

Calculations

The mole is the key concept for chemical calculations

DEFINITION: **The mole** is the amount of substance in grams that has the same number of particles as there are atoms in 12 grams of carbon-12.

DEFINITION: **Relative atomic mass** is the average mass of an atom compared to one twelfth of the mass of one atom of carbon-12

DEFINITION: **Relative molecular mass** is the average mass of a molecule compared to one twelfth of the mass of one atom of carbon-12

Avogadro's Number

There are 6.022×10^{23} atoms in 12 grams of carbon-12.

Therefore explained in simpler terms 'One mole of any specified entity contains 6.022×10^{23} of that entity':

For most calculations we will do at AS we will use the following 3 equations

Learn these equations carefully and what units to use in them

1. For pure solids and gases

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

Unit of Mass: grams
Unit of moles : mols

2. For gases

$$PV = nRT$$

Unit of Pressure (P): Pa
Unit of Volume (V): m^3
Unit of Temp (T): K
n= moles
R = 8.31

Converting temperature

$$^{\circ}\text{C} \rightarrow \text{K add } 273$$

3. For solutions

$$\text{Concentration} = \frac{\text{moles}}{\text{volume}}$$

Unit of concentration: mol dm^{-3} or M
Unit of Volume: dm^3

Converting volumes

$$\begin{aligned} \text{cm}^3 &\rightarrow \text{dm}^3 \div 1000 \\ \text{cm}^3 &\rightarrow \text{m}^3 \div 1000\ 000 \\ \text{dm}^3 &\rightarrow \text{m}^3 \div 1000 \end{aligned}$$

Note the different unit for volume

Typical mole calculations

Some Simple calculations using above equations

Example 1: What is the number of moles in 35g of CuSO_4 ?

$$\begin{aligned} \text{moles} &= \text{mass}/M_r \\ &= 35 / (63.5 + 32 + 16 \times 4) \\ &= 0.219 \text{ mol} \end{aligned}$$

Example 2: What is the concentration of solution made by dissolving 5g of Na_2CO_3 in 250 cm^3 water?

$$\begin{aligned} \text{moles} &= \text{mass}/M_r \\ &= 5 / (23.1 \times 2 + 12 + 16 \times 3) \\ &= 0.0472 \text{ mol} \\ \text{conc} &= \text{moles}/\text{Volume} \\ &= 0.0472 / 0.25 \\ &= 0.189 \text{ mol dm}^{-3} \end{aligned}$$

Example 3: What is the mass of Cl_2 gas that has a pressure of 100kPa, temperature 293K, volume 500 cm^3 . (R = 8.31)

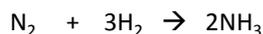
$$\begin{aligned} \text{moles} &= PV/RT \\ &= 100\ 000 \times 0.005 / (8.31 \times 293) \\ &= 0.205 \text{ mol} \end{aligned}$$

$$\begin{aligned} \text{Mass} &= \text{moles} \times M_r \\ &= 0.205 \times (35.5 \times 2) \\ &= 14.6 \text{ g} \end{aligned}$$

$$\begin{aligned} 100 \text{ kPa} &= 100\ 000 \text{ Pa} \\ 500 \text{ cm}^3 &= 0.005 \text{ m}^3 \end{aligned}$$

It is usually best to give your answers to 3sf

Converting quantities between different substances using a balanced equation



The balancing (stoichiometric) numbers are mole ratios
e.g. 1 mole of N_2 reacts with 3 moles of H_2 to produce 2 moles of NH_3

Typically we are given a quantity of one substance and are asked to work out a quantity for another substance in the reaction. Any of the above three equations can be used.

Step 1:

Use one of the above 3 equations to convert any given quantity into moles
Mass \rightarrow moles
PVT of gas \rightarrow moles
Conc and vol of solution \rightarrow moles

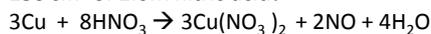
Step 2:

Use balanced equation to convert moles of initial substance into moles of second substance

Step 3

Convert moles of second substance into quantity question asked for using relevant equation
e.g. Moles, Mr \rightarrow mass
Mole, P, T gas \rightarrow vol gas
Moles, vol solution \rightarrow conc

Example 4: What mass of Copper would react completely with 150 cm^3 of 1.6M nitric acid?



Step 1: work out moles of nitric acid

$$\begin{aligned}\text{Moles} &= \text{conc} \times \text{vol} \\ &= 1.6 \times 0.15 \\ &= 0.24 \text{ mol}\end{aligned}$$

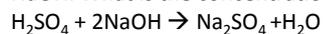
Step 2: use balanced equation to give moles of Cu

$$\begin{aligned}8 \text{ moles } \text{HNO}_3 &: 3 \text{ moles Cu} \\ \text{So } 0.24 \text{ HNO}_3 &: 0.09 \text{ (} 0.24 \times \frac{3}{8} \text{) moles Cu}\end{aligned}$$

Step 3: work out mass of Cu

$$\begin{aligned}\text{Mass} &= \text{moles} \times \text{Mr} \\ &= 0.09 \times 63.5 \\ &= 5.71\text{g}\end{aligned}$$

Example 5: 23.6 cm^3 of H_2SO_4 neutralised 25.0 cm^3 of 0.15M NaOH. What is the concentration of the H_2SO_4 ?



Step 1: work out moles of sodium hydroxide

$$\begin{aligned}\text{Moles} &= \text{conc} \times \text{vol} \\ &= 0.15 \times 0.025 \\ &= 0.00375 \text{ mol}\end{aligned}$$

Step 2: use balanced equation to give moles of H_2SO_4

$$\begin{aligned}2 \text{ moles NaOH} &: 1 \text{ moles } \text{H}_2\text{SO}_4 \\ \text{So } 0.00375 \text{ NaOH} &: 0.001875 \text{ moles } \text{H}_2\text{SO}_4\end{aligned}$$

Step 3 work out concentration of H_2SO_4

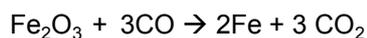
$$\begin{aligned}\text{conc} &= \text{moles} / \text{Volume} \\ &= 0.001875 / 0.0236 \\ &= 0.0794 \text{ mol dm}^{-3}\end{aligned}$$

% yield and % atom economy

$$\text{percentage yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100$$

$$\text{percentage atom economy} = \frac{\text{Mass of useful products}}{\text{Mass of all reactants}} \times 100$$

Example 6: What is the % atom economy for the following reaction where Fe is the desired product assuming the reaction goes to completion?



$$\begin{aligned}\% \text{ atom economy} &= \frac{(2 \times 55.8)}{(2 \times 55.8 + 3 \times 16) + 3 \times (12 + 16)} \times 100 \\ &= 45.8\%\end{aligned}$$

Other calculations

Empirical formulae

An empirical formula is the **simplest** ratio of atoms of each **element** in the compound.

General method

Step 1 : Divide each mass (or % mass) by the atomic mass of the element

Step 2 : For each of the answers from step 1 divide by the smallest one of those numbers.

Step 3: sometimes the numbers calculated in step 2 will need to be multiplied up to give whole numbers.

These whole numbers will be the empirical formula

The same method can be used for the following types of data:

1. masses of each element in the compound
2. percentage mass of each element in the compound

Example 7: Calculate the empirical formula for a compound that contains 1.82g of K, 5.93g of I and 2.24g of O

Step1: Divide each mass by the atomic mass of the element

$$\begin{array}{lll} \text{K} = 1.82 / 39.1 & \text{I} = 5.93/126.9 & \text{O} = 2.24/16 \\ = 0.0465 \text{ moles} & = 0.0467 \text{ moles} & = 0.14 \end{array}$$

Step 2 For each of the answers from step 1 divide by the smallest one of those numbers.

$$\begin{array}{lll} \text{K} = 0.0465/0.0465 & \text{I} = 0.0467/0.0465 & \text{O} = 0.14 / 0.0465 \\ = 1 & = 1 & = 3 \end{array}$$

Empirical formula = KIO_3

Molecular formula from empirical formula

A molecular formula is the **actual** number of atoms of each element in the compound.

From the relative molecular mass (M_r) work out how many times the mass of the empirical formula fits into the M_r .

Example 8 : work out the molecular formula for the compound with an empirical formula of $\text{C}_3\text{H}_6\text{O}$ and a M_r of 116

$\text{C}_3\text{H}_6\text{O}$ has a mass of 58

The empirical formula fits twice into M_r of 116

So molecular formula is $\text{C}_6\text{H}_{12}\text{O}_2$

Balancing ionic equations

Ionic equations need to be balanced both in terms of mass and charge

$\text{Fe}^{3+} + \text{Zn} \rightarrow \text{Fe}^{2+} + \text{Zn}^{2+}$ This is not balanced in terms of charge as there is a total reactant charge of +3 and product charge of +4

$2\text{Fe}^{3+} + \text{Zn} \rightarrow 2\text{Fe}^{2+} + \text{Zn}^{2+}$ This is now balanced in terms of atoms and charges