

## MOLES

- THE MOLE**
- the standard unit of amount of a substance ( **mol** )
  - the number of particles in a mole is known as **Avogadro's constant (  $N_A$  )**
  - Avogadro's constant has a value of  **$6.02 \times 10^{23} \text{ mol}^{-1}$** .
  - don't get too 'worked up' about it; it is only a very large number
    - after all, we use dozen (12); score (20); grand (1000) for certain numbers
    - 2 dozen (24) is twice 1 dozen (12) and 2 moles is twice as many as 1 mole

### RELATIVE MASS

#### **Relative Atomic Mass ( $A_r$ )**

The mass of an atom relative to that of the carbon 12 isotope having a value of 12.000

$$\text{or} \quad \frac{\text{average mass per atom of an element} \times 12}{\text{mass of an atom of } ^{12}\text{C}}$$

#### \* **Relative Molecular Mass ( $M_r$ )**

The sum of all the relative atomic masses present in a molecule

$$\text{or} \quad \frac{\text{average mass of a molecule} \times 12}{\text{mass of an atom of } ^{12}\text{C}}$$

**NB** \* **Relative Formula Mass** is used if the species is ionic

### MOLAR MASS

The mass of one mole of substance. units are  **$\text{g mol}^{-1}$**  or  **$\text{kg mol}^{-1}$** .

e.g. the molar mass of water is  $18 \text{ g mol}^{-1}$

**molar mass = mass of one particle x Avogadro's constant** ( $6.02 \times 10^{23} \text{ mol}^{-1}$ )

*Example* If 1 atom has a mass of  $1.241 \times 10^{-23} \text{g}$   
 1 mole of atoms will have a mass of  $1.241 \times 10^{-23} \text{g} \times 6.02 \times 10^{23} = 7.471 \text{g}$

**Q.1** Calculate the mass of... one mol of carbon-12 atoms

0.5 mol of oxygen-16 atoms

0.5 mol of oxygen-16 molecules.

[ mass of proton  $1.672 \times 10^{-24} \text{g}$ , mass of neutron  $1.674 \times 10^{-24} \text{g}$ , mass of electron  $9.109 \times 10^{-28} \text{g}$  ]

## MOLE CALCULATIONS

Substances      mass                      g            or      kg  
                          molar mass      g mol<sup>-1</sup>    or      kg mol<sup>-1</sup>

$$\text{moles} = \frac{\text{mass}}{\text{molar mass}}$$

*Example*      Calculate the number of moles of oxygen molecules in 4g

oxygen molecules have the formula O<sub>2</sub>

the relative mass will be 2 x 16 = 32 so the molar mass will be 32g mol<sup>-1</sup>

$$\text{moles} = \frac{\text{mass}}{\text{molar mass}} = \frac{4\text{g}}{32\text{g mol}^{-1}} \quad \text{ANS. } 0.125 \text{ mol}$$

**Q.2**      Calculate the number of moles in...

10g of Ca atoms

10g of CaCO<sub>3</sub>

4g of hydrogen atoms

4g of hydrogen molecules

Calculate the mass of...

2 mol of CH<sub>4</sub>

0.5 mol of NaNO<sub>3</sub>

6 mol of nitrogen atoms

6 mol of nitrogen molecules

Solutions      molarity      concentration / mol dm<sup>-3</sup>  
                          volume      dm<sup>3</sup> or cm<sup>3</sup>

$$\begin{aligned} \text{moles} &= \text{concentration} \times \text{volume} \\ &= \text{molarity} \times \text{volume in dm}^3 \\ &= \frac{\text{molarity} \times \text{volume in cm}^3}{1000} \end{aligned}$$

The **1000** takes into account that there are 1000 cm<sup>3</sup> in 1dm<sup>3</sup>

*Example 1*      Calculate the number of moles of sodium hydroxide in 25cm<sup>3</sup> of 2M NaOH

$$\begin{aligned} \text{moles} &= \frac{\text{molarity} \times \text{volume in cm}^3}{1000} \\ &= \frac{2 \text{ mol dm}^{-3} \times 25\text{cm}^3}{1000} \quad \text{ANS. } 0.05 \text{ mol} \end{aligned}$$

**Example 2** What volume of 0.1M H<sub>2</sub>SO<sub>4</sub> contains 0.002 moles ?

$$\begin{aligned} \text{volume in cm}^3 &= \frac{1000 \times \text{moles}}{\text{molarity}} \quad (\text{re-arrangement of above}) \\ &= \frac{1000 \times 0.002}{0.1 \text{ mol dm}^{-3}} \quad \quad \quad \mathbf{ANS. \ 20 \text{ cm}^3} \end{aligned}$$

**Example 3** 4.24g of Na<sub>2</sub>CO<sub>3</sub> is dissolved in water and the solution made up to 250 cm<sup>3</sup>. What is the concentration of the solution in mol dm<sup>-3</sup> ?

$$\begin{aligned} \text{molar mass of Na}_2\text{CO}_3 &= 106 \text{ g mol}^{-1} \\ \text{no. of moles in 250cm}^3 &= 4.24 \text{ g} / 106 \text{ g mol}^{-1} = 0.04 \text{ mol} \\ \text{no. of moles in 1000cm}^3 \text{ (1dm}^3) &= 0.16 \text{ mol} \end{aligned}$$

**ANS. 0.16 mol dm<sup>-3</sup>**

**Q.3** Calculate the number of moles in...

1dm<sup>3</sup> of 2M NaOH

250cm<sup>3</sup> of 2M NaOH

5dm<sup>3</sup> of 0.1M HCl

25cm<sup>3</sup> of 0.2M H<sub>2</sub>SO<sub>4</sub>

25cm<sup>3</sup> of 0.2M HCl

27.58cm<sup>3</sup> of 0.101M H<sub>2</sub>SO<sub>4</sub>

Calculate the concentration (in mol dm<sup>-3</sup>) of solutions containing

1 mol of HCl in 2dm<sup>3</sup>

0.2 mol of HCl in 2dm<sup>3</sup>

0.1 mol of NaOH in 250cm<sup>3</sup>

0.1 mol of H<sub>2</sub>SO<sub>4</sub> in 25cm<sup>3</sup>

## EMPIRICAL FORMULAE AND MOLECULAR FORMULAE

### Empirical Formula

**Description** Expresses the elements in a simple ratio (e.g. CH<sub>2</sub>).  
It can sometimes be the same as the molecular formula (e.g. H<sub>2</sub>O and CH<sub>4</sub>)

**Calculations** You need

- mass, or percentage mass, of each element present
- relative atomic masses of the elements present

**Example 1** Calculate the empirical formula of a compound containing C (48%), H (4%) and O (48%)

	<b>C</b>	<b>H</b>	<b>O</b>
1) Write out percentages (by mass)	48%	4%	48%
2) Divide by the relative atomic mass ... this gives a molar ratio	48/12	4/1	48/16
	4	4	3
3) If not whole numbers then scale up			
4) Express as a formula	<b>C<sub>4</sub>H<sub>4</sub>O<sub>3</sub></b>		

**Example 2** Calculate the empirical formula of a compound with C (1.8g), O (0.48g), H (0.3g)

	<b>C</b>	<b>H</b>	<b>O</b>
1) Write out ratios by mass	1.8	0.3	0.48
2) Divide by relative atomic mass (this gives the molar ratio)	1.8 / 12	0.3 / 1	0.48 / 16
	0.15	0.3	0.03
3) If not whole numbers then scale up - try dividing by smallest value (0.03)	5	10	1
4) Express as a formula	<b>C<sub>5</sub>H<sub>10</sub>O</b>		

### Molecular Formula

**Description** Exact number of atoms of each element in the formula (e.g. C<sub>4</sub>H<sub>8</sub>)

**Calculations** Compare empirical formula relative molecular mass. The relative molecular mass of a compound will be an exact multiple (x1, x2 etc.) of its relative empirical mass.

**Example** Calculate the molecular formula of a compound of empirical formula CH<sub>2</sub> and relative molecular mass 84.

$$\begin{aligned}
 \text{mass of CH}_2 \text{ unit} &= 14 \\
 \text{divide molecular mass (84) by 14} &= 6 \\
 \text{molecular formula} &= \text{empirical formula} \times 6 = \text{C}_6\text{H}_{12}
 \end{aligned}$$

## REACTING MASSES - THE LAW OF CONSERVATION OF MASS

**The masses of all the products = the masses of all the reactants**

In other words **The total mass of all the atoms in the products is the same as that of all the atoms in the reactants**

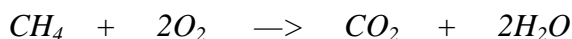
	<b>CaCO<sub>3</sub></b>	→	<b>CaO</b>	+	<b>CO<sub>2</sub></b>		
<i>Relative masses</i>	100	—	56		44		
<i>actual masses</i>	100g (1 mol)		56g (1 mol)		44g (1 mol)		
<i>if you started with</i>	25g (0.25 mol)		0.25 mol (14g)		0.25 mol (11g)		
	<b>CH<sub>4</sub></b>	+	<b>2O<sub>2</sub></b>	→	<b>CO<sub>2</sub></b>	+	<b>2H<sub>2</sub>O</b>
<i>Relative masses</i>	16		32		44		18
<i>actual masses</i>	16g		64g (2 mol)		44g		36g (2 mol)
<i>to make 88g CO<sub>2</sub></i>	<b>32g</b>		128g		<b>88g</b>		72g

### Q.4

a) What mass of CaSO<sub>4</sub> can be made from 112g of CaO?



b) What mass of carbon dioxide is made by burning 80kg of CH<sub>4</sub>?



c) How much NaOH is needed to make 42.5g of NaNO<sub>3</sub>?



d) Which gives a bigger mass of CO<sub>2</sub>: 200g of CaCO<sub>3</sub> or 32g of CH<sub>4</sub>?

[ A<sub>r</sub> values H = 1, C = 12, N = 14, O = 16, Na = 23, S = 32, Ca = 40, Cu = 63.5 ]

## YIELD AND PERCENTAGE YIELD

**YIELD** The mass you get

**PERCENTAGE YIELD** The mass you get compared with the maximum you ought to get

### Q.5

What mass of CuSO<sub>4</sub> can be made from 7.95g of CuO?



A student carried out this experiment. When they weighed the product, they found they had only made 7.20g of CuSO<sub>4</sub>.

i) What is the yield of CuSO<sub>4</sub> ?

ii) What is the percentage yield of CuSO<sub>4</sub> ?

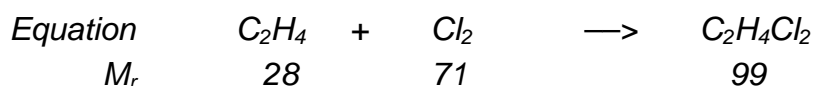
## ATOM ECONOMY

- Introduction
- in most reactions you only want to make one of the resulting products
  - **atom economy is a measure of how much of the products are useful**
  - a **high atom economy** means that there is **less waste**

$$\frac{\text{MOLECULAR MASS OF DESIRED PRODUCT}}{\text{SUM OF MOLECULAR MASSES OF ALL PRODUCTS}} \times 100$$

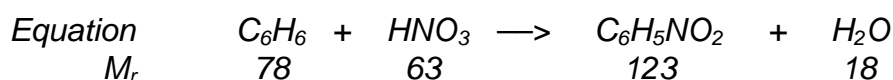
Example calculations

1. Formation of 1,2-dichloroethane,  $C_2H_4Cl_2$



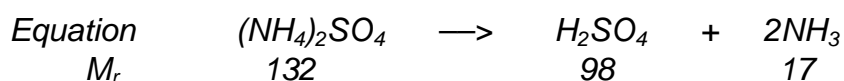
$$\begin{aligned} \text{atom economy} &= \frac{\text{molecular mass of } C_2H_4Cl_2}{\text{molecular mass of all products}} \times 100 \\ &= \frac{99}{99} \times 100 = \mathbf{100\%} \end{aligned}$$

2. Formation of nitrobenzene,  $C_6H_5NO_2$



$$\begin{aligned} \text{atom economy} &= \frac{\text{molecular mass of } C_6H_5NO_2}{\text{molecular mass of all products}} \times 100 \\ &= \frac{123}{123 + 18} \times 100 = \mathbf{87.2\%} \end{aligned}$$

3. Preparation of ammonia from the decomposition of ammonium sulphate



$$\begin{aligned} \text{atom economy} &= \frac{\mathbf{2 \times} \text{molecular mass of } NH_3}{\text{molecular mass of all products}} \times 100 \\ &= \frac{\mathbf{2 \times} 17}{98 + (2 \times 17)} \times 100 = \mathbf{25.8\%} \end{aligned}$$

Summary

- **addition** reactions will have **100% atom** economy
- **substitution** reactions will have **less than 100% atom** economy
- **elimination** reactions will have **less than 100% atom** economy
- **high atom economy = fewer waste materials**  
= **GREENER** and **MORE ECONOMICAL**

Notes

- the percentage yield of a reaction must also be taken into consideration
- some reactions may have a high yield but a low atom economy
  - some reactions may have a high atom economy but a low yield

## MOLAR GAS VOLUME (MOLAR VOLUME)

At rtp **The molar volume of any gas at rtp is  $24 \text{ dm}^3 \text{ mol}^{-1}$**  ( $0.024 \text{ m}^3 \text{ mol}^{-1}$ )  
**rtp** **R**oom **T**emperature and **P**ressure

At stp **The molar volume of any gas at stp is  $22.4 \text{ dm}^3 \text{ mol}^{-1}$**  ( $0.0224 \text{ m}^3 \text{ mol}^{-1}$ )  
**stp** **S**tandard **T**emperature and **P**ressure (**273K and  $1.013 \times 10^5 \text{ Pa}$** )

*example* 0.5g of a gas occupies  $250 \text{ cm}^3$  at rtp. Calculate its molar mass.

$250 \text{ cm}^3$	has a mass of	0.5g	
$1000 \text{ cm}^3 (1 \text{ dm}^3)$	has a mass of	2.0g	x4 to convert to $\text{dm}^3$
$24 \text{ dm}^3$	has a mass of	48.0g	x24 to convert to $24 \text{ dm}^3$

**ANSWER: The molar mass is  $48.0 \text{ g mol}^{-1}$**

**Q.6** Calculate the mass of...

- a)  $2.4 \text{ dm}^3$  of carbon dioxide,  $\text{CO}_2$  at rtp
- b)  $120 \text{ cm}^3$  of sulphur dioxide,  $\text{SO}_2$  at rtp
- c) 0.08g of a gaseous hydrocarbon occupies  $120 \text{ cm}^3$  at rtp. Identify the gas.

**Calculations** methods include using

- the ideal gas equation  $PV = nRT$
- the Molar Volume at stp

For 1 mole of gas  $PV = RT$

for n moles of gas  $PV = nRT$

(as moles = mass/molar mass)  $PV = \frac{mRT}{M}$

$$PV = nRT$$

$$PV = \frac{mRT}{M}$$

<i>where</i>	P pressure	Pascals ( <b>Pa</b> ) or <b><math>\text{N m}^{-2}</math></b>
	V volume	<b><math>\text{m}^3</math></b> (there are $10^6 \text{ cm}^3$ in a $\text{m}^3$ )
	n number of moles of gas	
	R gas constant	<b><math>8.31 \text{ J K}^{-1} \text{ mol}^{-1}</math></b>
	T temperature	<b>Kelvin</b> ( $\text{K} = ^\circ\text{C} + 273$ )
	m mass	<b>g</b> or <b>Kg</b>
	M molar mass	<b><math>\text{g mol}^{-1}</math></b> or <b><math>\text{Kg mol}^{-1}</math></b>

*Old units* **1 atmosphere** is equivalent to **760 mm/Hg** or  **$1.013 \times 10^5 \text{ Pa}$**  ( $\text{Nm}^{-2}$ )  
**1 litre ( $1 \text{ dm}^3$ )** is equivalent to  **$1 \times 10^{-3} \text{ m}^3$**

**Example 1** Calculate the number of moles of gas present in 500cm<sup>3</sup> at 100 KPa pressure and at a temperature of 27°C.

$$\begin{array}{lll}
 P & = 100 \text{ KPa} & = 100000 \text{ Pa} \\
 V & = 500 \text{ cm}^3 & \times 10^{-6} = 0.0005 \text{ m}^3 \\
 T & = 27 + 273 & = 300 \text{ K} \\
 R & = 8.31 \text{ J K}^{-1} \text{ mol}^{-1} & = 8.31
 \end{array}$$

$$PV = nRT \quad \therefore n = \frac{PV}{RT} = \frac{100000 \times 0.0005}{300 \times 8.31} = \mathbf{0.02 \text{ mol}}$$

**Example 2** Calculate the relative molecular mass of a vapour if 0.27g of gas occupy 400 cm<sup>3</sup> at a temperature of 227°C and a pressure of 100 KPa.

$$\begin{array}{lll}
 P & = 100 \text{ KPa} & = 100000 \text{ Pa} \\
 V & = 400 \text{ cm}^3 & \times 10^{-6} = 0.0004 \text{ m}^3 \\
 T & = 227 + 273 & = 500 \text{ K} \\
 m & = 0.27\text{g} & = 0.27\text{g} \\
 R & = 8.31 \text{ J K}^{-1} \text{ mol}^{-1} & = 8.31
 \end{array}$$

$$PV = \frac{mRT}{M} \quad \therefore M = \frac{mRT}{PV} = \frac{0.27 \times 500 \times 8.31}{100000 \times 0.0004} = \mathbf{28.04}$$

### Q.7

- Convert the following volumes into m<sup>3</sup>
  - a) 1dm<sup>3</sup>                      b) 250cm<sup>3</sup>                      c) 0.1cm<sup>3</sup>
- Convert the following temperatures into Kelvin
  - a) 100°C                      b) 137°C                      c) -23°C
- Calculate the volume of 0.5 mol of propane gas at 298K and 10<sup>5</sup> Pa pressure
- Calculate the mass of propane (C<sub>3</sub>H<sub>8</sub>) contained in a 0.01 m<sup>3</sup> flask maintained at a temperature of 273K and a pressure of 250kPa.



**Calculation** The volume of a gas varies with temperature and pressure. To convert a volume to that which it will occupy at stp (or any other temperature and pressure) one use the relationship which is derived from Boyle's Law and Charles' Law.

$$\frac{P_1 V_1}{T_1} = \frac{P_2 V_2}{T_2}$$

where  $P_1$  initial pressure  
 $V_1$  initial volume  
 $T_1$  initial temperature (in Kelvin)

$P_2$  final (in this case, standard) pressure  
 $V_2$  final volume (in this case, at stp)  
 $T_2$  final (in this case, standard) temperature (in Kelvin)

**Calculations** Convert the volume of gas to that at stp then scale it up to the molar volume. The mass of gas occupying 22.4 dm<sup>3</sup> (22.4 litres, 22400cm<sup>3</sup>) is the molar mass.

**Experiment** It is possible to calculate the molar mass of a gas by measuring the volume of a given mass of gas and applying the above equations.

**Methods**

- Gas syringe method
- Victor Meyer method
- Dumas bulb method

**Example** A sample of gas occupies 0.25 dm<sup>3</sup> at 100°C and 5000 Pa pressure. Calculate its volume at stp [273K and 100 kPa].

$P_1$ initial pressure	= 5000 Pa	$P_2$ final pressure	= 100000 Pa
$V_1$ initial volume	= 0.25 dm <sup>3</sup>	$V_2$ final volume	= ?
$T_1$ initial temperature	= 373K	$T_2$ temperature	= 273K

$$\text{thus} \quad \frac{5000 \times 0.25}{373} = \frac{100000 \times V_2}{273}$$

$$\text{therefore} \quad V_2 = \frac{273 \times 5000 \times 0.25}{373 \times 100000} = 0.00915 \text{ dm}^3 \quad (9.15 \text{ cm}^3)$$

**example** 1g of gas occupies 278cm<sup>3</sup> at 25°C and 2 atm pressure. Calculate its molar mass.

$$\text{i) convert to stp} \quad \frac{2 \times 278}{298} = \frac{1 \times V}{273} \quad \therefore V = \frac{278 \times 2 \times 273}{1 \times 298} = 509 \text{ cm}^3$$

ii) convert to molar volume	1g	occupies	509cm <sup>3</sup>	at stp
	1/509g	occupies	1cm <sup>3</sup>	
	22400 x 1/509g	occupies	22400cm <sup>3</sup>	

therefore 44g occupies 22.4 dm<sup>3</sup> at stp

**ANSWER: The molar mass is 44g mol<sup>-1</sup>**

## Gay-Lussac's Law of Combining Volumes

*Statement*     **“ When gases combine they do so in volumes that are in a simple ratio to each other and to that of any gaseous product(s) ”**

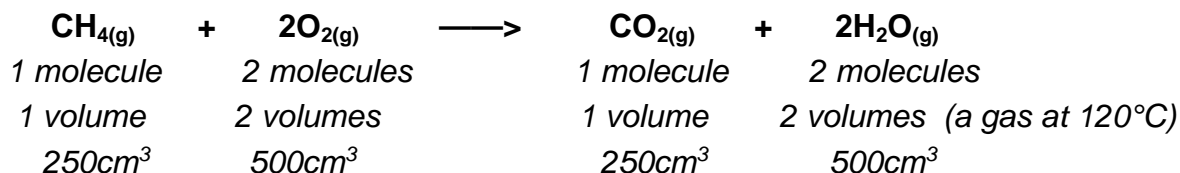
N.B. all volumes must be measured at the same temperature and pressure.

## Avogadro's Theory

*Statement*     **“ Equal volumes of all gases, at the same temperature and pressure, contain equal numbers of molecules ”**

**Calculations**     Gay-Lussac's Law and Avogadro's Theory are used for reacting gas calculations.

*example 1*     *What volume of oxygen will be needed to ensure that 250cm<sup>3</sup> methane undergoes complete combustion at 120°C ? How much carbon dioxide will be formed ?*

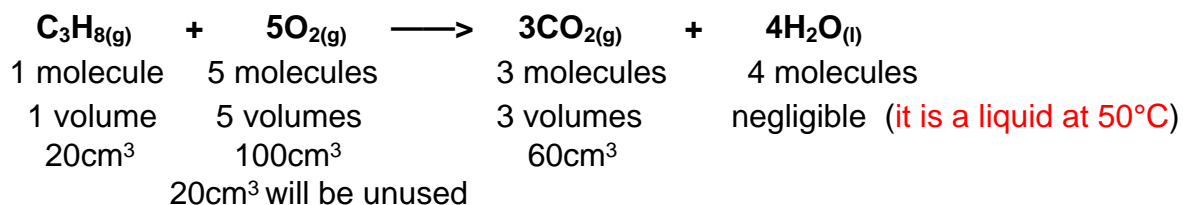


**ANS. 500cm<sup>3</sup> of oxygen and 250cm<sup>3</sup> of carbon dioxide.**

*Special tips*     An excess of one reagent is often included; e.g. excess O<sub>2</sub> ensures complete combustion

Check the temperature, and state symbols, to check which compounds are not gases. This is especially important when water is present in the equation.

*example 2*     *20cm<sup>3</sup> of propane vapour is reacted with 120cm<sup>3</sup> of oxygen at 50°C. Calculate the composition of the final mixture at the same temperature and pressure?*



**ANSWER 20cm<sup>3</sup> of unused oxygen and 60cm<sup>3</sup> of carbon dioxide.**

## ANSWERS TO QUESTIONS

- Q.1** 12.0858g 16.1144g 32.2288g
- Q.2**  $10/40 = 0.25 \text{ mol}$   $4/1 = 4 \text{ mol}$   
 $10/100 = 0.1 \text{ mol}$   $4/2 = 2 \text{ mol}$   
 $2 \times 16 \text{g} = 32 \text{g mol of CH}_4$   $0.5 \times 85 \text{g} = 42.5 \text{g}$   
 $6 \times 14 \text{g} = 84 \text{g}$   $6 \times 28 \text{g} = 168 \text{g}$
- Q.3** Calculate the number of moles in  
 2 mol  $0.5 \text{ mol}$   
 $0.5 \text{ mol}$   $0.005 \text{ mol}$  ( $5 \times 10^{-3}$ )  
 $2 \text{ mol dm}^{-3}$  ( $2 \text{ M}$ )  $0.4 \text{ mol dm}^{-3}$  ( $0.4 \text{ M}$ )  
 $0.4 \text{ mol dm}^{-3}$  ( $0.4 \text{ M}$ )  $4 \text{ mol dm}^{-3}$  ( $4 \text{ M}$ )  
 $0.4 \text{ mol dm}^{-3}$  ( $0.4 \text{ M}$ )  $4 \text{ mol dm}^{-3}$  ( $4 \text{ M}$ )
- Q.4** Calculate the mass of...  
 a) 276g (2 mol) b) 220g (5 mol) c) 20g (0.5 mol)  
 d) 2 mol  $\text{CaCO}_3$  gives 2 mol  $\text{CO}_2$ ; 2 mol  $\text{CH}_4$  gives 2 mol  $\text{CO}_2$  Both the same
- Q.5** What mass of  $\text{CuSO}_4$  can be made from 7.95g of CuO?  
 $\text{CuO} + \text{H}_2\text{SO}_4 \longrightarrow \text{CuSO}_4 + \text{H}_2\text{O}$   
 79.5g 159.5g  
 7.95g 15.95g  
 ANS 15.95g
- Q.6** Calculate the mass of...  
 a) 0.1 mol 4.4g  
 b)  $5 \times 10^{-3} \text{ mol}$  0.32g  
 c)  $M_r = 16$  Formula =  $\text{CH}_4$  (methane)
- Q.7** • Convert the following volumes into  $\text{m}^3$   
 a) 0.001 or  $1 \times 10^{-3} \text{ m}^3$  b) 0.00025 or  $2.5 \times 10^{-4} \text{ m}^3$  c)  $1 \times 10^{-7} \text{ m}^3$   
 • Convert the following temperatures into Kelvin  
 a) 373K b) 400K c) 250K  
 • Calculate the volume of 0.5 mol of propane gas at 298K and  $10^5 \text{ Pa}$  pressure  
 $V = (0.5 \times 298 \times 8.31) / 10^5 = 0.124 \text{ m}^3$   
 • Calculate the mass of propane ( $\text{C}_3\text{H}_8$ ) contained in a  $0.01 \text{ m}^3$  flask maintained at a temperature of 273K and a pressure of 250kPa.  
 $m = (44 \times 250000 \times 0.01) / (8.31 \times 273) = 48.49 \text{g}$