1. Empirical formula from combustion analysis

- **Empirical formula** are derived from **experimental** (empirical) data about the composition of a compound. An empirical formula shows the **simplest whole number ratio** of the **elements** in a compound.

Example 1 The analysis of a 2.4800 g sample of an organic compound showed it contained 0.6020 g of carbon, 1.7762 g of chlorine with the remainder being hydrogen. What is the empirical formula of the compound?

$m(H) = m(\text{compound}) - [m(C) + m(Cl)]$

$= 2.4800 - [0.6020 + 1.7762] = 0.1018\ g$

Since the compound contains only C, H and O then the sum of their masses must be 2.4800 g.

C	H	Cl	
C	H	Cl	List each element in the sample.
0.6020 g	0.1018 g	1.7762 g	List the mass of each element in the 2.480 g sample.
$\frac{0.6020}{12.01}$	$\frac{0.1018}{1.008}$	$\frac{1.7762}{35.45}$	Find the moles of each element by dividing the mass of each element my its molar mass.
0.05012	0.1010	0.05010	
$\frac{0.05012}{0.05010}$	$\frac{0.1010}{0.05010}$	$\frac{0.05010}{0.05010}$	To find the simplest mole ratio, divide each by the smallest value, ie 0.05010.
1.000	2.016	1.000	Thus the simplest whole number mole ratio of C:H:Cl is 1:2:1.

$\therefore$ the empirical formula is $\mathbf{CH_2Cl}$

The empirical formula CH_2Cl, shows this mole ratio.

Example 2 The complete combustion of a 3.648 g sample of a compound produced 7.137 g of carbon dioxide and 5.107 g of water. Find the compound's empirical formula if it contains the elements carbon, hydrogen and nitrogen only.

$n(CO_2) = \frac{m}{M} = \frac{7.137}{44.01} = 0.1622\ mol$ — Find the moles of CO_2.

$n(C) = n(CO_2) = 0.1622\ mol$ — Since there is one mole of C in every mole of CO_2.

$m(C) = n \times M = 0.1622 \times 12.01 = 1.948\ g$ — Since the carbon in CO_2 originated from the organic compound, this gives the mass of C in the sample.

$n(H_2O) = \frac{m}{M} = \frac{5.107}{18.016} = 0.2835\ mol$ — Find the moles of H_2O.

$n(H) = 2 \times n(H_2O) = 2 \times 0.2835 = 0.5669\ mol$ — There are two moles of H in every mole of H_2O.

$m(H) = n \times M = 0.5669 \times 1.008 = 0.5715\ g$ — Since the hydrogen in H_2O originated from the organic compound, this gives the mass of H in the sample.

$m(N) = 3.648 - [m(C) + m(H)]$

$= 3.648 - (1.949 + 0.5715) = 1.129\ g$ — The sample contains C, H and N only and has a total mass of 3.648 g.

C	H	N	
C	H	N	List each element in the compound.
1.948g	0.5713 g	1.129 g	List the mass of each element in the 3.648 g sample.
$\frac{1.948}{12.01}$	$\frac{0.5713}{1.008}$	$\frac{1.129}{14.01}$	Find the moles of each element, ie divide the mass of each element by its molar mass.
0.1622	0.5669	0.08058	To find the simplest mole ratio, divide by the smallest molar value, ie 0.08058.
2.013	7.036	1.000	

$\therefore$ the empirical formula is $\mathbf{C_2H_7N}$

The empirical formula C_2H_7N, shows this ratio.

2. Molecular formula

- The **molecular formula** shows the number of each type of atom present in **one molecule** of the substance.
- If the **molecular mass** and empirical formula of a compound are both known then the compound's **molecular formula** can be found.

Example 3 An organic compound has a molecular mass of 99.07 g mol^{-1} and an empirical formula of CH_2Cl. What is its molecular formula?

$M(CH_2Cl) = 12.01 + 1.008 \times 2 + 35.45 = 49.476 \text{ g mol}^{-1}$	Find the empirical formula mass from the known empirical formula CH_2Cl.
$\frac{\text{Molecular formula mass}}{\text{Empirical formula mass}} = \frac{99.07}{49.476} = 2.002$ $\therefore$ molecular formula $= \mathbf{C_2H_4Cl_2}$	Compare the molecular formula mass and empirical formula mass. The result 2, shows the M.F is twice the E F $\therefore$ double all empirical formula subscripts to obtain the molecular formula.

- **Molecular mass** can be found from empirical data for the **volume**, **pressure** and **temperature** of a **known mass** of gas. If the compound is normally a solid or liquid it would first need to be vaporised in order to make these measurements.

Example 4 A 3.429 g sample of organic compound is vaporised and found to occupy a volume of 1.130 L at 101.3 kPa and 398 K. Determine the compound's molecular formula if its empirical formula is CH_2Cl.

$PV = nRT$ *ie* $n = \frac{PV}{RT} = \frac{101.3 \times 1.130}{8.3145 \times 398} = 0.03461$ mol	Find the moles of gas using the ideal gas law.* Take care to use the correct value of R.
$n = \frac{m}{M}$ *ie* $M = \frac{m}{n} = \frac{3.429}{0.03461} = 99.07 \text{ g mol}^{-1}$	Find the molar mass of the gas.
$M(CH_2Cl) = 12.01 + 1.008 \times 2 + 35.45 = 49.476 \text{ g mol}^{-1}$	Determine the empirical formula mass from the empirical formula, ie CH_2Cl.
ratio $= \frac{\text{molecular formula mass}}{\text{empirical formula mass}} = \frac{99.07}{49.476} = 2.002$	Compare the molecular formula mass and empirical formula mass. This shows the molecular formula is twice the empirical formula.

$\therefore$ molecular formula $= \mathbf{C_2H_4Cl_2}$

* Alternatively, instead of using $n = PV/RT$, the gas volume at STP (V_{STP}) can be found using the combined gas law:

$$\frac{P_{STP} V_{STP}}{T_{STP}} = \frac{P_2 \times V_2}{T_2} \quad ie \quad V_{STP} = \frac{P_2 V_2 \times 273}{T_2 \times 101.3}$$

Then the moles of gas can be determined using the STP molar volume relationship:

$$n = \frac{V_{STP}}{22.4}$$