CHAPTER 6

QUANTITATIVE ASPECTS OF CHEMICAL CHANGE
1. **The Mole as an SI (Systéme International) unit**

   The mole is the SI unit for quantity of substance. It is one of the seven base units of the SI.

2. **Abbreviation of the unit**

   The official SI abbreviation of the unit mole is mol.

3. **The mole - mass relationship**

   3.1 One mole of any element is given by the relative atomic mass of the element expressed in grams.
      Examples: 1 mol of Na = 23 g
                 1 mol of C = 12 g
                 1 mol of Al = 27 g

   3.2 Certain elements exist not as individual atoms but as diatomic molecules. They are hydrogen (H₂); nitrogen (N₂); oxygen (O₂); fluorine (F₂); chlorine (Cl₂); bromine (Br₂) and iodine (I₂).
      Examples: 1 mol of O₂ = 32 g
                 1 mol of Cl₂ = 71 g

   3.3 One mole of any compound is given by the relative formula mass of the compound expressed in grams.
      Examples: 1 mol of KCl = (39) + (35.5) = 74.5 g
                 1 mol of Na₂CO₃ = (2 x 23) + (12) + (3 x 16) = 106 g

   3.4 The mole - mass relationship is summarised in the formula:

   \[
   n = \frac{m}{M}
   \]

   Where
   - \(n\) ~ number of moles of substance in mol
   - \(m\) ~ mass of sample of substance in g
   - \(M\) ~ molar mass of substance in g.mol\(^{-1}\)

   **Sample question 1:** What is the mass of 5 moles of sodium chloride (NaCl)?

   **Answer:**
   
   \[
   n = \frac{m}{M}
   \]
   therefore \(m = n \times M\)
   
   \(m = 5\ \text{mol} \times 58.5\ \text{g.mol}^{-1}\)
   \(m = 292.5\ \text{g}\)
Sample question 2: What is the molar mass of a substance if 3 moles of the substance have a mass of 75 g?

Answer: \[ n = \frac{m}{M} \] therefore \[ M = \frac{m}{n} = \frac{75\text{g}}{3\text{mol}} = 25\text{g.mol}^{-1} \]

4. **The Mole and the Avogadro constant**

4.1 *Avogadro’s Discovery*

In 1811 an Italian scientist, Amadeo Avogadro determined that 1 mole of any substance has a fixed number of elementary particles, namely: \( 6,023 \times 10^{23} \). (We round this number off to \( 6 \times 10^{23} \))

4.2 *Avogadro’s Constant*

The number above is called Avogadro’s Constant and is given the symbol \( N_A \).
\[ N_A = 6 \times 10^{23} \]

4.3 *Elementary Particles*

An elementary particle is defined as the smallest part of an element or a compound that can exist alone but still represent the element or compound.

Examples: The elementary particle in sodium is the **Na atom**.

The elementary particle in hydrogen is the **H\(_2\) molecule**.

The elementary particle in water is the **H\(_2\)O molecule**.

The elementary particle in sodium carbonate is a **unit** of **Na\(_2\)CO\(_3\)**.

Thus:

In 1 mol of sodium (23 g) there are **6 \times 10^{23} Na atoms**.

In 1 mol of hydrogen (2 g) there are **6 \times 10^{23} H\(_2\) molecules**.

In 1 mol of water (18 g) there are **6 \times 10^{23} H\(_2\)O molecules**.

In 1 mol of sodium carbonate (106 g) there are **6 \times 10^{23} units of Na\(_2\)CO\(_3\)**.
5. **The Mole and Gases**

Avogadro also determined that:

1 mol of ANY gas at STP occupies a volume of **22.4 dm$^3$**.

The molar volume of ANY gas at STP is given the symbol $V_m$

$$V_m = 22.4 \text{ dm}^3 \cdot \text{mol}^{-1}$$

**NOTE:** STP stands for Standard Temperature ($0 \degree C$) and Pressure (100 kPa).

Examples:

1 mole of nitrogen, N$_2$ (28 g) at a temperature of $0 \degree C$ and a pressure of 100 kPa occupies a volume of 22.4 dm$^3$.

1 mole of carbon dioxide, CO$_2$ (44 g) at a temperature of $0 \degree C$ and a pressure of 100 kPa occupies a volume of 22.4 dm$^3$.

For any gas at STP,

$$n = \frac{V}{V_m}$$

Where:

- $n$ ~ number of moles of gas
- $V$ ~ volume of gas sample
- $V_m$ ~ molar volume of gas (22.4 dm$^3$.mol$^{-1}$)

**NOTE:** The volume of the gas sample ($V$) must always be measured in dm$^3$

1 dm$^3$ = 0.001 m$^3$ = 1000 cm$^3$ = 1000 ml = 1 litre

Sample question: What mass of nitrogen gas would occupy 5.6 dm$^3$ at STP?

**Answer:**

$$n = \frac{V}{V_m} = \frac{5.6 \text{ dm}^3}{22.4 \text{ dm}^3 \cdot \text{mol}^{-1}} = 0.25 \text{ mol}$$

$$m = n \cdot M = 0.25 \text{ mol} \times 28 \text{ g/mol} = 7 \text{ g}$$
6. **The Mole and Percentage Composition of Substances**

The subscripts in a chemical formula give the mole ratio in which the elements combine.

Example: In 1 mol of potassium permanganate (KMnO$_4$) there are:
- 1 mole of K atoms
- 1 mole of Mn atoms
- 4 moles of O atoms

The mole ratio enables one to calculate the percentage composition, by mass, of the elements in the compound.

Sample question: Find the percentage composition, by mass, of each element in KMnO$_4$

Answer: Formula mass $= (39) + (55) + (4 \times 16) = 158 \text{ g.mol}^{-1}$

\[
\% \text{K} = \frac{39}{158} \times \frac{100}{1} = 24.68\%
\]

\[
\% \text{Mn} = \frac{55}{158} \times \frac{100}{1} = 34.81\%
\]

\[
\% \text{O} = \frac{64}{158} \times \frac{100}{1} = 40.51\%
\]

7. **The Mole and Empirical Formulae of Compounds**

7.1 The empirical formula of a compound gives the simplest mole ratio in which the elements of the compound combine.

Example: The empirical formula of sulphuric acid is H$_2$SO$_4$ and not, for example, H$_1$S$_{1\frac{1}{2}}$O$_2$ or H$_4$S$_2$O$_8$.

Sample question: A compound consists of, by mass, 29,11% sodium; 40,51% sulphur and 30,38% oxygen. What is the empirical formula of the substance?

Answer:

Step 1: Let the mass of a sample of the compound be 100 g.

Then:
- mass of Na in the 100 g sample $= 29,11$ g
- mass of S in the 100 g sample $= 40,51$ g
- mass of O in the 100 g sample $= 30,38$ g
Step 2: Convert mass quantities to mole quantities by dividing the given mass of each substance by its atomic mass (from the periodic table).

\[
\begin{align*}
n_{(\text{Na})} &= \frac{m}{M} = \frac{29.11\text{g}}{23\text{g.mol}^{-1}} = 1.27 \text{ mol} \\
n_{(\text{S})} &= \frac{m}{M} = \frac{40.51\text{g}}{32\text{g.mol}^{-1}} = 1.27 \text{ mol} \\
n_{(\text{O})} &= \frac{m}{M} = \frac{30.38\text{g}}{16\text{g.mol}^{-1}} = 1.9 \text{ mol}
\end{align*}
\]

Step 3: Simplify the mole ratio between the elements by dividing each mol value by the smallest mol value

\[
\begin{align*}
\text{Na} : & \quad \frac{1.27}{1.27} = 1 \\
\text{S} : & \quad \frac{1.27}{1.27} = 1 \\
\text{O} : & \quad \frac{1.9}{1.27} = 1.5
\end{align*}
\]

Step 4: Eradicate fractions by multiplying by a suitable coefficient
(NB: This step need not be done if you get whole number answers in step 3)

\[
\begin{align*}
\text{Na} : & \quad 2 \times 1 = 2 \\
\text{S} : & \quad 2 \times 1 = 2 \\
\text{O} : & \quad 2 \times 1.5 = 3
\end{align*}
\]

Step 5: The empirical formula may now be written: \( \text{Na}_2\text{S}_2\text{O}_3 \)

Sometimes percentage compositions, by mass, are not given but we still follow the same procedure when calculating the empirical formula.

Sample question: 4.6 g of an oxide of nitrogen contains 3.2 g of oxygen. Calculate the empirical formula of the compound.

Answer: 4.6 g is the total mass of the compound. 3.2 g of this mass consists of oxygen and the remaining 1.4 g consists of nitrogen.

\[
\begin{align*}
n_{(\text{N})} &= \frac{m}{M} = \frac{1.4\text{g}}{14\text{g.mol}^{-1}} = 0.1 \text{ mol} \\
n_{(\text{O})} &= \frac{m}{M} = \frac{3.2\text{g}}{16\text{g.mol}^{-1}} = 0.2 \text{ mol}
\end{align*}
\]

The empirical formula is thus \( \text{NO}_2 \)
7.2 Empirical formula simply tells us the ratio of the different elements in a compound, not the number of atoms of each element in the molecule. If we are given the molecular/formula mass, we can then work out the true formula.

In example above, if you were given that the formula mass of the oxide is 92 g.mol\(^{-1}\), and you were asked to find the true formula of the oxide then:

Calculate the mass of the empirical formula that you have determined.

For NO\(_2\) the mass = (14) + (2 x 16) = 46 g.mol\(^{-1}\)

Then divide the mass of the true formula by the mass of the empirical formula.

92 ÷ 46 = 2

Use this answer now to multiply the numbers in the empirical formula.

NO\(_2\) (x2) becomes N\(_2\)O\(_4\)

8. The Mole and Balanced Equations

The coefficients that balance a chemical equation indicate the mole ratios in which the reactants react and the products are formed.

The balanced equation will also tell us the minimum mass / volume of reagents that is required and the maximum mass / volume of product that may be formed from these reagents.

Example: 3H\(_2\) + N\(_2\) → 2NH\(_3\)

The coefficients tell us that 3 moles of hydrogen will react exactly with 1 mole of nitrogen to produce exactly 2 moles of ammonia.

The balanced equation also tells us that a minimum mass of 6 g of H\(_2\) and 28 g of N\(_2\) is required for the production of 34 g of ammonia.

The balanced equation also tells us that a minimum volume of 67.2 dm\(^3\) of H\(_2\) and 22.4 dm\(^3\) of N\(_2\) is required for the production of 44.8 dm\(^3\) of ammonia.

From this information, given by the balanced equation for any chemical reaction, we are able to calculate the number of moles / mass / volume required of reagent/s to produce a specific amount of product OR to calculate the number of moles / mass / volume of product that may be produced from a specific amount of reagent/s.

Sample question 1:
12 g of hydrogen reacts with an excess quantity (ie: more than what is required) of nitrogen. What is the maximum mass of ammonia that can be produced in this reaction?
Answer:

**Method 1**

Step 1: Convert any mass quantities into a mole quantity by dividing the mass of the given substance by its atomic/molecular mass.

\[ n_{(H_2)} = \frac{m}{M} = \frac{12 g}{2 g \cdot \text{mol}^{-1}} = 6 \text{ mol} \]

Step 2: Work with a ratio \(-\text{GOT : FIND}\)

The first numbers in the ratio come from the balanced equation.

The next set of numbers come from your answer to step 1.

\[
\begin{align*}
H_2 & : \text{NH}_3 \\
3 & : 2 \\
6 & : 4
\end{align*}
\]

Step 3: Use the ratio of the substance you had to FIND (in step 2) and multiply this by the atomic/molecular mass of the substance you have to find in order to calculate the mass reacted/produced.

\[ m = n \cdot M = 4 \text{ mol} \times 17 \text{ g \cdot mol}^{-1} = 68 \text{ g of ammonia} \]

**Method 2**

Step 1: Write down the balanced equation. Work out the mass of each substance.

\[
\begin{align*}
3H_2 & + N_2 \rightarrow 2\text{NH}_3 \\
6 \text{ g} & \quad 28 \text{ g} \quad 34 \text{ g}
\end{align*}
\]

Step 2: Calculate the mass of the required substance by using ratio and proportion.

\[
\begin{align*}
3H_2 & + N_2 \rightarrow 2\text{NH}_3 \\
6 \text{ g} & \rightarrow 34 \text{ g} \\
12 \text{ g} & \rightarrow z
\end{align*}
\]

Therefore (cross multiply)

\[ z = \frac{34 \times 12}{6} = 68 \text{ g of ammonia} \]

**Sample question 2:**

112 dm\(^3\) of nitrogen reacts with an excess quantity (ie: more than what is required) of hydrogen. What is the maximum volume of ammonia that can be produced at STP in this reaction?
Answer:

Method 1

Step 1: Convert any volume quantities into a mole quantity by dividing the given volume of the substance with the molar volume of any gas at STP.

Step 2: Work with a ratio ~ GOT : FIND
The first numbers in the ratio come from the balanced equation. The next set of numbers come from your answer to step 1.

\[
\begin{array}{ccc}
N_2 & : & NH_3 \\
1 & : & 2 \\
5 & : & 10 \\
\end{array}
\]

Step 3: Use the ratio of the substance you had to FIND (in step 2) and multiply this by the molar gas volume at STP in order to calculate the volume reacted/produced.

\[V = n.V_o = 10 \text{ mol x } 22.4 \text{ dm}^3\text{.mol}^{-1} = 224 \text{ dm}^3 \text{ of ammonia}\]

Method 2

Step 1: Write down the balanced equation. Work out the volume of each substance.

\[
\begin{align*}
3H_2 + N_2 & \rightarrow 2NH_3 \\
67.2 \text{ dm}^3 & + 22.4 \text{ dm}^3 & \rightarrow 44.8 \text{ dm}^3 \\
\end{align*}
\]

Step 2: Calculate the volume of the required substance by using ratio and proportion.

\[
\begin{align*}
3H_2 + N_2 & \rightarrow 2NH_3 \\
22.4 & \rightarrow 44.8 \\
112 & \rightarrow z \\
\end{align*}
\]

Therefore (cross multiply)

\[z = 44.8 \times 112 = 224 \text{ dm}^3 \text{ of ammonia}\]
Worksheet on Quantitative Aspects of Chemical Change

1. Calculate the mass of 1 mole of each of the following:
   a) lithium
   b) fluorine
   c) manganese(IV) oxide
   d) ammonium sulphate

2. How many moles are represented by each of the following:
   a) 36 g water
   b) 552 g silver carbonate

3. How many atoms are there in:
   a) 1 mol aluminium
   b) 3 mol nitrogen gas
   c) 3 mol water

4. Determine the volume of:
   a) 11 g carbon dioxide at STP
   b) 40 g neon at STP

5. Determine the percentage composition, by mass, of each element in the following compounds:
   a) CaC₂
   b) NH₄NO₃

6. Determine the empirical formula of the compounds which have the following percentage composition by mass:
   a) 63,5% Fe; 36,5% S
   b) 43,4% Na; 11,3 % C; 45,3% O
7. Balance each equation and then answer the question/s that follow:
   a) \( \text{NaOH} + \text{CO}_2 \rightarrow \text{Na}_2\text{CO}_3 + \text{H}_2\text{O} \)
      
      What mass of \( \text{CO}_2 \) is required for the production of 5 moles of \( \text{H}_2\text{O} \)?
   b) \( \text{S} + \text{KClO}_3 \rightarrow \text{SO}_2 + \text{KCl} \)
      
      192 g of sulphur reacts. What mass of KCl is produced?
   c) \( \text{Al} + \text{HCl} \rightarrow \text{AlCl}_3 + \text{H}_2 \)
      
      81 g of aluminium reacts with hydrochloric acid to produce aluminium chloride and hydrogen gas. The hydrogen produced is collected and subjected to a pressure of 100 kPa and a temperature of 0 °C. Under these conditions, what volume would it occupy?

8. Ammonium nitrate may be produced by reacting ammonia with nitric acid.

   The balanced equation for the reaction is:
   
   \[ \text{NH}_3 + \text{HNO}_3 \rightarrow \text{NH}_4\text{NO}_3 \]

   If 85 g of ammonia is reacted with an excess quantity of nitric acid, what mass of ammonium nitrate will be produced?

A turquoise powder (CuCO_3) was heated in the apparatus as represented in the diagram below. A colourless gas was produced and collected in a gas syringe. The gas was later shown to turn lime water from clear to white therefore confirming that it is carbon dioxide. The turquoise powder turned black. The test tube with powder was weighed before and after heating.

7.1 What mass change (in grams) occurred on heating.

7.2 What mass of colourless gas was collected in the syringe.

7.3 Calculate the number of moles of gas produced. Round off your answer to 5 decimal places.
7.4 Calculate the initial number of moles of copper (II) carbonate. Round off your answer to 5 decimal places. (5)

7.5 The black product is copper oxide. Write a balanced chemical equation for this reaction. (3)

7.6 State the Law of Conservation of mass. (2)

7.7 Apply the above law to confirm that you have written down the correct formula for copper oxide in your answer to (7.5). (6)

7.8 Identify the type of reaction which is taking place in the test tube above? (1)