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

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

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

Note the different unit for volume

3. For solutions

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

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

Converting temperature

$^oC \rightarrow$ K add 273

Converting volumes

$cm^3 \rightarrow dm^3 \div 1000$
$cm^3 \rightarrow m^3 \div 1000\ 000$
$dm^3 \rightarrow m^3 \div 1000$

Typical mole calculations

Some Simple calculations using above equations

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

moles = mass/Mr

= 35/ (63.5 + 32 +16 x4)

= 0.219 mol

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

moles = mass/Mr

= 5 / (23.1 x2 + 12 +16 x3)

= 0.0472 mol

conc= moles/Volume

= 0.0472 / **0.25**

= 0.189 mol dm^{-3}

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

100 kPa = 100 000 Pa
500 cm^3 = 0.005 m^3

moles = PV/RT

= 100 000 x 0.005 / (8.31 x 293)

= 0.205 mol

Mass = moles x Mr
= 0.205 x (35.5 x2)
= 14.6 g

It is usually best to give your answers to 3sf

Converting quantities between different substances using a balanced equation

$N_2 + 3H_2 \rightarrow 2NH_3$

The balancing (stoichiometric) numbers are mole ratios
e.g. 1 mole of N_2 reacts with 3 moles of H_2 to produce 2moles 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 → moles
PVT of gas → moles
Conc and vol of solution → 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 → mass
Mole, P, T gas → vol gas
Moles, vol solution → conc

Example 4: What mass of Copper would react completely with 150 cm^3 of 1.6M nitric acid?
$3Cu + 8HNO_3 \rightarrow 3Cu(NO_3)_2 + 2NO + 4H_2O$

Step 1: work out moles of nitric acid
Moles = conc x vol
= 1.6 x 0.15
= 0.24 mol

Step 2: use balanced equation to give moles of Cu
8 moles HNO_3 : 3 moles Cu
So 0.24 HNO_3 : 0.09 (0.24 x $^3/_8$) moles Cu

Step 3: work out mass of Cu
Mass = moles x Mr
= 0.09 x 63.5
=5.71g

Example 5: 23.6cm^3 of H_2SO_4 neutralised 25.0cm^3 of 0.15M NaOH. What is the concentration of the H_2SO_4?
$H_2SO_4 + 2NaOH \rightarrow Na_2SO_4 + H_2O$

Step 1: work out moles of sodium hydroxide
Moles = conc x vol
= 0.15 x 0.025
= 0. 00375 mol

Step 2: use balanced equation to give moles of H_2SO_4
2 moles NaOH : 1 moles H_2SO_4
So 0.00375 NaOH : 0.001875 moles H_2SO_4

Step 3 work out concentration of H_2SO_4
conc= moles/Volume
= 0.001875 / 0.0236
= 0.0794 mol dm^{-3}

% yield and % atom economy

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

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

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

$Fe_2O_3 + 3CO \rightarrow 2Fe + 3\,CO_2$

$$\%\text{ atom economy} = \frac{(2 \times 55.8)}{(2 \times 55.8 + 3\times16) + 3 \times (12+16)} \times 100$$

=45.8%

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

K = 1.82 / 39.1 = 0.0465 moles

I = 5.93/126.9 = 0.0467moles

O = 2.24/16 = 0.14

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

K = 0.0465/0.0465 =1

I = 0.0467/0.0465 = 1

O = 0.14 / 0.0465 = 3

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 (Mr) work out how many times the mass of the empirical formula fits into the Mr.

Example 8 : work out the molecular formula for the compound with an empirical formula of C_3H_6O and a M_r of 116

C_3H_6O has a mass of 58

The empirical formula fits twice into M_r of 116

So molecular formula is $C_6H_{12}O_2$

Balancing ionic equations

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

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

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