

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 **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 ($6.02 \times 10^{23} \text{ mol}^{-1}$)

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⁻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 O₂

the relative mass will be 2 x 16 = 32 so the molar mass will be 32g mol⁻¹

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

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

10g of Ca atoms

10g of CaCO₃

4g of hydrogen atoms

4g of hydrogen molecules

Calculate the mass of...

2 mol of CH₄

0.5 mol of NaNO₃

6 mol of nitrogen atoms

6 mol of nitrogen molecules

Solutions molarity concentration / mol dm⁻³
 volume dm³ or cm³

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

The **1000** takes into account that there are 1000 cm³ in 1dm³

Example 1 Calculate the number of moles of sodium hydroxide in 25cm³ 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_2SO_4 contains 0.002 moles ?

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

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 $mol \text{ dm}^{-3}$?

$$\begin{aligned} \text{molar mass of } Na_2CO_3 &= 106 \text{ g mol}^{-1} \\ \text{no. of moles in } 250 \text{ cm}^3 &= 4.24 \text{ g} / 106 \text{ g mol}^{-1} = 0.04 \text{ mol} \\ \text{no. of moles in } 1000 \text{ cm}^3 (1 \text{ dm}^3) &= 0.16 \text{ mol} \end{aligned}$$

ANS. 0.16 mol dm^{-3}

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

1 dm^3 of 2M NaOH

250 cm^3 of 2M NaOH

5 dm^3 of 0.1M HCl

25 cm^3 of 0.2M H_2SO_4

25 cm^3 of 0.2M HCl

27.58 cm^3 of 0.101M H_2SO_4

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

1 mol of HCl in 2 dm^3

0.2 mol of HCl in 2 dm^3

0.1 mol of NaOH in 250 cm^3

0.1 mol of H_2SO_4 in 25 cm^3

EMPIRICAL FORMULAE AND MOLECULAR FORMULAE

Empirical Formula

Description Expresses the elements in a simple ratio (e.g. CH₂).
It can sometimes be the same as the molecular formula (e.g. H₂O and CH₄)

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	C₄H₄O₃		

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	C₅H₁₀O		

Molecular Formula

Description Exact number of atoms of each element in the formula (e.g. C₄H₈)

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 CH₂ 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**

	CaCO₃	→	CaO	+	CO₂
<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)

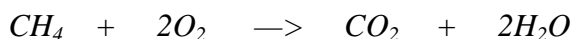
	CH₄	+	2O₂	→	CO₂	+	2H₂O
<i>Relative masses</i>	16		32		44		18
<i>actual masses</i>	16g		64g (2 mol)		44g		36g (2 mol)
<i>to make 88g CO₂</i>	32g		128g		88g		72g

Q.4

a) What mass of CaSO₄ can be made from 112g of CaO?



b) What mass of carbon dioxide is made by burning 80kg of CH₄?



c) How much NaOH is needed to make 42.5g of NaNO₃?



d) Which gives a bigger mass of CO₂: 200g of CaCO₃ or 32g of CH₄?

[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 CuSO₄ 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 CuSO₄.

i) What is the yield of CuSO₄ ?

ii) What is the percentage yield of CuSO₄ ?

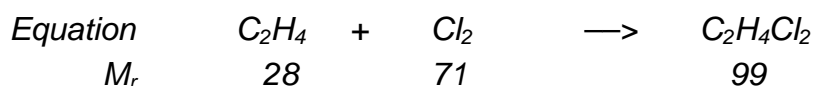
ATOM ECONOMY

- 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**

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

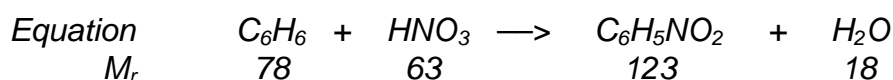
Example calculations

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



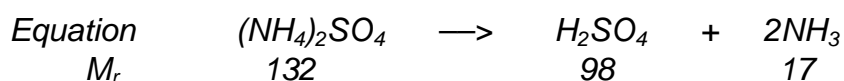
$$\begin{aligned} \text{atom economy} &= \frac{\text{molecular mass of } C_2H_4Cl_2}{\text{molecular mass of all products}} \times 100 \\ &= \frac{99}{99} \times 100 = \mathbf{100\%} \end{aligned}$$

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 cm^3 at rtp. Calculate its molar mass.

250 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 dm^3
24 dm^3	has a mass of	48.0g	x24 to convert to 24 dm^3

ANSWER: The molar mass is 48.0 g 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 120 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 (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	$8.31 \text{ J K}^{-1} \text{ mol}^{-1}$
	T	temperature	Kelvin ($\text{K} = ^\circ\text{C} + 273$)
	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 **$1.013 \times 10^5 \text{ Pa}$** (Nm^{-2})
1 litre (1 dm^3) is equivalent to **$1 \times 10^{-3} \text{ m}^3$**

Example 1 Calculate the number of moles of gas present in 500cm³ at 100 KPa pressure and at a temperature of 27°C.

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

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

Example 2 Calculate the relative molecular mass of a vapour if 0.2 g of gas occupy 400 cm³ at a temperature of 223°C and a pressure of 100 KPa.

$$\begin{aligned}
 P &= 100 \text{ KPa} && = 100000 \text{ Pa} \\
 V &= 400 \text{ cm}^3 && \times 10^{-6} = 0.0004 \text{ m}^3 \\
 T &= 223 + 273 && = 496 \text{ K} \\
 m &= 0.27 \text{ g} && = 0.27 \text{ g} \\
 R &= 8.31 \text{ J K}^{-1} \text{ mol}^{-1} && = 8.31
 \end{aligned}$$

$$PV = \frac{mRT}{M} \quad \therefore M = \frac{mRT}{PV} = \frac{0.27 \times 496 \times 8.31}{100000 \times 0.0004} = \mathbf{28.04}$$

Q.7

- Convert the following volumes into m³
 - a) 1dm³ b) 250cm³ c) 0.1cm³
- 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 10⁵ Pa pressure
- Calculate the mass of propane (C₃H₈) contained in a 0.01 m³ 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 dm³ (22.4 litres, 22400cm³) 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 dm³ 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

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

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

example 1g of gas occupies 278cm³ 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 ³	at stp
	1/509g	occupies	1cm ³	
	22400 x 1/509g	occupies	22400cm ³	

therefore 44g occupies 22.4 dm³ 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) ”**

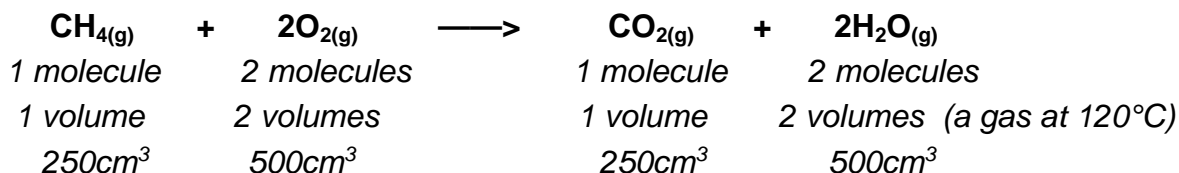
N.B. all volumes must be measured at the same temperature and pressure.

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 250cm³ methane undergoes complete combustion at 120°C ? How much carbon dioxide will be formed ?*

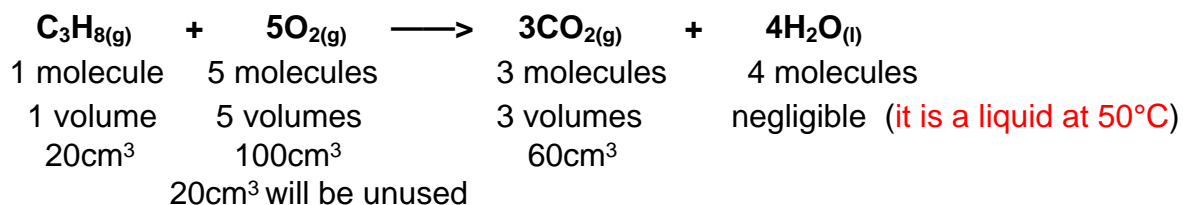


ANS. 500cm³ of oxygen and 250cm³ of carbon dioxide.

Special tips An excess of one reagent is often included; e.g. excess O₂ 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 *20cm³ of propane vapour is reacted with 120cm³ of oxygen at 50°C. Calculate the composition of the final mixture at the same temperature and pressure?*



ANSWER 20cm³ of unused oxygen and 60cm³ of carbon dioxide.