FACTFILE:
GCSE DAS CHEMISTRY: UNIT 2.6

Rewarding Learning

Quantitative Chemistry

Learning outcomes:

2.6.1 demonstrate knowledge and understanding of the terms **empirical formula, molecular formula**, hydrated, anhydrous and water of crystallisation;

2.6.2 demonstrate knowledge and understanding that water of crystallisation can be removed by heating to constant mass and any thermal decomposition may be carried out to completion by heating to constant mass;

2.6.3 calculate the relative formula mass of compounds containing water of crystallisation;

2.6.4 **determine the empirical formulae of simple compounds and determine the moles of water of crystallisation present in a hydrated salt from percentage composition, mass composition or experimental data;**

2.6.5 **calculate the concentration of a solution in mol/dm^3 given the mass of solute and volume of solution;**

2.6.6 **calculate the number of moles or mass of solute in a given volume of solution of known concentration;**

2.6.7 **calculate the atom economy of a reaction to form a desired product from the balanced equation:**

$$\text{Atom economy} = \frac{\text{mass of desired product}}{\text{total mass of products}} \times 100$$

Empirical formula and molecular formula

The empirical formula is the simplest whole number ratio of atoms of each element in a compound.

The molecular formula shows the actual number of atoms of each element present in a compound. It will be a simple multiple of the empirical formula. For example

molecular formula = C_4H_8 empirical formula = CH_2

molecular formula = CH_4 empirical formula = CH_4

To find the molecular formula from the empirical formula the relative formula mass is needed.

Example

A compound has relative formula mass 42 and empirical formula CH_2. What is the molecular formula of the compound?

Answer

A molecular formula is a multiple (n) of the empirical formula

$(CH_2)n = 42$

$(12 + 2 \times 1)n = 42$

$14n = 42$

$n = 3$

$(CH_2)n = (CH_2)_3 = C_3H_6$

Finding empirical formula.

1. Find the number of moles of each element in the compound using moles = $\frac{\text{mass (g)}}{A_r}$
2. Find the simplest ratio of moles (divide all the moles values by the smallest number of moles).

Example

Find the empirical formula of a compound which contains 50.05% sulfur, 49.95% oxygen.

Answer

In a sample of 100 g of this compound there is 50.05 g of sulfur, and 49.95 g of oxygen.

	sulfur	oxygen
Mass in grams	50.05	49.95
Moles = mass/A_r	$\frac{50.05}{32} = 1.56$	$\frac{49.95}{16} = 3.12$
Simplest ratio – divide by smallest number of moles (1.56)	$\frac{1.56}{1.56} = 1$	$\frac{3.12}{1.56} = 2$
Ratio	1	2
Formula	SO_2	

Water of crystallisation

Water of crystallisation is water which is chemically bonded into the crystal structure. Hydrated means the crystals contains water of crystallisation, and anhydrous means the substance does not contain water of crystallisation.

For example hydrated copper(II) sulfate contains five molecules of water of crystallisation for every one of copper(II) sulfate, the degree of hydration is five and the empirical formula is written $CuSO_4 \cdot 5H_2O$. When finding the relative formula mass of compounds containing water of crystallisation, the mass of the molecules of water of crystallisation must be included.

Experimental determination of mass of water of crystallisation in hydrated crystals

Water of crystallisation can be removed by heating to constant mass.

hydrated copper(II) sulfate	→	anhydrous copper(II) sulfate	+	water
$CuSO_4 \cdot 5H_2O$	→	$CuSO_4$	+	$5H_2O$

To heat to constant mass:

- Weigh the solid and container;
- Heat for a few minutes, cool then weigh;
- Repeat this until the mass does not change (at this point all of the water of crystallisation has been removed).

Example

In an experiment to find the mass of water of crystallisation in hydrated magnesium chloride $MgCl_2.xH_2O$ the following results were obtained.

Mass of empty crucible = 13.87g

Mass of crucible and hydrated magnesium chloride = 15.90g

Mass of crucible and anhydrous magnesium chloride = 14.82g

(i) Calculate the mass of the anhydrous magnesium chloride.

(ii) Calculate the number of moles of anhydrous magnesium chloride.

(iii) Calculate the mass of water of crystallisation removed.

(iv) Calculate the number of moles of water of crystallisation removed.

(v) Find x in the formula $MgCl_2.xH_2O$.

Answer

(i) To calculate the mass of anhydrous magnesium chloride, subtract the mass of the crucible (13.87 g) from the mass of the crucible and the anhydrous magnesium chloride (14.82 g)

$14.82 - 13.87 = 0.95$ g

(ii) M_r of anhydrous magnesium chloride = $24 + 2 \times 35.5 = 95$

$$\text{moles of anhydrous magnesium chloride} = \frac{\text{mass (g)}}{M_r} = \frac{0.95}{95} = 0.01 \text{ mol}$$

(iii) To calculate the mass of water, subtract the mass of the crucible and anhydrous magnesium chloride (14.82 g) from the mass of the crucible and hydrated magnesium chloride (15.90 g)

15.90 – 14.82 = 1.08 g

(iv) M_r of water = 18

$$\text{moles} = \frac{\text{mass (g)}}{M_r} = \frac{1.08}{18} = 0.06 \text{ mol}$$

(v)

	$MgCl_2$	H_2O
moles	0.01	0.06
ratio	1	6
formula	$MgCl_2.6H_2O$	

The value of x is 6

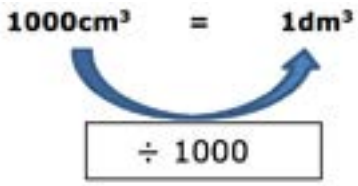
Thermal decomposition by heating to constant mass

Thermal decomposition is the breakdown of a solid using heat.

Sometimes a substance such as carbonates thermally decompose by the action of heat to produce a solid and a gas, which is released to the air and the mass decreases. To ensure the thermal decomposition goes to completion the solid is heated to constant mass. This means the solid is weighed, heated, cooled and reweighed until the mass no longer changes.

Concentration of solutions

The concentration of a solution is a measure of how much of a substance is dissolved in a given volume of water. Concentration is usually quoted in the units mol/dm^3 or g/dm^3.

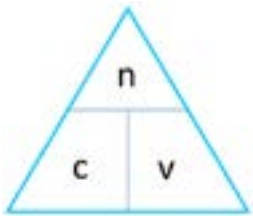


A concentrated solution will have a large number of **particles** of the solute in the solvent. A dilute solution will have a small number of particles of the solute in the solvent.

Concentration can be calculated using the following equation:

$$\text{concentration} = \frac{\text{number of moles}}{\text{volume (dm}^3\text{)}} \qquad c = \frac{n}{v}$$

This equation can be easily remembered using a triangle:



concentration = number of moles ÷ volume
number of moles = concentration × volume
volume = number of moles ÷ concentration

The units of concentration can be converted from mol/dm^3 to g/dm^3 using the following equation:

mol/dm^3 × RFM = g/dm^3

Example

What is the concentration in mol/dm^3 of a solution containing 11.1 g of $CaCl_2$ dissolved in 500 cm^3 of water?

Step 1: calculate the number of moles of solute (from unit 1 moles = $\frac{\text{mass (g)}}{M_r}$)

$$\text{moles of } CaCl_2 = \frac{\text{mass (g)}}{M_r} = \frac{11.1}{111} = 0.1 \text{ mol}$$

Step 2: convert the volume into dm^3

$$\text{Volume} = \frac{500}{1000} = 0.5 \text{ dm}^3$$

Step 3: substitute the values into the equation

$$\text{concentration} = \frac{\text{number of moles}}{\text{volume (dm}^3\text{)}} = \frac{0.1}{0.5} = 0.2 \text{ mol/dm}^3$$

Calculating moles or mass

The moles or mass of a substance dissolved in a solution can be calculated from a volume in cm^3 and concentration in mol/dm^3.

$$\text{moles} = \frac{\text{volume (cm}^3\text{) x concentration (mol/dm}^3\text{)}}{1000}$$

Example

Calculate the mass of calcium hydroxide dissolved in a 20.0 cm^3 of a 0.02 mol/dm^3 solution.

$$\text{moles} = \frac{\text{volume (cm}^3\text{) x concentration (mol/dm}^3\text{)}}{1000} = \frac{20.0 \text{ x } 0.02}{1000} \quad 0.004 \text{ mol}$$

M_r of calcium hydroxide = 40 + 2(16 + 1) = 74

mass of calcium hydroxide = moles × M_r = 0.004 × 74 = 0.296 g

Atom economy

Atom economy is essentially an efficiency calculation for a chemical reaction. It provides an indication of how much product is desired from the reaction and how much product is waste. The higher the atom economy of a reaction the 'greener' the process. Industrial processes need as high an atom economy as possible because it makes the process more sustainable and reduces the production of unwanted products – this saves on costs of disposal of these waste products.

Atom economy can be calculated using the following equation:

$$\text{Atom economy} = \frac{\text{mass of desired product}}{\text{total mass of products}} \times 100$$

Example

Iron is extracted from its ore using carbon. Find the atom economy of this reaction.

$2Fe_2O_3 + 3C \longrightarrow 4Fe + 3CO_2$

Step 1 – find the total M_r of iron atoms $4Fe = 4 \times 56 = 224$

Step 2 – find the total M_r of all products $4Fe = 224$; $3CO_2 = 3 \times 44 = 132$;

$224 + 132 = 356$

Step 3 – use the equation to calculate the atom economy

$$\text{Atom economy} = \frac{\text{mass of desired product}}{\text{total mass of products}} \times 100$$

$$\frac{224}{356} \times 100 = 62.9\%$$

A high atom economy is important in a reaction to prevent waste and to ensure sustainable development and to minimise loss of profit due to waste.

REVISION QUESTIONS

1. 3 g of hydrated zinc sulfate crystals are heated to constant mass. 1.68 g of the anhydrous salt remains. Find the formula of the hydrated crystals.

[4]

2. Determine the empirical formula of a compound with the following composition by mass: 36.0 % C, 4.0 % H, 28.0 % N and 32.0 % O.

[4]

3. Determine the empirical formula of a compound with the following composition by mass:
48.0 % C, 8.0 % H, 28.0 % N and 16.0 % O.
If this compound has an M_r of 200, what is its molecular formula?

[5]

4. Use the experimental data below to find the formula of the hydrated cobalt(II) chloride salt:

Mass of crucible	42.22 g
Mass of crucible and hydrated salt	44.60 g
Mass of crucible and anhydrous salt 1	43.95 g
Mass of crucible and anhydrous salt 2	43.42 g
Mass of crucible and anhydrous salt 3	43.42 g

[5]

5. A student reacted 0.438 g of strontium with 200 cm^3 of water.

$$Sr(s) + 2H_2O(l) \longrightarrow Sr(OH)_2(aq) + H_2(g)$$

(i) Calculate how many moles of Sr were reacted.

[2]

(ii) Calculate the concentration, in mol/dm^3, of the $Sr(OH)_2$ solution produced.

[2]

6. Calculate the atom economy when sodium is made from sodium chloride.

$$2NaCl \longrightarrow 2Na + Cl_2$$

[3]

7. Calculate the atom economy when hydrogen is produced from the reaction of zinc and hydrochloric acid.

$$Zn + 2HCl \longrightarrow ZnCl_2 + H_2$$

[3]