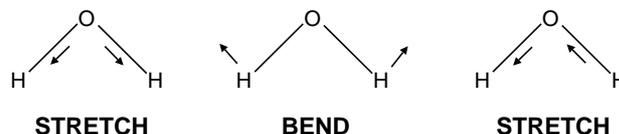


INFRA - RED SPECTROSCOPY

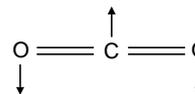
Introduction Different covalent bonds have different strengths due to the masses of different atoms at either end of the bond. As a result, the bonds vibrate at different frequencies (imagine two balls on either end of a spring). The frequency of vibration can be found by detecting when the molecules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

Various types of vibration are possible. **Bending** and **stretching** can be found in water molecules.

Each occurs at a different frequency.

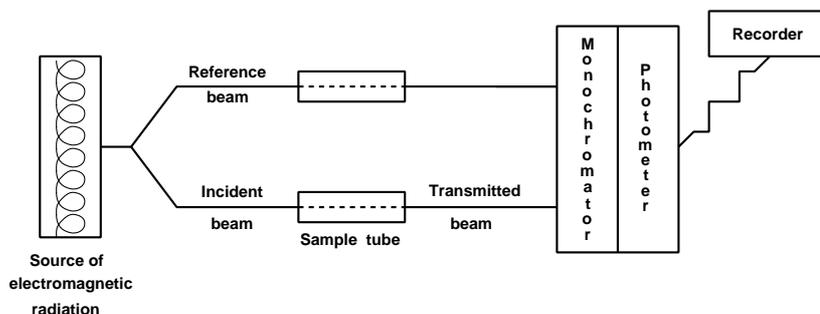


An equivalent **bend** at 667cm^{-1} occurs in a carbon dioxide molecule.



As molecules vibrate, there can be a change in the dipole moment of the molecule.

The Infra-red Spectrophotometer



Operation The intensity of the incident beam and reference beam is measured (they are the same). The intensity of the transmitted beam is also measured. The difference in intensity between the incidence beam and the transmitted beam is a measure of the amount of radiation absorbed by the sample. The frequency of radiation is examined continuously by the monochromator. In the photometer the relative intensities of the reference and transmitted beams are compared; the percentage of the reference beam found in the transmitted beam can be plotted as a function of frequency, or wavenumber.

Infra-red spectra

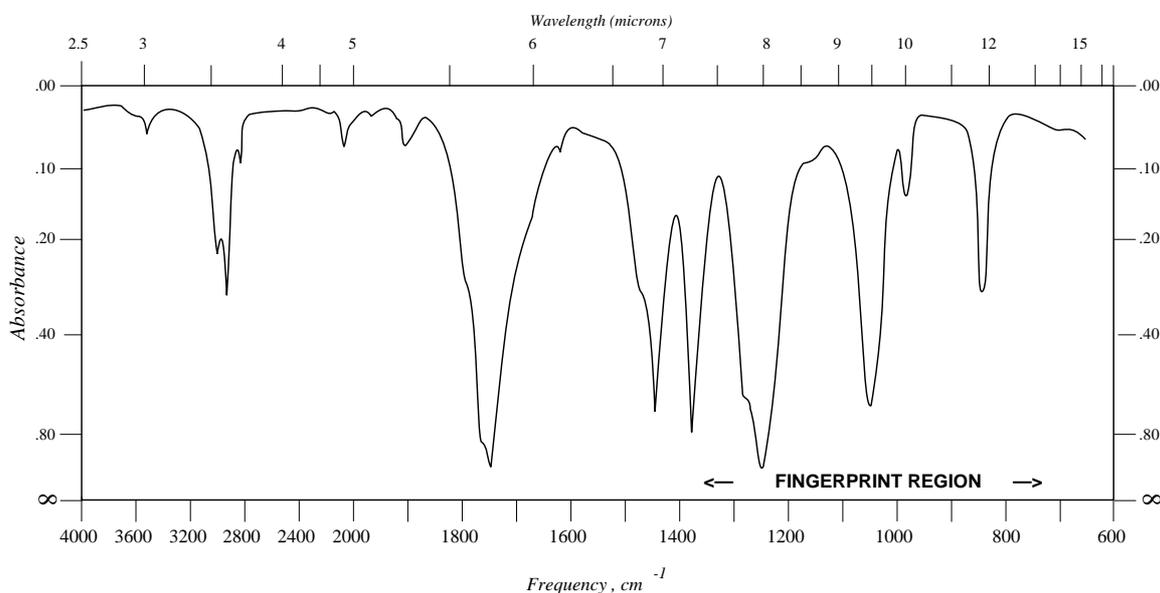
Interpretation Infra-red spectra are very complex due to the many types of vibration which occur in each molecule. Total characterisation of a substance based only on its IR spectrum is almost impossible unless one has computerised data handling facilities for comparison of the obtained spectrum with one in memory. However, the technique is useful when used in conjunction with other analytical methods such as nuclear magnetic resonance (nmr) spectroscopy and mass spectroscopy.

The position of a peak depends on the

- **bond strength**
 - **masses of the atoms** joined by the bond
- **strong bonds** and **light atoms** absorb at **lower wavenumbers**
- **weak bonds** and **heavy atoms** absorb at **high wavenumbers**

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

A typical IR spectrum



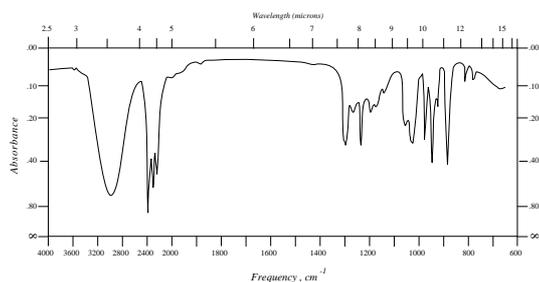
This is the IR spectrum of the ester, methyl ethanoate (*acetate*). An obvious feature is the strong signal between 1750 cm^{-1} and 1730 cm^{-1} due to the carbonyl group.

Fingerprint Region

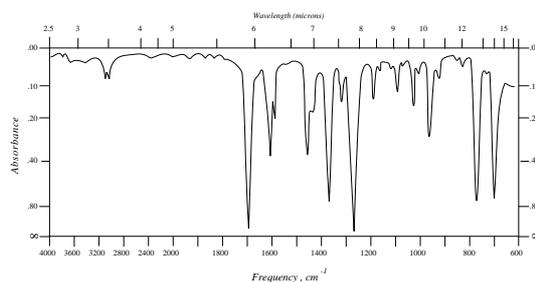
- organic molecules have a lot of C-C and C-H bonds within their structure
- spectra obtained will have peaks in the 1400 cm^{-1} to 800 cm^{-1} range
- this is referred to as the “**fingerprint**” region
- the pattern obtained is characteristic of a particular compound
the frequency of any absorption is also affected by adjoining atoms or groups.

One can **analyse the purity** of a substance by checking 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.



Typical spectrum of an ALCOHOL



Typical spectrum of a CARBONYL COMPOUND

CHARACTERISTIC ABSORPTION FREQUENCIES OF SOME FUNCTIONAL GROUPS

<i>Bond</i>	<i>Class of compound</i>	<i>Range, cm⁻¹</i>	<i>Intensity</i>	
C-H	Alkane	2965 - 2850	strong	
	CH ₃ -	1450	medium	
		1380	medium	
		1465	medium	
	CH ₂ -	3095 - 3010	medium	
		1000 - 700	strong	
	Alkyne	3300 (approx)	strong	
		Aldehyde	2900 - 2820	weak
			2775 - 2700	weak
C-C	Alkane	1200 - 700	weak	
C=C	Alkene	1680 - 1620	variable	
C≡C	Alkyne	2260 - 2100	variable	
C=O	Ketone	1725 - 1705	strong	
	Aldehyde	1740 - 1720	strong	
	Carboxylic acid	1725 - 1700	strong	
	Ester	1750 - 1730	strong	
	Amide	1700 - 1630	strong	
	Anhydride	1850 - 1800	strong	
C-O	Alcohol, ester, ether carboxylic acid	1300 - 1000	strong	
O-H	Alcohol (monomer)	3650 - 3590	variable, sharp	
	Alcohol (H-bonded)	3420 - 3200	strong, broad	
	Carbox. acid (H-bonded)	3300 - 3250	variable, broad	
N-H	Amine (1°), Amide (1°)	3500 (approx)	medium	
	Amine (2°), Amide (2°)	3500	medium	
C≡N	Nitrile	2260 - 2240	medium	
C-X	Fluoride	1400 - 1000	strong	
	Chloride	800 - 600	strong	
	Bromide	600 - 500	strong	
	Iodide	500 (approx)	strong	