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Unit 1

Moles and equations

Learning outcomes

You should be able to:

- define and use relative masses based on the ^{12}C scale
- define and use the mole and Avogadro's constant
- analyse simple mass spectra and use the data in relative atomic mass calculations
- define and use the terms *empirical* and *molecular formulae* and use experimental data to find them,
- write and construct equations and use them in performing mole calculations
- perform mole calculations involving solutions and gases,

This unit gathers together the basic chemistry calculations. You may need to refer to it as you revise other topics in later units.

1.01 Relative masses

An atom is the smallest part of an element that can exist and still retain the identity of the element. A molecule is a group of atoms bonded together and the smallest portion of an element or compound that can exist alone. A simple ion is an atom which has lost or gained one or more electrons. Atoms, molecules and ions are so small that their masses are far too small to measure directly on a balance. For most purposes, chemists use relative masses, which are the number of times heavier a particle is than (1/12) of the mass of one atom of carbon-12. Carbon-12 is the standard.

relative atomic mass,

$$A_r = \frac{\text{average mass of one atom of an element}}{(1/12)\text{ of the mass of one atom of } ^{12}\text{C}}$$

relative molecular mass,

$$M_r = \frac{\text{average mass of one molecule}}{(1/12)\text{ of the mass of one atom of } ^{12}\text{C}}$$

The relative molecular mass is the sum of all the relative atomic masses of the atoms making up the molecule.

If compounds are ionic, then '**relative formula mass**' is used instead of 'relative molecular mass'.

Atoms of an element always have the same number of protons in the nucleus but may have different numbers of neutrons. These atoms are called **isotopes** and have the same atomic number but a different mass number.

relative isotopic mass =

$$\frac{\text{mass of one atom of the isotope}}{(1/12)\text{ of the mass of one atom of } ^{12}\text{C}}$$

Relative masses are a ratio of two masses and have no units.

1.02 The mole and the Avogadro constant

To give an easy measurement of mass, a number of atoms is chosen so that their combined mass is equal to the relative atomic mass in grams. This number of atoms is called the **mole**.

> **TIP**
>
> Learn the relationships between mass and the mole.
>
> mass of one mole = M
>
> mass of n moles = m
>
> $n = \frac{m}{M}$
>
> $M = A_r$ in grams

The relative atomic mass is the weighted average of relative isotopic masses and may not be a whole number; relative isotopic masses are whole numbers.

a $12.0\,\text{g C} = 1\text{ mol of carbon;}$

$$3.0\,\text{g C} = \frac{3.0}{12.0}\text{ mol} = 0.25\text{ mol}$$

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b 24.3 g Mg = 1 mol of magnesium;

$$6.0\,\text{g Mg} = \frac{6.0}{24.3}\,\text{mol}$$
$$= 0.247\,\text{mol}$$

The number of atoms in 1 mole of carbon atoms equals the number of atoms in 1 mole of any other type of particle. The number of atoms in 1 mole is called the **Avogadro constant**.

The Avogadro constant, L, = $6.022 \times 10^{23}\,\text{mol}^{-1}$.

1 mol of carbon weighs 12.0 g and contains 6.022×10^{23} atoms

0.65 mol of carbon weighs 12.0×0.65 g and contains $0.65 \times 6.022 \times 10^{23}$ atoms

TIP

In mass calculations, make sure you use A_r values and not the atomic number.

1.03 Mass spectra and relative atomic mass calculations

A **mass spectrometer** is used to find the masses of atoms of individual isotopes; it produces a trace like the one for boron shown in Figure 1.01.

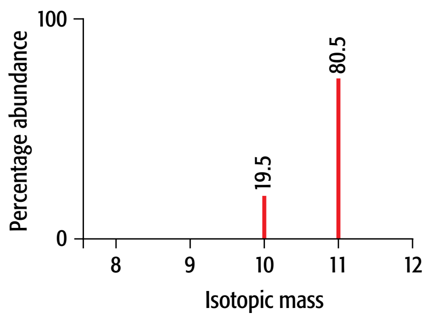

Figure 1.01 The mass spectrum for boron. The sum of the two percentage abundances = 100%.

Figure 1.01 shows two boron isotopes with relative isotopic masses of 10 and 11. The relative atomic mass for boron is the average of these values, taking account of the percentage abundances of each.

relative mass of 100 atoms of boron

$= \Sigma$ (relative isotopic mass × percentage abundance)

$$= (19.5 \times 10) + (80.5 \times 11)$$
$$= 1080.5$$
$$A_r[\text{boron}] = \frac{1080.5}{100}$$
$$= 10.81 \text{ (4 sig figs)}$$

Progress check 1.01

Be = 9.0; Mg = 24.3; Cr = 52.0; V = 50.9; Sc = 45.0; O = 16.0; Fe = 55.8

1 How many atoms are in the following:
   a 3.0 g of beryllium atoms?
   b 3.47 g of magnesium atoms?
   c 3.71 g of chromium atoms?

2 What is the mass of the following:
   a 6.022×10^{22} atoms of vanadium?
   b 3.011×10^{23} atoms of scandium?
   c 0.35 mol of O atoms?
   d 0.018 mol of iron?

3 The four isotopes of chromium and their abundancies are given in the table.

Mass numbers	50	52	53	54
% abundances	4.31	83.76	9.55	2.38

   a Sketch the mass spectrum for chromium and label the axes.
   b Work out A_r [chromium] to 3 sig figs from these values.

4 The mass spectrum for palladium is shown in Figure 1.02.

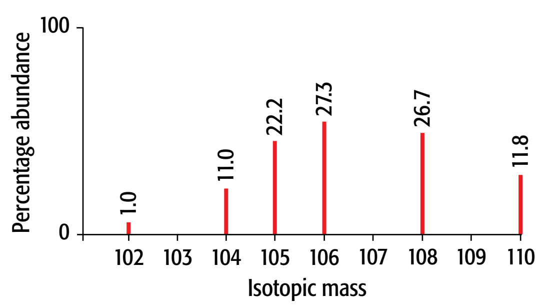

Figure 1.02

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a Label the axes of the spectrum.

b How many isotopes does palladium have?

c Work out the relative atomic mass of palladium using the values on the spectrum.

1.04 Empirical and molecular formulae

The **molecular formula** shows the actual number and types of atoms bonded together. Experimentally, you usually find the **empirical formula**, which is the simplest whole number ratio of all types of atoms bonded together. For example, the molecular formula of ethanoic acid is $C_2H_4O_2$ but its empirical formula is CH_2O. You can work out the empirical formula from the mass or the percentage mass of the elements combined together.

Worked example 1.01

0.50 g of compound **X** contains 0.30 g carbon, 0.133 g oxygen and the rest is hydrogen. What is the empirical formula of X?

How to get the answer:

Step 1: Find the mass of hydrogen combined = (0.50 − 0.30 − 0.133) g = 0.067 g

Step 2: Put the elements and their masses into a table.

Step 3: Divide the masses by the respective A_r values and insert in the table.

Step 4: Divide all values by the smallest of the values in Step 3 and put into the table.

Elements	Masses combined / g	Divide by A_r	Divide by the smallest value
C	0.30	$\frac{0.30}{12} = 0.025$	$\frac{0.025}{8.31 \times 10^{-3}} = 3$
O	0.133	$\frac{0.133}{16} = 8.31 \times 10^{-3}$	$\frac{8.31 \times 10^{-3}}{8.31 \times 10^{-3}} = 1$
H	0.067	$\frac{0.067}{1} = 0.067$	$\frac{0.067}{8.31 \times 10^{-3}} = 8$

Step 5: Write the empirical formula. X = C_3H_8O

Progress check 1.02

1 0.350 g of compound **Y** contains 0.142 g carbon, 0.0297 g hydrogen, 0.0831 g nitrogen and 0.0949 g oxygen. Find the empirical formula of Y.

2 What is the empirical formula of an oxide of iron which contains 72.3% Fe?

The molecular formula is an integral number of empirical formula units; the molecular formula can be found if you know both the empirical formula and the relative molecular mass.

Sample answer

Question:

a What is the empirical formula of a hydrocarbon containing 83.7% carbon? **[4]**

b If the M_r = 86, what is the molecular formula of the hydrocarbon? **[2]**

Answer: a

Element	%	Divide by A_r	Divide by the smallest	Convert to whole number by ×3
C	83.7	$\frac{83.7}{12} = 6.975$	$\frac{6.975}{6.975} = 1$	3
H	16.3	$\frac{16.3}{1} = 16.3$	$\frac{16.3}{6.975} = 2.34$	2.34 × 3 = 7
		[1 mark]	[1 mark]	[1 mark]

empirical formula = C_3H_7 **[1 mark]**

b $M_r[C_3H_7] = 43$

$\frac{86}{43} = 2$ **[1 mark]**

Two empirical formula units form the molecular formula, C_6H_{14}. **[1 mark]**

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1.05 Constructing equations

An equation is a shorthand way of describing a reaction using correct formulae for reactants and products.

For example, methane burns completely in oxygen to produce carbon dioxide and water. The equation becomes:

$$CH_4 + O_2 \longrightarrow CO_2 + H_2O$$

The equation needs to be balanced. Without changing the formulae, the numbers of molecules need to be adjusted so that the same number of atoms of each element are on the left-hand and right-hand sides of the arrow. In the above example, the carbon atoms balance but the hydrogen atoms need to be balanced:

$$CH_4 + O_2 \longrightarrow CO_2 + \mathbf{2}H_2O$$

and then the oxygen atoms need to be balanced:

$$CH_4 + \mathbf{2}O_2 \longrightarrow CO_2 + 2H_2O$$

Lastly, information on the physical state of reactants and products, using (g), (l), (s) or (aq), is inserted and any further information on conditions, such as temperature or pressure, is shown over the arrow:

$$CH_4(g) + 2O_2(g) \xrightarrow{\text{burn}} CO_2(g) + 2H_2O(l)$$

Progress check 1.03

Write correctly balanced equations for the following reactions.

Use formulae from this list:

$Cu(NO_3)_2$ HCl HNO_3 H_2O

Li_2CO_3 Li_2O NO NO_2 P_4

P_2O_5 O_2 $SiCl_4$ SiO_2

1 phosphorus burns in oxygen to produce phosphorus(V) oxide
2 silicon tetrachloride reacts with water to produce silica and hydrochloric acid
3 heating lithium carbonate produces carbon dioxide and lithium oxide
4 with concentrated nitric acid, copper produces nitrogen dioxide (nitrogen(IV) oxide) and water as well as copper nitrate
5 with dilute nitric acid, copper produces nitrogen monoxide (nitrogen(II) oxide) and water as well as copper nitrate

Balancing redox reactions using oxidation numbers is covered in Unit 7, section 7.

1.06 Mole calculations

A balanced equation shows the number of molecules and also the number of moles reacting and being produced.

a Reacting masses

As the number of moles is related to mass, a balanced equation can be used to calculate the masses reacting together and being produced in a reaction.

Worked example 1.02

What is the mass of magnesium oxide left when 1.00 g of magnesium carbonate is heated until there is no further reaction?

How to get the answer:

Step 1: Write the balanced equation:

$$MgCO_3(s) \longrightarrow MgO(s) + CO_2(g)$$

Step 2: Find the mole relationship:

1 mol $MgCO_3$ gives 1 mol MgO

Step 3: Work out $M_r[MgCO_3]$:

$[24.3 + 12.0 + (3 \times 16.0)] = 84.3$

Step 4: Work out how many moles you start with:

$$1.00\,g\ MgCO_3 = \frac{1.00}{84.3}\,mol\ MgCO_3$$
$$= 0.0119\,mol$$

Step 5: Use the mole relationship:

0.0119 mol $MgCO_3$ gives 0.0119 mol MgO

Step 6: Work out $M_r[MgO]$:

$24.3 + 16.0 = 40.3$

Step 7: Find the mass:

0.0119 mol MgO weighs $0.0119 \times 40.3\,g = 0.480\,g$

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b Reacting gas volumes

At constant pressure and temperature, the volume of a gas is proportional to the number of moles (see Unit 5, section 5). This means that 1.0 mol of every gas occupies the same volume. At room temperature and pressure, this volume is 24 dm^3.

For the reaction

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

the equation shows that equal numbers of moles and thus equal volumes of hydrogen and chlorine react together.

The volume of carbon dioxide formed when 0.50 g ethanol is completely burnt is found by using a balanced equation to get the mole ratio:

- $CH_3CH_2OH + 3O_2 \longrightarrow 2CO_2 + 3H_2O$
- 1 mol ethanol $\longrightarrow$ 2 mol CO_2
- M_r[ethanol] = 46, so number of moles $= \frac{0.50}{46} \longrightarrow 2 \times \frac{0.50}{46}$ mol CO_2
- volume $CO_2 = 2 \times \frac{0.50}{46} \times 24\ \text{dm}^3 = 0.522\ \text{dm}^3 = 522\ \text{cm}^3$

c Reacting solutions

The concentration of a solution is measured in mol dm^{-3}.

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

number of moles
= concentration in mol dm^{-3} × volume of solution in dm^3

For example, identify M when 0.281 g of the Group I hydroxide, MOH, dissolves to make 100 cm^3 of solution and a 10.0 cm^3 portion reacts exactly with 6.68 cm^3 of 0.075 mol dm^{-3} HC*l*:

- $MOH(aq) + HCl(aq) \longrightarrow MCl(aq) + H_2O(l)$
- number of moles HC*l*
  = concentration × volume
  = 0.075 mol dm^{-3} × 6.68 × 10^{-3} dm^3
  = 5.01 × 10^{-4}
- number of moles MOH in 10 cm^3 of solution
  = 5.01 × 10^{-4}
- number of moles MOH in 100 cm^3 of solution
  = 5.01 × 10^{-3}
- 0.281 g MOH contain 5.01 × 10^{-3} mol
- 1 mol MOH $= \frac{0.281}{5.01} \times 10^{-3}$ g = 56.1 g
- A_r[M] = 56.1 − 17 = 39.1
- M = potassium

d Combustion data calculations

An accurately known mass of an organic compound is burnt completely, to form CO_2 and H_2O. The volume or mass of carbon dioxide and the mass of water are accurately measured and the masses of C and H calculated. The empirical formula can then be worked out.

For example, Z contains carbon, hydrogen and oxygen. When 0.325 g Z is burnt completely, 265 cm^3 CO_2 and 0.149 g H_2O are produced. What is the empirical formula of Z?

- 265 cm^3 $CO_2 = \frac{265}{24\,000}$ mol = 0.0110 mol CO_2
- this contains 0.0110 mol C
- this weighs (0.0110 × 12) g = **0.132 g C**
- 0.149 g $H_2O = \frac{0.149}{18}$ mol H_2O = 8.28 × 10^{-3} mol H_2O
- this contains 0.0166 mol H = **0.0166 g H**
- mass O = (0.325 − 0.132 − 0.0166) g = **0.1765 g O**

Element	Mass / g	Divide by A_r	Divide by the smallest	×2
O	0.1765	$\frac{0.1765}{16} = 0.0110$	1	2
C	0.132	$\frac{0.132}{12} = 0.011$	1	2
H	0.0165	$\frac{0.0165}{1} = 0.0165$	1.5	3

- empirical formula = $C_2H_3O_2$

TIP

When working out reacting masses or gas volumes, always start with a correctly balanced equation.

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Progress check 1.04

1 What mass of $FeCl_3$ is formed if 1.12 g $FeCl_2$ is reacted with excess chlorine?

2 Magnesium nitride, Mg_3N_2, is decomposed by water to produce magnesium oxide and ammonia (NH_3). What mass of magnesium oxide is produced by decomposing 1.00 g of the nitride?

3 A sample of sodium sulfate, Na_2SO_4, is contaminated with sodium nitrate; 5.00 g of the contaminated sample is dissolved in water and then reacted with excess aqueous barium chloride; 5.74 g of solid barium sulfate, $BaSO_4$, is formed. What mass of sodium sulfate was in the contaminated sample?

4 Compound T contains carbon, hydrogen and oxygen only. On complete combustion, 0.450 g of T produces 360 cm^3 CO_2 and 0.27 g H_2O. Find the empirical formula of T.

5 Compound S contains carbon, hydrogen, oxygen and nitrogen. On complete combustion, 0.350 g of S produces 286 cm^3 CO_2, 71 cm^3 N_2 and 0.267 g H_2O. Find the empirical formula of S.

6 Aqueous barium chloride, $BaCl_2$, reacts with aqueous sulfuric acid, H_2SO_4, to produce a precipitate of barium sulfate and water. 10.0 cm^3 of a barium chloride solution requires 15.0 cm^3 of 0.0500 mol dm^{-3} H_2SO_4 for complete reaction. What is the concentration of the barium chloride solution in g dm^{-3}?

7 A solution of ethanoic acid, CH_3COOH, is contaminated by oxalic acid, $(COOH)_2$. Ethanoic acid is monobasic but oxalic acid is dibasic. 10.0 cm^3 of 0.0140 mol dm^{-3} NaOH requires 12.45 cm^3 of the contaminated ethanoic acid solution for complete reaction. The concentration of the ethanoic acid = 0.0100 mol dm^{-3}; what is the concentration of the oxalic acid?

Revision checklist

Check that you know the following:

- ☐ how to define and use 'relative atomic, isotopic, molecular and formula masses',
- ☐ how to use the mole and understand and use the concept of the Avogadro constant,
- ☐ how to analyse mass spectra in terms of isotopic abundances and calculate the relative atomic mass
- ☐ the definition, calculation and use of 'empirical' and 'molecular' formulae,
- ☐ how to construct balanced equations and use them to calculate reacting masses or gas volumes,
- ☐ how to work out the concentration of solutions and perform titration calculations

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Exam-style questions

1 Sodium carbonate crystals, $Na_2CO_3 \cdot xH_2O$, react with aqueous hydrochloric acid to form sodium chloride, carbon dioxide and water. 1.350 g of $Na_2CO_3 \cdot xH_2O$ crystals react completely with 25.0 cm^3 of 0.390 mol dm^{-3} HCl.

a i Write a balanced equation for the reaction. [2]

ii How many moles of HCl are used in the reaction? [1]

iii How many moles of $Na_2CO_3 \cdot xH_2O$ are used in the reaction? [1]

iv Work out x in the reaction. [3]

b What mass of $NaCl$ is formed in the reaction? [1]

c i What is the maximum volume of CO_2 (measured at room temperature and pressure) which can be produced by the reaction? [1]

ii Suggest why the actual volume of CO_2 would be less than your value in part c i. [1]

Total: 10

2 W is a dibasic acid which contains carbon, hydrogen and oxygen only.

a 1.50 g of W undergoes combustion analysis to form 1.73 dm^3 of CO_2 and 0.488 g H_2O. Work out the empirical formula of W. [6]

b 1.50 g of W was dissolved in water to make 1.00 dm^3 of solution. 10.0 cm^3 of this solution reacted exactly with 18.10 cm^3 of 0.0100 mol dm^{-3} NaOH.

i How many moles of NaOH were used? [1]

ii How many moles of W react with the NaOH in part b i? [1]

iii How many moles of W are contained in 1.50 g? [1]

iv What is the M_r of W? [1]

c Using your answers to parts a and b, what is the molecular formula of W? [2]

Total: 12

