2 Atoms, molecules and stoichiometry

Relative masses of atoms

There are more than 100 chemical elements, and each element is made up of its own kind of atoms. The atoms of different elements differ in size, and so have different masses. You saw in Chapter 1 that the atoms are made up of different sorts of and numbers of particles (Figure 2.1).

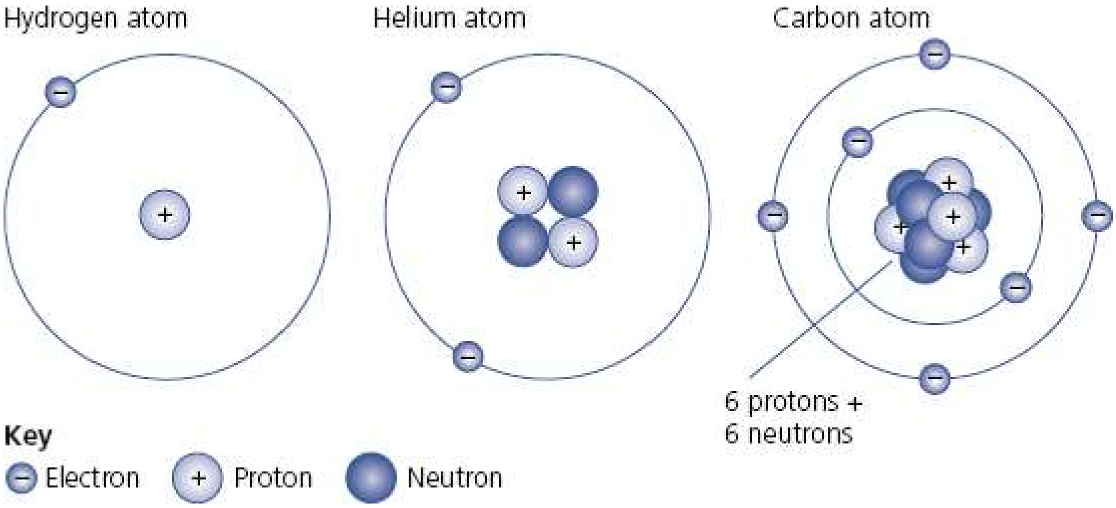

Figure 2.1 Atoms of hydrogen, helium and carbon

You should be able to identify:

- two types of particle in the **nucleus**, which is in the centre of the atom. The two particles in the nucleus are **protons** and **neutrons**. They have the same mass, but a proton has a single positive charge and a neutron has no charge.
- another type of particle that orbits the nucleus – these particles are called **electrons**. An electron has almost no mass but carries a single negative charge (Table 2.1).

Table 2.1

Particle	Relative mass	Relative charge
Proton	1	+1
Neutron	1	0
Electron	0	−1

NOW TEST YOURSELF

1 Make a copy of the table below. Use the Periodic Table to work out which particles are described in the table. The final entry needs some careful thought. Can you work out what is going on here?

	Protons	Neutrons	Electrons	Identity of species
a	11	12	11	$^{23}_{11}Na$
b	9	10	9	
c	16	16	16	
d	24	28	24	
e	18	20	17	

For AS Level you need to be able to distinguish between terms that relate to the masses of elements and compounds.

Mass related terms

Relative atomic mass, A_r, is defined as the mass of one atom of an element relative to one-twelfth of the mass of an atom of carbon-12, ^{12}C, which has a mass of 12.00 atomic mass units.

Relative isotopic mass is like relative atomic mass in that it deals with atoms. The difference is that we are dealing with different atoms of the same element. The isotopes of an element have the same number of protons, but different numbers of neutrons. Hence, isotopes of an element have different masses.

Relative molecular mass, M_r, is defined as the mass of one molecule of an element or compound relative to one-twelfth of the mass of an atom of carbon-12, ^{12}C, which has a mass of 12.00 atomic mass units.

Relative formula mass is used for substances that do not contain molecules, such as sodium chloride, NaCl, and is the sum of all the relative atomic masses of the atoms in the formula of the substance.

It is important to remember that because these are all *relative* masses, they have no units.

The mole

Individual atoms cannot be picked up or weighed, so we need to find a way of comparing atomic masses. One way is to find the mass of the same number of atoms of different types. Even so, the masses of atoms are so small that we need a huge number of atoms of each element to weigh. This number is called the **Avogadro constant**. It is equal to 6.02×10^{23} and is also referred to as **one mole**. The abbreviation for mole is 'mol'.

KEY TERM

A **mole** is Avogadro's number (6.02×10^{23}) of atoms or molecules.

You may wonder why such a strange number is used. It is the number of atoms of a substance that make up the relative atomic mass, A_r, in grams. The mass is measured relative to one-twelfth of the mass of a carbon atom, ^{12}C.

Mole calculations

You should be able to work out how many moles a given mass of an element or compound represents. To do that you need to know the relative atomic mass, A_r, of the element (or elements) present. You can get this information from the Periodic Table.

NOW TEST YOURSELF

2 How many moles of atoms do the following masses represent?

a 6 g of carbon, C

b 24 g of oxygen, O

c 14 g of iron, Fe

3 How many grams of substance are in the following amounts?

a 0.2 mol of neon, Ne

b 0.5 mol of silicon, Si

c 1.75 mol of helium, He

d 0.25 mol of carbon dioxide, CO_2

Empirical and molecular formulae

The **empirical formula** of a compound is its simplest formula. It shows the ratio of the numbers of atoms of the different elements in a compound.

You need to know how to use the composition by mass of a compound to find its empirical formula:

- Divide the mass (or percentage mass) of each element by its A_r.
- Use the data to calculate the simplest whole number ratio of atoms.

WORKED EXAMPLE

A chloride of iron contains 34.5% by mass of iron. Determine the empirical formula of the compound.

Answer

Element	% by mass (*m*)	A_r	m/A_r	Moles	Ratio
Fe	34.5	56	$\frac{34.5}{56}$	0.616	1
Cl	65.5	35.5	$\frac{65.5}{35.5}$	1.85	3

So the empirical formula of this chloride is $FeCl_3$.

NOW TEST YOURSELF

4 Work out the empirical formulae of the following compounds:

a compound A – composition by mass: 84.2% rubidium, 15.8% oxygen

b compound B – composition by mass: 39.1% carbon, 52.2% oxygen, 8.70% hydrogen

By contrast, the **molecular formula** of a compound shows the *actual number* of atoms of every element present in the compound. The molecular formula is always a multiple of the empirical formula.

WORKED EXAMPLE

A compound has the empirical formula CH_2O, and a molar mass of 60. What is its molecular formula?

Answer

You can see that the formula mass of the compound is:

$$(1 \times 12) + (2 \times 1) + (1 \times 16) = 30$$

Because the molar mass is 60, the molecular formula must be twice the empirical formula, $C_2H_4O_2$.

Writing and balancing equations

Chemical equations are a shorthand way of describing chemical reactions. Using the symbols of elements used in the Periodic Table ensures that they are understood internationally. Whenever you write a chemical equation there are simple rules to follow:

- Check the formula of each compound in the equation.
- Check that the overall equation balances.

- Try to visualise what is happening in the reaction. This will help you choose the correct **state symbol** – the state symbols are (s) for solid, (l) for liquid, (g) for gas and (aq) for an aqueous solution.

Suppose you want to write a chemical equation for the reaction between magnesium and dilute sulfuric acid. You can probably write a word equation for this from your previous studies of chemistry:

magnesium + sulfuric acid → magnesium sulfate + hydrogen

In symbols this becomes:

$$Mg + H_2SO_4 \rightarrow MgSO_4 + H_2$$

Counting up the numbers of each type of atom on each side of the arrow shows that they are equal – the equation is *balanced*.

You can include more detail about the states of the reactants and products and add the state symbols:

$$Mg(s) + H_2SO_4(aq) \rightarrow MgSO_4(aq) + H_2(g)$$

You might also remember that dilute sulfuric acid is a mixture of H^+ and SO_4^{2-} ions. So you can write an ionic equation showing just the changes in species (this word refers to a reactant or product that is not a chemical you can get from a bottle, e.g. sulfate ion, SO_4^{2-}), or chemical forms:

$$Mg(s) + 2H^+(aq) \rightarrow Mg^{2+}(aq) + H_2(g)$$

Writing and balancing complicated equations

A more complicated reaction is that between sodium carbonate and hydrochloric acid. You will have seen the mixture fizz in the laboratory:

sodium carbonate + hydrochloric acid → sodium chloride + carbon dioxide

Using symbols this becomes:

$$Na_2CO_3 + HCl \rightarrow NaCl + CO_2$$

Counting the atoms on each side of the arrow shows that there are ‘spare’ atoms of sodium, oxygen and hydrogen on the left-hand side and no hydrogen on the right-hand side. You can take care of the sodium by doubling the amount of sodium chloride formed, but what about the hydrogen and oxygen? Water is a compound of hydrogen and oxygen, so let us see what happens if water is added to the right-hand side:

$$Na_2CO_3 + 2HCl \rightarrow 2NaCl + CO_2 + H_2O$$

Doubling the amounts of HCl and NaCl now makes the equation balance. Adding the state symbols gives:

$$Na_2CO_3(s) + 2HCl(aq) \rightarrow 2NaCl(aq) + CO_2(g) + H_2O(l)$$

Notice that water is a liquid, not aqueous.

The ionic equation for this reaction is:

$$(Na^+)_2CO_3^{2-}(s) + 2H^+(aq) \rightarrow 2Na^+(aq) + CO_2(g) + H_2O(l)$$

Calculations using equations and the mole

Now that you understand moles and how to write balanced chemical equations, you can use these two ideas to calculate the quantities of substances reacting together and the amounts of products formed in reactions.

There are three main types of calculation you might be expected to perform:

- reacting masses (from formulae and equations)
- volumes of gases reacting or being produced
- volumes and concentrations of solutions of chemicals reacting

In each of these, use balanced chemical equations and the mole concept for quantities of chemical compounds.

Calculations involving reacting masses

Suppose copper(II) carbonate is heated. What mass of copper(II) oxide would be formed starting from 5.0 g of the carbonate?

Let us break the calculation down into simple stages.

1 Write the equation for the reaction:

$CuCO_3 \rightarrow CuO + CO_2$

2 Now work out the relative molecular mass of each of the substances involved:

$$CuCO_3 \rightarrow CuO$$
$$63.5 + 12 + (3 \times 16) \rightarrow 63.5 + 16$$
$$123.5\ g \rightarrow 79.5\ g$$

3 Finally, calculate the mass of CuO formed from 5.0 g of $CuCO_3$:

$$5.0\ g \rightarrow 5 \times \frac{79.5}{123.5}\ g = 3.2\ g$$

mass of CuO = 3.2 g

STUDY TIP

The starting mass of copper(II) carbonate is quoted to 2 significant figures, so you should give an answer to 2 significant figures. This idea is important in scientific calculations. You will also come across its use in practical work involving calculations.

NOW TEST YOURSELF

Try these calculations using the idea of reacting masses (remember to use the correct number of significant figures).

5 What mass of carbon dioxide is lost when 2.5 g of magnesium carbonate is decomposed by heating?

6 What mass of potassium chloride is formed when 2.8 g of potassium hydroxide is completely neutralised by hydrochloric acid?

7 What is the increase in mass when 6.4 g of calcium is completely burned in oxygen?

These questions are relatively straightforward. However, you might be asked to use mass data to determine the formula of a compound. The next worked example shows you how to do this.

WORKED EXAMPLE

When heated in an inert solvent, tin metal reacts with iodine to form a single orange-red solid compound. In an experiment, a student used 5.00 g of tin in this reaction. After filtering and drying, the mass of crystals of the orange compound was 26.3 g. Using this data, work out the formula of the orange compound.

Answer

First, calculate how much iodine was used in the reaction. Do this by subtracting the mass of tin from the final mass of the compound:

mass of iodine used = 26.3 g − 5.00 g = 21.3 g

Next, convert the masses of tin and iodine into the number of moles of each. Do this by dividing each mass by the relevant atomic mass:

$$\text{moles of tin} = \frac{5.00}{119} = 0.0420\,\text{mol}$$

$$\text{moles of iodine} = \frac{21.3}{127} = 0.168\,\text{mol}$$

As you can see, the ratio of the number of moles used shows that there are four times as many moles of iodine as there are of tin in the compound. So the formula of the orange-red crystals is SnI_4.

Calculations involving volumes of gases

- Not all chemical reactions involve solids. For reactions in which gases are involved it is more convenient to measure volumes than masses. You need a way of linking the volume of a gas to the number of particles it contains – in other words a way of converting volume to moles.
- In the early nineteenth century, Avogadro stated that equal volumes of gases at the same temperature and pressure contain equal numbers of molecules. One mole of a gas occupies 24 dm^3 at room temperature (25°C) and a pressure of 101 kPa (1 atm); or 22.4 dm^3 at standard temperature (273 K) and the same pressure (stp).
- This means that if you measure the volume of gas in dm^3 at room temperature and pressure, it can be converted directly to the number of moles present by dividing by 24.

The easiest way to see how this works is to look at an example. The reaction between hydrogen and chlorine forms hydrogen chloride:

$$H_2(g) + Cl_2(g) \rightarrow 2HCl(g)$$

It would not be easy to measure the reacting masses of the two gases. You could, however, measure their volumes. When this is done, we find that there is no overall change in volume during the reaction. This is because there are two moles of gas on the left-hand side of the equation and two moles of the new gas on the right-hand side.

Some reactions produce gases as well as liquids, and in others gases react with liquids to form solids, and so on. In these cases, you can use the above method combined with the method used the first calculation.

For example, 2.0 g of magnesium dissolves in an excess of dilute hydrochloric acid to produce hydrogen:

$$Mg(s) + 2HCl(aq) \rightarrow MgCl_2(aq) + H_2(g)$$

The equation shows that for every mole of magnesium used, 1 mole of hydrogen gas is formed.

Because 2.0 g of magnesium is $\frac{2.0}{24.3}$ mol, this means that $\frac{2.0}{24.3}$ mol of hydrogen gas should be formed.

Each mole of hydrogen occupies 24 dm^3 at room temperature and pressure, so:

$$\text{volume of hydrogen produced} = \frac{2.0}{24.3} \times 24\,dm^3 = 1.98\,dm^3$$

NOW TEST YOURSELF

Try the following calculations involving volumes of gas(es).

8 25 cm^3 of the gas propane, C_3H_8, is burned in an excess of oxygen to form carbon dioxide and water. What volume of oxygen reacts, and what volume of carbon dioxide is formed at room temperature and pressure? (You can assume that the water formed is liquid and has negligible volume.)

9 A sample of lead(IV) oxide was heated in a test tube:

$$2PbO_2(s) \rightarrow 2PbO(s) + O_2(g)$$

and the oxygen gas released was collected. What mass of the oxide would be needed to produce 80 cm^3 of oxygen at room temperature and pressure?

10 Carbon dioxide was bubbled into limewater (a solution of calcium hydroxide) and the solid calcium carbonate precipitated was filtered off, dried and weighed. If 0.50 g of calcium carbonate was formed, what volume of carbon dioxide, at room temperature and pressure, was passed into the solution?

$$Ca(OH)_2(aq) + CO_2(g) \rightarrow CaCO_3(s) + H_2O(l)$$

Calculations involving volumes and concentrations of solutions

- This type of calculation is particularly important because they often arise in the AS practical paper (see page 127 on practical work).
- The basic principles of the calculations are the same as those covered already, the only complication being that the reactants are in solution. This means that instead of dealing with masses, you are dealing with volumes of solutions of known concentration.

- Another way of dealing with this is to work how many **moles** of substance are dissolved in 1 dm^3 of solution – this is known as the **molar concentration**. Do not confuse this with **concentration**, which is the **mass** of substance dissolved in 1 dm^3.
- Think about a 0.1 mol dm^{-3} solution of sodium hydroxide. The mass of 1 mole of sodium hydroxide is (23 + 16 + 1) or 40 g. So a 0.1 mol dm^{-3} solution contains $40 \times 0.1 = 4.0$ g per dm^3.
- If you know the molar concentration of a solution and the volume that reacts with a known volume of a solution containing another reactant, you can calculate the molar concentration of the second solution using the equation for the reaction.

WORKED EXAMPLE

In a titration between dilute sulfuric acid and 0.1 mol dm^{-3} sodium hydroxide, 21.70 cm^3 of the sodium hydroxide was needed to neutralise 25.00 cm^3 of the dilute sulfuric acid. Using the following equation for the reaction, calculate the concentration of the acid in mol dm^{-3}.

$$H_2SO_4(aq) + 2NaOH(aq) \rightarrow Na_2SO_4(aq) + 2H_2O(l)$$

Answer

From the equation you can see that 1 mole of sulfuric acid requires 2 moles of sodium hydroxide for complete reaction. The number of moles of sodium hydroxide used is hydroxide used is $\frac{21.70}{1000} \times 0.1$..

This would neutralise

$$\frac{21.7 \times 0.1}{1000 \times 2}$$

moles of sulfuric acid.

This number of moles is contained in 25.00 cm^3 of sulfuric acid.

To get the number of moles in 1 dm^3, multiply this number by $\frac{1000}{25.00}$. This gives:

$$\frac{21.70 \times 0.1 \times 1000}{1000 \times 2 \times 25.00} = 0.0434\,\text{mol}\,\text{dm}^{-3}$$

Different types of salts

When we are looking at the formation of salts there are two different types – ones which contain water molecules in their crystals (**hydrated** salts) and ones which contain no water (**anhydrous** salts).

Dissolving copper(II) oxide in dilute sulfuric acid and crystallising the solution formed produces blue crystals of hydrated copper(II) sulfate.

$$CuO + H_2SO_4(aq) \rightarrow CuSO_4{\bullet}5H_2O + H_2O$$

If we gently heat these blue crystals we end up with a white powder called anhydrous copper(II) sulfate.

$$CuSO_4{\bullet}5H_2O \rightarrow CuSO_4 + 5H_2O$$

The water associated with the crystalline form and which is given off on heating is called **water of crystallisation**.

NOW TEST YOURSELF

The following calculations involving volumes and concentrations of solutions will give you practice in this important area of the syllabus.

11 In a titration, 27.60 cm^3 of 0.100 mol dm^{-3} hydrochloric acid neutralised 25.00 cm^3 of potassium hydroxide solution. Calculate the molar concentration of the potassium hydroxide solution and its concentration in g dm^{-3}.

12 A 0.2 mol dm^{-3} solution of nitric acid was added to an aqueous solution of sodium carbonate. 37.50 cm^3 of the acid was required to react completely with 25.00 cm^3 of the carbonate. Calculate the molar concentration of the carbonate.

REVISION ACTIVITY

a What is the mass of 0.05 mol of Na_2SO_4?

b What volume of 0.05 mol dm^{-3} H_2SO_4 is needed to exactly react with 25 cm^3 of 0.05 mol dm^{-3} NaOH to form a 0.05 mol dm^{-3} solution of Na_2SO_4?

c What volume of 0.05 mol dm^{-3} HCl would exactly neutralise the same volume of 0.05 mol dm^{-3} NaOH as in part b?

END OF CHAPTER CHECK

By now you should be able to:

- define relative masses of atoms and molecules based on carbon-12
- define the mole in terms of the Avogadro constant
- define and use empirical and molecular formulae
- calculate reacting masses and volumes of solutions and gases