightarrow C_2H_4 + C_8H_{18}$, or by dehydrating ethanol, $C_2H_5OH \rightarrow C_2H_4 + H_2O$.

(a) Calculate the atom economy for ethene by each route. [2]

(b) Suggest why the cracking route is less wasteful than its atom economy suggests. [1]

33. ★ Titanium is extracted by $TiCl_4 + 2Mg \rightarrow Ti + 2MgCl_2$.

(a) Calculate the atom economy for titanium. [1]

(b) Calculate the mass of by-product formed for each tonne of titanium. [2]

(c) The $MgCl_2$ is electrolysed to give magnesium and chlorine. Suggest why this makes the process greener. [1]

34. A process has a percentage yield of 95 % but an atom economy of 35 %.

(a) Distinguish between percentage yield and atom economy. [2]

(b) Explain why the process may still be considered inefficient. [1]

(c) State one other factor, apart from yield and atom economy, used to judge the efficiency of a process. [1]

35. ★ Paracetamol, $C_8H_9NO_2$, is made from 4-aminophenol, C_6H_7NO: $C_6H_7NO + C_4H_6O_3 \rightarrow C_8H_9NO_2 + CH_3COOH$. A student used 5.00 g of 4-aminophenol and 6.00 cm^3 of ethanoic anhydride, $C_4H_6O_3$ (density 1.08 g cm^{-3}), and obtained 4.85 g of paracetamol.

(a) Determine the limiting reactant. [2]

(b) Calculate the theoretical yield of paracetamol. [1]

(c) Calculate the percentage yield. [1]

(d) Calculate the atom economy. [1]

(e) Suggest how the overall waste from this process could be reduced. [1]

36. ★ A sealed 2.00 dm^3 vessel contains 0.290 g of butane and 1.60 g of oxygen. The butane is ignited and burns completely: $2C_4H_{10} + 13O_2 \rightarrow 8CO_2 + 10H_2O$. The vessel is then cooled to 25 °C, where the water is a liquid. Determine the amount of each gas left in the vessel and the final pressure. [4]

37. 50.0 cm^3 of 0.400 mol dm^{-3} NaOH(aq) is mixed with 30.0 cm^3 of 0.500 mol dm^{-3} H_2SO_4(aq). Identify the limiting reactant, and calculate the mass of sodium sulfate formed, the amount of excess acid, and the concentration of H^+(aq) in the final mixture. [4]

38. ★ Ibuprofen was first made by a six-step route with an atom economy of 40.0 %. A newer three-step route has an atom economy of 77.4 %.

(a) Calculate the mass of by-products formed per tonne of ibuprofen by each route. [2]

(b) Suggest two other advantages of the newer route. [2]

Part A: 17 marks · Part B: 83 marks · Total: 100 marks (about 2 hours)

8 Answers

Part A

1. C. Mg would need 0.80 mol HCl; HCl is limiting, giving 0.30/2 = 0.15 mol H_2.

2. B. 10 cm^3 N_2 needs 30 cm^3 H_2, so H_2 is limiting: 24 × 2/3 = 16 cm^3.

3. B. 0.10 mol NaOH reacts with only 0.05 mol H_2SO_4, so 0.06 mol acid is an excess. A and D have NaOH in excess; C is exactly stoichiometric.

4. B. O_2 is limiting: 6.0 mol O_2 reacts with 3.0 mol CH_4, leaving 1.0 mol.

5. A.

6. A. Water still in the product adds mass. B, C and D all lower the yield.

7. B. Theoretical = 8.0/28.06 × 46.08 = 13.1 g; 9.2/13.1 × 100 = 70 %.

8. D. 4.0/0.80 = 5.0 mol.

9. B. 0.80 × 0.50 = 0.40.

10. A. An addition reaction has only one product.

11. B. 56.08/100.09 × 100 = 56.0 %.

12. B. 100 − 40 = 60 %.

13. A.

14. A.

15. C. $n(H_2)$ = 0.990 mol, $n(O_2)$ = 1.000 mol; H_2 is limiting and uses 0.495 mol O_2, leaving 0.505 mol × 32.00 = 16.2 g.

16. B. CO is limiting: 6.0 mol CO uses 3.0 mol O_2, giving 6.0 mol CO_2; 1.0 mol O_2 remains; total 7.0 mol.

17. A. 2.02/(65.38 + 2 × 36.46) × 100 = 1.46 %.

Part B

18. (a) Fe: 0.600/2 = 0.300; Cl_2: 0.750/3 = 0.250, so Cl_2 is limiting [1]. (b) $n(FeCl_3)$ = 0.750 × 2/3 = 0.500 mol [1]; × 162.20 = 81.1 g [1]. (c) Fe used = 0.500 mol, so 0.100 mol of Fe is left [1].

19. (a) $n(H_2)$ = 10.0/2.02 = 4.95 mol; $n(N_2)$ = 50.0/28.02 = 1.784 mol [1]; 1.784 mol N_2 would need 5.35 mol H_2, so H_2 is limiting [1]. (b) $n(NH_3)$ = 4.95 × 2/3 = 3.30 mol [1]; × 17.04 = 56.2 g [1]. (c) N_2 used = 4.95/3 = 1.650 mol; left = 0.134 mol × 28.02 = 3.76 g; 56.2 + 3.76 = 60.0 g = 10.0 + 50.0 g [1].

20. (a) $n(C_2H_4)$ = 7.00/28.06 = 0.2495 mol; $n(Br_2)$ = 30.0/159.80 = 0.1877 mol [1]; 1 : 1, so Br_2 is limiting [1]. (b) 0.1877 × 187.86 = 35.3 g [1]. (c) 100 %: it is an addition reaction with only one product [1].

21. 50 cm^3 CH_4 needs 100 cm^3 O_2, so O_2 is limiting [1]; 40 cm^3 CH_4 reacts, giving 40 cm^3 CO_2 [1]; final gas = 40 cm^3 CO_2 + 10 cm^3 CH_4 = 50 cm^3 (water is liquid) [1].

22. (a) $CaCO_3(s) + 2HCl(aq) \rightarrow CaCl_2(aq) + H_2O(l) + CO_2(g)$ [1]. (b) $n(CaCO_3)$ = 1.00/100.09 = 9.99 × 10^{-3} mol; $n(HCl)$ = 0.800 × 0.0200 = 0.0160 mol [1]; the $CaCO_3$ would need 0.0200 mol HCl, so HCl is limiting [1]. (c) $n(CO_2)$ = 0.0160/2 = 8.00 × 10^{-3} mol; × 22.7 = 0.182 dm^3 (182 cm^3) [1]. (d) (9.99 − 8.00) × 10^{-3} = 1.99 × 10^{-3} mol × 100.09 = 0.199 g [1].

23. (a) $Pb^{2+}(aq) + 2I^-(aq) \rightarrow PbI_2(s)$ [1]. (b) $n(Pb^{2+})$ = 3.00 × 10^{-3} mol needs 6.00 × 10^{-3} mol I^-, but only 5.00 × 10^{-3} mol is present: I^- is limiting [1]. (c) $n(PbI_2)$ = 2.50 × 10^{-3} mol × 461.00 = 1.15 g [1]. (d) 0.968/1.1525 × 100 = 84.0 % [1].

24. (a) Any two: product lost on filter paper or glassware; some product stayed dissolved in the solution; side reactions; incomplete (or reversible) reaction; impure reactants [2]. (b) To heat to constant mass, making sure all the water/solvent has gone; otherwise the yield would be too high [1].

25. (a) $n(N_2)$ = 28.0 × 10^3/28.02 = 999 mol → 1998 mol NH_3 [1]; × 17.04 = 3.41 × 10^4 g = 34.1 kg [1]. (b) 5.10/34.1 × 100 = 15.0 % [1]. (c) The reaction is reversible and reaches equilibrium, so it cannot go to completion (unreacted gases are recycled) [1].

26. (a) $n(CuO)$ = 4.00/79.55 = 0.0503 mol; $n(H_2SO_4)$ = 1.00 × 0.0400 = 0.0400 mol [1]; 1 : 1, so H_2SO_4 is limiting [1]. (b) $M(CuSO_4 \cdot 5H_2O)$ = 249.72; 0.0400 × 249.72 = 9.99 g [1]. (c) 7.42/9.99 × 100 = 74.3 % [1]. (d) So that all of the acid reacts and none contaminates the crystals; the excess CuO is insoluble and is removed by filtration [1].

27. theoretical yield needed = 10.0/0.650 = 15.4 g [1]; M(C_4H_9Br) = 137.03, so n = 0.1123 mol [1]; mass of butan-1-ol = 0.1123 × 74.14 = 8.32 g [1].

28. $n(NH_3)$ = 1000/17.04 = 58.7 mol → 58.7 mol NO; theoretical = 58.7 × 30.01 = 1761 g [1]; × 0.960 = 1.69 × 10^3 g = 1.69 kg [1].

29. (a) 0.92 × 0.75 × 0.88 × 0.60 = 0.364 = 36.4 % [1]. (b) n(drug) = 50.0/206.28 = 0.2424 mol; starting material = 0.2424/0.3643 = 0.665 mol [1]; × 120.15 = 79.9 g [1]. (c) Each extra step multiplies the losses (and adds solvents, energy and waste), so fewer steps give a higher overall yield [1].

30. theoretical Al needed = 1.00/0.900 = 1.111 t [1]; 2 × 101.96 = 203.92 t of Al_2O_3 gives 4 × 26.98 = 107.92 t of Al [1]; Al_2O_3 needed = 1.111 × 203.92/107.92 = 2.10 t [1]; bauxite = 2.10/0.550 = 3.82 t [1].

31. (a) 120.38/(84.32 + 98.09) × 100 = 66.0 % [1]. (b) 120.38/(40.31 + 98.09) × 100 = 87.0 % [1]. (c) Route 2 [1]; any one other factor: cost or availability of the starting material; energy needed; rate; safety/toxicity; whether the by-product can be used [1].

32. (a) cracking: 28.06/142.32 × 100 = 19.7 % [1]; dehydration: 28.06/46.08 × 100 = 60.9 % [1]. (b) The other product, octane, is a valuable fuel, so it is not waste [1].

33. (a) 47.87/(189.67 + 2 × 24.31) × 100 = 20.1 % [1]. (b) 2 × 95.21 = 190.42 t of $MgCl_2$ per 47.87 t of Ti [1], so 3.98 t per tonne of Ti [1]. (c) The by-product is recycled: Mg is reused in the process and Cl_2 is used to make more $TiCl_4$, so less waste and fewer raw materials [1].

34. (a) Percentage yield compares the product obtained with the maximum possible (needs experimental data) [1]; atom economy compares the molar mass of the desired product with that of all the reactants, from the equation [1]. (b) Even at 95 % yield, about 65 % of the mass of the reactants ends up as by-products, so much raw material is wasted [1]. (c) Any one: rate; energy consumption; use of solvents or catalysts; toxicity of reagents or by-products; renewability of raw materials; cost [1].

35. (a) $n(C_6H_7NO)$ = 5.00/109.14 = 0.0458 mol; anhydride: 6.00 × 1.08 = 6.48 g → 6.48/102.10 = 0.0635 mol [1]; 1 : 1, so 4-aminophenol is limiting [1]. (b) 0.0458 × 151.18 = 6.93 g [1]. (c) 4.85/6.93 × 100 = 70.0 % [1]. (d) 151.18/(109.14 + 102.10) × 100 = 71.6 % [1]. (e) Any one: recover and use or sell the ethanoic acid by-product; recover the excess anhydride; improve the yield, e.g. by reducing losses in recrystallisation [1].

36. $n(C_4H_{10})$ = 0.290/58.14 = 4.99 × 10^{-3} mol needs 6.5 × 4.99 × 10^{-3} = 0.0324 mol O_2; $n(O_2)$ = 0.0500 mol, so butane is limiting [1]; O_2 left = 0.0500 − 0.0324 = 0.0176 mol [1]; CO_2 = 4 × 4.99 × 10^{-3} = 0.0200 mol (total 0.0375 mol of gas) [1]; $p = nRT/V$ = 0.0375 × 8.31 × 298/2.00 × 10^{-3} = 4.65 × 10^4 Pa (46.5 kPa) [1].

37. n(NaOH) = 0.0200 mol needs 0.0100 mol H_2SO_4; 0.0150 mol is present, so NaOH is limiting [1]; $n(Na_2SO_4)$ = 0.0100 mol × 142.05 = 1.42 g [1]; excess H_2SO_4 = 0.0150 − 0.0100 = 5.00 × 10^{-3} mol [1]; $n(H^+)$ = 2 × 5.00 × 10^{-3} = 0.0100 mol in 80.0 cm^3, so $[H^+]$ = 0.125 mol dm^{-3} [1].

38. (a) old route: 100/40.0 − 1 = 1.50 t [1]; new route: 100/77.4 − 1 = 0.292 t [1]. (b) Any two: fewer steps, so a higher overall yield; less energy and fewer solvents used; less hazardous waste to dispose of; catalysts that can be recovered and reused; cheaper and faster production [2].

Where this fits in Reactivity 2

- **Booklet 1** — 2.1.1–2.1.2: equations, reacting masses, gas volumes, titrations. **Booklet 2 (this booklet)** — 2.1.3–2.1.5: limiting reactant, yield, atom economy. Together they complete Reactivity 2.1.
- **Next:** Reactivity 2.2 — how fast? Rates of reaction. **Later:** Reactivity 2.3 — how far? Equilibrium explains why many yields can never reach 100 %.

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