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}**.
- 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

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 MASS

The mass of one mole of substance. units are **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 $\times$ 6.02×10^{23} = 7.471g

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 1.672×10^{-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}**

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

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

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

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

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*

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

$$= \frac{2\ mol\ dm^{-3} \times 25cm^3}{1000}$$

ANS. 0.05 mol

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

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

$$= \frac{1000 \times 0.002}{0.1 \text{ mol dm}^{-3}}$$

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 mol

no. of moles in 1000cm^3 (1dm^3) = 0.16 mol

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

25cm^3 of 0.2M HCl

27.58cm^3 of 0.101M H_2SO_4

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

1 mol of HCl in 2dm^3

0.2 mol of HCl in 2dm^3

0.1 mol of NaOH in 250cm^3

0.1 mol of H_2SO_4 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}

REACTING MASSES - THE LAW OF CONSERVATION OF MASS

The masses of all the prducts = 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**

	$CaCO_3$	——>	CaO	+	CO_2
Relative masses	100	—	56		44
actual masses	100g (1 mol)		56g (1 mol)		44g (1 mol)
if you started with	25g (0.25 mol)		0.25 mol (14g)		0.25 mol (11g)

	CH_4	+	$2O_2$	——>	CO_2	+	$2H_2O$
Relative masses	16		32		44		18
actual masses	16g		64g (2 mol)		44g		36g (2 mol)
to make 88g CO_2	**32g**		128g		**88g**		72g

Q.4

a) *What mass of $CaSO_4$ can be made from 112g of CaO?*

$CaO + H_2SO_4 \longrightarrow CaSO_4 + H_2O$

b) *What mass of carbon dioxide is made by burning 80kg of CH_4?*

$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$

c) *How much NaOH is needed to make 42.5g of $NaNO_3$?*

$NaOH + HNO_3 \longrightarrow NaNO_3 + H_2O$

d) *Which gives a bigger mass of CO_2; 200g of $CaCO_3$ or 32g of CH_4?*

[A_r 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 $CuSO_4$ can be made from 7.95g of CuO?*

$CuO + H_2SO_4 \longrightarrow CuSO_4 + H_2O$

A student carried out this experiment. When they weighed the product, they found they had only made 7.20g of $CuSO_4$.

i) *What is the yield of $CuSO_4$?* ii) *What is the percentage yield of $CuSO_4$?*

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, $C_2H_4Cl_2$

Equation	C_2H_4	+	Cl_2	—>	$C_2H_4Cl_2$
M_r	*28*		*71*		*99*

atom economy $= \dfrac{\text{molecular mass of } C_2H_4Cl_2}{\text{molecular mass of all products}} \times 100$

$= \dfrac{99}{99} \times 100 =$ **100%**

2. *Formation of nitrobenzene, $C_6H_5NO_2$*

Equation	C_6H_6	+	HNO_3	—>	$C_6H_5NO_2$	+	H_2O
M_r	*78*		*63*		*123*		*18*

atom economy $= \dfrac{\text{molecular mass of } C_6H_5NO_2}{\text{molecular mass of all products}} \times 100$

$= \dfrac{123}{123 + 18} \times 100 =$ **87.2%**

3. Preparation of ammonia from the decomposition of ammonium sulphate

Equation	$(NH_4)_2SO_4$	—>	H_2SO_4	+	$2NH_3$
M_r	*132*		*98*		*17*

atom economy $= \dfrac{\mathbf{2\ x}\ \text{molecular mass of } NH_3}{\text{molecular mass of all products}} \times 100$

$= \dfrac{2 \times 17}{98 + (2 \times 17)} \times 100 =$ **25.8%**

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 dm^3 mol^{-1}** (0.024 m^3 mol^{-1})

rtp Room Temperature and Pressure

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

stp Standard Temperature and Pressure (**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.6 *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

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

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

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

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

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	

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

Q.7

- *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.*

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

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

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

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}

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.**