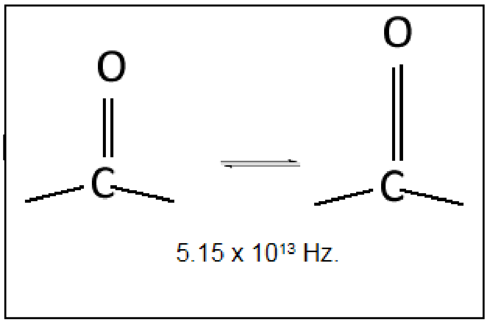
Lesson 1 IR spectroscopy

Click to revise IR

It is expected that students have revised IR by visiting the link above.

Molecules are not rigid, inflexible structures but can bend and stretch in many different ways, as the image of a water molecule shows on the link above. It is best to view the online IR section so that you can fully appreciate the movement of bonds which causes absorption of IR radiation. Covalent bonds in organic molecules are not rigid and behave more like springs. At room temperature, organic molecules are always changing shape ever so slightly, as their bonds undergo constant stretching, bending and twisting. These complex vibrations are not random and each one occurs at specific frequencies. This means that a molecule can only stretch and bend at certain 'allowed' frequencies. Take the carbonyl group from ketone, as shown on the right. It's stretching occurs at 5.15 X $10^{23}$ times every second at room temperature. If the molecule is exposed to electromagnetic radiation that matches the frequency of the carbonyl stretch, it will absorb this energy and increase the amount of stretch, but not the frequency of stretching. That is, each stretch will be longer while the rate remains at of 5.15 X $10^{23}$ per second. This takes the bond to a higher energy state. It turns out that the energy that bonds can absorb fall within the IR region of the electromagnetic spectrum.

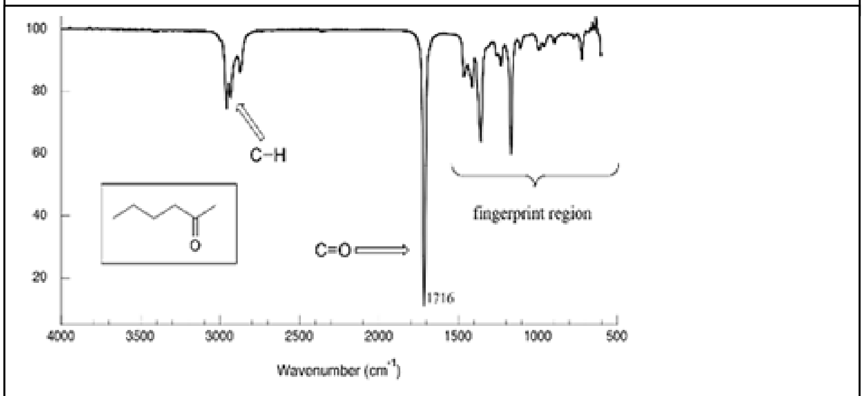



The frequency at which a particular bond type absorbs energy depends on the strength of the bond and the mass of each of the atoms on either side of the bond.

Molecules such as $Cl_2$ are IR inactive because they have no dipoles. Carbon dioxide, for example, although symmetrical, is IR active. When its bonds undergo an asymmetric stretch or bend the dipole moment of the molecule changes at a certain rate per second, known as its frequency measured in Hz. If this changing dipole frequency matches a frequency in the IR electromagnetic region then absorption of that particular IR frequency takes place. You will notice that IR absorption spectra graph absorbance or transmittance, on the Y-axis, against wavenumber, on the X-axis. Wavenumber is given as how many waves can fit into one centimetre hence its units are $cm^{-}$ . Frequency and wave number are related but the explanation is beyond the scope of this course.

An IR spectrum reveals the type of bond present and can also be used to identify a compound by its fingerprint region.

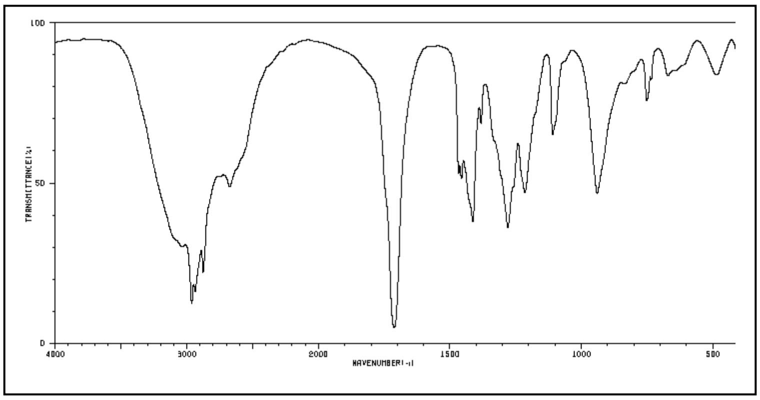
| Bond | Wave number ($cm^{-1}$) | Bond | Wave number ($cm^{-1}$) |
|---|---|---|---|
| C–Cl (chloroalkanes) | 600–800 | C=O (ketones) | 1680–1850 |
| C–O (alcohols, esters, ethers) | 1050–1410 | C=O (esters) | 1720–1840 |
| C=C (alkenes) | 1620–1680 | C–H (alkanes, alkenes, arenes) | 2850–3090 |
| C=O (amides) | 1630–1680 | O–H (acids) | 2500–3500 |
| C=O (aldehydes) | 1660–1745 | O–H (alcohols) | 3200–3600 |
| C=O (acids) | 1680–1740 | N–H (amines and amides) | 3300–3500 |



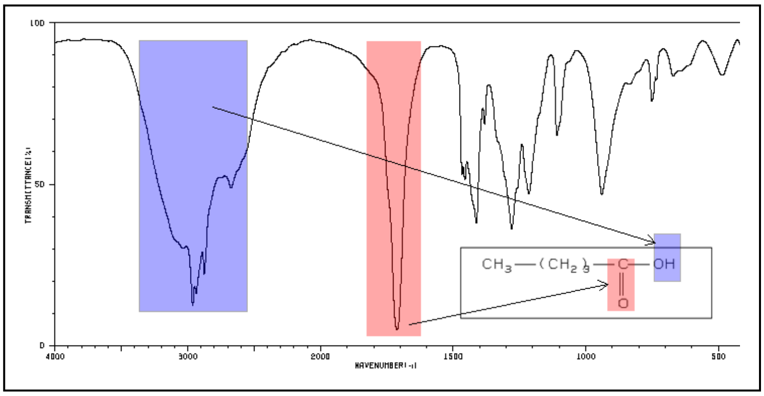
Example 1

Consider the IR spectrum on the right.

A researcher has two unlabelled bottles A and B that contain either pentanoic acid or pentanol.
Identify the compound in bottle A given its IR spectrum on the right.

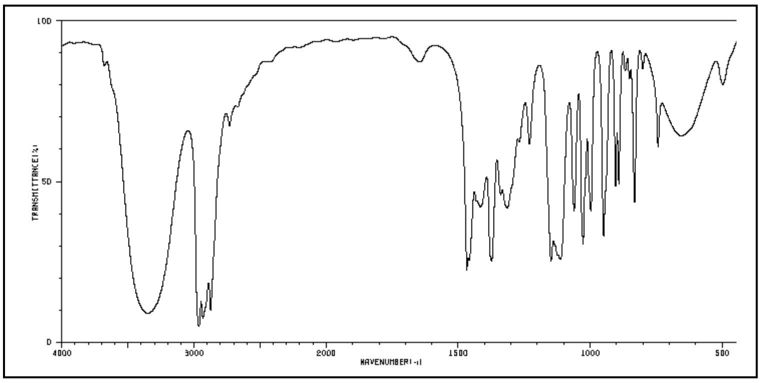



A strong absorption at 1700$cm^{-}$ indicates an acidic carbonyl group. The broad absorption band between 2500 – 3500 indicates an acidic OH.

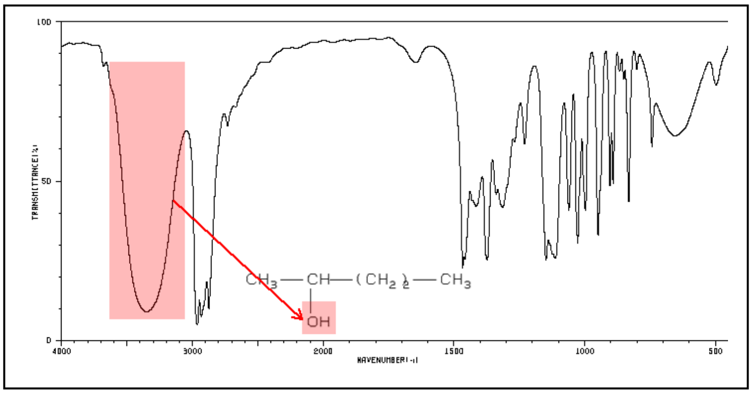



The substance in bottle B gives the IR spectrum shown on the right.

Identify the key feature that identifies the compound as the alcohol.

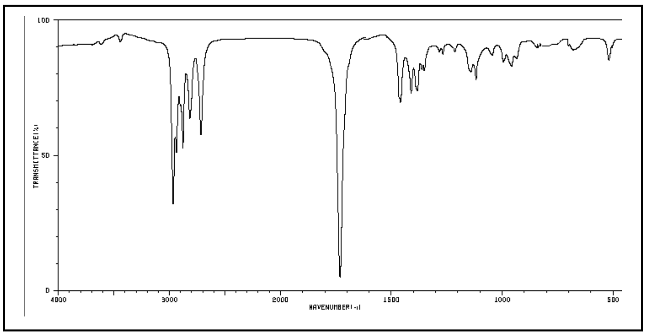



An absorption band between 3200 $cm^{-}$ and 3600 $cm^{-}$ is indicative of an alcohol OH group.



1) Which of the following molecules are IR active? Give a reason.
   $CO_2$ , $Cl_2$, $CH_4$.

2) A chemist wanted to identify the contents of a container. The IR spectrum of a pure sample taken from the bottle is shown on the right.
   Which of the two suspected compounds is present in the bottle.
   Butanol or butanal. Explain.



3) The frequency at which a particular bond absorbs IR radiation depends on what factors?

4) The IR spectrum of a compound with the molecular formula $C_4H_8O_2$ is shown on the right.
   Identify the molecule. Give reasons.