

FACTFILE: GCE CHEMISTRY

2.7 INFRARED SPECTROSCOPY



Learning Outcomes

Students should be able to:

- 2.7.1 explain that the absorption of infrared radiation arises from molecular vibrations;
- 2.7.2 demonstrate understand that groups of atoms within a molecule absorb infrared radiation at characteristic frequencies; and
- 2.7.3 use infrared spectra to deduce functional groups present in organic compounds given wavenumber data.

Electromagnetic radiation

Frequency is measured in hertz. Wavenumber is used for infrared radiation. Wavenumber is measured in cm^{-1} and calculated from wavelength in cm where wavenumber = $1/\text{wavelength}$.

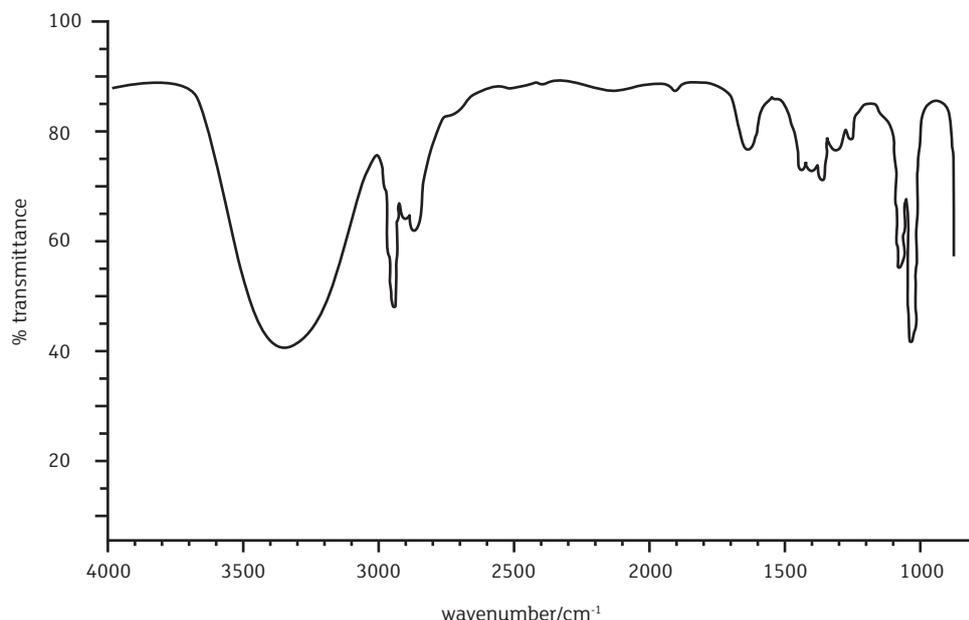
Ground state refers to a molecular vibration which is in the lowest possible energy state. Certain molecules can absorb electromagnetic radiation and be raised above the ground state. However, when a molecule absorbs infrared radiation (which has low energy), the bonds vibrate.

Energies in infrared radiation correspond to the energies involved in covalent **bond vibrations**.

Infrared spectroscopy is the study of how infrared radiation interacts with covalent bonds in molecules. The exact frequency of the infrared vibration depends on the nature of the bond that is vibrating. Some covalent bonds respond to infrared radiation more than others, resulting in increased bending or stretching of the covalent bonds which is picked up by the spectrometer. Different bonds in a covalent molecule absorb radiation of different frequencies which are normally measured as wavenumbers ($1/\text{wavelength}$). Wavenumber is the reciprocal of the wavelength and is measured in cm^{-1} . An infrared spectrum has a range from 4000 cm^{-1} to 600 cm^{-1} . The y axis is percentage transmittance. The dips are referred to as peaks. Some covalent bonds absorb infrared radiation particularly strongly; the table below shows infrared radiation data for some bonds.

Bond	Wavenumber / cm^{-1}
C—H	2850 – 3000
C=C	1450 – 1650
C=O	1650 – 1800
C—O	1000 – 1300
(alcohols) O—H	3200 – 3600
(carboxylic acids) O—H	2500 – 3000

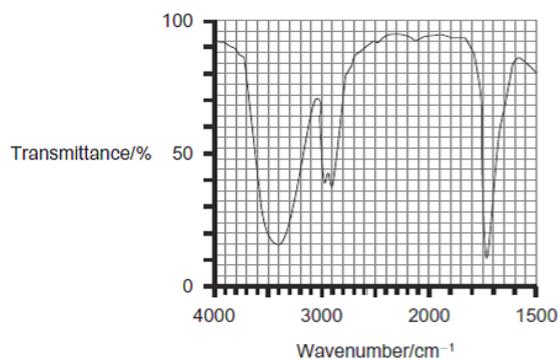
A typical infrared spectrum for ethanol is shown below.



The region below about 1300cm^{-1} is known as the fingerprint region. It contains a number of often over-lapping signals relating to specific bonds such as C-C and C-H in the sample molecule. The fingerprint region in an infrared spectrum is unique for each pure compound analysed.

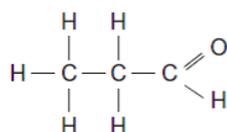
Above 1300cm^{-1} it is possible to identify individual signals corresponding to specific bonds which aids the elucidation of the structure of the compound. In the above spectrum, the broad peak at centred at 3400cm^{-1} is typical of an -OH group absorption in an alcohol. Note that a carboxylic acid has a peak at $1650 - 1800$ due to the presence of a C=O bond and another peak at $2500 - 3000$ due to the presence of an O—H bond.

3 Which one of the following molecules produces the infrared spectrum shown below?

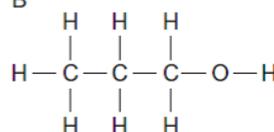


Bond	Wavenumber (cm ⁻¹)
O—H (alcohols)	3200–3700 strong broad
C—H	2700–3300 medium sharp
O—H (carboxylic acids)	2500–3200 strong broad
C=O	1680–1780 strong sharp

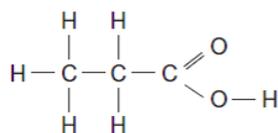
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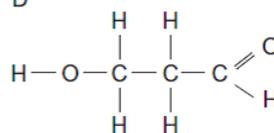
B



C



D



[1]

