

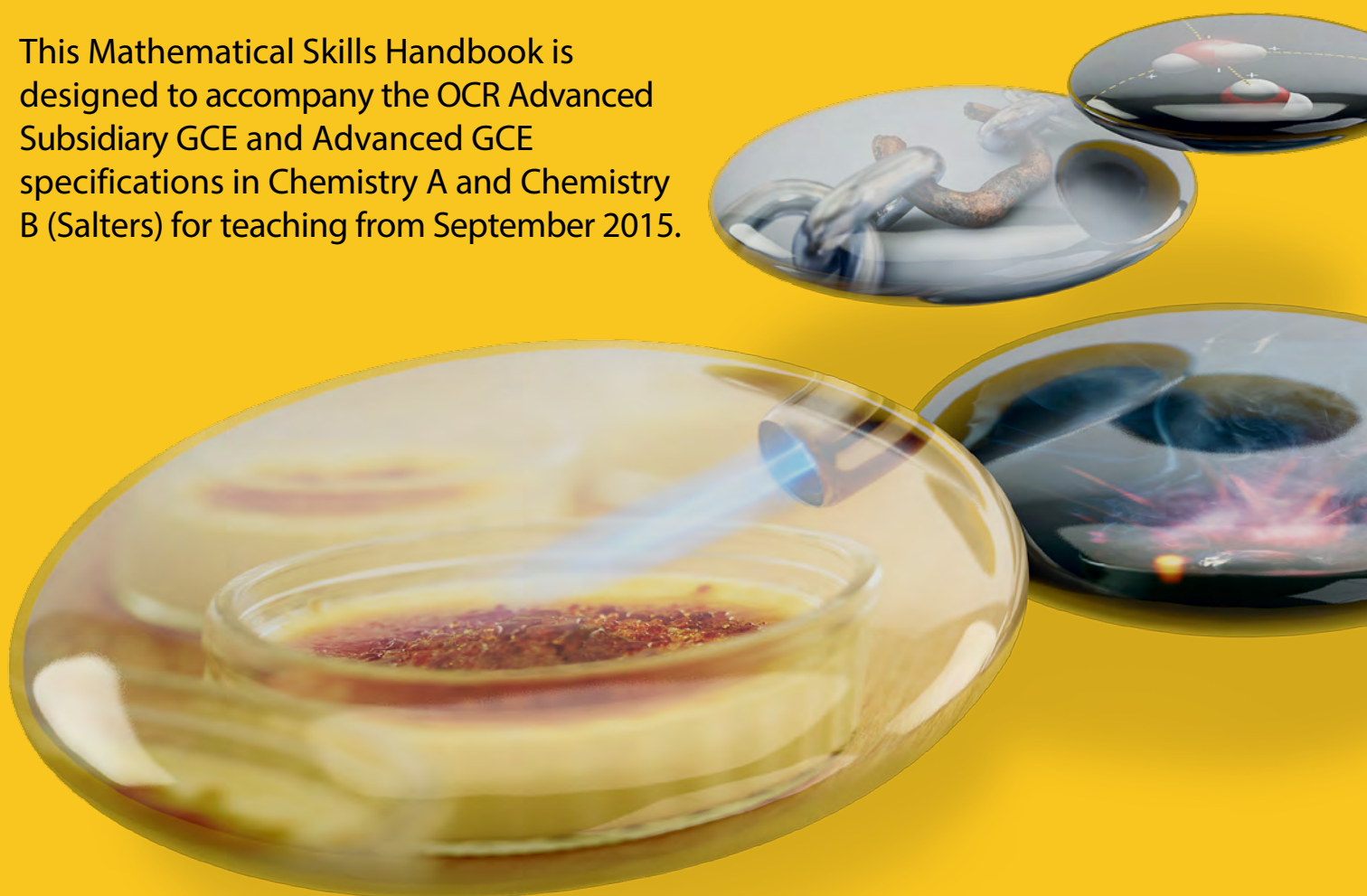
AS and A LEVEL

Mathematical Skills Handbook

CHEMISTRY A

CHEMISTRY B (SALTERS)

This Mathematical Skills Handbook is designed to accompany the OCR Advanced Subsidiary GCE and Advanced GCE specifications in Chemistry A and Chemistry B (Salters) for teaching from September 2015.



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Introduction

In order to be able to develop their skills, knowledge and understanding in A Level Chemistry, learners need to have been taught, and to have acquired competence in, the appropriate areas of mathematics relevant to the subject as indicated in Appendix 5e of the specification.

The assessment of quantitative skills will include at least 20% Level 2 (or above) mathematical skills for chemistry (see below for a definition of 'Level 2' mathematics). These skills will be applied in the context of the relevant chemistry.

This Handbook is intended as a resource for teachers to clarify the nature of the mathematical skills required by the specification, and indicate how each skill is relevant to the subject content of the specification.

The content of this Handbook follows the structure of the table in Appendix 5e of the specification, with each mathematical skill discussed in turn. The discussion of each skill begins with description and explanation of the mathematical concepts, followed by a demonstration of the key areas of the specification content in which the skill may be applied. For each skill, a number of examples are given of where the skill is used in the context of A Level Chemistry. These examples are not exhaustive; many skills may be used in a wide variety of contexts. Notes on common difficulties and misconceptions, as well as suggestions for teaching, may be included in either section as appropriate.

As this Handbook shows, all required mathematical skills can be covered along with the subject content in an integrated fashion. However, as assessment of the mathematical skills makes up a significant proportion of the overall assessment, OCR recommend that teachers aim to specifically assess learners' understanding and application of the mathematical concepts as a matter of course, in order to discover and address any difficulties that they may have. This is particularly relevant for learners who are not taking an A Level Mathematics qualification alongside A Level Chemistry.

Definition of Level 2 mathematics

Within A Level Chemistry, 20% of the marks available within written examinations will be for assessment of mathematics (in the context of chemistry) at a Level 2 standard, or higher. Lower level mathematical skills will still be assessed within examination papers, but will not count within the 20% weighting for chemistry.

The following will be counted as Level 2 (or higher) mathematics:

- application and understanding requiring choice of data or equation to be used
- problem solving involving use of mathematics from different areas of maths and decisions about direction to proceed
- questions involving use of A Level mathematical content (as of 2012) e.g. use of logarithmic equations.

The following will not be counted as Level 2 mathematics:

- simple substitution with little choice of equation or data and/or structured question formats using GCSE mathematics (based on 2012 GCSE mathematics content).

As lower level mathematical skills are assessed in addition to the 20% weighting for Level 2 and above, the overall assessment of mathematical skills will form greater than 20% of the assessment.

M0 – Arithmetic and numerical computation

M0.0 Recognise and make use of appropriate units in calculation

Learners should be able to:

- give measurements and results of calculations in the correct units
- convert between different units
- determine the units for particular constants.

Mathematical concepts

Units indicate what a given quantity is measured in. A measured quantity without units is meaningless, although note that there are some derived quantities in chemistry that do not have units, notably relative mass and pH.

At GCSE learners will have used various units of measurement and would be required to recognise appropriate units for common quantities. For example, whilst cm is appropriate for a length or distance, learners should be able to identify that cm^2 is used for area and cm^3 is used for volume. Learners will be expected to use this skill at AS and A Level as well.

Unit prefixes indicate particular multiples and fractions of units. A full list of SI unit prefixes is given in Table 1, with the prefixes that are most likely to be used within the A Level Chemistry course highlighted.

Table 1: SI unit prefixes

Factor	Name	Symbol	Factor	Name	Symbol
10^{24}	yotta	Y	10^{-1}	deci	d
10^{21}	zeta	Z	10^{-2}	centi	c
10^{18}	exa	E	10^{-3}	milli	m
10^{15}	peta	P	10^{-6}	micro	μ
10^{12}	tera	T	10^{-9}	nano	n
10^9	giga	G	10^{-12}	pico	p
10^6	mega	M	10^{-15}	femto	f
10^3	kilo	k	10^{-18}	atto	a
10^2	hecto	h	10^{-21}	zepto	z
10^1	deca	Da	10^{-24}	yocto	y

Learners would be expected to be able to convert between commonly encountered multiples without conversion 'facts' being given (e.g. $1 \text{ kg} = 10^3 \text{ g}$).

Converting between different multiples is a matter of multiplying by the appropriate factor. When converting a quantity q from a factor 10^a to a factor 10^b , the quantity needs to be multiplied by a factor 10^{a-b} .

For example, converting 7 mg (10^{-3} g) to kg (10^3 g) requires a multiplication by $10^{-3-3} = 10^{-6}$.
So, $7 \text{ mg} = 7 \times 10^{-6} \text{ kg}$.

In the AS and A Level assessments, candidates will be expected to be able to recognise and use compound units in the form mol dm^{-3} , rather than mol/dm^3 . This can be explained mathematically using the power laws (see Appendix A). The unit mol/dm^3 is another way of saying the unit is

$$\text{mol} \times \frac{1}{\text{dm}^3}$$

From the power laws

$$\frac{1}{x^3} = x^{-3}$$

and hence

$$\text{mol} \times \frac{1}{\text{dm}^3} = \text{mol} \times \text{dm}^{-3}$$

and hence the notation mol dm^{-3} .

Finding the units of a quantity may involve use of the power laws. Learners should be able to apply laws listed in Appendix A.

Within the OCR GCE Chemistry qualifications, learners will in general be expected to use and recognise standard SI units. For example, dm^3 is used rather than l (litre), although l and ml may be seen on glassware. Learners should be aware that

$$1 \text{ dm}^3 = 1 \text{ l}$$

$$1 \text{ cm}^3 = 1 \text{ ml}$$

$$1 \text{ dm}^3 = 10^3 \text{ cm}^3$$

The exception to use of SI units is the degree ($^\circ$) for angles, which is used in preference to the radian.

Note that kelvin (K) and degree Celsius ($^\circ\text{C}$) are both used for temperature. $\text{K} = 273 + ^\circ\text{C}$, and temperature differences are equivalent in both units.

While the pascal (Pa) is the SI – and therefore preferred – unit of pressure, the atmosphere (atm) is still in common usage and learners should be comfortable with both. Questions involving pressure calculations would usually involve all quantities expressed in the same unit.

The *Data Sheet* gives the conversion for 1 tonne to grams. Any other conversion to or from non-standard units that may be required in assessment would be provided in the question.

Contexts in chemistry

Amount of substance

Ensure that learners use the correct units for quantities associated with this topic. Correct use of units for amount of substance (mole, symbol 'mol') and molar mass (g mol^{-1}) can aid understanding of these often tricky concepts. Good understanding of units can in particular aid calculations, and removes the need to learn formulae such as $n = m / M$ (and its inversions) by rote. A learner who is aware of the units for amount of substance and molar mass can be shown how to deduce the calculation for a mass of substance.

For example, a question asks to give the mass in g of 0.48 mol Ca(OH)_2 . The molar mass of Ca(OH)_2 is 74.1 g mol^{-1} .

The data provided have the units mol and g mol⁻¹. To combine these units to give a value in g requires the calculation

$$\text{mol} \times \text{g mol}^{-1} = \text{g}$$

So $0.48 \text{ mol} \times 74.1 \text{ g mol}^{-1} = 36 \text{ g}$ (to 2 sig figs)

Once this principle is understood, it can be applied to any calculation. This method is ultimately more reliable and powerful than using formula triangles, which may be misremembered and can only be used for formulae that comprise three variables. A good understanding of units developed early on in the course will also stand learners in good stead for determining units of rate and equilibrium constants (see below), which is required at A Level.

Relative masses (isotopic, atomic, formula, molecular etc.) do not have units. For example, the relative atomic mass of magnesium is 24.3. This can cause confusion as the relative mass commonly has the same numerical value as the molar mass for a given species. This can lead learners to forget the units when using molar masses.

Learners will have to be able to interconvert between units for mass (e.g. g, kg and mg) and volume (cm³, dm³ and m³). Unit conversions may be required in order to express concentration correctly in mol dm⁻³, and will often play a part in ideal gas calculations.

Energetics

In enthalpy determination practicals, learners initially determine the energy given out or taken in in J, using $q = mc\Delta T$. This value is then used to calculate the enthalpy change for the reaction in kJ mol⁻¹. Learners must take care to convert between J and kJ in this calculation.

At A Level only, learners carry out calculations that combine entropy and enthalpy values. Here, they must be aware that entropy values are commonly given in J K⁻¹ mol⁻¹, while enthalpy values are commonly given in kJ mol⁻¹. Again, learners must take care to convert between the units.

Kinetics and equilibria

A Level candidates will be expected to be able to give correct units for rate constants and equilibrium constants. The units for these constants depend on the rate or equilibrium expression in question, as well as the units used to express reaction rate and concentration (rate is normally expressed in mol dm⁻³ s⁻¹ and concentration is normally expressed in mol dm⁻³).

The units for a rate constant can be determined by solving the rate equation for k (see Section M2.2), and substituting the units for the rate and concentration(s). The resulting expression then needs to be given in its simplest form, which may involve use of the power laws (see Appendix A).

For example, for the equation

$$\text{rate} = k[\text{A}]^2[\text{B}]$$

$$k = \frac{\text{rate}}{[\text{A}]^2[\text{B}]} = \frac{\text{mol dm}^{-3} \text{ s}^{-1}}{(\text{mol dm}^{-3})^2 (\text{mol dm}^{-3})}$$

To simplify the expression, the term 'mol dm⁻³' often cancels, as in

$$\begin{aligned} \frac{\cancel{\text{mol dm}^{-3}} \text{ s}^{-1}}{\text{mol}^2 \text{ dm}^{-6} \times \cancel{\text{mol dm}^{-3}}} &= \frac{\text{s}^{-1}}{\text{mol}^2 \text{ dm}^{-6}} \\ &= \text{dm}^6 \text{ mol}^{-2} \text{ s}^{-1} \quad \text{because } \frac{x^n}{x^m} = x^{n-m} \end{aligned}$$

Note that the convention in writing compound units is to put positive indices first.

Units for equilibrium constants can be determined in a similar way by substituting the units for concentration(s) into the equilibrium expression.

M0.1 Recognise and use expressions in decimal and ordinary form

Learners should be able to:

- use an appropriate number of decimal places in calculations
- perform calculations in standard and ordinary form
- convert between standard and decimal form, retaining significant figures.

Mathematical concepts

Decimal places in calculations

Measurements should be given to a number of decimal places appropriate to the apparatus (see Appendix 4 of the Practical Skills Handbook). When adding and subtracting measurements, the result should be quoted to the same number of decimal places. (Note that this is different from the rule used when combining different types of measurement, when the result of the calculation should be given to the lowest number of significant figures – see Section 1.1.)

For example:

$25.50\text{ }^{\circ}\text{C} - 8.30\text{ }^{\circ}\text{C} = 17.20\text{ }^{\circ}\text{C}$; answer given to the same number of decimal places (2), not lowest number of significant figures (3)

$5.458\text{ g} + 6.349\text{ g} = 11.807\text{ g}$; answer given to the same number of decimal places (3), not lowest number of significant figures (4)

Standard form

Standard form expresses a number as $a \times 10^b$, where $1 \leq a < 10$ and b is a $+/-$ integer.

For example

$$n(\text{NaCl}) = 6.559 \times 10^{-3} \text{ mol}$$

Some important constants in chemistry are either very large or very small. The standard form is a convenient way of expressing these numbers. Using standard form also reduces calculation errors.

Learners are expected to be able to recognise standard form and perform calculations with numbers given in standard form. Expression of final results in standard form is also required in some situations.

The following expressions for the amount of substance given above are *not acceptable*.

$$0.6559 \times 10^{-2} \text{ mol}$$

$$65.59 \times 10^{-4} \text{ mol}$$

These expressions are numerically equivalent to the standard form given above, but are not acceptable standard form.

The following equivalent expressions for the amount of substance are acceptable (unless a response in standard form is explicitly requested).

$$0.006559 \text{ mol}$$

$$6.559 \text{ mmol}$$

Whatever form numbers are given in, learners must use the appropriate number of decimal places or significant figures (as appropriate) in calculations. (A full treatment of significant figures is given in Section M1.1.) In the context of converting between standard and ordinary form, learners must appreciate that significant figures need to be retained. For example:

$$0.0050 \text{ mol dm}^{-3} = 5.0 \times 10^{-3} \text{ mol dm}^{-3}$$

Here the final zero in the expression on the left is a significant figure, and so must be retained in standard form. Situations such as the following are less clear cut:

$$14\,300 \text{ J} = 1.43(00) \times 10^4 \text{ J}$$

Here it is not clear whether the zeroes in the expression on the left are significant figures or not, though this would normally be clear from the context where conversion to standard form was required.

If a value such as 14 300 J emerges as the answer to a question where an appropriate number of significant figures is required, it may be safer to convert the answer to standard form (or in this case to kJ), so that it is unambiguous how many significant figures are being used.

Calculator use

Learners with access to a scientific calculator should be able to use it to convert between different decimal/standard form calculations, as well as enter numbers in standard form. Table 2 shows the required functions for common makes of calculator.

Table 2: Calculator functions for standard form

Calculator make	Convert decimal to standard	Enter numbers in standard form
Sharp	Change	EXP
Casio	S→D	$\times 10^x$

For other models encourage learners to investigate the appropriate functions for themselves.

It should be noted that calculators will not necessarily retain the correct number of decimal places required for the calculation. For example, 3.0×10^3 is correct to 2 significant figures, but once entered into a calculator the display could be 3×10^3 , which loses 1 significant figure.

Contexts in chemistry

There are a number of areas where learners will be required to recognise standard form. Use of standard form may on occasion be explicitly requested, and may sometimes be the most appropriate form to use for the answer – if it is a very big or small number, or to avoid ambiguity regarding the number of significant figures. This is may, for example, be relevant in any area of the specification that involves working with molar concentrations, the values for which are frequently much smaller than 1. A few representative examples of contexts are given below.

Measuring quantities by difference

This is the main area where learners need to consider the role of decimal places in addition and subtraction.

The most common quantities measured by difference in practical work are mass, temperature and volume (e.g. titres). The measurements made should be recorded to a specific number of decimal places, depending on the resolution of the instrument (see the Appendix 4 of the Practical Skills Handbook for more on this topic). When calculating the difference between the measurements, this number of decimal places should be maintained.

For example, a learner conducting an enthalpy investigation may record the following measurements:

initial temperature	22.5 °C
maximum temperature	29.5 °C
temperature difference	7.0 °C

The temperature difference is given to 1 decimal place, to match the resolution of the measured values. The '0' is significant, so must be included.

The Avogadro constant

Learners will have to use formulae involving the Avogadro constant, and use the constant to the appropriate number of significant figures. Note that the *Data Sheet* value of the constant is 6.02×10^{23} , i.e. to 3 significant figures.

Acids and bases

Appreciation of standard form is crucial in calculations involving concentrations of acids and bases and/or the ionic product of water, K_w .

Note that the *Data Sheet* value of K_w at 298 K is $1.00 \times 10^{-14} \text{ mol}^2 \text{ dm}^{-6}$, i.e. to 3 significant figures.

As an example, a learner may be asked to calculate the pH of water at body temperature (37 °C), given that K_w at that temperature is $2.38 \times 10^{-14} \text{ mol}^2 \text{ dm}^{-6}$:

$$K_w = [\text{H}^+][\text{OH}^-]$$

In water $[\text{H}^+] = [\text{OH}^-]$, so

$$K_w = [\text{H}^+]^2$$

$$[\text{H}^+] = \sqrt{2.38 \times 10^{-14}} = 1.57 \times 10^{-7} \text{ mol dm}^{-3}$$

M0.2 Use ratios, fractions and percentages

Learners should be able to:

- calculate a percentage of an amount
- use percentages in calculations to determine related quantities, such as reacting masses
- use ratios in calculations and to construct and balance equations.

Mathematical concepts

Ratios, fractions and percentages are related concepts. Many problems within chemistry will require learners to have a good understanding of the relationships between these concepts, and to use them in calculations.

The individual skills required will have been covered at GCSE, but they are used in new contexts here. While individual calculation steps based on ratio are not complicated – often requiring only a simple multiplication – they can easily be missed in multistep calculations.

'Percentage' means a 'number of parts per hundred'. As such, percentages are equivalent to fractions with the denominator 100:

$$10\% = \frac{10}{100} = \frac{1}{10}$$

In chemical contexts, percentages can often be thought of as a ratio. For example, in calculating the percentage yield for a reaction, the result tells us how the amount of product relates to the amount of reagent. If the yield is 27%, then the ratio of reactant to product is 100 : 27.

Learners will need to use the formula for calculating x as a percentage of y :

$$\text{percentage} = \frac{x}{y} \times 100\%$$

In some circumstances, this formula needs to be rearranged. For example, given that $x = 4.2$ and we know it is 38% of y , what is y ? This requires the formula in the arrangement:

$$y = \frac{100 \times 4.2}{38} = 11 \text{ (to 2 significant figures)}$$

Contexts in chemistry

Percentage yield and atom economy

Determination of % yield or atom economy requires a simple calculation of the form:

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

In more complex problems, the % yield may be given and used to calculate e.g. the required starting amount of a reactant.

These calculations are identical in form to the more general examples given above.

For %yield calculations the quantity used for the actual and theoretical yield can be (preferably) amount of substance, or mass, but it must be the same quantity for the two values. Problems in these calculations generally occur in the prior conversions to amount/mass rather than in the percentage calculation itself.

The form of the atom economy calculation is the same as for yield, but the quantity used is relative molecular mass. It is often quicker to divide the M_r of the useful product(s) by the total M_r of all products, rather than to calculate the total M_r of the reagents.

Percentage composition

Understanding of percentages and ratios are both required in percentage composition problems. These calculations usually follow a standard series of steps that learners often simply memorise; however, fully understanding the mathematical reasoning behind the process can help learners spot errors if they do occur, and tackle questions that approach the problem from an unfamiliar angle.

For example, an alkane is found to contain 82.8% by mass carbon, C, and 17.2% by mass hydrogen, H. To determine the formula of the alkane, the mathematical appreciation involved begins with the realisation that this effectively means that a 100 g sample of the alkane contains 82.8 g C and 17.2 g H.

Dividing these values by the relative atomic masses gives the amount of each element in the sample, and thus the molar ratio: 6.9 : 17.2 mol.

This ratio needs to be converted to a neater, whole number ratio to find the empirical formula. If both terms in a ratio are divided or multiplied by the same factor, the resulting ratio is equivalent to the original. In first instance, it is helpful to reduce the ratio so that the smallest term is 1, which is achieved by dividing both terms by the smallest term:

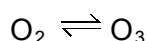
$$\frac{6.9}{6.9} : \frac{17.2}{6.9} \quad \therefore \quad 1 : 2.5$$

To turn 2.5 into a whole number requires multiplying by 2; this means the 1 must also be multiplied by 2 to maintain the ratio, giving C : H = 2 : 5, and an empirical formula of C₂H₅. In this case, the empirical formula is not an acceptable formula for an alkane, so the ratio must be multiplied again by an appropriate factor to achieve a molecular formula that fits the general formula for alkenes. In this case that is achieved by multiplying by 2 again, giving the formula C₄H₁₀.

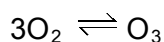
Balancing equations

Many methods for teaching balancing equations rely on mechanical technique that does not require understanding. Here, we present a way to demonstrate what is happening mathematically. The preferred approach is one where learners actually understand the processes and are left to develop their own techniques.

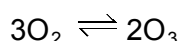
The key mathematical skill is understanding times tables and the use of common factors. Take for example the interconversion of molecular oxygen and ozone:



There are 2 atoms of oxygen on the left hand side, and 3 on the right. Mathematically speaking 2 and 3 are *coprime* (that is, their only common factor is 1). One side has to be adapted first to ensure that the numbers are not coprime. For example, if we multiply the left hand side of the equation with 2 atoms on by 3, there are now 6 atoms on the left and still 3 atoms on the left.



6 and 3 are not coprime, they have the common factor 3. The right hand side needs to be multiplied by 2 to get 6. The final equation is:

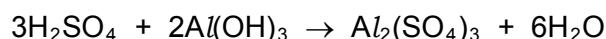


This type of proportional is taught for some from primary school but remains a very difficult concept to master for a lot of learners, especially those not taking mathematics at A level. A key approach is to talk through the problem in words. For example encourage learners to say to themselves: "What number multiplies 2 to 7?" "Err... there isn't one." "So, what if we multiply 7 by 2 and use 14 instead? Now what number multiplies 2 to 14?" "Ahh, that's 7...."

Whilst this approach may seem 'ad-hoc' it encourages learners to actually understand the processes rather than just following a set technique which relies little on mathematical understanding.

Amount of substance calculations

The ratios expressed in reaction equations are crucial in correctly navigating problems that relate to reacting masses. Learners need to understand what the numbers in a reaction equation mean. For example, the equation



Tells us that 3 mol sulfuric acid react with 2 mol aluminium hydroxide to produce 1 mol Al₂(SO₄)₃. If we have n mol Al(OH)₃, the minimum amount of H₂SO₄ required to fully react is $\frac{3}{2} \times n$, and the amount of Al₂(SO₄)₃ produced is $\frac{1}{2} \times n$.

Using these chemical ratios in calculations is normally mathematically straightforward, but it is a common error to forget this step.

M0.3 Estimate Results

Learners should be able to:

- make estimates of quantities by comparing to known reference values
- evaluate the effect of changing experimental parameters on measurable values.

Mathematical concepts

Estimating

Estimating is a valuable skill; if you are able to estimate an approximate answer to a calculation, it is easier to spot if you have made a mistake in carrying out the actual calculation. For example the calculation:

$$4.9/1.10$$

could be estimated as

$$5/1 = 5$$

This quick check can validate a learner's calculated answer of 4.45. However, if the calculation gives an answer of 0.45, the estimate will help to realise that a decimal point error has been made.

Estimating becomes easier if learners are familiar with the types of answers that are typical for a particular situation. Volumes, for example, can be hard to visualise. However, if learners understand that the molar gas volume (24.0 dm^3 at room temperature and pressure) is about the size of a decent-sized rucksack, this can be applied in estimates in calculations. Apparatus used to collect gas in a laboratory experiment is much smaller than this volume, so a calculation of the amount of gas should produce a number much smaller than 1 mol.

The effect of changing parameters

In investigating the effects different parameters have on outputs a good knowledge of the rules of mathematics is required. For example, take the fictional formula:

$$A = \frac{XY}{Z \times T^3}$$

The value of A will change as the variables in the formula are increased or decreased. The following rules are useful:

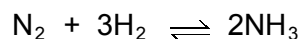
- The larger the numerator (value above the line), the larger the output. So, if either X or Y increases, A will increase.
- The larger the denominator (value below the line), the smaller the output. So, if either Z or T increases, A will decrease.
- The reverse is true in each case.

So in summary: A changes in the same direction as variables above the line, and in the opposite direction as variables below the line.

Contexts in chemistry

Equilibrium constants

Learners need to be able to estimate the effect of changing concentrations on the position of the equilibrium, knowing that the value of K_c stays the same. This depends on learners knowing how to construct the expression for K_c , e.g. for the equation:



$$K_c = \frac{[\text{NH}_3]^2}{[\text{N}_2][\text{H}_2]^3}$$

This expression is mathematically identical to the fictional formula for A given above.

If ammonia is removed from the reaction vessel, its concentration becomes smaller and thus the numerator decreases. This would cause the value for K_c to decrease, but the value for K_c must stay the same. Therefore, the system must shift to increase the numerator and decrease the denominator, to restore the value of K_c : the position of the equilibrium shifts to the right.

This can be distilled into general principles regarding the effects of changing concentrations, but learners must be able to explain shifts in equilibrium in terms of the effect of K_c .

M0.4 Use a calculator to use power, exponential and logarithm functions

Mathematical concepts

Learners should be able to:

- use a calculator to perform calculations involving powers of numbers, exponentials and logarithms.

The learners in your class will potentially own a wide range of calculator models, with different ways of entering and using powers. Symbols used include ' x^y ', ' 10^x ', ' $^{\wedge}$ ' and ' exp '. It is worth taking the time to become familiar with the different models used in your class, and that learners understand how to use these functions correctly. Also make sure they understand the different operations for e.g.:

$$3.6^3$$

and 3.6×10^3

A Level learners will need to use logarithm and inverse logarithm operations for base 10 and base e. To take the logarithm, the calculator button is usually ' $\log$ ' for base 10 logarithms, and ' $\ln$ ' for base e logarithms (natural logarithms).

To perform the inverse operation, some calculators use the ' inverse ' or ' shift ' operation combined with the ' $\log$ ' or ' $\ln$ ' key as required. Other calculators have separate functions for the inverse operations, which are ' 10^x ' for the inverse of a base 10 log, and ' e^x ' for the inverse of a natural log.

Contexts in chemistry

pH

pH uses a scale of log to base 10. The equation for calculating pH is

$$\text{pH} = -\log[\text{H}^+]$$

The pH of a solution is found applying the ' $\log$ ' function to the value for $[\text{H}^+]$.

The inverse formula is used to calculate $[H^+]$ from pH:

$$[H^+] = 10^{-\text{pH}}$$

$[H^+]$ is found by applying 'inverse + log', 'shift + log' or ' 10^x ' to the pH.

The Arrhenius equation

The Arrhenius equation expresses the exponential relationship between the rate constant, k , and the temperature, T :

$$k = Ae^{-E_a/RT}$$

To find k , the other quantities are simply substituted into the formula. Learners must calculate the coefficient $-E_a/RT$ first, apply the ' e^x ' function (or 'inverse/shift + ln'), and then multiply the result by the value for A .

The equation can be rearranged to produce a linear relationship:

$$\ln k = -E_a/RT + \ln A$$

The linear relationship is used to plot experimentally determined values for the rate constant against temperature, as $\ln k$ against $1/T$. See Section 3 for more detail on graphs.

Learners need to be able to determine the value of the pre-exponential factor A from such a graph. This involves reading the value of $\ln k$ at the y -axis intercept, or determining the intercept mathematically (see Section M3.3); this value is equal to $\ln A$. To determine the value for A , learners use ' e^x ' or 'inverse/shift + ln'.

M1 – Handling data

M1.1 Use an appropriate amount of significant figures

Learners should be able to:

- round to a given number of significant figures or decimal places
- report calculations to an appropriate number of significant figures
- understand that calculated results can only be reported to the limits of the measurement with the lowest resolution.

Mathematical concepts

Learners must understand that the lowest level of significant figures in the raw data provided for a calculation will determine the number of significant figures that should be given in the final answer. If there are 3 inputs to a particular calculation and they are quoted as being correct to 2, 3 and 4 significant figures, then the answer can only be quoted reliably correct to 2 significant figures. (Note though that if the calculation only involves addition and subtraction, decimal places should be taken into account rather than significant figures – see Section M0.1.)

In multi-step calculations, the results of intermediate steps should *not* be rounded. Unrounded intermediate values should be kept in the calculator, and rounding only performed after the final step.

Common rounding errors include:

- Forgetting to include zeroes where they are significant figures, rather than placeholders. For example, 4.99×10^5 rounded to 2 significant figures is 5.0×10^5 , not 5×10^5
- Confusing significant figures with decimal places. For example, giving an answer as 2.48 (2 decimal places) rather than 2.5 (2 significant figures).
- Rounding sequentially; for example rounding 2.4478 first to 2.45 and then to 2.5. This is incorrect; the number should be rounded in a single step, giving 2.4 to 2 significant figures.

The number of significant figures used to express particular values ultimately derives from the resolution of the measuring apparatus used to determine experimental values. See the Appendix 4 in the Practical Skills Handbook for more on this topic, including the appropriate number of decimal places to use for certain apparatus.

'Exact' numbers in calculations have no impact on the number of significant figures required in the results. Examples of exact numbers in chemistry include balancing numbers in equations.

Contexts in chemistry

Thinking about significant figures is important in any calculation, and learners should be particularly aware of the meaning of significant figures when performing calculations using experimentally determined values. A few representative examples of contexts are presented here.

Titration

In titrations, apparatus with high resolution are used throughout. This should be reflected in the number of significant figures used in the final answer. Rounding the final answer to a small number of significant figures defeats the object of performing a titration.

As an example: 25.00 cm^3 of an unknown solution of potassium carbonate (K_2CO_3) is titrated with $0.100 \text{ mol dm}^{-3} \text{ HCl}$. The titre is 22.70 cm^3 .

According to the data provided, the result of the calculation can be given to 3 significant figures. If asked to give the concentration of the potassium carbonate solution, the answer should be given as $0.0454 \text{ mol dm}^{-3}$.

Note that if the intermediate value for the amount of K_2CO_3 is rounded to 3 significant figures, the final calculated value is $0.0456 \text{ mol dm}^{-3}$. Thus, rounding in intermediate steps introduces an error. Rounding to the appropriate number of significant figures should only be done after the final step in the calculation.

Enthalpy determinations

This is a context where learners should take care – partially because the appropriate number of significant figures may be lower than expected (3 significant figures can become the ‘default’ for some learners), and partially because final answers expressed in joules can be very large. In order to avoid the ambiguity of whether zeroes are significant or not, it may be better to use standard form or convert to kJ.

The limiting values here would normally either be the volume of liquid or the temperature rise. If a temperature rise of less than 10°C is observed, using a thermometer with a resolution of 0.5°C , then the result of the final calculation can only be given to 2 significant figures.

M1.2 Find arithmetic means

Learners should be able to:

- find the arithmetic mean of a set of data in a list and in a table
- calculate weighted means
- understand the role outliers can have in a mean calculation and treat them accordingly.

Mathematical concepts

Means and weighted means

The mean is calculated using a simple formula:

$$\text{mean} = \frac{\sum x}{n}$$

where $\sum x$ is the sum of the data values and n is the number of data values.

Most learners will be familiar with this from GCSE and it is best taught as a rather ad-hoc message: ‘add them all up, divide by how many’. There are few misconceptions with this when dealing with raw, listed data as the calculations involved are quite simple.

However, the concept of weighted means is a little more tricky, as the values to be added up are not treated equally. Weighted means can be introduced starting from the regular mean calculation. For example, the mean of the values 2, 4, 4, 6 is calculated as

$$\frac{2 + 4 + 4 + 6}{4} = 4$$

This could also be written as

$$\frac{1}{4} \times 2 + \frac{1}{4} \times 4 + \frac{1}{4} \times 4 + \frac{1}{4} \times 6 = 4$$

which shows that each value has an equal weighting of 1/4, or 0.25. The total weight in the calculation must always be 1. The expression can be simplified to:

$$0.25 \times 2 + 0.5 \times 4 + 0.25 \times 6 = 4$$

What we have now is a *weighted* mean. The calculation produces the mean of the values of 2, 4 and 6, where the value of 4 is given twice as much weight as the other two values.

Weighted means are mainly used in chemistry when we know the percentage distribution of values. The above calculation would be applied to find the mean of a data set in which 25% of the values are 2, 50% are 4, and 25% are 6. The main application is in finding the atomic mass of an element based on isotopic abundances – see example below.

Outliers and selecting data

When treating experimental data, for example in recording the mean value of a number of measurements, learners must be able to identify outliers and decide whether exclude them from the calculation. It should be emphasised that there is no hard and fast rule on how to deal with outliers; they should be treated case by case. The detail of the mathematics involved to identify outliers goes way beyond the scope of A level Chemistry.

For experiments a simple checklist is this:

- was the suspected outlier recorded in error?
- was the suspected outlier recorded in different conditions to the other values?

If the answer to any of these questions is yes, then the outlier should be omitted from the data set and the mean should be calculated without this value. If a potential outlier is spotted at the time of the experiment then learners should question whether the experiment should be repeated.

For standard measurements, in particular titration data, common conventions are used to determine the measurements that should be used to calculate the mean experimental value – see example below.

Calculator use

Many different scientific calculators have a Statistics mode where the mean can be calculated automatically; learners studying A Level Biology may have been introduced to this mode. Whilst these functions are incredibly useful to gain full summary statistics (standard deviation, sum of squares, correlation coefficients etc.) the computational advantage of doing this for just the mean is nil. Learners can use this mode but will have to press just as many buttons and therefore have the same risk for error as if they perform the addition and division manually.

Contexts in chemistry

Calculating relative atomic mass

The relative atomic mass (A_r) of an element is calculated by finding the weighted mean of the relative isotopic masses. The weightings applied to each mass are determined by the isotopic abundances. The more there is of a particular isotope, the more its mass contributes to the final mean.

For example, the relative masses and abundances for the isotopes in a sample of bromine are given as

Isotopic mass	% abundance
85	72.17
87	27.83

Then

$$A_r = 85 \times \frac{72.17}{100} + 87 \times \frac{27.83}{100} = 85.56$$

Examples like this could be used to demonstrate the effect of using a weighted mean. If a simple mean of the two mass values were calculated, the result would be 86.

Note that the learners may have to extract the isotopic mass and % abundance values from mass spectra.

Calculating a mean titre

Calculating a mean titre may involve selecting the appropriate data to use in the calculation. Titration experiments should be repeated until results are found that are *concordant*, or roughly in agreement. Titres are considered concordant when they are within 0.1 cm³ of each other. If this cannot be achieved, the closest available values should be used to calculate the mean.

During a titration it is useful for learners to complete a results table such as this one:

	Trial	1 st run	2 nd run	3 rd run
Final reading / cm ³	22.90	45.40	43.05	22.55
Initial reading / cm ³	0.00	22.90	20.95	0.00
Titre	22.90	22.50	22.10	22.55

Looking at the titres, the 1st and 3rd runs are concordant, while the 2nd is 'out'. The mean titre is therefore

$$\frac{22.50 + 22.55}{2} = 22.525 \text{ cm}^3$$

N.B. This unrounded value for the mean titre should be used in further calculations.

M1.3 Identify uncertainties in measurements and use simple techniques to determine uncertainty when data are combined

Learners should be able to:

- appreciate that uncertainties exist when taking measurements
- determine absolute and relative uncertainties
- determine the uncertainty in the final value when adding or subtracting readings.

Mathematical concepts

When a measurement is taken there will always exist uncertainty regarding the true value. For example, the uncertainty in a Class B 250 cm³ volumetric flask is 0.2 cm³. This means that the actual volume measured with such a flask is somewhere between 249.8 cm³ and 250.2 cm³.

This uncertainty of 0.2 cm³ is the *absolute* uncertainty. The *relative* uncertainty is the ratio of the absolute uncertainty to the original measurement. In the case of the flask already described:

$$\frac{0.2}{250} \times 100\% = 0.08\%$$

When measurements are added or subtracted, the absolute uncertainties must be added to give the uncertainty in the combined measurement. For example, a thermometer graduated in divisions of 1 °C has an uncertainty of 0.5 °C in each measurement. The uncertainty in a temperature change, calculated from two measurements, is

$$0.5\text{ °C} + 0.5\text{ °C} = 1.0\text{ °C}$$

Say a temperature change is measured from a room temperature measurement of 21.0 °C to a maximum temperature of 67.5 °C, then the relative uncertainty is

$$\frac{1.0}{46.5} \times 100\% = 2.2\%$$

In general, the formula for calculating the relative uncertainty in a value calculated by difference is

$$\% \text{ uncertainty} = \frac{2 \times \text{absolute uncertainty}}{\text{quantity measured}} \times 100\%$$

In GCE Chemistry, learners do not need to be able to combine uncertainties in more complex operations, such as when multiplying or dividing.

Contexts in chemistry

The above principles explained through the example of volume and temperature measurements can be applied to any experimental results. Another example is provided taking the titration results used in Section M1.2.

The absolute uncertainty for a burette reading is $\pm 0.05\text{ cm}^3$. Therefore, the % uncertainty for the titre in the 3rd run is

$$\frac{2 \times 0.05}{22.55} \times 100\% = 0.4\%$$

M2 – Algebra

M2.1 Understand and use the symbols =, <, <<, >>, >, ∞, ~, ⇌

Learners should be able to:

- use these symbols appropriately and correctly in their given contexts
- understand these symbols in the contexts of formulae given.

Mathematical concepts

Learners should have had exposure to the symbols =, <, <<, >> and > from an early age, and should understand how and why they are used.

The symbol ∞ means 'is proportional to'. If two quantities *A* and *B* are *directly proportional* then the appropriate mathematical statement is

$$A \propto B$$

If the two quantities are *inversely proportional* then the appropriate relationship is:

$$A \propto \frac{1}{B}$$

The symbol ~ means 'is roughly equal to' or 'of the same order'. This symbol may be used in the context of approximations made in calculations of quantities, to indicate that a formula in which an approximation has been applied is 'roughly equal to' the original formula. For example in the expression for the dissociation constant of a weak acid:

$$K_a = \frac{[\text{H}^+(\text{aq})]^2}{[\text{HA}(\text{aq})] - [\text{H}^+(\text{aq})]} \sim \frac{[\text{H}^+(\text{aq})]^2}{[\text{HA}(\text{aq})]}$$

Here the approximation is that only a small proportion of HA dissociates, and therefore the concentration of H^+ produced is negligible in the denominator. The symbol ~ indicates that the expression following the approximation is roughly equal to the original expression.

The symbol ⇌ has a chemical rather than mathematical meaning, and is used in reaction equations to indicate that both forward and reverse reactions are occurring in a system.

Learners will be required to understand and use these symbols as they arise in various contexts. The more important aspect here is that learners *understand* the symbols when they are used; when answering questions learners are most likely to use = and ⇌ themselves. When describing mathematical relationships, learners would often be able to use descriptions in place of the symbols, for example stating that one constant is directly proportional to another rather than giving the formal mathematical statement. Conversely, learners might prefer to use symbols rather than descriptions for reasons of brevity. This is fine, but learners must be sure to use the correct symbol.

Contexts in chemistry

Equilibrium

The symbols $<$, $<<$, $>>$ and $>$ are used to describe the meaning of the value of the equilibrium constant, K_c :

- $K_c > 1$ means that the position of the equilibrium lies towards the products
- $K_c >> 1$ (of the order 10^{10}) means that the equilibrium lies fully on the side of the products – the reaction proceeds to completion
- $K_c < 1$ means that the position of the equilibrium lies towards the reactants
- $K_c << 1$ (of the order 10^{-10}) means that the equilibrium lies fully on the side of the reactants – no reaction takes place.

Note that the definitions involving $>>$ and $<<$ are only formally required in the Chemistry B (Salters) specification, not in Chemistry A.

Learners will need to be able to correctly interpret standard form (see Section M0.1) in this context. For example, they will need to understand the difference between 5.6×10^{-8} and 5.6×10^8 in terms of the sizes of these numbers.

Acids and bases

As noted above, the symbol $\sim$ is frequently used in this topic to indicate approximations made in weak acid calculations. $<<$ and $>>$ may also be used in this context. For example, the approximation

$$K_a = \frac{[\text{H}^+(\text{aq})]^2}{[\text{HA}(\text{aq})] - [\text{H}^+(\text{aq})]} \sim \frac{[\text{H}^+(\text{aq})]^2}{[\text{HA}(\text{aq})]}$$

can be made because $[\text{HA}(\text{aq})] >> [\text{H}^+(\text{aq})]$.

Rates

This is the main context in which learners may encounter the symbol $\propto$, in expressions for the order of reaction. For example

$$\text{rate} \propto [\text{A}]^2$$

means that the rate of reaction is proportional to the square of the concentration of A. In other words, the reaction is second order with respect to [A].

M2.2 Change the subject of the equation

Learners should be able to:

- rearrange an equation to change the subject.

Mathematical concepts

The most common equations to be rearranged can often be posed in the form of a formula triangle. This is where three quantities a , b and c are linked by the simple relationship:

$$a = bc$$

This is quite an easy equation to arrange for the other variables. For example dividing by b yields the formula for c :

$$c = \frac{a}{b}$$

whilst dividing by c will give the formula for b :

$$b = \frac{a}{c}$$

This mathematical principle should be familiar to learners. However, even learners who are comfortable with this area of mathematics may struggle with its application in the science classroom, because the equations are not presented in a familiar way. Learners may need help to see that e.g.

$$\text{mass} = \text{amount of substance} \times \text{molar mass} \quad (m = nM)$$

is equivalent to

$$a = bc$$

and

$$\ln k = -E_a/RT + \ln A$$

is equivalent to

$$y = ax + b$$

You may wish to discuss this application of algebra with maths teachers in your school, to ensure you can approach this skill in a way that help learners to make links between use of equations in science and what they have previously learnt in maths.

Contexts in chemistry

Amount of substance calculations

This is the area where learners will most frequently be required to use equations in different arrangements. Key equations that learners need to be able to manipulate include:

$$\text{amount of substance} = \frac{\text{mass}}{\text{molar mass}} \quad \left(n = \frac{m}{M}\right)$$

$$\text{amount of substance} = \frac{\text{volume}}{\text{molar gas volume}} \quad \left(n = \frac{V}{24.0}\right)$$

$$\text{amount of substance} = \text{concentration} \times \text{volume} \quad (n = cV)$$

$$\text{the ideal gas equation} \quad (pV = nRT)$$

Note that units are important in the application of these equations, in particular for volume. In $n = cV$ the volume takes units dm^3 , as the concentration will take units mol dm^{-3} . In the ideal gas equation, the volume takes units m^3 .

Longer, unstructured calculations may require using one or more of these equations multiple times, in different arrangements.

Learners who are able to grasp the mathematical principle of rearranging equations in this early stage of the course, as opposed to learning the different arrangements of each equation individually, will be able to apply this skill more confidently in other areas.

Rate equations

Rate equations take the form e.g.

$$\text{rate} = k[A]^x[B]^y$$

Calculation of the rate constant from rate and concentration data requires straightforward rearrangement by dividing by $[A]^x[B]^y$:

$$k = \frac{\text{rate}}{[A]^x[B]^y}$$

This is in effect the same operation as rearranging $a = bc$ to $b = a/c$, but many learners will need help spotting this.

The Arrhenius equation

Learners need to be able to determine the activation energy of a reaction from the gradient of a graph of $\ln k$ against $1/T$. The value of the gradient is equal to $-E_a/R$. Rearranging this give the expression for the activation energy:

$$E_a = -R \times \text{gradient}$$

The Arrhenius equation is provided on the *Data Sheet* in its exponential and linear form, and learners are not expected to be able to convert between the two. Indeed, the rearrangement – involving the use of natural logarithms – may be beyond learners not taking mathematics at A Level. The conversion is provided in Appendix B for reference, and could be used as a demonstration of principle, or for practise of rearranging skills, for more able learners.

M2.3 Substitute numerical values into algebraic equations using appropriate units for physical quantities

Learners should be able to

- substitute values into an expression to calculate a quantity from a formula.

Mathematical concepts

Learners should be aware of the principles from GCSE Mathematics but a few misconceptions may remain. The most common problem is their dealing with indices and negative quantities in formulae.

The expression x^2 , whilst innocuous enough, can cause issues when a negative number is substituted. Substituting $x = -2$ for example should be calculated as

$$(-2)^2 = 4$$

not

$$-2^2 = -4$$

There could be lots of confusion when substituting numbers of different signs.

The expression ‘two negatives make a positive’ is often over-used. Now it is *a/ways* true that two negatives multiplied/divided equal a positive, so

$$-3 \times -5 = +15$$

whilst if only one of them is negative then the answer is negative

$$2 \times -3 = -6$$

The over-use of this rule arises when addition is involved. For example:

$$-3 + -5$$

Learners could think that because there are two negatives being added then they become positive and the answer is

$$3 + 5 = 8$$

Actually for addition the changes occur only when the signs are the same in the 'middle' of the sum. In the above sum one of the signs in the 'middle' is negative so it becomes negative. So the above example should actually be read as '-3 minus 5' which is -8. However, in the formula:

$$-3 - -5$$

Here there are two negatives in the 'middle' and there it becomes a plus. Hence the sum is '-3 plus 5' which is +2.

Additionally, in the context of a formula such as $n = cV$ learners should be aware that the concentration is being *multiplied* to the volume despite the absence of a multiplication sign.

In general the laws of BIDMAS should be adhered to where the operations should be completed in the order of Brackets, Indices, Division & Multiplication, Addition & Subtraction.

Contexts in chemistry

Enthalpy change calculations

This topic shows up a number of errors that may occur in substituting values into equations.

Hess' law states that the total enthalpy change for a reaction is the same regardless of the route taken. If route 1 involves a single reaction with enthalpy change A , and route 2 involves two reactions with enthalpy changes B and C , then according to Hess' law:

$$A = B + C$$

Substitution of enthalpy values into this type of equation is ostensibly straightforward, and the mathematical steps involved are simple addition and subtraction, with some multiplication to take into account the stoichiometry of the reaction. Errors may occur in particular in dealing with the negative values.

Another form of enthalpy change calculation that is encountered early in the course is substituting experimental values into the equation $q = mc\Delta T$

This substitution is generally straightforward, though learners need to recognise that the value calculated from this expression has the unit J, and further operations are needed to determine a kJ mol^{-1} value for the reaction under investigation. See Section M0.0 for more about converting units.

Rate and equilibrium calculations

Calculations in these areas involve substituting values into rate equations and equilibrium constant expressions. This is largely a case of inserting the correct concentration values into the expression. Learners should take care if the concentration values used are in standard form, and if indices are present in the expressions – errors can easily be made when inputting these calculations into a calculator.

A worked example of a calculation of a rate constant is given in Section M2.4.

M2.4 Solve algebraic equations

Learners should be able to:

- solve algebraic equations.

Mathematical concepts

Solving an equation usually involves substituting values into a formula and realising that there is one unknown unaccounted for. Finding the value of this unknown is the same as solving the equation.

In order to calculate the unknown, it may be necessary to first rearrange the equation. Skills M2.2 and M2.3 are therefore often also needed in solving equations; indeed, the three skills are rarely encountered in isolation.

Take for example the formula:

$$E = U + pV$$

If we were to substitute some values in for E , U and p , the formula becomes an equation for V ; the only variable that remains unknown:

$$7 = 2 + 3V$$

To find V we have to 'unlock' what is happening to V . By this we mean we have to 'undo' the operations that link V to the other numbers. First we subtract the 2 from both sides to get the $3V$ by 'itself':

$$5 = 3V$$

To 'undo' the multiplication by 3 we divide by 3 and solve the equation:

$$V = \frac{5}{3} = 1.6666\ldots$$

Contexts in chemistry

Rate equations

The rate equation for the reaction between hydrogen and nitrogen monoxide is

$$\text{rate} = k[\text{H}_2(\text{g})][\text{NO}(\text{g})]^2$$

Calculation of the rate constant from given data involves rearranging the equation as described in Section M2.2, allowing the equation to be solved for k :

$$k = \frac{\text{rate}}{[\text{H}_2(\text{g})][\text{NO}(\text{g})]^2}$$

Given data can then be substituted into the expression, e.g.:

$$k = \frac{4.0 \times 10^{-3}}{3.0 \times 10^{-3} \times (4.0 \times 10^{-3})^2}$$

Many learners will reach for their calculators at this point, but note that the values are simple enough that much work can be done without the calculator. The term 4.0×10^{-3} appears in both numerator and denominator, and can be cancelled:

$$k = \frac{1}{3.0 \times 10^{-3} \times 4.0 \times 10^{-3}}$$

The terms in the denominator can now be collected using the multiplicative rule:

$$k = \frac{1}{1.2 \times 10^{-5}}$$

This can sometimes be a more reliable way of proceeding (as long as learners are fluent in power laws) than entering the entire expression into a calculator, as input errors are easily made.

The final division gives

$$k = 8.3 \times 10^4 \text{ dm}^6 \text{ mol}^{-2} \text{ s}^{-1} \text{ (to two significant figures)}$$

M2.5 Use logarithms in context with quantities that range over several orders of magnitude

Learners should be able to:

- perform calculations involving logarithms

Mathematical concepts

Logarithms are basically powers. If we take the following calculation:

$$10^2 = 100$$

this can be expressed as

the power of 10 that gives 100 is 2

or in formal notation

$$\log_{10} 100 = 2$$

and we usually drop the 10 as it is assumed to be base 10 unless stated otherwise:

$$\log 100 = 2$$

Logarithms provide a better scale when dealing with quantities that vary exponentially (get big/small very quickly). For example, imagine sketching a graph where the scale goes from 10, 100, 1000, 10 000, 100 000 and so on. This would be impossible to do on a standard graph. Taking the logarithms of these quantities gives 1, 2, 3, 4, 5, which is far more manageable to handle and to spot trends.

The natural logarithm is denoted by $\ln x$, which is shorthand for $\log_e x$. Here e is the mathematical constant approximately equal to 2.7182818. This number is of central importance in mathematics, and often occurs in situations where quantities change exponentially over time. Like π , which learners should be aware of, it is an irrational number, meaning it cannot be represented as a repeating decimal.

A note on significant figures

In numbers expressed as logarithms, the whole number represents the power of 10, and the decimal represents the value. So e.g. in the logarithmic number

$$2.86$$

the '2' represents the power of 10, and '.86' is the actual value. The whole number is thus *not* significant; the number above is given to 2 significant figures, not 3.

Given the result of a pH calculation

2.44977...

where the lowest number of significant figures in the data provided was 3, the final answer should be given as

2.450 (3 significant figures)

Contexts in chemistry

pH calculations

Logarithms are required in calculating the pH of an acidic solution. For example, a solution with $[\text{H}^+] = 0.0025 \text{ mol dm}^{-3}$ has pH

$$-\log 0.0025 = 2.60$$

The Arrhenius equation

Expressed as a linear relationship, the Arrhenius equation takes the form

$$\ln k = -E_a/RT + \ln A$$

which allows a manageable graph to be drawn showing the relationship between the rate constant and the temperature (see Section M3.3).

Learners need to be able to convert data for k and T (whether provided or experimentally determined) into the appropriate format for drawing such a graph, which includes taking the natural logarithm of the k values.

The y-axis intercept of the graph is equal to $\ln A$. Taking the inverse log of this value gives the value for A , the pre-exponential factor.

M3 – Graphs

M3.1 Translate information between graphical, numerical and algebraic forms

Learners should be able to:

- read, interpret and analyse data from graphs and spectra
- understand the relationship between two variables depicted on a graph in certain situations.

Mathematical concepts

There are several situations in GCE Chemistry where data may be presented graphically. Learners should be familiar with the types of graphical representations used, the conventions for variables used on the graph axes, and how to interpret the information provided in the graph.

Learners will need to be able to read co-ordinates for points on graphs. For some types of spectra, it is only necessary to read the x-axis co-ordinate to find the position of a relevant peak. For many other graph types, learners need to be able to read both x- and y-co-ordinates.

In chemistry, learners do not need an elaborate understanding of how to convert graphs into algebraic equations, but there are a few instances where learners should be able to judge the relationship between the plotted variables from the shape of the graph.

The following general graphs are useful for learners to know and recognise:

A graph showing a horizontal line parallel to the x-axis shows that the variable plotted on the y-axis is independent of the variable plotted on the x-axis. In mathematical terms, this relationship can be expressed as

$$y \propto x^0$$

or

$$y = \text{constant}$$

Where the constant in question is given by the y-axis value of any point on the line.

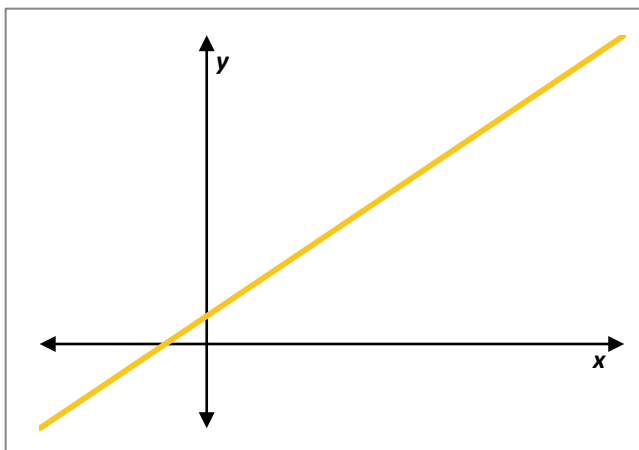
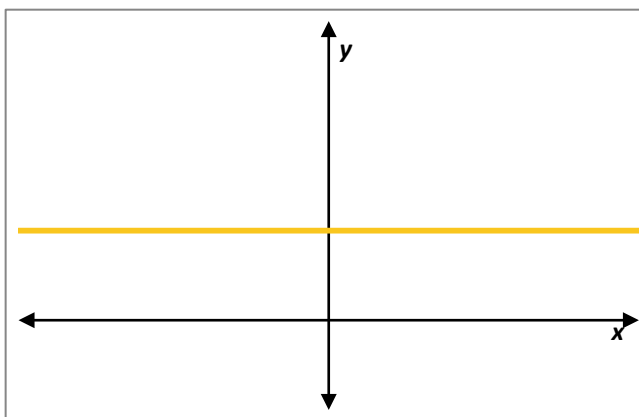
A non-horizontal straight line shows that the variable plotted on the y-axis is proportional to the variable plotted on the x-axis, or

$$y \propto x$$

In mathematical terms, this graph can be expressed as:

$$y = mx + c$$

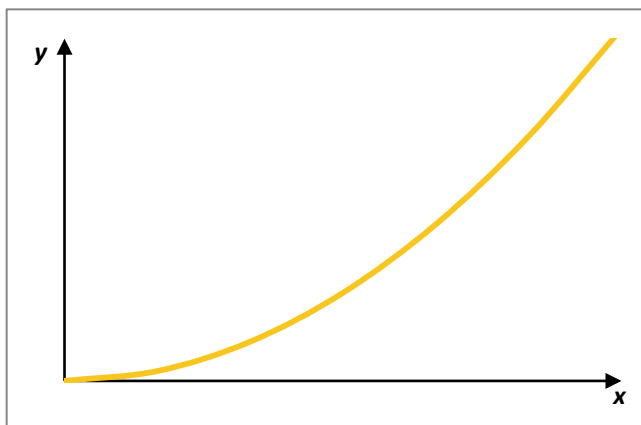
m is the gradient of the graph, and c is the value of the intercept on the y-axis.



A curved graph that passes through the origin indicates that the variable plotted on the y-axis is proportional to a power of the variable plotted on the x-axis that is greater than 1, or

$$y \propto x^n \text{ where } n > 1$$

Learners will not be required to determine the exact mathematical relationship of such graphs.



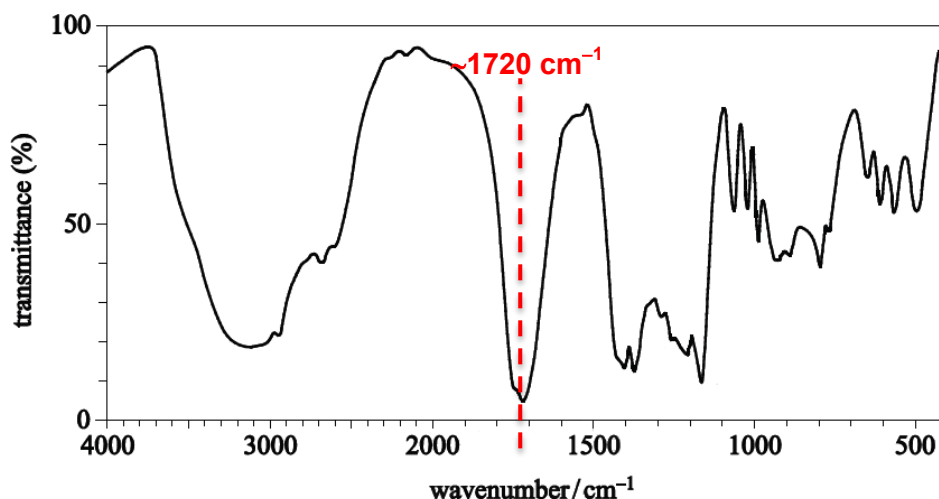
Contexts in chemistry

Interpreting and analysing spectra

Learners are expected to be able to interpret the information presented in mass, IR and NMR spectra.

IR spectra

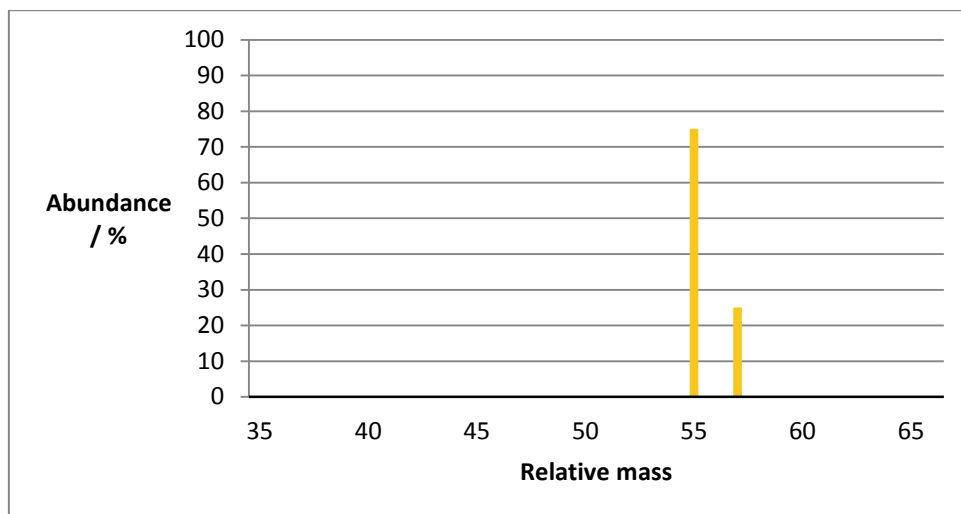
In IR spectra, learners must identify the position of peaks in the spectrum on the horizontal axis, and understand the significance of the presence or absence of peaks at certain values (using values provided e.g. in the *Data Sheet*). For example, the IR spectrum below has a peak at about 1720 cm^{-1} , which is a characteristic absorption for a C=O bond, indicating that the molecule under analysis contains a carbonyl group.



Note that the horizontal axis of IR spectra is non-standard. As in this example, the scale runs in the 'opposite' direction, from high to low. It is easy to get confused and think that a value to the right of '2000' on the scale will be a larger number. Also, the region between 4000 and 2000 cm^{-1} is more condensed than the region between 2000 and 500 cm^{-1} .

Mass spectra

In mass spectra, learners may have to identify the position of a peak on both the horizontal and vertical axes. For example, in using mass spectral data to calculate the relative atomic mass of an element, both the relative mass and the % abundance need to be read from the spectrum.



NMR spectra

Analysing NMR spectra may require:

- identification of the position of peaks on the horizontal axis; as for IR spectra, the scale runs in the 'opposite' direction
- identification of the splitting pattern of individual peaks (proton NMR only)
- determination of peak ratios from integration traces (proton NMR only)
- understanding of the significance of each of these.

In addition to analysing spectra, learners should be able to predict aspects of spectra for a given compound. This involves identifying certain data relating to the compound and 'visualising' the resulting spectrum.

Orders of reaction and rate equations

Graphical methods can be used to determine the order of reaction with respect to a particular reactant.

If the rate–concentration graph for reactant A in a reaction is a horizontal line, this shows that the rate is independent of [A]. This is expressed mathematically as

$$\text{rate} \propto [\text{A}]^0$$

$[\text{A}]^0 = 1$, so the above expression means that the rate is proportional to 1, i.e. constant. The order of reaction with respect to A is 0.

If the rate–concentration graph for reactant B is a straight line with a positive gradient, this shows the rate is directly proportional to the concentration of B, or

$$\text{rate} \propto [\text{B}]^1$$

The order of reaction with respect to B is 1.

If the order of reaction with respect to C is 2, then the rate–concentration graph will be a curve. However, many other reaction orders will give a curved graph, so the order cannot be determined immediately from the shape of the graph. It can be determined by mathematically analysing the graph, though learners will not be expected to do this in GCE Chemistry assessments.

If the reaction is second-order with respect to [C] this is expressed mathematically as

$$\text{rate} \propto [\text{C}]^2$$

Note that rate–concentration graphs for first and second order reactions must pass through the origin. The mathematical relation between the concentration of the reactant and the rate of reaction means that if the concentration is 0, the rate must also be 0.

First-order reactions can also be identified from concentration–time graphs through determination of the half-life. The half-life is the time it takes for the reactant concentration to reduce by half. If the half-life is constant throughout the reaction, i.e. measured from any point on the graph, then the reaction is first order with respect to the reactant.

Second-order reactions could also be identified through the half-life, although this is not a requirement in the GCE Chemistry specifications. In this case, the half-life will consistently double. So, if the first half-life is 30 seconds, the second will be 60 seconds, the third 120 seconds, and so on.

Once the orders towards all reactants have been determined, the rate equation can be constructed. For the reactants A, B and C described above, the rate equation would be

$$\text{rate} = k[\text{A}]^0[\text{B}]^1[\text{C}]^2 = k[\text{B}][\text{C}]^2$$

As $[\text{A}]^0$ is equal to 1 it is not included in the rate equation. $[\text{B}]^1$ is equal to $[\text{B}]$, so the index '1' is also not included.

M3.2 Plot two variables from experimental or other data

Learners should be able to:

- plot a graph from experiment or other data on paper or in a spreadsheet, including drawing lines of best fit
- extrapolation and interpolation.

Mathematical concepts

Plotting a graph should be a straightforward concept but the following guidelines are useful:

- Points plotted must be within 1 square of the correct value.
- Appropriate linear scale used on axes.
- Graph should make good use of available space.
- Scales should be 'sensible', i.e. using decimal or otherwise straightforward scale, not increments of 0.3 or something like that.
- Scales must be chosen so that all points fall within the graph area – points must not be plotted outside the graph area.
- Axes must be labelled, with units included.

In drawing lines (or curves) of best fit, the points plotted should **not** be connected. Rather, the best smooth line must be drawn that achieves a balance of points above and below the line.

Learners must realise when lines of best fit need to be drawn through the origin; this is the case for certain relationships, such as in rate–concentration graphs.

Interpolation is achieved through drawing lines of best fit; no formal method is required.

Extrapolation is required in some instances, for example to determine the intercept with the y-axis or in extrapolating cooling curves. Extrapolation is achieved by extending the line of best fit to the appropriate point.

Contexts in Chemistry

Rates experiments

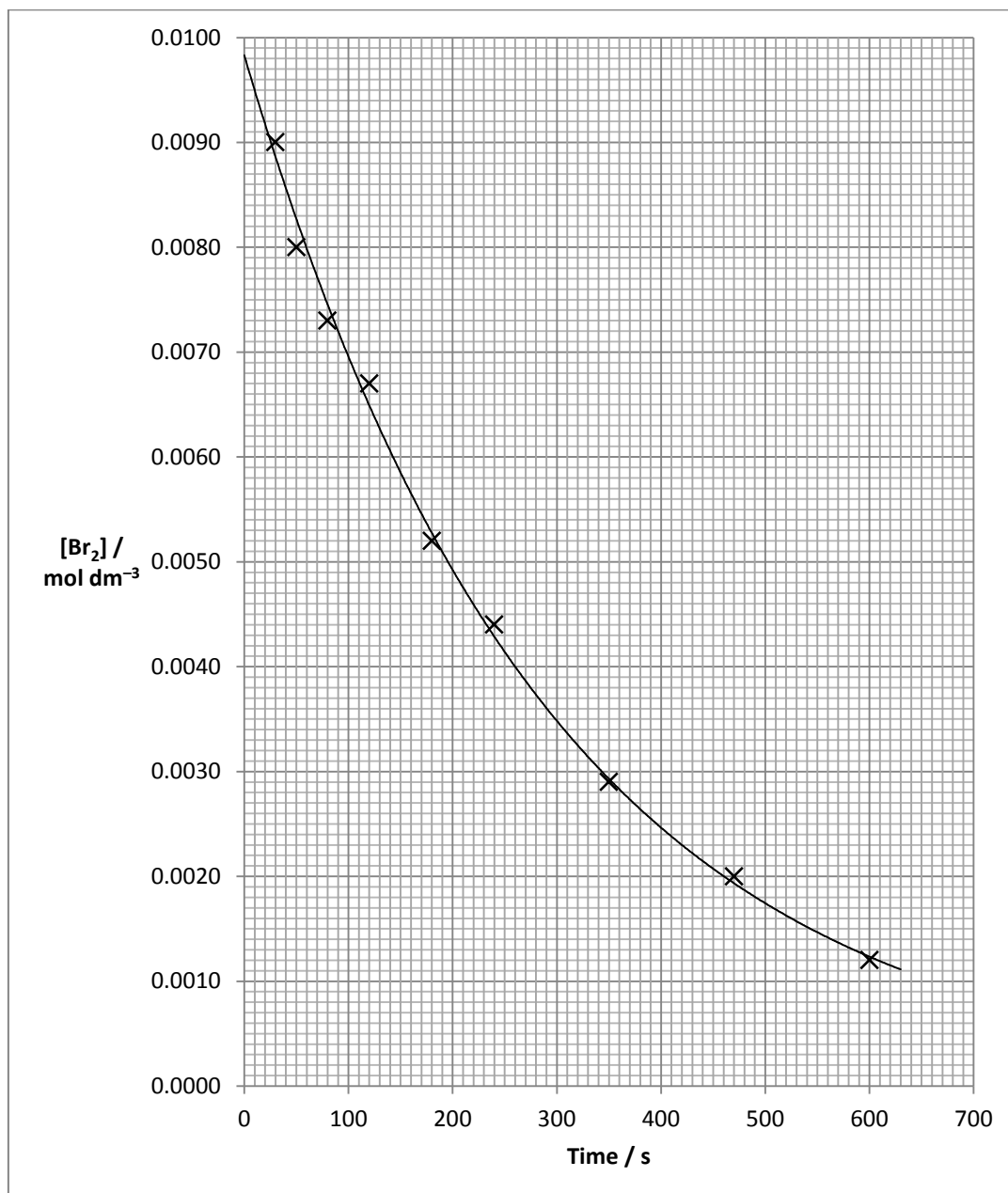
Data to be plotted would be recorded by learners themselves, or provided in a table such as below.

Time / s	30	50	80	120	180	240	350	470	600
[Br ₂] / mol dm ⁻³	0.0090	0.0080	0.0073	0.0067	0.0052	0.0044	0.0029	0.0020	0.0012

Suitable axis scales will depend on the size of the graph paper available, but sensible scales would be:

- 0–700 s, with 10 s per square, for the x-axis
- 0–0.0100 mol dm⁻³, with 0.0001 mol dm⁻³ per square, for the y-axis.

These scales would make excellent use of space on an A4-sheet of graph paper with 2 mm squares:



Calibration curves

A calibration curve is a technique whereby a relationship is established between two variables, so that the resultant curve can be used to establish a property of an unknown sample.

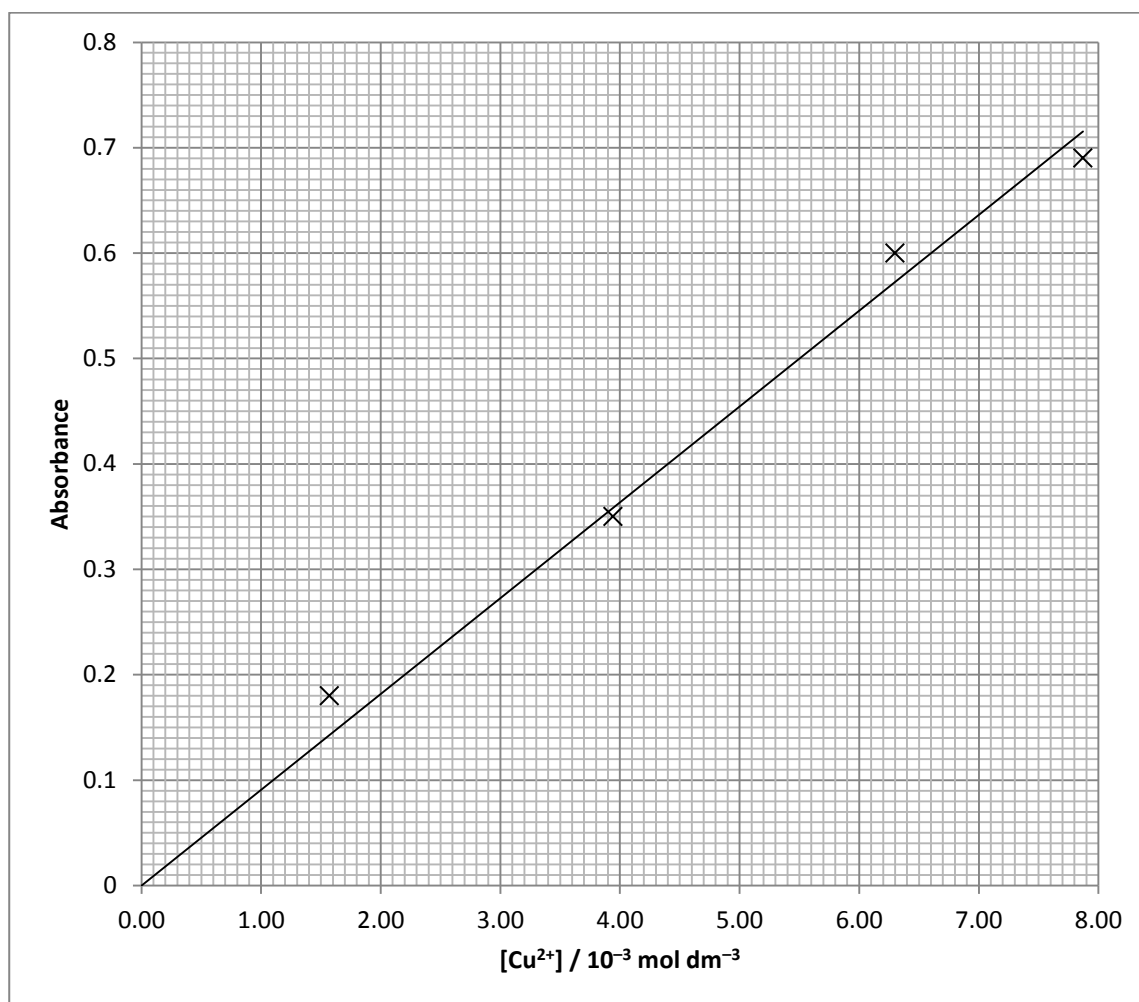
For example, in colorimetry, a calibration curve is used to establish the relationship between the absorption of a particular wavelength of light by a solution, and the concentration of a coloured solute. The following data might be produced for the absorption of solutions of copper(II) ions.

[Cu²⁺] / mol dm⁻³	1.57×10^{-3}	3.94×10^{-3}	6.30×10^{-3}	7.87×10^{-3}
Absorbance	0.18	0.35	0.60	0.69

Suitable axis scales would be:

- 0–8.00 × 10⁻³ mol dm⁻³, with 1 × 10⁻⁴ mol dm⁻³ per square, for the x-axis
- 0–0.8 absorbance units, 0.01 absorbance units per square, for the y-axis.

This would produce the following calibration curve:



Note that in this case the line of best fit is drawn through the origin, which would be appropriate if the colorimeter has been 'zeroed' using a reference solution without Cu²⁺ ions. Alternatively, an absorbance reading using such a solution might be taken – in that case the line of best fit should *not* pass through the origin. Learners should consider whether lines of best fit should pass through the origin.

The calibration curve is then used to determine the concentration of an unknown solution. If such a solution has an absorbance of 0.39, the concentration according to the line of best fit is $4.30 \times 10^{-3} \text{ mol dm}^{-3}$.

M3.3 Determine the slope and intercept of a linear graph

Learners should be able to:

- find the y-intercept of a linear graph
- find the gradient (slope) of a linear graph.

Mathematical concepts

The straightforward way to find the y-intercept is to examine where the line of the graph crosses the y-axis. However, this must be done at the point where $x = 0$ – this point is not always visible on an appropriately drawn graph (see Section M3.1 for comments on axis scales). In such cases, the y-intercept can be determined mathematically.

To find the gradient the following formula is useful:

$$\text{gradient} = \frac{\text{rise}}{\text{run}} \quad \left(= \frac{\Delta y}{\Delta x} \right)$$

The 'rise' represents the vertical step between 2 points, and the 'run' represents the horizontal step between the same two points. Both of these quantities could be negative and care has to be taken in these cases.

The principle is that two points are taken on the line of the graph. Measuring the horizontal distance between the points gives the run, and the vertical distance gives the rise. The division according to the formula above gives the gradient.

When determining the gradient of a graph plotted from experimental data, the points used must be on the line of best fit. Learners must **not** use two of the plotted points to determine the gradient.

Contexts in Chemistry

The Arrhenius equation

The Arrhenius equation gives an expression for the relation between the rate constant of a reaction and the temperature. The Arrhenius equation is stated as:

$$k = Ae^{\frac{-E_a}{RT}}$$

Taking the natural logarithm (see Section M2.4) of both sides of the equation, allows the expression to be written as:

$$\ln k = -\frac{E_a}{RT} + \ln A$$

Both the above expressions of the Arrhenius equation are given on the *Data Sheet*.

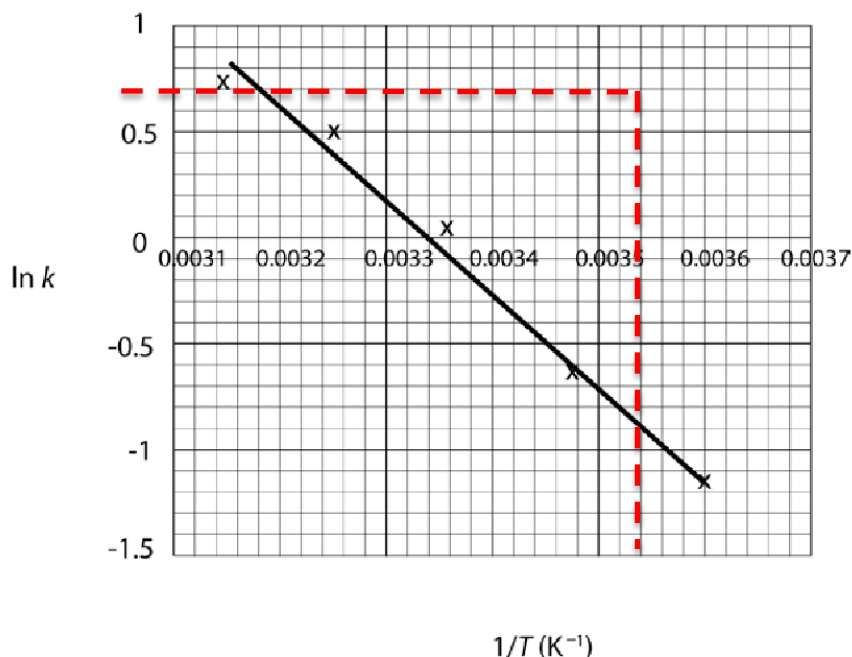
This can be thought of as

$$\ln k = -\frac{E_a}{R} \times \frac{1}{T} + \ln A$$

c.f. $y = mx + c$

Plotting $\ln k$ against $1/T$ thus produces a straight line in which the slope (m) is equal to $-E_a/R$ and the intercept (c) is equal to $\ln A$.

Consider for example the following graph. (Note that T is measured in kelvin.)



The gradient should be determined from two points on the line of best fit, for example the points indicated on the graph: (0.00314, 0.80) and (0.00352, -0.80).

$$\text{rise} = -0.80 - 0.80 = -1.60$$

$$\text{run} = 0.00352 - 0.00314 = 0.000380$$

$$\text{gradient} = \frac{-1.60}{0.000380} = -4.21 \times 10^3$$

The gradient is equal to $-E_a/R$ so

$$E_a = -\text{gradient} \times R$$

$$= -(-4.21 \times 10^3 \times 8.314) = 3.50 \times 10^5 \text{ J mol}^{-1} (= 35.0 \text{ kJ mol}^{-1})$$

(Note that E_a should be calculated using the unrounded value for the gradient.)

The intercept can, in this case, not be determined graphically. The line of best fit cannot be extrapolated to the point where it crosses the y-axis at $x = 0$.

$\ln A$ can be calculated mathematically by rearranging the linear Arrhenius equation

$$\ln k = -\frac{E_a}{R} \times \frac{1}{T} + \ln A$$

to

$$\ln A = \ln k + \frac{E_a}{R} \times \frac{1}{T}$$

and then substituting the calculated gradient value and any point from the graph, e.g.

$$\ln A = 0.80 + 4.21 \times 10^3 \times 0.00314 = 14.0$$

$$A = 1.23 \times 10^6$$

(The units for A will be the same as the units for k , and will depend on the reaction equation.)

M3.4 Calculate rate of change from a graph showing a linear relationship

Learners should be able to:

- calculate a rate of change from a linear graph.

Mathematical concepts

The gradient of a linear graph is always a measure of the rate of change between the two variables. The gradient of a linear graph with formula $y = mx + c$ basically measures the rate of change of y with respect to x . In words, the gradient expresses how quickly y changes as x changes.

A positive gradient means a quantity that increases as x increases whilst a negative gradient is a decreasing quantity as x increases.

The procedure for calculating a rate of change is therefore the same as for calculating the slope of a graph, as described in Section M3.3.

Contexts in Chemistry

Rate constants

The rate constant for a first-order reaction can be determined from the rate of change of a rate–concentration graph. This can be seen from the rate equation

$$\text{rate} = k[A]$$

which is mathematically equivalent to

$$y = ax$$

and therefore the rate constant k is equal to the gradient of the graph.

The gradient can be determined as described in M3.3.

M3.5 Draw and use the slope of the tangent to a curve as a measure of a rate of change

Learners should be able to:

- draw a tangent to a curve at a given point
- find the gradient of the tangent.

Mathematical concepts

For linear graphs, the gradient is the same throughout and hence the rate of change is easy to obtain (see previous sections). Non-linear graphs have an ever changing gradient and hence the rate of change will change from point to point. The rate of change at a particular point can be found mathematically using calculus, but this is not required in GCE Chemistry. Rather, a tangent is drawn by hand and eye to approximate the instantaneous rate of change at a particular point.

To draw a tangent accurately is tricky but there are a number of useful tips that can help:

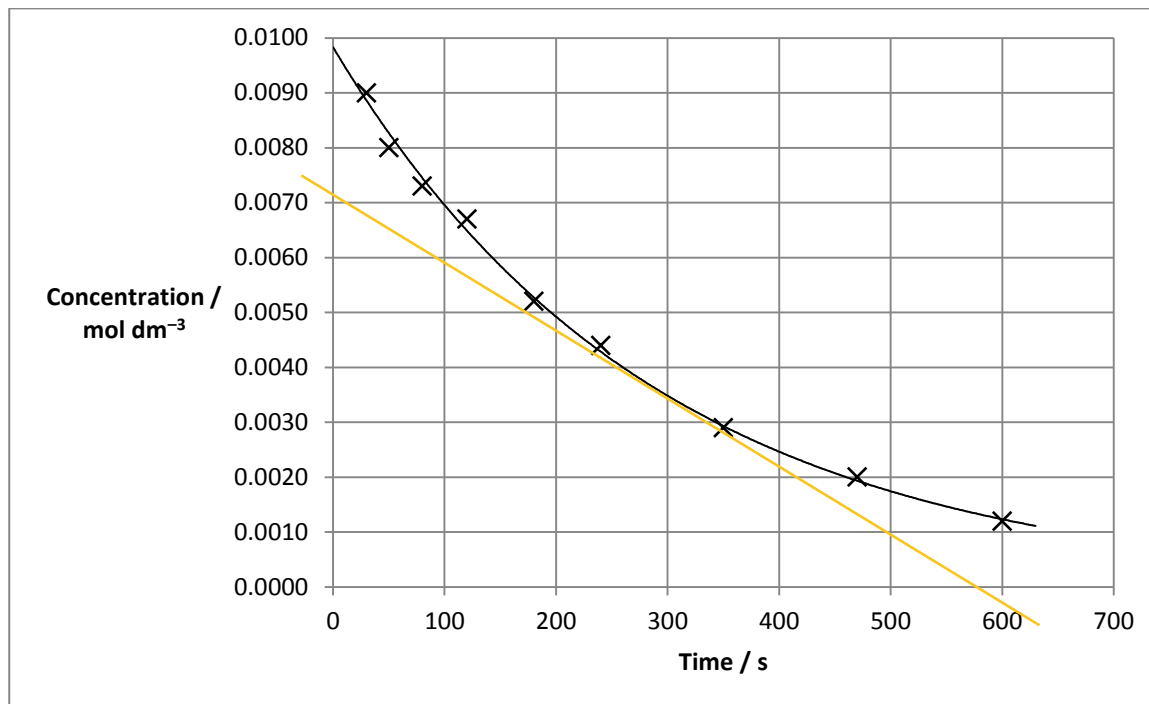
- Use a ruler and pencil. This sounds obvious, but many learners will not do this naturally.
- Line the ruler up to the point where the tangent is supposed to be taken.

- While aligning the ruler, make sure that in the vicinity of the point **none** of the line of the curve is covered by the ruler. The aim is to have all of the curve visible as the line is drawn, otherwise the tangent will not be accurate.

Contexts in Chemistry

Rates of reaction

Below is a typical concentration–time graph for a reaction.



To find the rate of reaction at 300 s, a tangent has to be drawn to approximate the gradient (which represents the rate) at that given time.

The gradient of the tangent is calculated as described in Section M3.3, by dividing the rise and the run between two points.

In this instance, it makes the calculations easier to take the x and y intercepts as the two points, which can approximately be read as (577,0) and (0,0.0071) respectively. The 'rise–run' calculation then becomes:

$$\text{gradient} = \frac{-0.0071}{577} = -1.2 \times 10^{-5}$$

and hence the rate of reaction at 300 s is $1.2 \times 10^{-5} \text{ mol dm}^{-3} \text{ s}^{-1}$. Note that while the gradient is negative (because the reactant is being used up over time), a rate of reaction is expressed as a positive number.

M4 – Geometry and trigonometry

M4.1 Use angles and shapes in regular 2-D and 3-D structures

Learners should be able to:

- predict/identify shapes of and bond angles within molecules.

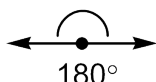
Mathematical concepts

Understanding shapes of molecules and bond angles is related to understanding of regular 2-D and 3-D structures. Learners do not need the full in-depth understanding of these mathematical principles described here in order to remember the basic facts, but it may help in their understanding and application of the principles to unfamiliar molecules.

2-D structures

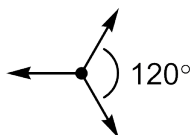
In 2-dimensional structures, or in a plane, the angle sum around a point is 360° .

If two lines emanate from a point, equally dividing the plane around that point, then each angle around that point is 180° :



Similarly, if three lines from a point equally divide the plane, then each angle is:

$$\frac{360}{3} = 120^\circ$$

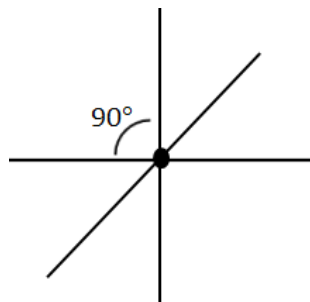


This principle can be applied to any arrangement around a point in a plane.

3-D structures

Learners must also consider angles within 3-dimensional shapes.

The octahedral arrangement can be thought of as being formed by points lying on three intersecting axes. This shows that all internal angles are 90° .



The bond angles in a tetrahedron are more complicated to calculate and require trigonometry. Learners merely have to recall the tetrahedral angle of 109.5° and do not need to be concerned

with the calculation. It is included in Appendix C as a background reference, and could be supplied to interested learners.

Contexts in chemistry

Structure and bonding

Learners are expected to be familiar with the following regular molecular shapes and angles:

linear (e.g. BeCl_2)	180°
trigonal planar (e.g. BF_3)	120°
tetrahedral (e.g. CH_4)	109.5°
octahedral (e.g. SF_6)	90°

Additionally, learners must understand certain molecular shapes that derive from a tetrahedral arrangement, but where one or two of the electron pairs surrounding the central atom are lone pairs rather than bonding pairs. This affects both the observed shape of the molecule, and the bond angle as the lone pairs repel more strongly than bonded pairs.

In this regard, learners should be familiar with the following shapes:

pyramidal, resulting from a central atom surrounded by three bonds and one lone pair; in NH_3 the bond angle resulting from the additional repulsion of the lone pair is 107°

non-linear, resulting from a central atom surrounded by two bonds and two lone pairs; in H_2O the bond angle resulting from the additional repulsion of the lone pair is 104.5°

M4.2 Visualise and represent 2-D and 3-D forms including 2-D representations of 3-D objects

M4.3 Understand the symmetry of 2-D and 3-D shapes

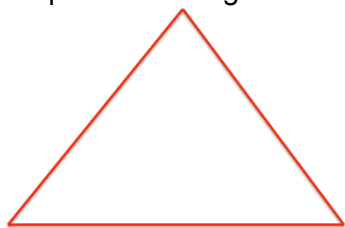
Learners should be able to:

- represent the 3-D shape of molecules in 2-D
- identify different representations of the same molecules
- draw and identify different forms of isomers
- identify chiral centres.

Mathematical concepts

Symmetry is a notoriously difficult topic to teach. It relies entirely on a learner's spatial awareness and reasoning. There are a few tricks that can help learners to improve. Symmetry is a measure of the ability of a shape to be 'messed around' with but still keep its essential structure the same.

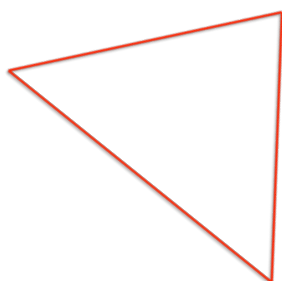
Take an equilateral triangle:



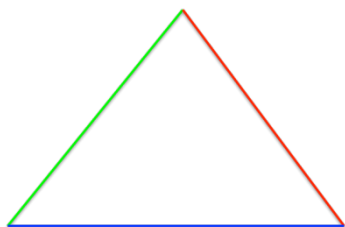
It displays a number of forms of symmetry.

- It has *rotational* symmetry: if you rotate it by 120° or 240° it looks the same.
- It has *mirror* symmetry: if you flip it about the vertical axis (or either of the other planes of symmetry) it looks the same.

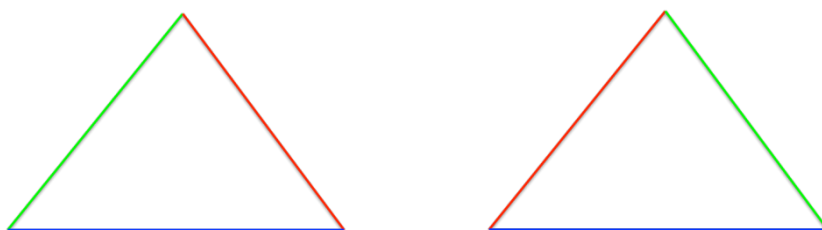
In the following diagram the triangle has been rotated to a different position, but its structure is still the same. It is identical to the first triangle, only its position is different. It can be rotated to make it look the same as the triangle above.



The following triangle is not symmetrical.



It cannot be rotated (unless by 360° , which takes it back to the starting point) or reflected to make it look the same. This has an effect on the nature of the mirror image of this triangle:



These triangles have the same position and structure. The colours are the same and in the same positions relative to each other. But the triangle on the right cannot be rotated in such a way as to produce the triangle on the left. The mirror images are *non-superimposable*.

In A Level Chemistry, learners need to apply these principles in 3 dimensions. If the 3-D shape of a molecule lacks symmetry, then its mirror image cannot be rotated so that it will look the same as the original (see below).

Looking at 3-D models can help to grasp the principle that molecules can be mirror images, but cannot be rotated so that they look the same. From there, learners must apply the principle to 2-D

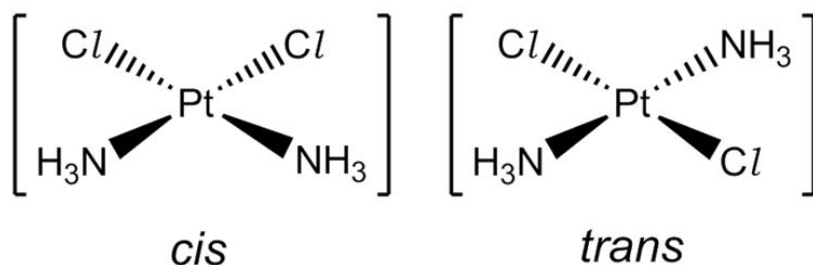
representations of molecules, bearing in mind that the 2-D representation may 'mask' any lack of symmetry.

Contexts in Chemistry

Organic structures

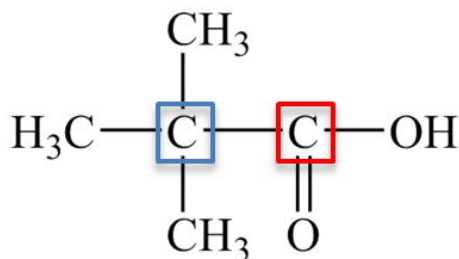
To represent any molecule on paper involves creating a 2-D representation of a 3-D shape. The issues involved hold true for all areas of chemistry, but the use of representations of molecules is most frequently encountered in the context of organic chemistry.

While it is possible to give a clear impression of the 3-D structure of a molecule using solid and dashed wedge bonds:



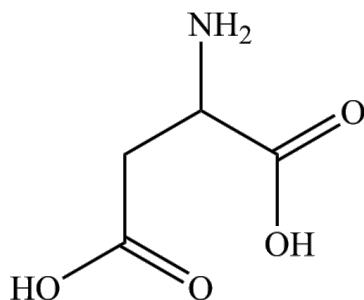
this is not commonly applied to full organic structures. Structural and skeletal formulae are simplified representations, which serve to highlight the connectivity within molecules rather than give a true impression of the 3-dimensional structure.

Structural formulae like this one:



are drawn as if all bond angles around the carbon atoms are 90°, and have a planar arrangement. This is clearly not a true representation of the actual structure. The four bonds around the carbon atom highlighted by the blue box are in reality in a tetrahedral arrangement, with a bond angle of 109.5°. The bonds around the carbon atom highlighted by the red box have a planar arrangement with bond angles of 120°.

Slightly different considerations apply to skeletal formulae:



In this structure, all bond angles are displayed as 120°. That is correct for the carbon atoms in the carboxylic acid groups, but not for the others, which have a tetrahedral arrangement. When examining skeletal formulae, learners need to mentally 'fill in' the implied hydrogen atoms in order to deduce the actual arrangement around an atom.

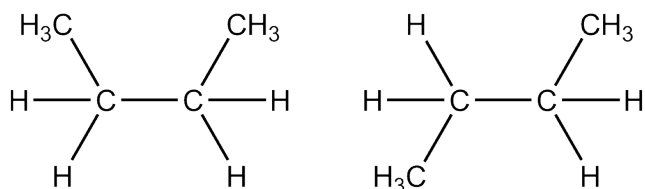
Isomerism

The two forms of stereoisomerism that learners are required to understand are *E/Z* isomerism and optical isomerism.

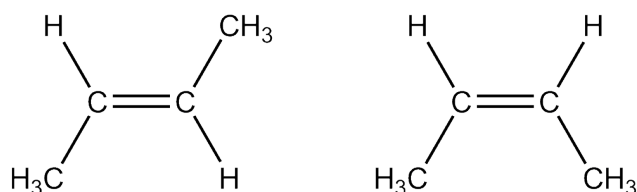
E/Z isomerism

E/Z isomerism arises due to the restriction in rotation around a double bond. It occurs when the two carbon atoms in a C=C bond are each bonded to two different groups.

The following alkanes are equivalent due to the rotation around the central C–C bond:

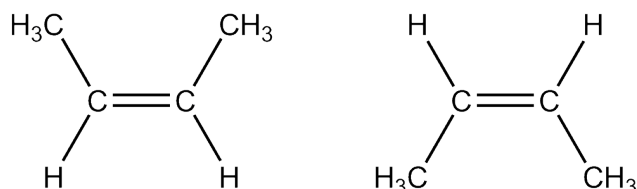


The single C–C bond means that rotation is possible. However, the following alkenes are stereoisomers because **no** rotation is possible around the C=C bond:



There is no way we can rotate the structure on the left so that we get the structure on the right.

As is the case for structural isomers, learners must realise that different diagrams may depict the same molecule, considering rotation of the whole molecule:

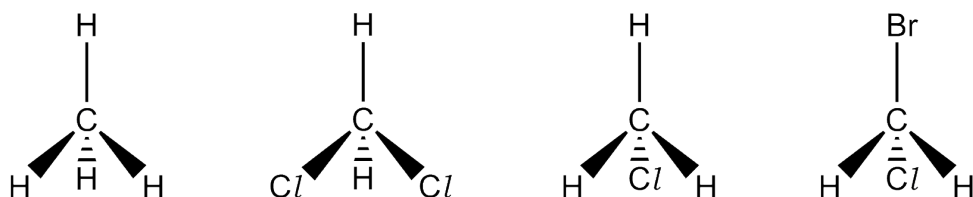


Here, if we rotate the molecule on the left by 180°, it looks like the molecule on the right. So, these two diagrams depict the same molecule.

Optical isomers

Optical isomers (enantiomers) are molecules that are non-superimposable mirror images of each other.

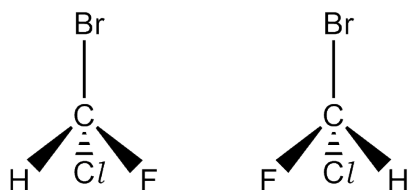
Optical isomers exist for molecules that have a structure that is asymmetrical. To appreciate this, it is helpful to start with how some molecules *are* symmetrical:



The molecules depicted above are all symmetrical. They are depicted so that the plane of symmetry runs down the vertical axis of each molecule. (Some have additional planes of symmetry.) The mirror images of all of these molecules looks identical to the original.

All of the molecules above have at least two identical groups attached to the central carbon.

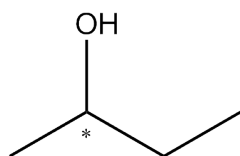
When a carbon is attached to four *different* groups, the molecule is not symmetrical:



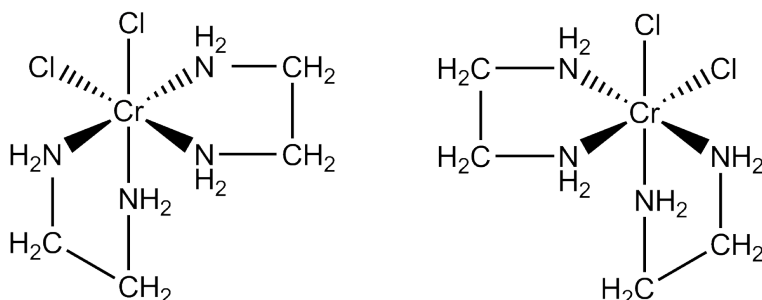
This molecule has no plane of symmetry. The mirror image does not look the same as the original, and cannot be rotated in such a way to make it look the same as the original – the mirror images are non-superimposable. Therefore, these molecules are enantiomers.

A carbon that is bonded to four different groups always results in a molecule that is asymmetrical. Such carbon atoms are called chiral centres.

Chiral centres can be determined from 2-D representations of molecules by examining the nature of the groups bonded to each carbon atom (this may require mentally 'filling in' the implied hydrogens). For example, in this diagram the carbon highlighted with an asterisk can be identified as a chiral centre:



Transition metal complexes can also exhibit optical isomerism due to the specific arrangements of ligands around the central ion, as in this example:



It is very hard to appreciate from the 2-D representation that these complexes are isomers. Handling 3-D models is invaluable here.

Appendix A – Key power laws

It is useful for learners to be aware of the following power laws to help in certain mathematical skills, as referenced in the text.

$$x^n \times x^m = x^{n+m} \quad \text{multiplicative rule}$$

$$\frac{x^n}{x^m} = x^{n-m} \quad \text{division rule}$$

$$(x^n)^m = x^{nm} \quad \text{power rule}$$

$$x^{-1} = \frac{1}{x^n} \quad \text{reciprocal rule}$$

$$x^{n/m} = \sqrt[m]{x^n} \quad \text{root rule}$$

Appendix B – Rearranging the Arrhenius equation

Given the exponential equation

$$k = Ae^{-E_a/RT}$$

Before we can 'get rid of' the exponential it is necessary to put the coefficient on the other side.

$$\frac{k}{A} = e^{-E_a/RT}$$

Now natural logs can be taken on each side.

$$\ln\left(\frac{k}{A}\right) = -\frac{E_a}{RT}$$

According to the log law

$$\log\left(\frac{A}{B}\right) = \log A - \log B$$

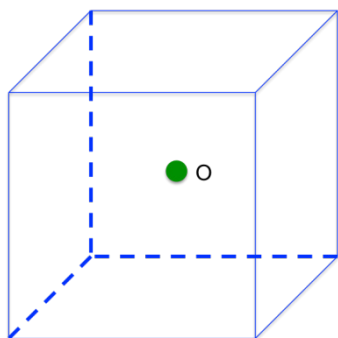
$$\ln k - \ln A = -\frac{E_a}{RT}$$

And finally

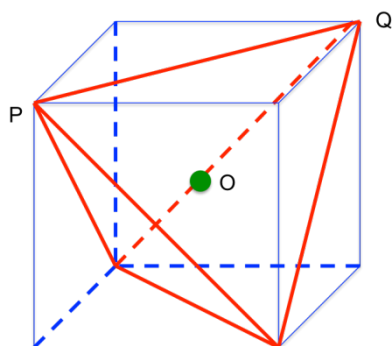
$$\ln k = -\frac{E_a}{RT} + \ln A$$

Appendix C – The tetrahedral bond angle

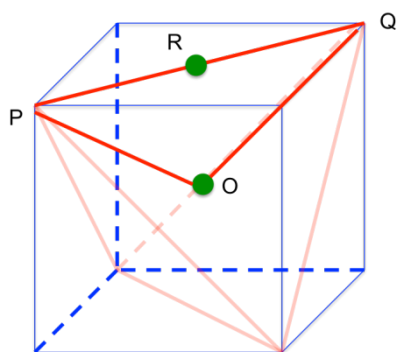
Take a cube of side length 2 with centre O:



Now imagine a tetrahedron with vertices on the vertices of the cube:



Then imagine the triangle OPQ:



The angle POQ is the tetrahedral angle. R is the midpoint of PQ.

The length of PQ can be calculated using Pythagoras:

$$\sqrt{2^2 + 2^2} = 2\sqrt{2}$$

Therefore the length of PR is $\sqrt{2}$. The length OR is 1, because O is the centre of the cube. Hence the triangle OPR is a right-angled triangle, and the angle POR can be found by trigonometry:

$$\angle POR = \tan^{-1} \frac{\sqrt{2}}{1} = \tan^{-1} \sqrt{2} \approx 54.75^\circ$$

Hence the bond angle POQ is $2 \times 54.75 \approx 109.5^\circ$.

OCR customer contact centre

General qualifications

Telephone 01223 553998

Facsimile 01223 552627

Email general.qualifications@ocr.org.uk



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