2B Analysis

Percentage yield:

Is the measure of conversion of reactants to products. It is a measure of the waste of the reactants

- When we think about reactions, we always think of them as going 100% to products.
- This is usually **not** the case due to:

1	**Equilibria:**	The reaction may not go to completion.
2	**Side reactions:**	This will produce 'by - products' reducing the amount of desirable product.
3	**Reactant purity:**	The reactants may be impure meaning you have started with less than you thought you did.
4	**Transfers:**	Every time you move your reactants / products from one place to another, you will leave some behind.
5	**Separation / purification:**	This inevitable results n the loss of product.

- Percentage yield is like a score in a test. It is an indication of what you achieved out of what you could have got:

$$\text{\% Yield} = \frac{\text{Actual amount of product (moles)}}{\text{Theoretical amount of product (moles)}} \times 100$$

The rules:

1. **Write a balanced chemical equation**
2. **Identify the limiting reactant**
3. **Calculate the theoretical amount of moles of product starting from the limiting reactant**
4. **Calculate the actual amount of moles of product obtained**
5. **Calculate % yield using the formula**

Examples:

A) Preparation of ethanoic acid:
A student reacted 9.20g of ethanol with and excess of sulphuric acid and sodium dichromate (the oxidising agent). The student obtained 4.35g of ethanoic acid. Calculate the % yield:

1) Write a balanced chemical equation:

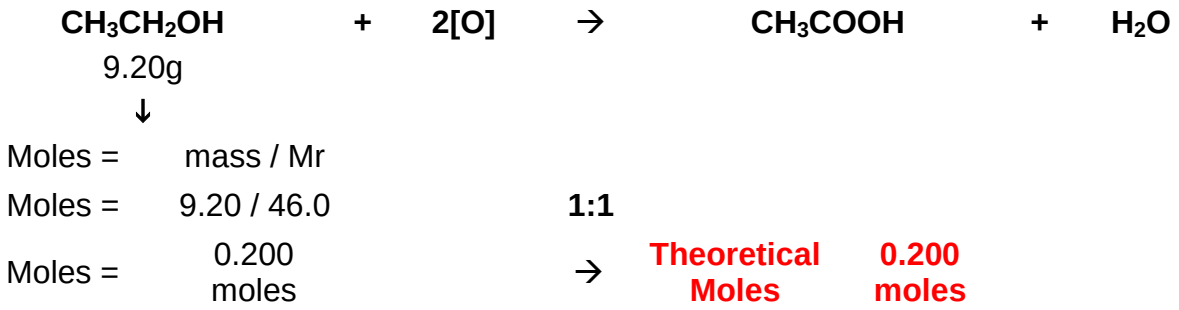
$$CH_3CH_2OH + 2[O] \rightarrow CH_3COOH + H_2O$$

2) Identify the limiting reactant

- You are told in the question that you have an excess of sulphuric acid and sodium dichromate.
- This means that the limiting reactant is ethanol.

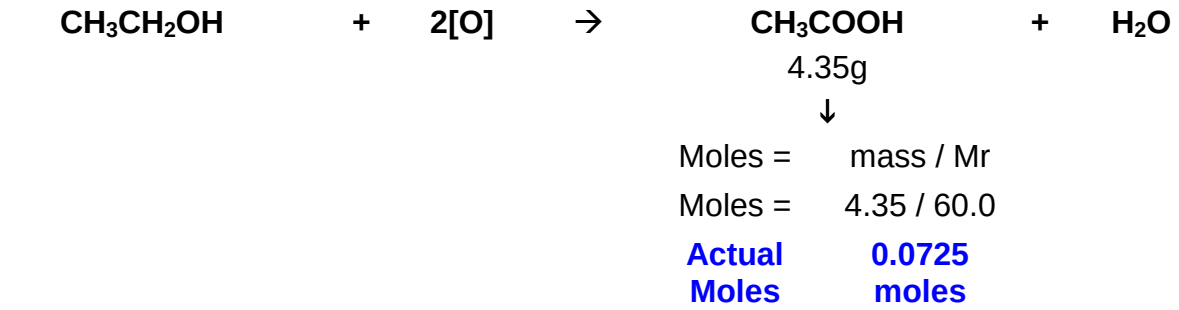
3) Calculate the theoretical amount of moles of product starting from the limiting reactant:

- Calculate the amount of moles of ethanoic acid you could have made:



4) Calculate the actual amount of moles of product obtained:

- Calculate the number of moles you actually made:



5) Calculate % yield using the formula:

$$\text{\% Yield} = \frac{\text{Actual number of moles}}{\text{Theoretical number of moles}} \times 100$$

$$= \frac{0.0725}{0.200} \times 100$$

$$= 36.25\%$$

B) Preparation of propyl methanoate

A student prepared propyl methanoate from propan - 1 - ol and methanoic acid.
The students reacted 3.00g of propan - 1 - ol witth 2.50g of methanoic acid in the presence of a sulphuric acid catalyst. He was disappointed to obtain only 1.75g of propyl methanoate.
Calculate the % yield of propyl methanoate:

1) Write a balanced chemical equation:

$$CH_3CH_2CH_2OH + HCOOH \rightarrow HCOOCH_2CH_2CH_3 + H_2O$$

2) Identify the limiting reactant

- You are given 2 starting amounts which means you have to work out which one is the limiting reactant:

$CH_3CH_2CH_2OH$ + **HCOOH** → **$HCOOCH_2CH_2CH_3$** + **H_2O**

3.00g 2.50g

↓ ↓

Moles =	mass / Mr	Moles =	mass / Mr
Moles =	3.00 / 60.0	Moles =	2.50 / 46.0
Moles =	**0.0500**		0.0543

- Propan - 1 - ol is the limiting reactant so the theoretical calculation must be made using this

3) Calculate the theoretical amount of moles of product starting from the limiting reactant:

- Calculate the amount of moles of ethanoic acid you could have made:

$CH_3CH_2CH_2OH$ + **HCOOH** → **$HCOOCH_2CH_2CH_3$** + **H_2O**

3.00g

↓

Moles =	mass / Mr			
Moles =	3.00 / 60.0	**1:1**		
Moles =	**0.0500**	→	**Theoretical Moles =**	**0.0500**

4) Calculate the actual amount of moles of product obtained:

- Calculate the number of moles you actually made:

$CH_3CH_2CH_2OH$ + **HCOOH** → **$HCOOCH_2CH_2CH_3$** + **H_2O**

3.00g 1.75g

↓ ↓

	Moles =	mass / Mr
	Moles =	1.75 / 88.0
	Actual Moles =	**0.0199**

5) Calculate % yield using the formula:

$$\text{\% Yield} = \frac{\text{Actual number of moles}}{\text{Theoretical number of moles}} \times 100$$

$$= \frac{0.0199}{0.050} \times 100$$

$$= 39.8\%$$

Questions P163 1-2

Atom economy:

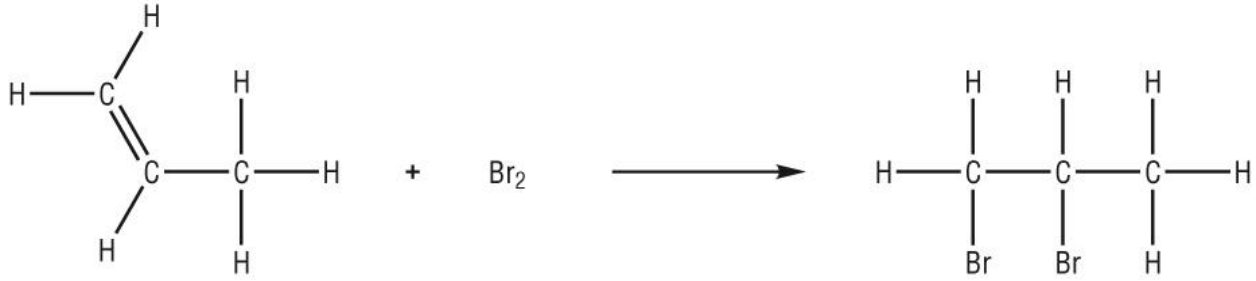
Is the measure of the waste associated with the products

- % yield tells us how much of our product is made from our starting materials but it doesn't take into account any undesirable or side products.
- Atom economy takes into account any wasteful by products too
- By products are considered wasteful as they are usually disposed of. This is costly and can cause environmental problems.
- A more efficient way of dealing with by products would be to sell them on to companies that would make use of them.

$$\text{Atom economy} = \frac{\text{Mr of the desired product}}{\text{Sum of Mr's of all products}} \times 100$$

Calculating atom economy:

A) Bromination of propene:



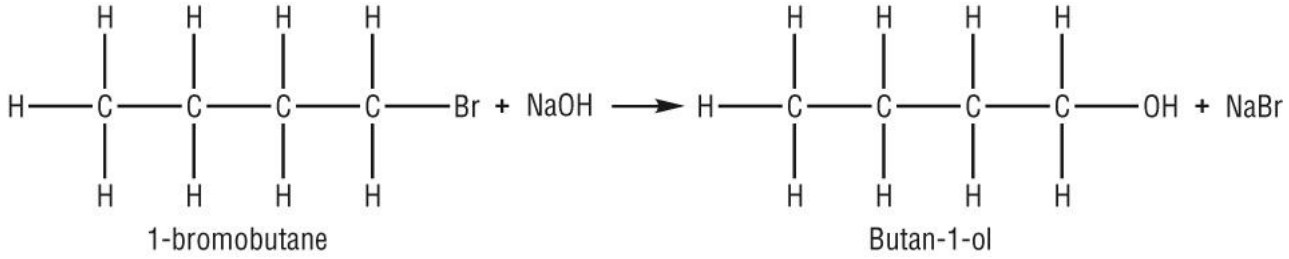
$$\text{Atom economy} = \frac{\text{Mr of the desired product}}{\text{Sum of Mr's of all products}} \times 100$$

$$= \frac{201.8}{201.8} \times 100$$

$$= 100\%$$

- Any reaction that gives only one product is very atom economic, addition reactions for example.

B) Preparation of butan - 1 - ol:



1-bromobutane Butan-1-ol

Atom economy = $\frac{\text{Mr of the desired product}}{\text{Sum of Mr's of all products}}$ x 100

= $\frac{74.0}{176.9}$ x 100

= **41.8%**

- This means that most of the starting materials ended up as waste.

Atom economy and type of reaction:

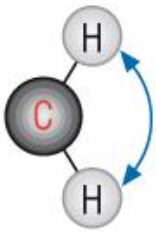
- Reactions having only one product have a high atom economy. The type of reactions giving only one product are **addition reactions**.
- Reactions giving more than one product have a low atom economy. The type of reactions giving more than one product are **substitution / elimination reactions**.
- To improve the atom economy for **substitution / elimination** reactions, a use for the undesired product should be found.
- If the undesired product is toxic, we have even bigger problems -disposal.

Questions P165 1-2

Infrared spectroscopy
Infrared radiation and molecules:

- All molecules absorb IR light.
- The IR light makes the bonds in a molecule vibrate (like the engine of a bus making the windows vibrate).
- Vibrations occur in one of 2 ways, a stretching vibration or a bending vibration:

The C–H bond stretches when it absorbs infrared radiation.

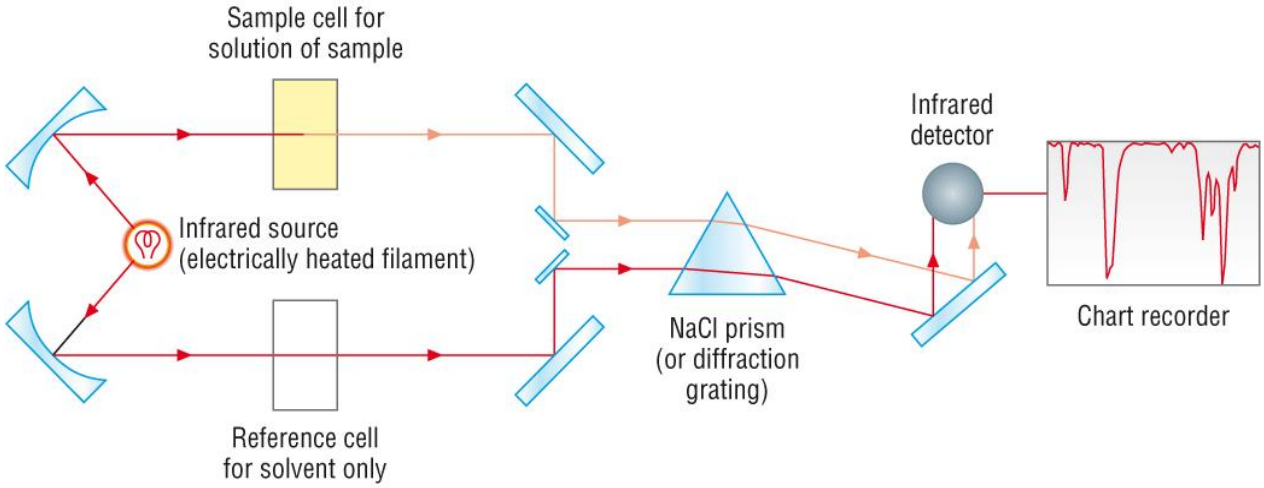


The C–H bond bends when it absorbs infrared radiation.

- Every bond vibrates at its own unique frequency depending on:

1) Bond strength
2) Bond length
3) Mass of atom at either end of the bond

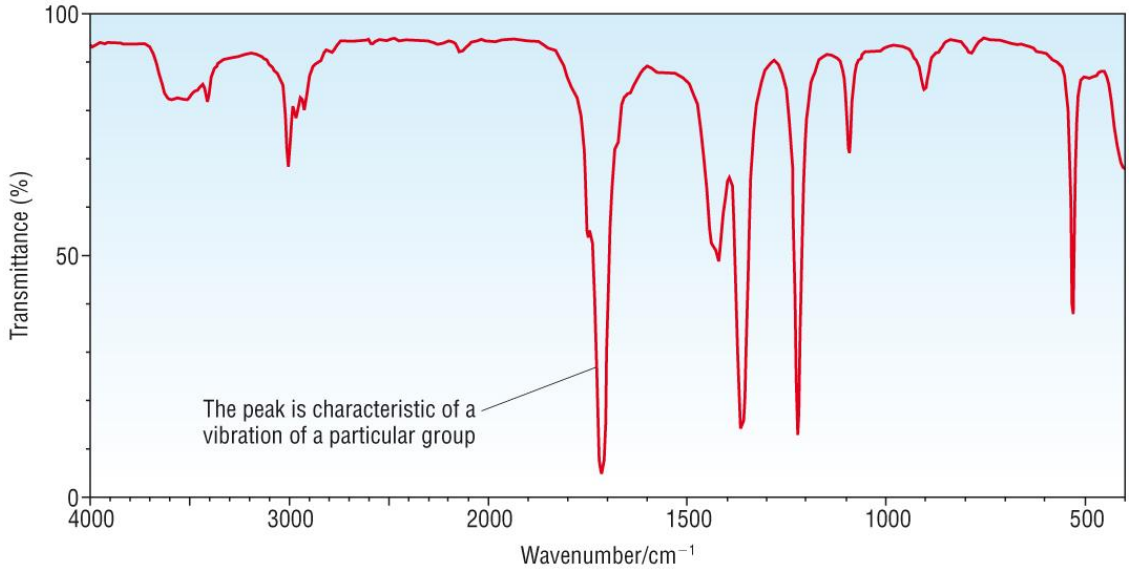
How it works:



- The full IR spectrum is passed through a sample.
- The frequencies are called wavenumbers - 300 - 4000cm^{-1}
- Some frequencies make some of the bonds in a molecule vibrate
- When these bonds vibrate they absorb energy from the IR light source.
- This means less IR light gets through the sample to the detector.
- Each absorbance peak is characteristic of a particular bond / atoms vibrating.
- A trace which we call a spectrum is produced.

What does the spectrum look like:

- The spectrum gives us **'peaks'** which are actually absorbance troughs.
- These troughs are caused by a frequency of IR light being absorbed from a bond vibrating bond.
- Each **'peak'** is characteristic to a specific bond / atoms



Applications of IR spectroscopy:

- It is used widely in forensic science analysing:

  - Paint fragments in hit and run offences
  - Monitor unsaturation in polymerisation
  - Drug analysis P167
  - Perfume quality control

Questions P167 1-3

Infrared spectroscopy: Functional groups

Identification of functional groups:

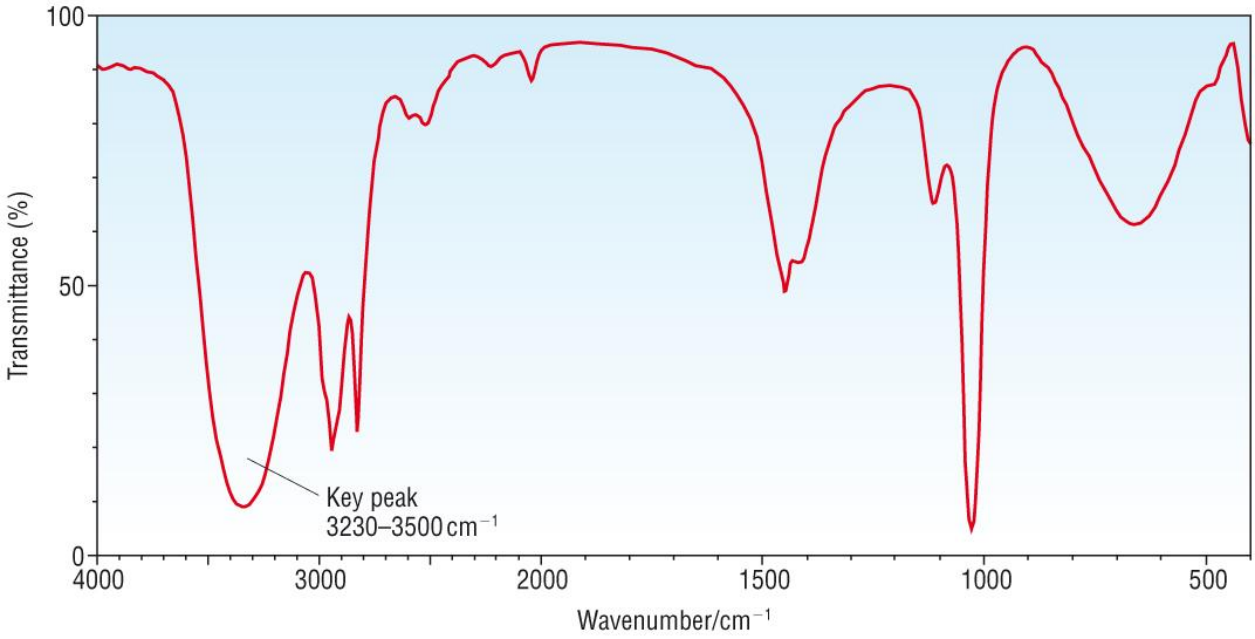
- We have just seen that the peak on an IR spectra are due to specific bonds (and atoms) vibrating or stretching.
- The frequency at which you find an absorbance peak is therefore unique to bonds and atoms at each end of the bond.
- This means that functional groups will give specific peaks.
- The groups you need to know are:

Bond	Functional group	Wavenumber
C=O	Aldehydes, ketones, carboxylic acids	1640 - 1750
C- H	Organic conpounds	2850 - 3100
O- H	Carboxylic acids	2500 - 3300 (very broad)
O- H	Alcohols (hydrogen bonded)	3200 - 3550 (broad)

- Do not get the peaks for C - H bonds confused with O - H bonds.

Alcohols:

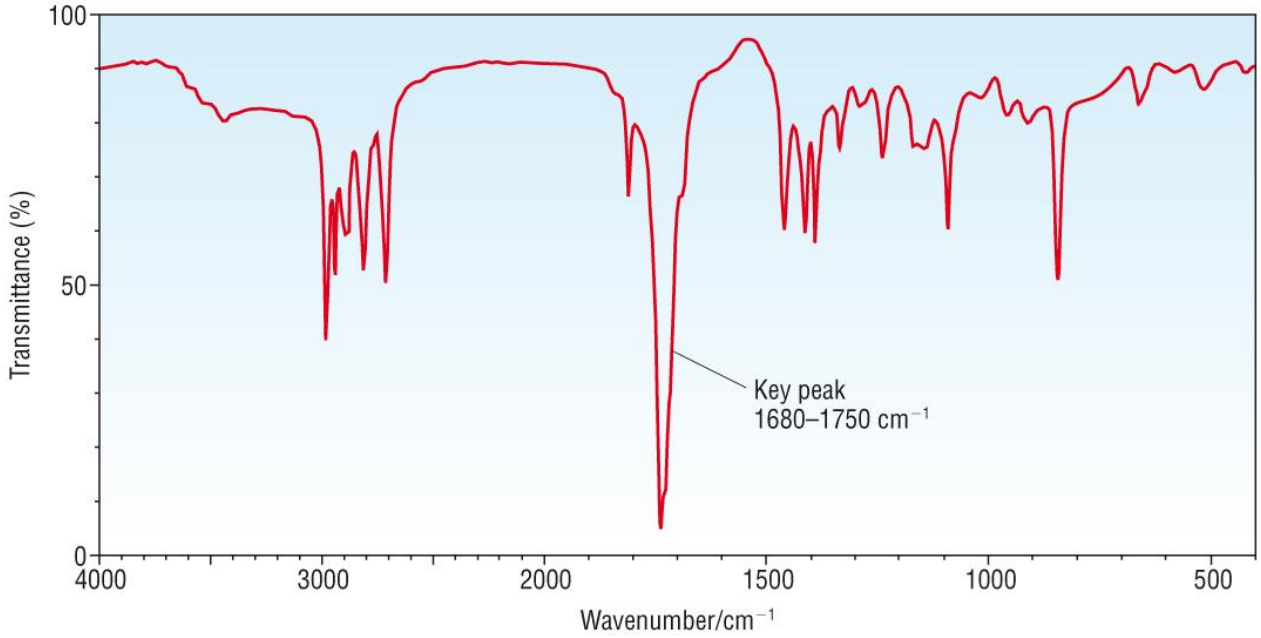
- The IR spectrum for methanol, CH_3OH is shown below:



- The peak at 3230 - 3500 represents an O - H group in alcohols.

Aldehydes and ketones:

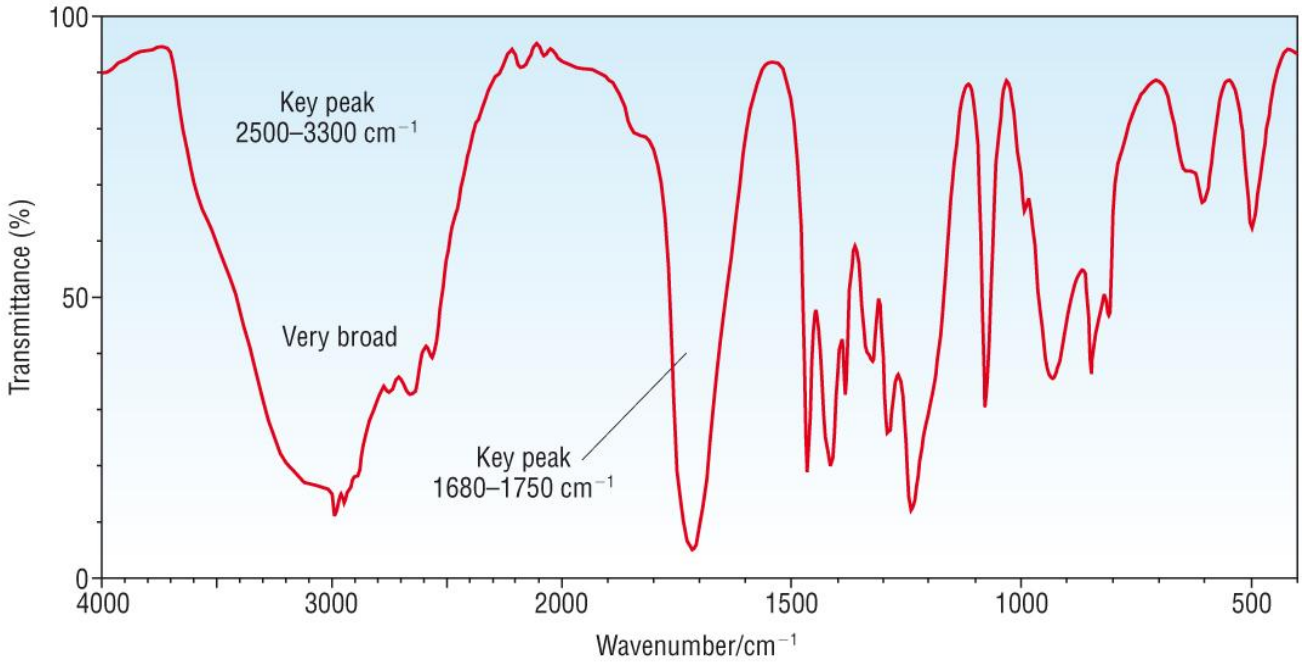
- The IR spectrum for propanal, CH_3CHO is shown below:



- The peak at 1680 - 1750 represents a C=O group in aldehydes and ketones.

Aldehydes and ketones:

- The IR spectrum for propanoic acid, CH_3CH_2COOH is shown below:



- The peak at 2500 - 3300 represents an O - H group in a carboxylic acid.
- The peak at 1680 - 1750 represents a C=O group in a carboxylic acid.

Questions P169 1-2

Mass Spectrometry

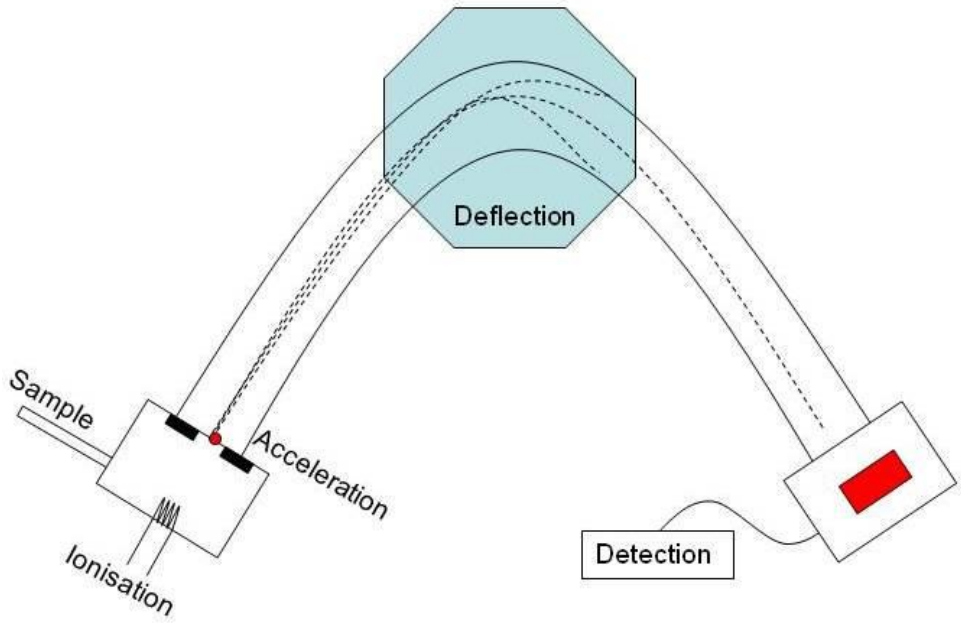
Uses of mass spectroscopy:

- First developed by JJ Thompson at the start of the 20th Century.
- It is used:
- To identify unknown compounds.
- To determine the abundance of isotopes
- To gain further information about the structure and chemical properties of molecules.

Examples:

- To examine patients breath while under anaesthetic.
- Detecting banned substances - steroids in athletes.
- Detecting traces of toxic chemicals in contaminated marine life

How a mass spectrometer works:

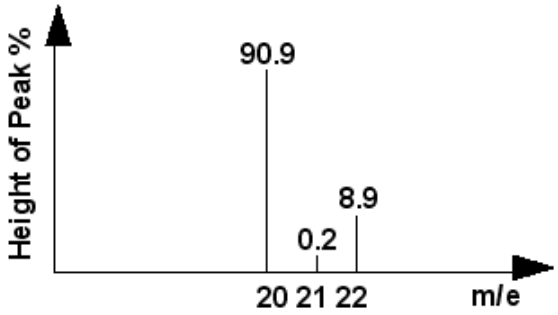


Deflection	Time of flight
• The sample is vaporised then **ionised = mass / charge**. • **Ionisation** is done by electron impact, chemical ionisation, electrospray or lasers. • Electroplates repel and **accelerate** the ion into the chamber. • A strong magnetic field **deflects** the beam of ions. • This is used to determine **mass / charge**. • The ion with a large mass is **deflected less** and hits the outer edge. • The ion with a small mass is **deflected most** hits the inside edge. • Only if the ion has the correct **mass / charge** ratio will it reach the **detector**. • The magnetic field strength can be varied to get a range of mass / charge readings.	• The sample is vaporised then **ionised = mass / charge**. • **Ionisation** is done by electron impact, chemical ionisation, electrospray or lasers. • Electroplates repel and **accelerate** the ion into the chamber. • A **short time of flight = small mass / charge** • A **long time of flight = large mass / charge** • The time taken to reach the detector determine the mass / charge of the ion.

Mass spectra of elements:

- One of the most important uses is to determine the isotopes present in a natural sample of an element.
- A mass spectrum shows the mass charge (the Ar) and the abundance as a %.
- This information can be used to determine the relative atomic mass:

From mass spectra



Use the formula:-

RAM = $\frac{(\% \times Ar) + (\% \times Ar) + \text{....etc}}{100}$

RAM = $\frac{(90.9 \times 20) + (0.2 \times 21) + (8.9 \times 22)}{100}$

RAM = 20.8

From table of data

RAM of silicon isotopes	% Abundance
28	92.2
29	4.7
30	3.1

Use the formula:-

RAM = $\frac{(\% \times Ar) + (\% \times Ar) + \text{....etc}}{100}$

RAM = $\frac{(92.2 \times 28) + (4.7 \times 29) + (3.1 \times 30)}{100}$

RAM = 28.1

Questions 1-2 P171

Mass spectrometry in organic chemistry

Mass spectrometry and molecules:

- Ionisation in a mass spectroscope is usually done by electron bombardment.
- Electron bombardment knocks another electron out of the molecule producing a positive **molecular ion**:

$$C_2H_5OH + e^- \rightarrow C_2H_5OH^+ + 2e^-$$

- This is called the **molecular ion, M^+**.
- The mass of the electron lost electron is negligible.
- The molecular ion has the same mass as the Mr of the molecule.
- As we have a mass and a charge we can use a mass spectrometer to determine the Mr (m/z).

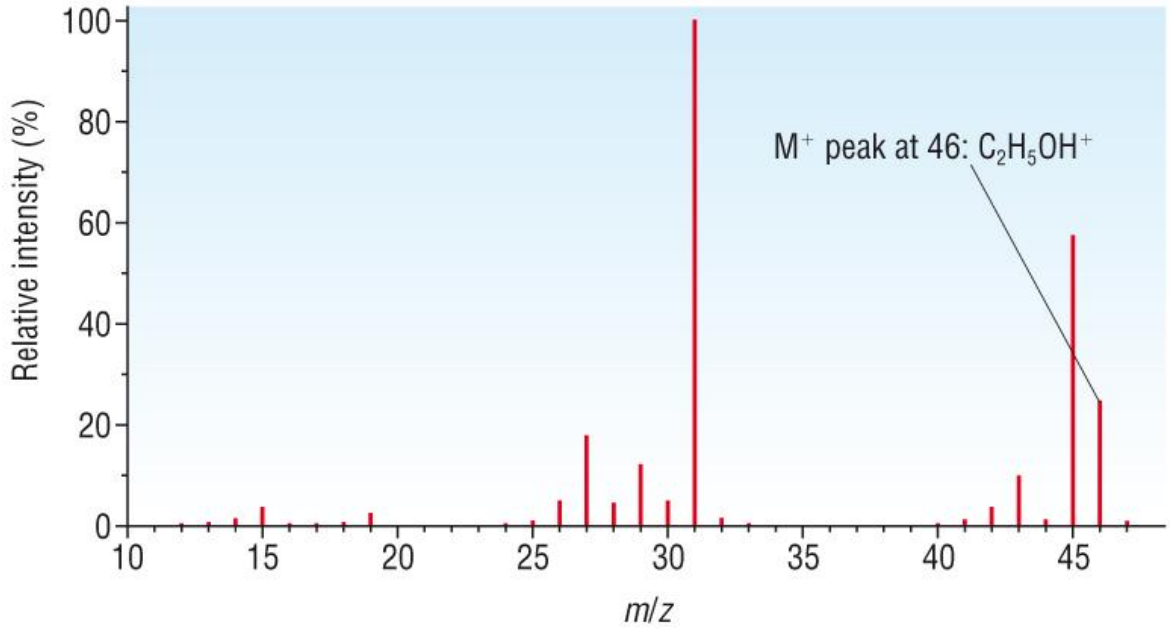
Fragmentation:

- Excess energy from the ionisation process causes bonds in the organic molecule to vibrate and weaken.
- This causes the molecule to split or **fragment** into smaller pieces.
- **Fragmentation** gives a positively charged molecular fragment ion and a neutral molecule:

$$C_2H_5OH^+ \rightarrow CH_3 + CH_2OH^+$$

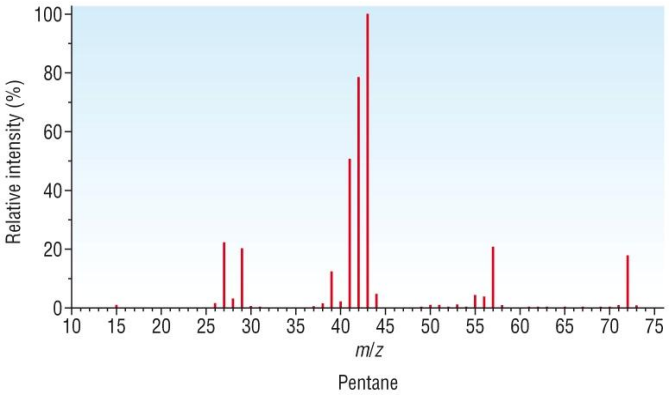
- The fragment ion, CH_2OH^+ has a mass and charge so we can use a mass spectrometer to determine the Mr (m/z) of that fragment.
- Fragment ions can be broken up further to give a range of m/z values.

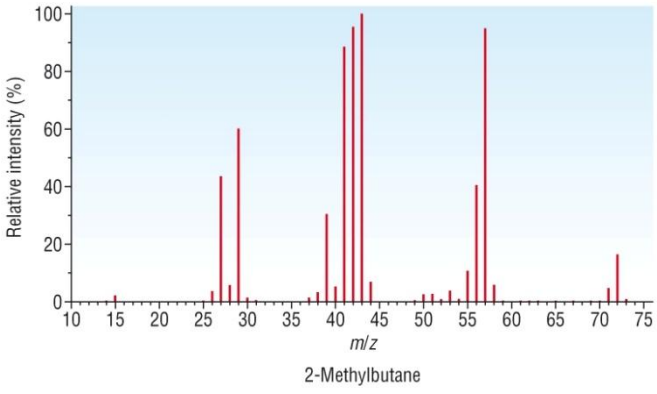
- The m/z values correspond to the Mr's of the molecule and its fragments.
- The Mr of the molecule is always the highest m/z value - ie this molecule has not been fragmented so it must have the highest Mr.
- The one below is for ethanol. It has a m/z of 46 which is also its Mr.



Fragmentation patterns:

- Mass spectroscopy is used to identify and determine the structures of unknown compounds.
- Although 2 isomers will have exactly the same $\mathbf{M^+}$ peak, the fragmentation patterns will be unique to that molecule, like a fingerprint.
- In practice mass spectrometers are linked to a database and the spectra is compared until an exact match is found:





- These are the mass spectra for pentane and a structural isomer of pentane, 2 methyl butane.
- The $\mathbf{M^+}$ peak is the same for each but the fragmentation patterns are different.

Questions 1-2 P173

Mass spectrometry: Fragmentation patterns

Identifying fragment ions:

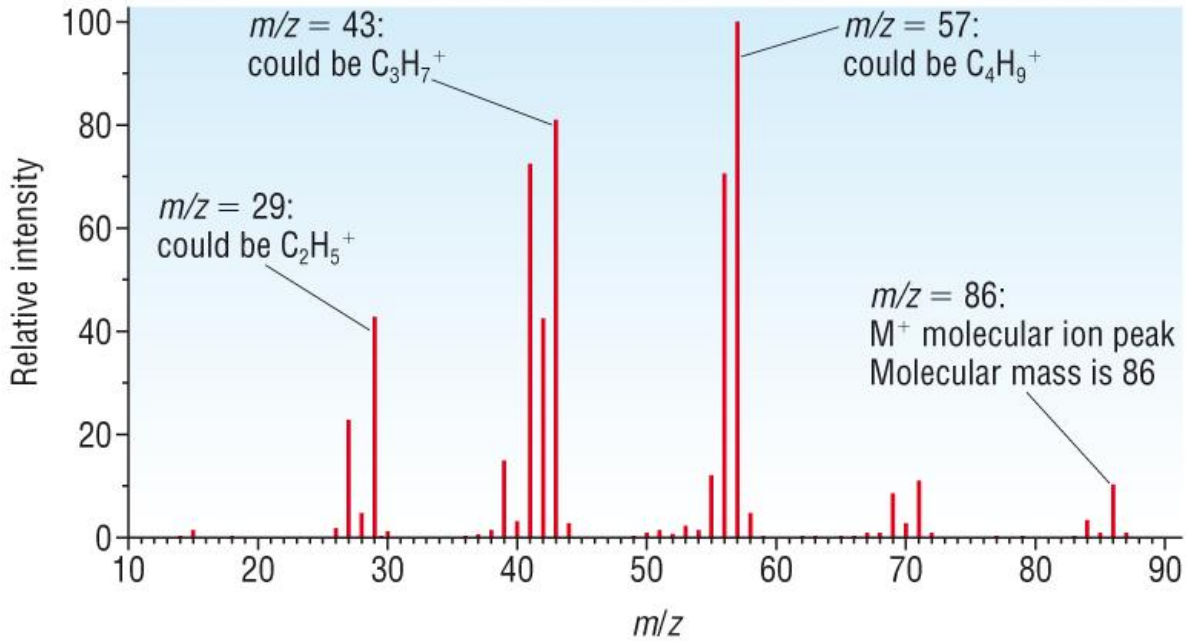
- When you look at a mass spectrum, other peaks seem to look more important than the **M^+** peak.
- These fragment peaks give clues to the structure of the compound.
- Even simple structures give common peaks that can be identified:

m/z value	Possible identity of the fragment ion
15	CH_3^+
29	$C_2H_5^+$
43	$C_3H_7^+$
57	$C_4H_9^+$
17	OH^+

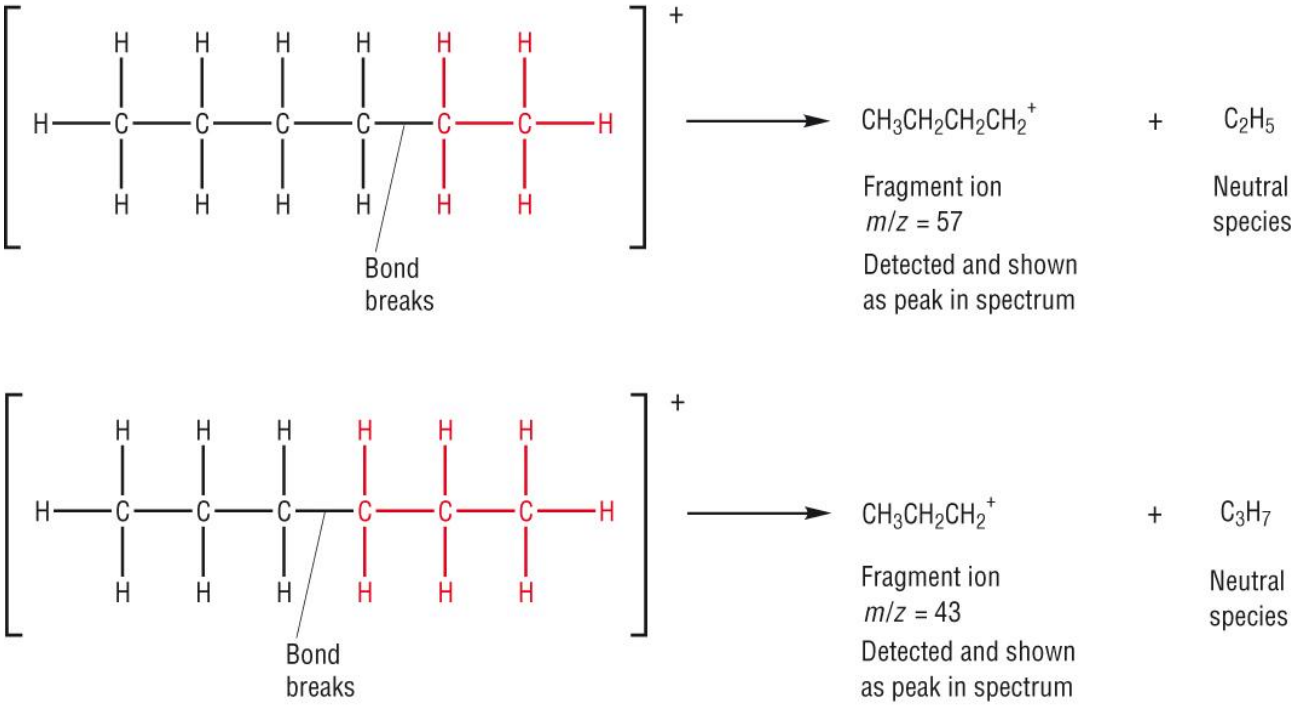
- Functional groups are a good place to start, OH = m/z of 17
- Some fragments are more difficult to identify as these will have undergone molecular rearrangement.

Identification of organic structures:

- A mass spectrum will not only tell you the Mr (from the **M^+** peak), but it can also tell you some of the structural detail.
- These peaks have been labelled with a letter:



- The mass spectrum above has been produced from hexane.
- The following reactions show how the molecule could fragment to form the fragment ions 57 and 43:



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