Chapter 2

Atoms, molecules and Stoichiometry

Counting atoms and molecules

There are two important definitions to remember in this chapter:

- Relative Atomic Mass, Ar, or an element:
  - Average mass of one atom relative to the mass of one atom of C^{12} which is considered to be 12 (atomic mass unit A.M.U)
- Relative Isotopic Mass of an Isotope of an element:
  - The mass of one atom of the isotope relative to that of one atom of C^{12}.

To calculate the Ar of an element we have to consider all the isotopes of the element and their abundance.

$$\boldsymbol{Ar = (\,isotopic\ mass\ \times abundance\%)}$$

Example, to find the relative atomic mass of chlorine:

Isotopes:

- Chlorine-35, abundance = 75.5%
- Chlorine-37, abundance = 24.5%

Therefore:

$$Ar = (35 \times \frac{75.5}{100} + 37 \times \frac{24.5}{100})$$

$$Ar = 35.5$$

The mass of different molecules are compared in a similar fashion. The *relative formula mass* (Mr) of a compound, is the mass of a molecule of the compound relative to the mass of an atom of carbon-12.

To find the relative Mr of a compound, we add up all the Ar's of the elements in the compound.

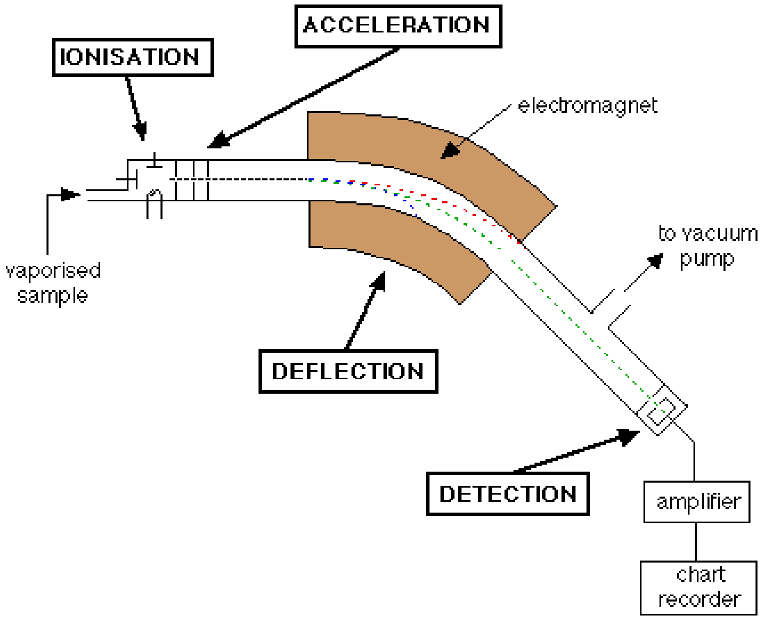
Example for CH_4:

$$Mr = 12 + (4 \times 1)$$

$$Mr = 16$$

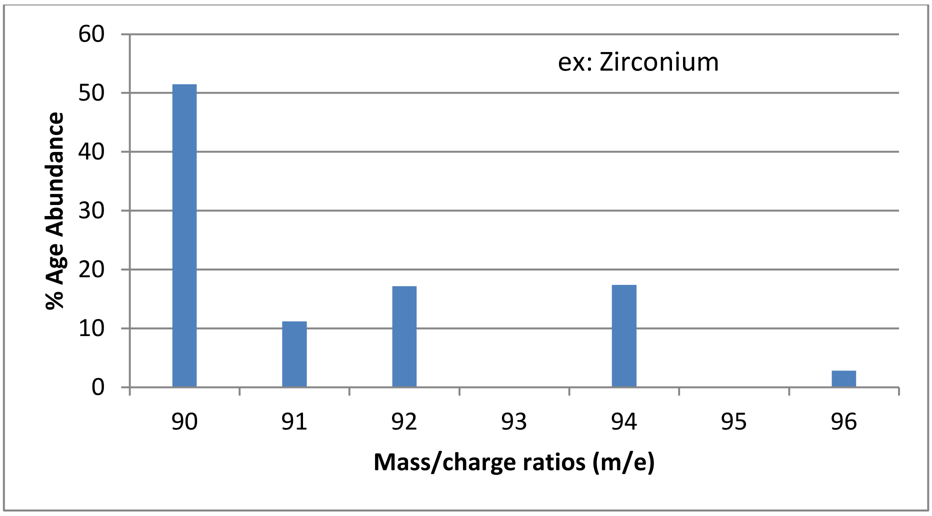
Determination of Ar from mass spectra

Ar is determined using an instrument called the mass spectrometer. The instrument is shown below:



Knowledge of the working of the mass spectrometer is **not** required by CIE.

The results of the mass spectrometer would be shown on a computer screen, as a chart of abundance against mass. For example, for zirconium:



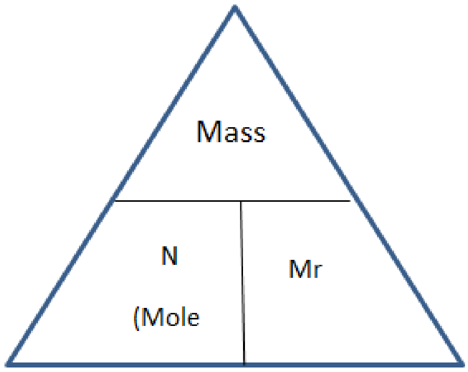
Counting chemical substances in bulk

The mole and Avogadro's constant

A <u>mole</u> of atoms is a quantity that contains <u>Avogadro's number</u> (6×10^{23}) of atoms.

Similarly,

- A Mole of molecules:
  - It is a quantity of the substance that contains Avogadro's number of molecules.
    (e.g. : a mole of ions … a mole of electrons)



In terms of mass,

A <u>mole</u> of atoms is a quantity in grams equal to the relative atomic mass.

For example, 1mol of S atoms weighs 32 grams.

<u>Relative Molecular Mass</u> (Mr) is the sum of atomic masses of all atoms in the molecule.

Examples are found in the book.

The empirical (simplest) formula & molecular formula:

- The Empirical Formula:

  Of a compound shows the simplest whole-number ratio of the elements in the compound

- The Molecular Formula:

  Of a compound shows the real number of each element in a molecule of a compound.

Example 1: SAQ 2.10 pg21

Q: Copper oxide has the following composition by mass: Cu = 0.635g ; O = 0.08g.

Calculate empirical formula of the oxide:

ANS:

Ar (Cu)	=63.5	Ar (O) =16
	<u>Cu</u>	<u>O</u>
	$\frac{0.635}{63.5}$	$\frac{0.08}{16}$

$\frac{0.01}{0.005}$ $\frac{0.005}{0.005}$

2 1

Cu_2O

Combustion analysis

The composition by mass of organic compounds can be found by combustion analysis. This involves the complete combustion in oxygen of a sample of a known mass.

In combustion analysis, all the carbon is converted to carbon dioxide and all the hydrogen into water.

These produced are carefully collected and weighed. Calculation gives the mass of carbon and hydrogen present.

If oxygen is also present, its mass is found by subtraction (elimination). Other elements require other methods.

- mass of C in a sample = mass of $CO_2 \times \frac{12}{44}$
- mass of H in a sample = mass of $H_2O \times \frac{2}{18}$

Example:

SAQ 2.11 pg22

Q: On complete combustion of 0.4g of a hydrocarbon (only H and C), 1.257g of CO_2 and 0.514g of H_2O were produced.

a) Find the Empirical formula of the hydrocarbon

ANS: Find C: $1.257 \times \frac{12}{44}$ Find H: $0.514 \times \frac{2}{18}$

C = 0.3428g H = 0.0571g

$\frac{0.3428}{12}$ $\frac{0.0571}{1}$

= 0.02856 = 0.0571

= 1 = 2

CH_2

b) If relative molecular mass of the hydrocarbon is 84, what is its molecular formula

ANS: mass of CH_2 = 14

$\frac{84}{14}$ = 6

So, the molecular formula is C_6H_{12}

Calculations involving reacting masses:

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

- molar mass of Fe_2O_3 = (2×56) + (3×16) = 160 g/mol

- one mole of Fe_2O_3 gives 2 moles of Fe.

160g of Fe_2O_3 gives (2×56) = 112g of iron

1000g of Fe_2O_3 gives 112 × $\frac{1000}{160}$ = 700g of iron

Example 1: SAQ 2.8 pg20

QUE: Calculate the mass of iron produced from 1000 tons of Fe_2O_3. How many tons of Fe_2O_3 would be needed to produce 1 ton of iron? If the iron ore contains 12% of Fe_2O_3, how many tons of ore are needed to produce 1 ton of iron?

ANS:

1) 1,000,000,000g of Fe_2O_3 gives 112 × $\frac{1000000000}{160}$ = 700,000,000g = 700 tons
2) 112 ×$\frac{X}{160}$ = 1,000,000, x = 1.43 tons
3) 1.43 × $\frac{100}{12}$ = 11.9 tons

Calculations involving concentration:

Concentration is how much solute is available in a specific volume of solution.

- Concentration by Mass:
  - how many grams of solute in 1 dm^3 solution. (unit is g/dm^3) (m/v)
- Concentration by Moles (Molar concentration):
  - How many moles of solute in 1 dm^3 solution (unit is $moles/dm^3$ (n/V)

Example 1:

QUE: What amount of NaOH is present in 24.0cm^3 of an aqueous 0.010 mol/dm^3?

ANS:

Convert the volume to dm^3

1dm^3 = 10 × 10 × 10cm^3 = 1000cm^3

24.0 cm^3 = $\frac{24.0}{1000}$dm^3

Amount of NaOH in 24.0cm^3 = $\frac{24.0}{1000}$ × 0.010mol

= 2.40 × 10^{-4}mol

Calculations involving gas volumes:

Equal volumes of different gases contain the same number of molecules under same conditions of temperature and pressure, and this number is Avogadro's Number.

The opposite is also true, equal numbers of molecules of different gases, under same conditions of temperature and pressure occupy the same volume.

At room temperature and pressure (r.t.p), one mole of any gas occupies approximately 24dm^3 (at s.t.p, this is 22.5dm^3).Reacting volumes of gases under same conditions of temperature and pressure can be used to determine the formula and stoichiometry of reaction.

Example 1:

QUE: 10cm^3 of hydrocarbon burned completely in 50cm^3 of oxygen produced 30cm^3 of CO_2 at r.t.p. Determine the formula of hydrocarbon and write a balanced equation of the reaction.

ANS:

	$HC_{(g)}$	+	$O_{2\,(g)}$	→	$CO_{2\,(g)}$	+	$H_2O_{(l)}$
Volume:	10cm^3 / 10		50cm^3/10		30cm^3/10		-
Gas Volume Ratio:	1	:	5	:	3		
Gas Mole Ratio:	1	:	5	:	3		

3 moles of C come from 3 moles of O_2 react with 3 moles of CO_2

5-3 = 2 moles of O_2 which react with hydrogen

$4H_2 + 2O_2 \rightarrow 4H_2O$

2 moles of O_2 react with 8 moles of H atoms, which gives C_3H_8

$$C_3H_{8\,(g)} + 5O_{2\,(g)} \rightarrow 3CO_{2\,(g)} + 4H_2O$$

Example 2: SAQ 2.21 pg27

QUE: 20cm^3 of gaseous hydrocarbon 'Y' burned completely in 60cm^3 of oxygen to produce water and 40cm^3 of CO_2 (@ r.t.p)

a) What is formula of hydrocarbon 'Y'
b) Write a balanced equation for the reaction.

ANS:

	$HC_{(g)}$	+	$O_{2\,(g)}$	→	$CO_{2\,(g)}$	+	$H_2O_{(l)}$
Volume:	20cm^3		60 cm^3		40 cm^3		--
Gas volume ratio:	1	:	3	:	2		
Gas mole ratio:	1	:	3	:	2		

$4C + 4O_2 \rightarrow$ 4 moles of Co_2

6-4= 2 moles to react with H_2

$8H + 2O_2 \rightarrow 4H_2O$

$C_4H_8/2$ gives $C_2H_4 + 3O_2 \rightarrow 2CO_2 + 2H_2O$

Summary:

Relative Atomic Mass, *Ar, or an element is the average mass of one atom relative to the mass of one atom of C^{12} which is considered to be 12 (atomic mass unit A.M.U).*

Relative Isotopic Mass *of an Isotope of an element the mass of one atom of the isotope relative to that of one atom of C^{12}.*

$$Ar = (\ isotopic\ mass\ \times abundance\%)$$

A ***mole*** *of atoms is a quantity that contains* ***Avogadro's number*** *(6×10^{23}) of atoms.*

$$Number\ of\ moles = \frac{Mass}{Mr}$$

Relative Molecular Mass *(Mr) is the sum of atomic masses of all atoms in the molecule*

The Empirical Formula *of a compound shows the simplest whole-number ratio of the elements in the compound*

The Molecular Formula *of a compound shows the real number of each element in a molecule of a compound.*

$$Mass\ of\ element = \frac{Ar\ of\ element}{Mr\ of\ compound} \times Mass\ of\ compound$$

$$Moles = Volume\ in\ dm^3\ \times Concentration$$

$$Concentration\ in\ gdm^{-3} = Concentration\ in\ moldm^{-3}\ \times Mr$$