EMPIRICAL FORMULA

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(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. The empirical formula CH_2Cl, shows this mole ratio.

∴ the empirical formula is **CH_2Cl**

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	

∴ the empirical formula is **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* $n = \frac{PV}{RT} = \frac{101.3 \times 1.130}{8.3145 \times 398} = 0.03461 \text{ mol}$

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.

$$\text{ratio} = \frac{\text{molecular formula mass}}{\text{empirical formula mass}} = \frac{99.07}{49.476} = 2.002$$

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:

$$\frac{P_{STP} V_{STP}}{T_{STP}} = \frac{P_2 \times V_2}{T_2} \quad ie \quad V_{STP} = \frac{P_2V_2 \times 273}{T_2 \times 101.3}$$

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

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

Set 21 Empirical formula

1. The characteristic odour of pineapple is largely due to an organic compound containing the elements carbon, hydrogen and oxygen. A 3.433 g sample of the compound was analysed and found to contain 2.130 g of carbon and 0.3575 g of hydrogen. Another 6.182 g sample of the compound was vaporised at 135 °C and filled a 2.25 L container at a pressure of 80.2 kPa.

   a. Determine the **empirical formula** for the compound.

   b. What is its **molecular formula**?

   c. The compound is known to be an ester of butanoic acid. What is its **IUPAC name**?

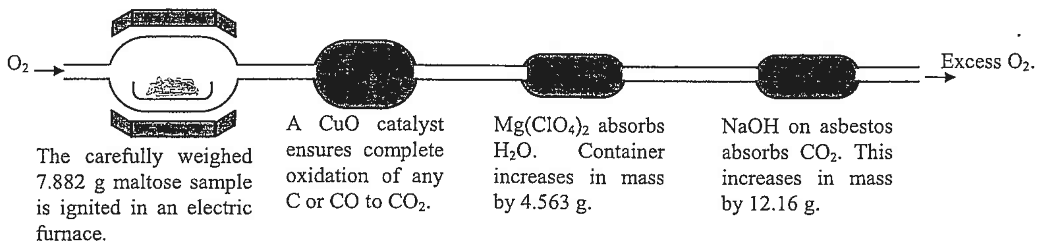
2. A particular hydrocarbon isolated from natural gas contains 85.66 % carbon with the remainder being hydrogen. At STP a 1.00 L sample of the gaseous compound was found to have a mass of 1.88 g.

   a. Determine the **empirical formula** of the hydrocarbon.

   b. What is its **molecular formula**?

   c. The hydrocarbon is found to rapidly decolourise a bromine water solution. What is its **IUPAC name**?

3. Maltose is a carbohydrate with a similar chemical composition to sucrose. It contains the elements carbon, hydrogen and oxygen. A 7.882 g sample of maltose is analysed by combustion analysis using an apparatus similar to that shown here.



   a. Using the data presented here determine the **empirical formula** for maltose.

   b. Another 3.115 g sample of the maltose was vaporised and found to occupy a volume of 324.2 mL at 165 °C and 101.9 kPa. What is the **molecular formula** for maltose?

4. The hydrocarbon used in a common gas lighter was analysed by burning a 5.249 g sample of the gas and collecting the resulting water vapour in a cold trap. This produced 8.198 g of water. Another 3.121 g sample of the compound was released into a sealed container and occupied a volume of 1.289 L at 23.5 °C and 102.5 kPa. What is the **molecular formula** of this hydrocarbon?

5. A 3.996 g sample of an organic compound containing the elements carbon, hydrogen and oxygen was completely burnt in oxygen. This produced 7.974 g of carbon dioxide and 3.264 g of water. A further 1.289 g sample of the compound was vaporised and occupied a volume of 446.8 mL at 185.5 °C and 125.4 kPa.

   a. Determine the **empirical formula**.

   b. What is its **molecular formula**?

   c. The unknown organic compound is found to react vigorously with sodium metal but shows no reaction with acidified potassium permanganate solution. What is its **IUPAC name**?

6. α-amino acids are the building blocks from which all proteins are made. One such amino acid is alanine. It contains the elements carbon, hydrogen, oxygen and nitrogen. To determine its empirical formula a 2.170 g sample was completely burnt in oxygen. The resulting carbon dioxide and water were collected and found to weigh 3.219 g and 1.537 g respectively. The nitrogen contained in the sample was released during combustion and collected as nitrogen gas. When isolated, the nitrogen gas had a volume of 300.3 mL at 102.1 kPa and 302.5 K.

   a. Determine the **empirical formula** for alanine.

   b. Further analysis showed alanine has a molar mass of **88.7 g mol^{-1}** and contains a **carboxylic acid** group and a **2° amino** group. Draw a possible **structure** for this α-amino acid.

7. Two chemistry students Bri and Scott were researching one of the chemical components of the rhubarb plant. They were able to extract a white crystalline solid from the stem tissue of the plant. Using various analytical techniques Bri determined that the crystalline solid contained **two carboxylic acid groups per molecule.** To find its empirical formula Scott dried a sample of the crystalline solid to ensure any water of crystallisation was driven off then weighed 10.79 g of the amorphous solid. This amorphous solid was completely burnt in excess oxygen producing 10.60 g of carbon dioxide and 2.136 g of water.

   a. Given the compound contains only carbon, hydrogen and oxygen, determine its **empirical formula.**
   b. A further 1.851 g sample of the compound was dissolved in water and made up to 250.0 mL in a volumetric flask. 20.00 mL samples of this solution were titrated with 0.2021 mol L^{-1} $NaOH$*(aq)*. On average 16.25 mL of $NaOH$*(aq)* was needed for equivalence. What is the **molecular formula**?
   c. Draw a possible **structure** for the compound.

8. A 4.413 g sample of a hydrocarbon is burnt in excess oxygen forming carbon dioxide and water. The resulting gases were bubbled through a solution of $NaOH$*(aq)* absorbing the CO_2*(g)* as Na_2CO_3*(aq)*. Adding $Ca(NO_3)_2$*(aq)* to this results in a precipitate of $CaCO_3$*(s)*. When washed and dried the $CaCO_3$*(s)* has a mass of 31.34 g.
   Another 4.485 g sample of the compound was vaporised and occupied a volume of 1.754 L at 76 °C and 129.5 kPa.

   a. Using this information determine the **empirical formula** of the hydrocarbon.
   b. What is its **molecular formula**?
   c. The unknown organic compound is found to slowly discolour a bromine water solution. Suggest a possible **IUPAC name** for the hydrocarbon?

Some empirical formula determinations will involve analysis data from **two different mass samples.** In situations like this it is advisable to use the given data to determine the **percentage composition** of each individual element in the compound. The percentage composition results can then be used to find the empirical formula.

9. Elementary analysis showed that an organic compound contained **carbon, hydrogen, nitrogen** and **oxygen** as its only constituents. A **1.279 g sample** of it was burned completely to form 1.600 g of carbon dioxide and 0.7700 g of water. Another separately weighed **1.625 g sample** of the compound was decomposed and released all of the nitrogen it contained as **nitrogen gas**. The nitrogen had a volume of 183.0 mL at 20.0 °C and 102.5 kPa. What is the empirical formula of the compound? (See margin note.)

10. Aspartame is a compound used as an artificial sweetener in foods and beverages. It contains the elements carbon, hydrogen, oxygen and nitrogen. To determine its empirical formula a **7.335 g sample** was completely burnt in oxygen. The resulting carbon dioxide and water were collected and found to weigh 15.36 g and 4.041 g respectively. A **second 4.719 g** aspartame sample was treated to convert the nitrogen it contained into ammonia (NH_3). The resulting ammonia was absorbed into 100.0 mL of 0.3559 mol L^{-1} HCl*(aq)*. The excess HCl*(aq)* was then titrated to equivalence using 28.18 mL of 0.1249 mol L^{-1} $NaOH$*(aq)*. Determine the **empirical formula** for aspartame.