Structure 1.4

IB CHEMISTRY SL

Structure 1.4.1

Understandings:

- The mole (mol) is the SI unit of amount of substance. One mole contains exactly the number of elementary entities given by the Avogadro constant.

Learning outcomes:

- Convert the amount of substance, *n*, to the number of specified elementary entities.

Additional notes:

- An elementary entity may be an atom, a molecule, an ion, an electron, any other particle or a specified group of particles.
- The Avogadro constant N_A is given in the data booklet. It has the units mol^{-1}.

The mole and amount of substance

- The mole, symbol mol, is the SI unit of amount of substance (*n*).
- It is a measure of the number of specified elementary entities (an elementary entity can refer to an atom, a molecule, an ion, an electron, or any other particle).
- One mole contains exactly 6.02×10^{23} elementary entities.
- This is numerically equal to the Avogadro constant (L or N_A) which is 6.02×10^{23} mol^{-1}.

Elementary entity	Number of elementary entities in one mole
Atoms	6.02×10^{23}
Molecules	6.02×10^{23}
Ions	6.02×10^{23}
Formula units	6.02×10^{23}

Structure 1.4.2

Understandings:

- Masses of atoms are compared on a scale relative to ^{12}C and are expressed as relative atomic mass A_r and relative formula mass M_r.

Learning outcomes:

- Determine relative formula masses M_r from relative atomic masses A_r.

Additional notes:

- Relative atomic mass and relative formula mass have no units.
- The values of relative atomic masses given to two decimal places in the data booklet should be used in calculations.

Relative atomic mass and relative formula mass

- Relative atomic mass, A_r, is the weighted average mass of the naturally occurring isotopes of an element relative to 1/12 the mass of an atom of carbon-12.
- The relative atomic mass scale is based on the isotope carbon-12 which has a mass of exactly 12 amu.
- Relative formula mass, M_r, is the weighted average mass of a substance relative to 1/12 the mass of an atom of ^{12}C.
- The M_r is the sum of the A_r of the atoms in a substance.
- Both relative atomic mass and relative formula mass do not have units.

Exercise: Calculate the relative formula masses of the following.

1. C_2H_5OH

2. CH_3COCH_3

3. $C_6H_{12}O_6$

4. KCl

5. $MgBr_2$

Structure 1.4.3

Understandings:

- Molar mass M has the units g mol^{-1}

Learning outcomes:

- Solve problems involving the relationships between the number of particles, the amount of substance in moles and the mass in grams.

Additional notes:

- The relationship $n = m/M$ is given in the data booklet.

Molar mass (*M*)

- The molar mass (M) is the mass of one mole of a substance in grams.
- The unit for molar mass is g mol^{-1}.
- The molar mass of a substance is numerically equal to its relative atomic mass.
- To convert A_r to M, multiply by the molar mass constant, M_u, which is approximately equal to 1 g mol^{-1}.

Example: Determine the molar mass of H_2O

H_2O is composed of 2 H atoms and 1 O atom. Find the relative atomic mass (A_r) of the elements from the periodic table and add them together. Multiply by the molar mass constant to get the molar mass.

$(2 \times 1.01) + (1 \times 16.00) = 18.02$

$18.02 \times 1 \text{ g mol}^{-1} = 18.02 \text{ g mol}^{-1}$

The molar mass of H_2O is 18.02 g mol^{-1}

Exercise: determine the molar mass of the following.

Substance	**Molar mass (g mol^{-1})**	**Substance**	**Molar mass (g mol^{-1})**	**Substance**	**Molar mass (g mol^{-1})**
H_2		CO_2		$CaCl_2$	
O_2		HCl		Al_2O_3	
Cl_2		CH_4		NH_4NO_3	
I_2		NH_3		$Al_2(SO_4)_3$	

Calculations involving amount (*n*), mass (*m*) and molar mass (*M*)

- To convert from mass (in g) to amount (in mol), divide the mass of the substance by its molar mass.

$$\textbf{amount (mol)} = \frac{\textbf{mass (g)}}{\textbf{molar mass (g mol}^{-1}\textbf{)}}$$

$$n(\text{mol}) = \frac{m\ (\text{g})}{M\ (\text{g mol}^{-1})} \qquad n = \frac{m}{M}$$

- This equation can be rearranged to find calculate (*m*) and molar mass (*M*):

$$m = n \times M \qquad M = \frac{m}{n}$$

Excercises:

1. Calculate the amount in mol of the following.

a. 30.00 g Mg

b. 75.00 g O_2

c. 26.93 g $CuSO_4$

d. 15.00 g NaOH

e. 1.78 g C_3H_8

f. 45.82 g $CaCl_2$

g. 98.36 g Al_2O_3

h. 173.81 g NH_4NO_3

i. 118.62 g $Al_2(SO_4)_3$

j. 261.04 g Fe_2O_3

2. Calculate the mass in grams of the following.

a. 3.00 mol Mg

b. 0.100 mol O_2

c. 0.400 mol $CuSO_4$

d. 9.84 mol NaOH

e. 0.270 mol C_3H_8

f. 0.600 mol $CaCl_2$

g. 3.56 mol Al_2O_3

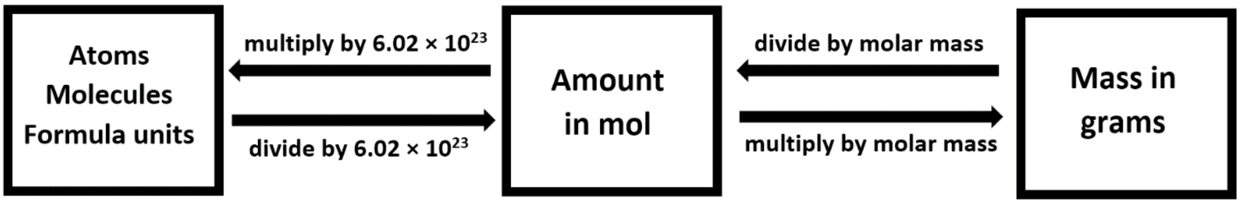
h. 2.40 mol NH_4NO_3

i. 0.850 mol $Al_2(SO_4)_3$

j. 0.0593 mol Fe_2O_3

The relationship between number of particles, amount in mol (*n*) and mass (*m*)

- One mole of any substance contains 6.02×10^{23} particles (atoms, molecules, formula units).
- The molar mass (*M*) of a substance is the mass (in g) of one mole of a substance.



Examples:

1. Calculate the number of H_2O molecules in 18.02 g of pure water.

First, convert to amount (in mol):

$$n = \frac{m}{M} \quad n = \frac{18.02}{18.02} = 1 \text{ mol } H_2O$$

Next, convert to number of molecules:

One mole of any substance contains 6.02×10^{23} molecules

1 mol of H_2O contains 6.02×10^{23} H_2O molecules

2. Calculate the mass of one molecule of H_2O.

One mole of H_2O (6.02×10^{23} H_2O molecules) has a mass of 18.02 g

One molecule of H_2O has a mass of $\frac{18.02}{6.02 \times 10^{23}} = 2.99 \times 10^{-23}$ g

3. Determine the number of H atoms in one mol of H_2O.

One molecule of H_2O is composed of 2 H atoms and 1 O atom.

One mole of H_2O has 6.02×10^{23} H_2O molecules

$2 \times 6.02 \times 10^{23} = 1.20 \times 10^{24}$ H atoms

Exercises:

1. Calculate the number of molecules in the following:

a. 0.500 mol CH_4

b. 0.750 mol SO_2

c. 1.08 mol C_2H_5OH

d. 2.50 mol C_3H_8

e. 1.45×10^{-3} mol NH_3

2. Calculate the **total** number of atoms in the following:

a. 0.500 mol CH_4

b. 0.750 mol SO_2

c. 1.08 mol C_2H_5OH

d. 2.50 mol C_3H_8

e. 1.45×10^{-3} mol NH_3

3. Calculate the number of hydrogen atoms in:

a. 0.750 mol CH_4

b. 1.24 mol C_2H_5OH

c. 0.913 mol C_3H_8

d. 2.45 mol C_5H_{10}

e. 6.90×10^{-4} mol NH_3

4. Calculate the number of ions in:

a. 1.00 mol of NaCl

b. 0.500 mol of Na_2O

c. 1.45 mol of $MgCl_2$

5. Calculate the following:

a. The number of ethanol molecules in a drop of ethanol (2.30×10^{-3} g).

b. The mass of one molecule of ethane (C_2H_6).

c. The amount (in mol) of O_2 that contains 1.80×10^{22} molecules.

d. The mass of 3.01×10^{23} molecules of H_2O

e. The number of iodine atoms in 0.835 mol of I_2

Structure 1.4.4

Understandings:

- The empirical formula of a compound gives the simplest ratio of atoms of each element present in that compound.
- The molecular formula gives the actual number of atoms of each element present in a molecule.

Learning outcomes:

- Interconvert the percentage composition by mass and the empirical formula.
- Determine the molecular formula of a compound from its empirical formula and molar mass.

Empirical formula and molecular formula

- Empirical formula is defined as the lowest whole number ratio of atoms in a compound.
- Molecular formula is the actual number of atoms in a compound.

Example:

- Butane has the molecular formula C_4H_{10}
- The empirical formula is C_2H_5 – how was this determined?

Exercise: State the empirical formula of the following compounds:

1. H_2O_2

2. C_2H_6

3. C_4H_8

4. $C_6H_{12}O_6$

5. $C_{20}H_{14}O_4$

Calculating empirical formula from percentage composition by mass

Example: The relative molecular mass of aluminium chloride is 267 and its composition by mass is 20.3% aluminium (Al) and 79.7% chlorine (Cl). Determine the empirical and molecular formula of aluminium chloride.

1. Check that the % add up to 100 %.

2. Divide the % of each element by its relative atomic mass.

3. Divide each number in part (2) by the smallest ratio - this will give you the empirical formula of the compound.

4. To find the molecular formula from the empirical formula determine the mass of the empirical formula and divide the molecular formula by the mass of the empirical formula.

Exercises:

1. Compound B has the following percentage composition by mass: C 26.7%, O 71.1% and H 2.2%. Calculate the empirical formula of compound B.

2. Compound C has the following percentage composition by mass: 48.6% C, 10.8% H, 21.6% O and 18.9% N. Calculate the empirical formula of compound C.

3. Determine the molecular formula of each of the following given the empirical formula and the relative molecular mass, M_r

   a. CH_2, $M_r = 70$

   b. OH, $M_r = 34$

   c. C_2H_5O, $M_r = 90$

4. An organic compound A contains 62.0% by mass of carbon, 24.1% by mass of nitrogen, the remainder being hydrogen.

a. Determine the percentage by mass of hydrogen and the empirical formula of A.

b. The relative molecular mass of A is 116. Determine the molecular formula of A.

Percentage composition by mass

- Percentage composition by mass is the percentage by mass of elements in a compound.

Example: Find the percentage by mass of carbon in ethanol (C_2H_5OH).

Exercises: Calculate the percentage by mass of carbon in the following.

1. CO_2

2. C_2H_6

3. $C_6H_5NO_2$

4. $C_6H_{12}O_6$

5. $C_6H_5COCH_3$

Calculating empirical formula from combustion analysis

Example: Menthol is an organic compound composed of C, H and O atoms. The complete combustion of 0.1005 g of menthol produces 0.2829 g of CO_2 and 0.1159 g of H_2O. Calculate the empirical formula of menthol.

1. Calculate the mass of carbon in CO_2 and convert to mol.

2. Calculate the mass of H in H_2O and convert to mol.

3. Calculate the mass of O by subtracting the mass of carbon and mass of hydrogen from the original mass of menthol. Convert to amount in mol.

4. Divide each amount by the smallest to get the lowest whole number ratio.

Structure 1.4.5

Understandings:

- The molar concentration is determined by the amount of solute and the volume of solution.

Learning outcomes:

- Solve problems involving the molar concentration, amount of solute and volume of solution.

Additional notes:

- The use of square brackets to represent molar concentration is required.
- Units of concentration should include g dm^{-3} and mol dm^{-3} and conversion between these.
- The relationship $n = CV$ is given in the data booklet.

Calculating the concentration of a solution

- The concentration of a solution can be expressed in mol dm^{-3} or g dm^{-3}.
- The equation for calculating concentration in mol dm^{-3} is shown below.
- In this equation, **volume must be in dm^3** (to convert from cm^3 to dm^3, divide by 1000).

$$c\ (\text{mol dm}^{-3}) = \frac{\text{amount of solute (mol)}}{\text{volume of solution (dm}^3\text{)}}$$

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

c = concentration in mol dm^{-3}
n = amount in mol
V = volume in dm^3

$$n = cV \qquad V = \frac{n}{c}$$

- The equation for calculating the concentration in g dm^{-3} is shown below.

$$c\ (\text{g dm}^{-3}) = \frac{\text{mass of solute (g)}}{\text{volume of solution (dm}^3\text{)}}$$

Example: 50.0 g of NaCl are dissolved in 100 cm^3 of water which is then made up to 500.0 cm^3 in a volumetric flask. Calculate the concentration of the solution in mol dm^{-3} and g dm^{-3}.

Exercises:

1. Calculate the concentration (in mol dm^{-3} and g dm^{-3}) of these solutions.

a. 10.6 g of sodium carbonate (Na_2CO_3) in 1.00 dm^3 of solution.

b. 117 g of sodium chloride (NaCl) in 5.00 dm^3 of solution.

c. 0.830 g of potassium iodide (KI) in 25.0 cm^3 of solution.

2. Calculate the amount (in mol) of solute in each of the following solutions.

a. 0.250 dm^3 of 0.400 mol dm^{-3} ammonium chloride solution.

b. 200.0 cm^3 of 0.800 mol dm^{-3} sodium carbonate solution.

c. 300.0 cm^3 of 4.00 mol dm^{-3} sodium hydroxide solution.

3. Calculate the mass of solute in the following solutions.

a. 2.00 dm^3 of 0.200 mol dm^{-3} potassium hydroxide (KOH) solution.

b. 200.0 cm^3 of 0.100 mol dm^{-3} sodium carbonate (Na_2CO_3) solution.

c. 25.0 cm^3 of 0.0500 mol dm^{-3} copper(II) sulphate ($CuSO_4 \cdot 5H_2O$) solution.

Structure 1.4.6

Understandings:

- Avogadro's law states that equal volumes of all gases measured under the same conditions of temperature and pressure contain equal numbers of molecules.

Learning outcomes:

- Solve problems involving the mole ratio of reactants and/or products and the volume of gases.

Avogadro's law

- Equal volumes of gases at the same temperature and pressure contain the same number of particles.
- At STP (273 K and 100 kPa):

Amount (mol)	1 mol H_2	1 mol N_2	1 mol O_2
Volume (dm^3)	22.7	22.7	22.7
Number of particles	6.02×10^{23}	6.02×10^{23}	6.02×10^{23}

Example: 40 cm^3 of CO reacts with 40 cm^3 of O_2. What volume of CO_2 is produced? What volume of the excess reactant remains?

$$2CO_{(g)} + O_{2(g)} \rightarrow 2CO_{2(g)}$$

Exercises:

1. What volume of sulfur trioxide, in cm^3, can be prepared using 40 cm^3 sulfur dioxide and 20 cm^3 oxygen gas by the following reaction? Assume all volumes are measured at the same temperature and pressure.

$$2SO_{2(g)} + O_{2(g)} \rightarrow 2SO_{3(g)}$$

2. 5 dm^3 of carbon monoxide, $CO_{(g)}$, and 2 dm^3 of oxygen, $O_{2(g)}$, at the same temperature and pressure are mixed together. What is the maximum volume of carbon dioxide, $CO_{2(g)}$, in dm^3, that can be formed? What volume of the excess reactant remains?

$$2CO_{(g)} + O_{2(g)} \rightarrow 2CO_{2(g)}$$

3. 100 cm^3 of ethene, C_2H_4, is burned in 400 cm^3 of oxygen, producing carbon dioxide and some liquid water. Some oxygen remains unreacted (excess).

$$C_2H_{4(g)} + 3O_{2(g)} \rightarrow 2CO_{2(g)} + 2H_2O_{(g)}$$

Calculate the volume of carbon dioxide produced and the volume of oxygen remaining.