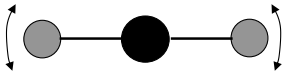
IR SPECTROSCOPY

- Infrared spectroscopy is a very important technique that can be used to analyse organic compounds.
- All covalent bonds vibrate at a characteristic frequency (stretching and contracting as well as bending vibrations are the commonest types).

stretching vibration



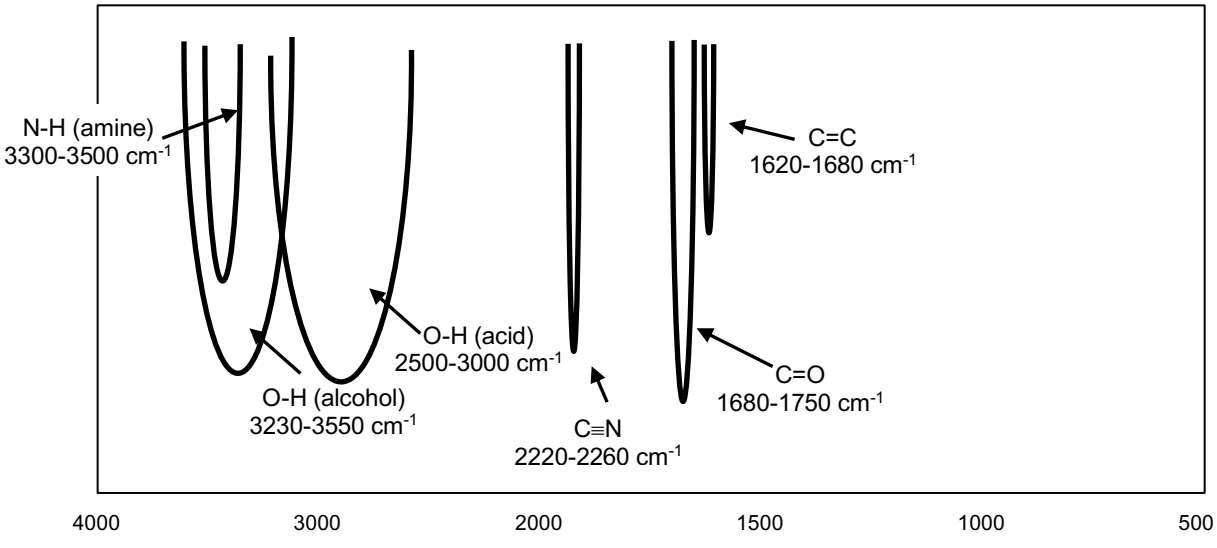
bending vibraion

- The frequency depends on the mass of the atoms in the bond, the bond strength, and the type of vibration.
- The frequencies at which they vibrate are in the infrared region of the electromagnetic spectrum.
- If infrared light is passed through the compound, it will absorb some or all of the light at the frequencies at which its bonds vibrate.
- Rather than using the actual values of the wavelength or frequency, the IR light is measured in wavenumbers [1/frequency (in cm)] because it gives convenient numbers in the range 4000 – 400 cm^{-1}
- There are two main things you need to be able to do with infra-red spectra:
  1) identify functional group signals (above 1500 cm^{-1}) – to identify functional groups
  2) use the "fingerprint" region (below 1500 cm^{-1}) – to identify specific compounds

1) Identifying functional group signals (above 1500 cm^{-1})

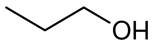
- This part of the spectrum is used to spot characteristic signals for functional groups (there are some below 1500 cm^{-1} but they are usually difficult to identify due to the high number of signals in that region of the spectrum).
- The table gives the wavenumber of some common bonds.
- It is also useful to remember that C-H bonds are all around 3000 cm^{-1}, but are C-H bonds on saturated C atoms are below 3000 cm^{-1} and those on unsaturated C atoms are above 3000 cm^{-1}
- However, there are some useful signals to look out for.

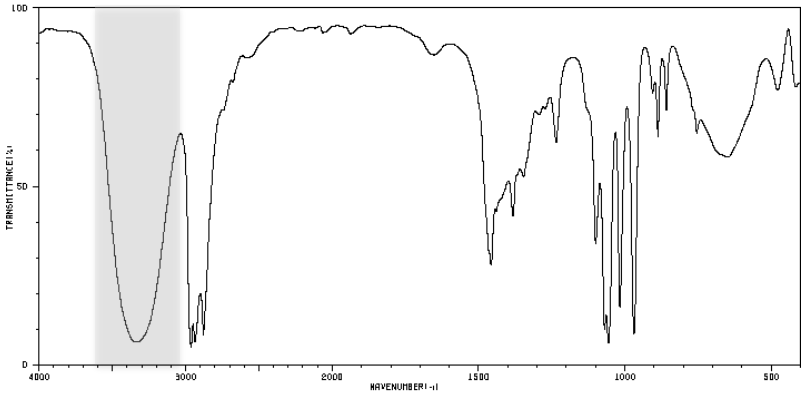
Bond	Wavenumber / cm^{-1}
N–H (amines)	3300 – 3500
O–H (alcohols)	3230 – 3550
C–H	2850 – 3300
O–H (acids)	2500 – 3000
C≡N	2220 – 2260
C=O	1680 – 1750
C=C	1620 – 1680
C–O	1000 – 1300
C–C	850 – 1100



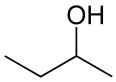
O–H alcohol	3230 – 3550 cm^{-1}	these are often very broad and obvious

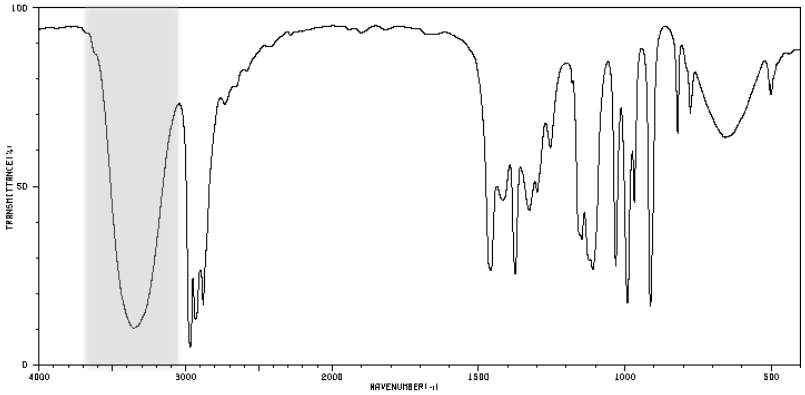
e.g. propan-1-ol





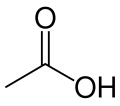
e.g. butan-2-ol

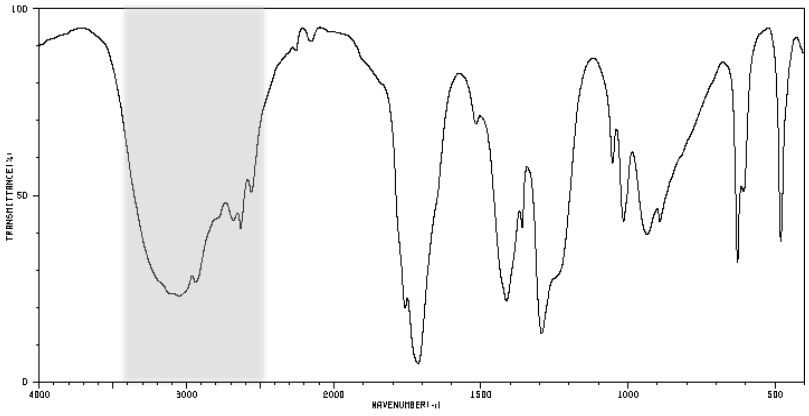




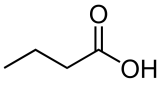
O–H acid	2500 – 3000 cm^{-1}	these are often very broad and obvious, but with C-H signals overlapping as well so making them “bumpy”

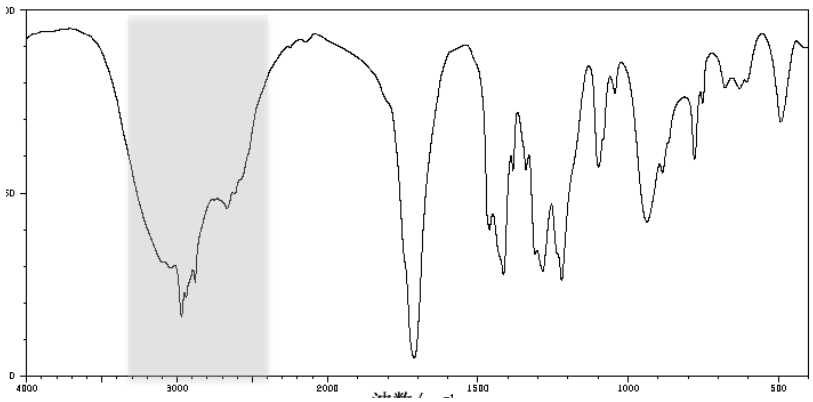
e.g. ethanoic acid





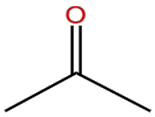
e.g. butanoic acid

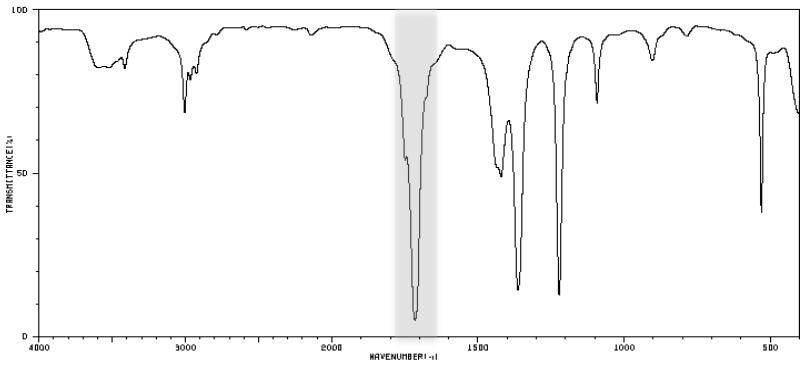




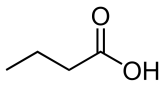
C=O	1680 – 1750 cm^{-1}	these are often narrow but very strong; they are found in aldehydes, ketones, acids, ester, amides, etc

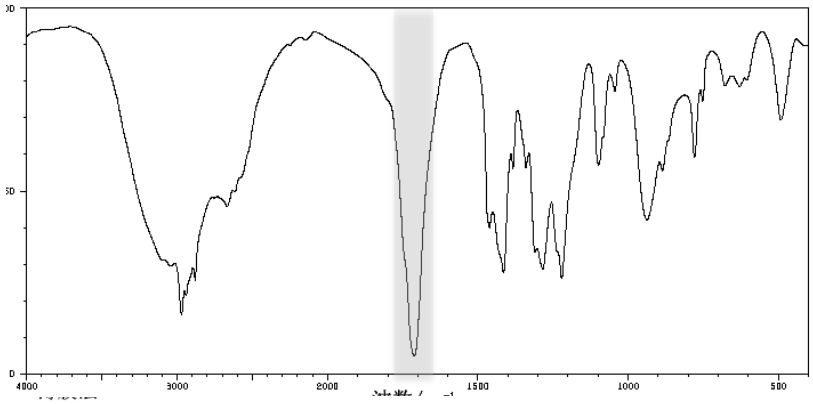
e.g. propanone



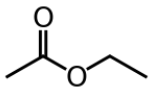


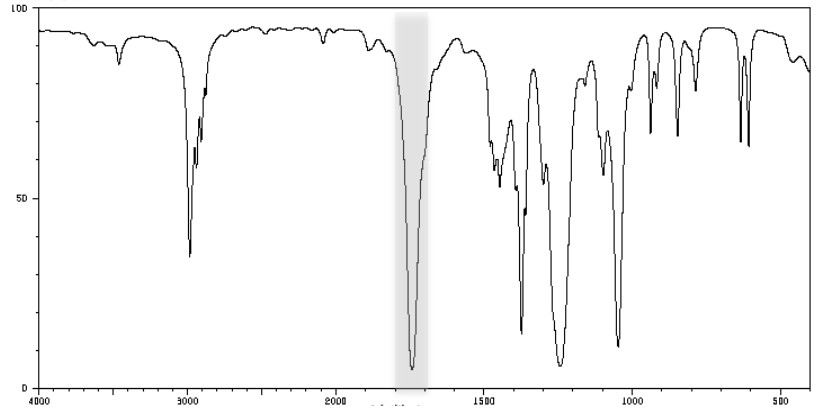
e.g. butanoic acid



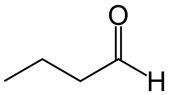


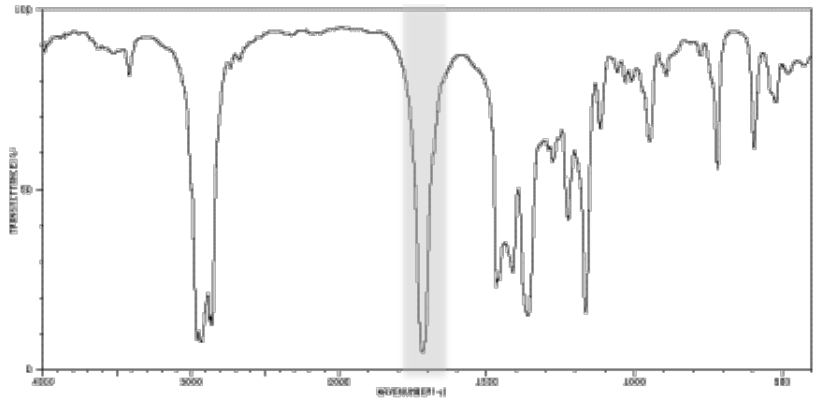
e.g. ethyl ethanoate





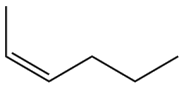
e.g. butanal

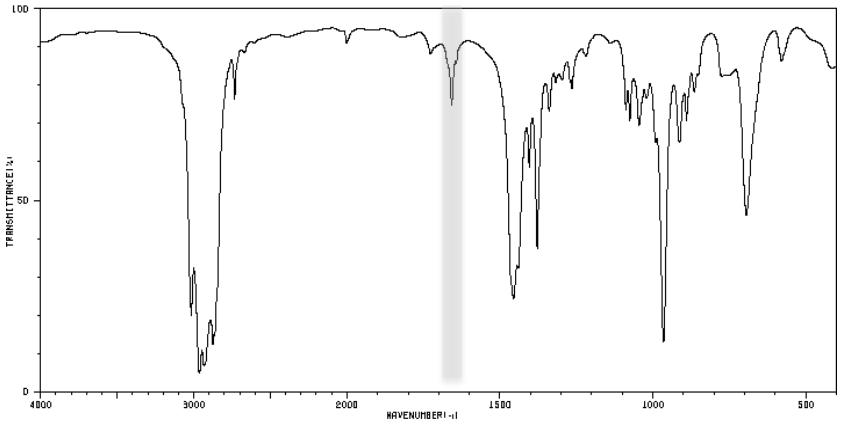




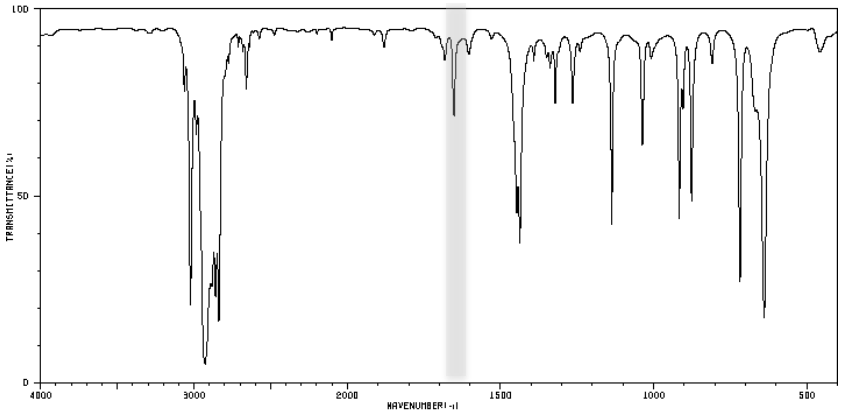
C=C	1620 – 1680 cm^{-1}	these are often narrow but relatively weak absorption

e.g. hex-2-ene



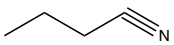


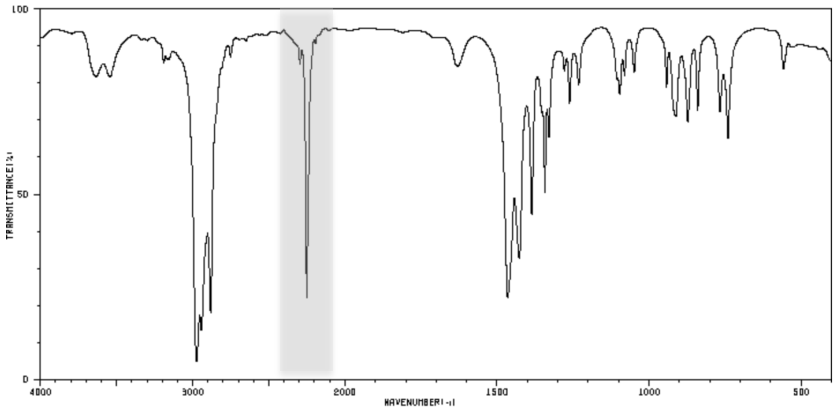
e.g. cyclohexene



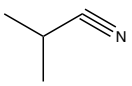
C≡N	2220– 2260 cm^{-1}	these are often narrow and strong

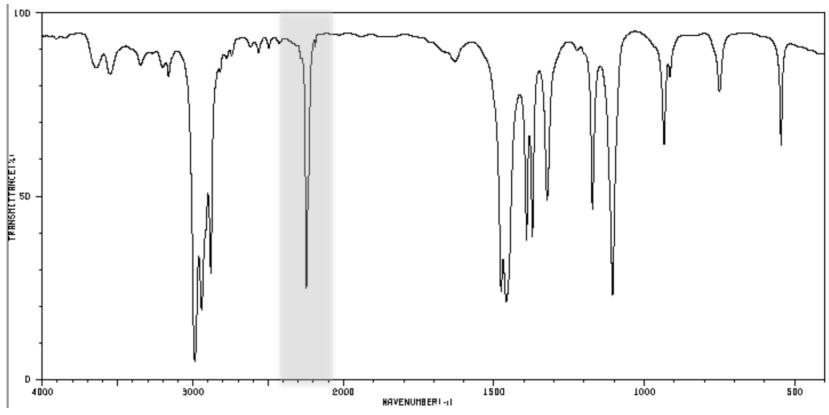
e.g. butanenitrile





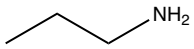
e.g. methylpropanenitrile

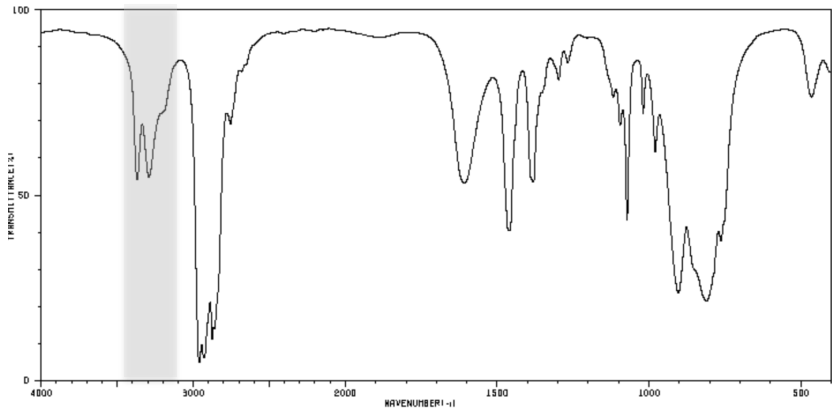




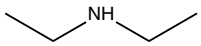
N–H (amines)	3300 – 3500 cm^{-1}	these are very obvious, large peaks; for primary amines (with NH_2 group) there are two peaks

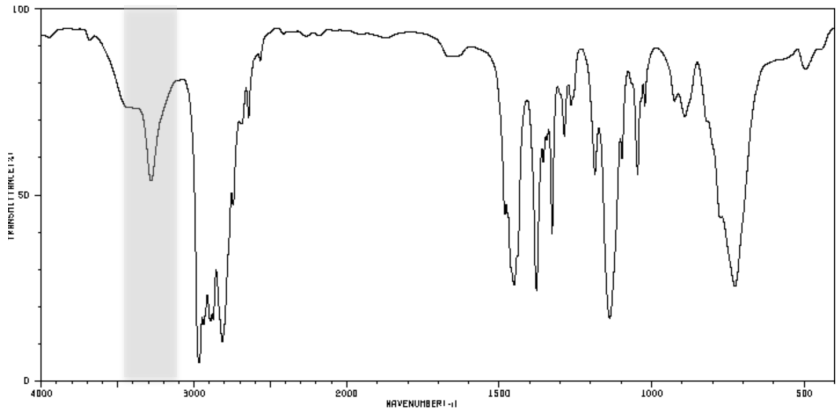
e.g. propylamine





e.g. diethylamine

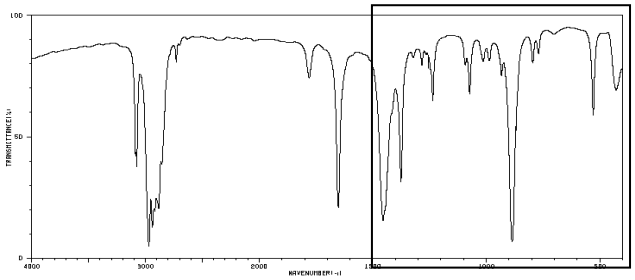


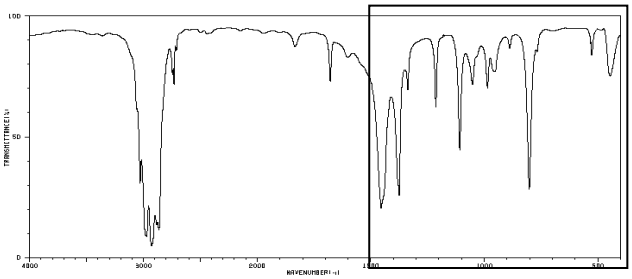


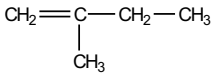
2) Using the "finger-print" region (below 1500 cm^{-1})

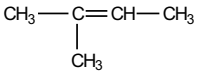
- This part of the spectrum is more complicated and contains many signals which means that we do not use it to identify functional groups.
- However, this part of the spectrum is unique for every compound, and so can be used as a "fingerprint". Comparison of the spectrum to that of known compounds can identify it.

  e.g. these two IR spectra are for 2-methylbut-1-ene and 2-methylbut-2-ene – these are very similar compounds but the fingerprint region of their IR spectra are very different









- This region can also be used to check if a compound is pure. If a comparison of the spectrum of a sample is made to the spectrum of the pure compound, they should be identical. If there are any extra peaks in the fingerprint region, they must be due to an impurity.