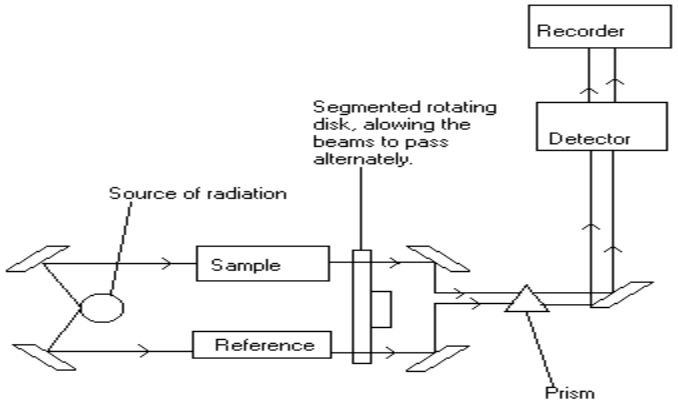
Infrared Spectroscopy [IR]

IR spectroscopy is a mainly qualitative analytical method based on the absorption of infrared light by analyte molecules. It is a powerful analytical tool as nearly all molecules absorb infrared light.
The covalent bonds in molecules bend, stretch, wag, twist and rock. The vibrational energy of the molecule caused by this bending and stretching is "quantised" into discrete vibrational energy levels. The frequency of IR light absorbed by the analyte have exactly the energy needed to promote molecules into different **vibrational energy levels.**
The energies [or frequencies] of IR absorbed by a molecule depend on the **kind of bonds** in the molecule [eg. O–H bonds absorb IR of a different frequency than that absorbed by C–H bonds] and the **overall structure of the molecule** [eg. O–H bonds in an alkanol will absorb in the range 3200 – 3600 cm^{-1}, whereas O–H bonds in a carboxylic acid will absorb in the range 2500 – 3300 cm^{-1}]

In IR spectroscopy the frequency is measured in **wavenumber** [**cm^{-1}**]. Wavenumber is the inverse of the wavelength measured in cm … what! Chemists are weird.

The Infrared Spectrometer

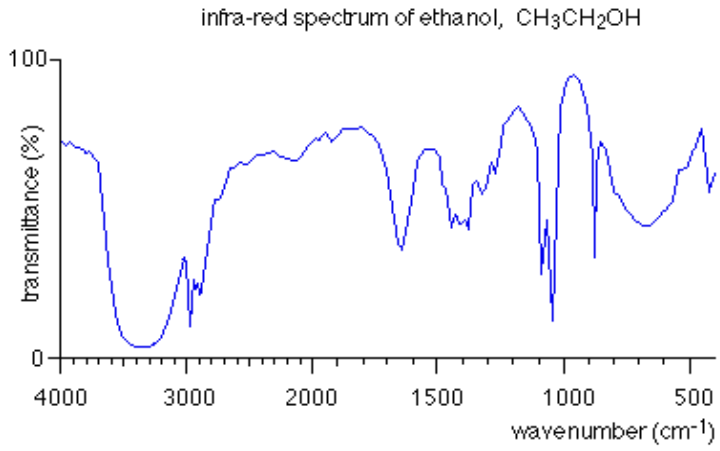


Infrared Absorption Data

Bond	Wavenumber [cm^{-1}]	Bond	Wavenumber [cm^{-1}]
C – Cl	700 – 800	O – H acid	2500 – 3300
C – C	750 – 1100	C – H alkane	2850 – 3100
C – O alkanol	1000 – 1300	C – H alkene	3000 – 3100
C = C alkene	1610 – 1680	N – H amine	3100 – 3500
C = O acid, ester	1670 – 1750	O – H alkanol	3200 – 3550

Chemists can use tables of wavenumbers to help identify the main functional groups present in an organic compound, or for positive identification, the whole spectrum can be compared to a computerized library of IR spectra.

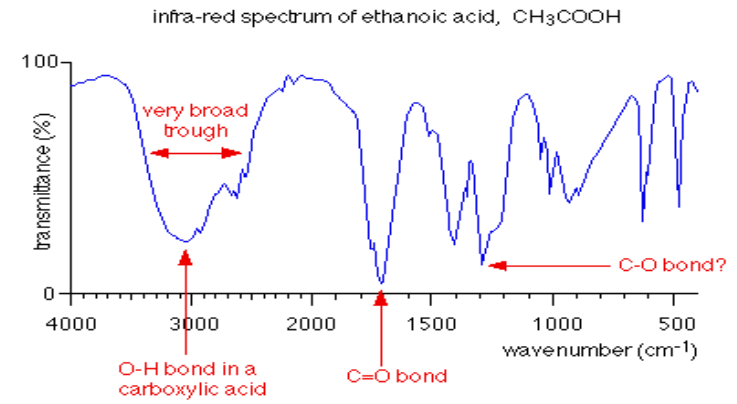
Interpreting an IR Spectrum



The broad peak [3000 – 3600 cm^{-1}] is an alkanol O–H .

The partially masked peak [2900 – 3000 cm^{-1}] is the C–H bond.

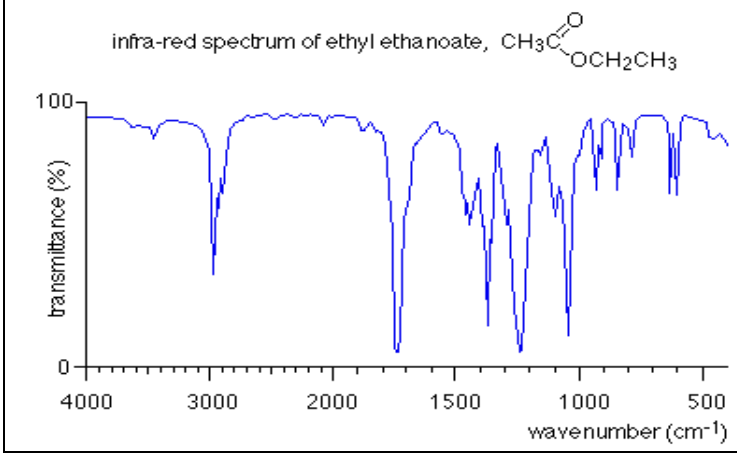
The twin peaks around 1050 cm^{-1} is the C–O bond.



The broad peak [2500 – 3300 cm^{-1}] is the O–H bond of a carboxylic acid.

The peak at about 1700 cm^{-1} is the C=O bond.

The peak at about 1300 cm^{-1} is probably the C–O bond.



The peak at 3000 cm^{-1} is not broad enough to be an O–H bond and is the C–H bond.

The peak at 1740 cm^{-1} is the C=O bond.

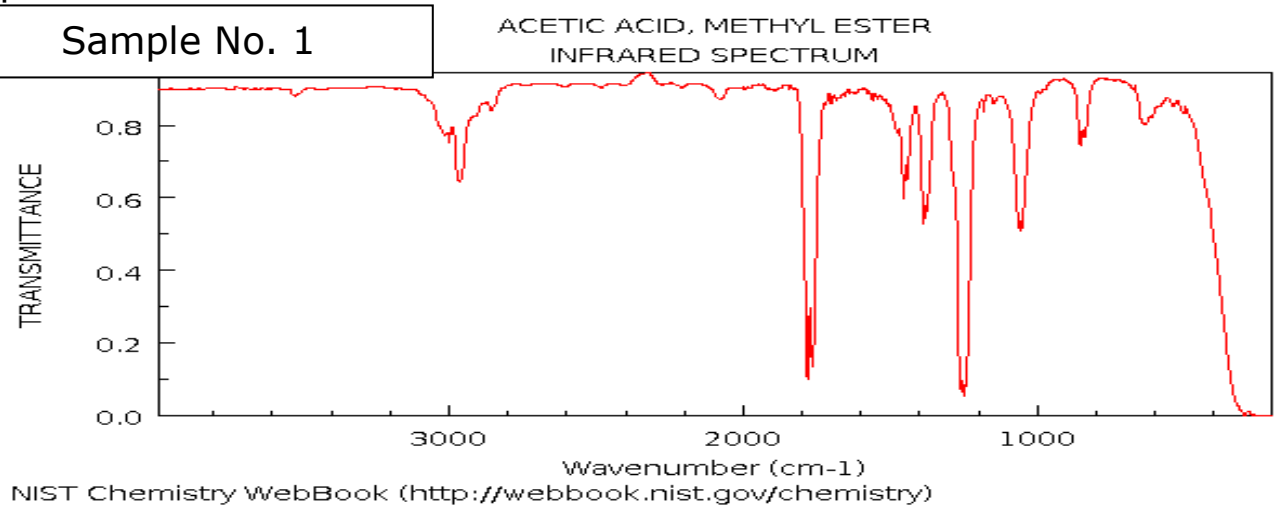
The peak at 1240 cm^{-1} is probably the C–O bond.

For the region to the right of the spectrum [500 – 1500 cm^{-1}], the complex collection of peaks makes identification of the functional groups difficult. However, this **fingerprint region** is unique to a compound and can be used for the positive identification of the compound utilizing a computerized library of IR spectra.

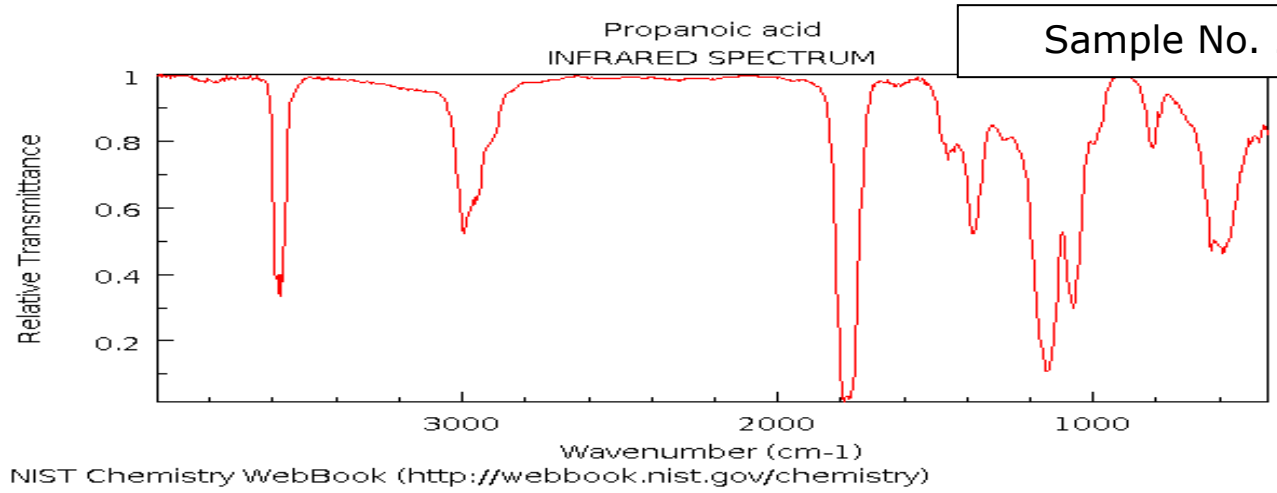
Example of Qualitative IR Spectroscopy

Propanoic acid [CH_3CH_2COOH] and methyl ethanoate [CH_3OCOCH_3] are structural isomers with the same molecular formula … $C_3H_6O_2$. A sample of each was analysed with an infrared spectrometer and the resulting IR spectra obtained.

Sample No. 1



Sample No. 2



The tabulated wavenumber data can be used to identify functional groups present in each sample and use this to identify them.

Sample	broad O–H peak ≈ 3000 cm^{-1}	C=O peak ≈ 1780 cm^{-1}
1	no	yes
2	yes	yes

Sample 2 has the broad O–H peak and must be propanoic acid, $CH_3CH_2CO\underline{OH}$. Sample 1, CH_3COOCH_3 has no hydroxyl –OH goup.