Cambridge (CIE) A Level Chemistry

Your notes

Infrared Spectroscopy

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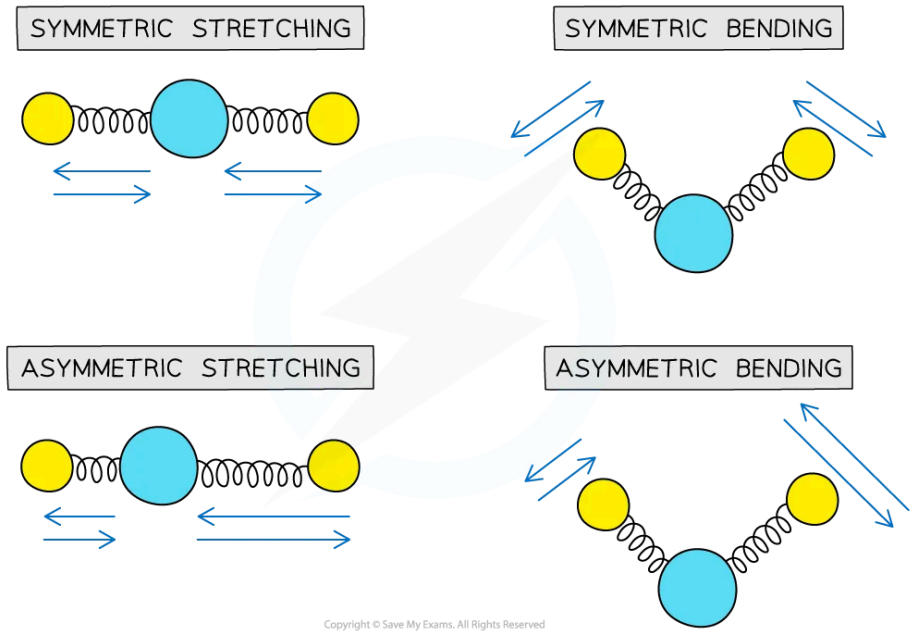
Interpreting IR Spectra

- **Infrared (IR) spectroscopy** is a technique used to identify compounds
  - It works by measuring how covalent bonds in molecules absorb infrared radiation
  - This absorption causes the bonds to vibrate in specific ways
- A **spectrophotometer** irradiates the sample with infrared waves
  - Then, it detects how much radiation is absorbed at each frequency
  - The resulting spectrum shows which types of bonds are present

Bond vibrations and absorption

- All **covalent bonds** behave like tiny **springs** rather than rigid bars
- Like springs, they can **vibrate in different ways**, such as stretching and bending



Different modes of vibration in molecules. Each mode has a characteristic frequency of vibration

- These vibrations occur at **specific frequencies** in the **infrared (IR)** region of the electromagnetic spectrum
- When IR radiation matches a bond's natural frequency, the bond **absorbs energy** and vibrates more strongly
- Each **vibration mode** (e.g. symmetric stretch, bending) has its own **characteristic frequency**

- These absorbed frequencies are expressed as **wavenumbers** (cm^{-1}), which are the **reciprocal of wavelength**

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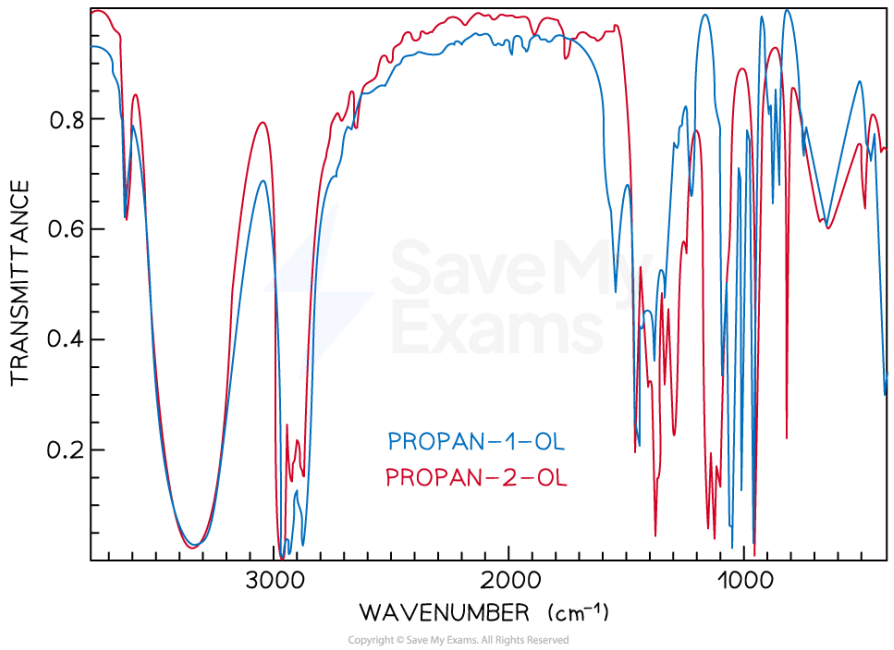
Absorption patterns and functional groups

- Each organic compound has a **unique IR spectrum**
  - Particularly in the region below 1500 cm^{-1}, known as the **fingerprint region**
- This region contains many small peaks caused by complex bond vibrations that are difficult to assign to specific groups
- However, comparing the fingerprint region to spectra from a database allows **exact identification** of a compound
- This is useful, for example, for identifying a particular isomer in a homologous series
  - They will all have the same functional groups but **different fingerprint regions**



The superimposed spectra of propan-1-ol and propan-2-ol show the same bonds above 1500 cm-1 but different fingerprint regions

- Each bond type absorbs within a **characteristic wavenumber range**
- Absorptions vary in **width** (broad or sharp) and **intensity** (strong or weak)
- For example:
  - O–H bonds in alcohols and carboxylic acids give **broad** peaks due to hydrogen bonding
  - C=O bonds in carbonyl compounds give **sharp**, strong peaks.
- Comparing an unknown IR spectrum with data for known compounds helps identify **functional groups**

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 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

Worked Example

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

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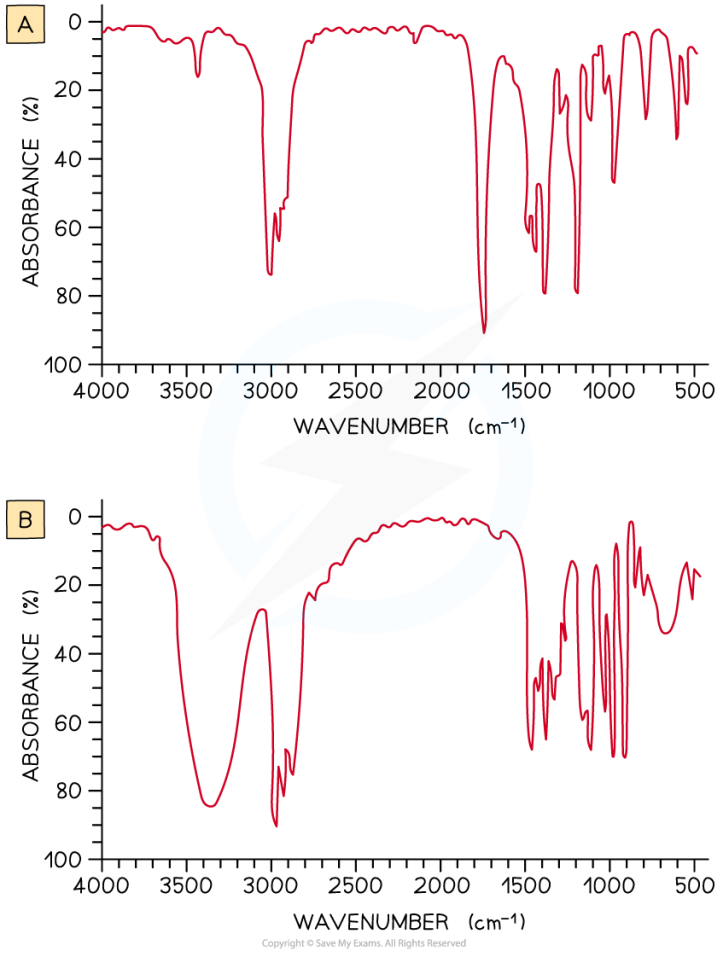

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Answer:

- 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.