

22.1 INFRARED SPECTROSCOPY

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Learning outcomes

Candidates should be able to:

1. analyse an infrared spectrum of a simple molecule to identify functional groups (see the Data section for the functional groups required)

Introduction

In **infrared spectroscopy**, a sample being analysed is irradiated (exposed to radiation) with electromagnetic waves in the infrared region of the electromagnetic spectrum. The machine used is called a *spectrophotometer*. It detects the intensity of infrared wavelengths that pass through the sample.

This analytical technique is particularly useful for organic chemists because all organic molecules absorb radiation in the infrared range of wavelengths. The energy absorbed corresponds to changes in the vibration of the bonds between atoms. The bonds can vibrate by stretching, bending and twisting. They have a natural frequency at which they vibrate. If we irradiate the molecules with energy that corresponds to this frequency, it stimulates larger vibrations and energy is absorbed. This is called the **resonance frequency** of that vibration.

Each type of vibration will absorb characteristic wavelengths of infrared radiation. Scientists often express these as the reciprocal of the wavelength, in a unit called *wavenumbers* (measured in cm^{-1}).

The presence of hydrogen bonding makes the absorbance of the O—H bonds in alcohols and carboxylic acids broad. By contrast, the C=O bond in carbonyl groups has a strong, sharp absorbance peak.

Characteristic infrared absorption frequencies for some selected bonds

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 hydroxy	2500–3000 3200–3600

Some examples:

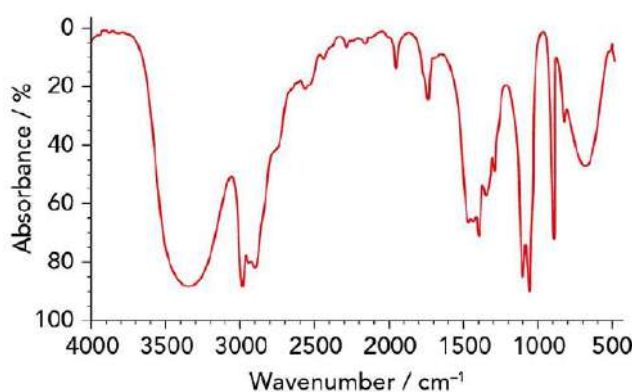


Figure: The infrared spectrum of ethanol, $\text{CH}_3\text{CH}_2\text{OH}$.

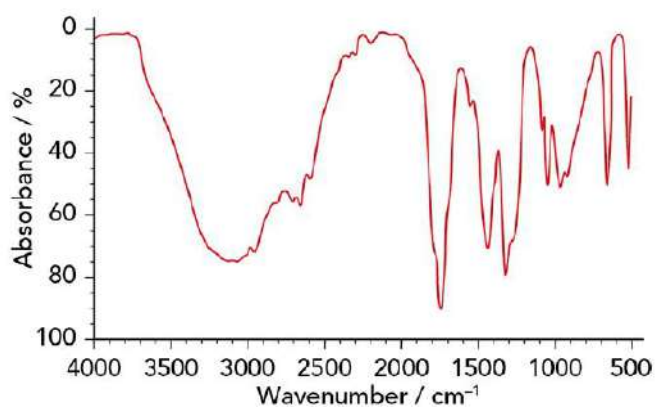


Figure: The infrared spectrum of ethanoic acid, CH_3COOH .

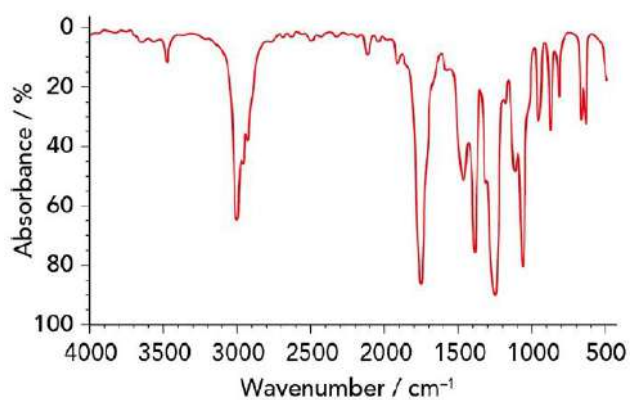


Figure: The infrared spectrum of ethyl ethanoate, $\text{CH}_3\text{COOCH}_2\text{CH}_3$.

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