# Infrared (I.R.)Spectroscopy

Infra-red spectrum provides information about functional groups present in the molecule

I.R. spectrum is obtained by exposing molecules to electromagnetic radiation of I.R. region.

When molecule is placed in magnetic field. Vibration of molecule take place. When these vibrations causes change in dipole moment, then that molecule become IR active

In past micron and micrometers are used as the units but nowadays wave number ($cm^{-1}$) is used.

A simple reciprocal relation is exist in wave number and wavelength

# Infrared (I.R.)Spectroscopy

## Principle of IR Spectroscopy

Molecule and atoms in molecule are continuously rotating , vibrating and moving from one point to another point. This require definite amount of energy.

When molecule exposed to IR radiations, molecule absorb IR radiation and get excited to higher vibrational energy level.

The type of IR wavelength absorbed by molecule depends on the type of the atoms and the chemical bonds present in the molecule. When these absorption are recorded, we get IR spectra.

# Infrared (I.R.)Spectroscopy

**Divisions of IR**

1) Near IR 12500-4000 $cm^{-1}$

2) IR 4000- 625 $cm^{-1}$

a) Functional group 4000-1300 $cm^{-1}$

b) Finger print 1300-909 $cm^{-1}$

c) Aromatic region 909-625 $cm^{-1}$

3) Far IR 625-50 cm-1

# Infrared (I.R.)Spectroscopy

## Subdivisions of Infrared Spectra

### 1) Functional group region (4000-1300 cm-1)

This part of spectrum contain absorption band due to stretching vibrations of functional groups such as –OH, -NH, -CH etc. Functional groups can be identified by this region

### 2) Finger print region (1430-910 cm-1)

This is the most complex part of I.R. spectra These absorption band due to stretching and bending vibrations. Each compounds have different spectra in finger print region.

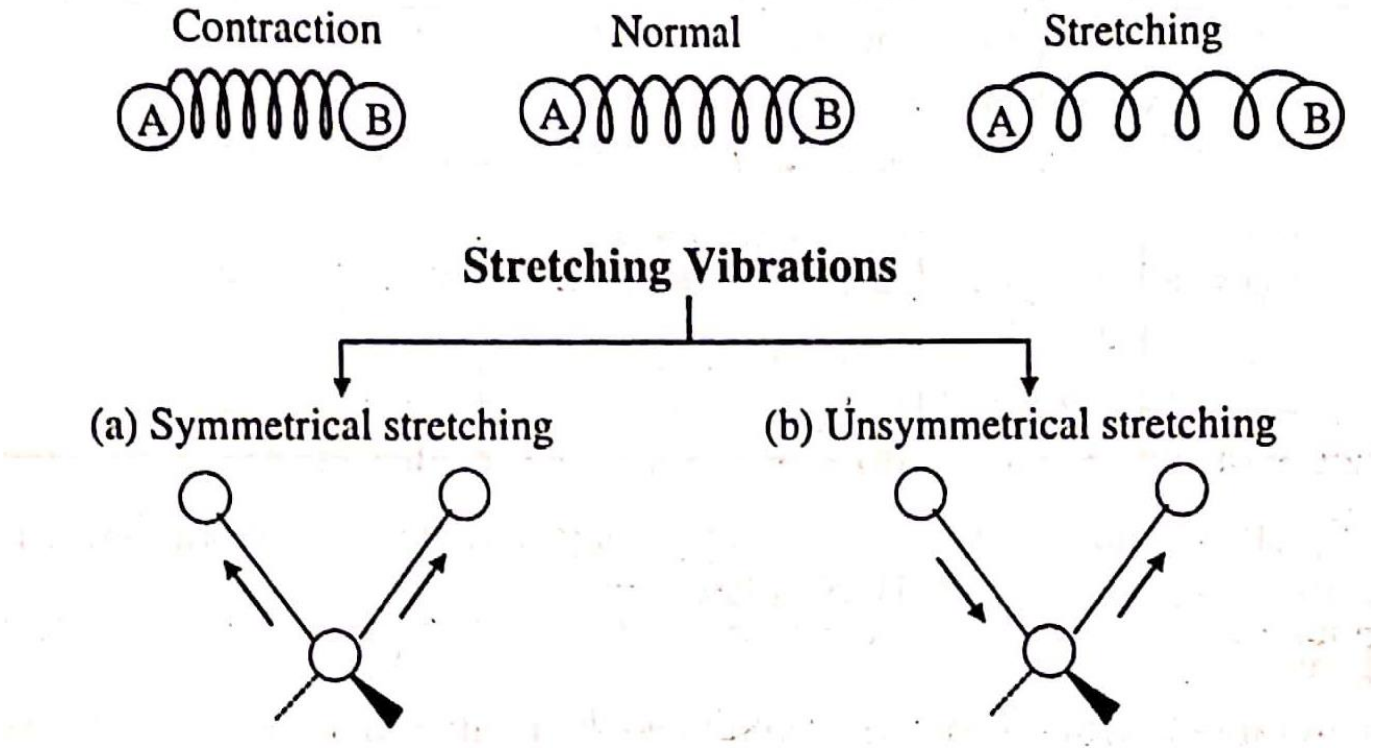
### 3) Aromatic region (910-650 cm-1)

Strong absorption in this region shows presence of aromatic character of compound

# Infrared (I.R.)Spectroscopy

## Modes of Vibration

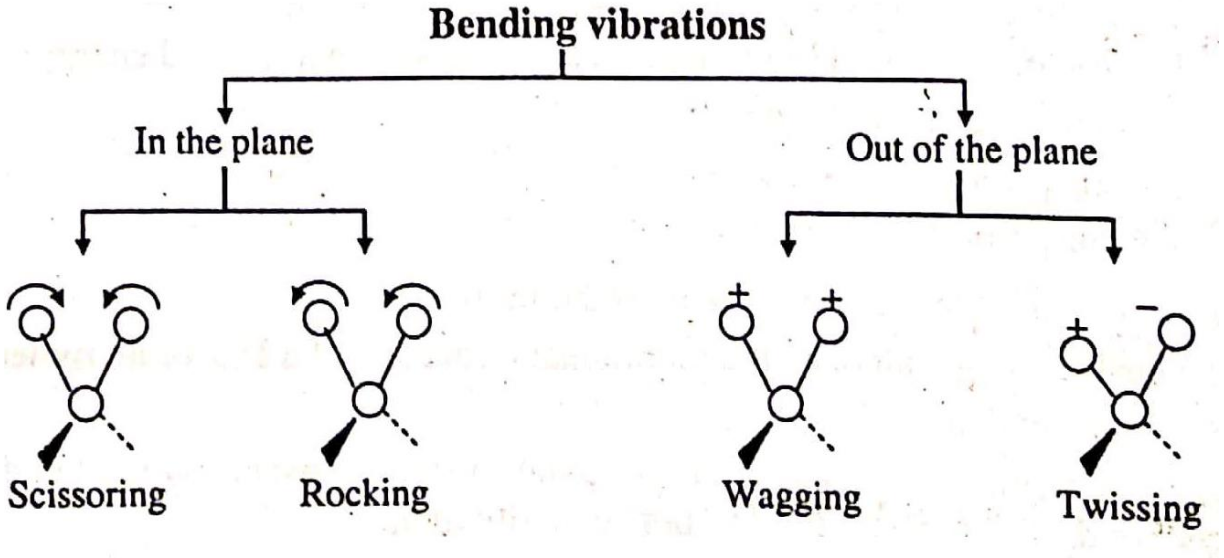
Stretching vibrations: These are characterized by change in inter nuclear distance.



# Infrared (I.R.)Spectroscopy

## Modes of Vibration

Bending vibrations: These are characterized by change in angle between covalent bonds.




**Bending vibrations**

Scissoring :

Both atoms move in opposite direction

Rocking :

Both atoms move in same direction

Wagging :

Both atoms move together either above or below the plane

Twisting :

One atom move above the plane while other atom move below the plane

# Infrared (I.R.)Spectroscopy

## Fundamental modes of vibrations

### For linear molecule:

( 3N-5 ) fundamental modes of vibrations

Example Carbon monoxide,

### For non linear molecule:

( 3N-6 ) fundamental modes of vibrations

Example water

( Where N is no. of atoms in molecule )

# Infrared (I.R.)Spectroscopy

| Sr. no. | Molecule | Linear /Non linear | Fundamental modes of vibrations |
|---|---|---|---|
| 1. | Benzene | Non linear | 30 |
| 2. | Water | Non linear | 03 |
| 3. | Methane | Non linear | 09 |
| 4. | Ammonia | Non linear | 06 |
| 5. | Nitrogen oxide | Linear | 01 |
| 6. | Carbon monoxide | Linear | 01 |
| 7. | Carbon dioxide | Linear | 04 |

# Infrared (I.R.)Spectroscopy

## Hooke's Law

Vibrational frequency of a bond is related to the masses of vibrating atoms and the force constant (f) of the vibrating bond.

$$\text{Vibrational frequency } \nu = \frac{1}{2\pi C}\sqrt{\frac{f}{\mu}} \qquad \text{.... (i)}$$

Where, $\nu$ = vibrational frequency in terms of $cm^{-1}$

$C$ = velocity of light $3 \times 10^{10}$ cm/sec.

$f$ = force constant of bond (dynes $cm^{-1}$) proportional to bond energy.

$\mu$ = reduced mass of atoms.

$$\text{i.e. } \mu = \frac{m_a \times m_b}{m_a + m_b} \qquad \text{.... (ii)}$$

where $m_a$ = mass of atom 'a' $m_b$ = mass of atom 'b'

# Infrared (I.R.)Spectroscopy

## Hooke's Law

1) Vibrational frequency is directly proportional to the force constant.(Stogner the bons, higher is the frequency)

2) Frequency is inversely proportional to reduced mass (u) (when reduced mass is small, frequency is more)

# Infrared (I.R.)Spectroscopy

**Example :** O–H $\mu = \frac{m_a \times m_b}{m_a + m_b} = \frac{16 \times 1}{16+1} = \frac{16}{17} = 0.94$

N–H $\mu = \frac{m_a \times m_b}{m_a + m_b} = \frac{14 \times 1}{14+1} = \frac{14}{15} = 0.93$

C–H $\mu = \frac{m_a \times m_b}{m_a + m_b} = \frac{12 \times 1}{12+1} = \frac{12}{13} = 0.92$

where as, C–C $\mu = \frac{m_a \times m_a}{m_a + m_a} = \frac{12 \times 12}{12+12} = \frac{144}{24} = 6.0$

Frequency

-OH, -NH, - CH from 3000-3600 $cm^{-1}$

C-C around 1100 $cm^{-1}$

**Relation between force constant, frequency and bond length :**

| Bond | Bond length | Force constant | Frequency |
|---|---|---|---|
| C–C | 1.54 A° | $5 \times 10^5$ dynes $cm^{-1}$ | ~ 1100 $cm^{-1}$ |
| C=C | 1.34 A° | $10 \times 10^5$ dynes $cm^{-1}$ | ~ 1650 $cm^{-1}$ |
| C≡C | 1.20 A° | $15 \times 10^5$ dynes $cm^{-1}$ | ~ 2200 $cm^{-1}$ |

# Infrared (IR)Absorption of some functional groups

| Functional group | Molecular motion | Wave number cm-1 |
|---|---|---|
| Alkanes | -C-H stretch | 2850-2950 |
| | -C-C- | 1100-1120 |
| Alkenes - | =C-H stretch | 3000-3100 |
| | -C=C stretch isolated | 1630-1699 |
| | -C=C stretch conjugated | 1610-1640 |
| | -C-H bend (monosubstituted) | 990 & 910 |
| | -C-H bend (disubstituted 1,1) | 890 |
| | -C-H bend (disubstituted E) | 960-980 |
| | -C-H bend (disubstituted Z) | 675-730 |
| | -C-H bend (Trisubstituted) | 800-840 |
| Alkynes | -C-H stretch | 3200-3310 |
| | C≡ C-H stretch | 2100-2140 |
| | C≡ C-C stretch | 2200-2260 |

# Infrared (IR)Absorption of some functional groups

| Functional group | Molecular motion | Wave number cm-1 |
|---|---|---|
| Aromatics | -C-H stretch | 3000-3020 |
| | -C=C Stretch | 1500-1600 |
| | -C-H bend (monosubstituted) | 690-710 &730-770 |
| | -C-H bend (ortho) | 735-770 |
| | -C-H bend (meta) | 750-810 |
| | -C-H bend (para) | 790-850 |
| Alcohols | -O-H stretch (free) | 3600-3650 |
| | -O-H stretch (bonded) | 3200-3500 |
| | -C-O stretch | 1260-1000 |
| Ethers | -C-O-C stretch | 1300-1000 |
| Aldehyde | -C-H stretch | 2700-2900 |
| | -C=O stretch | 1730-1740 |
| Ketone | -C=O stretch | 1705-1720 |

# Infrared (IR)Absorption of some functional groups

| Functional group | Molecular motion | Wave number cm-1 |
|---|---|---|
| Esters | -C=O stretch | 1730-1750 |
| Acid chloride | -C=O stretch | 1770-1815 |
| Halo Alkane | -C-X stretch | 500-750 |
| Anhydride | -C=O stretch | 1740-1850 |
| | -C-O stretch | 1000-1300 |
| Amines | -N-H stretch | 3300-3350 |
| Amides | -N-H stretch | 3300-3350 |
| | -C=O stretch | 1680-1700 |
| Nitriles | C=N stretch non conjugated | 2240-2260 |
| | C=N stretch conjugated | 2215-2240 |
| | -C=N- | 1590-1690 |
| Isocyanate | -N=C=O stretch | ~2270 |
| Isothiocyanate | -N=C=O stretch | ~2125 |
| Nitro group | -NO2 | 1370-1540 |

# Infrared (IR)Absorption of some functional groups

**Site of unsaturation**

*A) Compound containing CHO elements*

$$\text{Site of unsaturation} = \frac{(2 \times \text{no. of Carbon atoms} + 2) - (\text{no. of Hydrogen atoms})}{2}$$

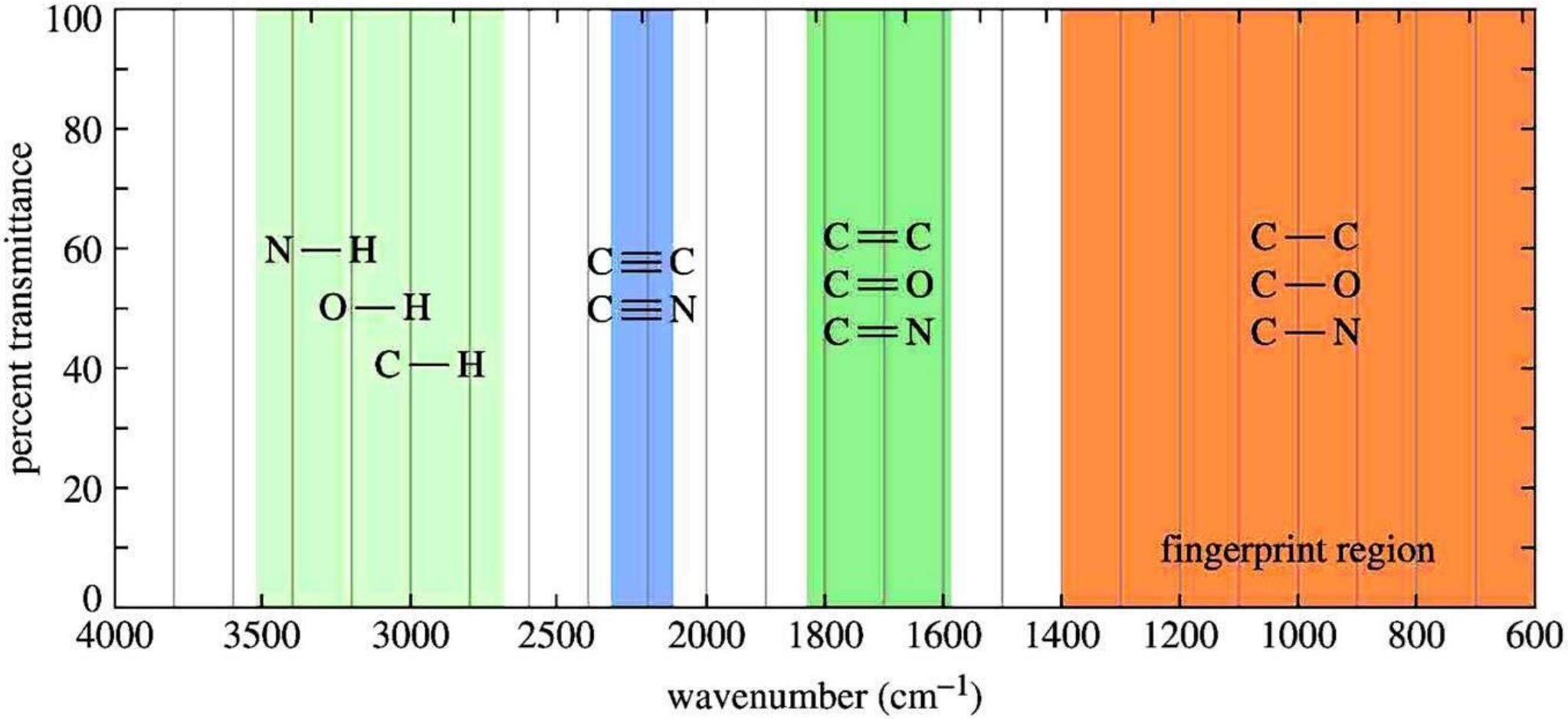
*B) Compound containing CHN elements*

$$\text{Site of unsaturation} = \frac{(2 \times \text{no. of Carbon atoms} + 2) - (\text{no. of Hydrogen atoms} - 1)}{2}$$

*C) Compound containing CHX elements*

$$\text{Site of unsaturation} = \frac{(2 \times \text{no. of Carbon atoms} + 2) - (\text{no. of Hydrogen atoms} + 1)}{2}$$

# Infrared (IR)Absorption of some functional groups




Graphics source: Wade, Jr., L.G. *Organic Chemistry*, 6th ed. Pearson Prentice Hall Inc., 2006

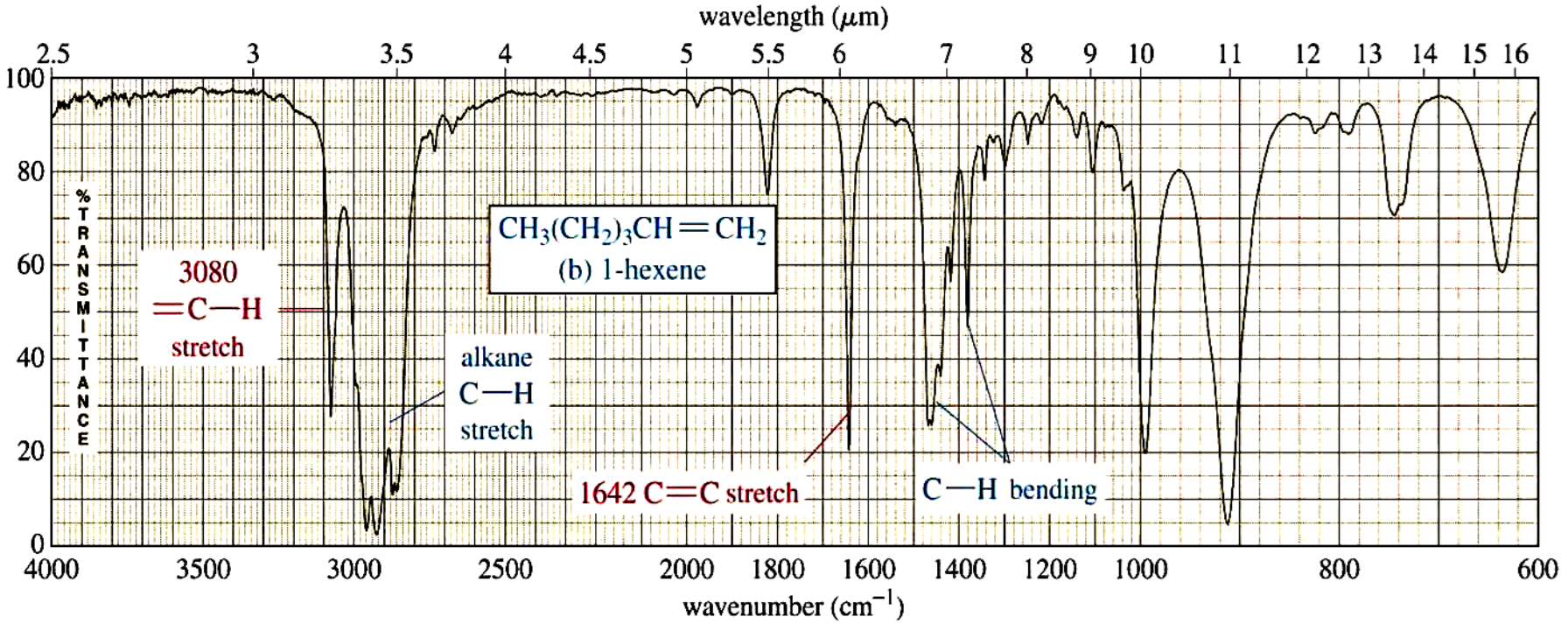
# Characteristics of IR Absorption of some functional groups

Alkanes

have no functional groups. Their IR spectrum displays only C-C ( 800-1200 $cm^{-1}$) and C-H ( 2850-3000 $cm^{-1}$) bond vibrations. Since most organic molecules have such bonds, hence less useful for structure determination.

Graphics source: Wade, Jr., L.G. *Organic Chemistry*, 6th ed. Pearson Prentice Hall Inc., 2006

# Characteristics of IR Absorption of some functional groups

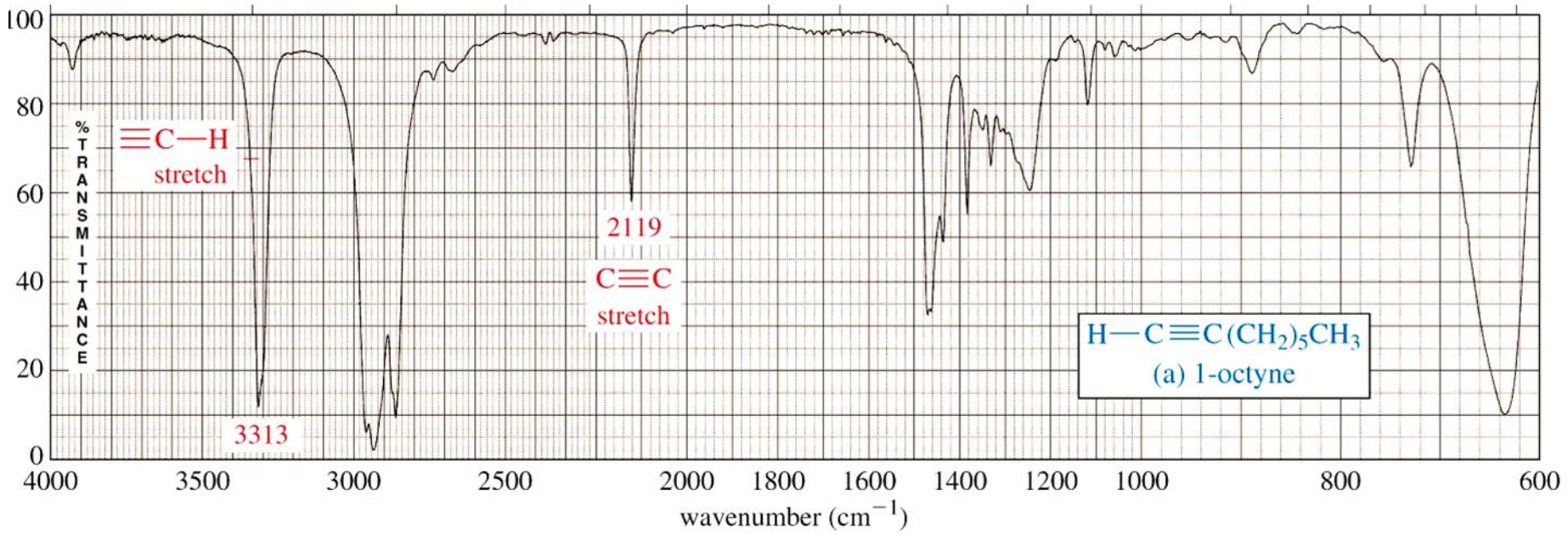



**Alkenes**

Alkenes show sharp, medium bands corresponding to the **C=C bond stretching vibration** at about **1600-1700 cm$^{-1}$** and also show a band for the =C-H bond stretch, appearing around **3000-3100 cm$^{-1}$** as shown below.

Graphics source: Wade, Jr., L.G. *Organic Chemistry*, 6th ed. Pearson Prentice Hall Inc., 2006

# Characteristics of IR Absorption of some functional groups




**Alkynes**

The most prominent band in alkynes corresponds to the **carbon-carbon triple bond**. It shows as a sharp, weak band at about **2100 -2260 cm$^{-1}$**. Terminal alkynes, have C-H bonds that weak band at about **3300 cm$^{-1}$** corresponding to the C-H stretch.

Graphics source: Wade, Jr., L.G. *Organic Chemistry*, 6th ed. Pearson Prentice Hall Inc., 2006

# Characteristics of IR Absorption of some functional groups

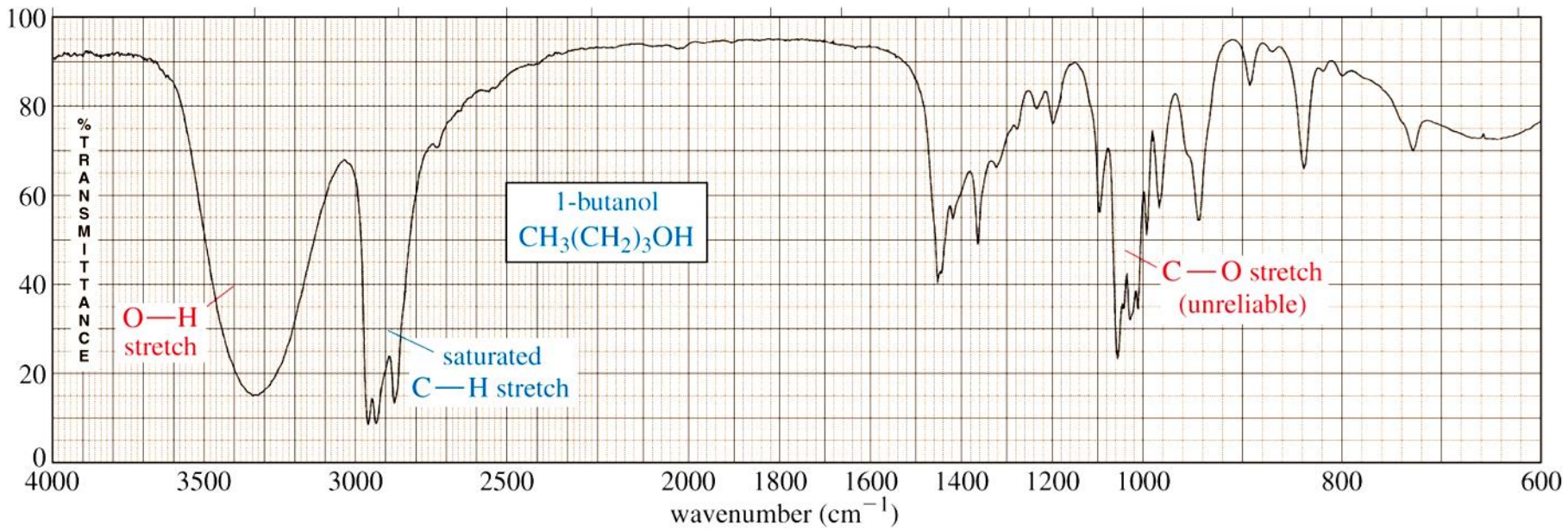
**Aromatic Hydrocarbon**

Aromatic hydrocarbons shows **carbon-carbon double bond** stretching frequency around **1500-1600 $cm^{-1}$**.

It shows =C-H bond stretching around **3000-3100 $cm^{-1}$**.

In these compound =C-H bond bending is observed around **675-710 $cm^{-1}$**.

# Characteristics of IR Absorption of some functional groups

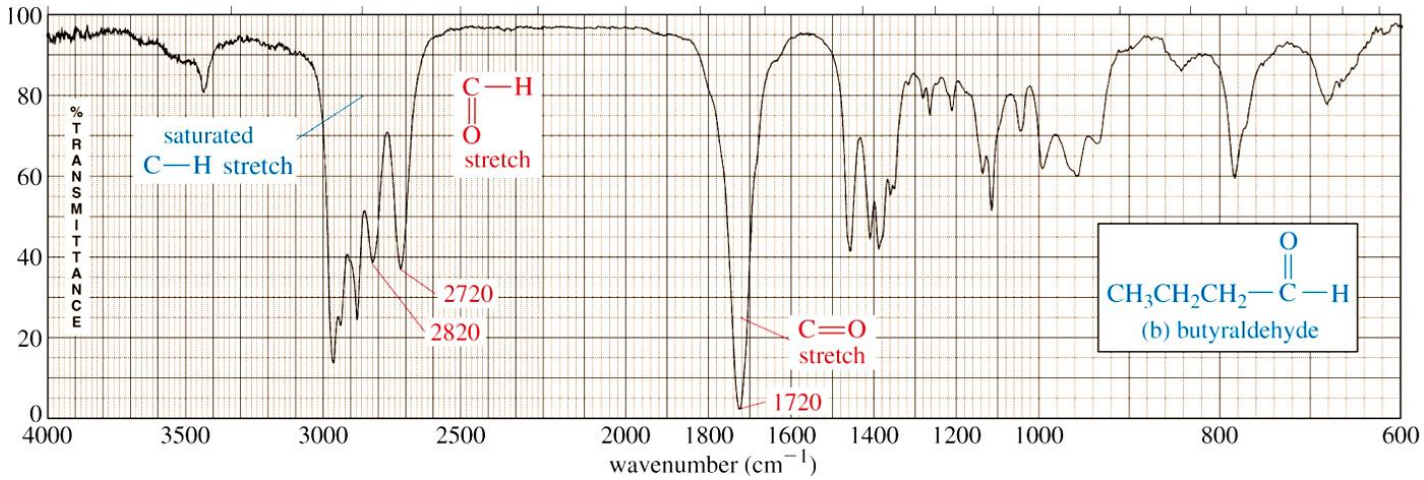


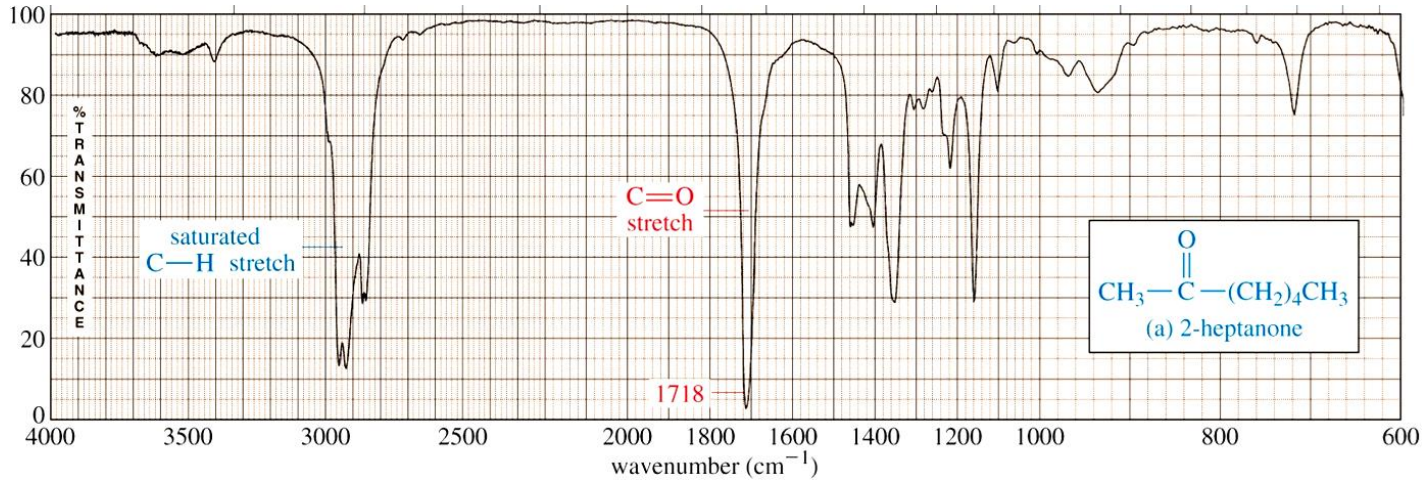

**Alcohols and Ethers** The most prominent band in alcohols is due to the **O-H bond**, and it appears as a strong, broad band around **3200 - 3600 $cm^{-1}$**. Another band for **C-O stretching** is observed around **1000 - 1200 $cm^{-1}$**.

Ethers They sow **C-O stretching** around **1000 - 1300 $cm^{-1}$**.

Graphics source: Wade, Jr., L.G. *Organic Chemistry*, 6th ed. Pearson Prentice Hall Inc., 2006

# Characteristics of IR Absorption of some functional groups



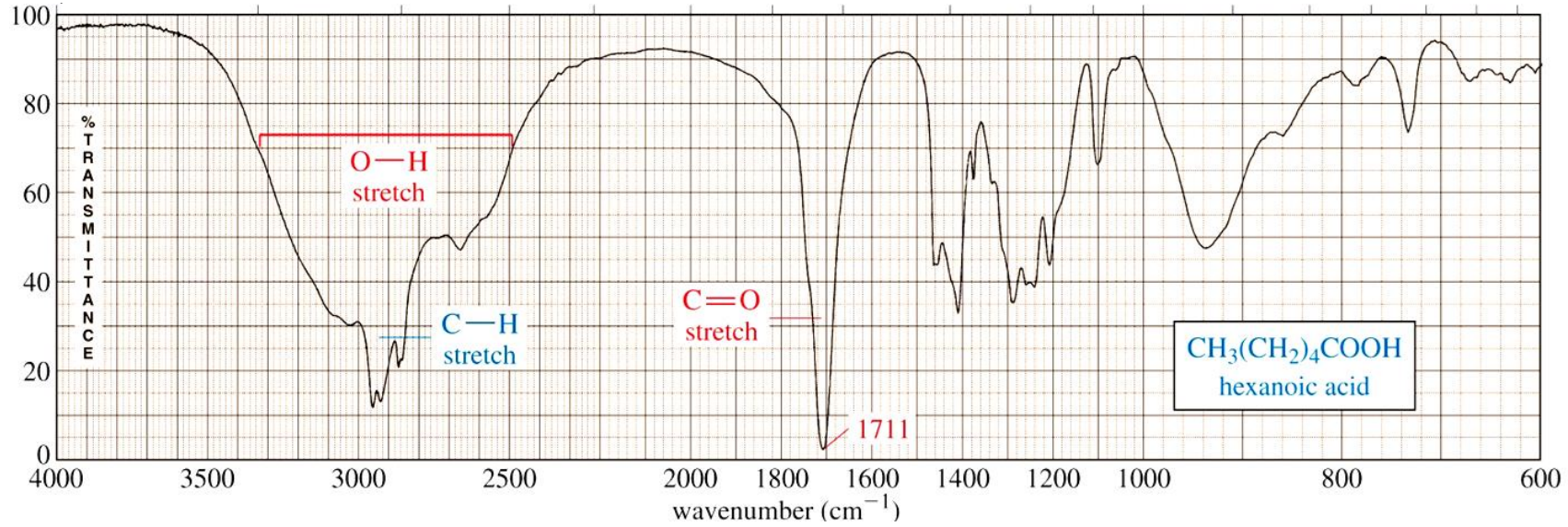




**Aldehydes** show a strong, prominent band around **1720 - 1740 cm$^{-1}$** for C=O stretching.
aldehydes also contain a C-H bond which show bands around **2700 - 2800 cm$^{-1}$**.

**Ketone** show a strong, prominent band around **1710 - 1715 cm$^{-1}$** for C=O stretching.

Graphics source: Wade, Jr., L.G. *Organic Chemistry*, 6th ed. Pearson Prentice Hall Inc., 2006

# Characteristics of IR Absorption of some functional groups

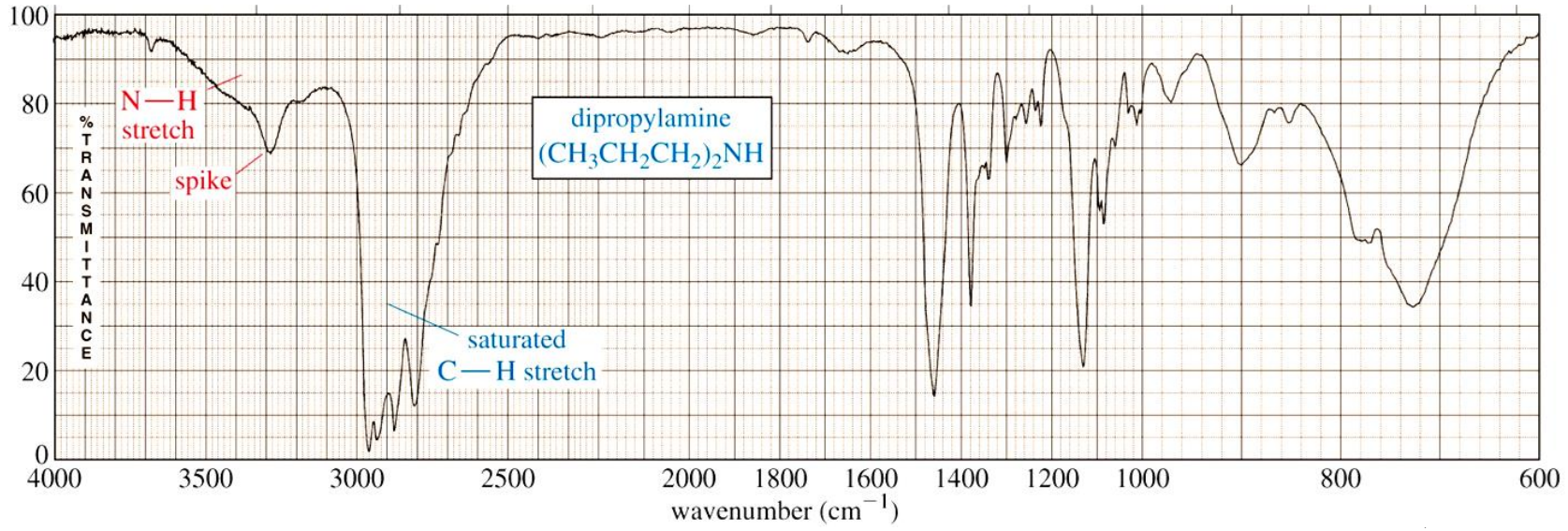



**A carboxylic acid** has both the **O-H bond** and the **C=O bond**. Therefore carboxylic acids show a very strong and broad band around **2400 - 3500 $cm^{-1}$** for the O-H stretch. Another band around **1710 $cm^{-1}$** is observed for the C=O stretch.

Ether shows **C=O stretching** band around **1730-1750 $cm^{-1}$ and –C-O stretching around 1000-1300 $cm^{-1}$ )**

Graphics source: Wade, Jr., L.G. *Organic Chemistry*, 6th ed. Pearson Prentice Hall Inc., 2006

# Characteristics of IR Absorption of some functional groups




**Amines**

The most characteristic band in amines is due to the **N-H bond stretch**, and it appears as a weak to medium. This band is observed in the range of about **3200 - 3600 $cm^{-1}$**.

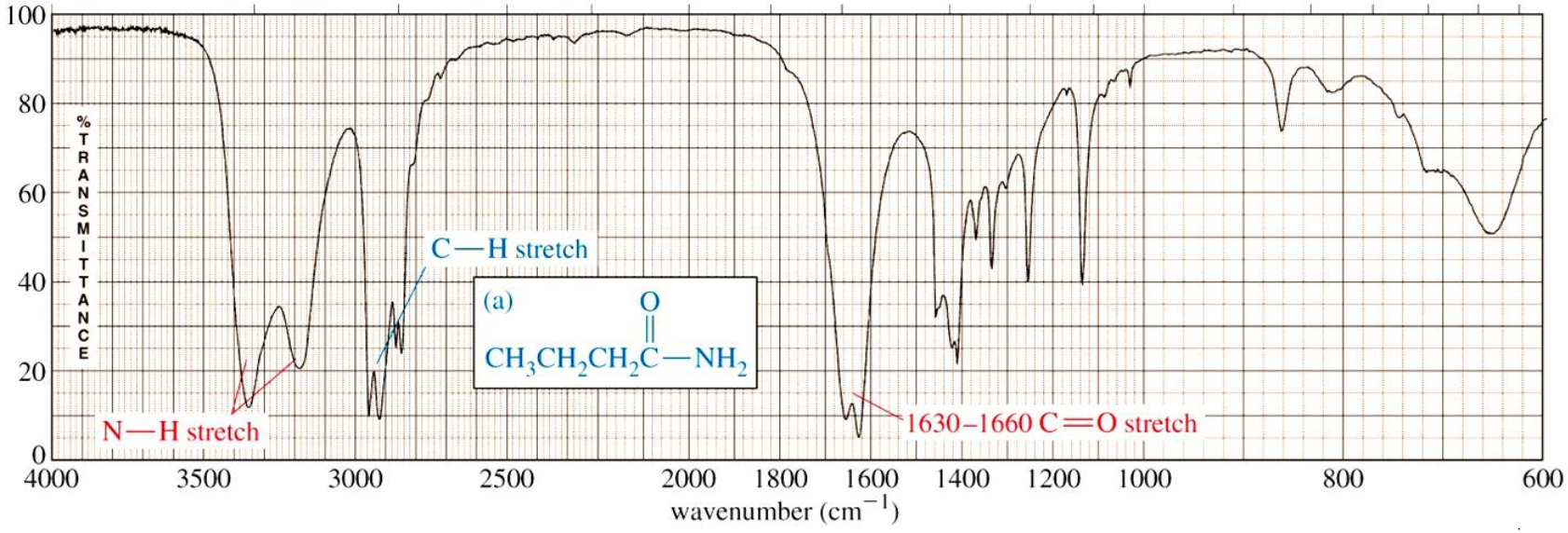
**Primary amines** have two N-H bonds, therefore they typically show two spikes.

**Secondary amines** have only one N-H bond, and show only one spike.

**Tertiary amines** have no N-H bonds, and therefore this band is absent.

Graphics source: Wade, Jr., L.G. *Organic Chemistry*, 6th ed. Pearson Prentice Hall Inc., 2006

# Characteristics of IR Absorption of some functional groups




Amide

functional group combines the features of amines and ketones because it has It shows both the **N-H bond** and the **C=O bond** stretching bands. The N-H stretch is observed in the range between **3100** and **3500 $cm^{-1}$** while C=O stretch is seen around **1710 $cm^{-1}$**

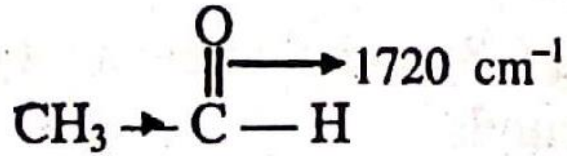
As with amines, primary amides show two spikes, whereas secondary amides show only one spike.

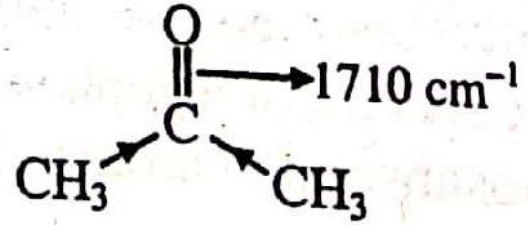
Graphics source: Wade, Jr., L.G. *Organic Chemistry*, 6th ed. Pearson Prentice Hall Inc., 2006

# Factors affecting IR frequencies

## (A) Inductive effects

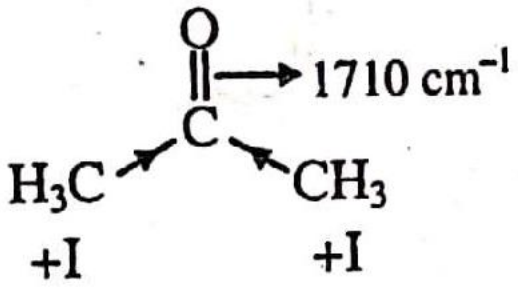
Groups which have electron donating inductive effects (+I), when attached to functional groups decrease the stretching frequency.

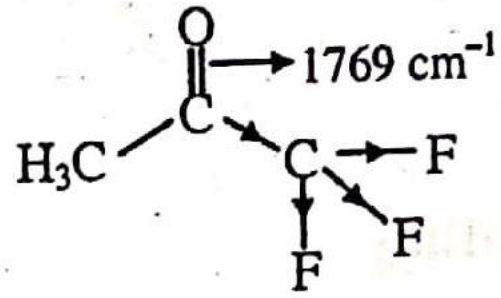


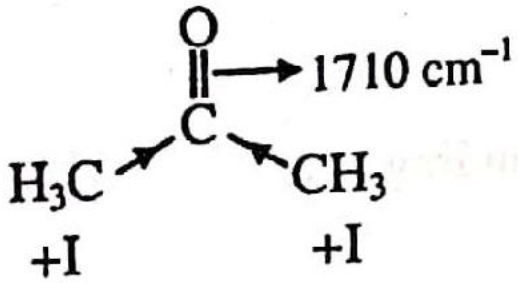

The additional +I effect in acetone decrease the carbonyl stretching frequency. The +I effect actually decrease the double bond character of the >C=O (or increase the single bond character of the carbon-oxygen bond)

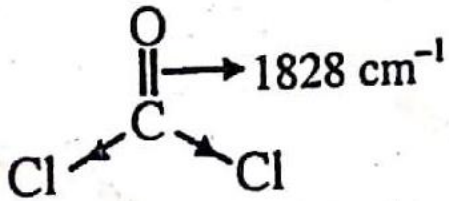
# Factors affecting IR frequencies

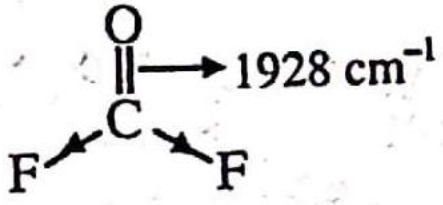



Strong –I effect




Strong –I effect

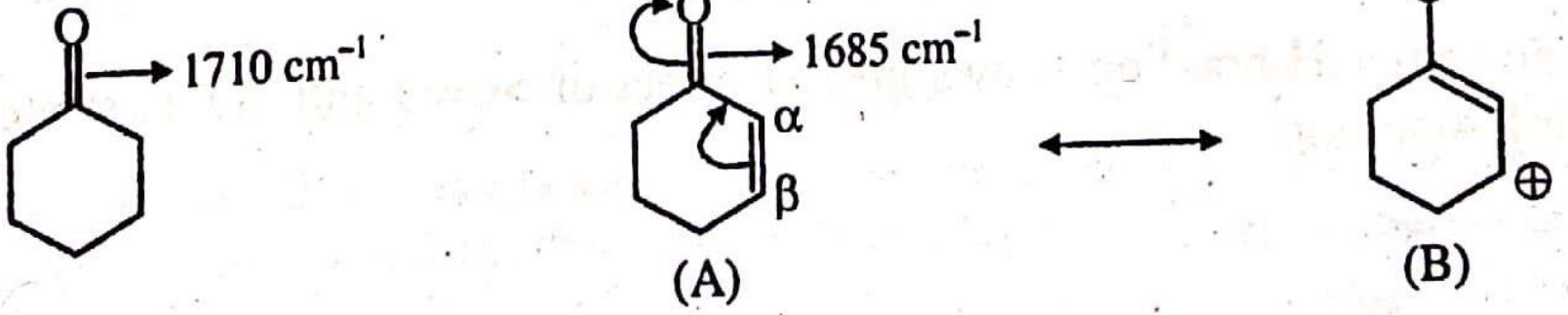
# Factors affecting IR frequencies

## (B) Resonance effects

### (i) Conjugated aldehydes and ketones

The groups which have electron donating resonance effects, (+R) when attached to functional groups, should decrease the stretching frequency and groups which have electron withdrawing resonance effects (–R) should increase the stretching frequency.

Consider the following molecules




(A) (B)

α : β unsaturated ketone

# Factors affecting IR frequencies

## (B) Resonance effects

### (i) Conjugated aldehydes and ketones

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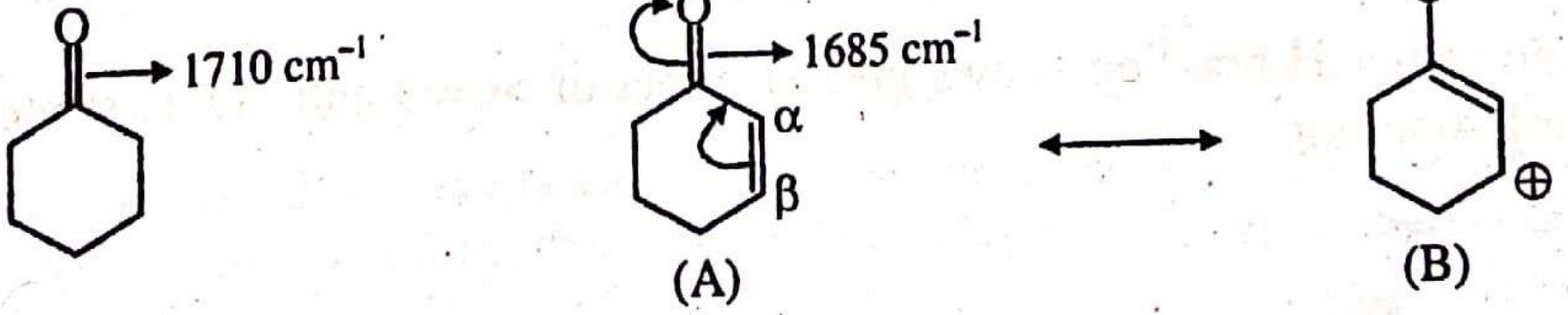
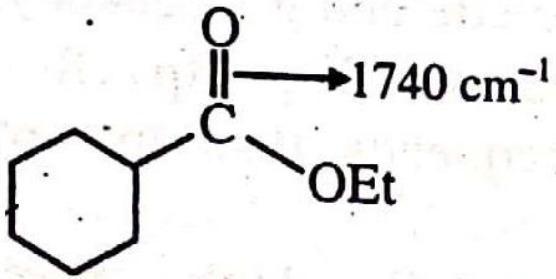
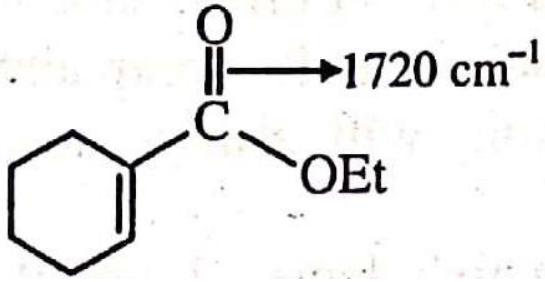


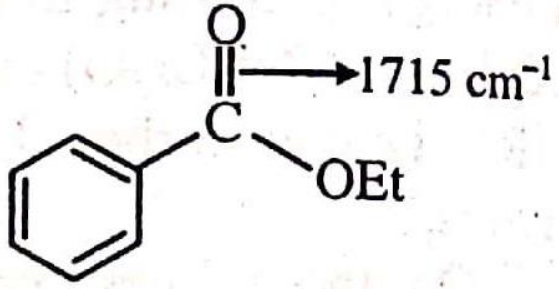

(A) (B)

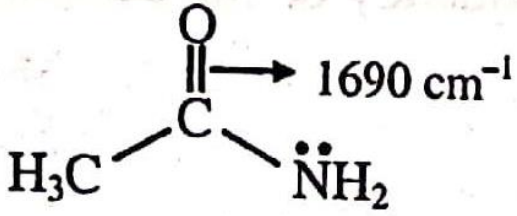
α : β unsaturated ketone

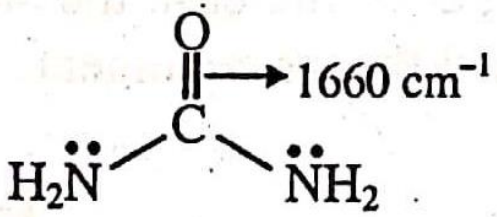
# Factors affecting IR frequencies

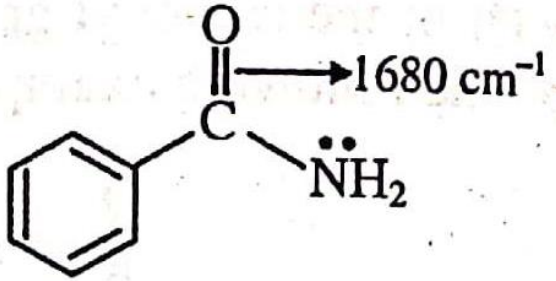


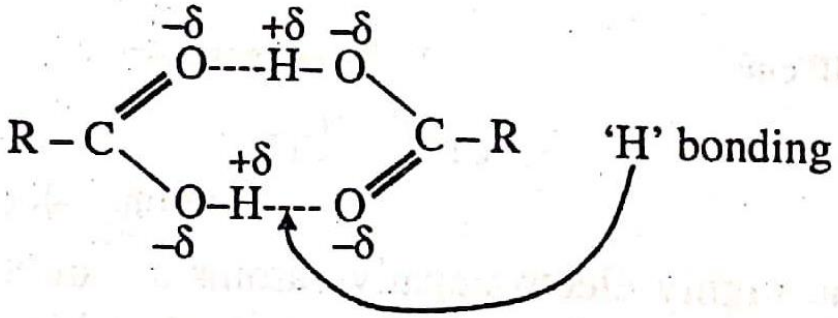



# Factors affecting IR frequencies

## (c) Hydrogen bonding

### (1) Carboxylic acids

Carboxylic acids in solid or pure liquid form usually exists in the dimeric form due to strong hydrogen bonding.




**Dimer of carboxylic acid**

The strong hydrogen bonding weakens the >C=O bond, thus lowering the >C=O absorption frequency. The appearance of the carbonyl stretching peak at 1721 $cm^{-1}$ indicates that the acid is largely in the hydrogen bonded, dimeric form.

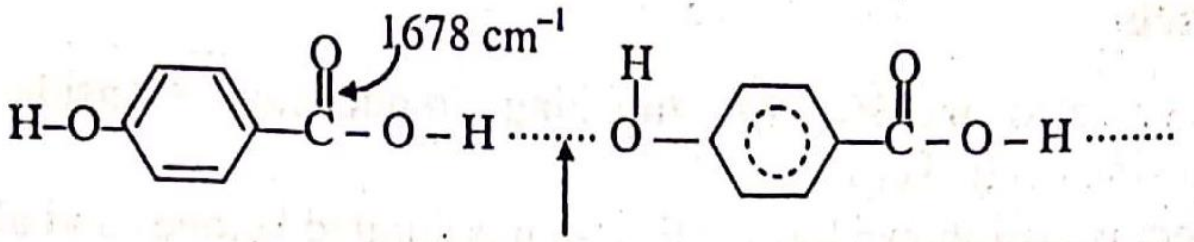
Due to H-bonding not only the >C=O frequency decreases but O–H stretching frequency also decreases. The O–H bond length increases due to H-bonding and hence its bond strength decreases.

# Factors affecting IR frequencies

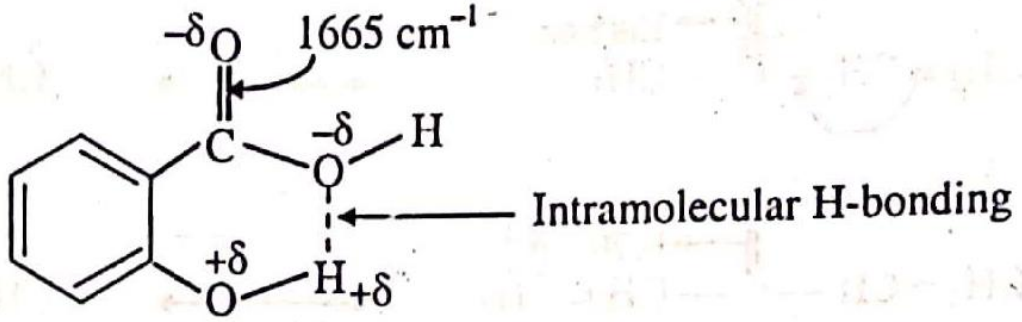
O–H H-bonded stretching 2700-2500 $cm^{-1}$

O–H free or without H-bonding – 3550 $cm^{-1}$

Intramolecular H-bonding shows greater effect of >C=O and –O–H stretching than intermolecular H-bonding




p-hydroxy benzoic acid **Intermolecular H-bonding**

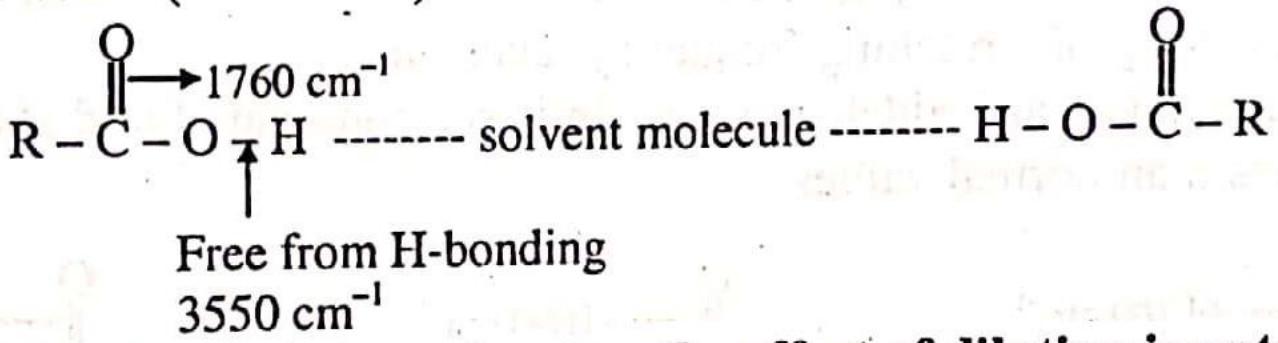



O-hydroxy benzoic acid

# Factors affecting IR frequencies

**Effects of dilution on hydrogen bonding :**

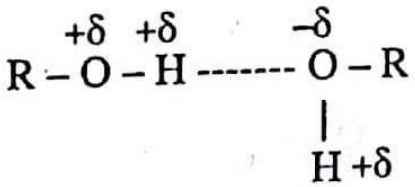
When the IR spectrum of acids is recorded with dilute solution (in aprotic solvents) the intermolecular H bonding effect decrease due to intervening solvent molecules. As a result, the O–H stretching frequency shifts to higher value (3550 $cm^{-1}$) and >C=O stretching also shifts to higher value (1760 $cm^{-1}$)



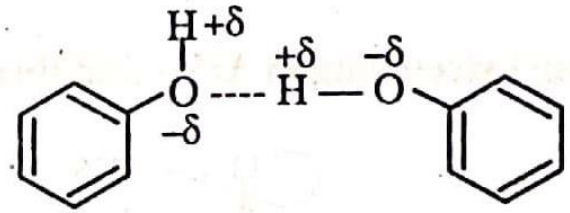

**However, if the H-bonding is intramolecular, the effect of dilution is not observed**

# Factors affecting IR frequencies

**(ii) Alcohols and Phenols** : Similar to acids, alcohols and phenols show strong H-bonding effects. H-bonded alcoholic OH groups show O–H peak in the range of 3200–3500 $cm^{-1}$

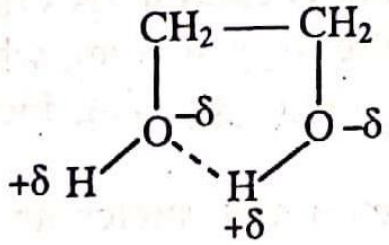


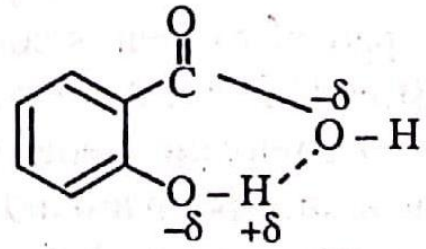
alcohols



phenols

Inter molecular H-bonding



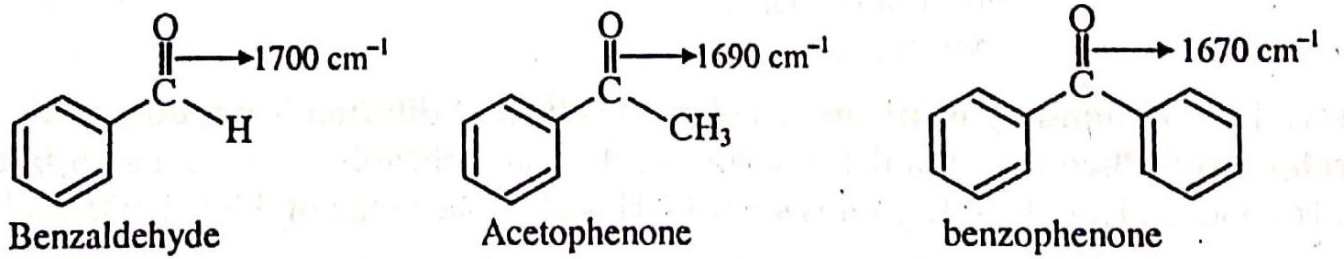


Intra molecular H-bonding

If IR spectrum of alcohols is measured in gas phase or in extremely dilute solution in aprotic solvents, the intermolecular H-bonding disappears and the –OH stretching frequency increase to 3650 $cm^{-1}$. Intramolecular H–bonds are however not affected as expected.

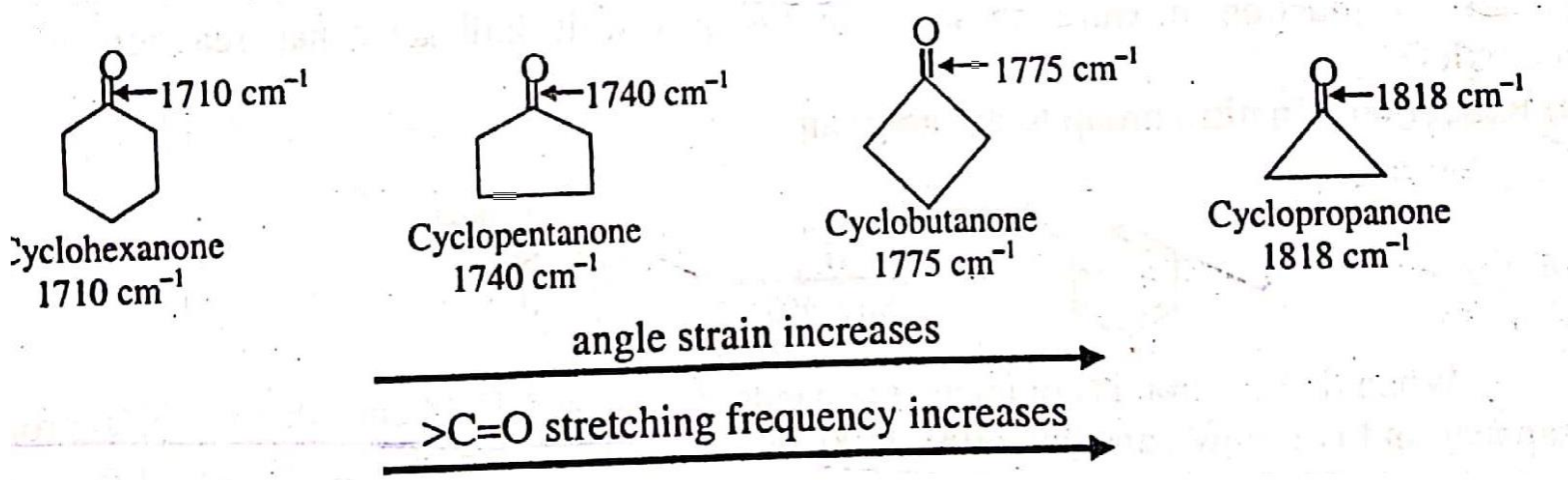
# Factors affecting IR frequencies

## d) Steric effect




## e) Angle strain /ring size

In below example as ring size decreases angle strain increases, which increase carbonyl stretching frequency.



# Structure Determination

**1) Molecular formula C3H6O**

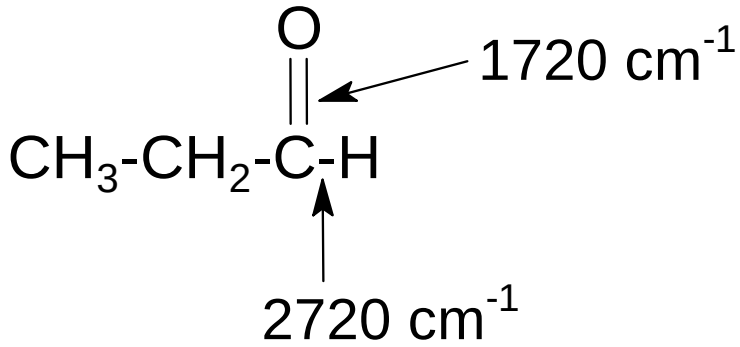
**IR band 1720 cm-1 ,2720 cm-1**

$$\text{Site of unsaturation} = \frac{(2 \times \text{no. of Carbon atoms} + 2) - (\text{no. of Hydrogen atoms})}{2}$$

$$= \frac{(2X3+2) - (6)}{2} = 1$$

IR band at 1720 cm-1 & 2720 cm-1 indicate presence of -CHO group

Hence structure of molecule is



# Structure Determination

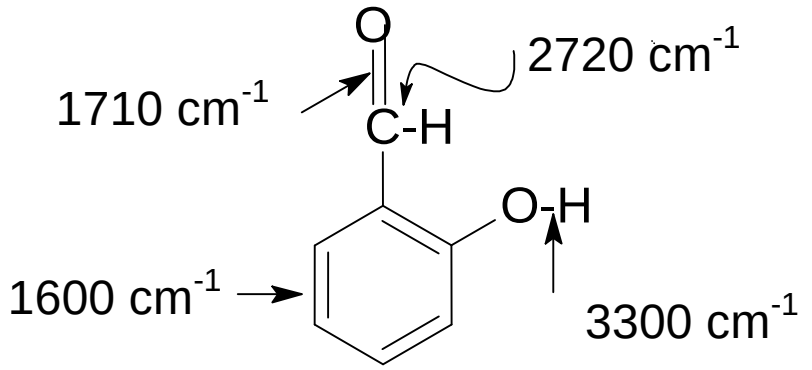
**2) Molecular formula $C_8H_8O_2$**

IR band 3300 $cm^{-1}$, 2720 $cm^{-1}$, 1710 $cm^{-1}$,1600 $cm^{-1}$
1505 $cm^{-1}$,760$cm^{-1}$

$$\text{Site of unsaturation} = \frac{(2 \times \text{no. of Carbon atoms} + 2) - (\text{no. of Hydrogen atoms})}{2}$$

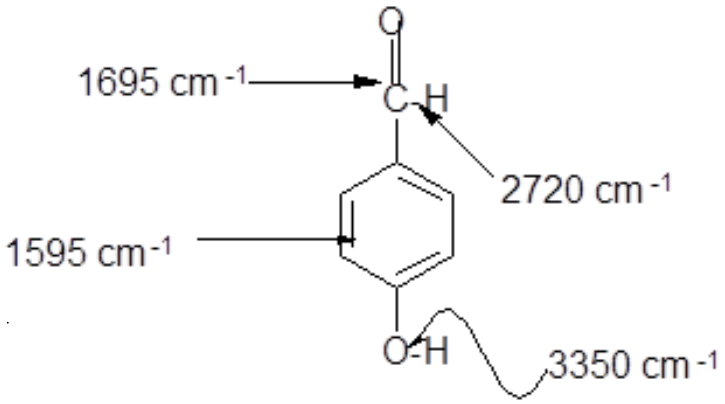
$$\frac{(2X8+2) - (8)}{2} = 5$$

Site of unsaturation is 5, hence benzene ring may present
IR band at 3300 $cm^{-1}$ indicate presence of -OH group
IR band at 1710 $cm^{-1}$ & 2720 $cm^{-1}$ indicate presence of -CHO group
IR band at 1600 $cm^{-1}$ & 1505 $cm^{-1}$ indicate presence of C=C group
IR band at 760$cm^{-1}$ indicate presence of ortho substituted benzene ring
Hence correct structure is



# Structure Determination

**3) Molecular formula $C_7H_6O_2$**




IR band 3350 $cm^{-1,}$ 2720 $cm^{-1,}$ 1695 $cm^{-1}$,1595 $cm^{-1}$
1490 $cm^{-1}$,850$cm^{-1}$

$$\text{Site of unsaturation} = \frac{(2 \times \text{no. of Carbon atoms} + 2) - (\text{no. of Hydrogen atoms})}{2}$$

$$\frac{(2X7+2) - (6)}{2} = 5$$

**Site of unsaturation is 5, hence benzene ring may present**

IR band at 3350 $cm^{-1}$ indicate presence of -OH group
IR band at 2720 $cm^{-1}$ & 1695 $cm^{-1}$ indicate presence of -CHO group
IR band at 1595 $cm^{-1}$ & 1490 $cm^{-1}$ indicate presence of -C=C- group
IR band at 850$cm^{-1}$ indicate presence of para substituted benzene ring
Hence structure of molecule is

# Structure Determination

**4) $C_3H_5N$**

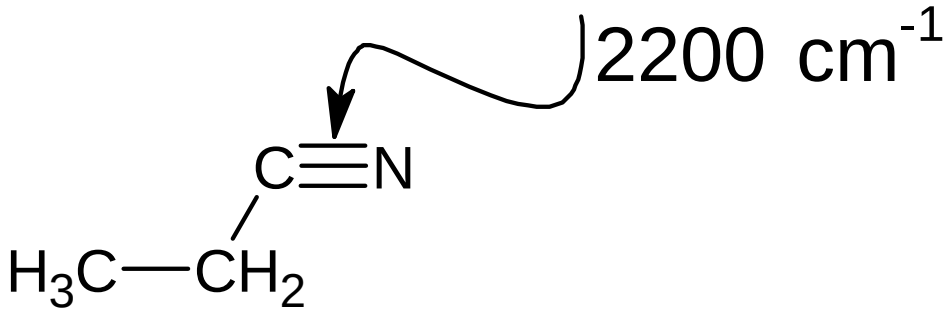
**IR band 2200 $cm^{-1}$**

$$\text{Site of unsaturation} = \frac{(2 \times \text{no. of Carbon atoms} + 2) - (\text{no. of Hydrogen atoms} - 1)}{2}$$

$$\frac{(2X3+2) - (5-1)}{2} = 2$$

IR band at 2200 $cm^{-1}$ indicate presence of -CN group

Hence correct structure is



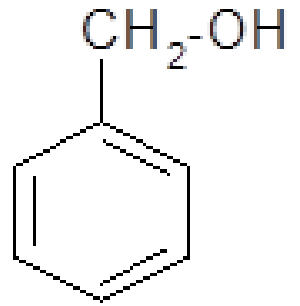
# Structure Determination

**5) Molecular formula $C_7H_8O$**

IR band 3300 $cm^{-1,}$ $^{1600}$ $cm^{-1}$,1490 $cm^{-1}$
690 $cm^{-1}$,760$cm^{-1}$

$$\text{Site of unsaturation} = \frac{(2 \times \text{no. of Carbon atoms} + 2) - (\text{no. of Hydrogen atoms})}{2}$$

$$\frac{(2X7+2) - (8)}{2} = 4$$




Site of unsaturation is 4, hence benzene ring may present
IR band at 3300 $cm^{-1}$ indicate presence of -OH group
IR band at 1600 $cm^{-1}$ & 1490 $cm^{-1}$ indicate presence of C=C group
IR band at 690$cm^{-1}$ & $^{690}cm^{-1}$ indicate presence of mono substituted benzene ring.
Hence correct structure is

# Structure Determination

6) Molecular formula

$C_6H_6O$

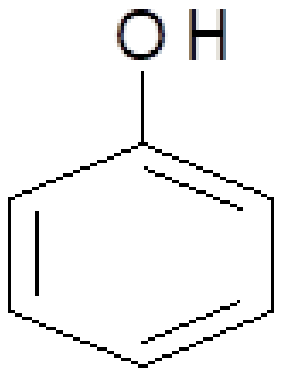
IR band 3300 $cm^{-1}$

1600 $cm^{-1}$,

1500 $cm^{-1}$,

760$cm^{-1}$,

690 $cm^{-1}$




7) Molecular formula

$C_3H_5N$

IR band 2200 $cm^{-1}$

$CH_3$-$CH_2$-CN

# Structure Determination

8) **Molecular formula** $C_3H_6O$

**(A)** IR band

1720 $cm^{-1}$

2720 $cm^{-1}$

**B)** IR band, 1620 $cm^{-1}$,

1140$cm^{-1}$,

990 $cm^{-1}$,

910$cm^{-1}$

**C)** IR band

3300 $cm^{-1}$,

1620 $cm^{-1}$,

990 $cm^{-1}$,

910 $cm^{-1}$

**D)** No band above 1500$cm^{-}$

$CH_3$-$CH_2$-CHO

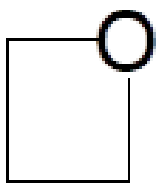
**A**

$CH_3$-O-CH=$CH_2$

**B**

$CH_2$=CH-$CH_2$-OH

**C**

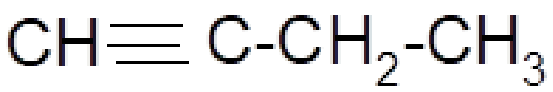


**D**

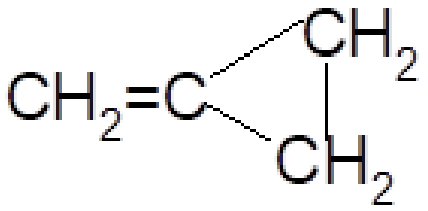
# Structure Determination

**9) Molecular formula $C_4H_6$**

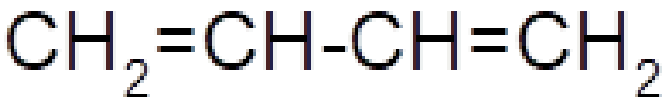
**(A)** IR band 3300 $cm^{-1}$
2100 $cm^{-1}$,



**B)** IR band 1620$cm^{-1}$,
890 $cm^{-1}$,



**C)** IR band, 1620 $cm^{-1}$,
910$cm^{-1}$,
990 $cm^{-1}$,
λ Max-217 nm

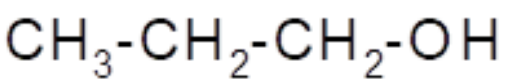


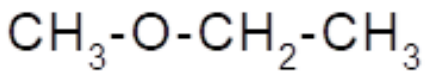
# Structure Determination

10) **Molecular formula $C_3H_8O$**

**(A)** IR band 3600cm$^{-1}$

**B)** IR band no band above 1500 cm$^{-1}$



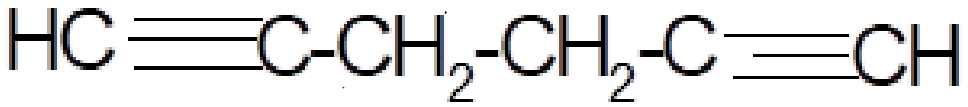


# Structure Determination

**11) Molecular formula $C_6H_6$**

IR band 3300 $cm^{-1}$

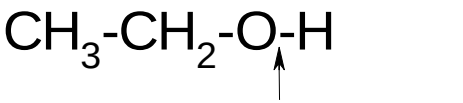
2100 $cm^{-1}$



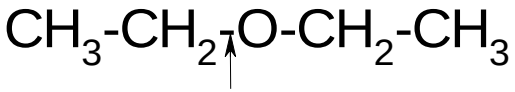
# Structure Determination

## Distinguish following pairs by IR spectroscopy

Ethanol & Diethyl ether




~3300 $cm^{-1}$

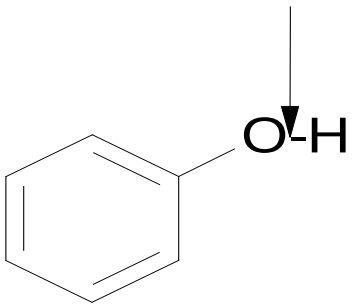



1300 -1000 $cm^{-1}$

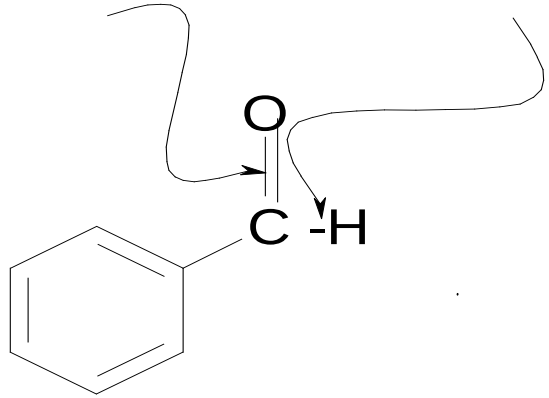
No band around 3300 $cm^{-1}$

Phenol & Acetaldehyde

~3300 cm-1



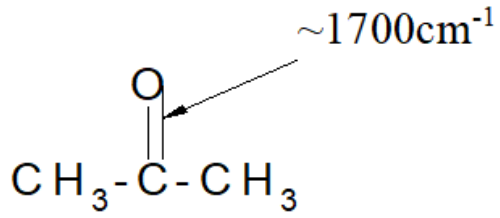

~1700 cm-1 ~ 2700cm-1

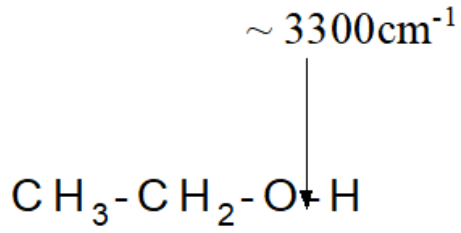


# Structure Determination

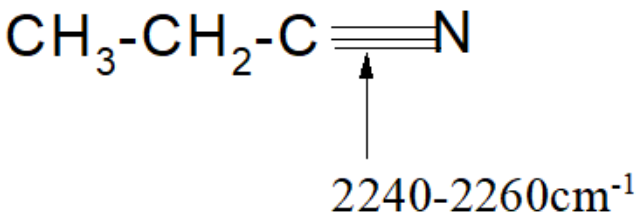
## Distinguish following pairs by IR spectroscopy

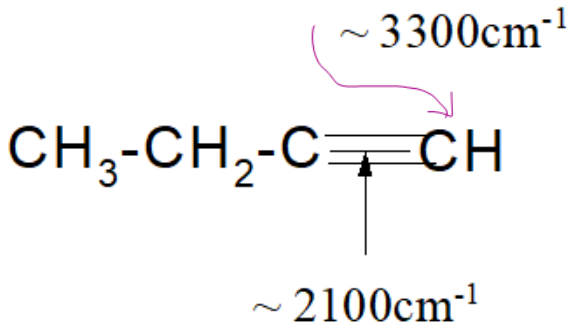
**3)Acetone & Ethyl alcohol**




4) Ethyl cyanide & Propyne

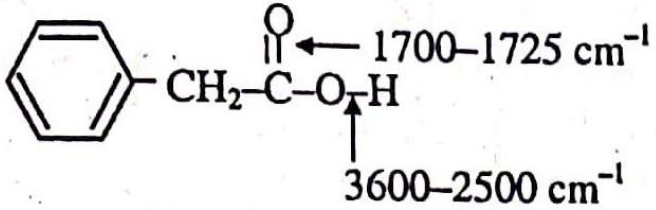


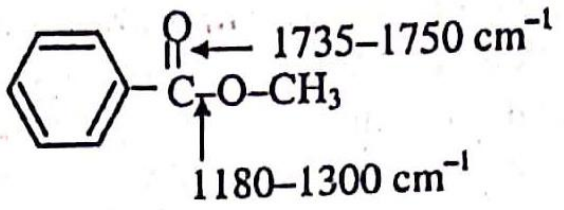
# Structure Determination

## Distinguish following pairs by IR spectroscopy

**Phenyl acetic acid and Methyl benzoate.**

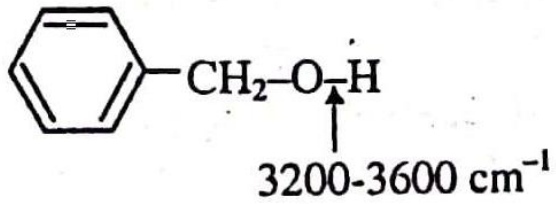



Phenyl acetic acid

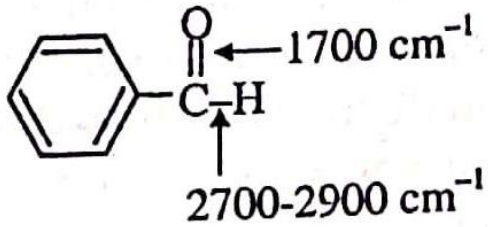



Methyl benzoate

**Benzyl alcohol and Benzaldehyde :**




Benzyl alcohol




Benzaldehyde

# Applications of IR spectroscopy

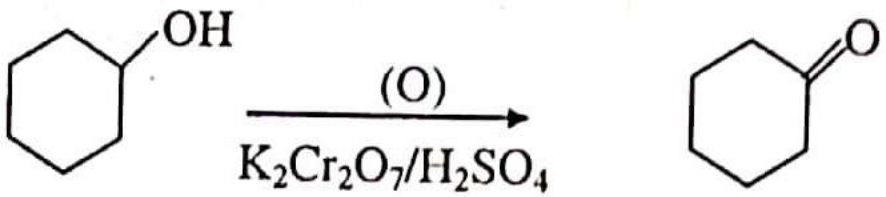
## 1) Structure Determination

Peaks in functional group region give information gives information regarding different functional groups present in the molecule. Peaks in aromatic region help to find out substitution patter present in aromatic compounds.

# Applications of IR spectroscopy

## 2) Study of Progress of Chemical reactions

(i) Oxidation of cyclohexanol to cyclohexanone.



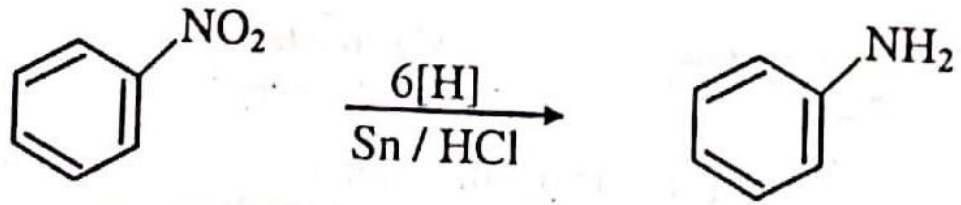

Initially only cyclohexanol is present and the IR spectrum will show O–H stretching peak at 3550 $cm^{-1}$.

When the reaction is complete the band at 3550 $cm^{-1}$ due to –OH stretching frequency disappears and a new band at 1710 $cm^{-1}$ due to ketonic group (C = O frequency) appears. If reaction mixture shows both the peaks, it indicates that reaction is still incomplete.

# Applications of IR spectroscopy

## 2) Study of Progress of Chemical reactions

(ii) Reduction of a nitro group to amino group.



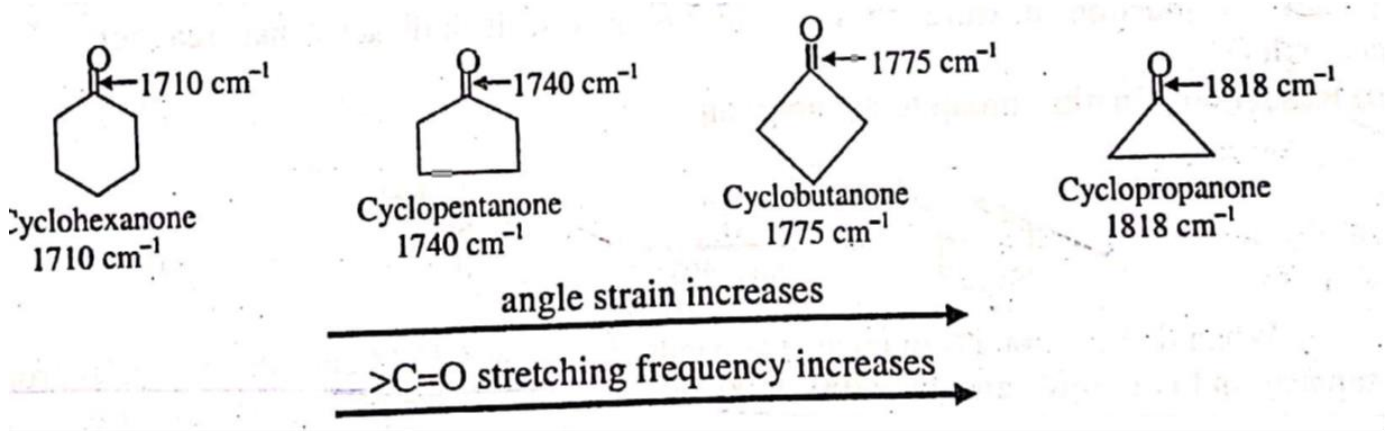

When the reaction is complete, the bands at 1540 and 1370 $cm^{-1}$ due to $-NO_2$ groups disappear and two new bands at 3300–3500 $cm^{-1}$ appears due to N–H stretching frequency, present in the final product.

## 3) Detection of hydrogen bonding

Free –OH appear at higher frequency ( 3600-3650 $cm^{-1}$) than bonded –OH (3200-3500 $cm^{-1}$)

# Applications of IR spectroscopy

## 4) Detection of ring size




## 5) Detection of Impurities

Small amount of impurity can be detected by carefully observing IR spectrum

Example Ketone in hydrocarbon