

Chemistry

Mole Calculations in Chemistry: The Unit Label Method

[MULTI-LEVEL]

Wilson Flood



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A number of courses are currently (summer 2004) being developed:

- effective use of ICT, including preparation of electronic worksheets in Word and in Excel, using RasMol and RasTop, getting familiar with using drawing packages, useful URLs, using whiteboards
- brushing up on demonstrations (with SSERC)
- assessment is for learning
- making chemistry attractive through the use of investigative approaches
- Intermediate 1 chemistry
- national assessment issues (with SQA).

With the initial support of BP, a website related to the project has been set up (www.scots.org.uk). As well as providing up-to-date information on all activities related to the project, the site is intended to share useful information for chemistry teachers, e.g. on all CPD activities, resources, useful websites, support for students, etc. Ideas for inclusion on the site should be sent to the name listed on the site or to Don Sutherland.

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Note on the use of cursive form of 'l'

The reader of this document will notice that I have adopted '*ℓ*' as the symbol for litre in the calculations instead of the more usual 'l'. The reason for this is that the units form part of the calculation before they are cancelled and I wanted the difference between a litre and the numeral 'l' in a calculation layout to be completely apparent.

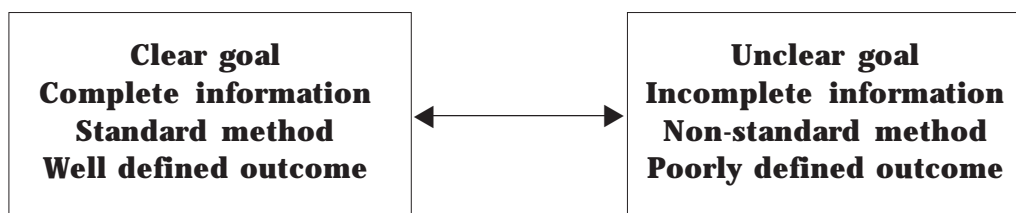
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SECTION 1**Introduction****1.1 Problem Solving**

Problems might be thought of as consisting of four dimensions:

- **Goal**
- **Information**
- **Method (of calculating)**
- **Outcome**

So we could think of the problem solving spectrum as stretching between two sets of dimensions:



As a generalisation, the more a problem has the left hand characteristics the more straightforward it tends to be. In school chemistry courses, as far as mole calculations are concerned, most problems have the left hand set of characteristics. It is clear what has to be calculated, complete information is given, and the answer, when found, will be unambiguous. Most of these problems can be solved using algorithms, i.e. standard methods which can be learned. Such a process is sometimes called closed problem solving and in this document such problems will be called calculations.

The right hand set of characteristics is sometimes referred to as open (or true) problem solving. This type of problem solving calculation is best practised when time is not at a premium and so it is more suited to the classroom or a tutorial, where there is opportunity for discussion, rather than in an examination.

It is possible to construct calculations where one or more of the dimensions is from the right hand set giving us something like a true problem. Here is an example:

**A mixture of zinc and magnesium with a total mass of 1 g was added to excess dilute hydrochloric acid. The volume of hydrogen gas produced was 548 cm³. Calculate the mass of magnesium in the sample.
(Take the molar volume of hydrogen = 24 l; relative atomic masses: Mg = 24.3; Zn = 65.4)**

The goal is clear, the information is complete, the outcome (or answer) is well defined when you arrive at it, but the method is non-standard. Doing this problem lets you experience truer problem solving than most chemical calculations allow. Go on, try it. The answer is on page 9, at the end of section 1.

This resource will not look at non-standard calculations: it is about an alternative standard method for doing mole calculations in chemistry.

1.2 Algorithms

In section 1.1, standard methods, or **algorithms**, are mentioned as applying to quantitative chemistry calculations involving the mole. You may be excused for asking, 'What algorithms are these?' since although there are tried and tested methods for carrying out mole calculations they vary quite a bit from one calculation to the next and might not be thought of as algorithms in the normal sense.

A fair proportion of school chemistry students finds difficulty with mole calculations. One cause may be weakness in arithmetic, especially in handling ratio and proportion. Another cause of difficulty may lie in the number of different factors that have to be correctly assembled in a mole calculation in order to arrive at a correct answer.

But what if there were another way of performing mole calculations, a way that got round difficulties of ratio and proportion? An algorithm has been developed for quantitative chemistry calculations; it is in wide use in other countries although it remains relatively unknown in Scotland. It is described in this resource.

1.3 The Problem with Chemistry Calculations

‘One orange costs 30 pence. How much would four oranges cost?’

Senior school students would not be expected to have much difficulty with the above ‘problem’, based as it is on simple ratio. So chemistry teachers are often at a loss to explain why chemistry calculations give so much difficulty since they too are based on ratio. However, the typical mole calculation is more complicated than the example above.

A more typical analogy of the chemistry calculation might be

‘Three pencils cost 84 pence. How much would five pencils cost?’

although an even better one might be

‘Three pencils cost 84 pence. How much would five pens cost if you know that seven pencils could be bought for the same price as four pens?’

In this example, we are dealing with multiple ratios which is what we normally have in mole calculations. This example is clearly more difficult than the first two and requires a little thought before we get to the correct answer. However, even then it is not that good an analogy since the mole calculation has even more dimensions of difficulty.

A simple mole calculation might consist of the student being supplied with a balanced equation along with the requirement to calculate a mass of product from a given mass of reactant. Performing this calculation will involve converting masses into moles, then using a mole ratio, and finally converting moles back into masses, something a little more complicated than pricing pencils. But the standard method we use to teach mole calculations is pretty much like the ‘orange’ approach and relies on students having the ability to ‘see’ the proportional relationship between the numbers.

To take a simple example:

What mass of zinc chloride would be formed by reacting 10 g of zinc with dilute hydrochloric acid?



After doing some work on mole ratios, the student might finally arrive at:

'65.4 g of Zn gives 136.4 g of ZnCl₂ so 10 g of Zn will give how many grams of ZnCl₂?'

The answer being $136.4 \times 10/65.4$ g of ZnCl₂ is obvious to some but gives difficulty to others. Errors often occur at setting up the ratio stage since the numbers lose their units in the calculation. There is also no way of checking whether the ratio has been set up properly other than by inspection of the magnitude of the answer obtained, a step often omitted by poor problem solvers.

1.4 The Unit Label Method

What we need is an algorithm that would allow mole calculations to be laid out in a consistent way, that would avoid the ratio difficulty, and would allow error checking. A method does exist: it is known as the Unit Label Method (you can also find it listed as the Factor Label Method or as Dimensional Analysis) and its use in a range of mole calculations is explained in the following sections.

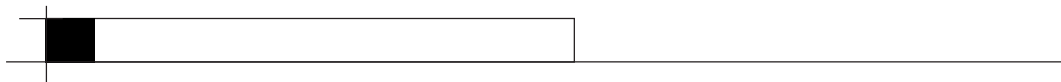
The fact that numbers in mole calculations represent quantities of substances is often overlooked. The Unit Label Method (or ULM) emphasises this. The quantities in question are defined by their units (g, kg, cm³, etc.) linked to chemical entities. In this way one gram of sodium is not equivalent to one gram of chlorine, for example. Understanding this simple idea drives the ULM.

It would be necessary to introduce the ULM gradually during the course of a chemistry programme, starting with relatively straightforward mole calculations in introductory courses and then moving on to more complicated examples in advanced courses. It would also be a matter of importance that all chemistry teachers in a given school adopted the method so that problems did not arise when students changed teachers.

Teaching the ULM would follow the usual procedure of worked example, followed by guided practice on the part of students (see **Section 4.11**). It might also be advisable to introduce the method in a non-chemistry context in the first instance as shown in the explanatory example.

As with calculations generally, at first acquaintance it is good practice for the student to lay out the calculation stepwise in some detail, but, as experience is gained, calculation steps may be combined to the extent to which students feel comfortable. In some of the examples that follow each step has been explained in some detail as a teacher might do but in some of the later examples steps have been combined to avoid tedium. However, for students, each new type of calculation would need to be explained in detail so no steps should be omitted on first encounter.

(Answer: The mass of magnesium in the sample was 0.292 g.)



SECTION 2

How to Use the Unit Label Method

The Unit Label Method (ULM) can be used to carry out a wide range of mole calculations. The method is useful in setting out calculations and in checking for set-up errors because if the unit of the final quantity is not correct, then the relationship of the numbers in the calculation and hence the answer must also be incorrect.

The Unit Label Method usually involves the following steps:

- In the calculation, you first identify what you are given (called here the '**given quantity**') and what you want to find out (called the '**required quantity**'). The 'given' and 'required' quantities must have units associated with them.
- You then identify what are called **conversion factors (CFs)**. Conversion factors *must* show units. They are ratios that show equivalences; for example, one mole of sodium is equivalent to 23 grams of sodium (**note: not just 23 grams**). In calculations involving balanced equations an additional CF is the **mole ratio (MR)**.
- Now you arrange the given quantity and the conversion factors in the calculation so that identical units cancel leaving you with the required quantity. The given quantity is normally on the top line (the numerator) at the left of the calculation and the required quantity will remain on the top line on completion of the calculation.
- Finally, perform the calculation.

Almost all mole calculations can be performed using this algorithm. As will be seen, calculations involving solutions are slightly different and require slight modification but once this is appreciated, they too become straightforward.

Basically all ULM calculations are laid out like this:

given quantity × **conversion factors** = **required quantity**

The number of conversion factors needed depends on the calculation to be performed.

As a simple memory aid this can be simplified to :

given \times CFs = required

In the ULM it is units and the chemical entities associated with them which cancel before setting up the final calculation. This emphasises an important point in chemistry which is worth repeating. Mole calculations are not just about numbers, they are about quantities of substances.

SECTION 3**Explanatory Example**

To illustrate the use of the method here is a simple example based on the following problem:

'A piece of wood is 29.8 inches in length. Convert this length into centimetres.'

(Use 1 in = 2.54 cm)

Using the four steps

1. Identify the given quantity and the required quantity

given quantity - 29.8 in
required quantity - ? cm

2. The equivalence is

1 in : 2.54 cm

and in the calculation the CF (conversion factor) could be written as one of two possible ratios, i.e.

$$\frac{1 \text{ in}}{2.54 \text{ cm}} \text{ or } \frac{2.54 \text{ cm}}{1 \text{ in}}$$

Both are appropriate but which should we use in the calculation?

The answer to the question is determined by the fact that the units of the required quantity **must** be on the top line of the fraction if the calculation is to make any sense and also by the fact that all other units must cancel.

Therefore the correct CF in this case is $\frac{2.54 \text{ cm}}{1 \text{ in}}$

3. We now have our given quantity from step 1 and we have the conversion factor from step 2 so the calculation is set up as follows:

$$\text{given} \times \text{CF} = \text{required}$$
$$\text{Length in centimetres} = 29.8 \cancel{\text{ in}} \times \frac{2.54 \text{ cm}}{1 \cancel{\text{ in}}}$$

Cancelling identical units leaves us with the basic calculation to perform.

4. Length in cm = $29.8 \times \frac{2.54 \text{ cm}}{1} = \underline{\underline{75.7 \text{ cm}}}$

Note that the units **must** be included when laying out the calculation since cancelling identical units leads us to the required answer. It also gives a method of error checking since if we are not left with the unit of the required quantity on the top line then the CFs must have been set up wrongly.

SECTION 4**Quantitative Calculations**

The types of mole calculation commonly encountered in Scottish NQ chemistry courses are as follows:

Standard Grade

empirical formula
masses and moles
solutions and moles
acid/base volumetric
masses, moles and equations

Intermediate 2

masses and moles
solutions and moles
acid/base volumetric
masses, moles and equations

Higher

redox titration
molar volume of gases
excess and limiting reactants
Avogadro constant calculations
mixed mole calculations – masses, gases, solutions – any 2 of in a calculation
Faraday calculations
enthalpy changes

Advanced Higher

complex mole combinations – mass, mole, titre, redox, empirical formula – any 2 or more of in a calculation

Examples of each of these types are given in the following sub-sections.

4.1 Simple mass-mole conversions; Avogadro constant

Example 1

What is the mass (in grams) of 0.60 moles of calcium?

given quantity - 0.60 mol Ca - NB: **not just mol**
 required quantity - ? g Ca - NB: **not just g**

The equivalence is 1 mol Ca : 40 g Ca

so the conversion factor could be $\frac{1 \text{ mol Ca}}{40 \text{ g Ca}}$ or $\frac{40 \text{ g Ca}}{1 \text{ mol Ca}}$

The right hand conversion factor is chosen in order to cancel identical units and leave the required units of grams of calcium on the top line.

Setting up the calculation:

given quantity \times conversion factor = required quantity

$$\text{g Ca} = 0.60 \cancel{\text{ mol Ca}} \times \frac{40 \text{ g Ca}}{1 \cancel{\text{ mol Ca}}} = 0.60 \times \frac{40 \text{ g Ca}}{1} = \underline{\underline{24 \text{ g Ca}}}$$

Example 2

How many moles of water are in 0.500 kg of water?

given quantity – 0.500 kg H₂O
 required quantity – ? mol H₂O

Conversion factors

Since molar mass is usually measured in grams we will need a conversion factor to convert kg H₂O to g H₂O, i.e.

conversion factor, CF(1) – 1 kg H₂O : 1000 g H₂O

conversion factor, CF(2) – 1 mol H₂O : 18 g H₂O

We convert kg H₂O to g H₂O using CF(1).

$$\text{So, g H}_2\text{O} = 0.500 \cancel{\text{ kg H}_2\text{O}} \times \frac{1000 \text{ g H}_2\text{O}}{1 \cancel{\text{ kg H}_2\text{O}}} = 500 \text{ g H}_2\text{O}$$

We can now convert g H₂O to mol H₂O using CF(2).

$$\text{moles of H}_2\text{O} = 500 \cancel{\text{ g H}_2\text{O}} \times \frac{1 \text{ mol H}_2\text{O}}{18 \cancel{\text{ g H}_2\text{O}}} = \frac{500}{18} \text{ mol H}_2\text{O} = \underline{\underline{27.8 \text{ mol H}_2\text{O}}}$$

The two separate steps can be combined into a single calculation.

The given quantity (kg H₂O) and the required quantity (mol H₂O) must be on the top line so the conversion factors must be arranged as follows:

$$\text{CF(1) - } \frac{1000 \text{ g H}_2\text{O}}{1 \text{ kg H}_2\text{O}} \text{ and CF(2) - } \frac{1 \text{ mol H}_2\text{O}}{18 \text{ g H}_2\text{O}} \text{ giving}$$

kg H₂O × CF(1) × CF(2) → mol H₂O as shown below
 (kg → g) (g → mol)

$$0.500 \cancel{\text{ kg H}_2\text{O}} \times \frac{1000 \cancel{\text{ g H}_2\text{O}}}{1 \cancel{\text{ kg H}_2\text{O}}} \times \frac{1 \text{ mol H}_2\text{O}}{18 \cancel{\text{ g H}_2\text{O}}} = 0.500 \times \frac{1000}{1} \times \frac{1}{18} \text{ mol H}_2\text{O}$$

$$= \underline{\underline{27.8 \text{ mol H}_2\text{O}}}$$

A common type of calculation asks students to calculate the number of chemical entities in a mass of substance.

Example 3

How many silver atoms are present in a ring of pure silver which has a mass of 3 g?

(Take: Avogadro constant = 6×10^{23} ; relative atomic mass of Ag = 108)

given quantity - 3 g Ag
required quantity - ? Ag atoms

We need two conversion factors: the first will convert 'g Ag' to 'mol Ag' and the second will convert 'mol Ag' to 'atoms Ag'.

conversion factor, CF(1) - 108 g Ag : 1 mol Ag

conversion factor, CF(2) - 1 mol Ag : 6×10^{23} atoms Ag

Arranging these we get:

$$\begin{aligned} \text{Number of atoms of Ag} &= 3 \cancel{\text{g Ag}} \times \frac{1 \cancel{\text{mol Ag}}}{108 \cancel{\text{g Ag}}} \times \frac{6 \times 10^{23} \text{ atoms Ag}}{1 \cancel{\text{mol Ag}}} \\ &= 3 \times \frac{1}{108} \times \frac{6 \times 10^{23}}{1} \text{ atoms Ag} \\ &= \underline{\underline{1.67 \times 10^{22} \text{ atoms Ag}}} \end{aligned}$$

4.2 Calculations involving reacting masses and/or moles only

In any chemical calculation involving balanced equations, moles and masses the arithmetic always employs the same steps which are:

given mass → given moles → required moles → required mass

The calculation could be one of four types:

- given and required are moles
- given is mass and required is moles
- given is moles and required is mass
- given and required are masses.

As with any calculation a correctly balanced equation is required.

Taking mass → mass calculations as our example we need the following information:

- a correctly balanced equation
- a given quantity
- mole-mass conversion factors (i.e. molar masses)
- mole-mole conversion factor (i.e. mole ratio)

in order to find a required quantity.

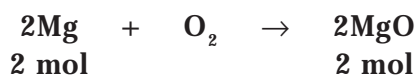
Mass → mole, mole → mass, and mole → mole calculations use exactly the same procedure but have fewer conversion factors.

It would be normal practice to have masses expressed in grams but other units can be used so long as the appropriate conversion factors are employed (see **Example 2** on page 17).

The next example shows the method applied to a typical calculation. The method is identical for all calculations of this type.

Example 4

How many grams of magnesium oxide would be produced by reacting completely 4.0 g of magnesium with oxygen?



given quantity - 4.0 g Mg
required quantity - ? g MgO

The calculation routine is:

1 **2** **3**

grams of Mg → moles of Mg → moles of MgO → grams of MgO

The calculation can be done as separate steps or as a combined calculation.

To illustrate the method we will look at the stepwise procedure first.

Step 1 – Calculate the number of moles of Mg that is equivalent to 4.0 g of Mg.

given quantity - 4.0 g Mg
required quantity - ? mol Mg

conversion factor, CF(1) – 24.3 g Mg (molar mass) : 1 mol Mg

This must have the form $\frac{1 \text{ mol Mg}}{24.3 \text{ g Mg}}$ to cancel with the given quantity.

$$\text{so moles of Mg} = 4.0 \text{ g Mg} \times \frac{1 \text{ mol Mg}}{24.3 \text{ g Mg}} = \underline{0.16 \text{ mol Mg}}$$

Step 2 – Calculate the number of moles of MgO produced from 0.16 mol of Mg.

given quantity - 0.16 mol Mg
required quantity - ? mol MgO

mole ratio conversion factor (MR) – 2 mol Mg : 2 mol MgO
(from balanced equation)

This must have the form $\frac{2 \text{ mol MgO}}{2 \text{ mol Mg}}$ to cancel with the unit of the given quantity.

$$\text{so moles of MgO produced} = 0.16 \cancel{\text{ mol Mg}} \times \frac{2 \text{ mol MgO}}{2 \cancel{\text{ mol Mg}}} = \underline{0.16 \text{ mol MgO}}$$

Step 3 – Calculate the number of grams of MgO equivalent to 0.16 mol of MgO.

given quantity – 0.16 mol MgO
 required quantity – ? g MgO

conversion factor, CF(2) – 1 mol MgO : 40.3 g MgO (molar mass)

This must have the form $\frac{40.3 \text{ g MgO}}{1 \text{ mol MgO}}$ to give the required unit on the top line.

$$\text{So, grams of MgO produced} = 0.16 \cancel{\text{ mol MgO}} \times \frac{40.3 \text{ g MgO}}{1 \cancel{\text{ mol MgO}}} = \underline{\underline{6.45 \text{ g MgO}}}$$

Once some practice has been gained with the method, some students should be able to combine the steps into a single calculation as shown below.

In setting out the conversion factors for a single calculation it is good practice to start with the 'given' and work towards the 'required' when this is possible.

conversion factor, CF(1) – 24.3 g Mg : 1 mol Mg
 mole ratio conversion factor, (MR) – 2 mol Mg : 2 mol MgO
 (from balanced equation)
 conversion factor, CF(2) – 1 mol MgO : 40.3 g MgO

Arranging so that identical units cancel, grams of MgO produced is given by

$$4.0 \text{ g Mg} \times \frac{1 \text{ mol Mg}}{24.3 \text{ g Mg}} \times \frac{2 \text{ mol MgO}}{2 \text{ mol Mg}} \times \frac{40.3 \text{ g MgO}}{1 \text{ mol MgO}}$$

CF(1) MR CF(2)

$$\rightarrow 4.0 \times \frac{1}{24.3} \times \frac{2}{2} \times \frac{40.3}{1} \text{ g MgO}$$

$$= \underline{\underline{6.45 \text{ g MgO}}}$$

It is identical units of chemical entities that cancel **not the numbers**. Only if the conversion factors are set up correctly can you end up with grams of MgO remaining and on the top line. With practice the method becomes routine since every calculation is essentially a variation on the same theme.

Identifying what goes on the top and bottom lines in the CFs may cause difficulty at first but this can be made easier if a systematic approach is taken. In the example above, CF(1) must have 'g Mg' on the bottom line to cancel with the given quantity; CF(2) must have 'g MgO' on the top line to give the required quantity; finally, the mole ratio conversion factor is determined from CF(1) and CF(2). It is probably least confusing if you place the 'required quantity' CF furthest to the right in the calculation layout whenever possible.

Using the grid method - an alternative way of laying out the calculation

Taking the example of the combined calculation above it is easy to see that some students could find difficulty in cancelling the terms. A grid method has been developed to reduce this problem.

With the grid method, instead of the multiplication signs and traditional numerators and denominators (top line and bottom line terms) the various quantities are placed in a grid that looks like this:

--	--	--	--

The number of cells in the grid will depend on the calculation to be performed. An advantage is that the grid can be built up as needed.

First, place the given quantity at the top left hand corner of the grid:

4.0 g Mg			
----------	--	--	--

and then add each of the conversion factors (and mole ratio) until you arrive at:

4.0 g Mg	1 mol Mg	2 mol MgO	40.3 g MgO
	24.3 g Mg	2 mol Mg	1 mol MgO

Like units of like entities are cancelled and the calculation completed. No multiplication signs are shown so it needs to be explained that top line numbers are multiplied together, then bottom line numbers are multiplied together, and then the bottom line answer is divided into the top line answer as usual.

4.3 Calculations involving mass and volume of gas

This type of calculation adds an additional CF if volumes of gases in cm^3 are to be converted into litres.

Example 5

In the reaction of lithium with water, what mass of lithium (in grams) would be required to produce 600 cm^3 of hydrogen?

(Take one mole of hydrogen = 24 l ; relative atomic mass of Li = 6.9).



given quantity - $600 \text{ cm}^3 \text{ H}_2$
 required quantity - $? \text{ g Li}$

Start converting from the 'given' and work towards the 'required'.

conversion factor, CF(1) - $1000 \text{ cm}^3 \text{ H}_2 : 1 \text{ l H}_2$

conversion factor, CF(2) - $24 \text{ l H}_2 : 1 \text{ mol H}_2$

conversion factor, MR - $1 \text{ mol H}_2 : 2 \text{ mol Li}$

conversion factor, CF(3) - $1 \text{ mol Li} : 6.9 \text{ g Li}$

The steps in the calculation are

1
2
3
4

$\text{vol H}_2 (\text{cm}^3) \rightarrow \text{vol H}_2 (\text{l}) \rightarrow \text{mol H}_2 \rightarrow \text{mol Li} \rightarrow \text{mass Li (g)}$

Step 1 - Convert the volume of hydrogen to litres of hydrogen using CF(1).

$$\text{l H}_2 = 600 \text{ cm}^3 \text{ H}_2 \times \frac{1 \text{ l H}_2}{1000 \text{ cm}^3 \text{ H}_2} = \underline{0.6 \text{ l H}_2}$$

Step 2 - Convert the volume of hydrogen to moles of hydrogen using CF(2).

$$\text{mol H}_2 = 0.6 \text{ l H}_2 \times \frac{1 \text{ mol H}_2}{24 \text{ l H}_2} = \underline{0.025 \text{ mol H}_2}$$

Step 3 – Convert moles of hydrogen to moles of lithium using MR.

$$\text{mol Li} = 0.025 \cancel{\text{ mol H}_2} \times \frac{2 \text{ mol Li}}{1 \cancel{\text{ mol H}_2}} = \underline{0.050 \text{ mol Li}}$$

Step 4 – Convert moles of lithium to grams of lithium using CF(3).

$$\text{g Li} = 0.050 \cancel{\text{ mol Li}} \times \frac{6.9 \text{ g Li}}{1 \cancel{\text{ mol Li}}} = \underline{0.345 \text{ g Li}}$$

Here is the calculation showing the steps combined:

$$600 \cancel{\text{ cm}^3 \text{ H}_2} \times \frac{1 \cancel{\text{ l H}_2}}{1000 \cancel{\text{ cm}^3 \text{ H}_2}} \times \frac{1 \cancel{\text{ mol H}_2}}{24 \cancel{\text{ l H}_2}} \times \frac{2 \cancel{\text{ mol Li}}}{1 \cancel{\text{ mol H}_2}} \times \frac{6.9 \text{ g Li}}{1 \cancel{\text{ mol Li}}}$$

CF(1) CF(2) MR CF(3)

$$\rightarrow 600 \times \frac{1}{1000} \times \frac{1}{24} \times \frac{2}{1} \times \frac{6.9}{1} \text{ g Li}$$

$$\rightarrow \frac{600 \times 2 \times 6.9}{1000 \times 24} \text{ g Li}$$

$$= \underline{0.345 \text{ g Li}}$$

Using the grid method, here is the calculation again showing the steps combined:

$600 \text{ cm}^3 \text{ H}_2$	$1 \cancel{\text{ l H}_2}$	$1 \cancel{\text{ mol H}_2}$	$2 \cancel{\text{ mol Li}}$	6.9 g Li
	$1000 \text{ cm}^3 \text{ H}_2$	$24 \cancel{\text{ l H}_2}$	$1 \cancel{\text{ mol H}_2}$	$1 \cancel{\text{ mol Li}}$

$$= \underline{0.345 \text{ g Li}}$$

4.4 Calculations involving solutions

Calculations involving solutions look slightly different from mass – mole conversions since solutions must be described in terms of both their volume and their concentration. Here are some examples. Most calculations of this type also need to use the 1 ℓ : 1000 cm³ equivalence.

Example 6

How many moles of potassium hydroxide (KOH) would be present in 250 cm³ of a KOH solution of concentration 0.4 mol ℓ⁻¹ ?

$$\text{given quantity} \quad - \quad 250 \text{ cm}^3 \text{ soln} \times \frac{0.4 \text{ mol KOH}}{1 \text{ ℓ soln}}$$

$$\text{required quantity} \quad - \quad ? \text{ mol KOH}$$

$$\text{conversion factor} \quad - \quad 1 \text{ ℓ soln} : 1000 \text{ cm}^3 \text{ soln}$$

Therefore the calculation becomes

$$250 \text{ cm}^3 \text{ soln} \times \frac{0.4 \text{ mol KOH}}{1 \text{ ℓ soln}} \times \frac{1 \text{ ℓ soln}}{1000 \text{ cm}^3 \text{ soln}}$$

$$= 250 \times \frac{0.4}{1} \times \frac{1}{1000} \text{ mol KOH}$$

$$= \underline{\underline{0.1 \text{ mol KOH}}}$$

If using the grid method, note that a solution would occupy three cells so the solution of potassium hydroxide in the above example would be written like this:

250 cm ³ soln	0.4 mol KOH
	1 ℓ soln

Up until Example 5 it had been possible to place cancelling units side by side in the calculation but this is not possible with calculations involving solutions. Note also that the presence of a solution is indicated by 'soln' in the unit. Since the chemical entity (KOH) is included with the 'mol'

unit it is not necessary to include it in the 'soln' unit also. While it might seem fussy to write 'soln' each time it helps to avoid confusion when dealing with calculations involving both volumes of solutions and volumes of gases (see **Example 11**).

Example 7

What mass (in g) of sodium hydroxide (NaOH) would be needed to make 2 l of a NaOH solution of concentration 0.2 mol l⁻¹ ?

$$\text{given quantity} \quad - \quad 2 \text{ l soln} \times \frac{0.2 \text{ mol NaOH}}{1 \text{ l soln}}$$

$$\text{required quantity} \quad - \quad ? \text{ g NaOH}$$

$$\text{conversion factor} \quad - \quad 1 \text{ mol NaOH} : 40 \text{ g NaOH}$$

Step 1 - Calculate the number of moles of NaOH needed.

$$\begin{aligned} \text{mol NaOH needed} &= 2 \text{ l soln} \times \frac{0.2 \text{ mol NaOH}}{1 \text{ l soln}} \\ &= 2 \times \frac{0.2 \text{ mol NaOH}}{1} \\ &= \underline{0.4 \text{ mol NaOH}} \end{aligned}$$

Step 2 - Convert moles of NaOH to grams of NaOH.

$$\begin{aligned} \text{g NaOH needed} &= 0.4 \text{ mol NaOH} \times \frac{40 \text{ g NaOH}}{1 \text{ mol NaOH}} \\ &= \underline{\underline{16 \text{ g NaOH}}} \end{aligned}$$

The two steps could have been combined in which case the calculation grid would have looked like this:

2 l soln	0.2 mol NaOH	40 g NaOH
	1 l soln	1 mol NaOH

Example 8

What volume (in ℓ) of $0.5 \text{ mol } \ell^{-1}$ solution could be made using 13.25 g of sodium carbonate, Na_2CO_3 ?

given quantity – $13.25 \text{ g Na}_2\text{CO}_3$

required quantity – $? \ell \text{ soln}$

Step 1 – Convert the mass of sodium carbonate into moles.

CF (1) – $1 \text{ mol Na}_2\text{CO}_3 : 106 \text{ g Na}_2\text{CO}_3$

$$\begin{aligned} \text{mol Na}_2\text{CO}_3 &= \frac{13.25 \text{ g Na}_2\text{CO}_3}{106 \text{ g Na}_2\text{CO}_3} \times \frac{1 \text{ mol Na}_2\text{CO}_3}{106 \text{ g Na}_2\text{CO}_3} \\ &= \underline{\underline{0.125 \text{ mol Na}_2\text{CO}_3}} \end{aligned}$$

Step 2 – Find the volume of solution that can be made using the concentration of the actual solution as a conversion factor.

CF (2) – $0.5 \text{ mol Na}_2\text{CO}_3 : 1 \ell \text{ soln}$

$$\begin{aligned} \text{vol soln } (\ell) &= \frac{0.125 \text{ mol Na}_2\text{CO}_3}{0.5 \text{ mol Na}_2\text{CO}_3} \times \frac{1 \ell \text{ soln}}{0.5 \text{ mol Na}_2\text{CO}_3} \\ &= \underline{\underline{0.250 \ell \text{ soln}}} \end{aligned}$$

4.5 Calculations involving volumetric analysis

Any volumetric calculation, acid/base or redox, may be carried out.

Example 9

20 cm³ of a solution of NaOH is exactly neutralised by 25 cm³ of a solution of HCl of concentration 0.5 mol ℓ⁻¹.

Calculate the concentration of the NaOH solution in mol ℓ⁻¹.



$$\text{given quantity} \quad - \quad 25 \text{ cm}^3 \times \frac{0.5 \text{ mol HCl}}{1 \text{ ℓ soln}}$$

$$\text{required quantity} \quad - \quad \frac{? \text{ mol NaOH}}{1 \text{ ℓ soln}}, \text{ i.e. concentration of NaOH soln}$$

The calculation steps are



Step 1 – Calculate moles of HCl in 25 cm³ soln using the conversion factor 1 ℓ soln : 1000 cm³ soln.

$$\begin{array}{l} \text{mol HCl} = \frac{25 \text{ cm}^3 \text{ soln}}{1000 \text{ cm}^3 \text{ soln}} \times \frac{0.5 \text{ mol HCl}}{1 \text{ ℓ soln}} \\ = \quad \underline{\underline{0.0125 \text{ mol HCl}}} \end{array}$$

Step 2 – Calculate number of moles of NaOH in 20 cm³ soln using the mole ratio – 1 mol HCl : 1 mol NaOH.

$$\begin{array}{l} \text{mol NaOH} = \frac{0.0125 \text{ mol HCl}}{1 \text{ mol HCl}} \times 1 \text{ mol NaOH} \\ = \quad \underline{\underline{0.0125 \text{ mol NaOH}}} \end{array}$$

Step 3 – Calculate the concentration of the NaOH solution in $\frac{\text{mol NaOH}}{1 \text{ l soln}}$

using the known concentration $\frac{0.0125 \text{ mol NaOH}}{20 \text{ cm}^3 \text{ soln}}$ and the conversion factor $1 \text{ l soln} : 1000 \text{ cm}^3 \text{ soln}$.

$$\begin{array}{l} \frac{\text{mol NaOH}}{1 \text{ l soln}} = \frac{0.0125 \text{ mol NaOH}}{20 \text{ cm}^3 \text{ soln}} \times \frac{1000 \text{ cm}^3 \text{ soln}}{1 \text{ l soln}} \\ = \frac{0.625 \text{ mol NaOH}}{1 \text{ l soln}}, \text{ i.e. the concentration is } 0.625 \text{ mol l}^{-1} \end{array}$$

With practice, the three steps can be combined into a single calculation. When this is done, the two l/cm^3 CFs cancel out and can be omitted, giving

$$\begin{array}{l} \frac{\text{mol NaOH}}{1 \text{ l soln}} = \frac{25 \text{ cm}^3 \text{ soln}}{1 \text{ l soln}} \times \frac{0.5 \text{ mol HCl}}{1 \text{ l soln}} \times \frac{1 \text{ mol NaOH}}{1 \text{ mol HCl}} \times \frac{1}{20.0 \text{ cm}^3 \text{ soln}} \\ = \frac{0.625 \text{ mol NaOH}}{1 \text{ l soln}} = \text{i.e. } 0.625 \text{ mol l}^{-1} \end{array}$$

This is certainly a quick way of doing a volumetric calculation but is only for the highly skilled. The volume of the given solution must always be in the top left cell. The algorithm here is comparing the two volumes in relation to the mole ratio.

Once again note that the volume unit uses the term ‘soln’ but, for the method to work, does not distinguish between different solutions. This is because the chemical entity is already described in the concentration unit. However, it is necessary to use ‘soln’ in order to distinguish between volumes of gas and volumes of solution as **Example 11** shows.

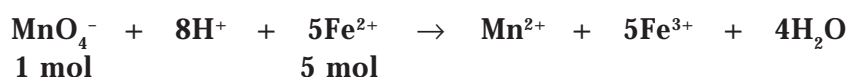
If we had been given the concentration of the NaOH solution and had been asked to calculate the volume needed to neutralise (in cm^3) then the grid would have this appearance, derived by a bit of old-fashioned cross-multiplying from the previous grid (see also **Example 10**).

25 cm ³ soln	0.5 mol HCl	1 mol NaOH	1 ℓ soln	= <u>20 cm³ soln</u>
	1 ℓ soln	1 mol HCl	0.625 mol NaOH	

Example 10

In **Example 9** the method is used to calculate a volume of solution of known concentration. This example also illustrates how conversion factors work equally well if the entities involved are merely ions rather than full chemical formulae.

The redox reaction between permanganate ions and iron(II) ions is:



What volume (in cm³) of permanganate solution of concentration 0.04 mol ℓ⁻¹ would react exactly with 30 cm³ of a solution of iron(II) which has a concentration of 0.3 mol ℓ⁻¹?

$$\text{given quantity} \quad - \quad 30 \text{ cm}^3 \text{ soln} \times \frac{0.3 \text{ mol Fe}^{2+}}{1 \text{ ℓ soln}}$$

$$\text{required quantity} \quad - \quad ? \text{ cm}^3 \text{ soln}$$

Conversion factors

$$1 \text{ ℓ soln} : 1000 \text{ cm}^3$$

$$1 \text{ mol MnO}_4^- : 5 \text{ mol Fe}^{2+}$$

The calculation steps are:

$$\text{vol Fe}^{2+} \xrightarrow{1} \text{mol Fe}^{2+} \xrightarrow{2} \text{mol MnO}_4^- \xrightarrow{3} \text{vol MnO}_4^-$$

Step 1

moles of Fe ²⁺	=	30 cm³ soln	0.3 mol Fe²⁺	1 ℓ soln
			1 ℓ soln	1000 cm ³ soln
	=	<u>0.009 mol Fe²⁺</u>		

Step 2

$$\begin{aligned} \text{moles of MnO}_4^- \text{ reacting} &= \frac{0.009 \text{ mol Fe}^{2+}}{5 \text{ mol Fe}^{2+}} \times \frac{1 \text{ mol MnO}_4^-}{1 \text{ mol MnO}_4^-} \\ &= \underline{0.0018 \text{ mol MnO}_4^-} \end{aligned}$$

Step 3

The volume of solution (in cm^3) of concentration $0.040 \text{ mol MnO}_4^- \ell^{-1}$ and containing $0.0018 \text{ mol MnO}_4^-$ is

$$\begin{aligned} &\frac{0.0018 \text{ mol MnO}_4^-}{0.04 \text{ mol MnO}_4^-} \times \frac{1 \ell \text{ soln}}{1 \ell \text{ soln}} \times \frac{1000 \text{ cm}^3 \text{ soln}}{1 \ell \text{ soln}} \\ &= \underline{45 \text{ cm}^3 \text{ soln}} \end{aligned}$$

Combining the steps into a single grid would give

$$\begin{aligned} &\frac{30 \text{ cm}^3 \text{ soln}}{1 \ell \text{ soln}} \times \frac{0.3 \text{ mol Fe}^{2+}}{5 \text{ mol Fe}^{2+}} \times \frac{1 \text{ mol MnO}_4^-}{1 \text{ mol MnO}_4^-} \times \frac{1 \ell \text{ soln}}{0.04 \text{ mol MnO}_4^-} \\ &= \underline{45 \text{ cm}^3 \text{ soln}} \end{aligned}$$

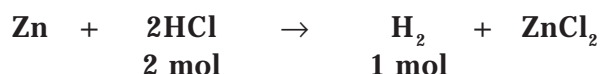
Once again the volume of the given solution goes to the top left cell of the grid.

4.6 Complex calculations involving solutions and molar volume of gas

Example 11

What volume (in ℓ) of hydrogen would be produced by completely reacting 60 cm^3 of hydrochloric acid of concentration $1.2 \text{ mol } \ell^{-1}$ with zinc?

(Take one mole of hydrogen = 24ℓ .)

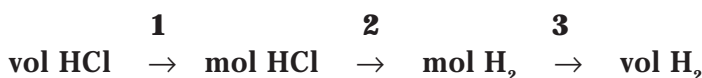


mole ratio – $2 \text{ mol HCl} : 1 \text{ mol H}_2$

given quantity – $60 \text{ cm}^3 \text{ soln} \times \frac{1.2 \text{ mol HCl}}{1 \ell \text{ soln}}$

required quantity – $? \ell \text{ H}_2$

The calculation steps are



Step 1 – Calculate the number of moles of HCl using the conversion factor $1 \ell : 1000 \text{ cm}^3$.

$$\begin{aligned} \text{moles of HCl} &= \frac{60 \text{ cm}^3 \text{ soln}}{1000 \text{ cm}^3 \text{ soln}} \times \frac{1.2 \text{ mol HCl}}{1 \ell \text{ soln}} \\ &= \underline{0.072 \text{ mol HCl}} \end{aligned}$$

Step 2 – Calculate the equivalent number of moles of hydrogen using the mole ratio.

$$\begin{aligned} \text{moles of hydrogen} &= \frac{0.072 \text{ mol HCl}}{2 \text{ mol HCl}} \times 1 \text{ mol H}_2 \\ &= \underline{0.036 \text{ mol H}_2} \end{aligned}$$

Step 3 – Calculate the volume of hydrogen produced using the conversion factor 1 mol H₂ : 24 l H₂

$$\begin{aligned} \text{vol of H}_2 &= \frac{0.036 \text{ mol H}_2}{1 \text{ mol H}_2} \times \frac{24 \text{ l H}_2}{1 \text{ mol H}_2} \\ &= \underline{\underline{0.864 \text{ l H}_2}} \end{aligned}$$

As in previous cases the separate steps can be combined into a single calculation.

$$\begin{aligned} \text{vol H}_2 &= \frac{60 \text{ cm}^3 \text{ soln}}{1000 \text{ cm}^3 \text{ soln}} \times \frac{1.2 \text{ mol HCl}}{2 \text{ mol HCl}} \times \frac{1 \text{ l soln}}{1 \text{ l soln}} \times \frac{1 \text{ mol H}_2}{1 \text{ mol H}_2} \times \frac{24 \text{ l H}_2}{1 \text{ mol H}_2} \\ &= \underline{\underline{0.864 \text{ l H}_2}} \end{aligned}$$

Note that in this calculation the unit ‘l H₂’ is distinct from ‘l soln’ and they do not cancel.

4.7 Calculations involving empirical formulae

Example 12

A compound containing only carbon, hydrogen and oxygen was analysed and was found to have the following percentage composition by mass:

carbon 54.4 %
hydrogen 9.1%
oxygen 36.5 %

Determine the empirical formula of the compound.

(Relative atomic masses: C = 12.0; H = 1.0; O = 16.0)

The percentage composition by mass is the equivalent of saying that in 100 g of the compound there are 54.4 g of carbon, 9.1 g of hydrogen and 36.5 g of oxygen.

Using the percentages, we are therefore able to determine the number of moles of each element in 100 g of the compound by using the relevant conversion factor for each element, i.e.

1 mol X : relative atomic mass of X in g.

The number of moles of each element in 100 g of compound is:

$$\text{mol C} = 54.4 \cancel{\text{ g C}} \times \frac{1 \text{ mol C}}{12.0 \cancel{\text{ g C}}} = 4.53 \text{ mol C}$$

$$\text{mol H} = 9.1 \cancel{\text{ g H}} \times \frac{1 \text{ mol H}}{1.0 \cancel{\text{ g H}}} = 9.10 \text{ mol H}$$

$$\text{mol O} = 36.5 \cancel{\text{ g O}} \times \frac{1 \text{ mol O}}{16.0 \cancel{\text{ g O}}} = 2.28 \text{ mol O}$$

The ratio of C:H:O is therefore **4.53 : 9.10 : 2.28** which simplifies to **2 : 4 : 1**.

Hence the empirical formula is **C₂H₄O**

The method can be adapted to calculate empirical formulae from combustion data or to calculate percentage composition from formulae.

Example 13

0.495 g of a compound containing only C, H, and O gave on complete combustion 0.991 g of CO₂ and 0.405 g of H₂O.

Calculate the empirical formula of the compound.

We first calculate the number of grams of C in the sample using the following conversion factors:

44 g CO₂ : 1 mol CO₂ – converts grams of carbon dioxide to moles of carbon dioxide

1 mol CO₂ : 1 mol C – converts moles of carbon dioxide to moles of carbon

1 mol C : 12 g C – converts moles of carbon to grams of carbon

and arrange them as follows:

$$\text{g C} = 0.991 \cancel{\text{g CO}_2} \times \frac{1 \cancel{\text{mol CO}_2}}{44 \cancel{\text{g CO}_2}} \times \frac{1 \cancel{\text{mol C}}}{1 \cancel{\text{mol CO}_2}} \times \frac{12 \text{ g C}}{1 \cancel{\text{mol C}}} = 0.270 \text{ g C}$$

Since this type of calculation would only be performed by senior students at AH level it could be simplified by the use of the equivalence 44 g CO₂ : 12 g C giving

$$\text{g C} = 0.991 \cancel{\text{g CO}_2} \times \frac{12 \text{ g C}}{44 \cancel{\text{g CO}_2}} = 0.270 \text{ g C}$$

Similarly, using the simplified method for H, the number of grams of H in the sample is given by

$$\text{g H} = 0.405 \cancel{\text{g H}_2\text{O}} \times \frac{2 \text{ g H}}{18 \cancel{\text{g H}_2\text{O}}} = 0.045 \text{ g}$$

Since we are told that this is a CHO compound the mass of oxygen in the sample must be the mass that remains when the sum of the masses of carbon and hydrogen is subtracted from the mass of the sample.

$$\text{g O} = 0.495 - (0.270 + 0.045) \text{ g O}$$

$$= 0.180 \text{ g O}$$

Now we calculate the number of moles of C, H and O in the sample.

$$\text{mol C} = 0.270 \text{ g C} \times \frac{1 \text{ mol C}}{12.0 \text{ g C}} = 0.0225 \text{ mol C}$$

$$\text{mol H} = 0.045 \text{ g H} \times \frac{1 \text{ mol H}}{1.0 \text{ g H}} = 0.0450 \text{ mol H}$$

$$\text{mol O} = 0.180 \text{ g O} \times \frac{1 \text{ mol O}}{16.0 \text{ g O}} = 0.0113 \text{ mol O}$$

The ratio of C:H:O is **0.0225 : 0.0450 : 0.0113** i.e. **2 : 4 : 1 approx**

Hence the empirical formula is, once again, **C₂H₄O**

Example 14

Calculate the percentage composition by weight of N in (NH₄)₂SO₄.

In effect we must calculate the mass of N in 100 g of (NH₄)₂SO₄.

We must also take note that there are two N atoms in the formula.

The conversion factors needed are:

132 g (NH₄)₂SO₄ : 1 mol (NH₄)₂SO₄ – converts grams of ammonium sulphate to moles

1 mol (NH₄)₂SO₄ : 2 mol N – converts moles of ammonium sulphate to moles of nitrogen combined in ammonium sulphate

1 mol N : 14 g N – converts moles of nitrogen to grams

In the calculation they are arranged as follows:

$$\begin{array}{c|c|c|c} 100 \text{ g (NH}_4\text{)}_2\text{SO}_4 & 1 \text{ mol (NH}_4\text{)}_2\text{SO}_4 & 2 \text{ mol N} & 14 \text{ g N} \\ \hline & 132 \text{ g (NH}_4\text{)}_2\text{SO}_4 & 1 \text{ mol (NH}_4\text{)}_2\text{SO}_4 & 1 \text{ mol N} \end{array} = 21.2 \text{ g N}$$

Therefore the percentage composition by weight of N is **21.2%**.

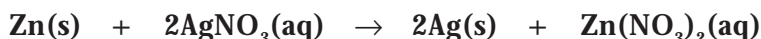
(This calculation could have been carried out stepwise. First, we could have calculated the mass of nitrogen in one mole of ammonium sulphate and then converted this mass into a percentage.)

4.8 Calculations involving limiting and excess reactants

Calculations of this type have two 'given' quantities.

Example 15

A strip of zinc metal weighing 2.00 g is placed in an aqueous solution containing 10.00 g of silver nitrate. The reaction that occurs is



- (a) Determine which reactant is in excess.
 (b) Calculate how many grams of silver will be formed.

- (a) Determine which reactant is in excess.

given quantity - 2.00 g Zn
 required quantity - ? mol Zn
 CF(1) - 1 mol Zn : 65.4 g Zn

and

given quantity - 10.00 g AgNO₃
 required quantity - ? mol AgNO₃
 CF(2) - 1 mol AgNO₃ : 170 g AgNO₃

$$\text{mol Zn} = 2.00 \cancel{\text{g Zn}} \times \frac{1 \text{ mol Zn}}{65.4 \cancel{\text{g Zn}}} = 2.00 \times \frac{1 \text{ mol Zn}}{65.4} = \underline{3.06 \times 10^{-2} \text{ mol Zn}}$$

$$\text{mol AgNO}_3 = 10.00 \cancel{\text{g AgNO}_3} \times \frac{1 \text{ mol AgNO}_3}{170 \cancel{\text{g AgNO}_3}} = \underline{5.88 \times 10^{-2} \text{ mol AgNO}_3}$$

The mole ratio conversion factor for complete reaction is
 1 mol Zn : 2 mol AgNO₃.

Moles of AgNO₃ needed to react with 3.06×10^{-2} mol Zn would be

$$3.06 \times 10^{-2} \cancel{\text{mol Zn}} \times \frac{2 \text{ mol AgNO}_3}{1 \cancel{\text{mol Zn}}} = 6.12 \times 10^{-2} \text{ mol AgNO}_3$$

Since there is only 5.88×10^{-2} mol of AgNO₃ available it is the AgNO₃ that is the limiting reactant and so the zinc metal is in excess.

(b) Calculate how many grams of silver will be formed.

The mass of silver formed will be determined by the limiting reactant which is AgNO_3 .

given quantity $5.88 \times 10^{-2} \text{ mol AgNO}_3$
 required quantity ? g Ag

mole ratio $2 \text{ mol AgNO}_3 : 2 \text{ mol Ag}$
 CF(3) $1 \text{ mol Ag} : 108 \text{ g Ag}$

$$\begin{aligned} \text{g Ag formed} &= 5.88 \times 10^{-2} \text{ mol AgNO}_3 \times \frac{2 \text{ mol Ag}}{2 \text{ mol AgNO}_3} \times \frac{108 \text{ g Ag}}{1 \text{ mol Ag}} \\ &= \underline{\underline{6.35 \text{ g Ag}}} \end{aligned}$$

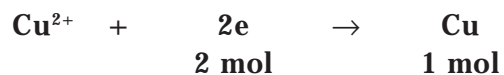
The ULM is at its most elegant with stoichiometric calculations. It can be extended to cover calculations involving the Faraday constant and heats of reaction but in these cases the given and required quantities may sometimes be conversion factors and this introduces an extra layer of difficulty. Examples 16 and 17 and Problems 17 and 18 give some flavour of the challenges involved.

4.9 Calculations involving the Faraday constant

Example 16

4825 C of electricity was passed through a solution containing copper (II) ions.

What mass of copper (in grams) would be deposited at the negative electrode?



given quantity – 4825 C

required quantity – ? g Cu

Conversion factors

96500 C : 1 mol e⁻ – converts coulombs to moles of electrons

2 mol e⁻ : 1 mol Cu – converts moles of electrons to moles of copper

1 mol Cu : 63.5 g Cu – converts moles of copper to grams of copper

$$\begin{aligned} \text{g Cu formed} &= \frac{4825 \text{ C}}{96500 \text{ C}} \times \frac{1 \text{ mol e}^-}{2 \text{ mol e}^-} \times \frac{1 \text{ mol Cu}}{1 \text{ mol Cu}} \times \frac{63.5 \text{ g Cu}}{1 \text{ mol Cu}} \\ &= \underline{\underline{1.59 \text{ g Cu}}} \end{aligned}$$

4.10 Calculations involving enthalpy changes

The example given shows the method applied to an enthalpy of combustion calculation.

Example 17

Complete combustion of 2g of an organic compound released 67.2 kJ of energy.

Calculate the relative formula mass of the compound given that its molar enthalpy of combustion is 2016 kJ mol⁻¹.

This calculation is a non-standard application of the method since the required quantity is a conversion factor, i.e. how many grams of compound is equivalent to one mole, i.e.

$\frac{x \text{ g compound}}{1 \text{ mol compound}}$ where x is the relative formula mass

given quantity $\Delta H_c = -2016 \text{ kJ mol}^{-1}$ written as $\frac{-2016 \text{ kJ}}{1 \text{ mol compound}}$

conversion factor 2 g compound: -67.2 kJ written as $\frac{2 \text{ g compound}}{-67.2 \text{ kJ}}$

required quantity = given x conversion factor

$$\begin{aligned} &= \frac{-2016 \cancel{\text{ kJ}}}{1 \text{ mol compound}} \times \frac{2 \text{ g compound}}{-67.2 \cancel{\text{ kJ}}} \\ &= \frac{-2016 \times 2 \text{ g compound}}{-67.2 \times 1 \text{ mol compound}} \\ &= \frac{60 \text{ g compound}}{1 \text{ mol compound}} \end{aligned}$$

Relative formula mass of compound = 60 (amu)

The method can be extended to calculations involving heating masses of water and noting the temperature rise but it then becomes essential that the unit for the specific heat capacity of water ($\text{kJ kg}^{-1} \text{C}^{-1}$) is fully shown. The specific heat capacity is itself a conversion factor and would be

written as $\frac{4.18 \text{ kJ}}{1 \text{ kg H}_2\text{O} \times 1 \text{ C}}$.

In this final example we have had to manufacture a way of reaching the answer. With practice a wider range of calculations can be carried out using the ULM.

4.11 Teaching calculations in chemistry – a few tips

1. Teaching calculations takes time. It should not be rushed.
2. Because of the way we learn things, teaching calculations is best done using a stepwise, gradual approach. Rather than spend a week on calculations and then not revisit the topic until just before the examination it is more productive to introduce a calculation topic, give some practice in the process, and then set time aside to return to it from time to time over the next few weeks. Learning often occurs at second or third encounter because, at first encounter, the mind is too busy trying to assemble the new information and make sense of it all.

3. The method known as

see one → try one → do one

should be applied when teaching chemistry calculations, that is to say, the teacher explains, with the usual questioning, how to carry out a new type of calculation. The class then attempts a calculation with close support from the teacher. Once the teacher is satisfied that most students are reasonably confident further calculations can be attempted with support being provided where necessary.

4. The difficulty of a calculation type should advance by small steps when teaching it. This is because, before an algorithm has been taught, any problem is non-standard to the learner and is therefore inherently difficult. Once taught, knowing how to apply the algorithm correctly removes much (although not all) of the difficulty.

To take an example, suppose that the reacting masses calculation is being introduced. In explaining the method it would be advisable to use as simple a balanced equation as possible, like

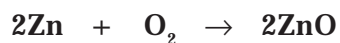


After explaining how to do the calculation the students should attempt one. The equation chosen should be something similar, say

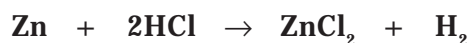


Students should gain confidence since they can perform the calculation simply by substituting terms.

From there students should progress gradually to more and more complicated equations, adding one layer of complexity at a time, for example



and then



With each step students should become more confident in applying the algorithm and eventually the point is reached where students can apply the algorithm to any calculation of a given type.

A similar process should be gone through with each type of calculation.

4.12 Sample calculations

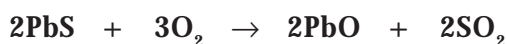
These calculations are intended for teachers to practise the method.

Outline solutions to these calculations using the ULM are provided. The solutions have been determined using the following relative atomic masses.

Ag	107.9	Fe	55.8	O	16.0
Al	27.0	H	1.0	P	31.0
C	12.0	K	39.1	Pb	207.2
Cl	35.5	Mg	24.3	S	32.1
Cr	52.0	N	14.0	Ti	47.9
F	19.0	Na	23.0		

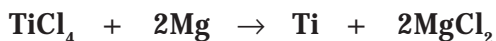
The Avogadro Constant was taken to be 6×10^{23} .

1. What is the mass (in grams) of 0.5 mol of K_2SO_4 ?
2. How many moles of aluminium carbonate, $Al_2(CO_3)_3$, are present in 4.68 g of the substance?
3. What is the mass of 10^{23} molecules of H_2O ?
4. Lead oxide is produced when lead sulphide is heated in oxygen.



What mass of oxygen would react exactly with 95.72 g of PbS?

5. Titanium(IV) chloride can be converted to titanium by reacting it with an excess of magnesium.

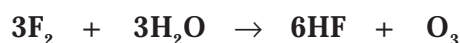


What mass of titanium could theoretically be obtained from 37.98×10^4 kg of titanium(IV) chloride?

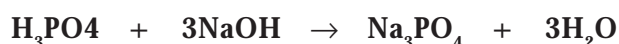
6. Under conditions in which the molar volume of hydrogen is 24.0 ℓ, what volume of hydrogen would be required to produce 8.4 g of cyclohexane from cyclohexene?



7. Under conditions in which the molar volume of ozone, O₃, is 22.4 ℓ, what volume of ozone would be produced by reacting 0.95 g of fluorine with excess steam?

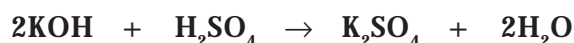


8. A sample of a compound containing sulphur and phosphorus only and weighing 22 g was found to contain 9.6 g of sulphur. What is the empirical formula of the compound?
9. What is the empirical formula of the organic compound, a sample of which was found to contain 0.451 g of carbon, 0.0376 g of hydrogen, and 0.202 g of oxygen only?
10. How many moles of potassium hydroxide, KOH, would be present in 240 cm³ of a solution of concentration 0.65 mol ℓ⁻¹?
11. How many grams of FeCl₂ would be needed to make 600 cm³ of a solution of concentration 0.5 mol ℓ⁻¹?
12. A sample of liquid containing phosphoric acid (and no other acids) was completely neutralised by 21.6 cm³ of 0.5 mol ℓ⁻¹ sodium hydroxide solution.



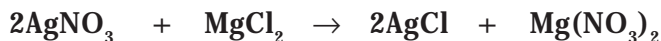
What mass (in grams) of phosphoric acid was in the sample?

13. 48.8 cm³ of a solution of potassium hydroxide of concentration 0.5 mol ℓ⁻¹ exactly neutralised 25 cm³ of sulphuric acid solution.



Calculate the concentration of the acid.

14. 40 cm³ of a 0.08 mol ℓ⁻¹ solution of silver(I) nitrate solution was added to 46 cm³ of a 0.3 mol ℓ⁻¹ solution of magnesium chloride.



What mass (in g) of silver(I) chloride would be formed?

15. $\text{Cr}_2\text{O}_7^{2-} + 14\text{H}^+ + 6\text{e}^- \rightarrow 2\text{Cr}^{3+} + 7\text{H}_2\text{O}$



60 cm³ of an acidified dichromate(VI) solution with a concentration 0.05 mol ℓ⁻¹ was titrated against a 0.6 mol ℓ⁻¹ Fe²⁺ solution. What volume of Fe²⁺ solution would be required to reach the end point of this titration?

16. Under conditions in which the molar volume of ammonia gas is 22.4 ℓ, what volume of ammonia gas (in ℓ) would be required to neutralise 80 cm³ of a 0.025 mol ℓ⁻¹ solution of sulphuric acid?



17. A total of 210 C was passed through a solution of dilute sulphuric acid and 26 cm³ of hydrogen gas was collected at the negative electrode.

Calculate the volume of one mole of hydrogen gas (in litres) under the prevailing conditions of temperature and pressure.

18. 50 cm³ of a solution of HCl was exactly neutralised by 50 cm³ of a NaOH solution. The temperature rise in the resulting solution was 13.6 C.

Given that the enthalpy of neutralisation for HCl and NaOH is -57 kJ per mole of H₂O formed, calculate the concentration of the acid in moles per litre.

Assume all solutions have a density of 1 g per cm³. Ignore the mass of any water formed.

4.13 Solutions to calculations**Problem 1**

$$\text{Mass} = 0.5 \text{ mol K}_2\text{SO}_4 \times \frac{174.3 \text{ g K}_2\text{SO}_4}{1 \text{ mol K}_2\text{SO}_4}$$

Problem 2

$$\text{Mol Al}_2(\text{CO}_3)_3 = 4.68 \text{ g Al}_2(\text{CO}_3)_3 \times \frac{1 \text{ mol Al}_2(\text{CO}_3)_3}{234 \text{ g Al}_2(\text{CO}_3)_3}$$

Problem 3**Step 1**

$$\text{Mol H}_2\text{O} = 10^{23} \text{ molecules H}_2\text{O} \times \frac{1 \text{ mol H}_2\text{O}}{6 \times 10^{23} \text{ molecules H}_2\text{O}}$$

Step 2

$$\text{Mass H}_2\text{O} = 0.167 \text{ mol H}_2\text{O} \times \frac{18 \text{ g H}_2\text{O}}{1 \text{ mol H}_2\text{O}}$$

(Note: 'molecules' could be abbreviated to 'molec' but *not* 'mol' or 'mols')

Problem 4**Step 1**

$$\text{Mol PbS} = 95.72 \text{ g PbS} \times \frac{1 \text{ mol PbS}}{239.3 \text{ g PbS}}$$

Step 2

$$\text{Mol O}_2 = 0.4 \text{ mol PbS} \times \frac{3 \text{ mol O}_2}{2 \text{ mol PbS}}$$

Step 3

$$\text{Mass O}_2 = 0.6 \text{ mol O}_2 \times \frac{32 \text{ g O}_2}{1 \text{ mol O}_2}$$

Problem 5*Step 1*

$$\text{Mass TiCl}_4 \text{ in g} = 37.98 \times 10^4 \text{ kg TiCl}_4 \times \frac{1000 \text{ g TiCl}_4}{1 \text{ kg TiCl}_4}$$

Step 2

$$\text{Mol TiCl}_4 = 37.98 \times 10^7 \text{ g TiCl}_4 \times \frac{1 \text{ mol TiCl}_4}{189.9 \text{ g TiCl}_4}$$

Step 3

$$\text{Mol Ti} = 2 \times 10^6 \text{ mol TiCl}_4 \times \frac{1 \text{ mol Ti}}{1 \text{ mol TiCl}_4}$$

Step 4

$$\text{Mass Ti} = 2 \times 10^6 \text{ mol TiCl}_4 \times \frac{47.9 \text{ g Ti}}{1 \text{ mol Ti}}$$

(This answer could be converted to kg using the CF for g and kg.)

Problem 6*Step 1*

$$\text{Mol C}_6\text{H}_{12} = 8.4 \text{ g C}_6\text{H}_{12} \times \frac{1 \text{ mol C}_6\text{H}_{12}}{84 \text{ g C}_6\text{H}_{12}}$$

Step 2

$$\text{Mol H}_2 = 0.1 \text{ mol C}_6\text{H}_{12} \times \frac{1 \text{ mol H}_2}{1 \text{ mol C}_6\text{H}_{12}}$$

Step 3

$$\text{Vol H}_2 = 0.1 \text{ mol H}_2 \times \frac{24 \text{ l H}_2}{1 \text{ mol H}_2}$$

Problem 7**Step 1**

$$\text{Mol F}_2 = 0.95 \text{ g F}_2 \times \frac{1 \text{ mol F}_2}{38 \text{ g F}_2}$$

Step 2

$$\text{Mol O}_3 = 0.025 \text{ mol F}_2 \times \frac{1 \text{ mol O}_3}{3 \text{ mol F}_2}$$

Step 3

$$\text{Vol O}_3 = 0.0083 \text{ mol O}_3 \times \frac{22.4 \text{ l O}_3}{1 \text{ mol O}_3}$$

Problem 8

$$\text{Mol S} = 9.6 \text{ g S} \times \frac{1 \text{ mol S}}{32 \text{ g S}}$$

$$\text{Mol P} = 12.4 \text{ g P} \times \frac{1 \text{ mol P}}{31 \text{ g P}}$$

$$\text{P} : \text{S} = 0.4 : 0.6 = 2 : 3$$

Problem 9

$$\text{Mol C} = 0.451 \text{ g C} \times \frac{1 \text{ mol C}}{12 \text{ g C}}$$

$$\text{Mol H} = 0.0376 \text{ g H} \times \frac{1 \text{ mol H}}{1 \text{ g H}}$$

$$\text{Mol O} = 0.202 \text{ g O} \times \frac{1 \text{ mol O}}{16 \text{ g O}}$$

$$\text{C} : \text{H} : \text{O} = 0.038 : 0.038 : 0.013 = 3 : 3 : 1$$

Problem 10

$$\text{Mol KOH} = 240 \text{ cm}^3 \text{ soln} \times \frac{0.65 \text{ mol KOH}}{1 \text{ l soln}} \times \frac{1 \text{ l soln}}{1000 \text{ cm}^3 \text{ soln}}$$

Problem 11*Step 1*

$$\text{Mol FeCl}_2 = 600 \text{ cm}^3 \text{ soln} \times \frac{0.5 \text{ mol FeCl}_2}{1 \text{ l soln}} \times \frac{1 \text{ l soln}}{1000 \text{ cm}^3 \text{ soln}}$$

Step 2

$$\text{Mass FeCl}_2 = 0.3 \text{ mol FeCl}_2 \times \frac{126.8 \text{ g FeCl}_2}{1 \text{ mol FeCl}_2}$$

Problem 12*Step 1*

$$\text{Mol NaOH} = 21.6 \text{ cm}^3 \text{ soln} \times \frac{0.5 \text{ mol NaOH}}{1 \text{ l soln}} \times \frac{1 \text{ l soln}}{1000 \text{ cm}^3 \text{ soln}}$$

Step 2

$$\text{Mol H}_3\text{PO}_4 = 0.0108 \text{ mol NaOH} \times \frac{1 \text{ mol H}_3\text{PO}_4}{3 \text{ mol NaOH}}$$

Step 3

$$\text{Mass H}_3\text{PO}_4 = 0.0036 \text{ mol H}_3\text{PO}_4 \times \frac{98 \text{ g H}_3\text{PO}_4}{1 \text{ mol H}_3\text{PO}_4}$$

Problem 13*Step 1*

$$\text{Mol KOH} = 48.8 \text{ cm}^3 \text{ soln} \times \frac{0.5 \text{ mol KOH}}{1 \text{ l soln}} \times \frac{1 \text{ l soln}}{1000 \text{ cm}^3 \text{ soln}}$$

Step 2

$$\text{Mol H}_2\text{SO}_4 = 0.0244 \text{ mol KOH} \times \frac{1 \text{ mol H}_2\text{SO}_4}{2 \text{ mol KOH}}$$

Step 3

$$\begin{aligned} \text{Concn H}_2\text{SO}_4 &= \frac{0.0122 \text{ mol H}_2\text{SO}_4}{25 \text{ cm}^3 \text{ soln}} \times \frac{1000 \text{ cm}^3 \text{ soln}}{1 \text{ l soln}} \\ &= \underline{\underline{0.488 \text{ mol l}^{-1}}} \end{aligned}$$

Problem 14**Step 1**

$$\begin{aligned} \text{Mol AgNO}_3 &= 40 \text{ cm}^3 \text{ soln} \times \frac{0.08 \text{ mol AgNO}_3}{1 \text{ l soln}} \times \frac{1 \text{ l soln}}{1000 \text{ cm}^3 \text{ soln}} \\ &= 3.2 \times 10^{-3} \text{ mol AgNO}_3 \end{aligned}$$

Step 2

$$\begin{aligned} \text{Mol MgCl}_2 &= 46 \text{ cm}^3 \text{ soln} \times \frac{0.3 \text{ mol MgCl}_2}{1 \text{ l soln}} \times \frac{1 \text{ l soln}}{1000 \text{ cm}^3 \text{ soln}} \\ &= 1.38 \times 10^{-2} \text{ mol MgCl}_2 \end{aligned}$$

AgNO₃ is limiting reactant

Step 3

$$\text{Mol AgCl} = 3.2 \times 10^{-3} \text{ mol AgNO}_3 \times \frac{2 \text{ mol AgCl}}{2 \text{ mol AgNO}_3}$$

Step 4

$$\text{Mass AgCl} = 3.2 \times 10^{-3} \text{ mol AgCl} \times \frac{143.4 \text{ g AgCl}}{1 \text{ mol AgCl}}$$

Problem 15**Step 1**

$$\text{Mol Cr}_2\text{O}_7^{2-} = 60 \text{ cm}^3 \text{ soln} \times \frac{0.05 \text{ mol Cr}_2\text{O}_7^{2-}}{1 \text{ l soln}} \times \frac{1 \text{ l soln}}{1000 \text{ cm}^3 \text{ soln}}$$

Step 2

$$\text{Mol Fe}^{2+} = 3 \times 10^{-3} \text{ mol Cr}_2\text{O}_7^{2-} \times \frac{6 \text{ mol Fe}^{2+}}{1 \text{ mol Cr}_2\text{O}_7^{2-}}$$

Step 3

$$\text{Vol soln} = 1.8 \times 10^{-2} \text{ mol Fe}^{2+} \times \frac{1 \text{ l soln}}{0.6 \text{ mol Fe}^{2+}} \times \frac{1000 \text{ cm}^3 \text{ soln}}{1 \text{ l soln}}$$

Problem 16**Step 1**

$$\text{Mol H}_2\text{SO}_4 = 80 \text{ cm}^3 \text{ soln} \times \frac{0.025 \text{ mol H}_2\text{SO}_4}{1 \text{ l soln}} \times \frac{1 \text{ l soln}}{1000 \text{ cm}^3 \text{ soln}}$$

Step 2

$$\text{Mol NH}_3 = 2 \times 10^{-3} \text{ mol H}_2\text{SO}_4 \times \frac{2 \text{ mol NH}_3}{1 \text{ mol H}_2\text{SO}_4}$$

Step 3

$$\text{Vol NH}_3 = 4 \times 10^{-3} \text{ mol NH}_3 \times \frac{22.4 \text{ l NH}_3}{1 \text{ mol NH}_3}$$

Problem 17

The working of this problem is a little trickier since it is non standard. You are given one CF, that between volume and coulombs, and asked to calculate another, that between one mole of hydrogen and its volume.

$$\text{CF} = 1 \text{ mol H}_2 : 2 \text{ mol e}^- \quad (1 \text{ mol e}^- = 96\,500 \text{ C})$$

$$\text{CF} = 26 \text{ cm}^3 \text{ H}_2 : 210 \text{ C}$$

$$\begin{aligned} \text{Vol H}_2 &= \frac{26 \text{ cm}^3 \text{ H}_2}{210 \text{ C}} \times \frac{96\,500 \text{ C}}{1 \text{ mol e}^-} \times \frac{2 \text{ mol e}^-}{1 \text{ mol H}_2} \times \frac{1 \text{ l H}_2}{1000 \text{ cm}^3 \text{ H}_2} \\ &= \frac{23.9 \text{ l H}_2}{1 \text{ mol H}_2} \end{aligned}$$

Volume of one mole of hydrogen is 23.9 l.

Problem 18

This is a challenging problem irrespective of the manner of tackling it but it breaks down into three simple steps.

Step 1 – energy released

$$\frac{-4.18 \text{ kJ}}{1 \text{ kg H}_2\text{O} \times 1 \text{ }^\circ\text{C}} \times 0.1 \text{ kg H}_2\text{O} \times 13.6 \text{ }^\circ\text{C}$$

$$= -5.69 \text{ kJ}$$

Step 2 – moles of water formed and hence moles of HCl present

$$-5.69 \text{ kJ} \times \frac{1 \text{ mol H}_2\text{O}}{-57 \text{ kJ}} \times \frac{1 \text{ mol HCl}}{1 \text{ mol H}_2\text{O}}$$

$$= 0.1 \text{ mol HCl}$$

Step 3 – concentration of HCl

$$\frac{0.1 \text{ mol HCl}}{50 \text{ cm}^3 \text{ soln}} \times \frac{1000 \text{ cm}^3 \text{ soln}}{1 \text{ } \ell \text{ soln}}$$

$$= \underline{\underline{2 \text{ mol } \ell^{-1}}}$$