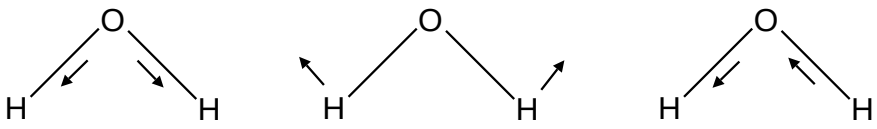
INFRA-RED SPECTROSCOPY

Introduction Infra-red spectroscopy is one of a variety of modern analytical techniques used to indentify unknown chemicals. Used in conjuction with **nuclear magnetic resonance spectroscopy (nmr)** and **mass spectrometry**, the identity of any organic molecule can be found.

How it works Covalent bonds have different strengths due to the masses of different atoms at either end of the bond. As a result, the bonds vibrate at different frequencies (imagine two balls on either end of a spring) . The frequency of vibration can be found by detecting when the molecules absorb electro-magnetic radiation.

Various vibrations are possible. **Bending** and **stretching** are two such examples and can be found in water molecules. Each one occurs at a different frequency.



Symmetric stretching | Bending | Asymmetric stretching

Infra-red spectra

Interpretation Infra-red spectra are complex due to the many types of vibration in molecules.

The position of a peak depends on
- **bond strength**
- **masses of the atoms** joined by the bond

- **strong bonds** and **light atoms** absorb at **high wavenumbers**
- **weak bonds** and **heavy atoms** absorb at **low wavenumbers**

Fingerprint Region The technique is widely used in the analysis of the structure of organic compounds. As these tend to have a lot of C-C and C-H bonds within their structure, spectra obtained will have peaks in the 1400 cm^{-1} to 800 cm^{-1} range. This region is referred to as the **"fingerprint"** region as the pattern obtained is characteristic of a particular compound. The frequency of any absorption is also affected by adjoining atoms or groups.

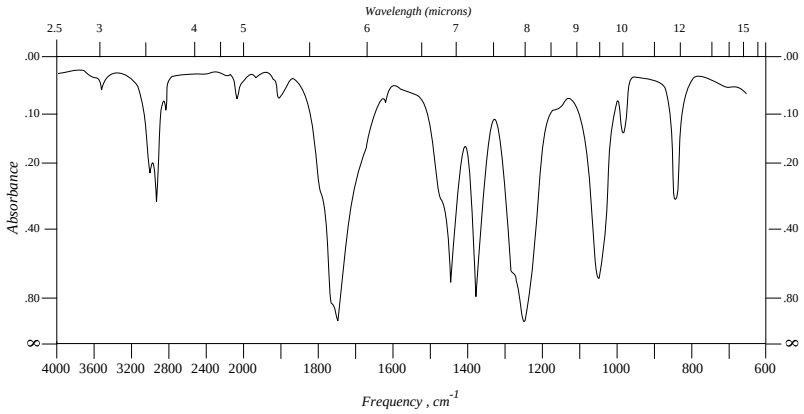
One can also analyse the purity of a substance by checking the spectrum for unwanted peaks. The presence of a strong absorption due to a C=O bond can tell if an alcohol has been oxidised to the equivalent carbonyl compound.

The spectrum

Vertical axis	**Absorbance**	stronger the absorbance the larger the peak.
Horizontal axis	**Frequency** or Wavelength	**wavenumber** (waves per centimetre) / **cm^{-1}** microns (μ); 1 micron = 1000 nanometres

A typical IR spectrum

This is the IR spectrum of the ester, methyl ethanoate *(acetate)*. An obvious feature is the strong signal between 1750 cm^{-1} and 1730 cm^{-1} due to the carbonyl group.



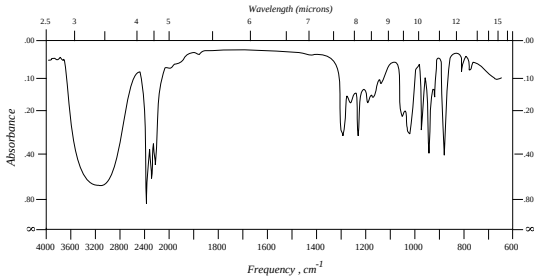
IDENTIFICATION USING INFRA RED SPECTROSCOPY

Compound Compare the compound's IR spectrum with one on a computer database

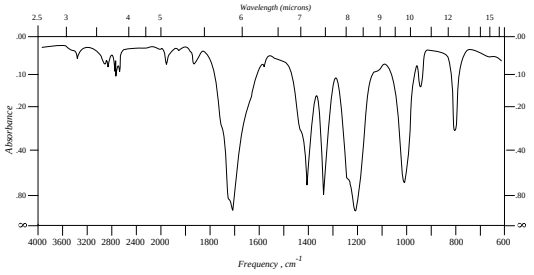
Functional Groups The presence of certain absorptions can be used to identify functional groups.

BOND	COMPOUND	ABSORBANCE	RANGE
O-H	alcohols	broad	3200 cm^{-1} to 3550 cm^{-1}
O-H	carboxylic acids	very broad	2500 cm^{-1} to 3300 cm^{-1}
C=O	ketones, aldehydes, acids	strong and sharp	1640 cm^{-1} to 1750 cm^{-1}

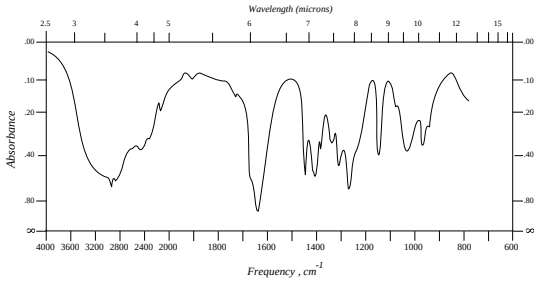
ALCOHOL
O-H absorption



ALDEHYDE / KETONE
C=O absorption



CARBOXYLIC ACID
O-H absorption
C=O absorption



Other

- **Monitoring air pollution** (e.g. CO and NO from car emissions)
- In **breathalysers** by monitoring the amount of ethanol in breath

GLOBAL WARMING

Greenhouse gases	CARBON DIOXIDE	CO_2	contains	C=O bonds
	WATER VAPOUR	H_2O	contains	O-H bonds
	METHANE	CH_4	contains	C-H bonds

The 'Greenhouse Effect' of a given gas is dependent on its...

- **atmospheric concentration**
- **ability to absorb infrared radiation**

Introduction

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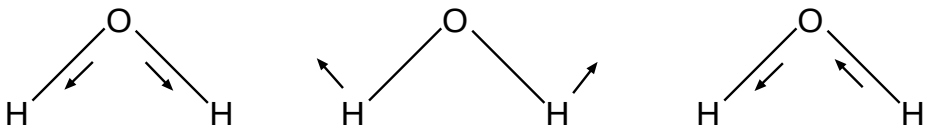
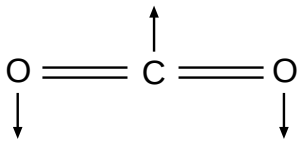
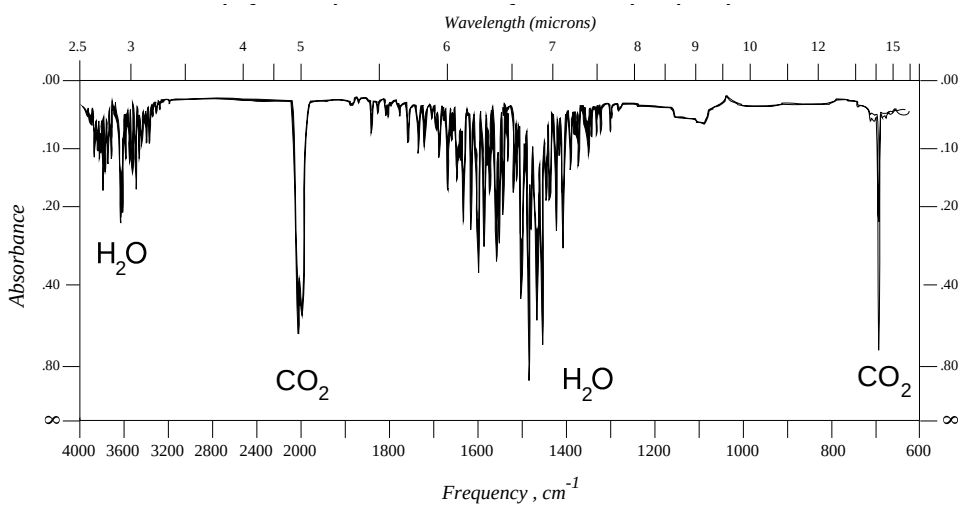


Symmetric stretching | Bending | Asymmetric stretching

Bending in a carbon dioxide molecule



The frequencies lie in the INFRA RED part of the electro-magnetic spectrum and can be detected using **infra red spectroscopy**.



It is the absorption of infra red radiation by atmospheric gases such as methane, carbon dioxide and water vapour that contributes to global warming.