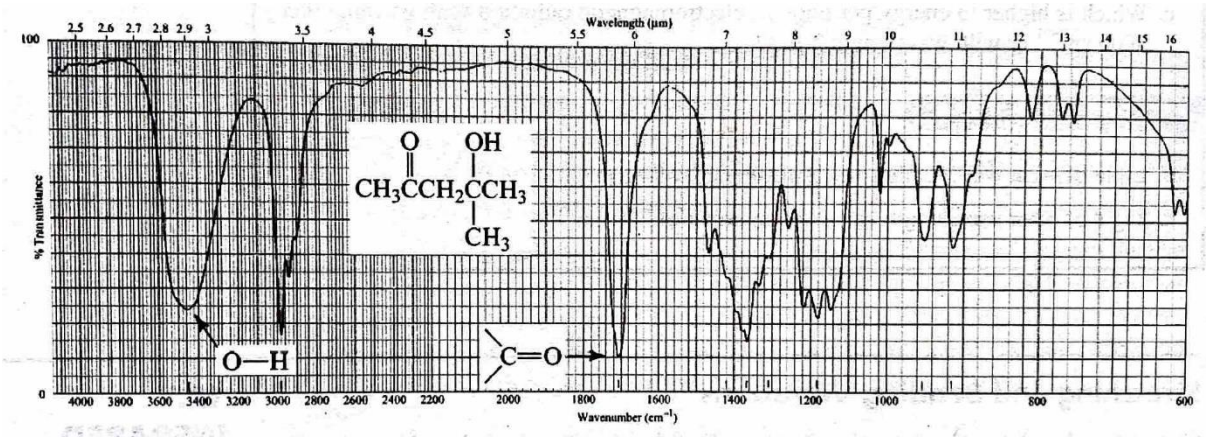
Infrared spectroscopy

Organic molecules are constantly vibrating. The bond vibrates with both stretching and bending motions .Electromagnetic radiation with wavenumbers from 4000 to 600 $cm^{-1}$ has just the right energy to correspond to stretching and bending vibrations in organic molecules.



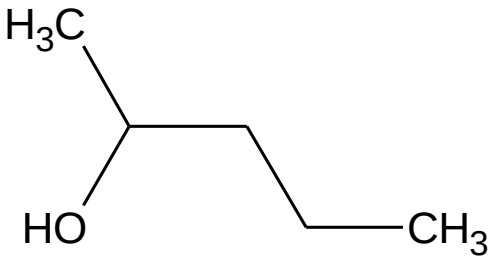

The Infrared spectrum of 4-hydroxy-4-methyl-2-pentanone

Functional group region

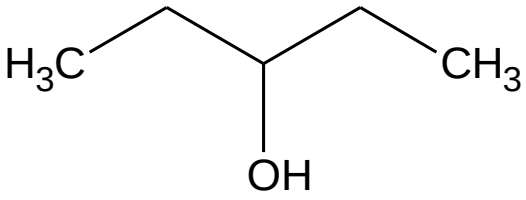
An IR spectrum can be divided into 2 areas. The left-hand two-thirds of an IR spectrum (4000-1400 $cm^{-1}$)is where most of the functional groups show absorption bands. This is called the functional group region.

Finger print region

The right- hand third (1400-600 $cm^{-1}$) is called the fingerprint region. The overall pattern in the fingerprint region is characteristic of the compound as a whole because each compound shows a unique pattern in this region.

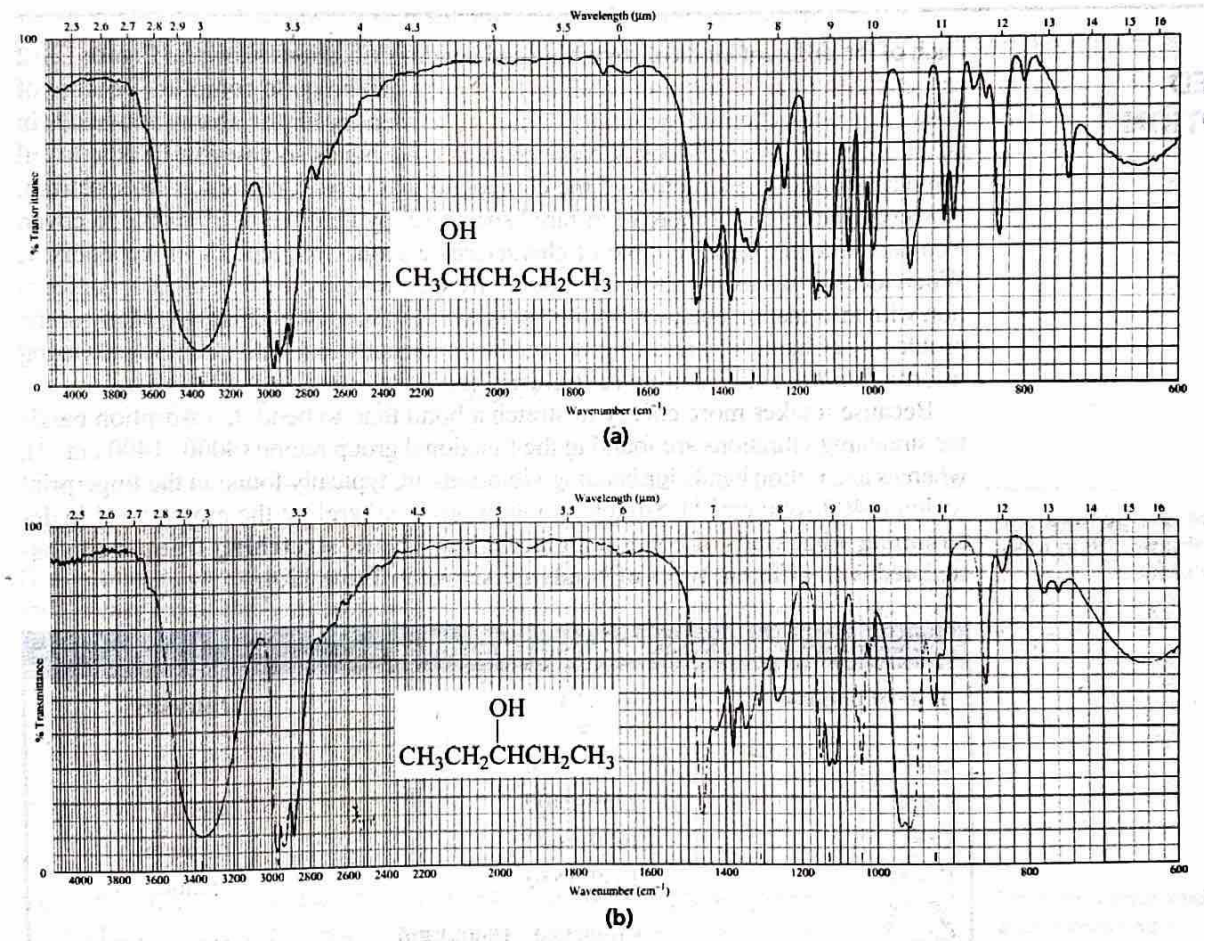



2-pentanol




3-pentanol

For example 2-pentanol and 3-pentanol have the same functional groups, so they show the same absorption bands in the functional group region. Their fingerprint regions are different, however because the compounds are different so a compound can be positively identified by comparing its fingerprint region with the fingerprint region of the actual spectrum of the compound.



From the above we can see the characteristic bands in the fingerprint region of these 2 compounds.

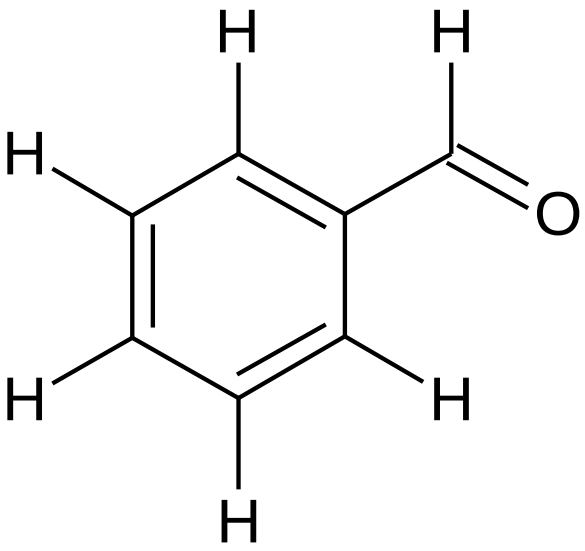
Characteristic IR absorption bands

| Bond | Compound type | Frequency range $cm^{-1}$ |
|---|---|---|
| C-H | alkanes | 2850-2960<br>1350-1470 |
| C-H | alkenes | 3020-3080(m)<br>675-1000 |
| C-H | Aromatic rings | 3000-3100(m)<br>675-870 |
| C-H | alkynes | 3300 |

| Bond | Compound type | Frequency range $cm^{-1}$ |
|---|---|---|
| C=C | alkenes | 1640-1680(v) |
| C=C | alkynes | 2200-2260(v) |
| C=C | Aromatic rings | 1500,1600(v) |

| Bond | Compound type | Frequency range $cm^{-1}$ |
|---|---|---|
| C-O | Alcohols, ethers, carboxylic acids ,esters | 1080-1300 |
| C=O | Aldehydes, ketones, carboxylic acids, esters | 1690-1760 |
| O-H | Monomeric alcohols, phenols<br>Hydrogen bonded alcohols, phenols<br>Carboxylic acids | 3610-3640(v)<br>3200-3600(broad)<br>2500-3000(broad) |
| N-H | Amines | 3300-3500(m) |
| C-N | Amines | 1180-1360 |
| C=N | Nitriles | 2210-2260(v) |
| $-NO_2$ | Nitro compounds | 1515-1560<br>1345-1385 |

Characteristic IR absorption bands for Benzaldehyde




C=O: 1690-1760 $cm^{-1}$

C=C aromatic:1500,1600 $cm^{-1}$

C-H aromatic:3000-3100 $cm^{-1}$

# Applications of Infrared spectroscopy

## 1.Functional group analysis

The presence or absence of absorption bands help in predicting the presence of certain functional groups in the compound. The presence of oxygen reveals that the group present may be –OH, C=O, COOR, -COOH but an absorption band between 3600-3200 $cm^{-1}$ limits the possibilities. The band in this region may be due to O-H str.

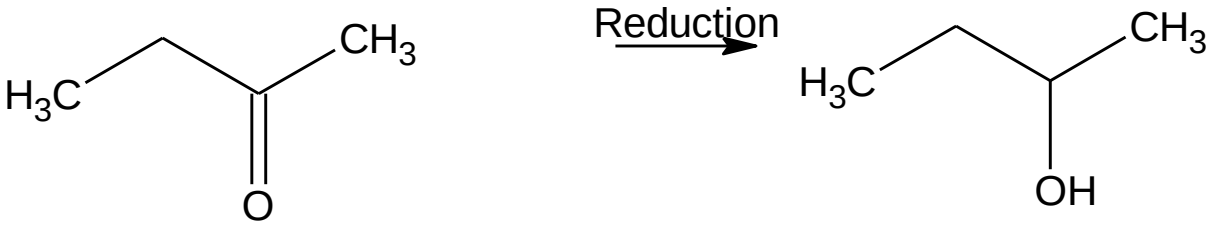
## 2.Detection of purity of a sample

Infra-red spectroscopy is also useful in the detection of impurity in a compound by comparing its spectrum with the spectrum of the authentic sample of the compound. Moreover a pure sample always consists of sharp peaks and bands while impure sample will consist of poor bands and also some additional bands.

## 3.Establishing the identity of an unknown compound

This technique helps to establish the structure of an unknown compound. All major functional groups absorb at their characteristic wavenumbers, from the data available due to absorption frequencies, the probable structure can be predicted. If some chemical data is available it can lead to the confirmation of the structure.

## 4.Studying the progress of a chemical reaction




Butan-2-one

1710 $cm^{-1}$

Butan-2-ol

3300$cm^{-1}$

The technique is quite useful to studying chemical reactions. Consider the reduction of a saturated aliphatic ketone to form secondary alcohol. Ketone forms a strong band at about 1710 $cm^{-1}$.When it is subjected to reduction, it forms Butan-2-ol which absorbs at 3300$cm^{-1}$ due to O-H stretching. The progress of the reaction can be studied from time to time and the reduction will be complete when a strong band due to C=O str will be missing and only a band due to O-H str is present.