SL IB Chemistry

Your notes

Tool 3: Mathematics

Contents

* Applying General Mathematics in Chemistry
* Using Units, Symbols & Numerical Values in Chemistry
* Processing Uncertainties in Chemistry
* Graphing in Chemistry

Your notes

Applying General Mathematics in Chemistry

Applying General Mathematics in Chemistry

Using arithmetic and algebraic calculations in chemistry

- Chemistry often requires the use of calculations, which can include:
  - Decimals
    - Most chemical calculations use decimals, e.g. the concentration of a chemical
  - Fractions
    - These are most commonly used in uncertainty calculations
    - Most scientific calculators will initially give answers as fractions
      - Make sure you know where the S⇔D button is so that you convert the fraction into a decimal
  - Percentages
    - There are many percentage calculations, including percentage yield, percentage atom economy, percentage change, percentage difference, percentage error and percentage uncertainty
  - Ratios
    - These are commonly used in moles calculations where the stoichiometry of the balanced chemical equation is not 1 : 1, e.g.
$$H_2SO_4 + 2NaOH \rightarrow Na_2SO_4 + 2H_2O$$

  - Reciprocals
    - These are most obvious in gas laws, using $1/V$, and concentration versus rate graphs, using $1/T$
      - For more information about gas laws, see our revision notes in the Ideal Gases topic
      - For more information about concentration and rates, see our revision notes in the How Fast? The Rate of Chemical Change topic
  - Logarithmic functions
    - These are most obvious in pH and Arrhenius calculations
      - For more information about pH, see our revision note on The pH Scale
      - For more information about Arrhenius, see our revision note on The Arrhenius Equation
  - Exponential functions (Additional Higher level)
    - This is most obvious in Arrhenius calculations
- Section 1 of the Data Booklet contains a list of the mathematical equations that you are expected to be able to manipulate and work with
  - **Careful:** This is not an exhaustive list – there are other equations that you will be expected to know that are not given in Section 1 of the Data Booklet, e.g. percentage yield

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💡 **Examiner Tip**

- Make sure your final answers are written as proper numbers, not left as fractions
  - Leaving them as fractions will typically lose you a mark

Your notes

What is the mean average?

- The mean average is often just called the "average"
- It is the **total** of all the values **divided** by the **number of values**, i.e. add all the numbers together and divide by how many there are
- For example, two common isotopes of chlorine are chlorine-35 and chlorine-37, which exist in a 3 : 1 ratio
    - The information shows that there are three chlorine-35 atoms for every one chlorine-37 atom
    - Overall, there is a total of four atoms to be considered in the calculation
    - So, the mean average = $\dfrac{35 + 35 + 35 + 37}{4}$ = 35.5
- Problems with the mean average occur when there are anomalous results
    - These should not be included in a mean average calculation

What mean average calculations are in chemistry?

- Two main calculations in chemistry that involve mean average calculations are:
    - Calculating relative atomic mass from isotopic abundance data
        - For more information, see our revision note on Isotopes
    - Calculating average titres as part of a titration calculation
        - These calculations will typically have values that should not be considered because they are not concordant

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✏️ Worked example

Calculate the average titre for the following experimental results.

Rough titre / cm^3	Titre 1 / cm^3	Titre 2 / cm^3	Titre 3 / cm^3	Titre 4 / cm^3
15.50	14.90	15.15	14.95	14.95

Answer:

- The **three** values that are used for the mean average calculation are:
    - **14.90**
    - **14.95**
    - **14.95**
- The rough titre should never be used in the mean average calculation
- Any results that are not concordant are considered to be outlying / anomalous results and should not be included in the mean average calculation
- So, the average titre = $\dfrac{14.90 + 14.95 + 14.95}{3}$ = **14.93 cm³**

Your notes

Range

- The range can only be applied to numerical data
- It is a measure of how spread out the data is, which means that it is the difference between the highest and lowest values
  - You can remember this as "Hi – Lo"
- It can be expressed as:
  - A range of values
    - e.g. 9.2 – 8.4
  - A single value
    - e.g. 9.2 – 8.4 = 0.8
- The range can be affected when the highest and / or lowest data are anomalous results themselves

What is scientific notation?

- **Scientific notation** is also known as **standard form**
- It is a system of writing and working with very large or very small numbers
  - For example, Avogadro's number 602 000 000 000 000 000 000 000 is 6.02×10^{23} in scientific notation
- Numbers in scientific notation are written as:

$$a \times 10^n$$

- They follow these rules:
  - **a** is a number above 1 and below 10
  - For large numbers, **n** is an integer that is greater than 0
    - i.e It shows how many times **a** is multiplied by 10
  - For small numbers, **n** is an integer that is less than 0
    - i.e It shows how many times **a** is divided by 10
  - $n < 0$ for small numbers i.e how many times a is divided by 10
- For example:

Applying scientific notation to numbers

$$300000000 = 3 \times 10^8$$

$$0.00002 = 2 \times 10^{-5}$$

The scientific notation for numbers greater than 1 has the x 10 raised to a positive power while the scientific notation for numbers less than 1 has the x 10 raised to a negative power

- When rounding a number in standard form to a certain number of significant figures, only the value of **a** is rounded (the $\times 10^n$ value will not be significant)
  - For example, 4.37×10^6 to 2 significant figures is 4.4×10^6

Orders of magnitude

- When a number is expressed to an **order of 10**, this is an **order of magnitude**
  - Example: If a number is described as 3×10^8 then that number is actually $3 \times 100\ 000\ 000$
  - The order of magnitude of 3×10^8 is just $\mathbf{10^8}$
- Orders of magnitude follow rules for rounding
  - The order of magnitude of 6×10^8 is $\mathbf{10^9}$ as the magnitude is **rounded up**
- A quantity is **one order of magnitude larger** than another quantity if it is about **ten times larger**
  - Similarly, **two orders of magnitude** would be **100 times larger**, or 10^2
- In chemistry, orders of magnitude can be very large or very small

Approximation and estimation

- Approximation and estimation are both methods used to obtain values that are close to the true or accurate values
  - While they share some similarities, they have distinct characteristics and are used in different contexts

Approximation

- Approximation involves finding a value that is close to the actual value of a quantity
  - It may not necessarily be very precise or accurate
- It is often used when an exact calculation is challenging or time-consuming and a reasonably close value is sufficient
- Approximations are typically quick and easy to calculate
- For example, the pH of a strong acid is commonly accepted as being between pH 1.0 and pH 3.0
  - A reasonable approximation would be to say that the pH of a strong acid is pH 1.0
  - The approximation is not exact, but it is reasonable as well as being aligned with a value that most people accept as a strong acid

Estimation

- Estimation involves making an educated guess or assessment based on available information or data
- It is used when the true value of a quantity is unknown or cannot be directly measured
- For example, estimating the percentage yield of an industrial reaction involves:
  - Taking a known amount of reactant
  - Calculating the theoretical mass of the product that should be made
  - Completing the reaction and measuring the mass of the product that is made
  - Performing the percentage yield calculation
  - The percentage yield calculation is correct for that amount of reactant under the specific reaction conditions used but can be applied to the industrial reaction to give an estimated percentage yield

Appreciate when some effects can be ignored and why this is useful

- During calculations using acid and base dissociation constants the assumption made is that the value of [H⁺] = [HA]
  - Or the concentration of hydrogen ions is the same as the concentration of the acid
- This is because
  - The weak acid has a low degree of dissociation so you can assume the concentration of the acid is the same value at equilibrium and use it in the expression for K_a
    - $CH_3COOH \rightleftharpoons CH_3COO^- + H^+$
    - A point to remember is that K_a values are different depending on the acid, so the degree of dissociation also varies. Therefore the error using this assumption for some acids will be larger than others
  - All the H⁺ ions are assumed to come from the acid as water will contribute a very small number of H⁺ ions
- So the K_a expression:

$$K_a = \frac{[H^+][A^-]}{[HA]}$$

can be simplified to

$$K_a = \frac{[H^+]^2}{[HA]}$$

  - Remember to give the full expression in an exam when asked

Percentage change and percentage difference

- Percentage change and percentage difference are commonly used to express the relative change between two values
  - They are useful for comparing experimental results, determining reaction yields and analysing other chemical data

Percentage change

- Percentage change is used to express the relative change between an initial value and a final value
- It is calculated using the following formula:

$$\text{Percentage Change} = \frac{(\text{Final Value} - \text{Initial Value})}{\text{Initial value}} \times 100$$

> ✏️ **Worked example**
>
> During the course of a chemical reaction, the initial of chemical species **A** increases from 0.05 mol dm⁻³ to 0.08 mol dm⁻³.
>
> Calculate the percentage change in concentration.
>
> **Answer:**
>
> - Percentage change = $\dfrac{(\text{Final Value} - \text{Initial Value})}{\text{Initial value}} \times 100$
>
> - Percentage change = $\dfrac{(0.08 - 0.05)}{0.05} \times 100 = 60\%$
>
> - So, the concentration of the chemical species increased by 60% during the reaction

Percentage difference

- Percentage difference is used to compare two values to determine how much they differ from each other as a percentage
- It is calculated using the following formula:

$$\text{Percentage Difference} = \dfrac{(\text{value 1} - \text{value 2})}{(\text{average of value 1 and value 2})} \times 100$$

Your notes

> ✏️ **Worked example**
>
> The melting points of different samples **B** and **C** are measured:
>
> - **B** = 75°C
> - **C** = 81°C
>
> Calculate the percentage difference in melting points.
>
> **Answer:**
>
> - Percentage difference = $\dfrac{(\text{value } 1 - \text{value } 2)}{(\text{average of value 1 and value 2})} \times 100$
>
> - Percentage difference = $\dfrac{(75 - 81)}{((75 + 81)/2)} \times 100$
>
> - Percentage difference = $\dfrac{-6}{78} \times 100$ = –7.69%
>
>   - When calculating percentage difference, you can ignore the minus sign in front of the calculation
> - So, the melting points of **B** and **C** differ by 7.69%

Percentage Error

- Percentage error is used to express the difference between a final calculated answer and an accepted or literature value
- It is calculated using the following formula

$$\text{Percentage error} = \frac{\text{accepted value} - \text{experimental value}}{\text{accepted value}} \times 100$$

- You should be able to comment on any differences between the experimental and literature values

Your notes

> ✏️ **Worked example**
>
> Experimental results showed the enthalpy of combustion of propan-1-ol to be -1.5×10^3 kJ mol^{-1}.
>
> The literature value for this enthalpy change is -2021 kJ mol^{-1}. Calculate the percentage error.
>
> **Answer:**
>
> - Percentage error = $\dfrac{\text{accepted value} - \text{experimental value}}{\text{accepted value}} \times 100$
>
> - Percentage error = $\dfrac{2021 - 1500}{2021} \times 100 = \textbf{25\%}$

Percentage uncertainty

- **Percentage uncertainties** are a way to compare the significance of an **absolute uncertainty** on a measurement
  - This is not to be confused with **percentage error**, which is a comparison of a result to a literature value
- It is calculated using the following formula

$$\text{Percentage uncertainty} = \frac{\text{absolute uncertainty}}{\text{measured value}} \times 100$$

Diagram with examples of percentage uncertainty calculations for common laboratory apparatus

Your notes
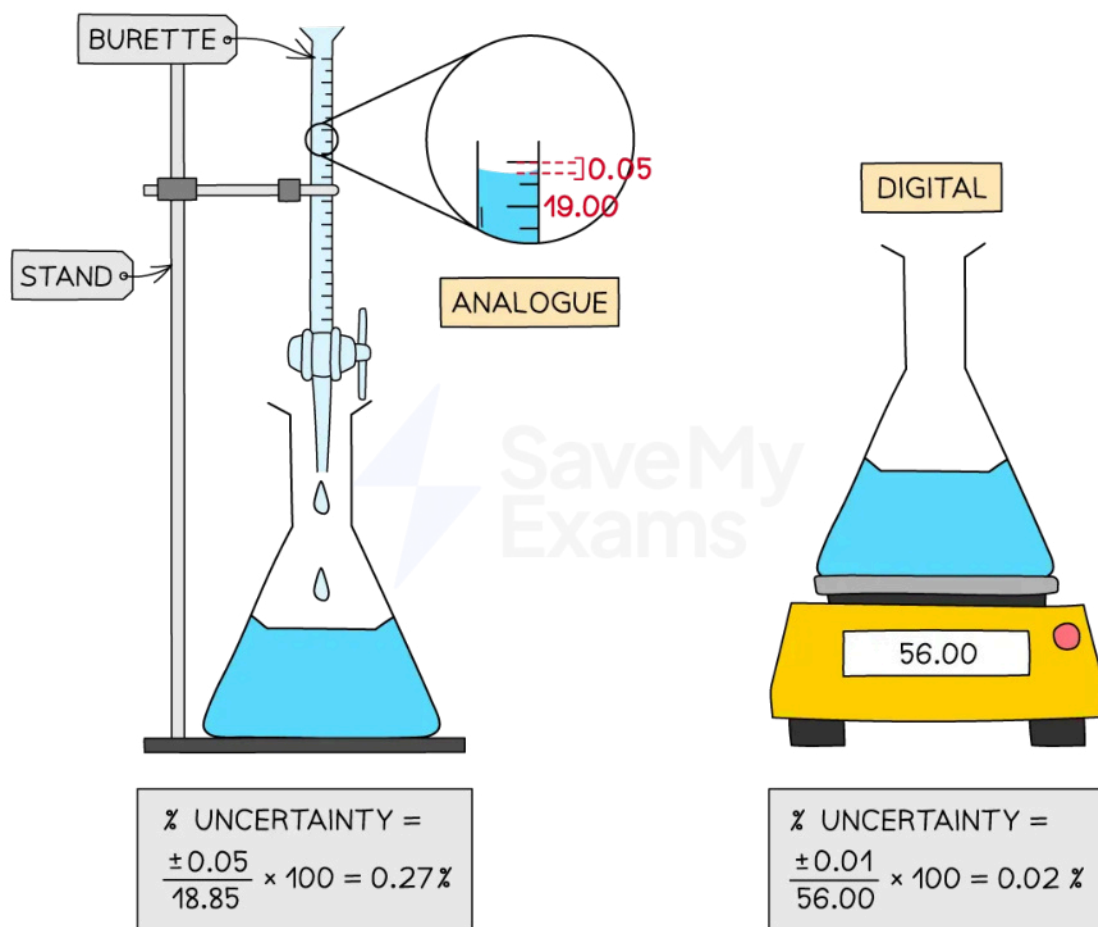
The absolute uncertainty for analogue measurements is ± half a division and for digital measurements is ± the last significant division

- For more information about uncertainties, see our revision note on Processing Uncertainties in Chemistry

> 💡 **Examiner Tip**
>
> - Percentage uncertainty can be reduced by:
>   - Using equipment with a smaller uncertainty
>   - Increasing the measured value, e.g. using a sample with greater mass or volume

Mathematical skills linked to graphs and tables

- There are several specification points linked to graphs and tables

Your notes

- For more information about working specifically with graphs, see our revision note on Graphing in Chemistry
- These include, but are not limited to, being able to:
  - Distinguish between qualitative and quantitative data, incorporating continuous and discrete variables
  - Understand direct and inverse proportionality, as well as positive and negative correlations between variables
  - Determine rates of change from tabulated data

Qualitative and quantitative data

- **Qualitative** data usually describes something in words, not numbers
  - For example:
    - Copper sulfate solution is blue
    - A more dilute copper sulfate solution is pale blue, while a more concentrated copper sulfate solution is a darker blue

- **Quantitative** data uses numbers to count / measure something
  - For example:
    - The neutralisation of 25.0 cm^3 sodium hydroxide by 25.0 cm^3 hydrochloric acid increases the temperature of the system by 2.5 °C

- **Discrete** data is quantitative
  - It consists of separate, distinct and countable values
  - For example:
    - The stoichiometric coefficients representing the relative number of molecules or atoms involved in the reaction are discrete values and must be integers
    - Electrons can only occupy certain discrete energy levels, e.g. 1s, 2s, etc

- **Continuous** data is also quantitative
  - It is based on measurements and can include decimal numbers or fractions
  - This allows for an infinite number of values
  - For example:
    - The temperature of an exothermic reaction as time progresses
    - The volume of gas produced during the thermal decomposition of calcium carbonate

Direct and inverse proportionality

- There are a number of terms that are commonly applied to trends, particularly in graphs

- **Directly proportional**
  - This applies to a trend that has a clearly **linear** relationship
  - Mathematically, this can be described as y = kx, where k can be positive or negative
  - In most situations, it is clear that k is positive
  - This means that the relationship can be described as "**when one variable increases, the other increases**" or "if x doubles, then y doubles"

Your notes

- A **directly** proportional relationship is always a **straight line through the origin** with a fixed gradient

- **Inversely proportional**
  - Mathematically, this can be described as $y = \dfrac{k}{x}$, where k can be positive or negative
  - This means that the relationship can be described as "**when one variable increases, the other decreases**" or "if x doubles, then y halves"
  - When plotted, inverse proportionality is **not a straight line** and **does not pass through the origin**

- **Positive correlation**
  - This term is best applied to the gradient of a graph
  - The gradient of the graph is positive / slopes or curves upwards
  - It describes a relationship where as x increases, y also increases

- **Negative correlation**
  - This term is, also, best applied to the gradient of a graph
  - The gradient of the graph is negative / slopes or curves downwards
  - It describes a relationship where as x increases, y decreases

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💡 **Examiner Tip**

- **Careful:** A common mistake made by students is to describe any graph with a straight line going diagonally upwards as directly proportional
  - This is not correct because direct proportionality **must** go through the origin
  - A graph that does not go through the origin can correctly be described as proportional, but it is not directly proportional

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Determine rates of change from tabulated data

- To determine rates of change from tabulated data, you can use the average rate of change or gradient, if the data has been plotted as a graph
- The average rate of change between two points on a graph or in a table is:

$$\text{Rate of change} = \frac{\text{the change in the dependent variable } (y - \text{axis})}{\text{the change in the independent variable } (x - \text{axis})}$$

Your notes

✏️ Worked example

An experiment is run to measure the amount of chemical **Y** produced as time progresses:

Time / seconds	10	20	30	40	50
Amount of Y / cm^3	3.0	7.0	10.0	14.0	18.0

Calculate the rate of change for this reaction between 10 and 30 seconds.

Answer:

- Rate of change = $\dfrac{\text{the change in the dependent variable } (y-\text{axis})}{\text{the change in the independent variable } (x-\text{axis})}$

- Rate of change = $\dfrac{(10.0-3.0)}{(30-10)} = 0.35\ \text{cm}^3\,\text{s}^{-1}$

- So, on average, the amount of **Y** increases by 3.5 cm^3 every 10 seconds over the interval from t = 10 to t = 30 seconds

Your notes

Using Units, Symbols & Numerical Values in Chemistry

Using Units, Symbols & Numerical Values in Chemistry

International System of Units (SI)

- In science, there are 7 base SI units which are used to measure various physical quantities

SI Base Units Table

Quantity	SI base unit	Symbol
length	metre	m
mass	kilogram	kg
time	second	s
temperature	Kelvin	K
amount of substance	mole	mol
current	Ampere	A
luminous intensity	candela	cd

- These base SI units form the foundation for measuring various properties and quantities in chemistry and other sciences
- Other common units can be derived from these base units for specific applications, but they are all based on the International System of Units (SI)
  - Concentration, **c** [mol dm^{-3}]
  - Joules, **J** [N m]
  - Molar mass, **M$_r$** [g mol^{-1}]
  - Pascals, **Pa** [kg / m s^2]

Table of common units in chemistry

Quantity	Unit	Abbreviation
energy	joule	J

Your notes

pressure	pascal	Pa
electrical charge	coulomb	C
enthalpy	kilojoules per mole	$kJ\,mol^{-1}$
entropy	joules per Kelvin	$J\,K^{-1}$
potential difference	volts	V
concentration	moles per cubic decimetre	$mol\,dm^{-3}$

Prefixes

- Measurements of physical quantities can require very large and very small values, for example:
    - The diameter of an atom is about 10^{-10} m or 0.0000000001 m
    - One mole of a substance contains 6.02×10^{23} or 602 000 000 000 000 000 000 000 particles
- Powers of ten are numbers that can be achieved by multiplying 10 times itself
- These come under two categories of units:
    - **Multiples** e.g. 10^2, 10^3
    - **Sub-multiples** e.g. 10^{-1}, 10^{-2}
- Each power of ten is defined by a prefix, the most common ones used in chemistry are listed in the table below
    - The complete list of prefixes can be found in Section 3 of the data booklet

Table of common prefixes in chemistry

Prefix	Abbreviation	Power of ten
kilo-	k	10^3
centi-	c	10^{-2}
milli-	m	10^{-3}
micro-	μ	10^{-6}
nano-	n	10^{-9}

pico-	p	10^{-12}

Your notes

Example conversions

- A mass of 5.2 kg
  - 5.2 kg = 5.2 **kilo**grams = 5.2 x 10^3 = 5200 grams
- The diameter of an aluminium atom is 184 pm
  - 184 pm = 184 **pico**metres = 184 x 10^{-12} m
  - Correctly given in standard form, this is a value of 1.84 x 10^{-10} m
- The energy required to heat 10 dm^3 of liquid water at constant pressure from 0 °C to 100 °C is approximately 4.2 MJ
  - 4.2 MJ = 4.2 **mega**joules = 4.2 x 10^6 = 4 200 000 J

Symbols in chemistry

- There is a large number of symbols used in chemistry:
  - State symbols
    - e.g. solid (s), liquid (l), gas (g)
  - Chemical symbols – from the Periodic Table, Section 7 of the data booklet
    - e.g. lithium = Li, carbon = C, Copper = Cu
  - Physical constants - given in Section 2 of the data booklet
    - e.g. Planck's constant = h, the speed of light in a vacuum = c
  - Terms in equations - relevant equations are given in Section 1 of the data booklet
    - e.g. $n = CV$, where n is the number of moles, C is the concentration and V is the volume
  - Units for quantities
    - e.g. specific heat capacity measured in $J\,g^{-1}\,K^{-1}$
  - Other abbreviations used in chemistry
    - e.g. STP for standard temperature and pressure

- While the data booklet can assist with using the correct symbols, it is essential to know the symbols specifically linked to physical constants, terms in equations and units for quantities
  - For example, the letter c, depending on capitalisation (c or C), could represent:
    - The speed of light in a vacuum in the $c = f\lambda$ equation
    - The specific heat capacity in the $Q = mc\Delta T$ equation
    - Concentration in the $n = CV$ equation
    - The units of electrical charge
    - The prefix centi-, e.g. cm^3
    - The centigrade / Celsius units of temperature
    - The chemical symbol for carbon
    - The symbol for combustion in the enthalpy of combustion term ΔH_c^{θ} term (if subscripts are included)

What are significant figures?

- Significant figures must be used when dealing with quantitative data

Your notes

- Significant figures are the digits in a number that are **reliable** and **absolutely necessary** to indicate the quantity of that number
- There are some important **rules** to remember for significant figures
  - All non-zero digits are significant
  - Zeros between non-zero digits are significant
    - 4107 (4.s.f.)
    - 29.009 (5.s.f)
  - Zeros that come before all non-zero digits are not significant
    - 0.00079 (2.s.f.)
    - 0.48 (2.s.f.)
  - Zeros after non-zero digits within a number without decimals are not significant
    - 57,000 (2.s.f)
    - 640 (2.s.f)
  - Zeros after non-zero digits within a number with decimals are significant
    - 689.0023 (7.s.f)
- When rounding to a certain number of significant figures:
  - Identify the significant figures within the number using the rules above
  - Count from the first significant figure to the specified number
  - Use the next number as the 'rounder decider'
  - If the decider is 5 or greater, increase the previous value by 1
- The same approach can be applied to decimal places, although significant figures are more common

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✏️ Worked example

Write 1.0478 to 3 significant figures.

Answer:

1. Identify the significant figures
   - They are all significant figures
2. Count to the specified number
   - The question says to 3 significant figures, so the fourth digit is the 'rounder decider'
   - 1.04**7**8
3. Round up or down
   - 1.05

💡 Examiner Tip

- Exam questions sometimes state:
  - To give an answer to a certain number of significant figures, commonly 3
  - To give an answer to an appropriate number of significant figures
- Make sure you keep an eye out for this as it can be an easy and frustrating mark to lose after all your hard work in the calculation

Your notes

An appropriate number of significant figures

- The appropriate number of significant figures depends on:
  - The precision of the measurement
  - The limitations of the equipment used to make the measurement
- When performing calculations involving measured values, it's essential to maintain the proper number of significant figures throughout the calculation to avoid rounding errors
  - An easy way to avoid rounding errors is to continue using the calculator value until the final answer
  - **Tip:** Avoid rounding any calculation to 1 significant figure during a calculation as this typically introduces rounding errors and can sometimes, automatically, lose you a mark
- In the final result, the number of significant figures should not exceed the value with the least number of significant figures used in the calculation

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✏️ Worked example

Calculate the number of moles in 35.75 cm^3 of a 0.015 mol dm^{-3} solution of HCl. Give your answer to an appropriate number of significant figures.

Answer:

- Convert 35.75 cm^3 to dm^3
  - $\dfrac{35.75}{1000}$ = 0.03575 dm^3
- Moles = concentration x volume
  - Moles = 0.015 x 0.03575 = 5.3625 x 10^{-4}
- The volume is given to 4 significant figures
- The concentration is given to 2 significant figures
  - Therefore, the appropriate number of significant figures is 2
- So, the final answer is **5.36 x 10^{-4} moles**

💡 Examiner Tip

- For numbers such as the Avogadro constant and Gas constant, the number of significant figures is not limited by measurement precision but rather by the definition of the constant itself
- In these cases, use the defined number of significant figures provided for that constant
  - e.g. Avogadro = 6.02 x 10^{23} mol^{-1} has 3 significant figures

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Your notes

Processing Uncertainties in Chemistry

Processing Uncertainties in Chemistry

What is uncertainty?

- Uncertainty is **quantitative** indication of the quality of the result
  - It is the difference between the **actual** reading taken (caused by the equipment or techniques used) and the **true value**
  - It is a range of values around a measurement within which the true value is expected to lie and is an **estimate**
- Uncertainties are **not** the same as errors
  - Errors arise from equipment or practical techniques that cause a reading to be different from the true value
- Uncertainties in measurements are recorded as a range (±) to an appropriate level of precision

Table showing different uncertainties

	Uncertainty
in a reading	± half the smallest division
in a measurement	at least ±1 smallest division
in repeated data	half the range i.e. ± ½ (largest – smallest value)
in digital readings	± the last significant digit (unless otherwise quoted)

Types of uncertainty

- Uncertainty is grouped into three main types:
  - **Absolute uncertainty**

    - The actual amount by which the quantity is uncertain
    - e.g. if v = 5.0 ± 0.1 cm, the absolute uncertainty in v is 0.1 cm
  - **Fractional uncertainty**

    - The absolute uncertainty divided by the quantity itself
    - e.g. if v = 5.0 ± 0.1 cm, the fractional uncertainty in v is $\dfrac{0.1}{5.0} = \dfrac{1}{50}$
  - **Percentage uncertainty**

    - The ratio of the expanded uncertainty to the measured quantity on a scale relative to 100%

- This is calculated using the following formula:

$$\text{Percentage uncertainty} = \frac{\text{uncertainty}}{\text{measured value}} \times 100$$

How to calculate absolute, fractional and percentage uncertainty
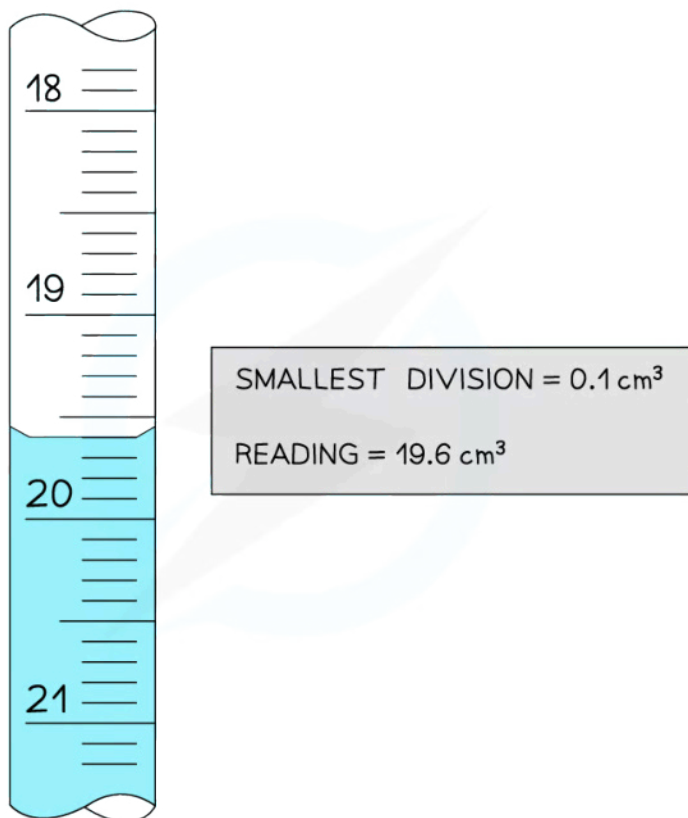
SMALLEST DIVISION = 0.1 cm^3

READING = 19.6 cm^3

The key pieces of information from this burette reading are the smallest division and the reading

- The uncertainties in this reading are:
  - Absolute
    - Uncertainty = $\dfrac{0.1}{2}$ = 0.05 cm^3
    - Reading = $19.6 \pm 0.05 \text{ cm}^3$
  - Fractional
    - Uncertainty = $\dfrac{\text{uncertainty}}{\text{value}}$ = $\dfrac{0.1}{19.6}$ = $\dfrac{1}{196} \text{ cm}^3$
  - Percentage

Your notes

- Uncertainty = $\dfrac{\text{uncertainty}}{\text{value}} \times 100 = \dfrac{0.1}{19.6} \times 100 = 0.5\%$
- Reading = $19.6 \pm 0.5\% \text{ cm}^3$

Propagating uncertainties in processed data

- Uncertainty propagates in different ways depending on the type of calculation involved

Adding or subtracting measurements

- When you are adding or subtracting two measurements then you add together the **absolute** measurement uncertainties
- For example,
  - Using a balance to measure the initial and final mass of a container
  - Using a thermometer for the measurement of the temperature at the start and the end
  - Using a burette to find the initial reading and final reading
- In all of these examples, you have to read the instrument twice to obtain the quantity
  - If each time you read the instrument the measurement is 'out' by the stated uncertainty, then your final quantity is potentially 'out' by twice the uncertainty

Multiplying or dividing measurements

- When you multiply or divide experimental measurements then you **add** together the **percentage uncertainties**
- You can then calculate the **absolute uncertainty** from the sum of the percentage uncertainties

Exponential measurements (HL only)

- When experimental measurements are raised to a power, you multiply the fractional or percentage uncertainty by the power

The coefficient of determination, R^2

- The **coefficient of determination** is a **measure of fit** that can be applied to lines and curves on graphs
- The coefficient of determination is written as R^2
- It is used to evaluate the fit of a trend line / curve:
  - **$R^2 = 0$**
    - The dependent variable cannot be predicted from the independent variable.
    - R^2 is usually greater than or equal to zero
  - **R^2 between 0 and 1**
    - The dependent variable can be predicted from the independent variable, although the degree of success depends on the value of R^2
    - The closer to 1, the better the fit of the trend line / curve
  - **$R^2 = 1$**
    - The dependent variable can be predicted from the independent variable
    - The trend line / curve is perfect
    - **Note:** This does not guarantee that the trend line / curve is a good model for the relationship between the dependent and independent variables
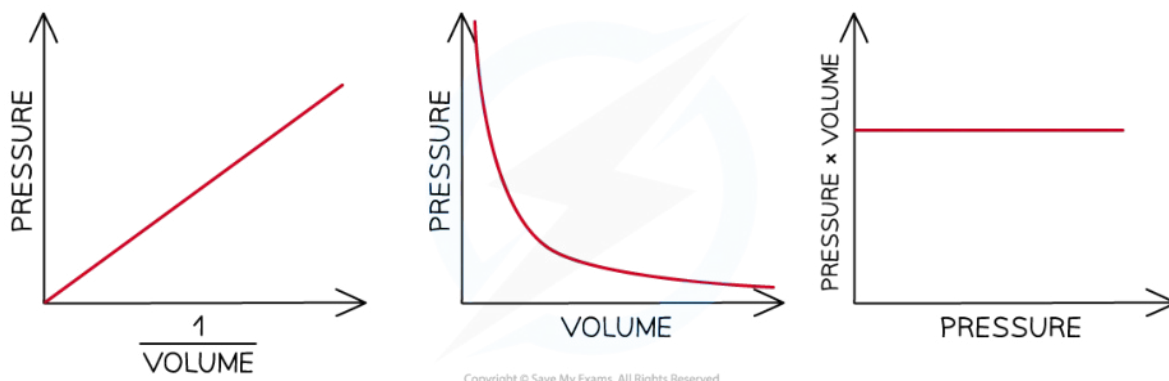
Your notes

Graphing in Chemistry

Graphing in Chemistry

Sketch graphs

- **Sketch graphs** are a way to represent qualitative trends where the variables shown are often **proportional** or **inversely proportional**
- Sketch graphs do not have scales or data points, but they must have labels as these examples from the Gas Laws show:

Sketch graphs of Boyle's Law

*Sketched graphs show relationships between variables*

Graphical Relationships

- In the first sketch graph above you can see that the relationship is a straight line going through the origin
  - This means as you double one variable the other variable also doubles so we say the independent variable is **directly proportional** to the dependent variable
- The second sketched graph shows a shallow curve which is the characteristic shape when two variables have an **inversely proportional** relationship
- The third sketched graph shows a straight horizontal line, meaning as the independent variable (x-axis) increases the dependent variable does not change or is **constant**

🔵 **Worked example**

Which graph shows the correct relationship between the number of moles of a gas, n, and the temperature, T, at constant pressure and volume?
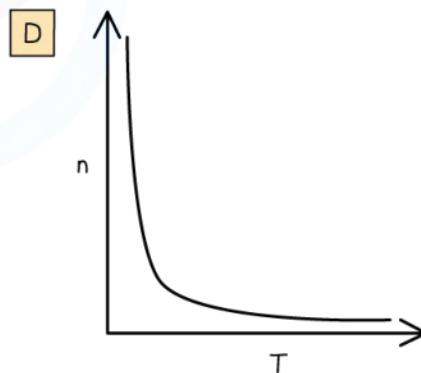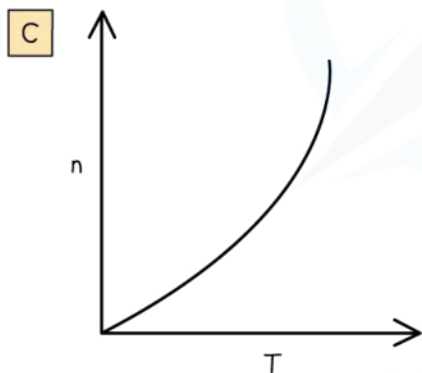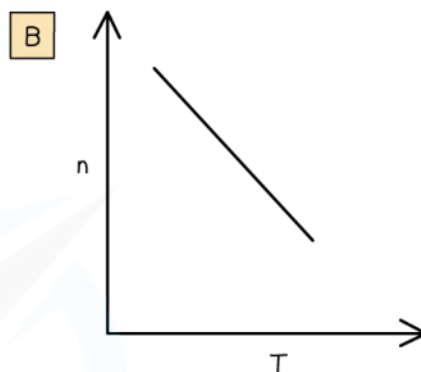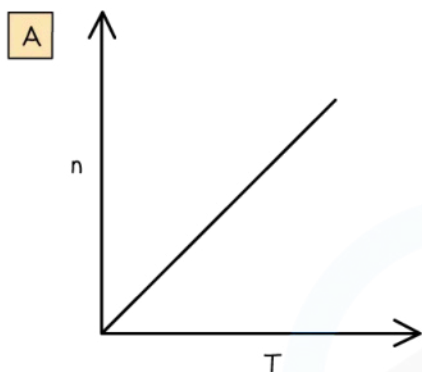
Answer:

- The correct option is **D**
  - The ideal gas equation is $PV = nRT$
  - If P, V and R are constant then $PV / R = nT$, which is a constant
  - n must be inversely proportional to T, which gives graph **D**

General guidance on drawing graphs

- The types of graphs that students are expected to be able to draw include:
  - Bar charts
  - Histograms
  - Scatter graphs
  - Line / curve graphs
- Graphs need to have:
  - Clear title

- Labelled axes
- Units on the axes
- Appropriate linear scales without any jumps
  - This means the plotted graph must occupy at least half or more of the sheet or grid
  - A rough rule of thumb is that if you can double the scale and still fit all the points on, then your scale is not appropriate
- Clearly shown data points
  - The most common convention is to use small crosses to show the data points

Graph of concentration versus time
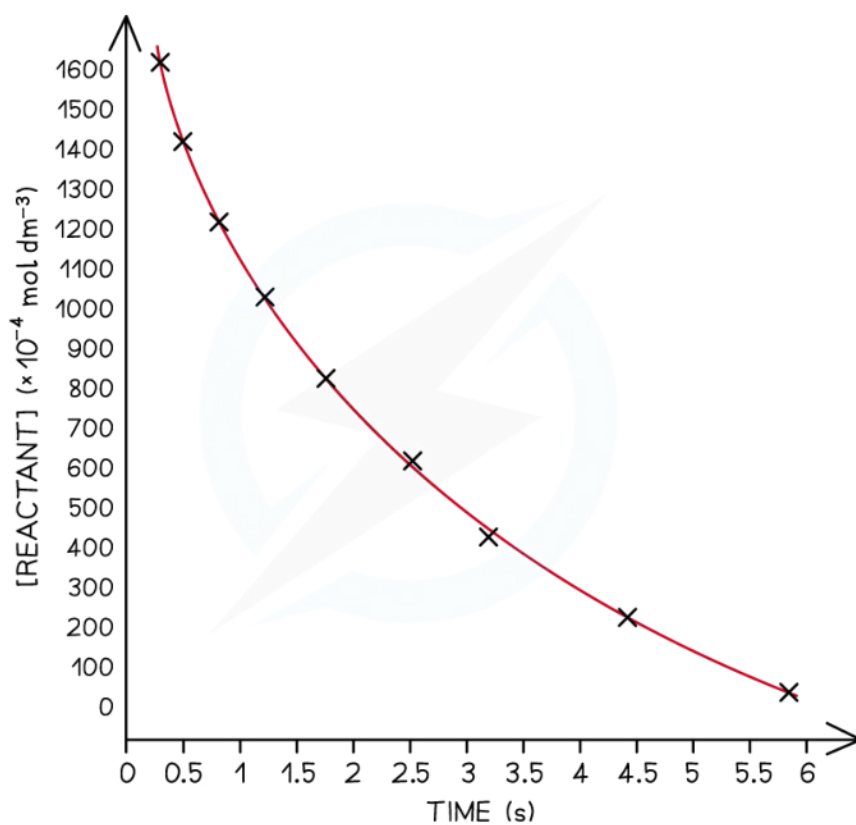
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Graphs must show appropriate scales, labelling and units. The independent variable usually goes on the x-axis and the dependent variable on the y-axis

- **Remember:** The independent variable is the one you control or manipulate and the dependent variable is the one that changes as a result of your manipulation
- Always draw data points in pencil as it makes it easier to make corrections and adjustments

Best Fit Lines

- Students often confuse the term **lines of best fit** with straight lines

- **Lines of best fit** can be straight lines or curves (just like the example above) and:
  - They show the trend of the data
    - It does not have to go through all the points, but shows the general trend
  - They must go through the majority of the points
  - Where the data is scattered the points should be evenly distributed on either side of the **best fit line**
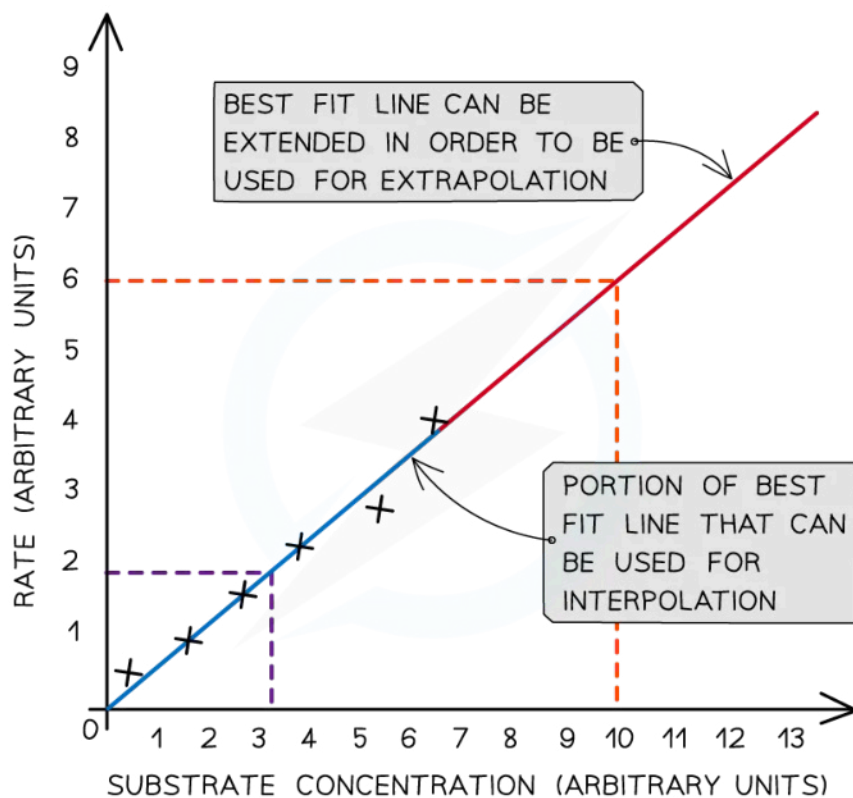
Extrapolation and interpolation

- **Extrapolation** is the term used to describe the process of extending a line of best fit

Extrapolation on a temperature correction graph

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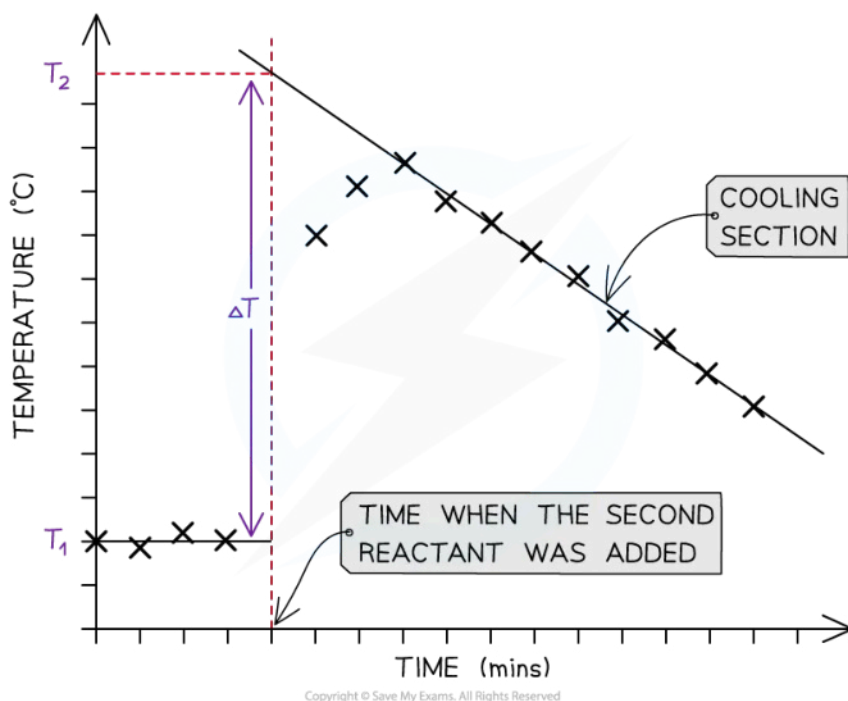
This temperature correction graph from a calorimetry investigation shows how the two best fit lines are extrapolated to find the maximum temperature rise

- **Interpolation** is the term used to describe the process of assuming a trend line applies between two points

Extrapolation and interpolation on a graph

✏️
Your notes

Interpolation uses the line of best fit within the plotted points and extrapolation extends the best fit line beyond the plotted points

---

💡 **Examiner Tip**

- You will have to decide if the origin, point (0,0) should be included as a data point
- If it does, it will be a good place to anchor the graph as it will be the most accurate data point


Other features of graphs

Gradient

- The gradient of a graph can be found by:
  - For straight-line graphs
    - Draw a triangle
    - Then, use the equation for a straight line
  - For curves
    - Draw a **tangent** to the graph, using a ruler to line up against the curve at the point where the gradient is to be measured
    - Then, use the equation for a straight line to calculate the gradient

How to draw a tangent to a curve

Your notes
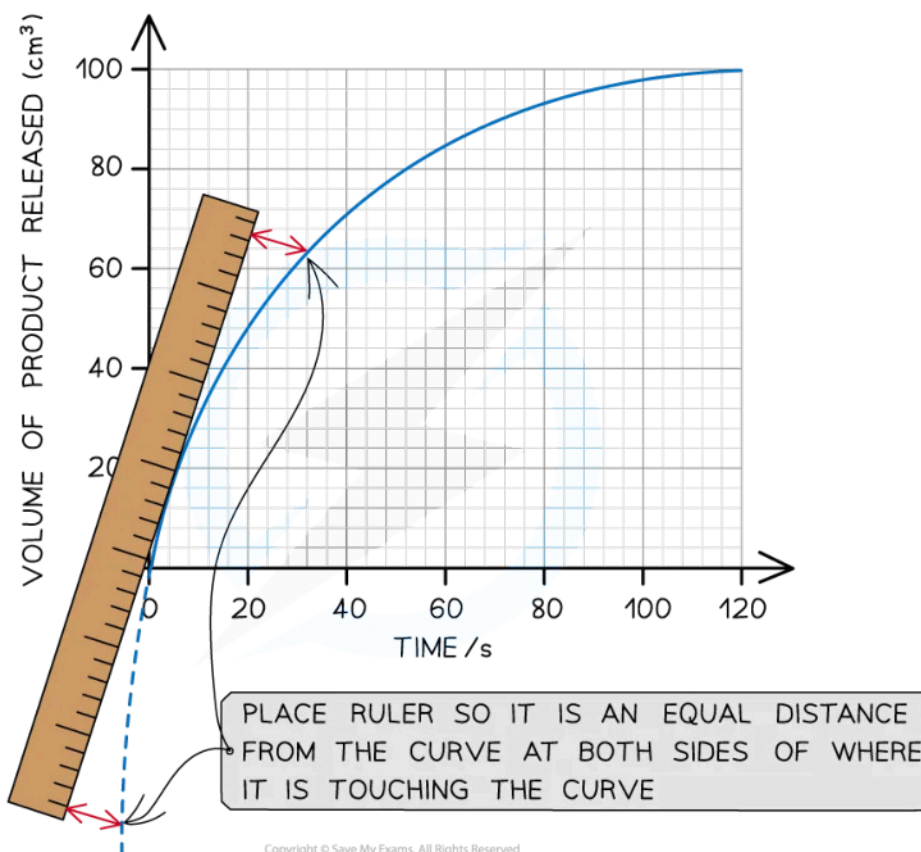
Lining up a ruler against the curve is essential to drawing a tangent accurately

- The triangle should be as large as possible to minimise precision errors
- The equation for a straight line is **y = mx + c**, where:
    - **y = dependent variable**
    - **x = independent variable**
    - **m = slope**
    - **c = y–intercept**
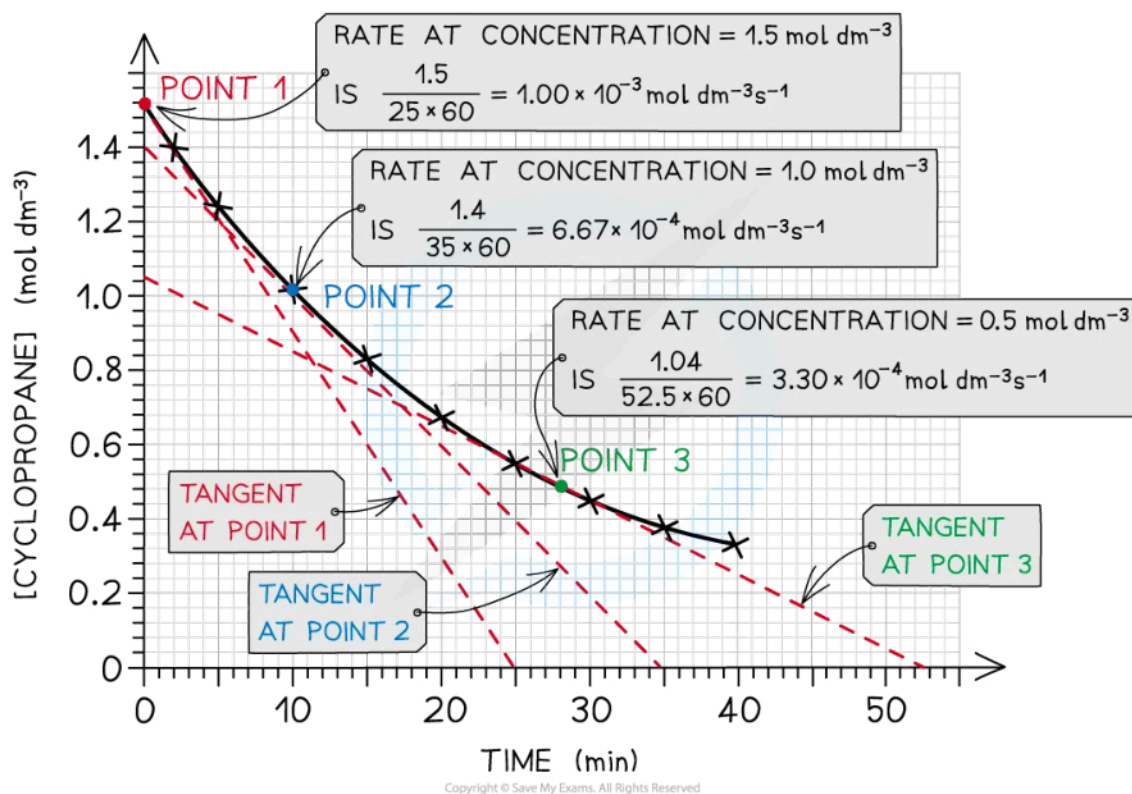- Therefore, the **gradient** or slope, **m = Δy / Δx**

Changes in gradient

- Graphs with curves of best fit have changing gradients
- This means that multiple gradients can be calculated to show:
    - The progressing rate of a reaction
    - The effects of factors, such as concentration, on the rate of reaction
   **A rate kinetics graph illustrating the calculation of rates from a curve**

RATE AT CONCENTRATION = 1.5 mol dm^{-3} IS $\dfrac{1.5}{25 \times 60}$ = 1.00 × 10^{-3} mol dm^{-3}s^{-1}

RATE AT CONCENTRATION = 1.0 mol dm^{-3} IS $\dfrac{1.4}{35 \times 60}$ = 6.67 × 10^{-4} mol dm^{-3}s^{-1}

RATE AT CONCENTRATION = 0.5 mol dm^{-3} IS $\dfrac{1.04}{52.5 \times 60}$ = 3.30 × 10^{-4} mol dm^{-3}s^{-1}

The gradient can be found at different points on a curve. Each rate has been multiplied by 60 to convert it from minutes^{-1} to seconds^{-1}

Intercepts

- Intercepts are the points where a line / curve of best fit crosses an axis on a graph
- The most common use of intercepts is in graphs of free energy versus temperature

Graph of free energy versus temperature for the synthesis of ammonia

Your notes

GRADIENT $m = -\Delta S = 0.0994 \, kJ/K/mol$

$y = 0.0994x - 46.153$
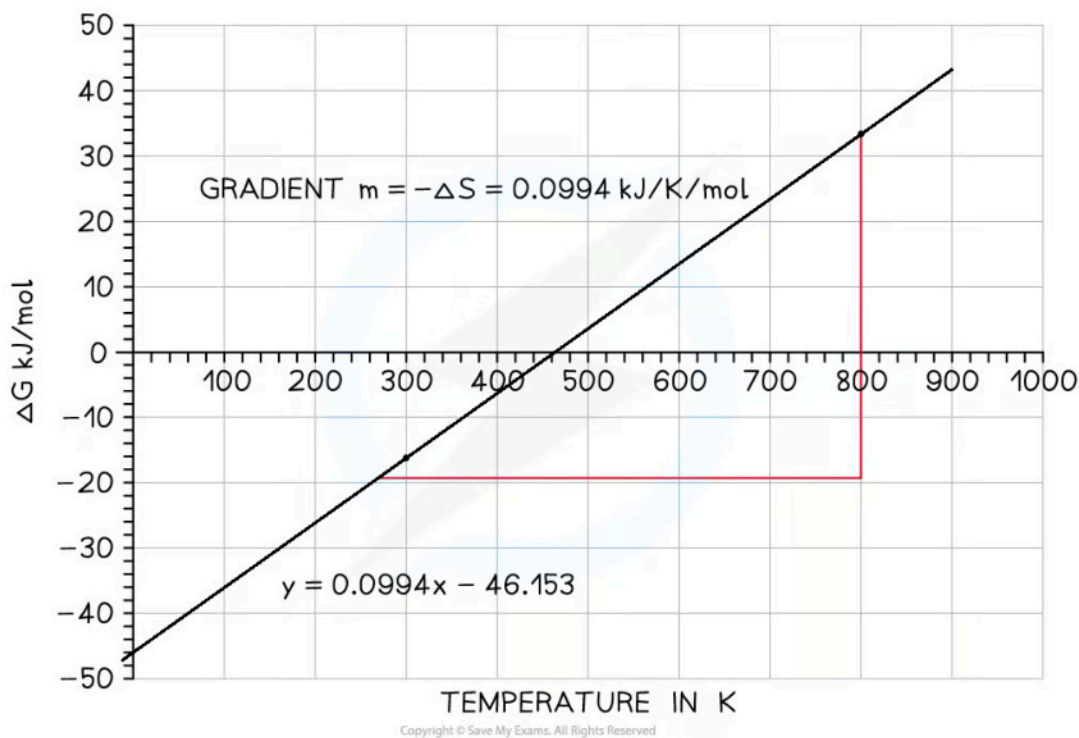
TEMPERATURE IN K

The x-intercept shows the temperature when the reaction ceases to be feasible, in this case at 460 K (187 °C) and the y-intercept shows that the reaction is exothermic as the extrapolated value is approximately –46 kJ mol^{-1}
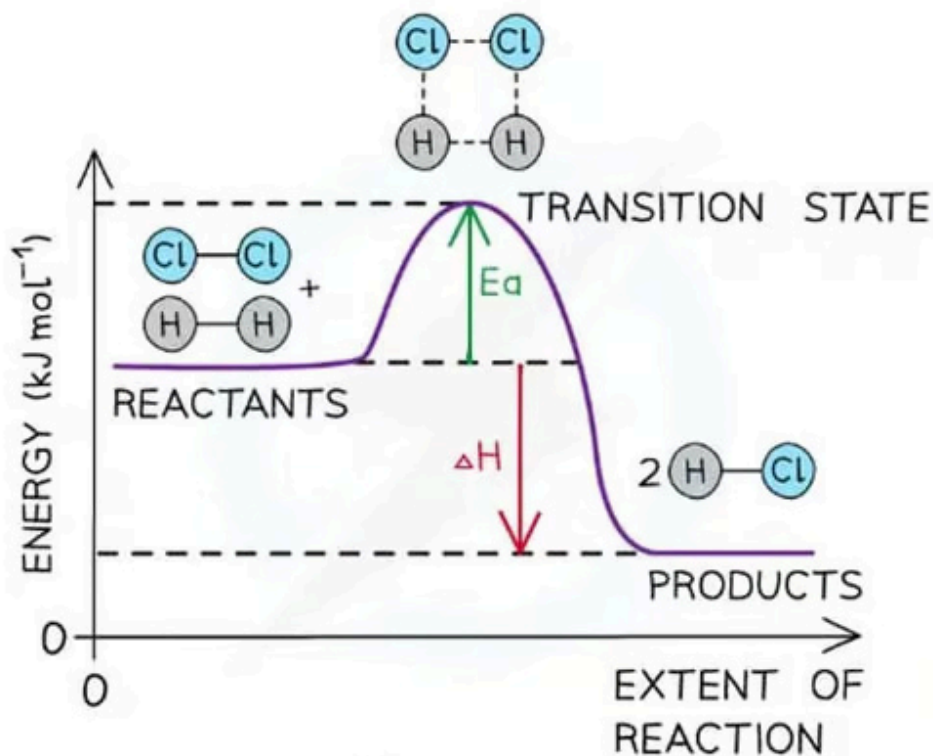
Maxima and minima

- The **maxima** and **minima** are the highest and lowest points respectively
  - Maxima - the gradient goes from positive to 0 to negative
  - Minima - the gradient goes from negative to 0 to positive
- A literal application of maxima and minima is in energy profile diagrams

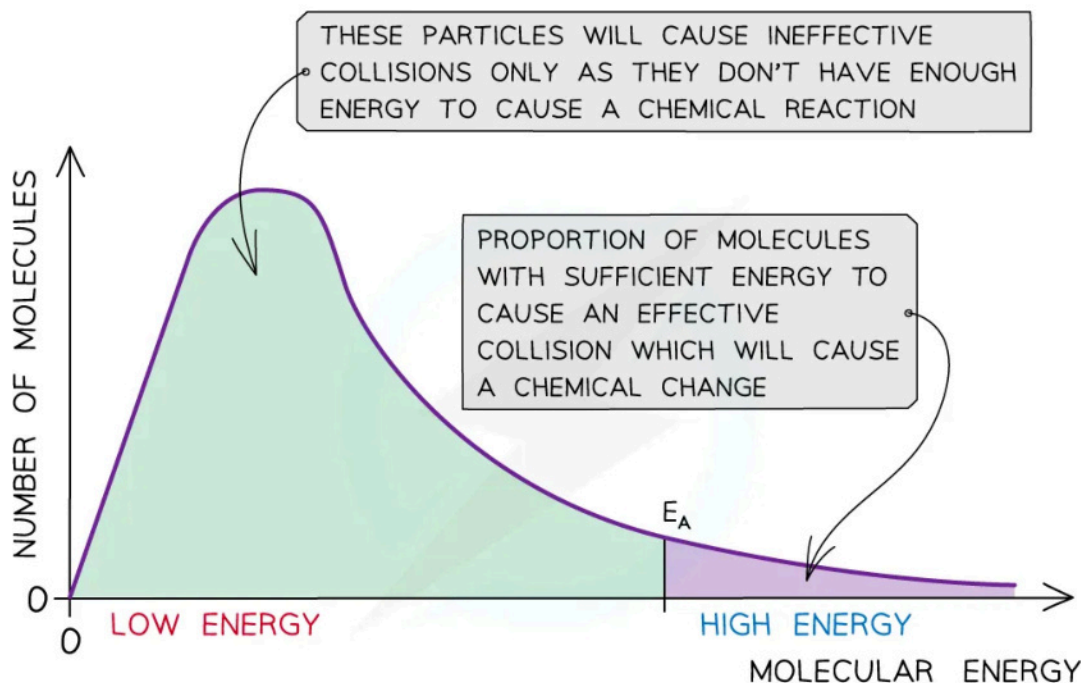**The energy profile diagram for $H_2 + Cl_2 \rightarrow 2HCl$**

Maxima represent the energy of the transition state and minima represent the energy of the reactants and products

Areas

- A common use of areas of graphs in chemistry is Maxwell–Boltzmann curves

A Maxwell–Boltzmann distribution curve

The total area under the curve represents the total number of molecules / particles, while the E_a line further divides this area into particles with and without the minimum activation energy to react

Uncertainty bars

- The uncertainty in a measurement can be shown on a graph as an uncertainty bar
  - This bar is drawn above and below the point and shows the uncertainty in that measurement
- Uncertainty bars are plotted on graphs to show the absolute uncertainty of values plotted
  - Usually, these bars will be in the vertical direction, for y-values but they can be plotted horizontally, for x-values
- The size of the uncertainty bar can be used as an indication of the amount of error / uncertainty in the measurement

Graph to show uncertainty bars
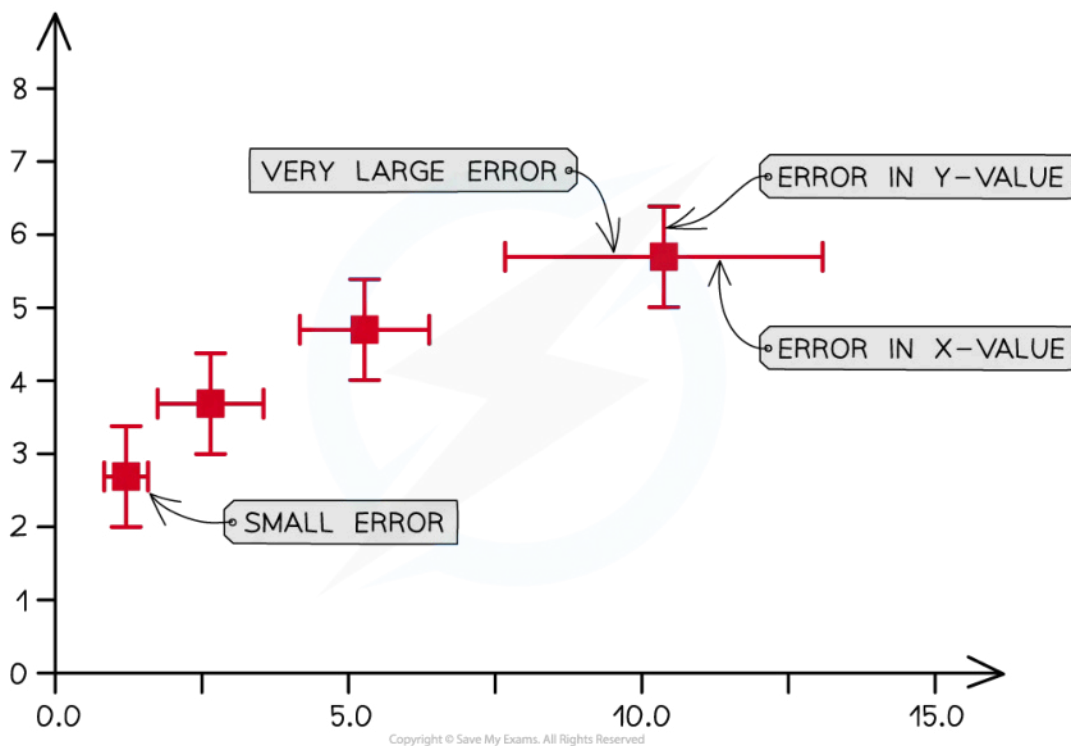
Uncertainty bars show the error / uncertainty in a specific measurement