IB Chemistry DP

11. Measurements & Data Processes

**CONTENTS**

11.1 Spectroscopic Identification

11.1.1 Index of Hydrogen Deficiency

Index of Hydrogen Deficiency

- The **degree of unsaturation** or **index of hydrogen deficiency** provides information about the number of double or triple bonds in a molecule
- The **IHD** is the number of hydrogen molecules, H_2, needed to convert the molecule to the corresponding saturated, non-cyclic molecule
- There are two ways to solve **IHD** problems. One way is to draw the structure and identify rings and double and triple bonds, counting each one as an **IHD** value of 1.
- The second way is to use a formula,
  - For a compound containing C_xH_y, **IHD = (2x+2−y)/2**
  - This is a little complicated, since for the formula to work you need to:
    - ignore O and S
    - count halogens as hydrogen
    - add one C and one H for every nitrogen in the formula
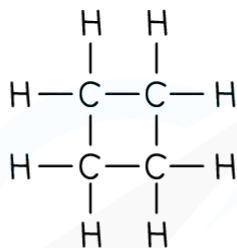
C_5H_{12}

H H
| |
H—C—C—H
| |
H—C—C—H
| |
H H
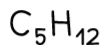
$IHD = (2x + 2 - y)/2$
$= (10 + 2 - 12)/2$
$= 0$

ALKANE
• SATURATED
• NO RINGS

$IHD = (2x + 2 - y)/2$
$= (8 + 2 - 8)/2$
$= 1$

CYCLOALKANE
• 1 RING

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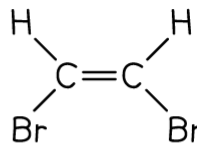
$IHD = (2x + 2 - y)/2$
$= (4 + 2 - 4)/2$
$= 1$

SUBSTITUTED ALKENE
• 1 DOUBLE BOND

$IHD = (2x + 2 - y)/2$
$= (10 + 2 - 8)/2$
$= 2$

DIENE
• 2 DOUBLE BONDS

$IHD = (2x + 2 - y)/2$
$= (8 + 2 - 4)/2$
$= 3$

CYCLIC DIENE
• 1 RING
• 2 DOUBLE BONDS

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C_6H_5OH
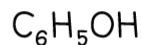
$IHD = (2x + 2 - y)/2$
$= (12 + 2 - 6)/2$
$= 4$

PHENOL
• AROMATIC RING
• 3 DOUBLE BONDS

Index of Hydrogen Deficiency Examples

> **?** **Worked Example**
>
> Deduce the Index of Hydrogen Deficiency in ethyne, C_2H_2, methyl benzene, $C_6H_5CH_3$, and propanone, CH_3COCH_3

Answer:

Answer 1: Ethyne, C_2H_2 **IHD = 2**

TRIPLE BOND

$$H-C\equiv C-H \ + \ 2H_2 \longrightarrow$$

$$IHD = (2x + 2 - y)/2$$
$$= (4 + 2 - 2)/2$$
$$= 2$$

FULLY SATURATED
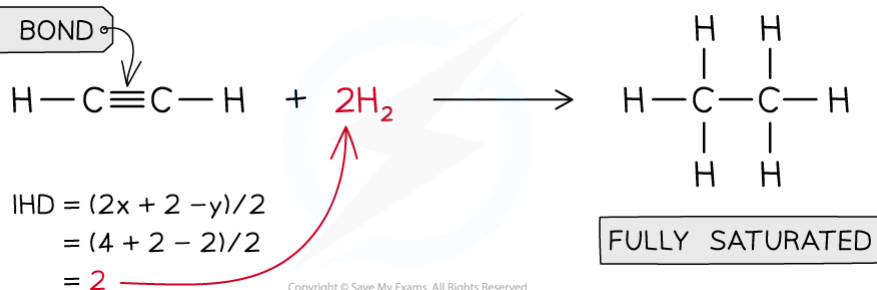
Answer 2: Methylbenzene, $C_6H_5CH_3$, **IHD = 4**

1 RING
3 DOUBLE BONDS

$$+ \ 4H_2 \longrightarrow$$

$$IHD = (2x + 2 - y)/2$$
$$= (14 + 2 - 8)/2$$
$$= 4$$

FULLY SATURATED
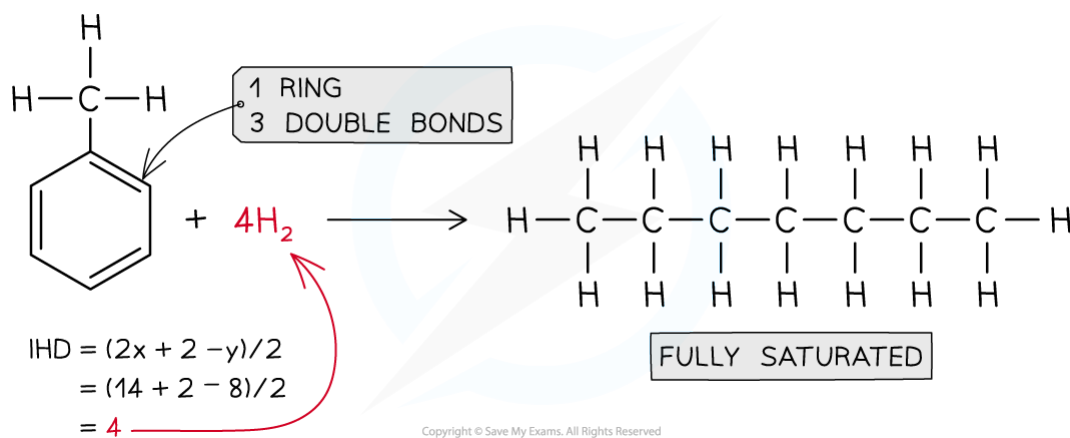
Answer 3: Propanone, CH_3COCH_3 **IHD = 1**

$$+ \ H_2 \longrightarrow$$

$$IHF = (2x + 2 - y)/2$$
$$= (6 + 2 - 6)/2$$
$$= 1$$

FULLY SATURATED
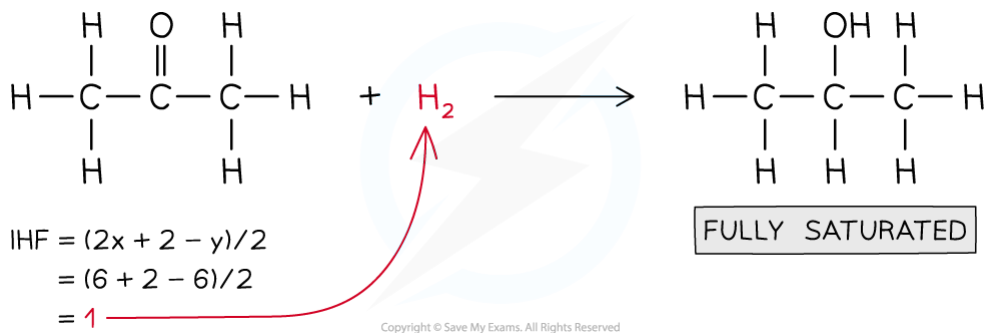
💡 Exam Tip

Drawing out the structure is a much faster way to solve IHD problems, but using the formula is helpful when you are struggling to draw the structure

11.1.2 Mass Spectrometry

Determining Molecular Mass

- When a compound is analysed in a mass spectrometer, vaporised molecules are bombarded with a beam of high-speed electrons
- These knock off an electron from some of the molecules, creating **molecular ions:**

Electron bombardment

MOLECULE $\longrightarrow$ MOLECULE$^+_\bullet$ + e$^-$

Molecular ion

- The relative abundances of the detected ions form a **mass spectrum**: a kind of molecular fingerprint that can be identified by computer using a spectral database
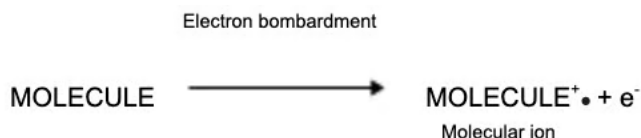- The peak with the highest *m/e* value is the molecular ion (**M⁺**) peak which gives information about the **molecular mass** of the compound
- This value of m/z is equal to the **relative molecular mass** of the compound

The M+1 peak

- The **[M+1]** peak is a smaller peak which is due to the natural abundance of the isotope **carbon-13**
- The height of the **[M+1]** peak for a particular ion depends on how many carbon atoms are present in that molecule; The more carbon atoms, the larger the **[M+1]** peak is
  - For example, the height of the **[M+1]** peak for an hexane (containing six carbon atoms) ion will be greater than the height of the **[M+1]** peak of an ethane (containing two carbon atoms) ion

YOUR NOTES
↓

❓ Worked Example

Determine whether the following mass spectrum belongs to propanal or butanal

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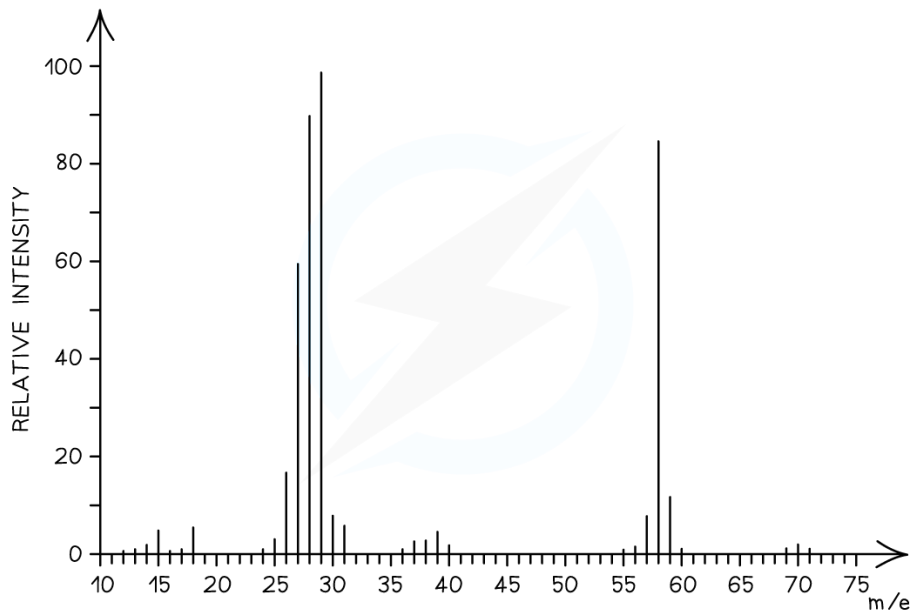
Answer:

- The mass spectrum corresponds to **propanal** as the molecular ion peak is at $m/e = 58$
- Propanal arises from the $CH_3CH_2CHO^+$ ion which has a molecular mass of 58
- Butanal arises from the $CH_3CH_2CH_2CHO^+$ ion which has a molecular mass of 72

Fragmentation Patterns

- The molecular ion peak can be used to identify the **molecular mass** of a compound
- However, different compounds may have the same molecular mass
- To further determine the structure of the unknown compound, **fragmentation analysis** is used
- Fragments may appear due to the formation of **characteristic fragments** or the **loss of small molecules**
  - For example, a peak at 29 is due to the characteristic fragment $C_2H_5^+$
  - Loss of small molecules give rise to peaks at 18 (H_2O), 28 (CO), and 44 (CO_2)

Alkanes

- Simple alkanes are fragmented in mass spectroscopy by breaking the C–C bonds
- *M/e* values of some of the common alkane fragments are given in the table below

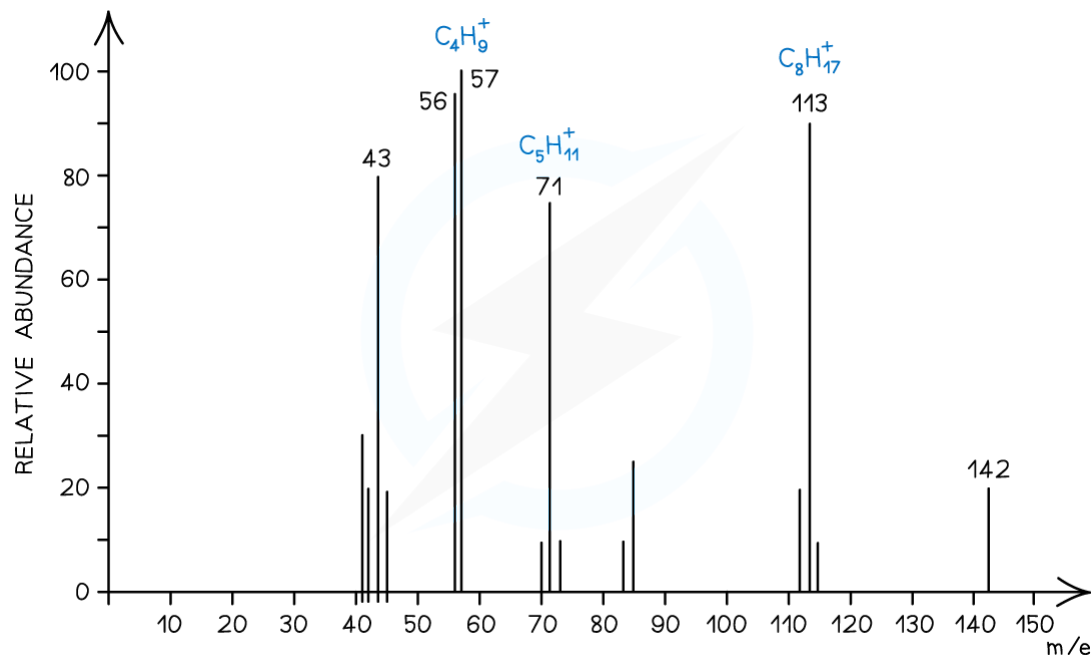### *m/e* values of Fragments Table

Fragment	m/e
CH_3^+	15
$C_2H_5^+$	29
$C_3H_7^+$	43
$C_4H_9^+$	57
$C_5H_{11}^+$	71
$C_6H_{13}^+$	85

YOUR NOTES
↓

Mass spectrum showing fragmentation of alkanes

Halogenoalkanes

- Halogenoalkanes have often multiple peaks around the molecular ion peak
- This is caused by the fact that there are different isotopes of the halogens

Alcohols

- Alcohols often tend to lose a **water molecule** giving rise to a peak at **18 below the molecular ion**
- Another common peak is found at m/e value 31 which corresponds to the CH_2OH^+- fragment
- For example, the mass spectrum of propan-1–ol shows that the compound has fragmented in four different ways:
  - Loss of H to form a $C_3H_7O^+$ fragment with $m/e = 59$
  - Loss of a water molecule to form a $C_3H_6^+$ fragment with $m/e = 42$
  - Loss of a C_2H_5 to form a CH_2OH^+ fragment with $m/e = 31$
  - And the loss of CH_2OH to form a $C_2H_5^+$ fragment with $m/e = 29$

> 💡 Exam Tip
>
> A table of mass spectral fragments lost is included in the IB Chemistry Data Booklet Section 28 so you don't need to learn all the likely fragments

**11.1.3 Nuclear Magnetic Resonance Spectroscopy**

How NMR works

- **Nuclear Magnetic Resonance (NMR)** spectroscopy is used for analysing organic compounds
- Only atoms with **odd mass numbers** show signals on **NMR** spectra and have the property of **nuclear spin**
- In ^{1}**H NMR**, the magnetic field strengths of protons in organic compounds are measured and recorded on a spectrum
- Samples are irradiated with radio frequency energy while subjected to a strong magnetic field
- The nuclei can align themselves with or against the magnetic field
- Protons on different parts of a molecule (in different molecular environments) absorb and emit (**resonate**) different radio frequencies
- All samples are measured against a reference compound – **Tetramethylsilane (TMS)**
  - TMS shows a single sharp peak on an **NMR** spectrum, at a value of zero
  - Sample peaks are then plotted as a 'shift' away from this reference peak
  - This gives rise to 'chemical shift' values for protons on the sample compound
  - Chemical shifts are measured in **parts per million (ppm)**

Features of a NMR spectrum

- An **NMR** spectrum shows the intensity of each peak against their chemical shift
- The area under each peak is proportional to the number of protons in a particular environment
- The height of each peak shows the intensity/absorption from protons
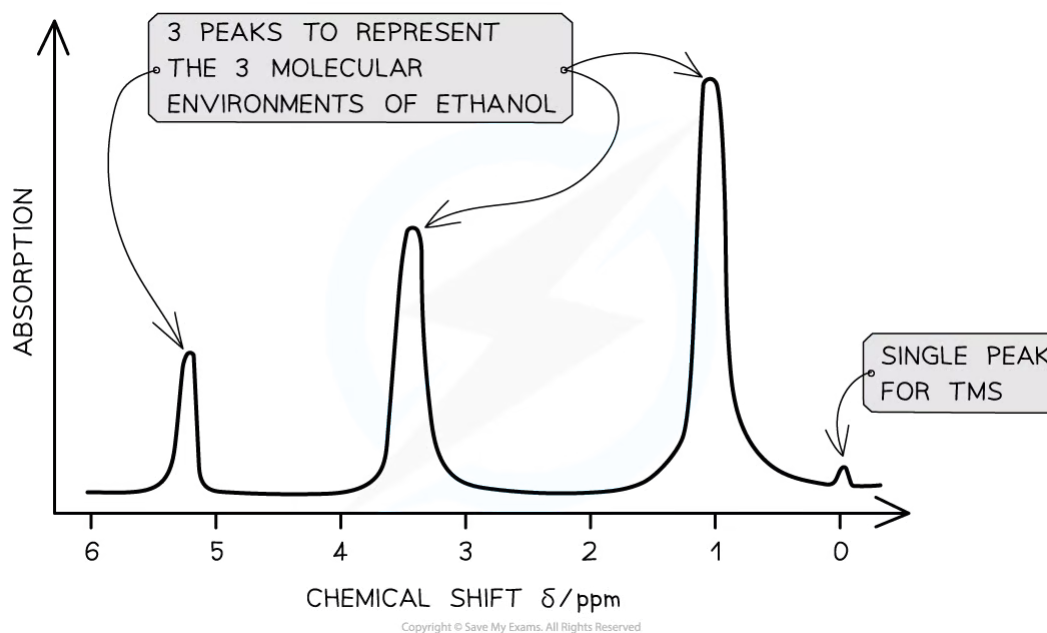
A low resolution ^{1}H NMR for ethanol showing the key features of a spectrum

Chemical Environments

Chemical environments

- Hydrogen atoms of an organic compound are said to reside in different chemical environments
  - Eg. Methanol has the molecular formula CH_3OH
  - There are 2 environments: $-CH_3$ and $-OH$

- The hydrogen atoms in these environments will appear at 2 different chemical shifts
- Different types of protons are given their own range of chemical shifts

| Aldehyde	HCOR	9.3 − 10.5
Alcohol	ROH	0.5 − 6.0
Phenol	Ar − OH	4.5 − 7.0
Carboxylic acid	RCOOH	9.0 − 13.0
Alkyl amine	R − NH −	1.0 − 5.0
Aryl amine	Ar − NH$_2$	3.0 − 6.0
Amide	RCONHR	5.0 − 12.0

💡 **Exam Tip**

Typical proton chemical shift values are given in Section 27 of the IB Chemistry Data Booklet. The values alone do not identify specific protons as the values occur over a range that is sometimes overlapping, but they can be used in combination with other structural information to help confirm a feature

Interpreting an NMR Spectrum

- Protons in the same environment are chemically equivalent
- Each peak on a NMR spectrum relates to protons in the same environment
- Peaks on a low resolution NMR spectrum refers to environments of an organic compound
  - Eg. Ethanol has the molecular formula CH_3CH_2OH
  - This molecule as 3 separate environments: $-CH_3$, $-CH_2$, $-OH$
  - So 3 peaks would be seen on its spectrum at 1.2 ppm ($-CH_3$), 3.7 ppm ($-CH_2$) and 5.4 ppm ($-OH$)
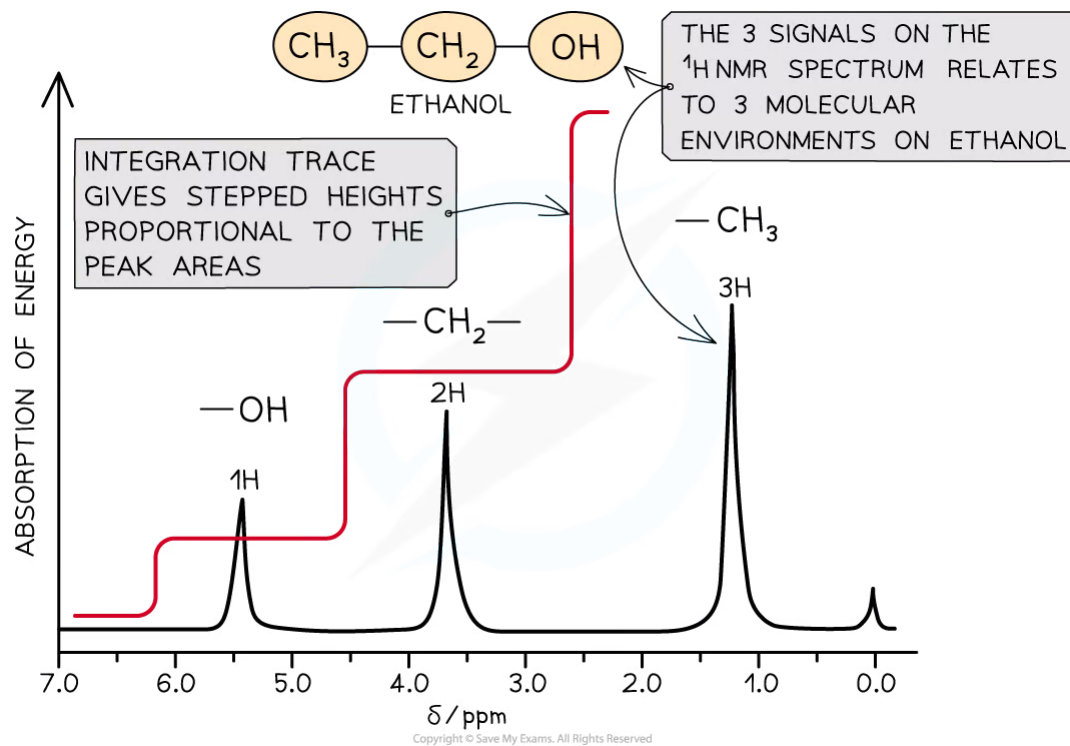
A low resolution NMR spectrum with integration trace

- The area under each peak is determined by computer and an **integration trace** overlaid on the spectrum
- The **integration trace** has stepped lines whose steps are in the same proportion as the peak areas
- This makes it easier to determine the relative abundance of the different proton environments

? Worked Example

Which of the following features can be found from a ^{1}H NMR spectrum?

    A. The total mass of hydrogen atoms present

B. The number of different hydrogen environments

C. The frequency vibration of C–O bonds

D. The first ionization energy of hydrogen

Answer:

The correct option is **B**.

- An NMR spectrum can tell you about the type of hydrogen environments and the relative proportion of the Hs in those environments

How IR Spectroscopy works

- All **covalent bonds** act rather like springs, as opposed to rigid bars
- Like springs, the bonds can vibrate in a number of different ways
- The frequency of vibration occurs in the **infra-red region** of the **electromagnetic spectrum**
- If an organic molecule is irradiated with **infra-red energy** that matches the **natural vibration frequency** of its bonds, it absorbs some of that energy and the amplitude of vibration increases
- This is known as **resonance**
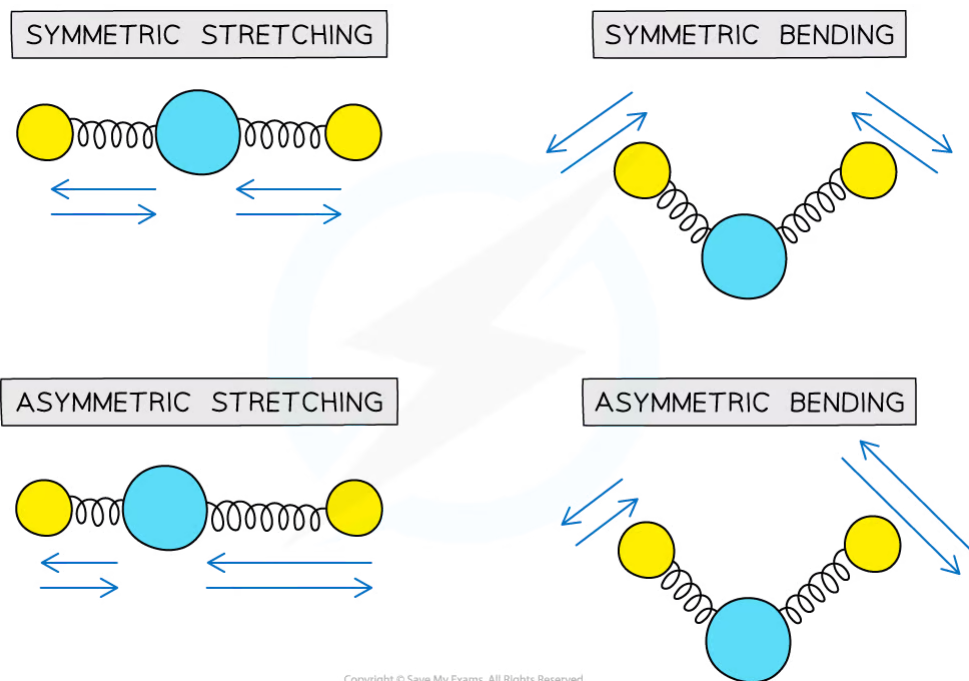
Different modes of vibration in molecules. Each mode has a characteristic frequency of vibration

Infrared (IR) spectroscopy

- **Infrared (IR) spectroscopy** is a technique used to identify compounds based on changes in **vibrations** of atoms when they **absorb** IR of certain **frequencies**
- A **spectrophotometer** irradiates the sample with IR radiation and then detects the **intensity** of **IR radiation** absorbed by the molecule
- **IR energy** is absorbed only if a molecule has a **permanent dipole** that changes as it vibrates
  - Symmetrical molecules such as O_2 or H_2, are therefore **IR inactive**

- The **resonance frequency** is the specific frequency at which the bonds will vibrate
- Rather than displaying frequency, an **IR spectrum** shows a unit called **wavenumber**
  - **Wavenumber** is the reciprocal of the **wavelength** and has units of **cm^{-1}**

- Characteristic absorptions can be matched to specific bonds in molecules

○ This enables chemists to determine the **functional groups** present

Absorption Range of Bonds

Bond	Functional groups containing the bond	Characteristic infrared absorption range (in wavenumbers) (cm^{-1})
C−O	Hydroxy, ester	1040−1300
C=C	Aromatic compound, alkene	1500−1680
C=O	Amide carbonyl, carboxyl ester	1640−1690 1670−1740 1710−1750
C≡N	Nitrile	2200−2250
C−H	Alkane	2850−2950
N−H	Amine, amide	3300−3500
O−H	Carboxyl, hydroxyl	2500−3000 3200−3600

• Due to some absorption bands overlapping each other, other analytical techniques such as **mass spectroscopy** should be used alongside **IR spectroscopy** to identify an unknown compound
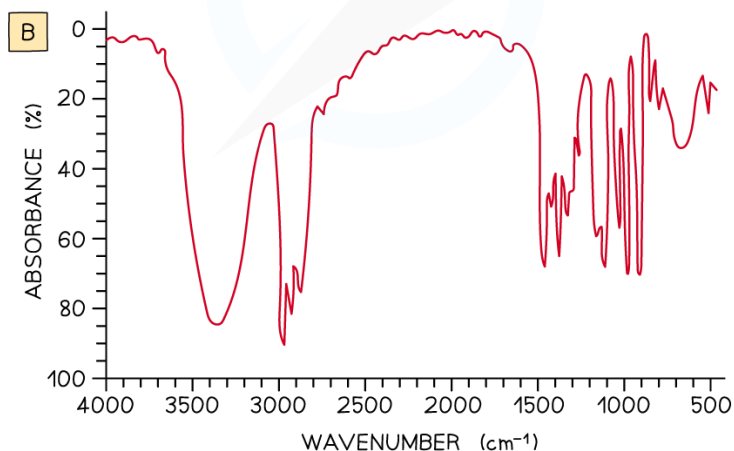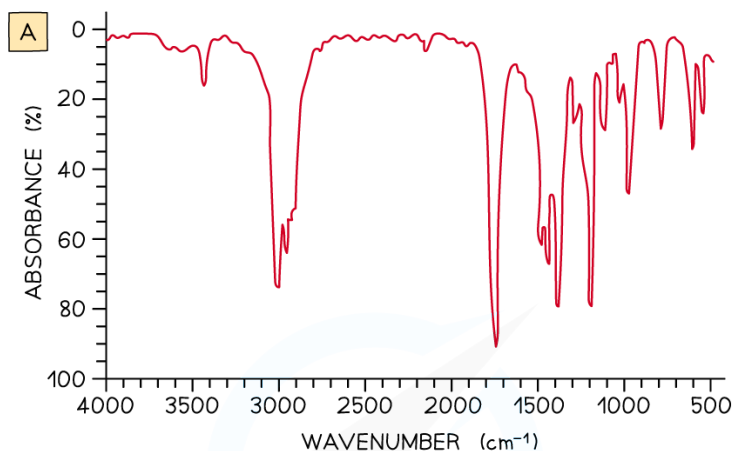
Interpreting an IR Spectrum

- The best way to understand how to interpret an **IR spectrum** is by looking at examples and becoming familiar with the characteristic features of an **IR spectrum**

❓ Worked Example

Examine the two spectra shown and determine which one belongs to propan-2–ol and which one belongs to propanone

---

Answer:

- IR spectrum **A** is **propanone** and spectrum **B** is **propan–2–ol**.
- In IR spectrum **A** the presence of a strong, sharp absorption around 1710 cm^{-1} corresponds to the characteristic C=O, carbonyl, group in a ketone.
- In spectrum **B** the presence of a strong, broad absorption around $3200–3500$ cm^{-1} suggests that there is an alcohol group present, which corresponds to the -OH group in propan-2–ol.

Fingerprint Region

YOUR NOTES
↓

- The region below about 1500 cm^{-1} is called the **fingerprint region** and is unique to every molecule
- It has many peaks that can be difficult to assign
- These peaks represent the complex vibrational interactions that occur between different bonds within a molecule
- The value of the **fingerprint region** is in being able to compare the **IR spectrum** to a known compund from a database and coming up with an exact match
- This is particularly useful, for example, in identifying a specific member of a **homologous series**
  - All members of the series will show the same type of bonds present, but no two molecules will have the same fingerprint region

💡 Exam Tip

Infrared data is found in Section 26 of the IB Chemistry Data Booklet so there is no need to learn specific wavenumber ranges of bonds

11.2 Synoptic Data Handling & Graphical Skills

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 1ºC, the uncertainty would be $\pm0.5\,°C$
    - 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
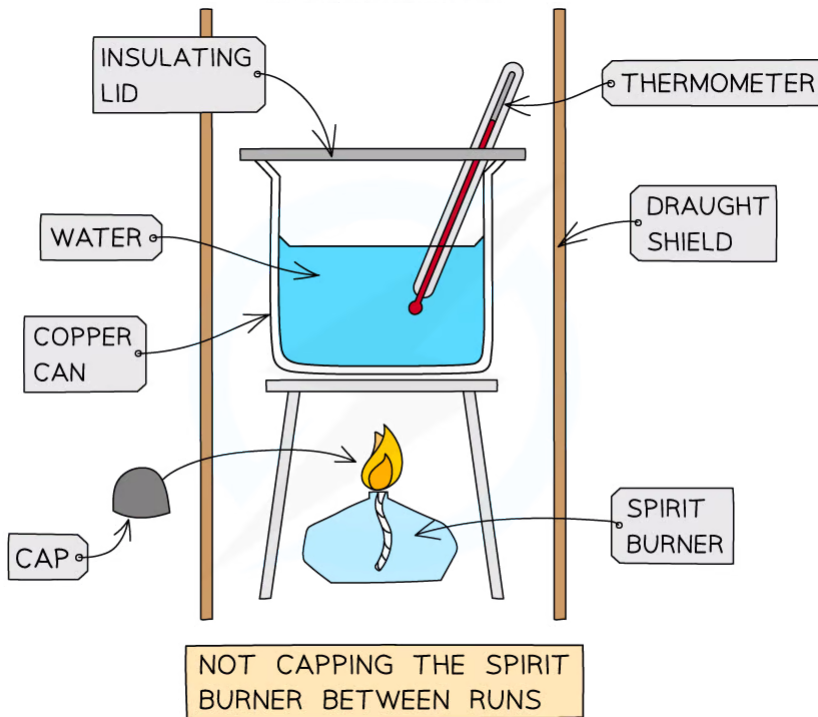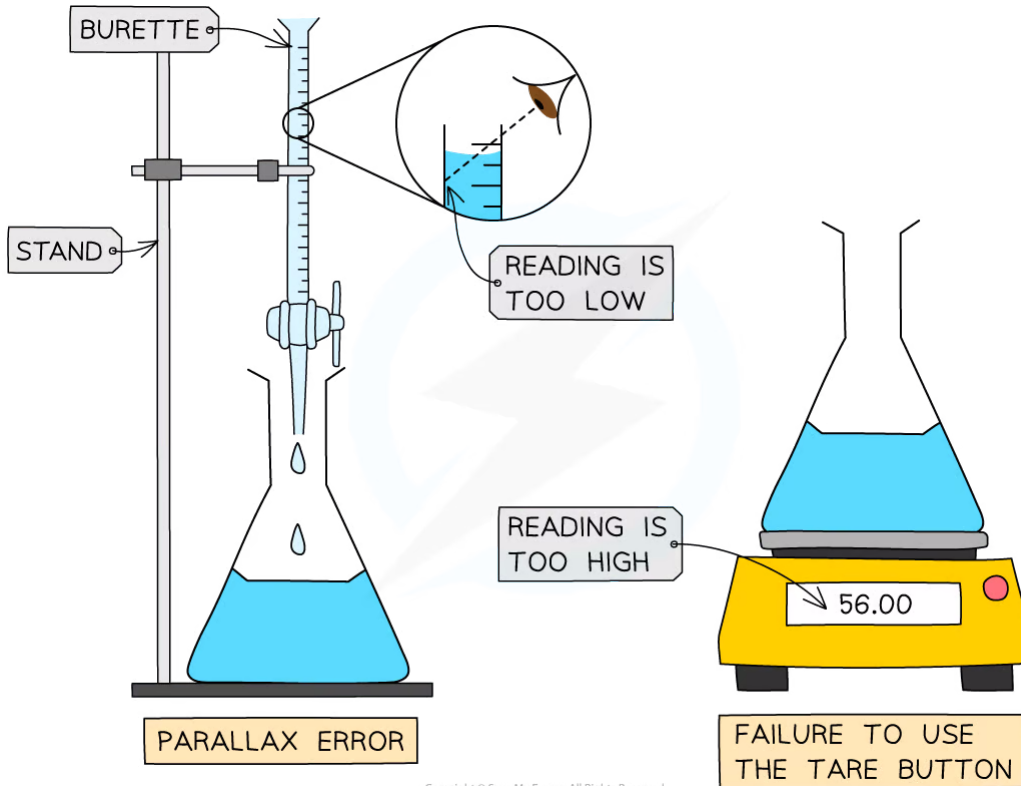
Types of Errors

- 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

INSULATING
LID

THERMOMETER

WATER

DRAUGHT
SHIELD

COPPER
CAN

CAP

SPIRIT
BURNER

NOT CAPPING THE SPIRIT
BURNER BETWEEN RUNS

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:

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

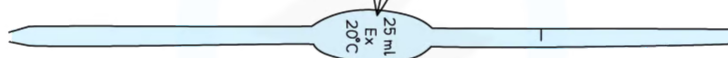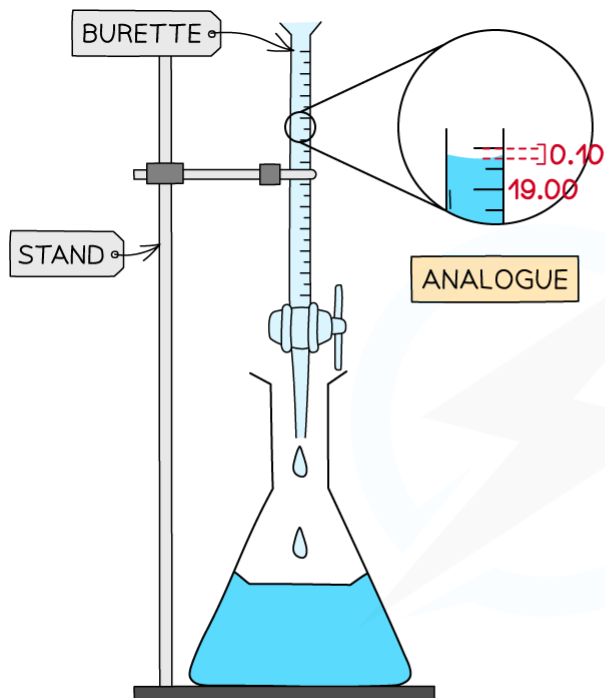- Some examples of percentage uncertainty calculations for common laboratory apparatus:

ANALOGUE

PIPETTES WILL USUALLY HAVE THE UNCERTAINTY PRINTED ON THEM

25 ml
Ex
20°C

A VOLUMETRIC PIPETTE

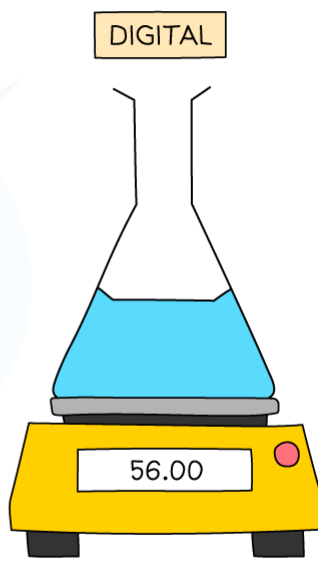$$\% \text{ UNCERTAINTY} = \frac{\pm 0.08}{25.00} \times 100 = 0.32 \%$$

BURETTE

STAND

☐ 0.10
19.00

ANALOGUE

DIGITAL

56.00

$$\% \text{ UNCERTAINTY} = \frac{\pm 0.05}{19.00} \times 100 = 0.26 \%$$

$$\% \text{ UNCERTAINTY} = \frac{\pm 0.01}{56.00} \times 100 = 0.02 \%$$

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

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**:

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
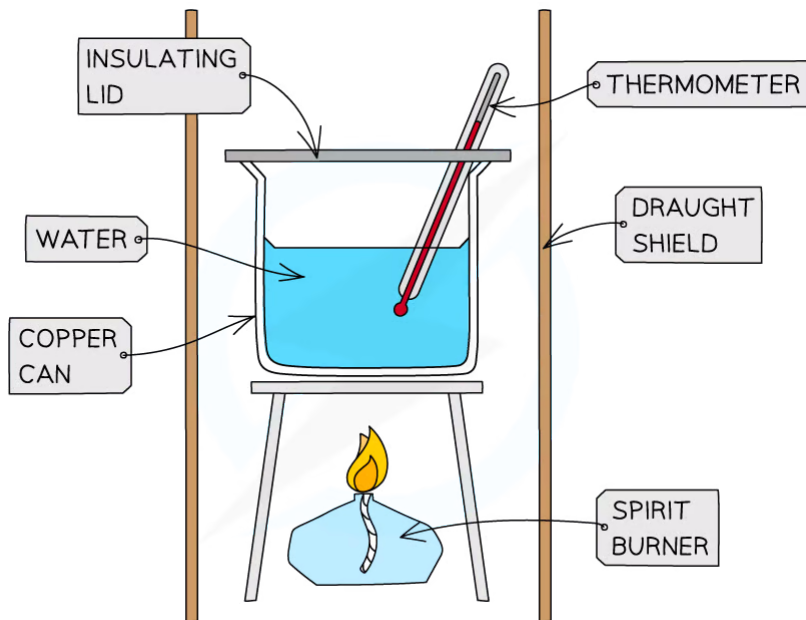

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You should be able to state what the impact would be of not using a draught shield in a simple combustion calorimetry experiment

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
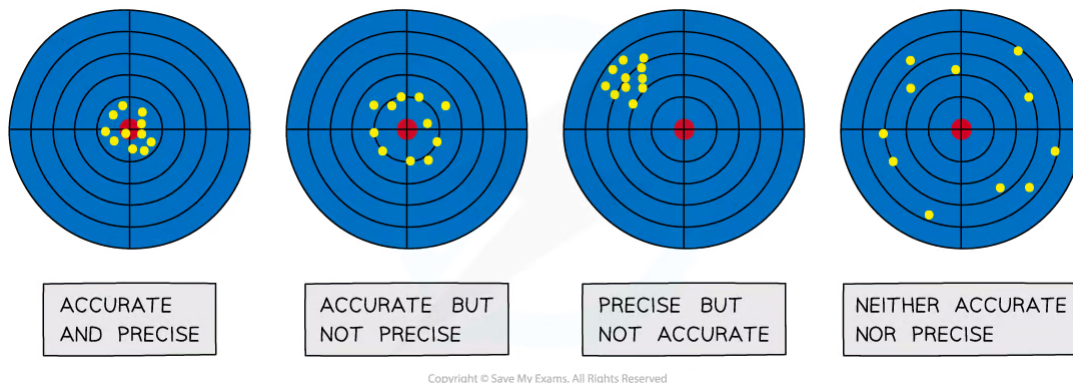
Accuracy and precision in target shooting

- 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.

YOUR NOTES
↓

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 x c x ΔT

q = 200 g x 4.18 J g^{-1}K^{-1} x 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

ΔH = q ÷ n = –25 080 J ÷ 0.01702 mol = – 1 473 560 J = –1 474 kJ = **–1.5 x 10^3 kJ**

Answer 2:

Using the formula

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

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

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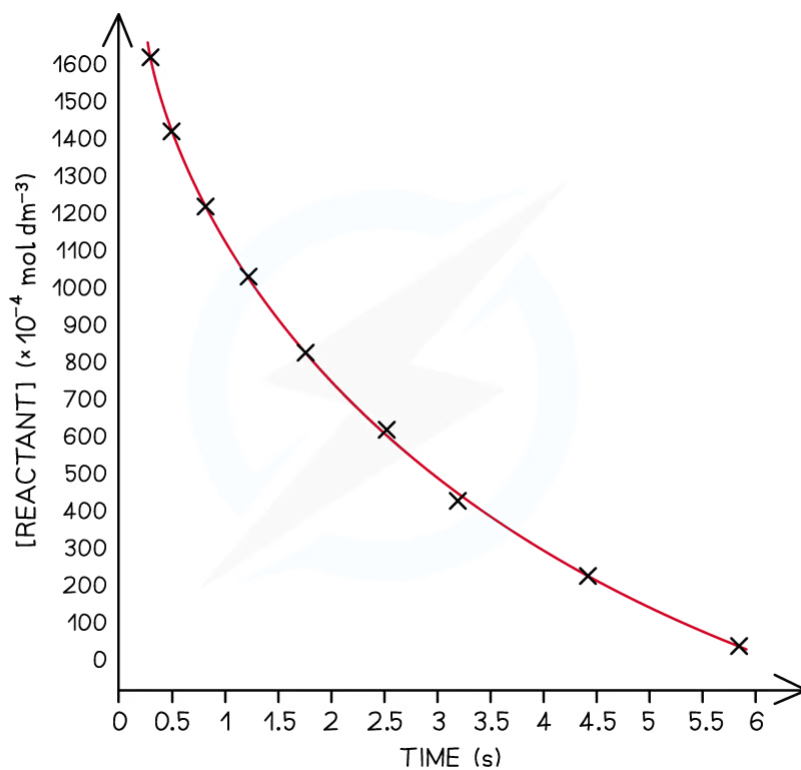
Graphs must shows appropriate scales, labelling and units. The independent variable usually goes on the x-axis and the dependent variable on the y-axis

- 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:
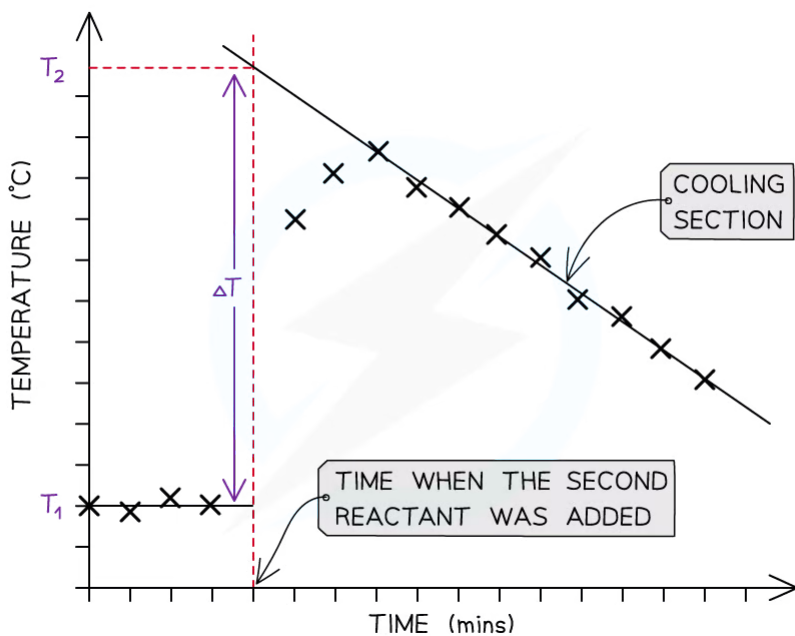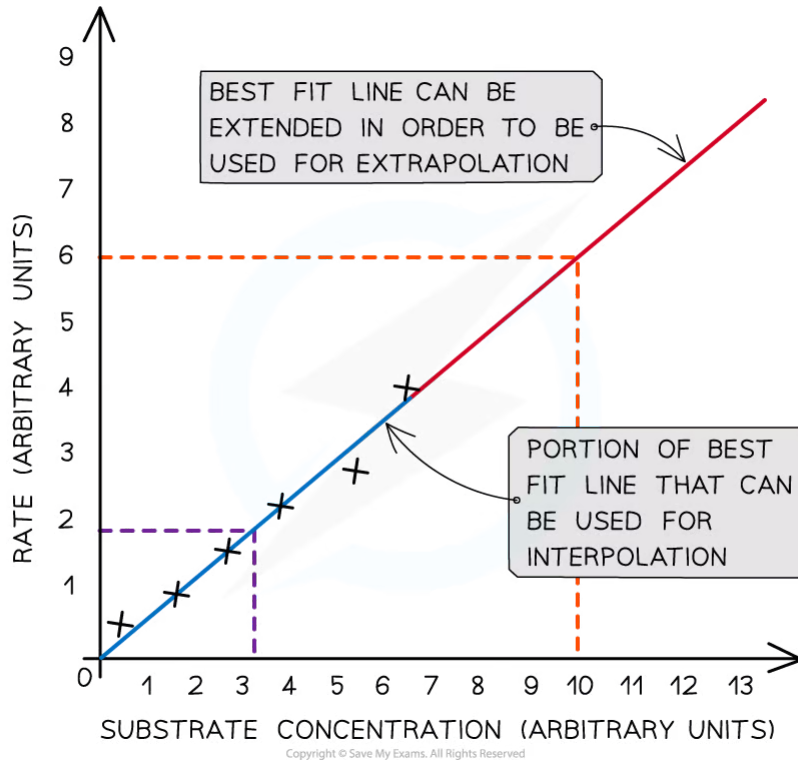

Extrapolation on a temperature correction graph

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

YOUR NOTES
↓

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

11.2.6 Analysing Graphs
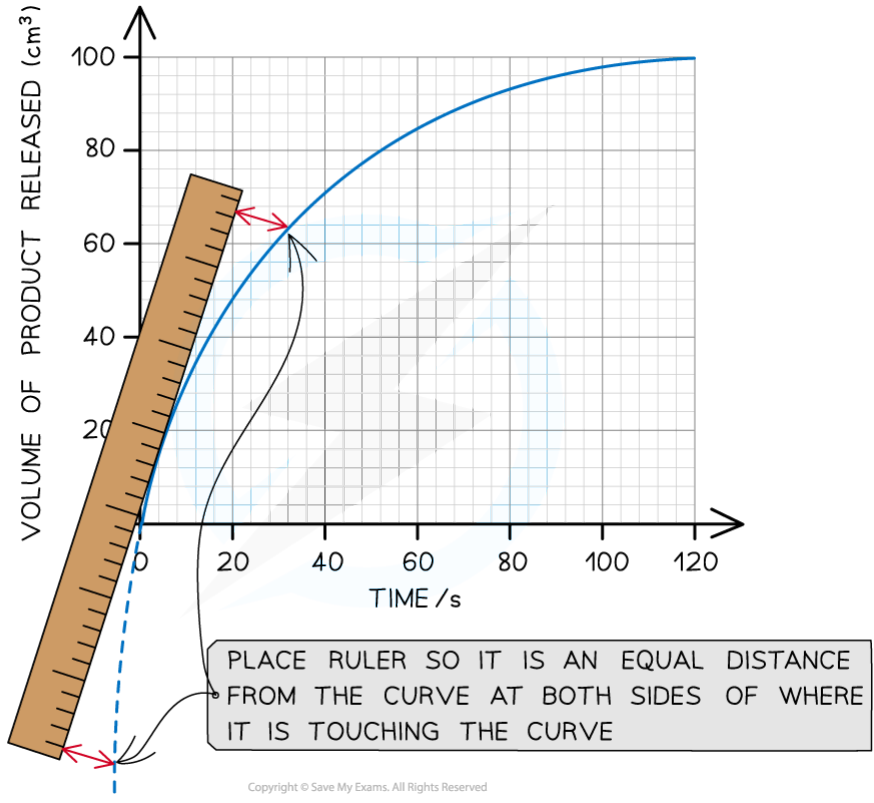
Analysing Graphs

- The **gradient** of a graph can be found by:
  - In the case of a straight line graph: using a triangle and the equation for a straight line
  - In the case of a curve: drawing a **tangent** to the graph

- 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**

- The **gradient** or **slope** is therefore : **m = Δy/Δx**
- This example from Kinetics illustrates the calculation of rates from a curve
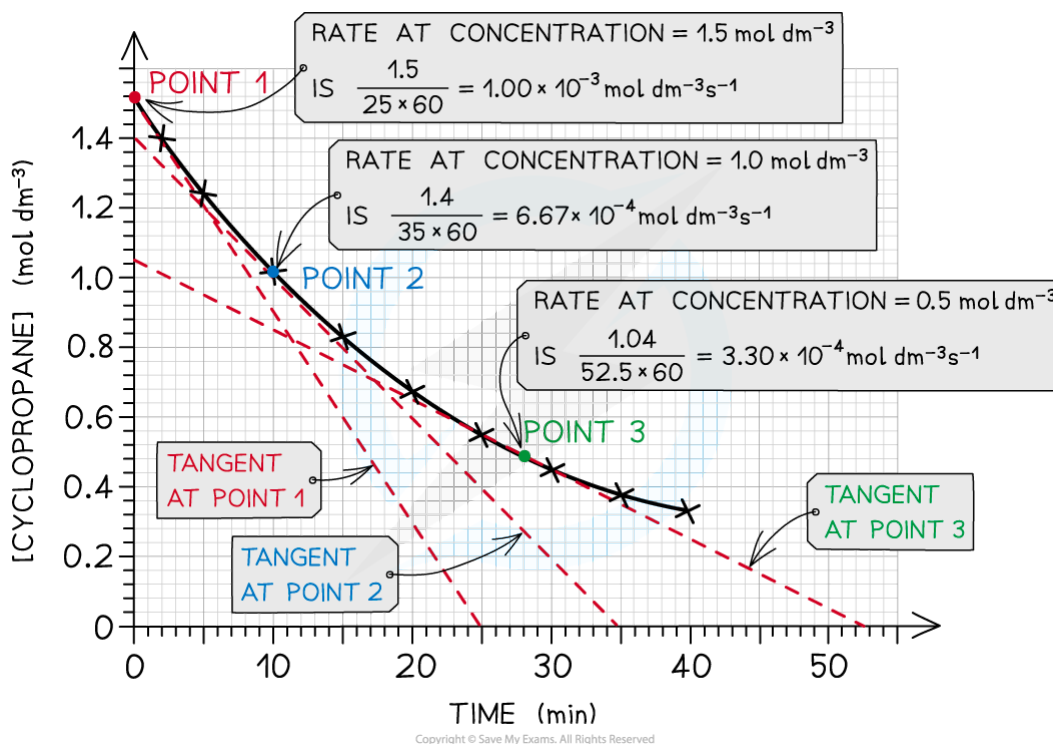
The gradient can be found at different points on a curve. Here it has been multiplied by 60 to convert it from minutes^{-1} to seconds^{-1}

- In the case of curves you will need a ruler to line up against the curve at the point you want to measure the gradient:

YOUR NOTES
↓

3

PLACE RULER SO IT IS AN EQUAL DISTANCE FROM THE CURVE AT BOTH SIDES OF WHERE IT IS TOUCHING THE CURVE

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

💡 **Exam Tip**

Be careful that you process the units correctly when finding the gradient. The gradient unit is the y-unit divided by the x-unit, so in the example above the gradient of the curve is measured in $cm^3 \, s^{-1}$

Sketched Graphs

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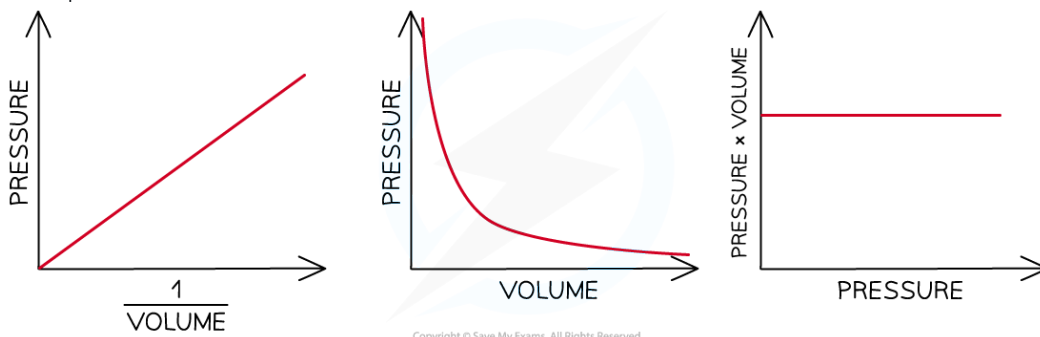
Sketched graphs show relationships between variables

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?

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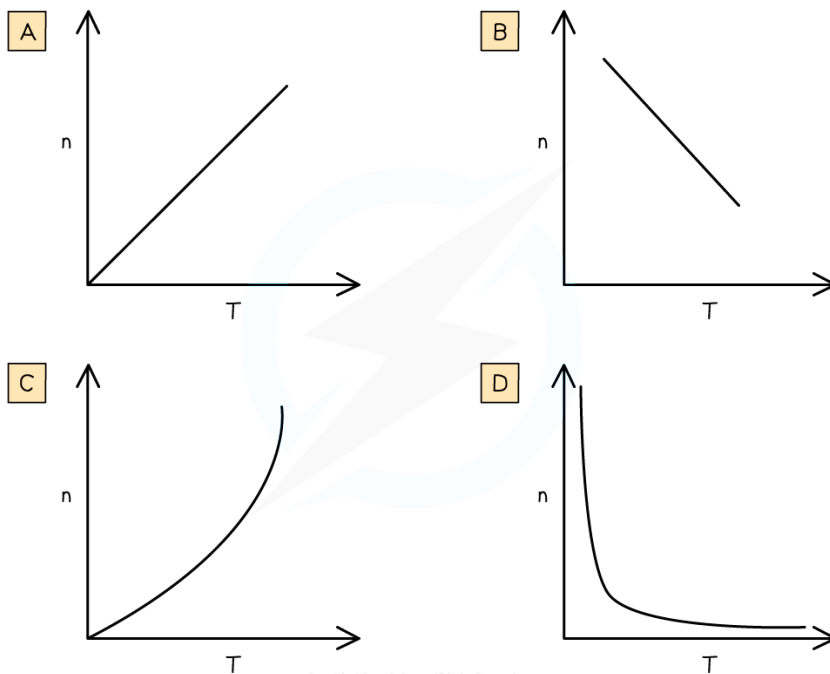
Answer:

The correct option is **D**

- The Ideal Gas Equation is PV = nRT.
- If P, V and R are constant then PV/R = nT = a constant
- n must be inversely proportional to T, which gives graph D