

AS 91161: Carry out quantitative analysis

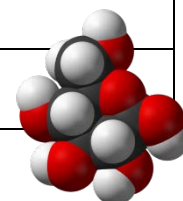
DETERMINING EMPIRICAL AND MOLECULAR FORMULAE

The **empirical formula is the simplest whole number ratio of atoms** in a compound. The **molecular formula is the same as or a multiple of the empirical formula**, and is based on **the actual number of atoms of each type in the compound**. For example, if the empirical formula of a compound is C_3H_8 , its molecular formula may be C_3H_8 , C_6H_{16} , etc. An empirical formula is often calculated from elemental composition data.

Determine the empirical and molecular formula for a compound with 40.0% C, 6.72% H, 53.3% O, and a molar mass of 180 g mol^{-1} .

$$M(\text{C}) = 12.0 \text{ g mol}^{-1}, M(\text{H}) = 1.00 \text{ g mol}^{-1} \text{ and } M(\text{O}) = 16.0 \text{ g mol}^{-1}$$

	C	H	O
Write the percentage as a mass	40.0 g	6.72 g	53.3 g
Calculate amount in mol; ($n = m/M$)	$40.0/12.0$ = 3.33	$6.72 / 1.00$ = 6.72	$53.3 / 16.0$ = 3.33
Divide each answer by the smallest number to get a ratio	$3.33/3.33 = 1$	$6.72 / 3.33 = 2$	$3.33/3.33 = 1$
x2 or x3 etc only IF numbers are not approx. whole numbers	n/a here (as 1:2:1)		
Write the empirical formula	CH_2O		
Molar mass of empirical formula	$M(\text{CH}_2\text{O}) = 12.0 + (2 \times 1.00) + 16.0 = 30 \text{ g mol}^{-1}$		
Divide molar mass (molecular formula) by molar mass (empirical formula) to find a multiple	$180 / 30 = 6$		
Write the molecular formula (empirical formula x multiple)	$\text{CH}_2\text{O} \times 6$ $\text{C}_6\text{H}_{12}\text{O}_6$		



Guaifenesin is a drug sold over the counter to assist the bringing up of phlegm from the airways in respiratory tract infections. Determine the empirical and molecular formulas of guaifenesin from the following percentage composition data. 60.6% C, 7.07% H, 32.3% O. The molecular mass of guaifenesin is 198 g mol^{-1} .

	C	H	O
Write the percentage as a mass	60.6 g	7.07 g	32.3 g
Calculate amount in mol; ($n = m/M$)	$60.6/12.0 = 5.05$	$7.07/1.00 = 7.07$	$32.3/16.0 = 2.02$
Divide each answer by the smallest number to get a ratio	$5.05/2.02 = 2.5$	$7.07/2.02 = 3.5$	$2.02/2.02 = 1$
x2 or x3 etc only IF numbers are not approx. whole numbers	2.5×2 5	3.5×2 7	1×2 2
Write the empirical formula	$\text{C}_5\text{H}_7\text{O}_2$		
Molar mass of empirical formula	$M(\text{C}_5\text{H}_7\text{O}_2) = (5 \times 12.0) + (7 \times 1.00) + (2 \times 16.0) = 99 \text{ g mol}^{-1}$		
Divide molar mass of molecular formula by molar mass of empirical formula to find a multiple	$198/99 = 2$		
Write the molecular formula (empirical formula x multiple)	$\text{C}_{10}\text{H}_{14}\text{O}_4$		