

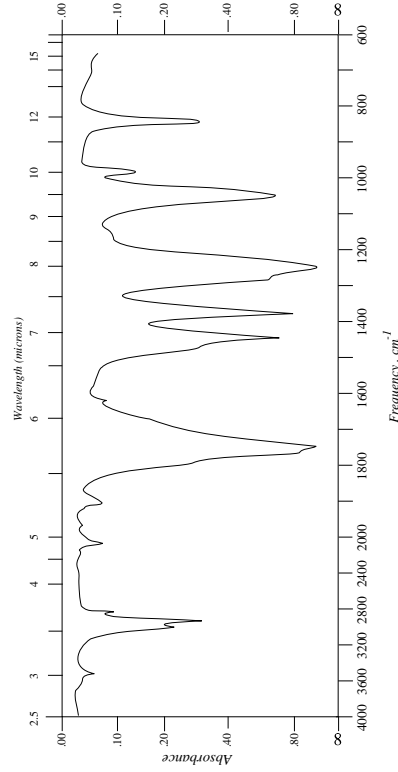
# SPECTROSCOPY

## AT A GLANCE

- **Infra-red spectroscopy**
- **Nuclear magnetic resonance (NMR) spectroscopy**
- **Mass spectrometry**

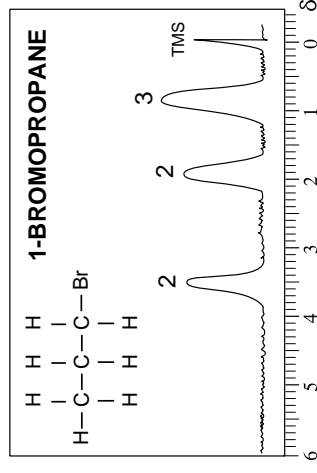
### INFRA RED

- **chemical bonds vibrate at different frequencies**
- the frequency is found by detecting when molecules absorb radiation
- the frequency of any absorption is affected by adjoining atoms
- spectra are complex due to the many vibrations occurring
- correlation charts may be used to assign peaks
- each molecule gives a unique spectrum
- characterisation of a substance involves **comparison of spectra**
- organic molecules tend to have a lot of C-C and C-H bonds
- spectra will thus have many peaks in the 1400  $\text{cm}^{-1}$  to 800  $\text{cm}^{-1}$  range
- this region of the spectrum is referred to as the **“fingerprint” region**
- typical absorptions occur at about 3500  $\text{cm}^{-1}$  for O-H bonds  
1750  $\text{cm}^{-1}$  for C=O bonds



### NUCLEAR MAGNETIC RESONANCE - NMR

- produces **information about hydrogen atoms** in molecules
- a liquid sample is spun in a magnetic field
- **hydrogen atoms in different environments** respond differently to the field
- each different environment produces a different signal at a different chemical shift
- tetramethylsilane provides the reference signal at  $\delta = 0$
- the **area under each peak** (signal) is proportional to the number of hydrogens



### MASS SPECTROMETRY

- the process is similar to that used to gather information about isotopes
- **gaseous molecules are ionised, accelerated and deflected**
- the **amount of deflection depends on m/z** - mass/charge ratio
- each molecule undergoes **fragmentation** into smaller particles
- each peak in the spectrum is due to a charged fragment with a certain **m/z value**
- the final peak is due to the **molecular ion** which has the **largest m/z value**
- the m/z value of the molecular ion is **used to calculate the relative molecular mass**

