Empirical and Molecular Formulae Map

AQA A-level Chemistry · 3.1.2 Amount of substance: empirical and molecular formulae

1 Empirical formula

3.1.2.4 i

- **Simplest whole-number ratio** of atoms
- $C_6H_{12}O_6 \rightarrow CH_2O$
- $C_2H_6 \rightarrow CH_3$
- Ionic compounds: always empirical
- From experiment, not drawn



2 From masses

3.1.2.4 iv

- Mass of each element
- Oxygen = mass gained
- Divide by A_r: **moles**
- **Divide by the smallest**
- Mg 0.243 g + O 0.160 g: MgO

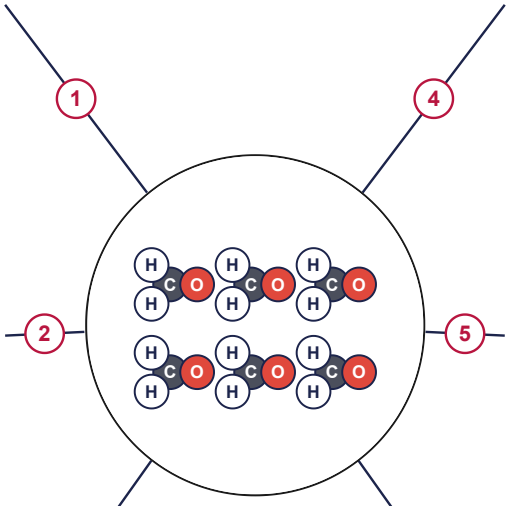


3 From percentages

3.1.2.4 iv

- Take **100 g**: % becomes g
- Missing element **by difference**
- Keep 3 s.f. until the end
- C 40.0, H 6.7, O 53.3 %: CH_2O
- Na 32.4, S 22.6, O 45.0 %: Na_2SO_4





4 Awkward ratios

3.1.2.4 iv

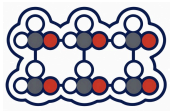
- .5: × 2; .33 or .67: × 3
- .25 or .75: × 4; .2 or .4: × 5
- Multiply **every** value
- Never round 1.5
- Fe 1 : 1.5 → Fe_2O_3



5 Molecular formula

3.1.2.4 ii–iii, v

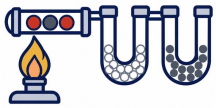
- **Actual** atoms in one molecule
- n = M_r ÷ empirical mass
- Multiply every subscript by n
- M_r from M^+ or M = m ÷ n
- $CH_2O \times 6 = C_6H_{12}O_6$



6 Combustion analysis

3.1.2.4 v

- All C → CO_2: n(C) = n(CO_2)
- All H → H_2O: n(H) = **2** × n(H_2O)
- O **by difference** in mass
- Then the ratio, then M_r
- 0.880 g CO_2 + 0.450 g H_2O: C_2H_5



From data to molecular formula

empirical formula mass × n = M_r; n is always a whole number

Compound	Data	Empirical	M_r	Molecular
glucose	C 40.0 %, H 6.7 %, O 53.3 %	CH_2O	180	$C_6H_{12}O_6$
ethanoic acid	C 40.0 %, H 6.7 %, O 53.3 %	CH_2O	60	$C_2H_4O_2$
butane	0.880 g CO_2, 0.450 g H_2O	C_2H_5	58	C_4H_{10}
benzene	C 92.3 %, H 7.7 %	CH	78	C_6H_6
cyclopentane	C 85.7 %, H 14.3 %	CH_2	70	C_5H_{10}
ethyl ethanoate	M^+ at m/z 88	C_2H_4O	88	$C_4H_8O_2$

Worked examples

From masses

- 2.80 g Fe, 1.20 g O
- 0.0502 : 0.0750 = 1 : 1.5
- **Fe_2O_3**

By difference

- C 54.5 %, H 9.1 %: O 36.4 %
- 4.54 : 9.1 : 2.28
- **C_2H_4O**

Molecular

- CH_2Cl = 49.5
- M^+ at m/z 99: × 2
- **$C_2H_4Cl_2$**

M_r values come from mass spectra and from pV = nRT (solutions and gases).

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