9. Finding the empirical formula or molecular formula

- The empirical formula of a compound is the simplest whole number ratio of atoms of each element in the compound. It can be the same as the compound's molecular formula - but not always.
- Molecular formula: It is a chemical formula that gives the total number of atoms of each element in each molecule of a substance.

Example1:

8 Hydrocarbons are compounds which contain only carbon and hydrogen.

(a) 20 cm^3 of a gaseous hydrocarbon was burned in 120 cm^3 of oxygen, which is in excess. After cooling, the volume of the gases remaining was 90 cm^3. Aqueous sodium hydroxide was added to remove carbon dioxide, 30 cm^3 of oxygen remained. All volumes were

(iii) Complete the following.

volume of gaseous hydrocarbon = ...cm^3

volume of oxygen used = ...cm^3

volume of carbon dioxide formed = ...cm^3 [2]

(iv) Use the above volume ratio to find the mole ratio in the equation below and hence find the formula of the hydrocarbon.

.....$C_xH_y(g)$ + ...$O_2(g)$ → .....$CO_2(g)$ + ...$H_2O(l)$

hydrocarbon formula = ... [2]

Solution:

Volume of the gaseous hydrocarbon=20cm^3

Volume of oxygen used= (Total O_2)-(Left O_2)=120cm^3-30cm^3=90cm^3

Volume of CO_2 formed =90cm^3-30cm^3=60cm^3

Hence experimental mole ratio:

	C_xH_y	:	O_2	:	CO_2	:	H_2O
	20	:	90	:	60		
Reduced mole ratio	2	:	9	:	6	:	6

Careful observation tells us that there are 18 oxygen to the left ($9O_2$) , so there must be not more than 18 oxygen atoms to the right. 6 CO_2 has 12 oxygen atoms. So the only possible coefficient of H_2O to the right is 6.

Balanced equation is: $2C_xH_y$: $9O_2$: $6CO_2$: $6H_2$

Also; $2C_x$=6 ; Hence x= 3

and $2H_y$=12 Hence y=6

Required formula= C_3H_6

Empirical formula :Example2:

[O/N/06-P3-Q6]

6 An ore of copper is the mineral, chalcopyrite. This is a mixed sulphide of iron and copper.

(a) Analysis of a sample of this ore shows that 13.80 g of the ore contained 4.80 g of copper, 4.20g of iron and the rest sulphur.
Complete the table and calculate the empirical formula of chalcopyrite.

	copper	iron	sulphur
composition by mass / g	4.80	4.20	
number of moles of atoms			
simplest mole ratio of atoms			

[3]

The empirical formula is

..... [1]

Solution:

No of moles:

Copper= 4.80/63=0.076

Iron = 4.20/56 =0.075

Sulfur= [13.80-(4.80+4.20)]/32=0.15

Simplest mole ratio =	**Copper**	:	**Iron**	:	**Sulfur**
Divide by smallest no of moles	0.076/0.075	:	0.075/0.075	:	0.15/0.075
	1.01 rounded off to 1.00	:	1	:	2

Empirical formula is: $CuFeS_2$

Empirical formula: Example 3 [O/N/08-P31-Q4]

(b) Benzene contains 92.3% of carbon and its relative molecular mass is 78.

(i) What is the percentage of hydrogen in benzene?

..... [1]

(ii) Calculate the ratio of moles of C atoms: moles of H atoms in benzene.

.....

..... [2]

(iii) Calculate its empirical formula and **then** its molecular formula.

The empirical formula of benzene is .....

The molecular formula of benzene is ..... [2]

Solution:

- **Percentage of benzene= 100-92.3=7.7%**

Ratio of moles of *C* and H is:

	C	:	H
• Moles=mass/M_r	92.3/12=7.69=7.7		7.7/1=7.7
Smallest mole ratio	7.7/7.1=1	:	7.7/7.1=1

- **Ratio of moles of *C* and H is 1:1**
- **Empirical formula is: *CH***

M_r of Benzene=78---given,

Hence the Mr(*C*) + Mr(H) = M_r Benzene

x(12) + x(1) =78

13x=78

x=78/13=6

Hence required molecular formula is 6 x *CH* = C_6H_6

Empirical formula: Example 4 [O/N/14-V33-Q2B]

(b) Compound X is a hydrocarbon. It contains 85.7% of carbon. The mass of one mole of X is 84 g.

(i) What is the percentage of hydrogen in the compound ?

..... [1]

(ii) Calculate the empirical formula of X. Show your working.

empirical formula = ... [3]

(iii) What is the molecular formula of compound X?

..... [1]

Solution:

- **Percentage of hydrogen= 100-85.7=14.3%**
- **Empirical formula of X**

	C	:	H
Moles =Mass/M_r	85.7/12=7.14		14.3
Small whole number mole ratio	7.14/7.14=1	:	14.3/7.14=2.00

Empirical formula= CH_2

- **Molecular formula of compound X**

Mr(C_xH_{2x})=84

Mr (C) + Mr (H) = Mr compound X

12x + 1(2x) = 84

14x = 84

x = 84/14 = 6

Molecular formula of compound=C_6H_{12}

10: Finding the moles of water in a molecule of a given hydrated salt

(c) Insoluble salts are made by precipitation. An equation for the preparation of barium sulfate is given below.

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$$BaCl_2(aq) + MgSO_4(aq) \rightarrow BaSO_4(s) + MgCl_2(aq)$$

This reaction can be used to find x in the formula for hydrated magnesium sulfate $MgSO_4.xH_2O$.

A known mass of hydrated magnesium sulfate, $MgSO_4.xH_2O$, was dissolved in water. Excess aqueous barium chloride was added. The precipitate of barium sulfate was filtered, washed and dried. Finally it was weighed.

Mass of hydrated magnesium sulfate = 1.476 g

Mass of barium sulfate formed = 1.398 g

The mass of one mole of $BaSO_4$ = 233 g

The number of moles of $BaSO_4$ formed = ... [1]

The number of moles of $MgSO_4.xH_2O$ = ... [1]

The mass of one mole of $MgSO_4.xH_2O$ = ... g [1]

The mass of one mole of $MgSO_4$ = 120 g

The mass of xH_2O in one mole of $MgSO_4.xH_2O$ = ... [1]

x = ... [1]

Solution:

- **Moles of $BaSO_4$ formed= Mass of $BaSO_4/M_r$=1.398/233=0.006**
- **Number of moles of $MgSO_4.xH_2O$=0.006**

[Mole ratio from the standard equation is: 1: 1:1:1]

Mole ratio for experiment is: 0.006 : 0.006 : 0.006 : 0.006]

- **Mass of 1 mole of $MgSO_4.xH_2O$ means the M_r of $MgSO_4.xH_2O$**
  =Mass of $MgSO_4.xH_2O$÷ moles
  =1.476÷0.006 =246g

Mass of 1 mole of $MgSO_4$=120g

Mass of xH_2O in one mole of $MgSO_4.xH_2O$ = 246g-120g=126g

- **x=**
  Mass of 1 mole of H_2O= 18g

Mass of x moles of H_2O = 126g

18x=126 ; x =126/18 =7 . Hence x=7