CHAPTER 2: Atoms, Molecules and Stoichiometry

2.1 Mass of Atoms and Molecules
2.2 Mass Spectrometer
2.3 Amount of Substance
2.4 Empirical Formula and Molecular Formula
2.5 Stoichiometry and Equations

Learning outcomes:

(a) define and use the terms relative atomic, isotopic, molecular and formula masses, based on the C-12 scale.
(b) define and use the term mole in terms of the Avogadro constant.
(c) analyse mass spectra in terms of isotopic abundances [knowledge of the working of the mass spectrometer is not required].
(d) calculate the relative atomic mass of an element given the relative abundances of its isotopes, or its mass spectrum.
(e) define and use the terms empirical and molecular formulae.
(f) calculate empirical and molecular formulae, using combustion data or composition by mass.
(g) write and/or construct balanced equations.
(h) perform calculations, including use of the mole concept, involving:
(i) reacting masses (from formulae and equations).
(ii) volumes of gases (e.g. in the burning of hydrocarbons).
(iii) volumes and concentrations of solutions.
When performing calculations, candidates' answers should reflect the number of significant figures given or asked for in the question. When rounding up or down, candidates should ensure that significant figures are neither lost unnecessarily nor used beyond what is justified.
(i) deduce stoichiometric relationships from calculations such as those in (h).

2.1 Mass of Atoms and Molecules

Concept of relative mass

1) Relative mass is an indication of how heavy is an atom compared to another atom which is used as a standard model.

2) Relative mass is expressed in atomic mass unit(a.m.u).

3) C-12 was chosen to be the standard model because:
   i. it is the most abundant isotope of carbon
   ii. it is a solid, easy to handle and easily available

4) C-12 was assigned a mass of exactly 12 a.m.u.. This is known as C-12 scale.

5) For example, an atom which is 3.5 times heavier than a C-12 atom would have a relative mass of (3.5 x 12) = 42 a.m.u.. That means, this atom is 42 times heavier than the mass of (1/12 x the mass of C-12 atom).

Relative isotopic mass

1) *Relative isotopic mass* is the mass of an isotope measured on a scale in which a carbon-12 atom has a mass of exactly 12 units.

Relative atomic mass, Ar

1) *Relative atomic mass, Ar* is the weighted average relative masses of all its isotopes measured on a scale in which a carbon-12 atom has a mass of exactly 12 units.

$$\boxed{\text{Relative atomic mass, Ar} = \frac{\text{Average mass of one atom of the element}}{\text{Mass of one atom of carbon-12}} \times 12}$$

Example:

Ratio of Cl-35 to Cl-37 is 3:1. If you have 4 typical atoms of chlorine, total mass is $(35 \times 3) + (37 \times 1) = 142$. So, the average mass of the isotopes is $142/4 = 35.5$.

This implies that 35.5 is the **relative atomic mass** of chlorine while 35 is the **relative mass** of Cl-35 and 37 is the **relative mass** of Cl-37.

Relative molecular mass, Mr

1) *Relative molecular mass, Mr* is the weighted average of the masses of the molecules measured on a scale in which a carbon-12 atom has a mass of exactly 12 units.

2) It should only be applied to substances which exist as molecules.

3) It is found by adding up all the relative atomic masses of all the atoms present in the molecule.

4) Examples:
   i. Mr (H_2O) = 2(1) + 16 = 18
   ii. Mr ($CHCl_3$) = 12 + 1 + 3(35.5) = 119.5

Relative formula mass, Mr

1) *Relative formula mass, Mr* is the weighted average of the masses of the formula units measured on a scale in which a carbon-12 atom has a mass of exactly 12 units.

2) It works for both ionic and covalent compounds.

3) Examples:
   i. Mr (NaCl) = 23 + 35.5 = 58.5
   ii. Mr ($CuSO_4 \cdot H_2O$) = 64 + 32+ 4(16) +5[2(1) + 16] = 249.5

2.2 Mass Spectrometer

What is mass spectrometer?

1) A mass spectrometer is used to determine:
   a. relative isotopic mass
   b. relative abundance of isotopes
   c. relative atomic mass
   d. relative molecular mass
   e. structural formula of compounds

Determination of relative atomic mass using mass spectrometer

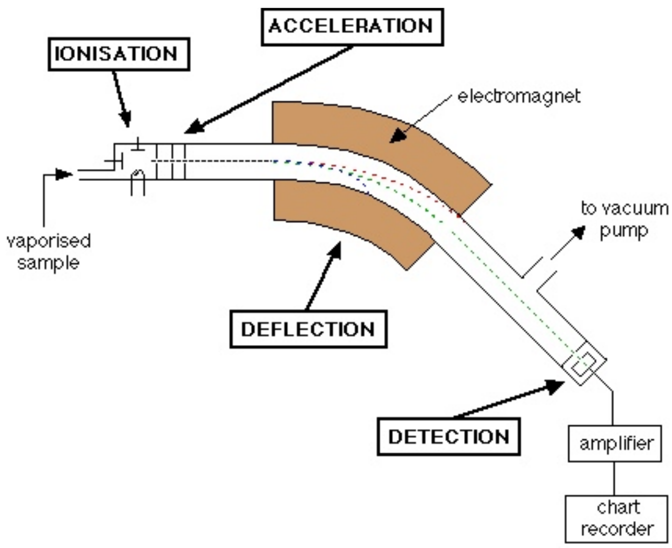
1) Five steps:
   i. Vaporisation
      - atoms are vaporised to form **gaseous atom**.

   ii. Ionisation
      - gaseous atoms are bombarded with high energy electrons to form positive ions.

   iii. Acceleration
      - the ions are accelerated so that they have the same kinetic energy.

   iv. Deflection
      - ions are deflected by a magnetic field. The amount of deflection depends on:
         1) the mass of the ion
         2) the amount of positive charge on it
      - **the larger the mass, the smaller the deflection.**
      - **the higher the charge, the larger the deflection.**
      - the two factors combine into **mass/charge ratio** (**m/e or m/z**).
      - the smaller the value of m/e, the larger the deflection

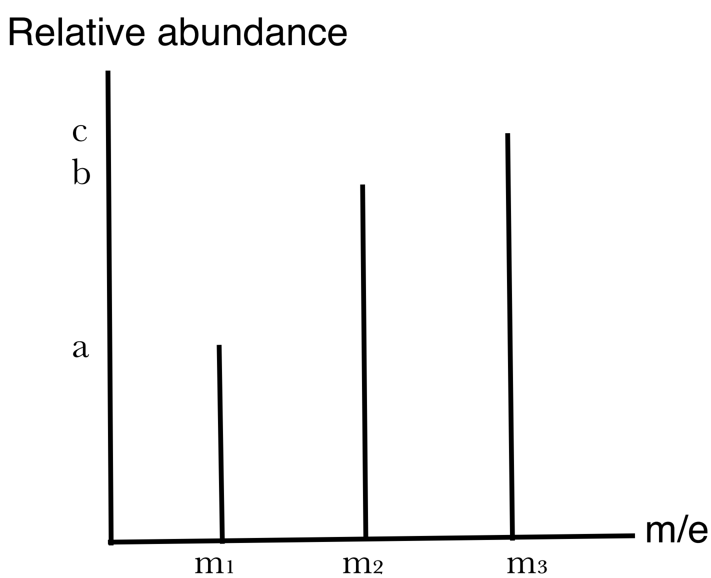
   v. Detection
      - the beam of ions are detected electrically.
      - the data are fed into the computer and the mass spectrum is produced.



Side note

1) Ionisation chamber is **vacuum** so that the ions produced can run freely without knocking air molecules.

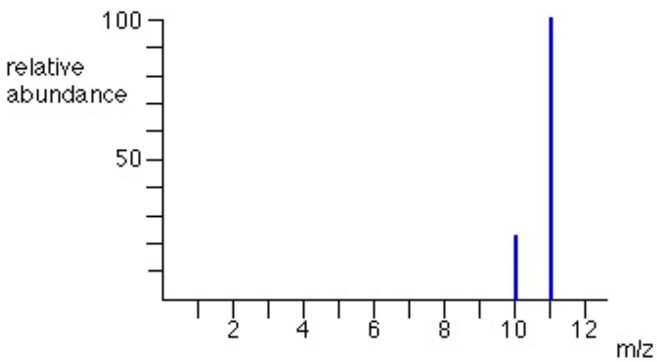
Mass spectrum (How to calculate relative atomic mass, Ar from it?)



$$Ar = \frac{(m_1 \times a) + (m_2 \times b) + (m_3 \times c)}{a + b + c}$$

Example:

The mass spectrum of boron, B is as shown, given the relative abundances:
B-10 : 23
B-11 : 100



$$Ar = \frac{(23 \times 10) + (100 \times 11)}{23 + 100}$$

$$= 10.8$$

2.3 Amount of Substance

The mole and the Avogadro's constant

1) A *mole* of a substance is the amount of substance that contains the same amount of stated elementary units as there are atoms in 12 g of C-12.

2) The number of atoms is 12 g of C-12 is 6.02×10^{23} . This number is also known as the **Avogadro's constant, *L***.

3) Examples:
   i. 1 mol of He contains 6.02×10^{23} He **atoms**.
   ii. 1 mol of CO_2 contains 6.02×10^{23} CO_2 **molecules** but $3 \times (6.02 \times 10^{23})$ **atoms**.
   iii. 1 mol of NaCl contains 6.02×10^{23} NaCl units, Na^+ and Cl^- ions.

Moles and mass

$$\text{No. of mole / mol} = \frac{\text{Mass / g}}{\text{Molar mass / g mol}^{-1}}$$

Moles and volumes

1) Volume occupied by a gas depends on the amount of gas, temperature and pressure. In other words the volume of a gas is not fixed.

2) *Avogadro's law* states that for equal volumes of all gases, under the same conditions, contain the same number of moles.

3) Hence, equal number of moles of any gas, under the same conditions, would occupy the same volume. It does not depend on the nature of gas.

4) At room temperature of 20 ℃ and a pressure of 1 atm, one mole of any gas occupies 24 dm^3.

5) At standard temperature and pressure (s.t.p), which is 0 ℃ and 1 atm, one mole of any gas occupies 22.4 dm^3.

$$\text{No.of mole / mol} = \frac{\text{Volume of a gas / dm}^3}{\text{Molar volume / dm}^3\text{ mol}^{-1}}$$

6) i. Complete combustion of hydrocarbon produces water and carbon dioxide. The general equation is as follow:

$$C_xH_y + \left(x + \frac{y}{4}\right) O_2 \rightarrow xCO_2 + \left(\frac{y}{2}\right) H_2O$$

ii. In incomplete combustion, the possible products are carbon dioxide, carbon monoxide, carbon soot and water.

Moles and concentration of solutions

1) A *solution* is a homogeneous mixture of two or more substance.

2) The substance presents in small quantity is called the solute while the substance present is larger quantity is called the solvent.

3) *Concentration* is the amount of solute present in a fixed quantity of solution.

4) Concentration is expressed in terms of g dm^{-3}. Concentration in mol dm^{-3} is called molar concentration or **molarity**.

$$\text{Concentration / g dm}^{-3} \quad \frac{\text{Mass of solute / g}}{\text{Volume of solution / dm}^{3}}$$

$$\text{Molarity / mol dm}^{-3} \quad \frac{\text{Concentration / g dm}^{-3}}{\text{Molar mass of solute / g mol}^{-1}}$$

$$\text{No. of moles / mol} = \frac{\text{Volume / cm}^{3} \ \times \ \text{Molarity / mol dm}^{-3}}{1000}$$

2.4 Empirical Formula and Molecular Formula

Percentage composition by mass

$$\text{Percentage composition by mass / \%} = \frac{\text{Ar x No.of mole of that element}}{\text{Molar mass of compound}} \times 100\%$$

Empirical formula

1) *Empirical formula* is a chemical formula that shows the simplest ratio of the atoms that combine to form a molecule.

2) Steps to find empirical formula:
   i. Find the mass of each element.
   ii. Find the number of mole of each element (divide by its Ar).
   iii. Find the simplest ratio (divide by the smallest number).
   iv. Construct the empirical formula using the simplest ratio.

   [If a decimal or fraction exists, round up or eliminate the fraction]
   [Never assume a formula]

3) Some facts:
   i. The formula for an ionic compound is always its empirical formula.
   ii. The empirical formula and molecular formula for simple inorganic molecules are often the same.
   iii. Organic molecules have different empirical and molecular formula.

Molecular formula

1) *Molecular formula* is a chemical formula that shows the actual number of atoms that combine to form the compound.

2) In order to deduce the molecular formula of a compound, we need to know:
   i. the relative formula mass of the compound.
   ii. the empirical formula of the compound.

Principle of conservation of mass

1) Mass is neither created nor destroyed during a chemical reaction. Therefore the total mass of the reactants is equal to the total of the products in a closed system.

2) For example, the total mass of iodine in the reactants is equal to the total mass of iodine in the products.

3) This can be used to solve problems in calculating the empirical formula.

2.5 Stoichiometry and Equations

Stoichiometry

1) Stoichiometry is the proportion of things either reacting or combining.

2) In compounds, it refers to the ratio in which the atoms are combined together. For example, water, H_2O has a stoichiometry of 2 hydrogen to 1 oxygen.

3) It also refers to the reacting proportions in a chemical equation. For example:

$$2H_2 + O_2 \rightarrow 2H_2O$$

The stoichiometry shows that 2 moles of hydrogen react with 1 mole of oxygen to form 2 moles of water.

Ionic equations

1) Steps to construct net ionic equations:
   i. Write the balanced molecular equation.
   ii. Write the complete ionic equation by splitting it into ions(if possible).
   iii. Cancel out the spectator ions. (Spectator ions are ions that present in the mixture but do not participate in the reaction.)
   iv. Write down the 'leftovers', that is the net ionic equation.

Chemical equation: $HCl_{(aq)} + NaOH_{(aq)} \rightarrow NaCl_{(aq)} + H_2O_{(l)}$

Complete ionic equation: $H^+\cancel{Cl^-}_{(aq)} + \cancel{Na^+}OH^-_{(aq)} \rightarrow \cancel{Na^+}\cancel{Cl^-}_{(aq)} + H_2O_{(l)}$

Net ionic equation: $H^+_{(aq)} + OH^-_{(aq)} \rightarrow H_2O_{(l)}$

FAQ 1: When to split compounds into ions?

1) Only split aqueous ionic compounds. For example, NaCl(aq) and HCl(aq)
2) Do not split solid ionic compounds and covalent compounds, as well as metals. For example, NaCl(s), H_2O(l), Mg(s) and HCl(g)

FAQ 2: How to identify spectator ions?

1) The ions present on both sides of the equation are spectator ions.