<u>Topic 12a – Analytical Techniques</u> <u>Revision Notes</u>

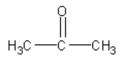
1) Infrared spectroscopy

- Absorption of infrared radiation causes covalent bonds to vibrate
- The frequencies that are absorbed can be used to identify the presence of certain bonds
- The absorptions you need to know are:

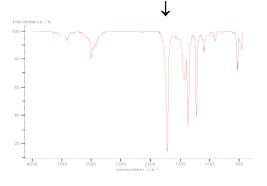
a)	C=0	1680 - 1750 cm ⁻¹
b)	-OH in alcohols	3230 - 3550 cm ⁻¹
c)	-OH in carboxylic acids	2500 - 3300 cm ⁻¹ (broad peak)
d)	C=C	1620 – 1680 cm ⁻¹

- The section of the spectrum below 1500 cm⁻¹ is known as the fingerprint region
- This allows identification of a molecule by finding a match with a spectrum in a database

Example 1 – propanone



Of the absorptions mentioned above, only the C=O peak will be present in propanone's IR spectrum:

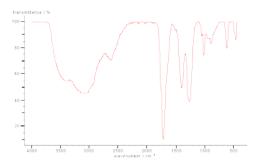


Example 2 – Ethanoic acid

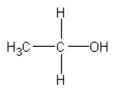


Of the peaks mentioned above, the -OH in acids and the C=O peaks will be present in ethanol's IR spectrum:

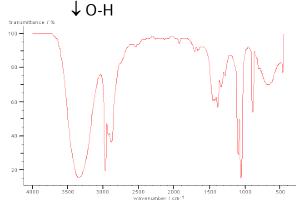
↓ O-H ↓ C=O



Example 3 – ethanol



Of the absorptions mentioned above, the –OH in alcohols peak will be present in ethanol's IR spectrum:



a) Global Warming

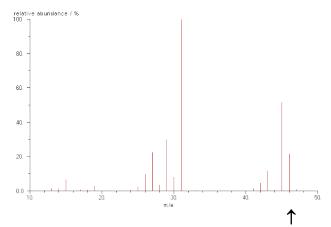
- In the troposphere, various gases absorb infrared radiation and keep the atmosphere warm
- Infrared radiation is absorbed by C=O bonds in CO₂, O-H bonds in H₂O and C-H bonds in methane
- The warming effect (or 'Greenhouse Effect') of a given gas depends on its concentration in the atmosphere, its ability to absorb infrared radiation and the time taken for it to break down
- Increased concentrations of greenhouse gases, like CO₂, contributes global warming because of the increased absorption of IR radiation
- Global warming has undesirable effects such as climate change and the melting of polar ice-caps and consequent rise in sea level which could flood low-lying areas. It is, therefore, important to control global warming resulting from increased concentrations of greenhouse gases

2) Mass spectrometry

- Mass spectrometry is a technique for measuring the masses of particles accurately
- In a mass spectrometer an electron is knocked off an organic molecule to create a molecular ion
- The molecular ion produces the peak furthest to the right (or highest m/z) in the spectrum

• The accurate mass of the molecular ion can be used to determine the molecular formula of an unknown compound

Example – ethanol



• The molar mass of ethanol is 46.0 The molecular ion peak is indicated by the arrow