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 **6.02×10^{23} mol^{-1}**.

MOLAR MASS The mass of one mole of substance. It has units of **g mol^{-1}** or **kg mol^{-1}**.

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

molar mass = mass of one particle x Avogadro's constant (6.02×10^{23} mol^{-1})

Example *If 1 atom has a mass of* *1.241×10^{-23}g*

1 mole of atoms will have a mass of *1.241×10^{-23}g x 6.02×10^{23} = 7.471g*

Q.1 *Calculate the mass of one mole of carbon-12 atoms. [mass of proton 1.672×10^{-24}g, mass of neutron 1.674×10^{-24}g, mass of electron 9.109×10^{-28}g]*

MOLE CALCULATIONS

Substances mass	**g**	or	**kg**
molar mass	**g mol^{-1}**	or	**kg mol^{-1}**

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

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

oxygen molecules have the formula O_2
the relative mass will be 2 x 16 = 32 so the molar mass will be 32g mol^{-1}

$$moles = \frac{mass}{molar\ mass} = \frac{4g}{32g\ mol^{-1}}$$

ANS. 0.125 mol

Q.2 *Calculate the number of moles in*

10g of Ca atoms *10g of $CaCO_3$*
4g of hydrogen atoms *4g of hydrogen molecules*

Calculate the mass of...

2 mol of CH_4 *0.5 mol of $NaNO_3$*
6 mol of nitrogen atoms *6 mol of nitrogen molecules*

Solutions molarity concentration / **mol dm^{-3}**
volume **dm^3** or **cm^3**

moles = concentration x volume

= molarity x volume in dm^3

= $\frac{\text{molarity x volume in cm}^3}{1000}$

The 1000 takes into account that there are 1000 cm^3 in 1dm^3

Example 1 *Calculate the number of moles of sodium hydroxide in 25cm^3 of 2M NaOH*

moles = $\frac{\text{molarity x volume in cm}^3}{1000}$

= $\frac{2 \text{ mol dm}^{-3} \text{ x } 25\text{cm}^3}{1000}$ ***ANS. 0.05 mol***

Example 2 *What volume of 0.1M H_2SO_4 contains 0.002 moles ?*

volume in cm^3 = $\frac{\text{1000 x moles}}{\text{molarity}}$ *(re-arrangement of above)*

= $\frac{1000 \text{ x } 0.002}{0.1 \text{ mol dm}^{-3}}$ ***ANS. 20 cm^3***

Example 3 *4.24g of Na_2CO_3 is dissolved in water and the solution made up to 250 cm^3. What is the concentration of the solution in mol dm^{-3} ?*

molar mass of Na_2CO_3 = 106g mol $^{-1}$
no. of moles in 250cm^3 = 4.24g / 106g mol $^{-1}$ = 0.04 moles
no. of moles in 1000cm^3 (1dm^3) = 0.16 moles ***ANS. 0.16 mol dm^{-3}.***

Q.3 *Calculate the number of moles in*

1dm^3 of 2M NaOH *250cm^3 of 2M NaOH*

5dm^3 of 0.1M HCl *25cm^3 of 0.2M H_2SO_4*

Calculate the concentration (in moles dm^{-3}) of solutions containing

0.2 moles of HCl in 2dm^3 *0.1 moles of NaOH in 25cm^3*

EMPIRICAL FORMULAE AND MOLECULAR FORMULAE

Empirical Formula

Description Expresses the elements in a simple ratio (e.g. CH_2).
It can sometimes be the same as the molecular formula (e.g H_2O and CH_4)

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%)*

	C	**H**	**O**
1) Write out percentages (by mass)	*48%*	*4%*	*48%*
2) Divide by the relative atomic mass	*48/12*	*4/1*	*48/16*
... this gives a molar ratio	*4*	*4*	*3*
3) If not whole numbers then scale up			
4) Express as a formula	**$C_4H_4O_3$**		

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

	C	**H**	**O**
1) Write out ratios by mass	*1.8*	*0.3*	*0.48*
2) Divide by relative atomic mass	*1.8 / 12*	*0.3 / 1*	*0.48 / 16*
(this gives the molar ratio)	*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	**$C_5H_{10}O$**		

Molecular Formula

Description Exact number of atoms of each element in the formula (e.g. C_4H_8)

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_2 and relative molecular mass 84.*

mass of CH_2 unit = 14
divide molecular mass (84) by 14 = 6
molecular formula = empirical formula x 6 = C_6H_{12}

MOLAR MASS CALCULATIONS

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

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

* ***Relative Molecular Mass (M_r)*** The sum of all the relative atomic masses present in a molecule

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

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

MOLAR VOLUME

At rtp **The molar volume of any gas at rtp is 24 dm^3 mol^{-1}** (0.024 m^3 mol^{-1})

rtp **R**oom **T**emperature and **P**ressure

At stp **The molar volume of any gas at stp is 22.4 dm^3 mol^{-1}** (0.0224 m^3 mol^{-1})

stp **S**tandard **T**emperature and **P**ressure (**273K and 1.013 x 10^5 Pa**)

example *0.5g of a gas occupies 250cm^3 at rtp. Calculate its molar mass.*

250 cm^3	*has a mass of 0.5g*	
1000 cm^3 (1dm^3)	*has a mass of 2.0g*	*x4 to convert to dm^3*
24 dm^3	*has a mass of 48.0g*	*x24 to convert to 24dm^3*

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

Q.4 *Calculate the mass of...*

a) 2.4 dm^3 of carbon dioxide, CO_2 at rtp

b) 120 cm^3 of sulphur dioxide, SO_2 at rtp

c) 0.08g of a gaseous hydrocarbon occupies 120cm^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 $PV = nRT$

PV = n R T

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

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

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

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

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

P = 100 KPa = 100000 Pa
V = 500 cm^3 x 10^{-6} = 0.0005 m^3
T = 27 + 273 = 300 K
R = 8.31 J K^{-1} mol^{-1} = 8.31

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

Example 2 *Calculate the relative molecular mass of a vapour if 0.2 g of gas occupy 400 cm^3 at a temperature of 223°C and a pressure of 100 KPa.*

P = 100 KPa = 100000 Pa
V = 400 cm^3 x 10^{-6} = 0.0004 m^3
T = 227 + 273 = 500 K
m = 0.27g = 0.27g
R = 8.31 J K^{-1} mol^{-1} = 8.31

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

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.

$$\frac{P_1V_1}{T_1} = \frac{P_2V_2}{T_2}$$

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^3 (22.4 litres , 22400cm^3) 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^3 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^3	V_2	*final volume*	= ?
T_1	*initial temperature*	= 373K	T_2	*temperature*	= 273K

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

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

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^3 methane undergoes complete combustion at 120°C ? How much carbon dioxide will be formed ?*

$CH_{4(g)}$	+	$2O_{2(g)}$	——>	$CO_{2(g)}$	+	$2H_2O_{(g)}$
1 molecule		*2 molecules*		*1 molecule*		*2 molecules*
1 volume		*2 volumes*		*1 volume*		*2 volumes (a gas at 120°C)*
250cm^3		*500cm^3*		*250cm^3*		*500cm^3*

ANS. 500cm^3 of oxygen and 250cm^3 of carbon dioxide.

Special tips An excess of one reagent is often included; e.g. excess O_2 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^3 of propane vapour is reacted with 120cm^3 of oxygen at 50°C. Calculate the composition of the final mixture at the same temperature and pressure?*

$C_3H_{8(g)}$	+	$5O_{2(g)}$	——>	$3CO_{2(g)}$	+	$4H_2O_{(l)}$
1 molecule		5 molecules		3 molecules		4 molecules
1 volume		5 volumes		3 volumes		negligible (it is a liquid at 50°C)
20cm^3		100cm^3		60cm^3		
		20cm^3 will be unused				

ANSWER 20cm^3 of unused oxygen and 60cm^3 of carbon dioxide.

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

i) convert to stp

$$\frac{2 \times 278}{298} = \frac{1 \times V}{273} \qquad V = \frac{278 \times 2 \times 273}{1 \times 298} = 509\ cm^3$$

ii) convert to molar volume

	1g	occupies	509cm^3	at stp
	1/509g	occupies	1cm^3	
	22400 x 1/509g	occupies	22400cm^3	
therefore	44g	occupies	22.4 dm^3	at stp

ANSWER: The molar mass is 44g mol^{-1}

Q.5

- *Convert the following volumes into m^3*

  a) 1dm^3 *b) 250cm^3* *c) 0.1cm^3*

- *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 10^5 Pa pressure*

- *Calculate the mass of propane (C_3H_8) contained in a 0.01 m^3 flask maintained at a temperature of 273K and a pressure of 250kPa.*

ANSWERS TO QUESTIONS

Q.1 2.0089×10^{-23}g,

Q.2

10/40 = 0.25 mol	10/100 = 0.1 mol
4/1 = 4 mol	4/2 = 2 mol
2 x 16g = 32gmol of CH_4	0.5 x 85g = 42.5g
6 x 14g = 84g	6 x 28g = 168g

Q.3 *Calculate the number of moles in*

2 mol	0.5 mol
5 mol	0.005 mol (5×10^{-3})
0.1 mol dm^{-3}	4 mol dm^{-3}

Q.4 *Calculate the mass of...*

a) 0.1 mol 4.4g

b) 5×10^{-3} mol 0.32g

c) $M_r = 16$ Formula = CH_4

Q.5

- Convert the following volumes into m^3

  a) 0.001 or $1 \times 10^{-3}\ m^3$ b) 0.00025 or $2.5 \times 10^{-4}\ m^3$ c) $1 \times 10^{-7}\ m^3$

- Convert the following temperatures into Kelvin

  a) 373K b) 400K c) 250K