2.1.3 Amount of Substance

The Mole (symbol = mol)

The mole is used as the unit for the amount of a substance.
A mole of substance contains the Avogadro constant, N_A, of particles. N_A is approximately 6.02×10^{23} $mol^{-1.}$
N_A is defined as the number of particles per mole.

Molar mass is the mass per mole of a substance, in grams mol^{-1}.

Molar gas volume is the gas volume per mole. In dm^3 mol^{-1}

Empirical formula of a compound shows the simplest whole number ratio of the atoms of each element present.

Molecular formula shows the actual number of atoms of each element present in a molecule of the compound.

Empirical and Molecular Formulae

Calculating empirical and molecular formulae
e.g. A compound contains 82.76% carbon and 17.24% hydrogen. Find its empirical formula.

Moles C 82.76/12.0 : H 17.24/1.0
= 6.897 : 17.24

Divide by the smallest number of moles, 6.897
= 1 : 2.4996
= 2 : 5
Empirical formula is C_2H_5

(This calculation can also be done if you are given the quantities of elements in grams.)

If the compound has molar mass 58, find its molecular formula.
Molar mass of EF = 29
Molar mass of compound = 2x molar mass of EF

Molecular formula is C_4H_{10}

Anhydrous and Hydrated Salts

Anhydrous salts are the compounds left after removing the **water of crystallisation** from a **hydrated salt,** e.g. Hydrated copper (II) sulphate is blue. Heating drives off the **water of crystallisation** as steam leaving a white solid, **anhydrous** copper(II) sulphate.

$$\mathbf{CuSO_4.5H_2O \rightarrow CuSO_4 + 5H_2O}$$

Calculating the formula of a hydrated salt:
0.942 g of $MgSO_4$ gave 0.461 g of residue after heating.

$MgSO_4$	:	H_2O	
0.461	:	0.481 (0.942-0.461)	
0.461/120.4	:	0.481/18	
3.83×10^{-3}	:	0.0267	
1	:	7	therefore $MgSO_4.7H_2O$

The Ideal Gas Equation

pV = nRT

where

p= pressure in pascals (Pa)

V = volume in m^3 (note 1 m^3 = 1000 dm^3 = 1,000,000 cm^3)

n = number of moles

T = Temperature in Kelvin (K)

R = gas constant (you will be given this, 8.31 J K^{-1} mol^{-1})

Mole calculations

A) For masses : moles = mass / molar mass

B) For volumes of gases : moles = volume (dm^3) / 24.0 at RTP

C) For solutions : moles = volume (dm^3) x concentration (mol dm^{-3})

Concentrations may be in mol dm^{-3} or g dm^{-3}. To convert from one to the other use A) above.
Concentration of 2 mol dm^{-3} means 2 moles of solid dissolved in 1 dm^3 of **solution** (not water).

Calculating quantities from equations:
1) Calculate moles of the known chemical using one of the three formulae above.
2) Calculate moles of the unknown chemical from the balanced equation.
3) Calculate mass, volume or concentration of unknown chemical using A), B), or C) above.

You need to be able to carry out structured titration calculations (from 2.1.4 Acids)

The terms concentrated and dilute are used as qualitative descriptions for the concentration of a solution.

Percentage Yields and Atom Economy

$$\% \text{ yield} = \frac{\text{actual mass}}{\text{theoretical mass}} \times 100 \quad \text{or} \quad \frac{\text{actual moles}}{\text{theoretical moles}} \times 100$$

$$\text{Atom Economy} = \frac{\text{molecular mass of desired products}}{\text{sum of molecular masses of all products}} \times 100$$

Addition reactions have an atom economy of 100 %, whereas substitution reactions are less efficient.

Chemical processes with a high atom economy produce fewer waste materials.

A reaction may have a high percentage yield but a low atom economy.