

1.3 – Chemical calculations II

5. Empirical and molecular formulae

Molecular formula: The actual number of atoms of each element present in the molecule.

Empirical formula: The simplest whole number ratio/proportion of elements present.

Example: A hydrocarbon (M_r 58) contains 4.80 g carbon and 1.01 g hydrogen. Calculate the empirical formula and molecular formula of the hydrocarbon.

	C	H
Moles ($\frac{\text{Mass}}{A_r}$)	$\frac{4.80}{12.0}$	$\frac{1.01}{1.01}$
→	0.40	1.00
Divide by the smaller	$\frac{0.40}{0.40}$	$\frac{1.00}{0.40}$
→	1	2.5 do not round up!
Multiply by two to get whole numbers	→ 2	5
Empirical formula	→ C_2H_5	

Mass of empirical formula = $(2 \times 12.0) + (5 \times 1.01) = 29.05$

Number of units in a molecule = $\frac{58}{29.05} = 1.992 \approx 2$

Molecular formula → $2 \times$ empirical formula → C_4H_{10}

Note: You can also use an empirical formula style calculation to find λ in a water of crystallisation calculation.

6. Volumes of gases

At standard temperature and pressure (stp) [273 K, 1 atm] one mole of any gas occupies a volume of 22.4 dm^3 . This value is called the molar gas volume (V_m).

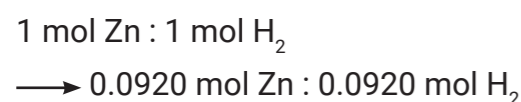
Example: What volume of hydrogen is formed, at stp, when 6.00 g of zinc reacts with excess sulfuric acid?



Step 1 – Calculate the moles of the substance you have information about – zinc in this case.

$$\text{moles zinc} = \frac{6.00}{65.4} = 0.0920 \text{ mol}$$

Step 2 – Use the balanced equation to find out the mole ratio of zinc to hydrogen and deduce the moles of hydrogen formed.



Step 3 – Calculate the volume of this number of moles of hydrogen gas at stp.

$$\text{volume of hydrogen} = 0.0920 \times 22.4 = 2.061 \text{ dm}_3$$

Note: Molar gas volume is 24.5 dm^3 at 25°C (298K) and 1 atm - room temperature and pressure (rtp).

7. Changes of conditions affecting gases

$$\frac{p_1V_1}{T_1} = \frac{p_2V_2}{T_2}$$

If a gas that was originally at p_1 , V_1 and T_1 has a condition changed, e.g. temperature, then the above equation can be used to see how another factor changes, e.g. volume.

p is pressure and V is volume (for this equation it does not matter which units are used as long as they are the same for $_1$ and $_2$). T is temperature (you must change $^\circ\text{C}$ into K (+273)).

If a question states, for example, that the temperature remains the same then you can use $p_1V_1 = p_2V_2$ to solve the calculation.

8. The ideal gas equation

In an ideal gas:

- the particles are of a negligible size
- the particles move with rapid, random motion
- collisions between particles are perfectly elastic
- there are no intermolecular forces.

$$pV = nRT$$

To use this equation, you **must use the following units:**

p → pressure → Pa or Nm^{-2}

V → volume → m^3

n → number of moles → mol

R → molar gas constant → $8.31 \text{ J mol}^{-1} \text{ K}^{-1}$ (data booklet)

T → temperature → K

Conversions:

$$1 \text{ kPa} = 1 \times 10^3 \text{ Pa}$$

$$1 \text{ atm} = 1.01 \times 10^5 \text{ Pa (data booklet)}$$

$$1 \text{ cm}^3 = 1 \times 10^{-6} \text{ m}^3$$

$$1 \text{ dm}^3 = 1 \times 10^{-3} \text{ m}^3$$

Example: Calculate the number of moles in 200 cm^3 of a gas at 25°C and at a pressure of 100 kPa.

$$p = 100 \text{ kPa} \longrightarrow 100 \times 10^3 \text{ Pa}$$

$$V = 200 \text{ cm}^3 \longrightarrow 200 \times 10^{-6} \text{ m}^3$$

$$T = 25^\circ\text{C} \longrightarrow 298 \text{ K}$$

$$pV = nRT \longrightarrow n = \frac{pV}{RT}$$

$$n = \frac{(100 \times 10^3) \times (200 \times 10^{-6})}{8.31 \times 298}$$

$$n = 0.808 \text{ mol (correct to 3 sig. figs)}$$

Note: A zero does not count as a significant figure until it has a non-zero number in front of it.

9. Calculations involving solutions

$$\text{moles} = \text{volume (dm}^{-3}\text{)} \times \text{concentration (mol dm}^{-3}\text{)}$$

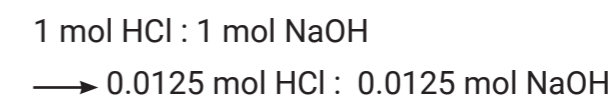
Example: During a titration, 25.00 cm^3 of $0.500 \text{ mol dm}^{-3}$ hydrochloric acid was exactly neutralised by 35.00 cm^3 of sodium hydroxide solution. Calculate the concentration of the sodium hydroxide solution.



Step 1 – Calculate the moles of the substance you have information about – hydrochloric acid in this case.

$$\begin{aligned} \text{moles HCl} &= \frac{\text{volume (cm}^3\text{)}}{1000} \times \text{concentration} \\ &= \frac{25.00}{1000} \times 0.500 = 0.0125 \text{ mol} \end{aligned}$$

Step 2 – Use the balanced equation to find out the mole ratio of HCl to NaOH and deduce the moles of NaOH that reacted.



Step 3 – Calculate the concentration of sodium hydroxide.

$$\begin{aligned} \text{concentration of NaOH} &= \frac{\text{moles}}{\text{volume (dm}^3\text{)}} = \frac{0.0125}{0.035} \\ &= 0.357 \text{ mol dm}^{-3} \end{aligned}$$

10. Converting a concentration from mol dm^{-3} to g dm^{-3}

$$\text{g dm}^{-3} = \text{concentration (mol dm}^{-3}\text{)} \times M_r$$

11. Atom economy and percentage yield

$$\text{atom economy} = \frac{\text{mass of required product}}{\text{total mass of reactants}} \times 100$$

Note: Don't forget to use any associated balancing numbers.

$$\text{percentage yield} = \frac{\text{mass of product obtained}}{\text{maximum theoretical mass}} \times 100$$

Note: Often the theoretical mass is not given directly in the question and will need to be calculated.

12. Percentage error

An error is usually taken as **half** of the smallest division on the apparatus. In chemistry, we usually measure the difference between two values so that we have two readings with an error of half a division, adding up to an overall error of one division.

Burette: Error of 0.05 cm^3 per reading so overall error 0.1 cm^3 .

Example: What is the percentage error when 24.30 cm^3 of a solution is measured from a burette?

$$\text{percentage error} = \frac{0.1}{24.30} \times 100 = 0.41\%$$

Note: Percentage errors decrease as the amount measured increases, so using larger amounts decreases the percentage error.