1.3 – Chemical calculations II

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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 ($\frac{Mass}{A_r}$)		$\frac{4.80}{12.0}$	$\frac{1.01}{1.01}$	
	⟶	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 × 12.0) + (5 × 1.01) = 29.05

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

Molecular formula ⟶ 2 × empirical formula ⟶ C_4H_{10}

Note: *You can also use an empirical formula style calculation to find χ 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 dm³. 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?*

$$Zn + H_2SO_4 \longrightarrow ZnSO_4 + H_2$$

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

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

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

1 mol Zn : 1 mol H_2

⟶ 0.0920 mol Zn : 0.0920 mol H_2

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

volume of hydrogen = 0.0920 × 22.4 = 2.061 dm_3

Note: *Molar gas volume is 24.5 dm³ 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 $\mathbf{p_1}$, $\mathbf{V_1}$ and $\mathbf{T_1}$ 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 °C into K (+273).

If a question states, for example, that the temperature remains the same then you can use $\mathbf{p_1V_1 = p_2V_2}$ 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 J mol^{-1} K^{-1} (data booklet)
T ⟶ temperature ⟶ K

Conversions:

1 kPa = 1 × 10^3 Pa
1 atm = 1.01 × 10^5 Pa (data booklet)
1 cm³ = 1 × 10^{-6} m³
1 dm³ = 1 × 10^{-3} m³

Example: *Calculate the number of moles in 200 cm³ of a gas at 25°C and at a pressure of 100 kPa.*

p = 100 kPa ⟶ 100 × 10^3 Pa
V = 200 cm³ ⟶ 200 × 10^{-6} m³
T = 25°C ⟶ 298 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 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

moles = volume (dm^{-3}) × concentration (mol dm^{-3})

Example: *During a titration, 25.00 cm³ of 0.500 mol dm^{-3} hydrochloric acid was exactly neutralised by 35.00 cm³ of sodium hydroxide solution. Calculate the concentration of the sodium hydroxide solution.*

$$HCl + NaOH \longrightarrow NaCl + H_2O$$

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

moles HCl = $\frac{volume\ (cm^3)}{1000}$ × concentration

= $\frac{25.00}{1000}$ × 0.500 = 0.0125 mol

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

1 mol HCl : 1 mol NaOH

⟶ 0.0125 mol HCl : 0.0125 mol NaOH

Step 3 – Calculate the concentration of sodium hydroxide.

concentration of NaOH = $\frac{moles}{volume\ (dm^3)}$ = $\frac{0.0125}{0.035}$

= 0.357 mol dm^{-3}

10. Converting a concentration from mol dm⁻³ to g dm⁻³

g dm^{-3} = concentration (mol dm^{-3}) × M_r

11. Atom economy and percentage yield

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

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

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

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 cm³ per reading so overall error 0.1 cm³.

Example: *What is the percentage error when 24.30 cm³ of a solution is measured from a burette?*

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

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