4 Stoichiometry – chemical calculations

FOCUS POINTS

- ★ How can I calculate the mass of products in a reaction?
- ★ What is relative atomic mass?
- ★ How is a mole and the Avogadro constant useful in balancing calculations?
- ★ How can I determine the formula of a compound?

In this chapter, you will learn how to calculate the masses of products formed in a chemical reaction, when told the quantity of reactants you start with, and also how to calculate the mass of starting materials you need to produce a certain mass of product. These are the type of calculations your teacher does before they write the methods for student practicals. Have you ever thought how your teachers were able to get it right every time?

We will look at the amounts of substances used and formed during reactions involving solids, gases and solutions. You need to know whether you actually got the right amount of product in your experiment, and we will also look at how well a reaction went.

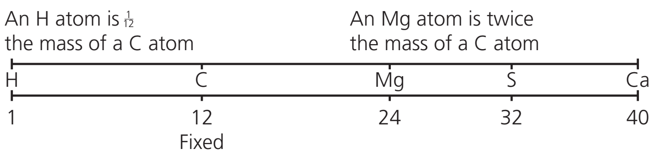
By the end of this chapter we hope that you will be confident in using numbers and balanced chemical reactions to help you to discover these things.

4.1 Relative atomic mass

There are at present 118 different elements known. The atoms of these elements differ in mass because of the different numbers of protons, neutrons and electrons they contain. The actual mass of one atom is very small. For example, the mass of a single atom of sulfur is around:

0.000 000 000 000 000 000 000 053 16 g

Such small quantities are not easy to work with and, as you saw in Chapter 3, a scale called the **relative atomic mass, A_r,** scale is used. In this scale, an atom of carbon is given a relative atomic mass, A_r, of 12.00. All other atoms of the other elements are given a relative atomic mass compared to that of carbon.



▲ **Figure 4.1** The relative atomic masses of the elements H, C, Mg, S and Ca

Key definition

Relative atomic mass, A_r, is the average mass of the isotopes of an element compared to 1/12th of the mass of an atom of ^{12}C.

Reacting masses

Chemists often need to be able to show the relative masses of the atoms involved in a chemical process.

? Worked example

What mass of carbon dioxide would be produced if 6 g of carbon was completely burned in oxygen gas?

$$C + O_2 \rightarrow CO_2$$

Instead of using the actual masses of atoms, we use the relative atomic mass to help us answer this type of question.

In this example we can work out the **relative molecular mass, M_r,** of molecules such as O_2 and CO_2 using the relative atomic masses of the atoms they are made from. The relative molecular mass is the sum of the relative atomic masses of all those elements shown in the **molecular formula** of the substance. The molecular formula of oxygen is O_2 and it shows that one molecule of oxygen contains two oxygen atoms. Each oxygen atom has a relative atomic mass of 16, so O_2 has a relative molecular mass of $2 \times 16 = 32$.

The molecular formula of carbon dioxide is CO_2 and it shows that in one molecule of carbon dioxide there is one carbon atom and two oxygen atoms. The carbon atom has a relative atomic mass of 12 and each oxygen atom has a relative atomic mass of 16, so CO_2 has a relative molecular mass of 12 + (2 × 16) = 44.

Key definitions

The **molecular formula** of a compound is defined as the number and type of different atoms in one molecule.

Relative molecular mass, M_r, is the sum of the relative atomic masses. Relative formula mass, M_r, is used for ionic compounds.

Relative formula mass, M_r, is used for ionic compounds

So we can now use the equation to answer the question: What mass of carbon dioxide would be produced if 6 g of carbon was completely combusted?

$$C + O_2 \rightarrow CO_2$$

12 32 44

We can convert these relative masses to actual masses by adding mass units, g, which gives:

$$C + O_2 \rightarrow CO_2$$

12 32 44

12 g 32 g 44 g

The above calculation shows that if 12 g of carbon was burned completely then 44 g of carbon dioxide gas would be formed. So, 6 g of carbon burning would result in the formation of 22 g of carbon dioxide gas.

Test yourself

1 What mass of carbon dioxide gas would be produced if 10 g of calcium carbonate reacted with an excess of hydrochloric acid?

2 What mass of sulfur dioxide would be produced if 64 tonnes of sulfur was completely reacted with oxygen gas?

Chemists often need to know how much of a substance has been formed or used up during a chemical reaction. This is particularly important in the chemical industry, where the substances being reacted (the reactants) and the substances being produced (the products) may be worth a great deal of money. Waste costs money!

To solve this problem, the chemical industry needs a way of counting atoms, ions or molecules. As atoms, ions and molecules are very tiny particles, it is impossible to measure out a dozen or even a hundred of them. Instead, chemists weigh out a very large number of particles.

This number is 6.02×10^{23} atoms, ions or molecules and is called Avogadro's constant after the famous Italian scientist Amedeo Avogadro (1776–1856). An amount of substance containing 6.02×10^{23} particles is called a **mole** (often abbreviated to mol).

Key definition

The **mole**, symbol mol, is the unit of amount of substance. 1 mole contains 6.02×10^{23} particles, e.g. atoms, ions, molecules. This number is called the Avogadro constant.

4.2 Calculating moles

In Chapter 3, we looked at how we can compare the masses of all the other atoms with the mass of carbon atoms. This is the basis of the relative atomic mass scale. Chemists have found by experiment that if you take the relative atomic mass of an element in grams, it always contains 6.02×10^{23} or 1 mole of its atoms.

Moles and elements

For the elements we can see that, for example, the relative atomic mass (A_r) of iron is 56, so 1 mole of iron is 56 g. Therefore, 56 g of iron contains 6.02×10^{23} atoms.

The A_r for aluminium is 27. In 27 g of aluminium it is found that there are 6.02×10^{23} atoms. Therefore, 27 g of aluminium is 1 mole of aluminium atoms.

So, we can calculate the mass of a substance present in any number of moles using the relationship:

$$\text{mass (in grams)} = \text{number of moles} \times \text{molar mass of the element}$$

The molar mass of an element or compound is the mass of 1 mole of the element or compound and has units of g/mol.

So, a mole of the element magnesium is 6.02×10^{23} atoms of magnesium and a mole of the element carbon is 6.02×10^{23} atoms of carbon (Figure 4.2).

a A mole of magnesium **b** A mole of carbon

▲ **Figure 4.2**

Worked example

Calculate the number of atoms of carbon in:

a 0.5 moles
b 0.1 moles.

Molar mass of carbon contains 6.02×10^{23} atoms of carbon so 0.5 moles would contain half of this amount:

Atoms of carbon in 0.5 moles = $6.02 \times 10^{23} \times 0.5 = 3.01 \times 10^{23}$ atoms

In a similar way:

Atoms of carbon in 0.1 moles = $6.02 \times 10^{23} \times 0.1 = 6.02 \times 10^{22}$ atoms

Worked example

What mass of hydrogen gas would be produced if 46 g of sodium was reacted with water?

First write down the balanced chemical equation:

$$2Na + 2H_2O \rightarrow 2NaOH + H_2$$

Next find the relative atomic mass of sodium (from the Periodic Table (p. 135)) and work out the relative formula masses of water, sodium hydroxide and hydrogen gas. The term **relative formula mass** is used when the compound is ionic, in this case sodium hydroxide. It is used and calculated in the same way as we have used relative molecular mass for covalently bonded compounds, such as water and hydrogen.

Relative atomic mass of sodium is 23.

Relative molecular mass of water, H_2O, is (2 × 1) + 16 = 18

Relative formula mass of sodium hydroxide is 23 + 16 + 1 = 40

Relative molecular mass of hydrogen gas, H_2, is 2 × 1 = 2

Now write these masses under the balanced chemical equation taking into account the numbers used to balance the equation.

2Na	+	$2H_2O$	→	2NaOH	+	H_2
2 × 23 = 46		2 × 18 = 36		2 × 40 = 80		2

These relative masses can now be converted into actual or reacting masses by putting in mass units, for example, grams.

2Na	+	$2H_2O$	→	2NaOH	+	H_2
2 × 23 = 46		2 × 18 = 36		2 × 40 = 80		2
46 g		36 g	→	18 g		2g

So the answer to the question of what mass of hydrogen would be produced if 46 g of sodium was reacted with water is 2 g.

Worked example

Calculate the mass of **a** 2 moles of iron and **b** 0.25 mole of iron. (A_r: Fe = 56)

a mass of 2 moles of iron
= number of moles × relative atomic mass (A_r)
= 2 × 56
= 112 g

b mass of 0.25 mole of iron
= number of moles × relative atomic mass (A_r)
= 0.25 × 56
= 14 g

If we know the mass of the element, then it is possible to calculate the number of moles of that element using:

$$\text{number of moles} = \frac{\text{mass of the element}}{\text{molar mass}}$$

Worked example

Calculate the number of moles of aluminium present in **a** 108 g and **b** 13.5 g of the element. (A_r: Al = 27)

a number of moles of aluminium

$$= \frac{\text{mass of aluminium}}{\text{molar mass of aluminium}}$$

$$= \frac{108}{27}$$

= 4 moles

b number of moles of aluminium

$$= \frac{\text{mass of aluminium}}{\text{molar mass of aluminium}}$$

$$= \frac{13.5}{27}$$

= 0.5 mole

4.3 Moles and compounds

The idea of the mole can also be used with compounds (Figure 4.3).

▲ **Figure 4.3** 1 mole of water (H_2O) (left) and 1 mole of ethanol (C_2H_5OH) (right) in separate measuring cylinders

For example, consider the molar mass of water (H_2O) molecules (A_r: H = 1; O = 16).

From the formula of water, H_2O, you will see that 1 mole of water molecules contains 2 moles of hydrogen (H) atoms and 1 mole of oxygen (O) atoms. The molar mass of water molecules is therefore:

$$(2 \times 1) + (1 \times 16) = 18 \text{ g}$$

The molar mass of a compound is called its molar mass: it has units of g/mol. If you write the molar mass of a compound without any units then it is the relative molecular mass (M_r). So the relative molecular mass of water is 18.

Now follow these examples to help you understand more about moles and compounds.

Worked example

What is **a** the molar mass and **b** the relative molecular mass, M_r, of ethanol, C_2H_5OH? (A_r: H = 1; C = 12; O = 16)

a 1 mole of C_2H_5OH contains 2 moles of carbon atoms, 6 moles of hydrogen atoms and 1 mole of oxygen atoms. Therefore:

molar mass of ethanol = (2 × 12) + (6 × 1) + (1 × 16)
= 46 g/mol

b The relative molecular mass of ethanol is 46.

Worked example

What is **a** the molar mass and **b** the relative molecular mass of nitrogen gas, N_2? (A_r: N = 14)

a Nitrogen is a diatomic gas. Each nitrogen molecule contains two atoms of nitrogen. Therefore:
molar mass of N_2 = 2 × 14
= 28 g/mol

b The relative molecular mass of N_2 is 28.

The mass of a compound found in any number of moles can be calculated using the relationship:

$$\text{mass of compound} = \text{number of moles of the compound} \times \text{molar mass of the compound}$$

Worked example

Calculate the mass of **a** 3 moles and **b** 0.2 moles of carbon dioxide gas, CO_2. (A_r: C = 12; O = 16)

a 1 mole of CO_2 contains 1 mole of carbon atoms and 2 moles of oxygen atoms. Therefore:
molar mass of CO_2 = (1 × 12) + (2 × 16)
= 44 /mol

mass of 3 moles of CO_2 = number of moles × molar mass of CO_2
= 3 × 44
= 132 g

b mass of 0.2 mole of CO_2 = number of moles × molar mass of CO_2
= 0.2 × 44
= 8.8 g

If we know the mass of the compound, then we can calculate the number of moles of the compound using the relationship:

$$\text{number of moles of compound} = \frac{\text{mass of compound}}{\text{molar mass of the compound}}$$

Worked example

Calculate the number of moles of magnesium oxide, MgO, in **a** 80 g and **b** 10 g of the compound. (A_r: O = 16; Mg = 24)

a 1 mole of MgO contains 1 mole of magnesium atoms and 1 mole of oxygen atoms. Therefore:
molar mass of MgO = (1 × 24) + (1 × 16) = 40 g/mol
number of moles of MgO in 80 g

$$= \frac{\text{mass of MgO}}{\text{molar mass of MgO}} = \frac{80}{40}$$

= 2 moles

b number of moles of MgO in 10 g

$$= \frac{\text{mass of MgO}}{\text{molar mass of MgO}} = \frac{10}{40}$$

= 0.25 mole

Moles and gases

Many substances exist as gases. If we want to find the number of moles of a gas, we can do this by measuring the volume rather than the mass.

Chemists have shown by experiment that 1 mole of any gas occupies a volume of approximately 24 dm^3 (24 litres) at room temperature and pressure (r.t.p.). This quantity is also known as the molar gas volume, V_m.

Therefore, it is relatively easy to convert volumes of gases into moles and moles of gases into volumes using the following relationship:

$$\text{number of moles of a gas} = \frac{\text{volume of the gas (in dm}^3\text{ at r.t.p)}}{24\ \text{dm}^3}$$

or

$$\text{volume of a gas (in dm}^3\text{ at r.t.p.)} = \text{number of moles of gas} \times 24\ \text{dm}^3$$

We will use these two relationships to help us answer some questions concerning gases.

Worked example

Calculate the number of moles of ammonia gas, NH_3, in a volume of 72 dm^3 of the gas measured at r.t.p.

$$\text{number of moles of ammonia} = \frac{\text{volume of ammonia in dm}^3}{24\ \text{dm}^3}$$

$$= \frac{72}{24} = 3$$

? Worked example

Calculate the volume of carbon dioxide gas, CO_2, occupied by **a** 5 moles and **b** 0.5 mole of the gas measured at r.t.p.

a volume of CO_2 = number of moles of CO_2 × 24 dm^3
= 5 × 24 = 120 dm^3

b volume of CO_2 = number of moles of CO_2 × 24 dm^3
= 0.5 × 24 = 12 dm^3

The volume occupied by 1 mole of any gas must contain 6.02 × 10^{23} molecules. Therefore, it follows that equal volumes of all gases measured at the same temperature and pressure must contain the same number of molecules. This hypothesis was also first put forward by Amedeo Avogadro and is called **Avogadro's Law.**

Moles and solutions

Chemists often need to know the concentration of a solution. Sometimes **concentration** is measured in grams per cubic decimetre (g/dm^3), but more often concentration is measured in moles per cubic decimetre (mol/dm^3).

Key definition

Concentration can be measured in g/dm^3 or mol/dm^3.

When 1 mole of a substance is dissolved in water and the solution is made up to 1 dm^3 (1000 cm^3), a 1 molar (1 mol/dm^3) solution is produced. Chemists do not always need to make up such large volumes of solution.

A simple method of calculating the concentration uses the relationship:

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

It is very easy to change a volume given in cm^3 into one in dm^3 by simply dividing the volume in cm^3 by 1000. For example, 250 cm^3 is 0.25 dm^3.

? Worked example

Calculate the concentration (in mol/dm^3) of a solution of sodium hydroxide, NaOH, which was made by dissolving 10 g of solid sodium hydroxide in water and making up to 250 cm^3. (A_r: H = 1; O = 16; Na = 23)

1 mole of NaOH contains 1 mole of sodium, 1 mole of oxygen and 1 mole of hydrogen. Therefore:

molar mass of NaOH = (1 × 23) + (1 × 16) + (1 × 1)
= 40 g

$$\text{number of moles NaOH in 10 g} = \frac{\text{mass of NaOH}}{\text{molar mass of NaOH}}$$

$$= \frac{10}{40} = 0.25$$

$$\left(250\ \text{cm}^3 = \frac{250}{1000}\ \text{dm}^3 = 0.25\ \text{dm}^3\right)$$

$$\text{concentration of the NaOH solution} = \frac{\text{number of moles of NaOH}}{\text{volume of solution (dm}^3)}$$

$$= \frac{0.25}{0.25} = 1\ \text{mol/dm}^3$$

Sometimes chemists need to know the mass of a substance that has to be dissolved to prepare a known volume of solution at a given concentration. A simple method of calculating the number of moles, and so the mass of substance needed, is by using the relationship:

$$\text{number of moles} = \text{concentration (in mol/dm}^3) \times \text{volume in solution (in dm}^3)$$

? Worked example

Calculate the mass of potassium hydroxide, KOH, that needs to be used to prepare 500 cm^3 of a 2 mol/dm^3 solution in water. (A_r: H = 1; O = 16; K = 39)

number of moles of KOH
= concentration of solution (mol/dm^3) × volume of solution (dm^3)

$$= 2 \times \frac{500}{1000} = 1$$

1 mole of KOH contains 1 mole of potassium, 1 mole of oxygen and 1 mole of hydrogen. Therefore:

molar mass of KOH
= (1 × 39) + (1 × 16) + (1 × 1)
= 56 g

Therefore:

mass of KOH in 1 mole (500 cm^3 of 2 mol/dm^3) = 56 g

Test yourself

Use these values of A_r to answer the questions below.

H = 1; C = 12; N = 14; O = 16; Ne = 20; Na = 23; Mg = 24; S = 32; Cl = 35.5; K = 39; Fe = 56; Cu = 63.5; Zn = 65

1 mole of any gas at r.t.p. occupies 24 dm^3.

3 Calculate the number of moles in:
- **a** 2 g of neon atoms
- **b** 4 g of magnesium atoms
- **c** 24 g of carbon atoms.

4 Calculate the number of atoms in 1 mole of:
- **a** calcium
- **b** carbon dioxide
- **c** methane.

5 Calculate the mass of:
- **a** 0.1 mol of oxygen molecules
- **b** 5 mol of sulfur atoms
- **c** 0.25 mol of sodium atoms.

6 Calculate the number of moles in:
- **a** 9.8 g of sulfuric acid (H_2SO_4)
- **b** 40 g of sodium hydroxide (NaOH)
- **c** 720 g of iron(II) oxide (FeO).

7 Calculate the mass of:
- **a** 2 mol of zinc oxide (ZnO)
- **b** 0.25 mol of hydrogen sulfide (H_2S)
- **c** 0.35 mol of copper(II) sulfate ($CuSO_4$).

8 Calculate the number of moles at r.t.p. in:
- **a** 2 dm^3 of carbon dioxide (CO_2)
- **b** 240 dm^3 of sulfur dioxide (SO_2)
- **c** 20 cm^3 of carbon monoxide (CO).

9 Calculate the volume of:
- **a** 0.3 mol of hydrogen chloride (HCl)
- **b** 4.4 g of carbon dioxide
- **c** 34 g of ammonia (NH_3).

10 Calculate the concentration of solutions containing:
- **a** 0.2 mol of sodium hydroxide dissolved in water and made up to 100 cm^3
- **b** 9.8 g of sulfuric acid dissolved in water and made up to 500 cm^3.

11 Calculate the mass of:
- **a** copper(II) sulfate ($CuSO_4$) which needs to be used to prepare 500 cm^3 of a 0.1 mol/dm^3 solution
- **b** potassium nitrate (KNO_3) which needs to be used to prepare 200 cm^3 of a 2 mol/dm^3 solution.

12 How many atoms are there in:
- **a** 0.25 moles of aluminium
- **b** 0.15 moles of magnesium?

13 How many moles of calcium contain 1.204×10^{24} atoms?

4.4 Calculating formulae

If we have 1 mole of a compound, then the formula shows the number of moles of each element in that compound. For example, the formula for lead(II) bromide is $PbBr_2$. This means that 1 mole of lead(II) bromide contains 1 mole of lead ions and 2 moles of bromide ions. If we do not know the formula of a compound, we can find the masses of the elements present experimentally, and we can then use these masses to work out the formula of that compound.

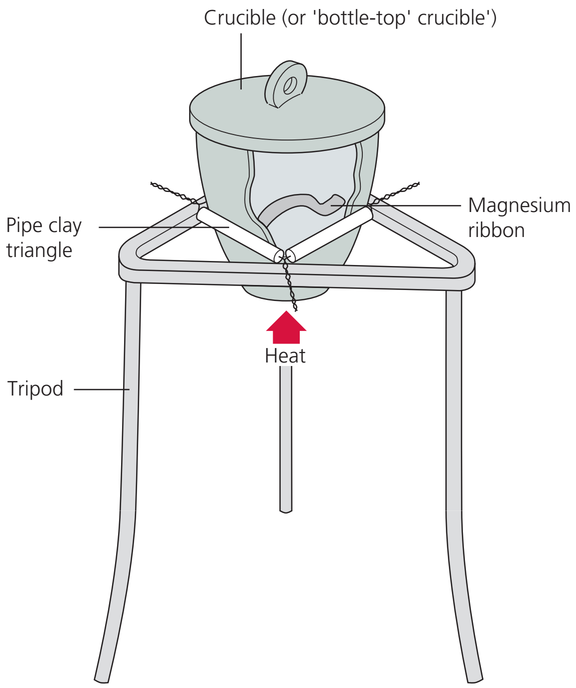
Practical skills

Experiment to find the formula of magnesium oxide

For safe experiments/demonstrations which are related to this chapter, please refer to the *Cambridge IGCSE Chemistry Practical Skills Workbook*, which is also part of this series.

Safety

- Eye protection must be worn.
- Take care when handling hot apparatus.



▲ **Figure 4.4** Apparatus used to determine magnesium oxide's formula

If a known mass of magnesium ribbon is heated strongly in a crucible (or 'bottle-top' crucible) with a lid, it reacts with oxygen to form magnesium oxide.

magnesium + oxygen → magnesium oxide

To allow oxygen into the crucible, the lid needs to be lifted briefly during the heating process.

To heat to constant mass:

- Heat strongly for 5 minutes, then the crucible and contents should be allowed to cool and reweighed.
- The above step should be repeated until a constant mass is obtained.

When the magnesium is heated, it can be seen that:

- the shiny magnesium metal burns brightly to form a white powder, magnesium oxide
- the powder is very fine and when the lid is lifted it can be seen to rise out of the crucible (which is the reason the lid is lifted only briefly).

Table 4.1 Data from the magnesium oxide experiment

Mass of crucible	14.63 g
Mass of crucible and magnesium	14.87 g
Mass of crucible and magnesium oxide	15.03 g

From these data we can find the formula of magnesium oxide by following these steps:

1. Calculate the mass of magnesium metal used in this experiment.
2. Calculate the mass of oxygen which reacts with the magnesium.
3. Calculate the number of moles of magnesium used.
4. Calculate the number of moles of oxygen atoms which react with the magnesium.
5. Determine the simplest ratio of moles of magnesium to moles of oxygen.
6. Determine the simplest formula for magnesium oxide.

This formula is the **empirical formula** of the compound.

Key definition

The **empirical formula** of a compound is the simplest whole number ratio of the different atoms or ions in a compound.

7. Why is it important to lift the lid briefly while heating the crucible?
8. What are the main sources of error in this experiment?

Worked example

In an experiment, an unknown organic compound was found to contain 0.12 g of carbon and 0.02 g of hydrogen. Calculate the empirical formula of the compound. (A_r: H = 1; C = 12)

	C	H
Masses (g)	0.12	0.02
Number of moles	$\frac{0.12}{12} = 0.01$	$\frac{0.02}{1} = 0.02$
Ratio of moles	1	2
Empirical formula	CH_2	

From our knowledge of covalent bonding (Chapter 3, p. 38) we know that a molecule of this formula cannot exist. However, molecules with the following formulae do exist: C_2H_4, C_3H_6, C_4H_8 and C_5H_{10}. All of these formulae show the same ratio of carbon atoms to hydrogen atoms, CH_2, as our unknown. To find out which of these formulae is the actual formula for the unknown organic compound, we need to know the molar mass of the compound.

Using a mass spectrometer, the relative molecular mass (M_r) of this organic compound was found to be 56. We need to find out the number of empirical formulae units present:

M_r of the empirical formula unit

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

$= 14$

Number of empirical formula units present

$$= \frac{M_r \text{ of compound}}{M_r \text{ of empirical formula unit}} = \frac{56}{14}$$

$= 4$

Therefore, the actual formula of the unknown organic compound is $4 \times CH_2 = C_4H_8$.

This substance is called butene. C_4H_8 is the **molecular formula** for this substance and shows the actual numbers of atoms of each element present in one molecule of the substance.

Key definition

The **molecular formula** of a compound is the number and type of different atoms in one molecule.

Sometimes the composition of a compound is given as a percentage by mass of the elements present. In cases such as this, the procedure shown in the next example is followed.

Worked example

Calculate the empirical formula of an organic compound containing 92.3% carbon and 7.7% hydrogen by mass. The M_r of the organic compound is 78. What is its molecular formula? (A_r: H = 1; C = 12)

	C	H
% by mass	92.3	7.7
Masses in 100 g	92.3 g	7.7 g
Number of moles	$\frac{92.3}{12} = 7.7$	$\frac{7.7}{1} = 7.7$
Ratio of moles	1	1
Empirical formula	CH	

M_r of the empirical formula unit CH

$= 12 + 1$

$= 13$

Number of empirical formula units present

$$= \frac{M_r \text{ of compound}}{M_r \text{ of empirical formula unit}} = \frac{78}{13}$$

$= 6$

The molecular formula of the organic compound is $6 \times CH = C_6H_6$. This is a substance called benzene.

Test yourself

Use the following values of A_r to answer the questions below: H = 1; C = 12; O = 16; Ca = 40.

14 Determine the empirical formula of an oxide of calcium formed when 0.4 g of calcium reacts with 0.16 g of oxygen.

15 Determine the empirical formula of an organic hydrocarbon compound which contains 80% by mass of carbon and 20% by mass of hydrogen. If the M_r of the compound is 30, what is its molecular formula?

4.5 Moles and chemical equations

When we write a balanced chemical equation, we are indicating the numbers of moles of reactants and products involved in the chemical reaction. Consider the reaction between magnesium and oxygen.

$$\text{magnesium} + \text{oxygen} \rightarrow \text{magnesium oxide}$$

$$2Mg(s) + O_2(g) \rightarrow 2MgO(s)$$

This shows that 2 moles of magnesium react with 1 mole of oxygen to give 2 moles of magnesium oxide.

Using the ideas of moles and masses we can use this information to calculate the quantities of the different chemicals involved.

$2Mg(s)$	+	$O_2(g)$	$\rightarrow$	$2MgO(s)$
2 moles		1 mole		2 moles
2 × 24		1 × (16 × 2)		2 × (24 + 16)
= 48 g		= 32 g		= 80 g

You will notice that the total mass of reactants is equal to the total mass of product. This is true for any chemical reaction and it is known as the **Law of conservation of mass**. This law was understood by the Greeks but was first clearly formulated by Antoine Lavoisier in 1774. Chemists can use this idea to calculate masses of products formed and reactants used in chemical processes before they are carried out.

Solids

Worked example

Lime (calcium oxide, CaO) is used in the manufacture of lime mortar: a mixture of lime, sand, aggregate and water. It is used as a binding material when building with brick. Lime is manufactured in large quantities in Europe (Figure 4.5) by heating limestone (calcium carbonate, $CaCO_3$).

▲ **Figure 4.5** A rotary kiln for burning (calcining) limestone into lime, located in Moha, Belgium

The equation for the process is:

$CaCO_3(s)$	$\rightarrow$	$CaO(s)$	+	$CO_2(g)$
1 mole		1 mole		1 mole
40 + 12 + (3 × 16)		40 + 16		12 + (2 × 16)
= 100 g		= 56 g		= 44 g

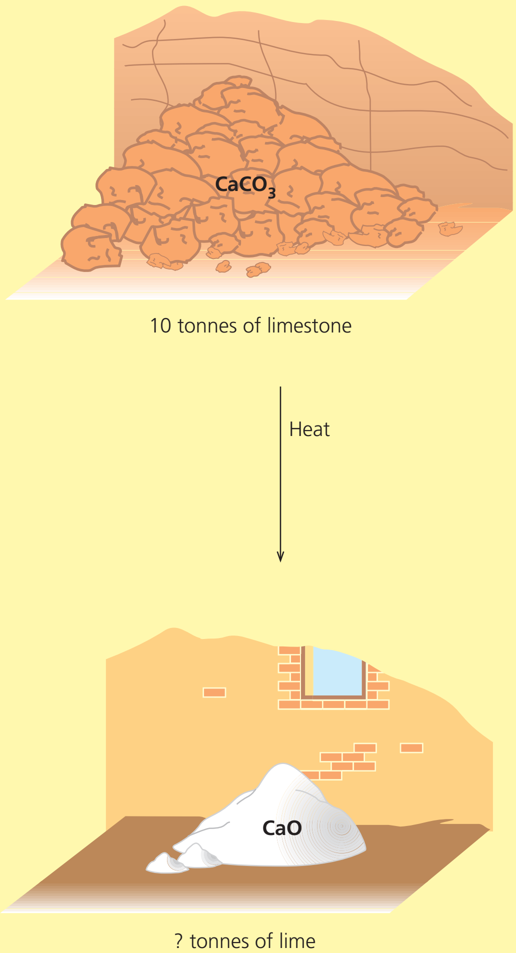
Calculate the amount of lime produced when 10 tonnes of limestone are heated (Figure 4.6). (A_r: C = 12; O = 16; Ca = 40)

1 tonne (t) = 1000 kg

1 kg = 1000 g

From this relationship between grams and tonnes we can replace the masses in grams by masses in tonnes:

$CaCO_3(s)$	$\rightarrow$	$CaO(s)$	+	$CO_2(g)$
100 t		56 t		44 t
10 t		5.6 t		4.4 t



▲ **Figure 4.6** How much lime is produced?

The equation now shows that 100 t of limestone will produce 56 t of lime. Therefore, 10 t of limestone will produce 5.6 t of lime.

Gases

Many chemical processes involve gases. The volume of a gas is measured more easily than its mass. This example shows how chemists work out the volumes of gaseous reactants and products needed using Avogadro's Law and the idea of moles.

Worked example

Some rockets use hydrogen gas as a fuel. When hydrogen burns in oxygen it forms water vapour. Calculate the volumes of **a** O_2(g) used and **b** water, H_2O(g), produced if 960 dm³ of hydrogen gas, H_2(g), was burned in oxygen. (A_r: H = 1; O = 16) Assume 1 mole of any gas occupies a volume of 24 dm³.

$2H_2(g)$	+	$O_2(g)$	→	$2H_2O(g)$
2 moles		1 mole		2 moles
2 × 24		1 × 24		2 × 24
= 48 dm³		= 24 dm³		= 48 dm³

Therefore:

(×2)	96 dm³	48 dm³	96 dm³
(×10)	960 dm³	480 dm³	960 dm³

When 960 dm³ of hydrogen is burned in oxygen:

a 480 dm³ of oxygen is required and

b 960 dm³ of H_2O(g) is produced.

Solutions

Worked example

Chemists usually carry out reactions using solutions. If they know the concentration of the solution(s) they are using, they can find out the quantities reacting.

Calculate the volume of 1 mol/dm³ solution of H_2SO_4 required to react completely with 6 g of magnesium. (A_r: Mg = 24).

number of moles of magnesium

$$= \frac{\text{mass of magnesium}}{\text{molar mass of magnesium}} = \frac{6}{24}$$

= 0.25

Mg(s)	+	H_2SO_4(aq)	→	$MgSO_4$(aq)	+	H_2(g)
1 mole		1 mole		1 mole		1 mole
0.25 mol		0.25 mol		0.25 mol		0.25 mol

So 0.25 mol of H_2SO_4(aq) is required. Using:

volume of H_2SO_4(aq) (dm³)

$$= \frac{\text{moles of } H_2SO_4}{\text{concentration of } H_2SO_4 \text{ (mol/dm}^3\text{)}} = \frac{0.25}{1}$$

= 0.25 dm³ or 250 cm³

Worked example

40 cm³ of 0.2 mol/dm³ solution of hydrochloric acid just neutralised 20 cm³ of sodium hydroxide solution in a titration (Chapter 8, p. 128).

What is the concentration of sodium hydroxide solution in g/dm³ used in this neutralisation reaction?

number of moles of HCl used

= concentration (mol/dm³) × volume (dm³) = 0.2 × 0.04

= 0.008

HCl(aq)	+	NaOH(aq)	→	NaCl(aq)	+	H_2O(l)
1 mole		1 mole		1 mole		1 mole
0.008 mol		0.008 mol		0.008 mol		0.008 mol

You will see that 0.008 mole of NaOH was present. The concentration of the NaOH(aq) is given by:

concentration of NaOH (mol/dm3)

$$= \frac{\text{number of moles of NaOH}}{\text{volume of NaOH (dm}^3\text{)}} = \frac{0.008}{0.02}$$

(volume of NaOH in dm³ $= \frac{20}{1000} = 0.02$)

= 0.4 mol/dm³

Now we have the concentration in mol/dm³, we can easily convert this in g/dm³ using the relationship below:

Concentration of a solution in g/dm³ = concentration in mol/dm³ × molar mass of the substance

So the concentration of the NaOH in g/dm³ = 0.4 × (23 + 16 + 1)
= 16g/dm³

Percentage yield

Chemical reactions rarely produce the predicted amount of product from the masses of reactants in the reaction as they are not 100% efficient.

An example of this is the reaction of carbon with oxygen to produce carbon dioxide gas.

$$C(s) + O_2(g) \rightarrow CO_2(g)$$

The equation for the reaction states that 1 mole of carbon reacts with oxygen to give 1 mole of carbon dioxide gas.

If you burn 12 g, 1 mole, of carbon to make CO_2, then the amount of carbon dioxide expected is 44 g, 1 mole of CO_2. The theoretical yield of carbon dioxide from this reaction is 44 g. This only occurs, however, if the reaction is 100% efficient.

In reality, the mass of carbon dioxide you will get will be less than 44 g, because another reaction can also occur between carbon and oxygen. Some of the carbon reacts to make carbon monoxide, CO.

$$2C(s) + O_2(g) \rightarrow 2CO(g)$$

The **percentage yield** of the reaction is based on the amount of carbon dioxide that is actually produced against what should have been produced if the reaction were 100% efficient.

For example, if 12 g of carbon was burned in excess oxygen and only 28 g of carbon dioxide was produced, the percentage yield can be worked out:

$$\text{percentage yield of carbon dioxide} = \frac{28}{44} \times 100$$

$$= 63.6\%$$

In general:

$$\text{percentage yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100$$

Percentage composition

Percent composition is used to describe the percent by mass of each element in a compound. It is found by dividing the mass of a particular element in the compound by the molar mass and then multiplying by 100 to give a percentage.

For example, the percentage composition of magnesium oxide, MgO, can be found by using the calculations shown below.

The molar mass of MgO is 24 + 16 = 40 g

Of this, 24g is magnesium and 16g is oxygen.

$$\%Mg = \frac{24}{40} \times 100 = 60\%$$

$$\%O = \frac{16}{40} \times 100 = 40\%$$

Percentage purity

In Chapter 2 (p. 14), we saw that the **purity** of a substance is very important. If a factory makes medicines or chemicals used in food then the purity of the product is crucial, as the impurities may harm the people using the medicine or eating the food.

$$\text{percentage purity} = \frac{\text{mass of the pure product}}{\text{mass of the impure product obtained}} \times 100\%$$

Sodium hydrogencarbonate, $NaHCO_3$, is used in the manufacture of some toothpastes and as a raising agent in food production. The purity of this substance can be obtained by measuring how much carbon dioxide is given off.

Worked example

84 g of sodium hydrogencarbonate was thermally decomposed and 11.5 dm^3 of carbon dioxide gas was collected at room temperature and pressure (r.t.p.).

The equation for the reaction is:

$$\underset{\text{2 moles}}{2NaHCO_3(s)} \rightarrow Na_2CO_3(s) + H_2O(g) + \underset{\text{1 mole}}{CO_2(g)}$$

Step 1: Calculate the relative formula mass of sodium hydrogencarbonate (A_r: Na = 23; C = 12; O = 16; H = 1)

The relative formula mass of $NaHCO_3$ = 84

Step 2: 2 moles of $NaHCO_3$ produces 1 mole of CO_2.

168 g of $NaHCO_3$ would give 44 g of CO_2, which would have a volume of 24 dm^3 at r.t.p.

84 g of $NaHCO_3$ should give 12 dm^3 of CO_2 at r.t.p.

Hence the mass of $NaHCO_3$ in the sample was

$$84 \times \frac{11.5}{12} = 80.5 \text{ g}$$

Step 3: Calculate the percentage purity.

There is 80.5 g of sodium hydrogencarbonate in the 84 g sample.

$$\text{percentage purity} = \frac{80.5}{84} \times 100\% = 95.8\%$$

In a chemical reaction, not all the reactants are always completely used up. Usually one of the reactants will remain at the end of the reaction because it has nothing to react with. This is the excess reactant. The reactant which has been completely used up and does not remain at the end of the reaction is called the limiting reactant. The amount of product that can be obtained is determined by the limiting reactant. This is often the case when acids are used to make salts by their reactions with bases or carbonates (see Chapter 8, p. 122). An excess of the base or carbonate is used to ensure the acid has completely reacted. The acid would be the limiting reactant as it determines the amount of the salt produced.

In a chemical reaction, it is important to be able to determine which reactant is the limiting reactant as this will allow you to find the maximum mass of products which can be produced.

Worked example

How much copper(II) oxide could be formed if 16 g of copper reacted with 20 g of oxygen gas?

Step 1: Write down the balanced chemical equation for the reaction.

$$2Cu(s) + O_2(g) \rightarrow 2CuO(s)$$

2 moles 1 mole 2 moles

Step 2: Convert the mass of each reactant into moles:

Moles of Cu used = 16/64 = 0.25 moles

Moles of O_2 used = 20/(2×16) = 0.625 moles

Step 3: Now look at the ratio of the moles in the balanced equation:

2 moles of Cu would react with 1 mole of O_2

0.25 moles of Cu would react with 0.25/2 = 0.125 moles of O_2

So Cu will be the limiting reactant because it would be used up, but there would be 0.625 – 0.125 = 0.5 moles of O_2 remaining at the end of the reaction. The oxygen would have been used in excess.

Step 4: Now we know which is the limiting reactant, we can use the mole ratio between it and the product to find the mass of copper(II) oxide we could produce.

0.25 moles of Cu would give 0.25 moles of CuO

Mass of CuO which could be produced = 0.25 × (64 + 16) = 20 g

Test yourself

Use the following A_r values to answer the questions below: O = 16; Mg = 24; S = 32; K = 39; Cu = 63.5.

16 Calculate the mass of sulfur dioxide produced by burning 16 g of sulfur in an excess of oxygen.

17 Calculate the mass of sulfur which, when burned in excess oxygen, produces 640 g of sulfur dioxide.

18 Calculate the mass of copper required to produce 159 g of copper(II) oxide when heated in excess oxygen.

19 A rocket uses hydrogen as a fuel. Calculate the volume of hydrogen used to produce 24 dm^3 of water ($H_2O(g)$).

20 Calculate the volume of 2 mol/dm^3 solution of sulfuric acid required to react with 24 g of magnesium.

21 20 cm^3 of 0.2 mol/dm^3 solution of hydrochloric acid just neutralised 15 cm^3 of potassium hydroxide solution in a titration (see Chapter 8, p. 128). What is the concentration of potassium hydroxide solution used in this neutralisation reaction?

22 Calculate the percentage composition of ammonium nitrate, NH_4NO_3.

23 What is the maximum mass of magnesium oxide that could be produced if 48 g of magnesium reacted with 38 g of oxygen gas?

Revision checklist

After studying Chapter 4 you should be able to:

- ✔ Define and, given data, calculate the molecular and empirical formula of a compound.
- ✔ Describe the terms relative atomic, molecular and formula mass.
- ✔ State that the mole is the unit of amount of substance and that it contains 6.02×10^{23} particles.
- ✔ Carry out calculations to find masses, moles, volumes and concentrations in reactions using solids gases and solutions.
- ✔ State that concentration has units of g/dm^3 and mol/dm^3, and convwert between them.
- ✔ Calculate percentage yield and purity.
- ✔ Calculate the percentage composition of a compound.

Exam-style questions

Use the data in the table below to answer the questions.

Element	A_r
H	1
C	12
N	14
O	16
Na	23
Mg	24
Si	28
S	32
Cl	35.5
Fe	56

1 Calculate the mass of:
  a 1 mole of:
    i chlorine molecules
    ii iron(III) oxide
  b 0.5 moles of:
    i magnesium nitrate
    ii ammonia.

2 Calculate the volume occupied, at r.t.p., by the following gases. (1 mole of any gas occupies a volume of 24 dm^3 at r.t.p.)
  a 12.5 moles of sulfur dioxide gas
  b 0.15 mole of nitrogen gas

3 Calculate the number of moles of gas present in the following:
  a 36 cm^3 of sulfur dioxide
  b 144 dm^3 of hydrogen sulfide.

4 Use the following experimental information to determine the empirical formula of an oxide of silicon.

Mass of crucible = 18.20 g

Mass of crucible + silicon = 18.48 g

Mass of crucible + oxide of silicon = 18.80 g

5 **a** Calculate the empirical formula of an organic liquid containing 26.67% of carbon and 2.22% of hydrogen, with the rest being oxygen.
  b The M_r of the liquid is 90. What is its molecular formula?

6 Iron is extracted from its ore, hematite, in a blast furnace. The main extraction reaction is:

$$Fe_2O_3(s) + 3CO(g) \rightarrow 2Fe(s) + 3CO_2(g)$$

  a Identify the reducing agent in this process.
  b Give the oxide of iron shown in the equation.
  c Explain why this is a redox reaction.
  d Calculate the mass of iron which will be produced from 640 tonnes of hematite.