CIE AS Chemistry

Your notes

22.1 Infrared Spectroscopy

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Infrared Spectroscopy

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Interpreting IR Spectra

- **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 electromagnetic waves in the infrared region and then detects the **intensity** of the wavelength of IR radiation which goes through the sample
- All organic molecules absorb IR radiation and depending on which energies of radiation are absorbed, bonds between atoms will vibrate by **stretching**, **bending** and **twisting**
- The molecules will only vibrate at a specific frequency
- The **resonance frequency** is the specific frequency at which the molecules will vibrate to stimulate larger vibrations
- Depending on the rest of the molecule, each vibration will absorb specific wavelengths of IR radiation which are also shown as the **reciprocal** of the wavelength
  - This unit is called the **wavenumber** (cm^{-1})
- Particular absorbances have characteristic **widths** (broad or sharp) and **intensities** (strong or weak)
  - For example, hydrogen bonds cause the O-H bonds in alcohols and carboxylic acids to be **broad** whereas the C-O bond in carbonyl (C=O) groups have a strong, sharp absorbance peak
- The energies absorbed by different functional groups are given as a range and an unknown compound can be identified by comparing its IR spectrum to the IR spectrum of a known compound

Absorption range of bonds table

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	1640 - 1690
	Carbonyl, carboxyl	1670 - 1740
	Ester	1710 - 1750
C ≡ N	Nitrile	2200 - 2250
C-H	Alkane	2850 - 2950
N-H	Amine, amide	3300 - 3500

O–H	Carboxyl	2500 - 3000
	Hydroxyl	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


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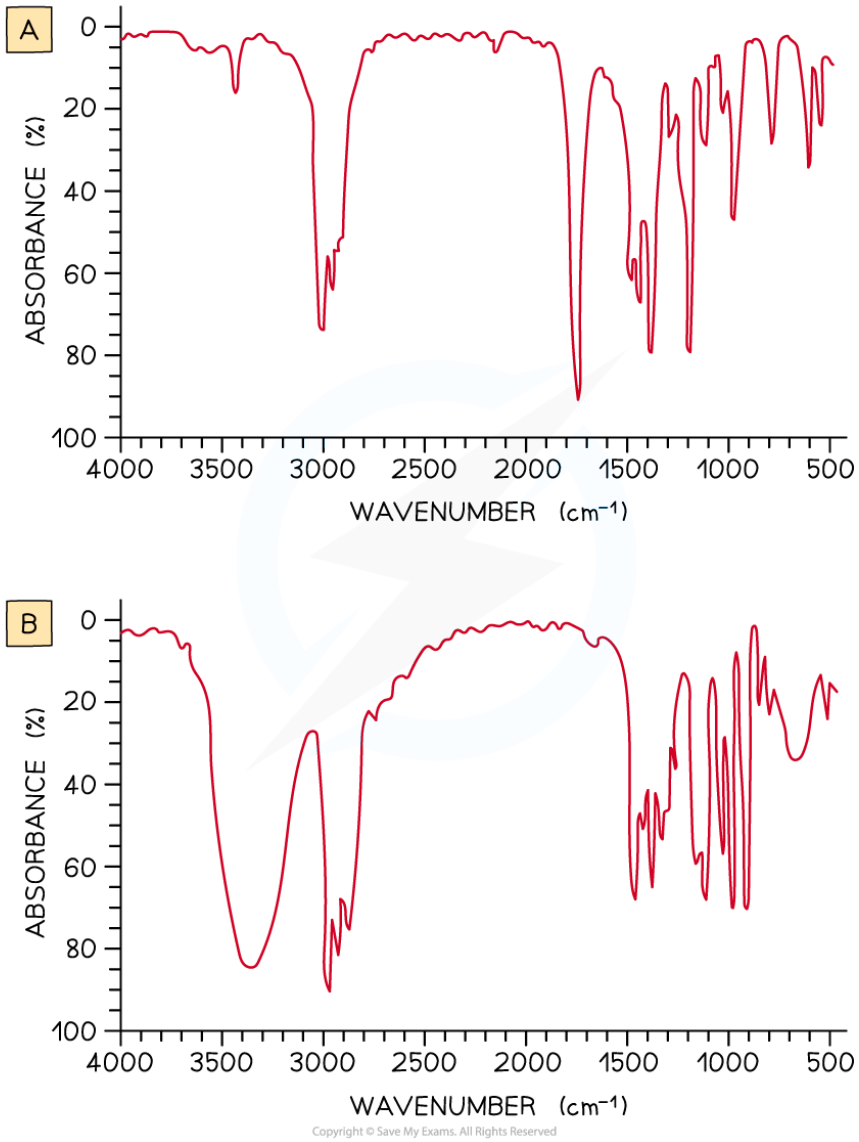
Worked example

Look at the two infrared spectra below and determine which one corresponds to propanone and which one to propan-2-ol.



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.

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- 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.


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