CAIE Chemistry A-level

2: Atoms, Molecules and Stoichiometry

Notes

Relative Atomic Masses of Atoms and Molecules

It is important that you learn the following definitions:

- **Unified atomic mass:** 1/12 the mass of an atom of carbon-12.
- **Relative atomic mass**: the weighted average mass of an atom of an element compared with 1/12 of the mass of an atom of carbon-12.
- **Relative isotopic mass**: the mass of an atom of an isotope compared to 1/12 of the mass of an atom of carbon-12.
- **Relative molecular mass**: the weighted average mass of one molecule of an element or compound compared with 1/12 of the mass of an atom of carbon-12.
- **Relative formula mass**: the weighted average mass of one unit of a substance compared with 1/12 of the mass of an atom of carbon-12.

The Mole and the Avogadro Constant

One mole is the **amount** of any substance that contains as many particles as there are carbon atoms in **exactly 12 g of carbon-12**. One mole of any substance will always contain exactly the same number of particles. **Avogadro's constant** is the **number of particles in one mole** of any substance. The particles could represent **atoms**, **ions** or **molecules**. Avogadro's constant is equal to 6.02×10^{23}.

Therefore, there exists the following relationship:

Number of particles = Avogadro's constant x moles

<u>Example</u>
How many atoms are there in 0.250 moles of carbon?
Number of atoms $= 0.250 \times 6.02 \times 10^{23}$
$= 1.51 \times 10^{23}$ *atoms*
The answer must be given in as many significant figures as were given in the question.

Formulae

Formulae for Ionic Compounds

The **chemical formula** for ionic compounds can be constructed by ensuring the **charges** on the constituent ions are **balanced**. The compound must have a **neutral charge** overall.

The ionic **charge** of an ion can sometimes be **deduced** by the position of the element in the **periodic table**. However, this is not possible for all elements since some elements form ions with **different charges**. The following points can be obtained from the periodic table:

- **Metals**, found on the left of the periodic table, will lose electrons to form **positive ions**.
- **Non-metals**, found on the right of the periodic table, will gain electrons to form **negative ions**.
- **Group 1** metals all form positive ions with a **+1 charge** since they all lose one electron to form a stable electron configuration. In the same way, **Group 2** elements all form positive ions with a **+2 charge**.
- The first four halide ions, in **Group 7**, all form ions with a **-1 charge** since they all gain one electron to form a stable electron configuration.

The charge on an ion can be represented as a **charge next to the chemical symbol** or by **roman numerals** at the end of the chemical name. If an element forms multiple ions, roman numerals are used at the end of the name to **distinguish which ion has formed**.

For example, **iron** can form **two ions**: Fe^{2+} and Fe^{3+}. If the Fe^{2+} ion reacts with a SO_4^{2-} sulfate ion, the compound will be named iron(II) sulfate. The roman numerals distinguish the presence of the +2 charged iron ion.

The following **common ions** should be learnt. They will help you when writing the formulae of ionic compounds:

Nitrate: NO_3^-
Carbonate: CO_3^{2-}
Sulfate: SO_4^{2-}
Hydroxide: OH^-
Ammonium: NH_4^+
Bicarbonate: HCO_3^-
Phosphate: PO_4^{3-}
Zinc: Zn^{2+}
Silver: Ag^+

<u>Example</u>
What is the chemical formula for the ionic compound magnesium hydroxide?

Magnesium is in Group 2 of the periodic table so it forms the ion Mg^{2+}. The hydroxide ion is one of the common ions shown above, which we know is OH^-. Since the hydroxide ion only has a 1- charge we need two of them to balance out the 2+ charge on the magnesium ion. This gives the formula $Mg(OH)_2$.

Ionic compounds can be described as **hydrous** or **anhydrous**. A compound is hydrous if it contains water within its structure, whereas a compound is anhydrous if it contains no water within its structure. If there are **water molecules** present within **crystal structures**, then the water molecules are described as **water of crystallisation.**

Balanced Equations

For equations to be balanced there must be the **same number of each atom** on both sides.

Example

Balance the equation: $C_3H_8 + O_2 \rightarrow CO_2 + H_2O$

First balance the carbon atoms by placing a 3 in front of the CO_2 product:

$$C_3H_8 + O_2 \rightarrow \mathbf{3}CO_2 + H_2O$$

Next, balance the hydrogen atoms by placing a 4 in front of the H_2O product:

$$C_3H_8 + O_2 \rightarrow \mathbf{3}CO_2 + \mathbf{4}H_2O$$

Finally, balance the oxygen atoms by placing a 5 in front of the O_2 reactant:

$$C_3H_8 + \mathbf{5}O_2 \rightarrow \mathbf{3}CO_2 + \mathbf{4}H_2O$$

It can be useful to also include **state symbols** in reaction equations so it is clear what might be observed during the reaction.

There are four state symbols:

- (s) - solid
- (l) - liquid
- (g) - gas
- (aq) - aqueous (dissolved in water)

Ionic Equations

Ionic equations show just the **reacting particles** that undergo a change during the reaction and not the **spectator species**. As with normal chemical equations, it must be balanced. The reacting species are shown as **dissociated ions.**

Example: $Ag^+_{(aq)} + Cl^-_{(aq)} \rightarrow AgCl_{(s)}$

Empirical and Molecular Formulae

- **Empirical formula**: the simplest whole number ratio of atoms of each element in a compound.
- **Molecular formula**: the actual number of atoms of each element in a compound.

Calculating Empirical Formulae

1. Divide the mass (or percentage by mass) of each element by its molar mass to calculate the molar ratio.
2. Divide each number in the ratio by the smallest number to get the simplest ratio of elements.
3. If the ratio contains decimal numbers, multiply it as appropriate to obtain whole numbers.

<u>Example</u>

A 10 g compound contains 5.65 g potassium, 0.870 g carbon and 3.48 g oxygen. Find the empirical formula.

First calculate the moles of each element:

Moles of potassium = 5.65 ÷ 39.1 = 0.145

Moles of carbon = 0.870 ÷ 12 = 0.0725

Moles of oxygen = 3.48 ÷ 16 = 0.218

Divide all of the moles by the smallest mole value (0.0725) we get the ratio 2:1:3 of K:C:O.

Therefore, we have the empirical formula: K_2CO_3

Calculating Molecular Formulae

To **calculate** molecular formula, calculate the **relative formula mass** of the **empirical formula** and then divide the relative formula mass of the compound by this empirical formula mass value. This will show **how many times larger** the molecular formula is than the empirical formula.

<u>Example</u>

A compound has the empirical formula HO and the relative formula mass is 34. What is the molecular formula?

Empirical formula mass = 16 + 1 = 17

34/17 = 2 so the molecular formula is H_2O_2.

Reacting Masses and Volumes

When completing calculations in chemistry, quantities should be given to the **same number of significant figures** as the **least accurate measured quantity**. So if the values are given to 2 significant figures then the answer should also be given to 2 significant figures.

Calculations Involving Reacting Masses:

Molar mass is the mass per mole of a substance and can be calculated by **adding the relative atomic masses** of all the atoms in a formula. To calculate the number of moles using mass and molar mass:

Number of moles = mass (g) ÷ molar mass

This equation can be used to calculate the **mass of products** produced in a reaction:

<u>Example</u>

What is the mass of iron oxide produced if 30.4 g of iron is burnt in air?

$$4Fe + 3O_2 \rightarrow 2Fe_2O_3$$

The Mr of Fe is 55.8 so the number of moles of iron in 30.4 g is:

30.4 ÷ 55.8 = 0.545 moles

The equation shows that 4 moles of Fe give 2 moles of Fe_2O_3 *so 0.545 moles of Fe will give 0.273 moles of* Fe_2O_3 *(found by dividing the moles by 2).*

The Mr of Fe_2O_3 *is 2(55.8)+3(16)=159.6 so the mass of* Fe_2O_3 *produced is:*

0.273 x 159.6 = 43.6 g (3.s.f)

Percentage Yield

The percentage yield indicates how much of the maximum amount of product you obtained during an **experiment**. A **low** percentage yield could indicate an **incomplete reaction**, or the loss of product during **purification**.

$$\% \text{ yield} = \frac{\text{Experimental mass} \times 100}{\text{Theoretical mass}}$$

Calculations Involving Volumes of Gases

At the **same temperature and pressure**, one mole of any gas will occupy the **same volume**. At room temperature and pressure, this is 24 dm^3. Room temperature and pressure is **298K** and **1 atm.**

This relationship gives the following equation that can be used to work out the volume of a gas if its amount (number of moles) is known and vice versa.

$$\text{Volume of gas } (dm^3) = 24 \times \text{Number of moles}$$
(At room temperature & pressure)

Calculations Involving Concentrations and Volumes of Solutions

Concentration is the **amount of solute** dissolved in a **given volume of solution**. The concentration of a solution can be measured in **mol dm^{-3}** and **g dm^{-3}** which can be calculated using the following equations:

$$\textbf{Concentration (mol dm}^{-3}\textbf{)} = \frac{\text{Number of moles (mol)}}{\text{Volume } (dm^3)}$$

$$\textbf{Concentration (g dm}^{-3}\textbf{)} = \frac{\text{Mass (g)}}{\text{Volume } (dm^3)}$$

Calculations Involving Excess and Limiting Reagents

The **limiting reagent** is the reactant that gets **used up completely**, since it limits how much product is formed. The **reagent in excess** is the reactant which is **not used up** once the reaction has finished.

The limiting reagent is used to calculate **how much product will be formed** from a reaction:

1. Determine the balanced chemical equation for the reaction given.
2. Calculate the moles of each reactant using the equation and the masses which took places in the reaction.
3. Calculate the mole ratio and compare this to the balanced equations ratio.
4. Use the limiting reagent to calculate the amount of product that will be produced.

Example:
Calculate how much product is formed from the reaction when 2.85 g of aluminium reacts with 4.18 g of chlorine. Identify the limiting reagent.

The balanced equation is: $2Al + 3Cl_2 \rightarrow 2AlCl_3$
Al has an Mr of 27.0 so the number of moles of Al in 2.85 g is:
Number of moles = $2.85 \div 27 = 0.106$
Cl_2 *has an Mr of 71.0 so the number of moles of* Cl_2 *in 4.18 g is:*
Number of moles = $4.18 \div 71 = 0.0589$
Aluminium and chlorine react in a 2:3 ratio.
We would need $2(0.106) \div 3 = 0.0707$ *moles of chlorine to react with aluminium completely. Since we do not have this many moles of chlorine, we have found that chlorine is the limiting reagent.*
Therefore, chlorine determines the amount of product formed:
Cl_2 *and* $AlCl_3$ *are in a 3:2 ratio so* $2(0.0589 \div 3) = 0.0393$ *moles of* $AlCl_3$ *are formed. The Mr of* $AlCl_3$ *is 133.5 so the mass of* $AlCl_3$ *formed is:*
$0.0393 \times 133.5 = 5.24$ *g*

Stoichiometry

Stoichiometry is the **relationship** between the number of moles of **reactants** and number of moles of **products** of a reaction. A **balanced chemical equation** can be used to find the stoichiometry of a reaction. Stoichiometric relationships can be deduced by using the various **calculations** outlined above.