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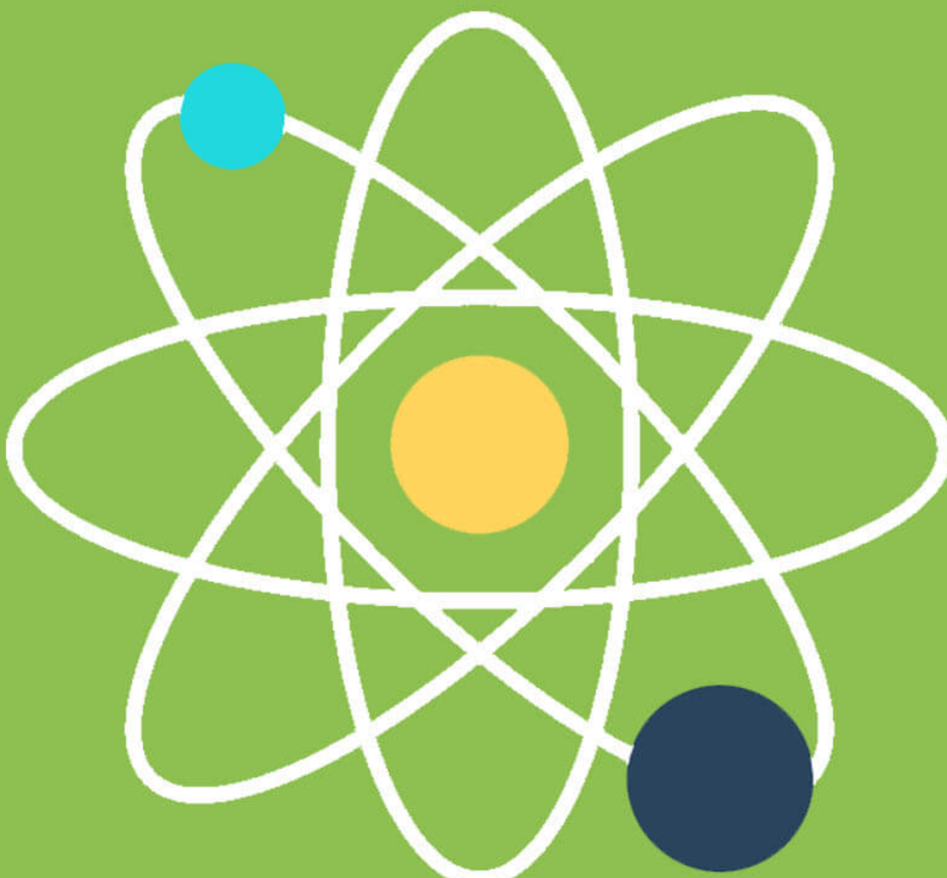
11.2 Synoptic Data Handling & Graphical Skills



IB Chemistry - Revision Notes

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11.2.1 Recording Data

Qualitative & Quantitative data

- When recording results of experiment, both **quantitative** and **qualitative** data should be obtained
- **Quantitative data** is obtained from measurements whereas **qualitative data** is non-numerical information that comes from observations
- **Quantitative data** is always associated with random errors/uncertainties, determined by the apparatus, and by human limitations such as reaction time
- Where there are several items of data you should record your data in a table with appropriate **headings** and **units**:

Data Table showing headings and units

Measurement	$[CaCO_3]$ (mol dm^{-3})	$[Cl^-]$ (mol dm^{-3})	$[H^+]$ (mol dm^{-3})	Initial rate of reaction (mol dm^{-3}s^{-1})
1	0.0250	0.0125	0.0125	4.38×10^{-6}
2	0.0375	0.0125	0.0125	6.63×10^{-6}
3	0.00625	0.0250	0.0250	2.19×10^{-6}

Uncertainties

- **Uncertainties** are the same as **random errors**
- **Uncertainties** express the confidence to which the measurement can be taken
- Treatment of **uncertainties** depends on the type of instrument used

Using analogue instruments

- Any instruments that have an **analogue scale**, the uncertainty is taken as **half the smallest division** on the scale
- For example,
  - A thermometer that reads to 1°C, the uncertainty would be ±0.5 °C
  - A burette that reads to 0.10 mL, the uncertainty would be ±0.05 mL

Using digital instruments

- Any instruments that have a **digital scale**, the uncertainty is taken as the **smallest division** on the scale
- For example,
  - An electronic balance that reads to 0.01 g, the uncertainty would be ±0.01 g

Other uncertainties

- Other sources of uncertainty can arise where the judgement of the experimenter is needed to determine a changing property
- For example,
  - Judging the end point of a **titration** by looking at the colour of the **indicator**
  - Controlling a stopwatch in a rate of reaction experiment
  - Deciding when to extinguish the flame in an **enthalpy of combustion** experiment
- These uncertainties are very difficult to quantify, but they should be commented on as a source of error in an **evaluation**

Exam Tip

Notice that when recording the measurement you should always record it to the same level of precision as the uncertainty. The measurement cannot be any more or less precise than the uncertainty. Even though a burette reads to 0.1 mL, it must be recorded as 0.10 mL, so the last digit is always a 0 or a 5

11.2.2 Processing Errors

Types of Errors

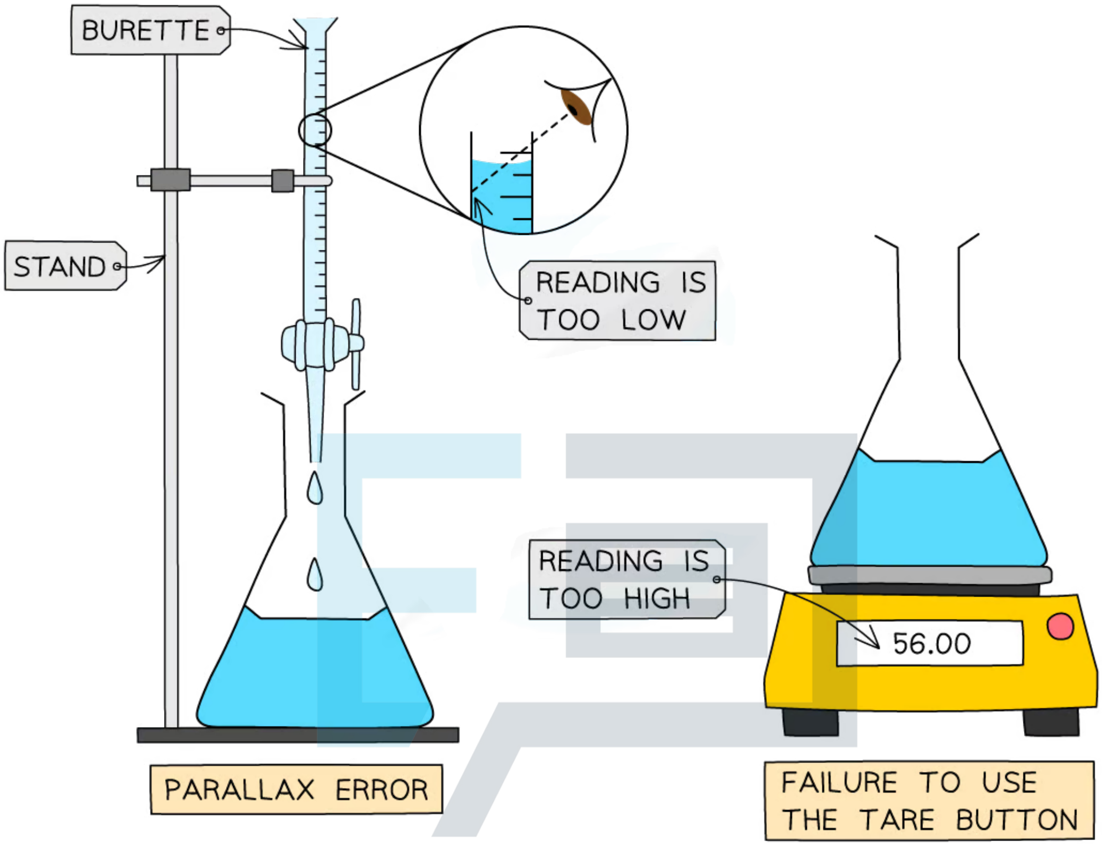
- An error is the difference between a value or quantity obtained in an experiment and an accepted or literature value for an experiment
- There are two types of errors in experiments, **random errors** and **systematic errors**

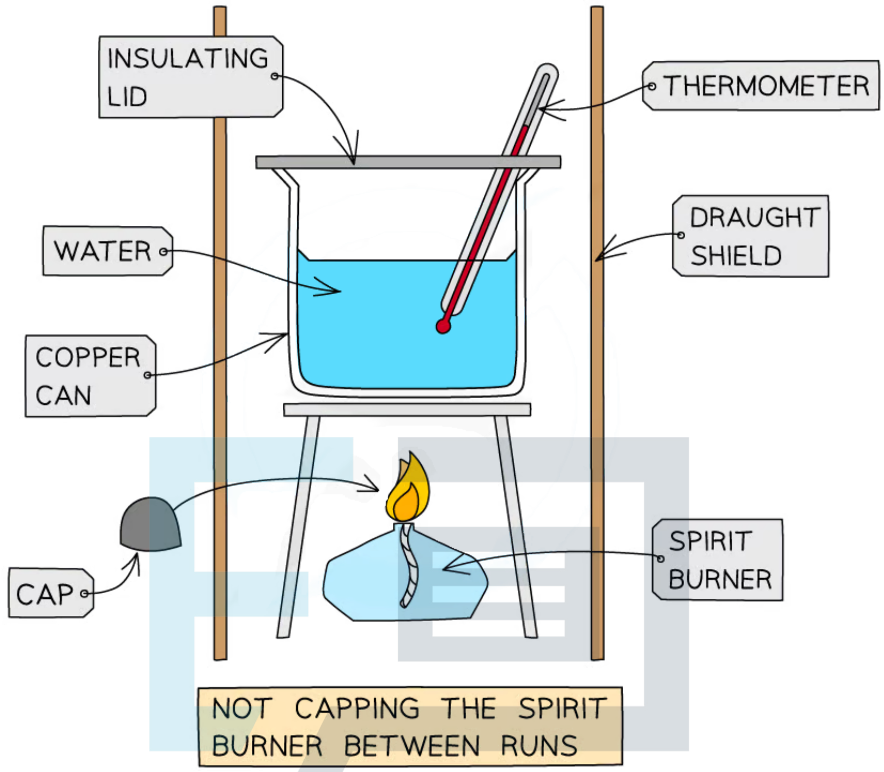
Random Errors

- When you are reading an instrument and estimate the final digit, there is an equal chance that you may read it slightly too high or slightly too low
  - This is a **random error**
- **Random errors** are can be affected by:
  - How easily the instrument or scale is to read
  - The person reading the scale poorly
  - Changes in the environment, for example
    - fluctuations in the temperature of the lab
    - air currents in the room
- **Random errors** will pull a result away from an accepted value in either direction (either too high or too low)

Systematic Errors

- **Systematic errors** are errors that occur as a result of a faulty or poorly designed experimental procedure
- **Systematic errors** will always pull the result away from the accepted value in the **same** direction (always too high or always too low)
- For example,
  - If you forget to zero an electronic balance (using the tare button) the mass weighings will always be higher than they should be
  - If you don't read the volume in a burette at eye level, the volumes will always be smaller than they should be due to a parallax error
  - If you fail to keep a cap on a spirit burner in a calorimetry experiment, the alcohol will evaporate and give you a larger mass loss


BURETTE
STAND
READING IS TOO LOW
READING IS TOO HIGH
56.00
PARALLAX ERROR
FAILURE TO USE THE TARE BUTTON



Systematic errors

Propagation of Errors

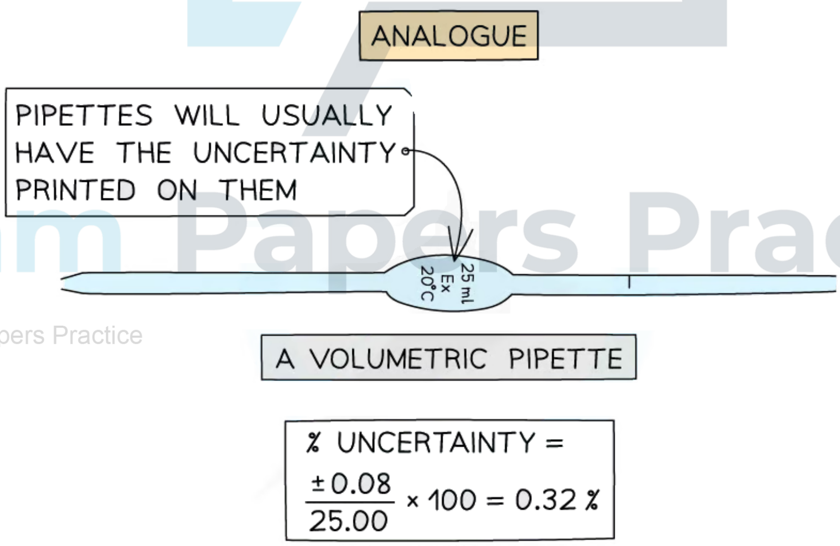
- **Propagation of errors** means the processing of errors so they are reflected appropriately in a final calculation based on experiment results
- There are a number of rules and processes to follow, beginning with **percentage uncertainty**

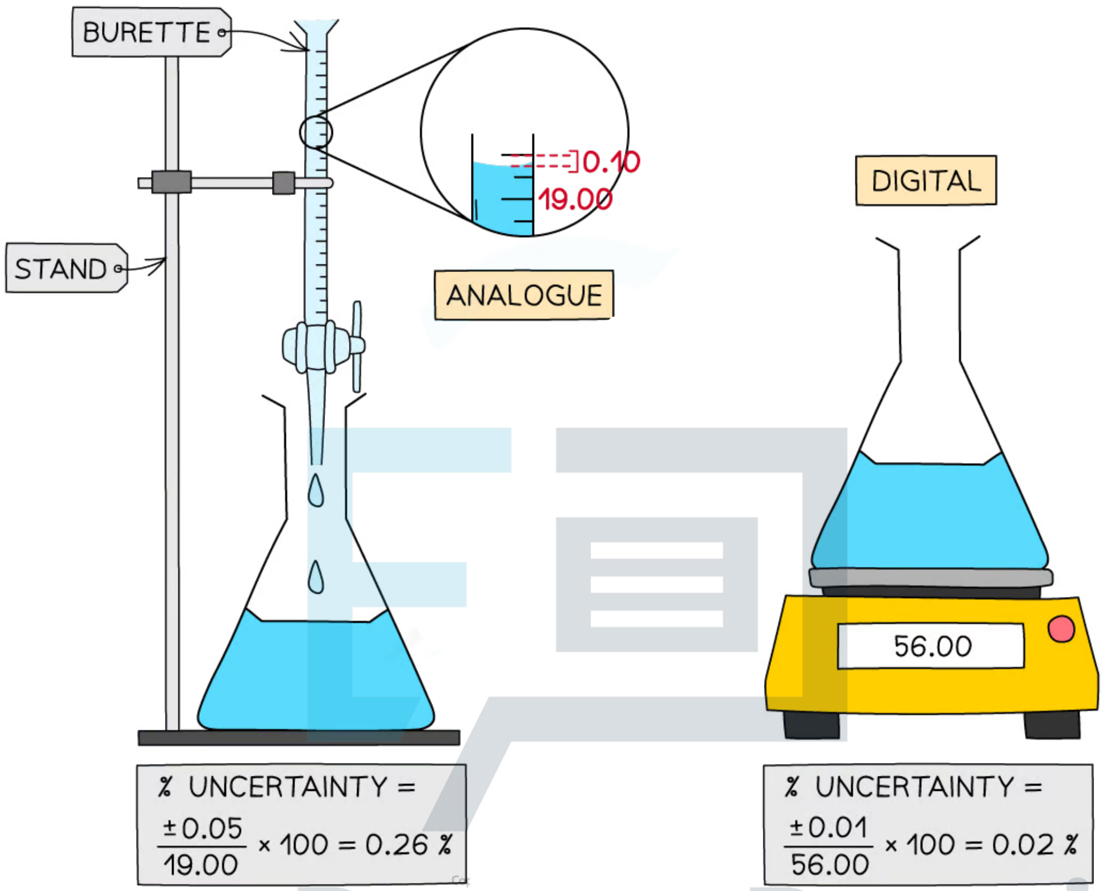
Percentage Uncertainties

- **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
- The formula for calculating percentage uncertainty is as follows:

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

- Some examples of percentage uncertainty calculations for common laboratory apparatus:





Calculating Percentage Uncertainty

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 these examples you have to read the instrument **twice** to obtain the quantity
- If each you 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

Exam Tip

If you are multiplying or dividing data you should quote the answer to the same number of significant figures as the least precise data.

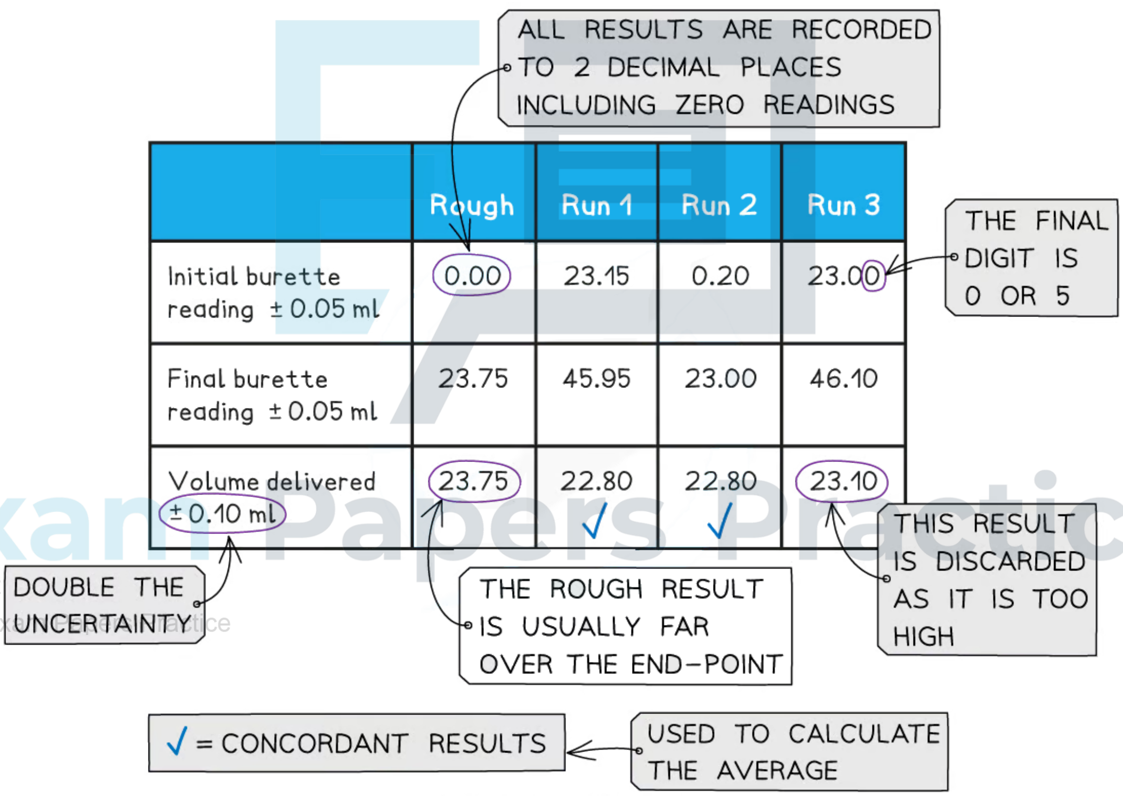
When you add or subtract data you should use the same number of decimal places as the least precise data value

11.2.3 Reducing the Impact of Errors

Reducing Errors

- **Random errors** can be reduced by repeated trials and measurements
- Multiple measurements when averaged will reduce the impact of a **random error** on the average
  - The more readings you have the lower the possibility that a **random error** will skew the results

- If you spot a **random error** in a data table then you can omit it in the calculation of an average
- For example, in a **titration** you can leave out results that are not concordant when finding the average **titre**:



	Rough	Run 1	Run 2	Run 3
Initial burette reading ± 0.05 ml	0.00	23.15	0.20	23.00
Final burette reading ± 0.05 ml	23.75	45.95	23.00	46.10
Volume delivered ± 0.10 ml	23.75	22.80 √	22.80 √	23.10

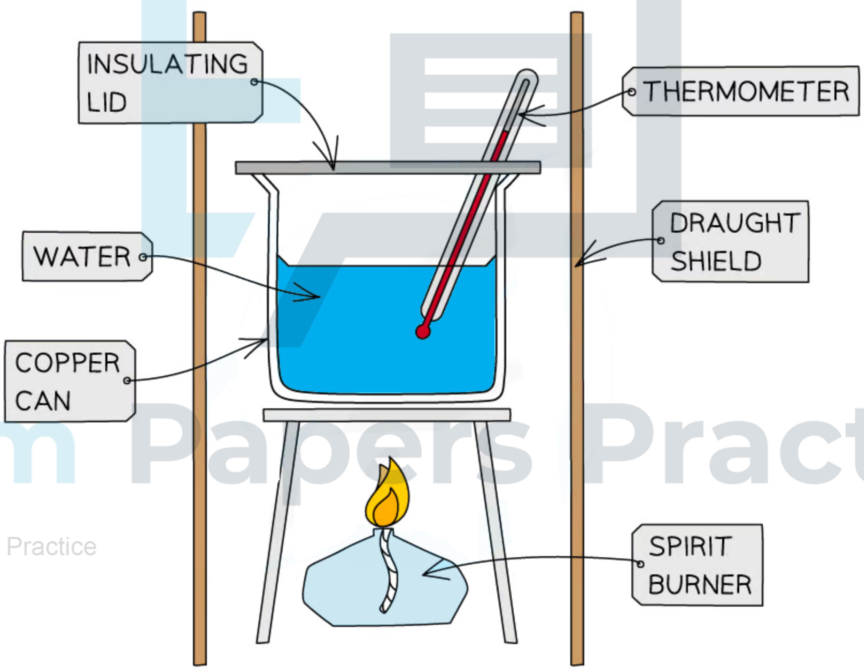
Calculating the average volume delivered in a titration should not include non-concordant volumes. Run 3 (and the Rough run) is omitted from the calculation of the average volume delivered

- **Systematic errors** cannot be reduced by repetition
- **Systematic errors** can only be reduced by changing the procedure and making sure you are using the instruments correctly

- If you cannot actively reduce **systematic errors** you must still try to identify them and comment on them in your evaluation

Impact of Errors

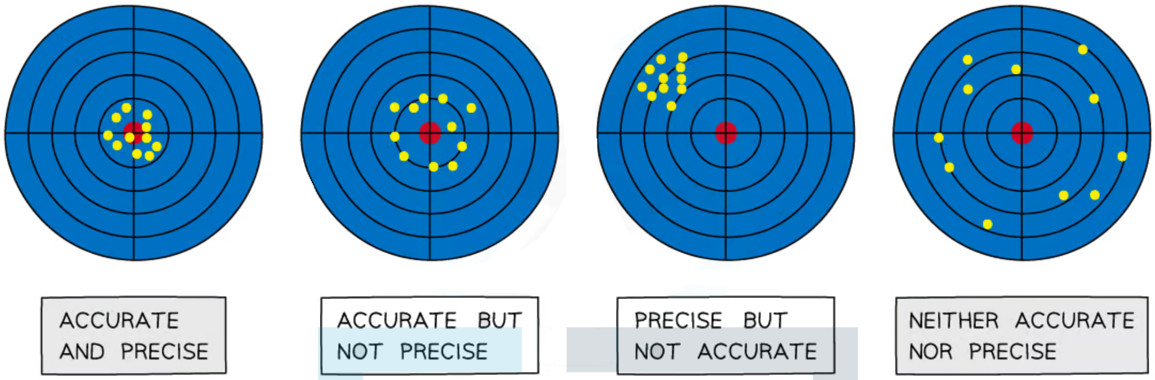
- A skill that is very important in data processing is the ability to discuss the **impact** of different types of errors on an experimental conclusion
- This is an integral part of the **Internal Assessment**, but it can also be examined in the written exam papers
- You should always evaluate **random errors** and **systematic errors** in an investigation
- This includes assessing the relative impact of errors, for example:
  - Whether a particular error has a major or minor effect on the final result
  - Which errors produce the largest impact on a final result



You should be able to state what the impact would be of not using a draught shield in a simple combustion calorimetry experiment

Accuracy & Precision

- **Accuracy** is how close you are to an accepted value
- **Precision** is a measure of how many decimal places you can express your results to
- Imagine you are shooting at a target: the following results show the difference between these concepts



Accuracy and precision in target shooting

- In practical chemistry terms, if you have a literature value for a final calculation, then it is very easy to compare how close you got to the literature value, in other words how **accurate** you were
  - For example in enthalpy of combustion experiments, did you get close to the Data Book value?
- Sometimes you can control precision by changing instrument
  - For example if you change from a two decimal place to three decimal place balance, you are making your measurements more **precise**

Worked example

Which of the following procedures could be used to reduce the random uncertainty while performing a titration?

A. Changing the burette

B. Reading the burette at eye level to the meniscus

C. Repeating the titration

D. Changing the indicator for the titration

Answer

The correct option is **C**.

Random errors can be reduced by repetition. All the other procedures would only affect systematic errors.

11.2.4 Percentage Error

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

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

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

Worked example

1.023 g of propan-1-ol (M = 60.11 g mol^{-1}) was burned in a spirit burner and used to heat 200 g of water in a copper calorimeter. The temperature of the water rose by 30 °C.

1. Calculate the enthalpy of combustion of propan-1-ol using this data.
2. The literature value for this enthalpy change is -2021 kJ mol^{-1}. Calculate the percentage error and comment on your findings

Answer 1:

Step 1: Calculate q

$q = m \times c \times \Delta T$

$q = 200\ g \times 4.18\ J\ g^{-1} K^{-1} \times 30\ K = -25\ 080\ J$

Step 2: Calculate the amount of propan-1-ol burned

moles = mass ÷ molar mass = 1.023 g ÷ 60.11 g mol^{-1} = 0.01702 mol

Step 3: Calculate ΔH

$\Delta H = q \div n = -25\ 080\ J \div 0.01702\ mol = -1\ 473\ 560\ J = -1474\ kJ =$ **-1.5×10^3 kJ**

Answer 2:

Using the formula

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

$$\text{percentage error} = \frac{2021 - 1500}{2021} \times 100\% = \mathbf{25\%}$$

Heat losses are likely to be the largest source of error in this experiment

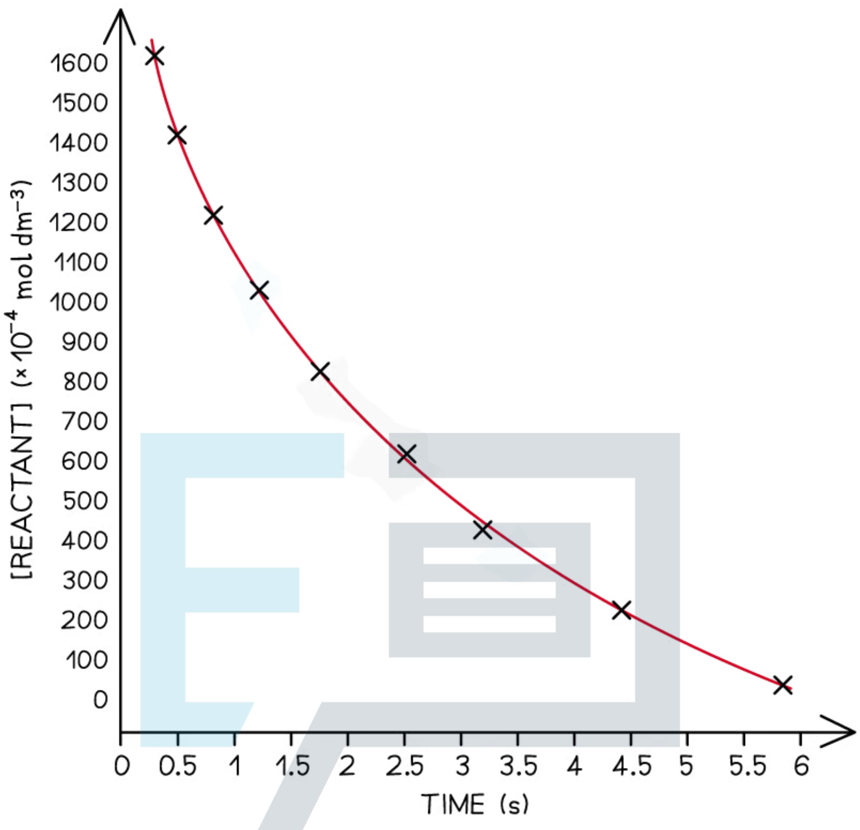
11.2.5 Drawing Graphs

Drawing Graphs

General guidance on drawing 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

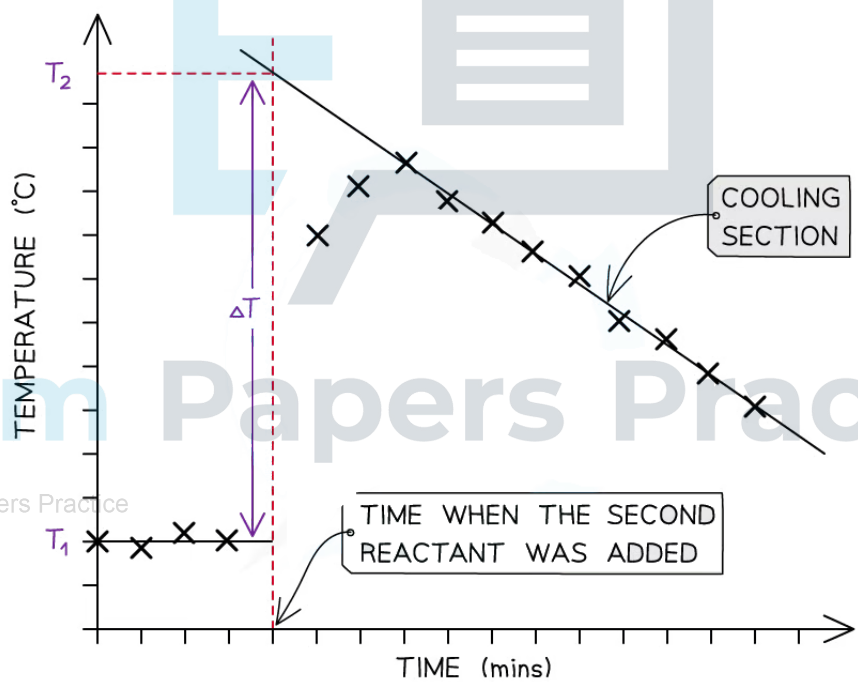


Graphs must shows appropriate scales, labelling and units. The independent variable usually goes on the x-axis and the dependent variable on the y-axis

- 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

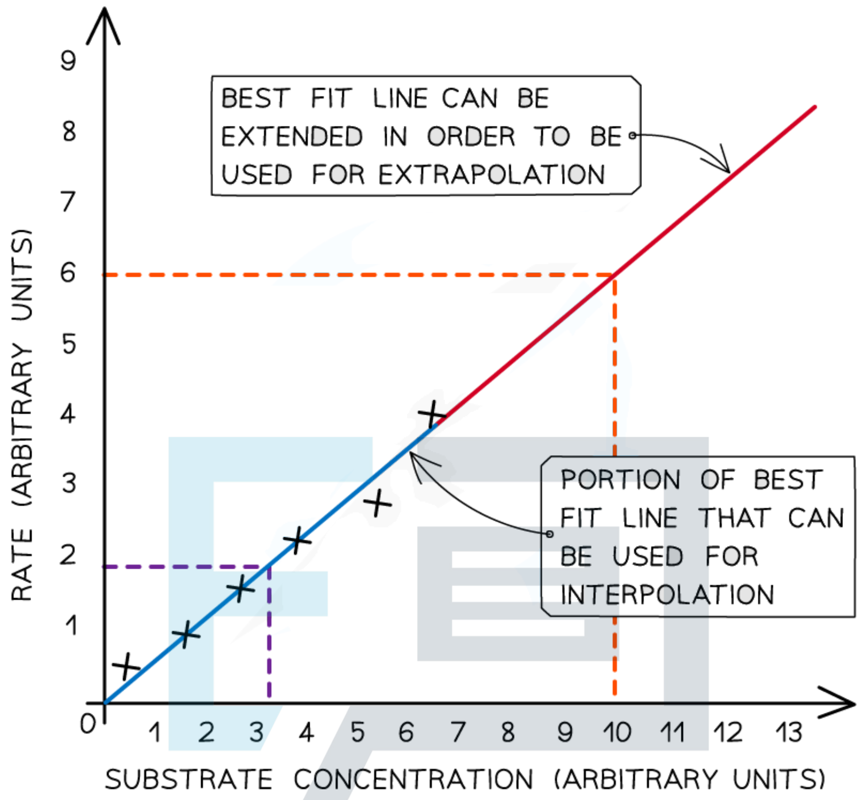
Best Fit Lines

- 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**
- Sometimes the **best fit line** has to be extended to find a value from a graph
  - This is called **extrapolation** as this example shows from a temperature correction graph in a calorimetry investigation where the cooling section is extrapolated to find the maximum temperature rise:



Extrapolation on a temperature correction graph

- **Interpolation** is the term used to describe the process of assuming a trend line applies between two points as this example below shows:



The difference between extrapolation and interpolation on a graph

Exam Tip

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