# Infrared Spectroscopy

## Part “1”

## Introduction and principles

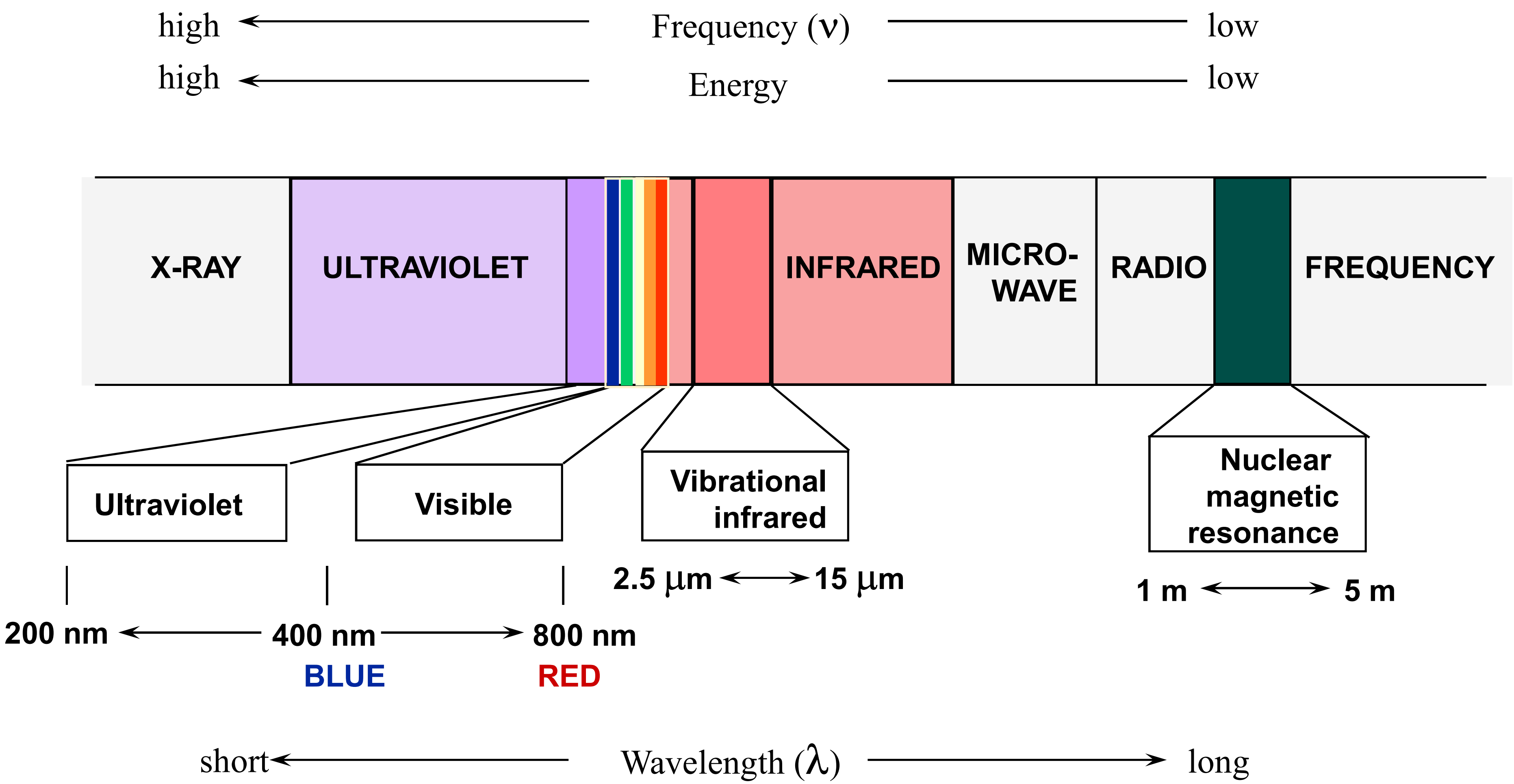
# WHAT IS IR RADIATION

- Natural infrared-

Sunlight, at an effective temperature of 5,780 kelvins, is composed of nearly thermal-spectrum radiation that is slightly more than half infrared.

sunlight provides an irradiance of just over 1 kilowatts per square meter at sea level. Of this energy, 527 watts is infrared radiation, 445 watts is visible light, and 32 watts is ultraviolet radiation.

# The Electromagnetic Spectrum



high ← Frequency ($\nu$) low

high ← Energy low

X-RAY

ULTRAVIOLET

INFRARED

MICRO-WAVE

RADIO

FREQUENCY

Ultraviolet

Visible

Vibrational infrared

Nuclear magnetic resonance

2.5 µm ⟷ 15 µm

1 m ⟷ 5 m

200 nm ← 400 nm → 800 nm

BLUE

RED

short ← Wavelength ($\lambda$) → long

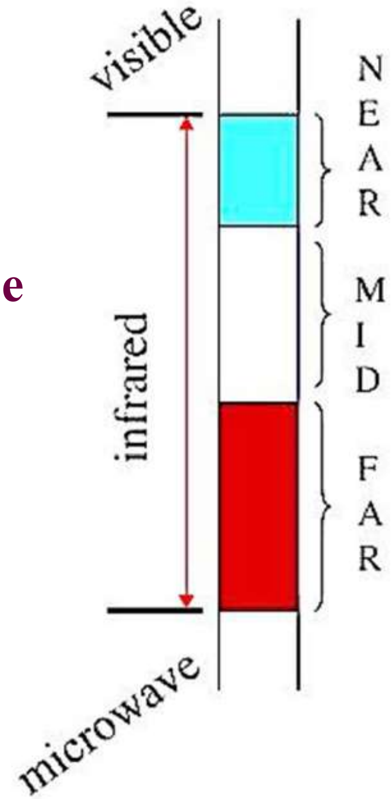
# IR regions

## IR region subdivided into 3 sub-regions

A. Near IR region (Nearest to the visible)

780 nm to 2.5 μm (12,800 to 4000 $cm^{-1}$)

**(overtones region)**



B. Mid IR region

2.5 to 50 μm (4000 – 200 $cm^{-1}$)

**The mid IR region is of greatest practical use to the organic compounds.**

C. Far IR region

50 to 1000 μm (200 – 10$cm^{-1}$)

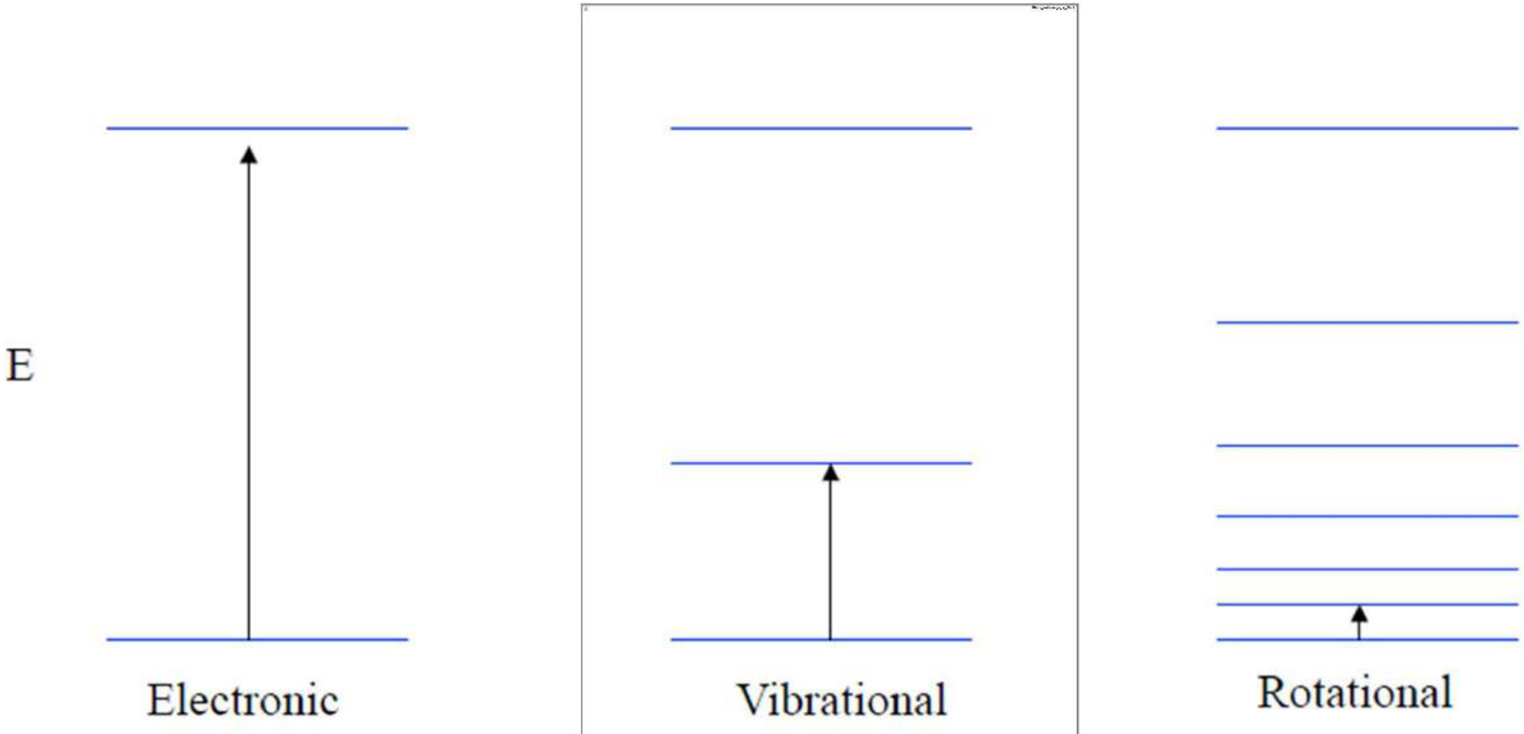
# Use of IR spectra

- Identification of functional groups on a molecule – this is a very important tool in organic chemistry.
- Corresponding with a known sample's IR spectrum confirms the identity of the compound.
- Since absorbance follows Beer's Law, can do quantitative analysis.
- IR alone cant determine the structure
- Some signals may be ambiguous.

**NOTES:-**

1. Since most "types" of bonds in covalent molecules have roughly the same energy, i.e., C=C and C=O bonds, C-H and N-H bond; ;they show up in similar regions of the IR spectrum.
2. Remember all organic functional groups are made of multiple bonds and therefore show up as multiple IR bands (peaks)

# Different energy means different effect

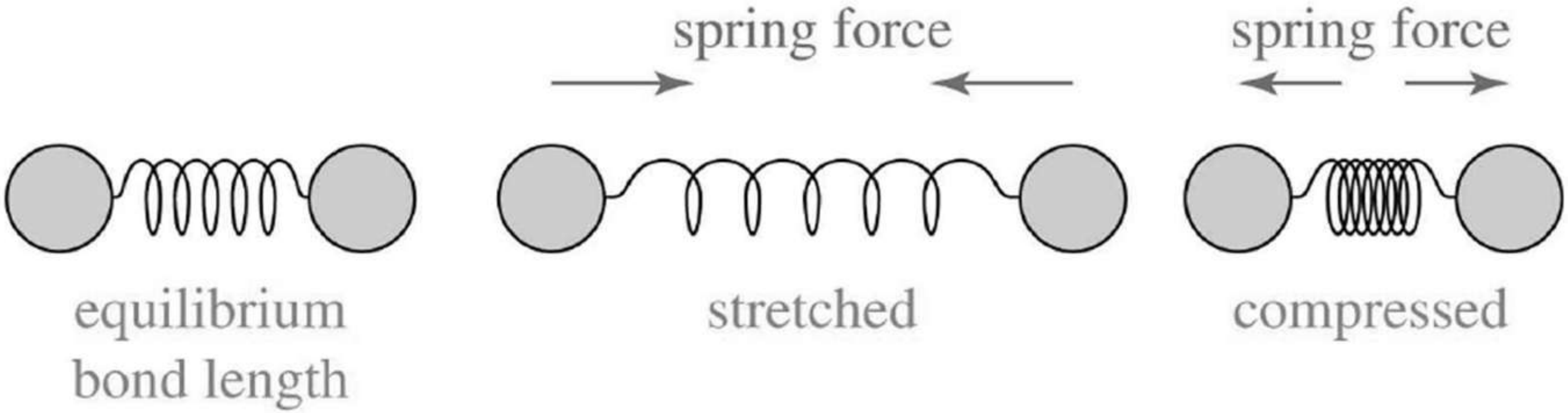


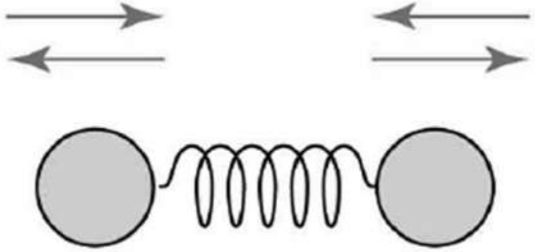
- Electronic transitions: UV-visible
- Vibrational transitions: IR
- Rotational transitions: Radio

**IR influence**

# Molecular Vibrations

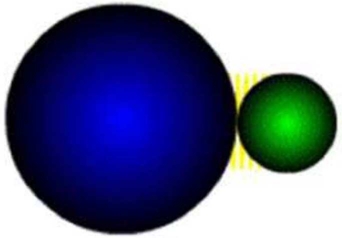
Covalent bonds vibrate at only certain allowable frequencies.





# Principle of IR spectroscopy

- Molecules are made up of atoms linked by chemical bonds. The movement of atoms and the chemical bonds like like spring and balls (vibration)



Vibration of a Diatomic Molecule
Approximates an Oscillating Spring

- This characteristic vibration are called Natural frequency of vibration.

- When energy in the form of infrared radiation is applied then it causes the vibration between the atoms of the molecules and when,

Applied infrared frequency = Natural frequency of vibration

Then, Absorption of IR radiation takes place and a peak is observed.

Different functional groups absorb characteristic frequencies of IR radiation. Hence gives the characteristic peak value.

Therefore, IR spectrum of a chemical substance is a finger print of a molecule for its identification.

# Infrared Spectroscopy

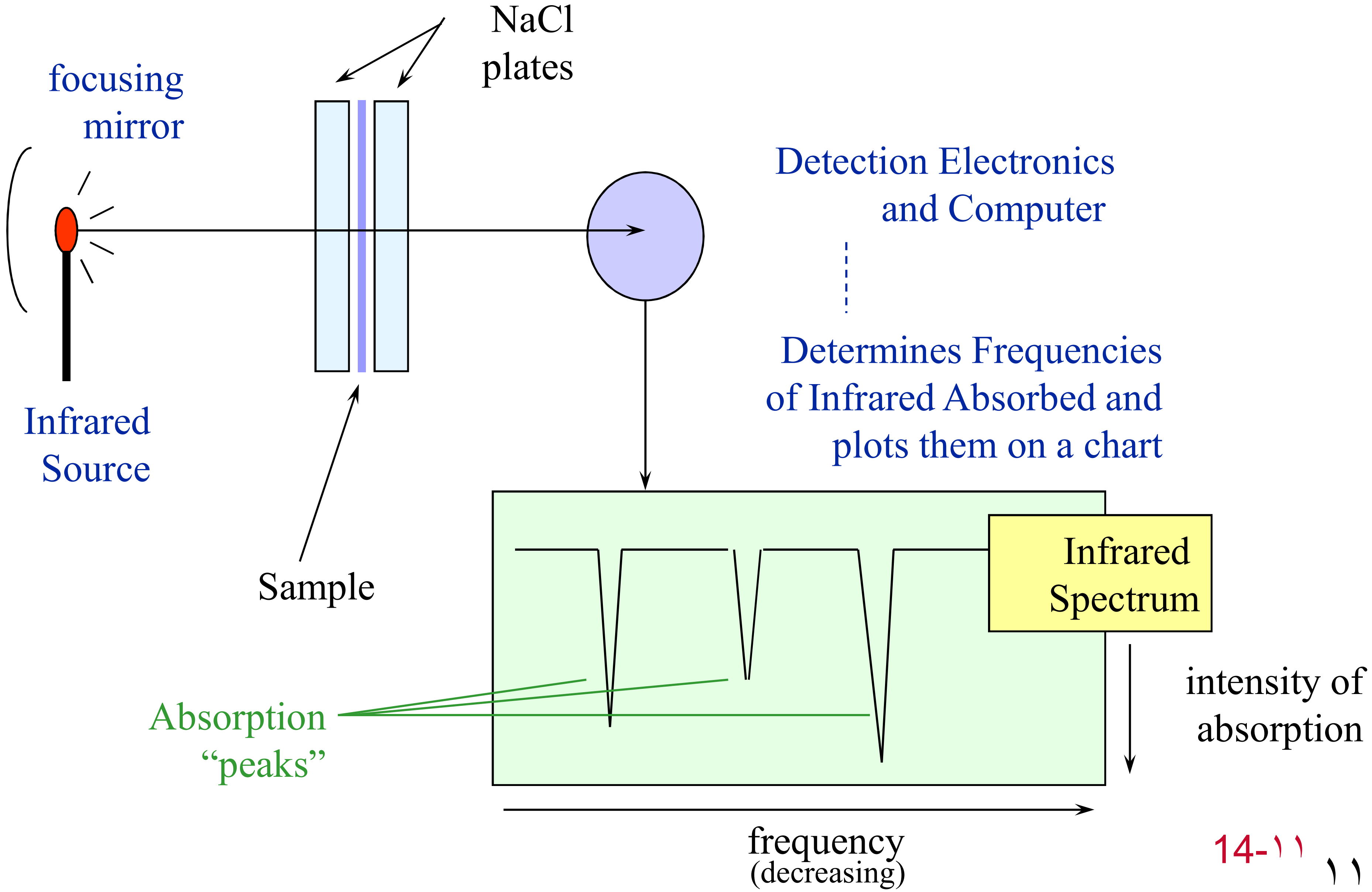
## Background

- Absorption of IR light causes changes in the vibrational motions of a molecule (from $V_0$ to $V_1$ ............ $V_f$)
- The different vibrational modes available to a molecule include stretching and bending modes.

- When the frequency of IR light matches the frequency of a particular vibrational mode, the IR light is absorbed, causing the amplitude of the particular bond stretch or bond bend to increase.

- The vibrational modes of a molecule are quantized, so they occur only at specific frequencies which correspond to the frequency of IR light.

# Simplified Infrared Spectrophotometer



focusing
mirror

NaCl
plates

Detection Electronics
and Computer

Determines Frequencies
of Infrared Absorbed and
plots them on a chart

Infrared
Source

Sample

Infrared
Spectrum

Absorption
“peaks”

intensity of
absorption

frequency
(decreasing)

# The unit used on an IR spectrum is
# Wavenumbers $\bar{\nu}$

$$\bar{\nu} = \text{wavenumbers } (\text{cm}^{-1}) = \frac{1}{\lambda}$$

wavelength (cm)

$\nu$ = frequency = $\bar{\nu}\,C$

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

or

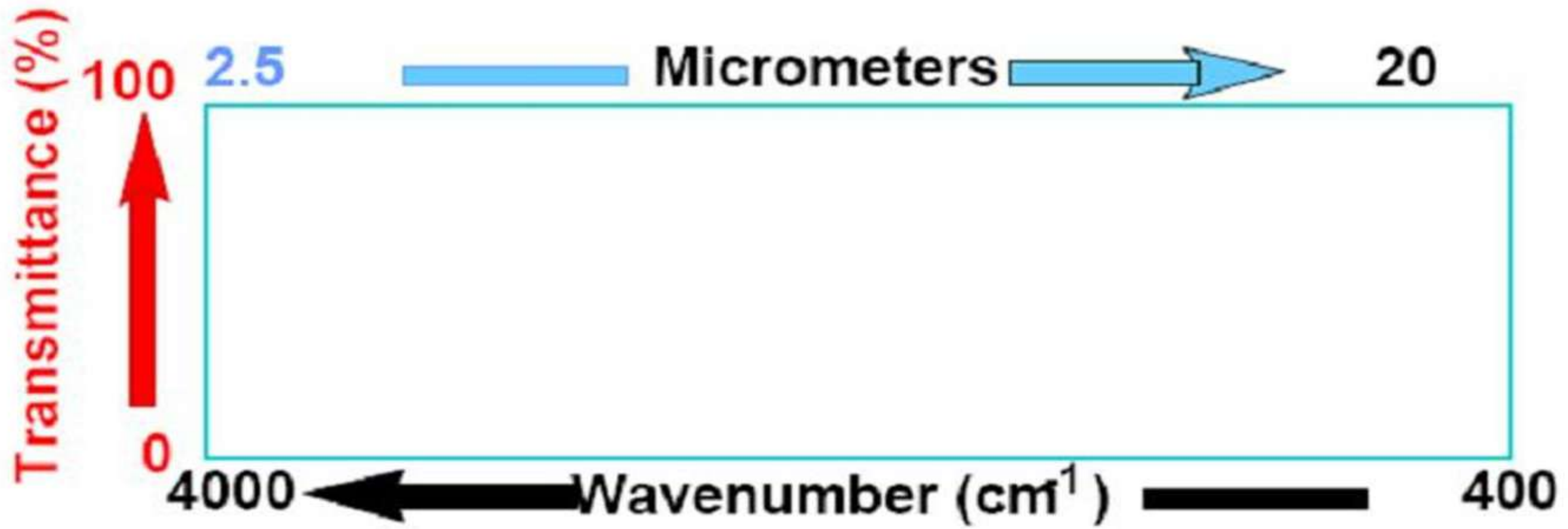
$$\nu = \left(\frac{1}{\lambda}\right) C = \frac{C}{\lambda}$$

$$\frac{\text{cm/sec}}{\text{cm}} = \frac{1}{\text{sec}}$$

wavenumbers are directly proportional to frequency

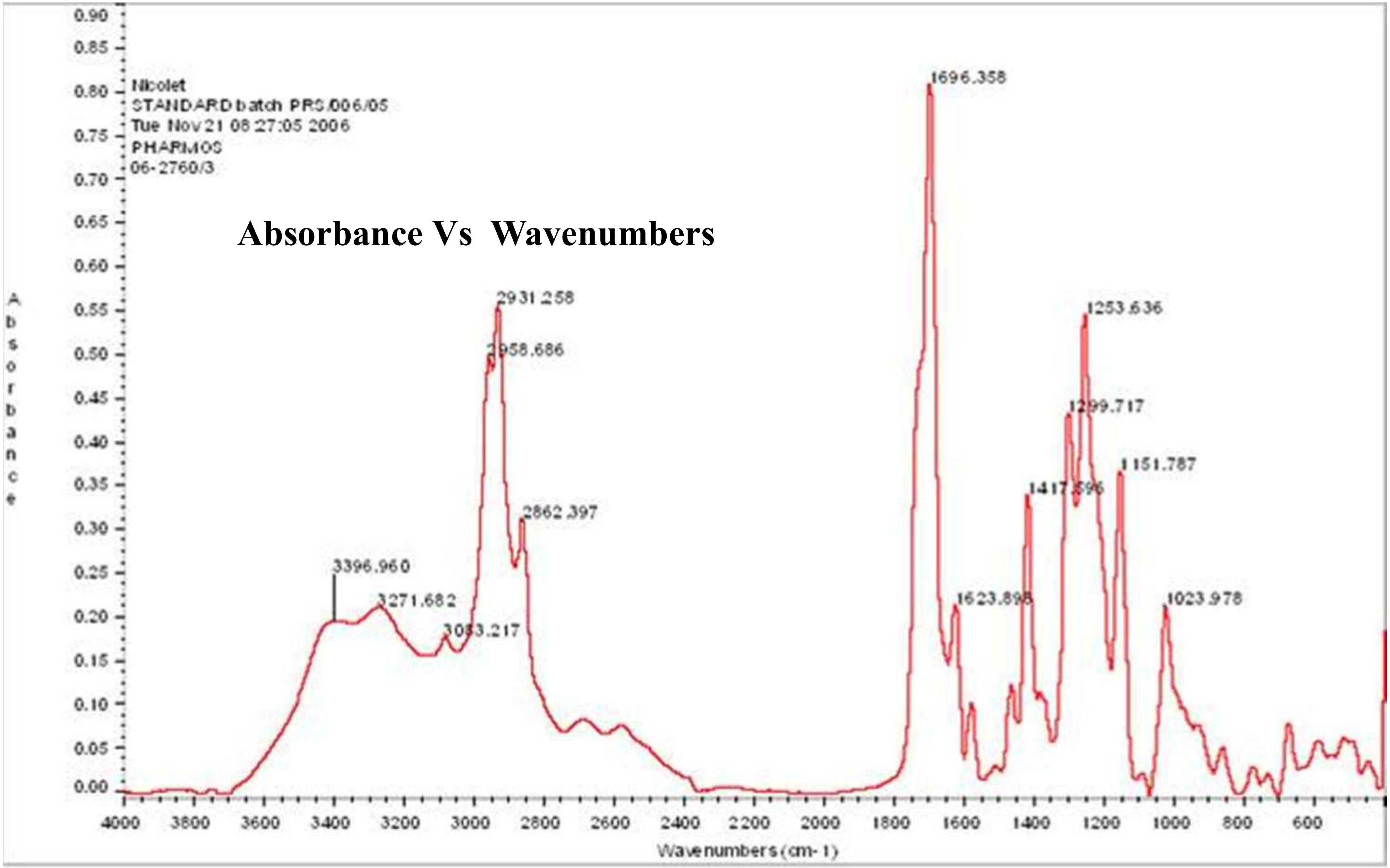
# The IR Chart

## *Spectrum*



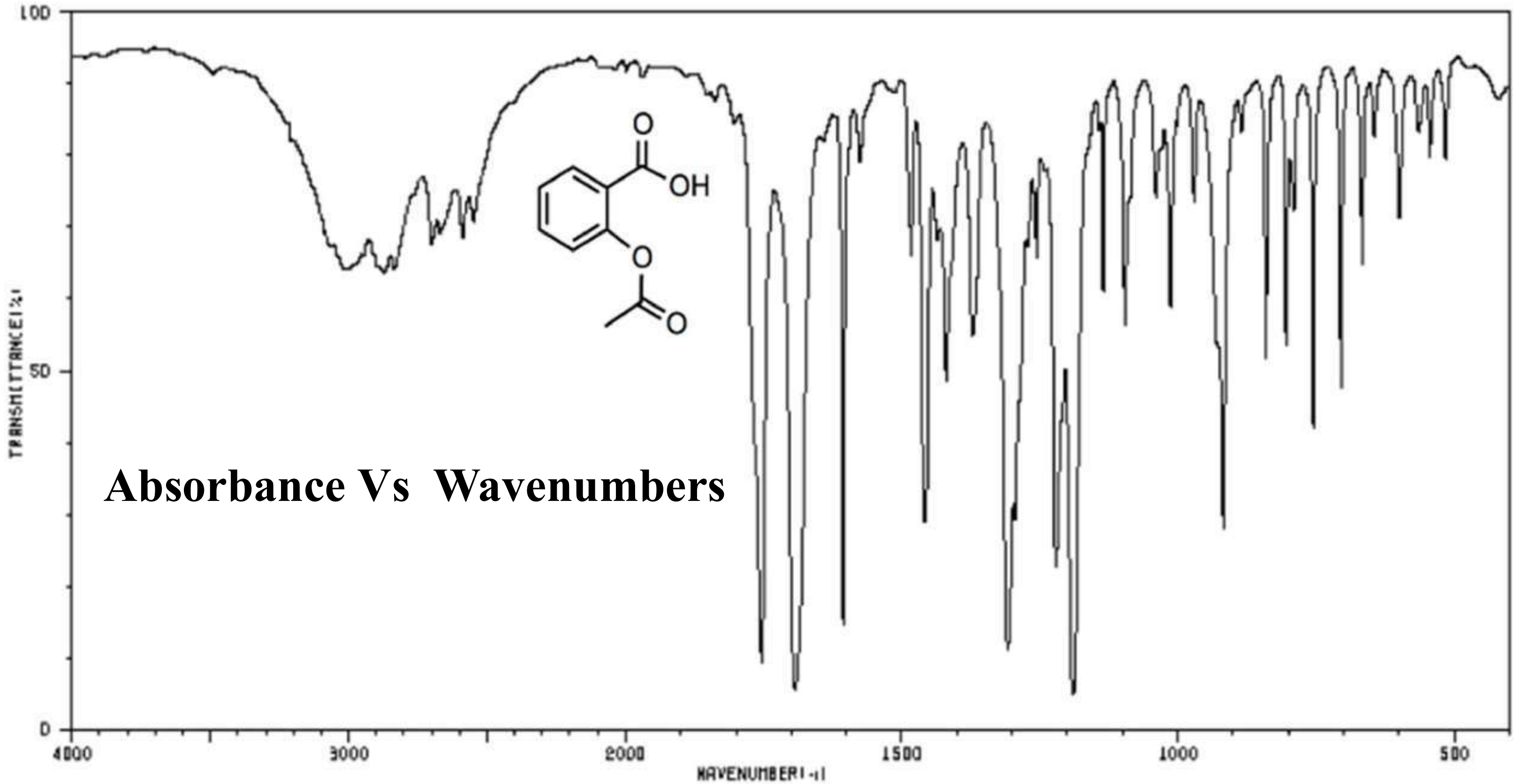
Please “know” this

**Y axis might be Transmittance (T) or Absorbance (A); the T is most common**



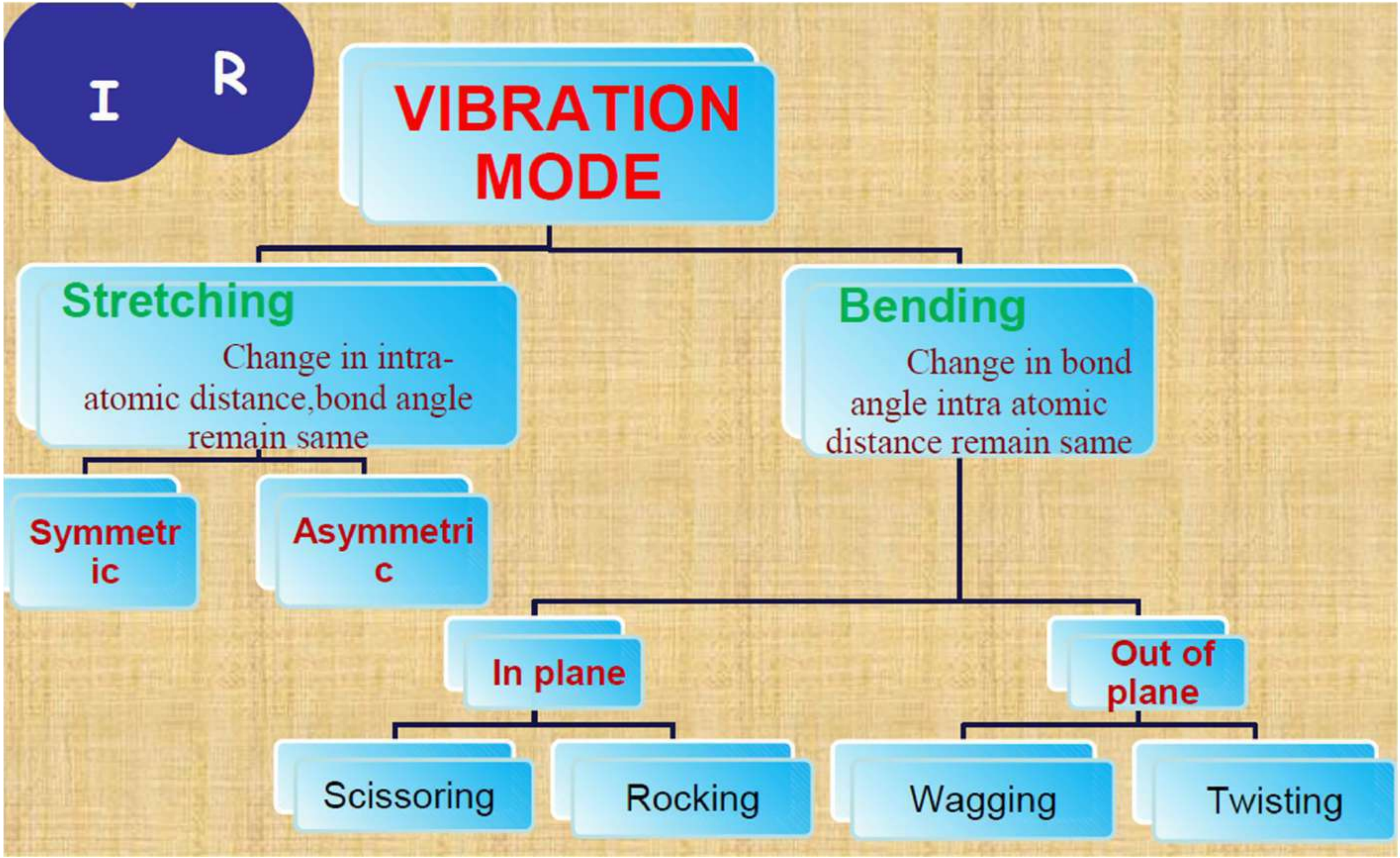
**Absorbance Vs Wavenumbers**

[redacted]



Absorbance Vs Wavenumbers

15. (5 pts.) Assign the peaks in the infrared spectrum of salicylic acid (below) with frequencies greater than



I R

VIBRATION MODE

**Stretching**

Change in intra-atomic distance,bond angle remain same

**Bending**

Change in bond angle intra atomic distance remain same

**Symmetric**

**Asymmetric**

**In plane**

**Out of plane**

Scissoring

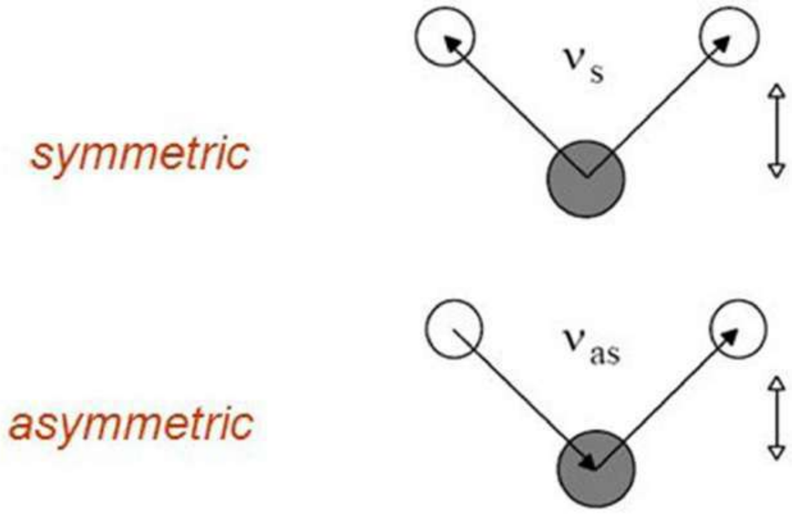
Rocking

Wagging

Twisting

## iii.) Types of Molecular Vibrations

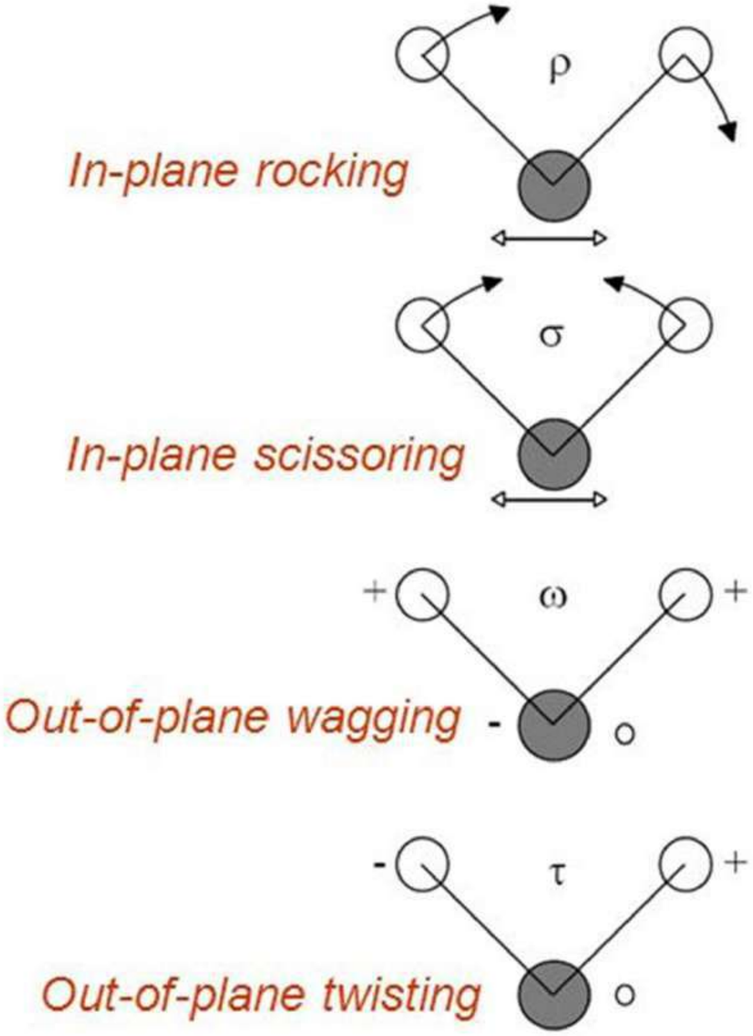
### Bond Stretching



*symmetric*

*asymmetric*

### Bond Bending



*In-plane rocking*

*In-plane scissoring*

*Out-of-plane wagging*

*Out-of-plane twisting*

# Degrees of freedom and molecular vibrations

**Linear molecule D.o.F= 3N-5**

**[$CO_2$ (3X3-5)=4]**

**Non-Linear molecule D.o.F= 3N-6**

**[$H_2O$ (3X3-6)=3]**

# Video

# Infrared Spectroscopy

## Part 1“B”

## Introduction and principles

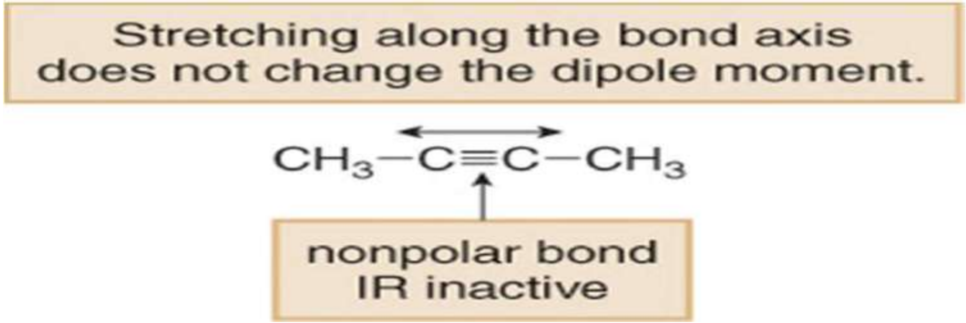
# DO ALL COMPOUNDS ARE CLASSIFIED AS IR ACTIVE ?!!!

**NO !!**

# Raman

# IR Absorption Conditions

- Only Polar bonds are IR active and can show a clear absorption in the IR spectrum
- Symmetrical nonpolar bonds do not absorb in the IR. This type of vibration is said to be IR inactive.
- For a bond to absorb in the IR, there must be a change in dipole moment during the vibration.
- For these non polar compounds Raman spectroscopy can do the job



Stretching along the bond axis does not change the dipole moment.

$CH_3-C\equiv C-CH_3$

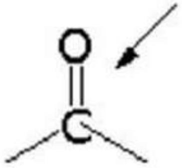
nonpolar bond
IR inactive

# INFRARED ACTIVE BONDS

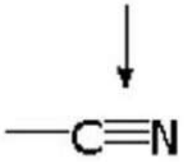
Not all covalent bonds display bands in the IR spectrum. **Only polar bonds do so. These are referred to as IR active**.

The intensity of the bands depends on the magnitude of the **dipole moment** associated with the bond in question:

- Strongly polar bonds such as carbonyl groups (C=O) produce strong bands.
- Medium polarity bonds and asymmetric bonds produce medium bands.
- Weakly polar bond and symmetric bonds produce weak or non observable bands.

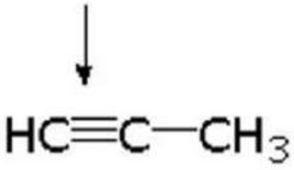


STRONG



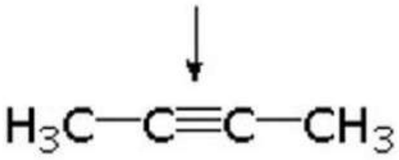
$-C\equiv N$

MEDIUM



$HC\equiv C-CH_3$

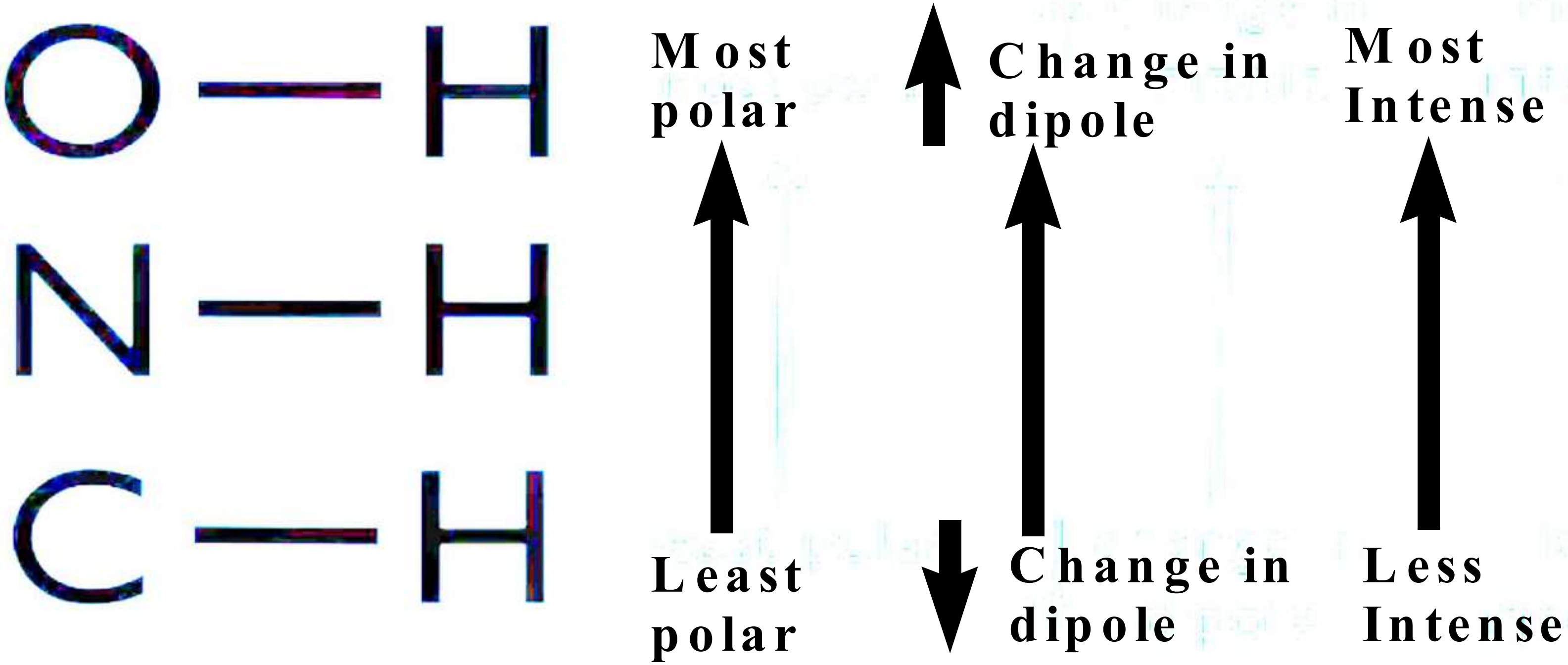
WEAK



$H_3C-C\equiv C-CH_3$

NOT
OBSERVABLE

# Increasing polarity means more absorption



Most polar

Change in dipole

Most Intense

Least polar

Change in dipole

Less Intense

# Factors that influence in determining the locations of the spectrum peaks various

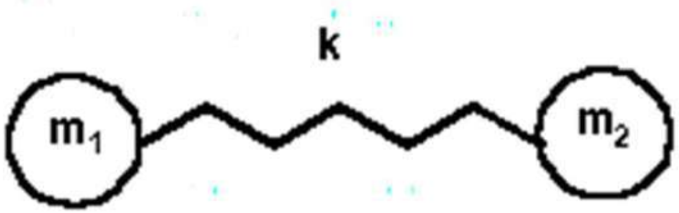
1. Atomic Masses

Frequency decreases with increasing atomic mass.

C-H > C-C > C-O > C-Cl > C-Br

3000 1200 1100 750 650

# Hooke's law



$$\bar{\upsilon} = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}} \qquad \mu = \frac{m_1 . m_2}{m_1 + m_2}$$

$\bar{\upsilon}$ = frequency

$\mu$ = reduced mass

Two factors affect the IR absorption according to Hookes law

1- bond strength (Directly proportional)

2- Atomic mass (Inversely proportional)

# IR Stretching Frequencies of two bonded atoms:

## What Does the Frequency, ν, Depend On?

$$\nu = \frac{1}{2\pi}\sqrt{\frac{k}{m_r}}$$

$$m_r = \frac{m_1 m_2}{m_1 + m_2}$$

**ν = frequency**
**k = spring strength (bond stiffness)**
**$m_r$ = reduced mass (mass of largest atom)**

## 2. Bond Strength

**Frequency increases with increasing bond energy.**

$C{\equiv}C \;>\; C{=}C \;>\; C{-}C$

2150 1650 1200

## 3. The coupling between bonds different groups.

| $C{=}O$ | $O{=}C{=}O$ |
|---|---|
| 1800 to 1650 | 2350 |

## 4. stereochemistry effects.

## 5. Solvents, Temperature and Sample state.

# Band Intensity

1- The greater the dipole moment, the greater change in dipole moment when a band stretches.

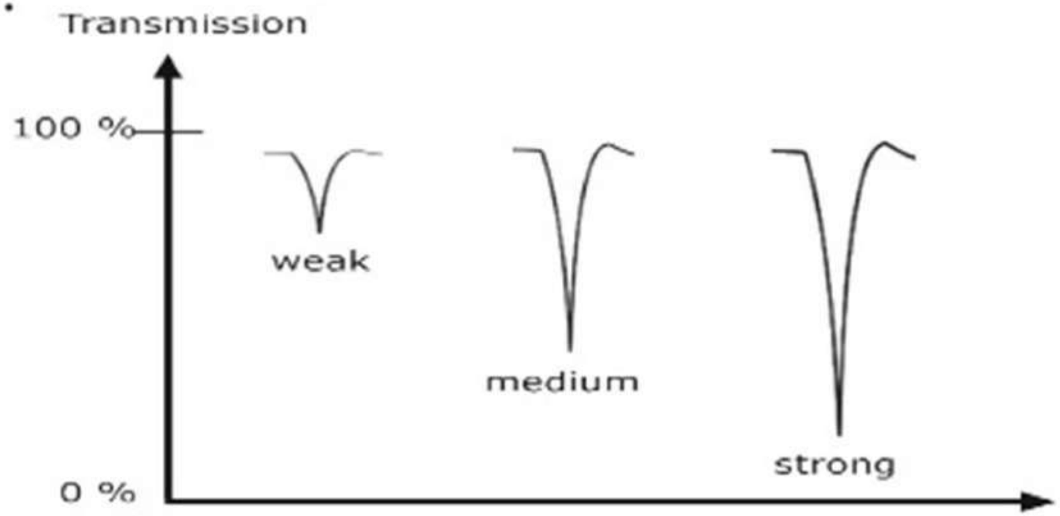
2- The greater the change in dipole moment, the more intense the absorption band.

# INFRARED ABSORPTION BANDS

| | | |
|---|---|---|
| POSITION | REDUCED MASS | LIGHT ATOMS HIGH FREQUENCY |
| | BOND STRENGTH (STIFFNESS) | STRONG BONDS HIGH FREQUENCY |
| STRENGTH | CHANGE IN ‘POLARITY’ | STRONGLY POLAR BONDS GIVE INTENSE BANDS |
| WIDTH | HYDROGEN BONDING | STRONG HYDROGEN BONDING GIVES BROAD BANDS |

# CLASSIFICATION OF IR BANDS

- IR bands can be classified as **strong** (s), **medium** (m), or **weak** (w), depending on their relative intensities in the infrared spectrum.
- A strong band covers most of the *y*-axis. A medium band falls to about half of the *y*-axis, and a weak band falls to about one third or less of the *y*-axis.



# Describing IR Absorptions

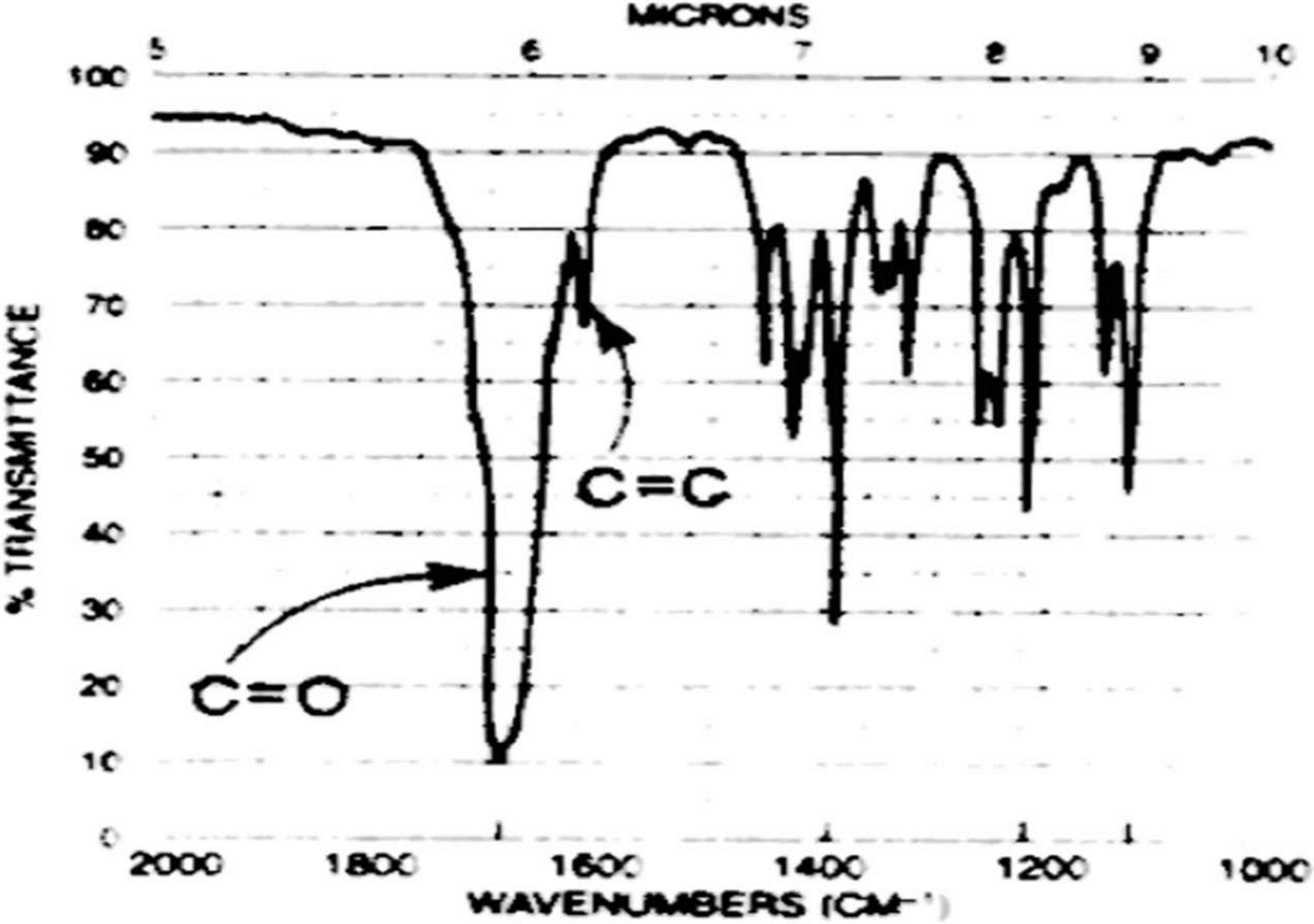
IR absorptions are described by their frequency and appearance.

- *Frequency* ($\nu$) is given in wavenumbers ($cm^{-1}$)
- *Appearance* is qualitative: intensity and shape
- conventional abbreviations:

| | |
|---|---|
| vs | very strong |
| s | strong |
| m | medium |
| w | weak |
| br | broad |
| sh | sharp or shoulder |

# Intensity of C=O vs C=C

**Don’t get confused=Don’t miss-match**

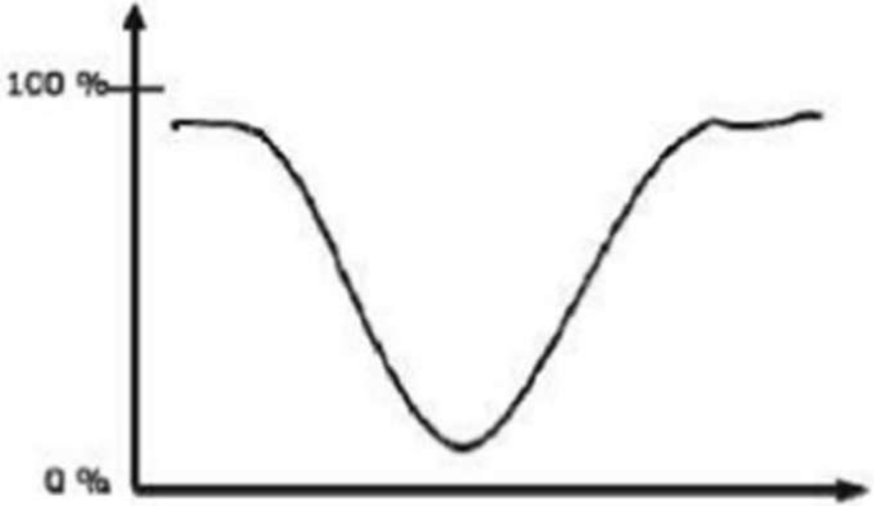


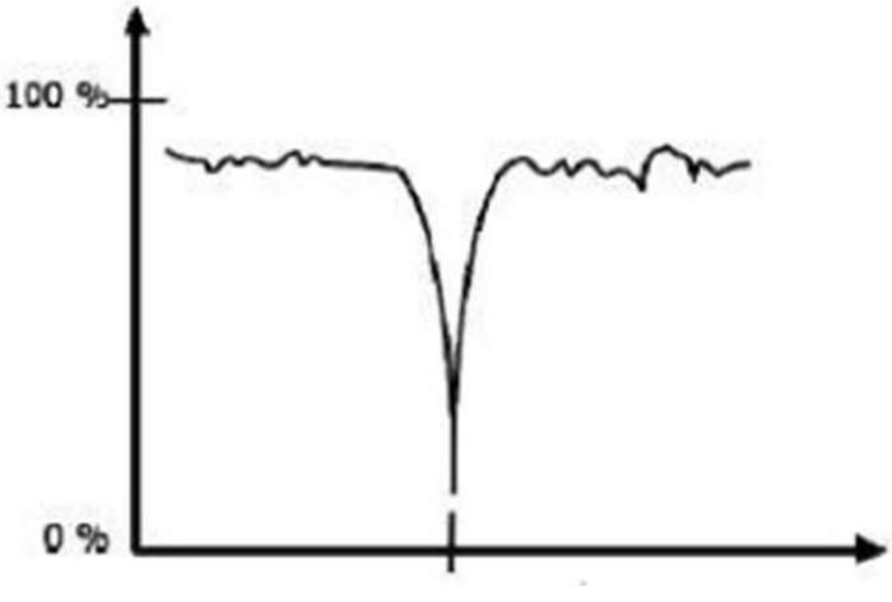
# INFRARED BAND SHAPES

Infrared band shapes come in various forms. Two of the most common are **narrow and broad.**

- **Narrow bands** are thin and pointed, like a dagger.
- **Broad bands** are wide and smoother.

A typical example of a broad band is that displayed by **O-H bonds**, such as those found **in alcohols and carboxylic acids**, as shown below.





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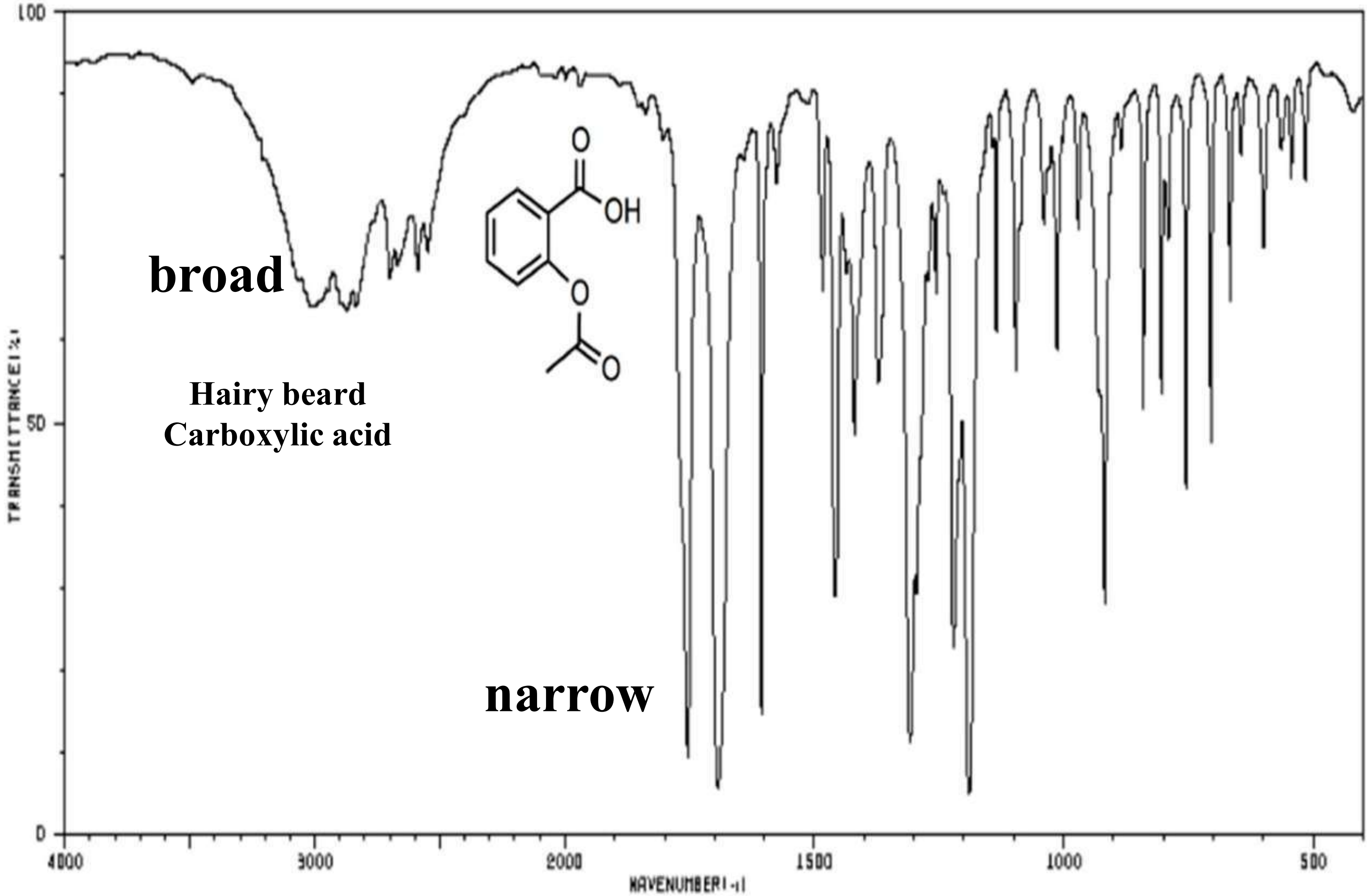


**broad**

**Hairy beard**
**Carboxylic acid**

**narrow**

15. (5 pts.) Assign the peaks in the infrared spectrum of salicylic acid (below) with frequencies greater than

# Infrared Spectroscopy

## Part “2”

## Absorption regions

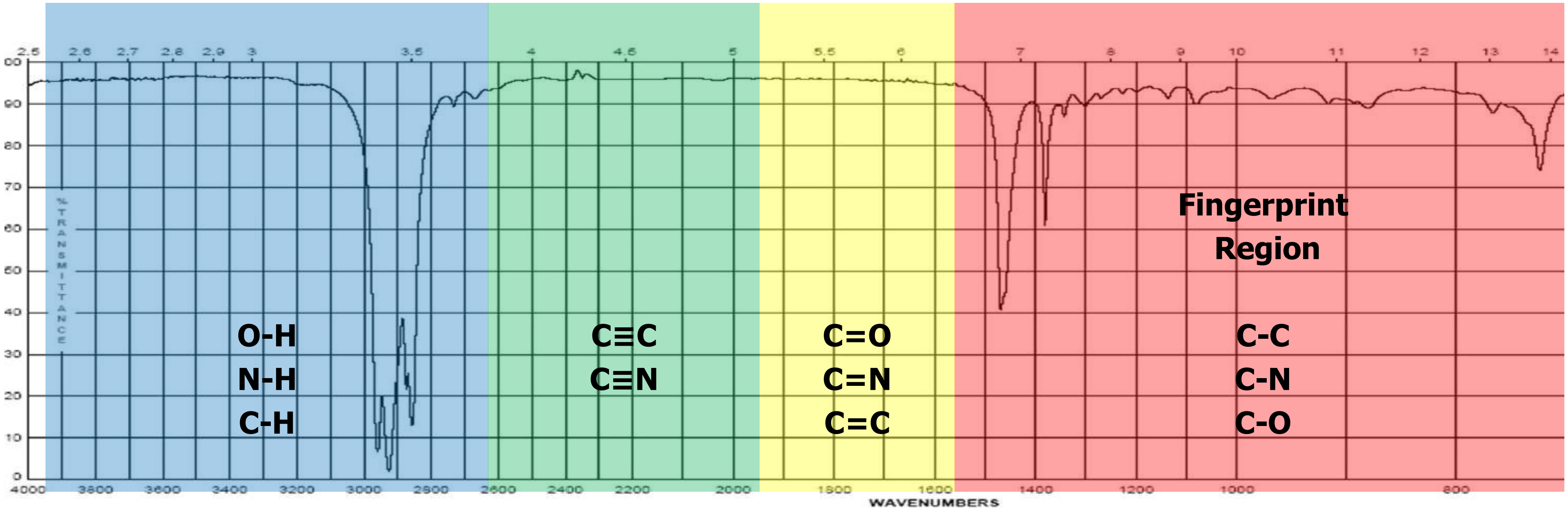
# IR Absorption Regions

**In general, the IR spectrum can be split into four regions for interpretation:**

- **4000 – 2500 $cm^{-1}$:** **Absorption of single bonds formed by hydrogen and other elements e.g. O–H, N–H, C–H**
- **2500 – 2000 $cm^{-1}$:** **Absorption of triple bonds e.g. C≡C, C≡N**
- **2000 – 1500 $cm^{-1}$:** **Absorption of double bonds e.g. C=C, C=O**
- **1500 – 400 $cm^{-1}$:** **This region often consists of many different, complicated bands, called the fingerprint region. It is rarely used for identification of particular functional groups.**

# The four primary regions of the IR spectrum

Bonds to H | Triple bonds | Double bonds | Single Bonds



**O-H**
**N-H**
**C-H**

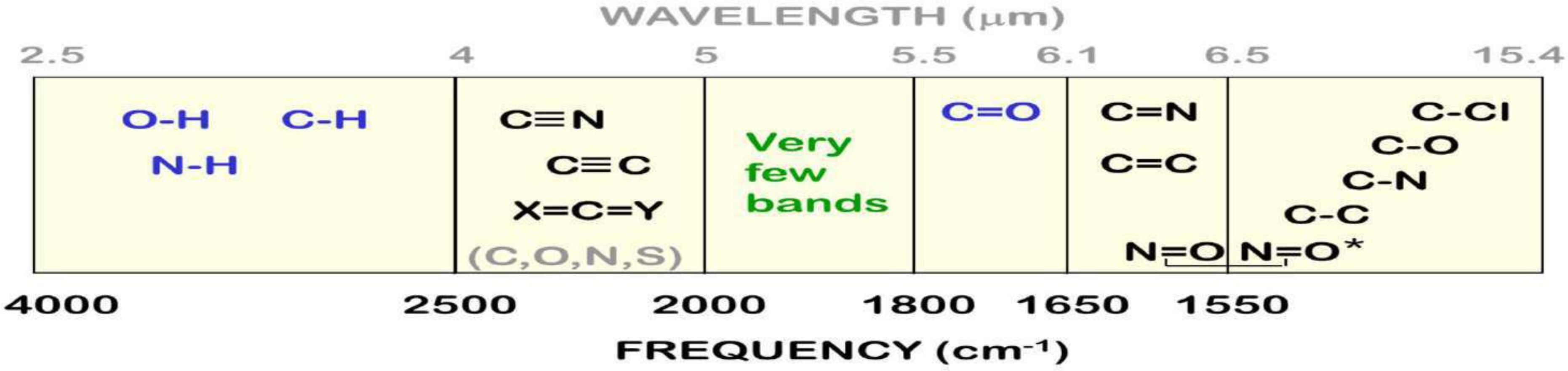
**C≡C**
**C≡N**

**C=O**
**C=N**
**C=C**

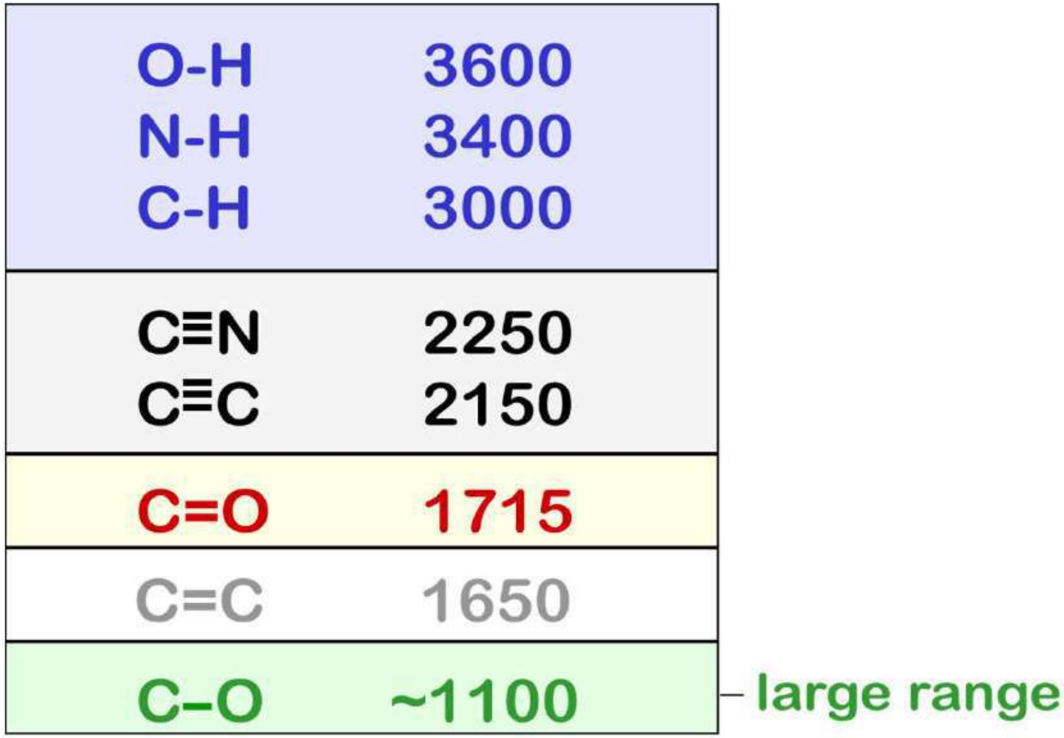
**Fingerprint Region**

**C-C**
**C-N**
**C-O**

4000 $cm^{-1}$ | 2700 $cm^{-1}$ | 2000 $cm^{-1}$ | 1600 $cm^{-1}$ | 600 $cm^{-1}$



# Base Values
# (+/-10 $cm^{-1}$)

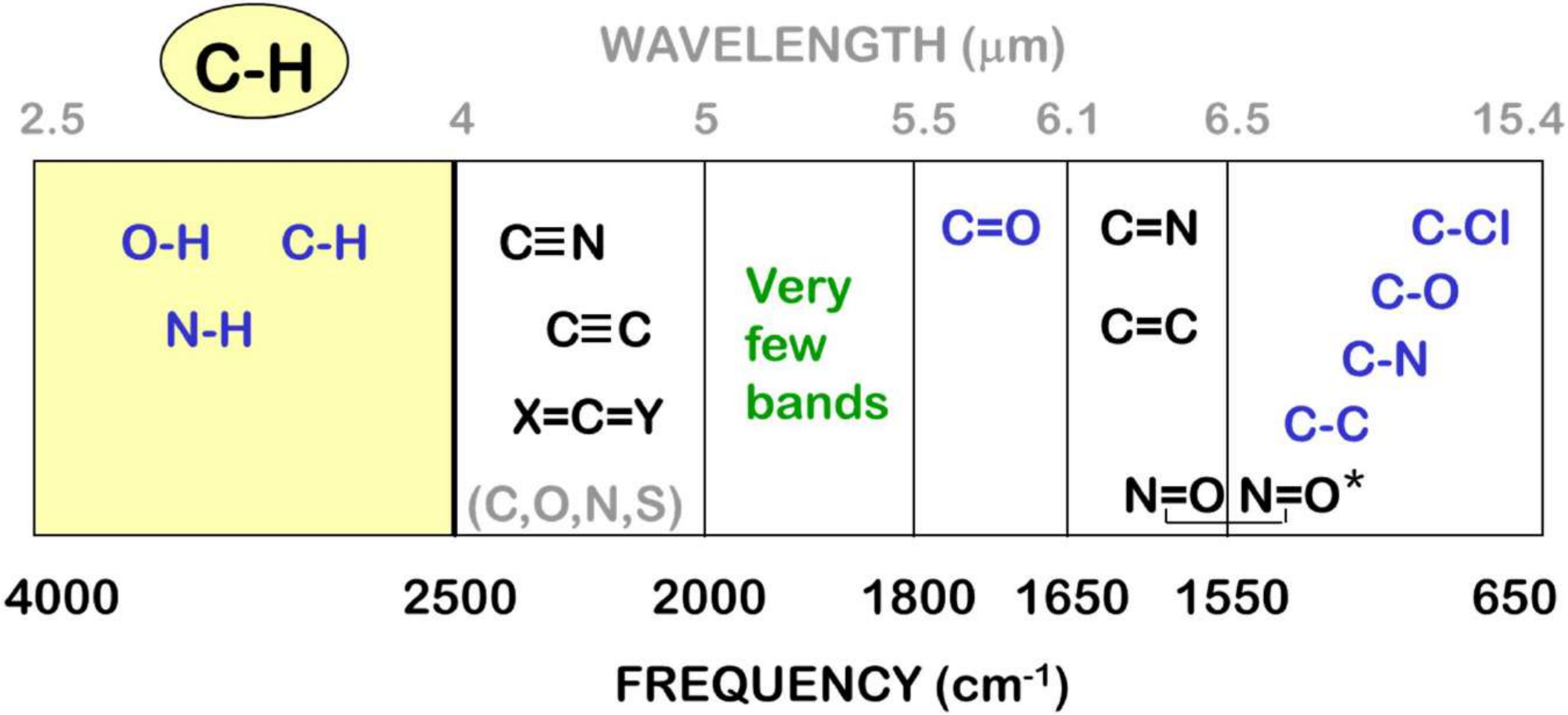


| | |
|---|---|
| O-H | 3600 |
| N-H | 3400 |
| C-H | 3000 |
| C≡N | 2250 |
| C≡C | 2150 |
| C=O | 1715 |
| C=C | 1650 |
| C–O | ~1100 |

large range

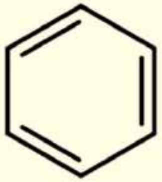
# The C-H Stretching Region

## Base Value = 3000 $cm^{-1}$



increasing frequency (cm$^{-1}$)

3300 3100 3000 2900



≡C-H =C-H -C-H

sp-1s $sp^2$-1s $sp^3$-1s

2850 2750

-CH=O
(weak)

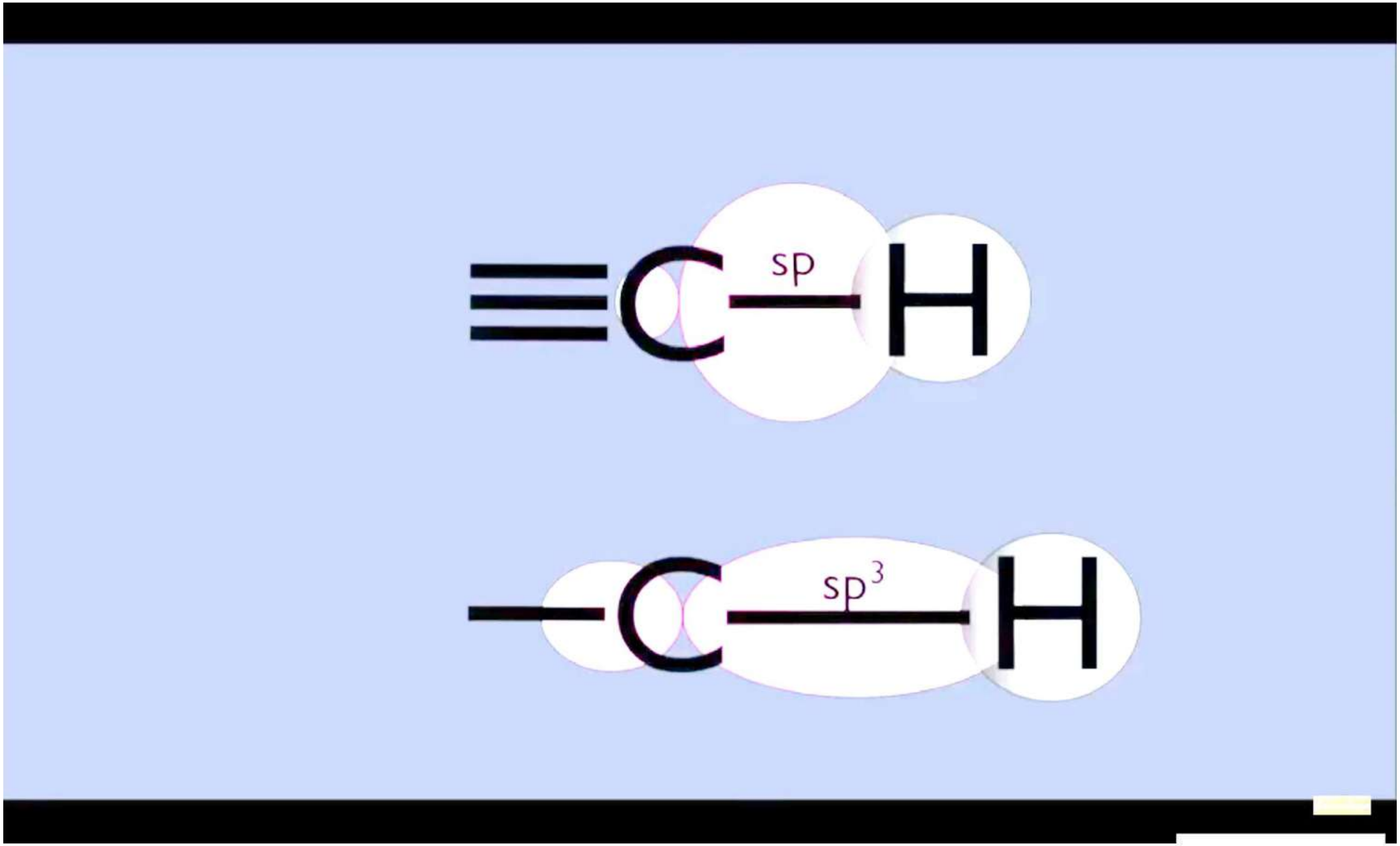
aldehyde

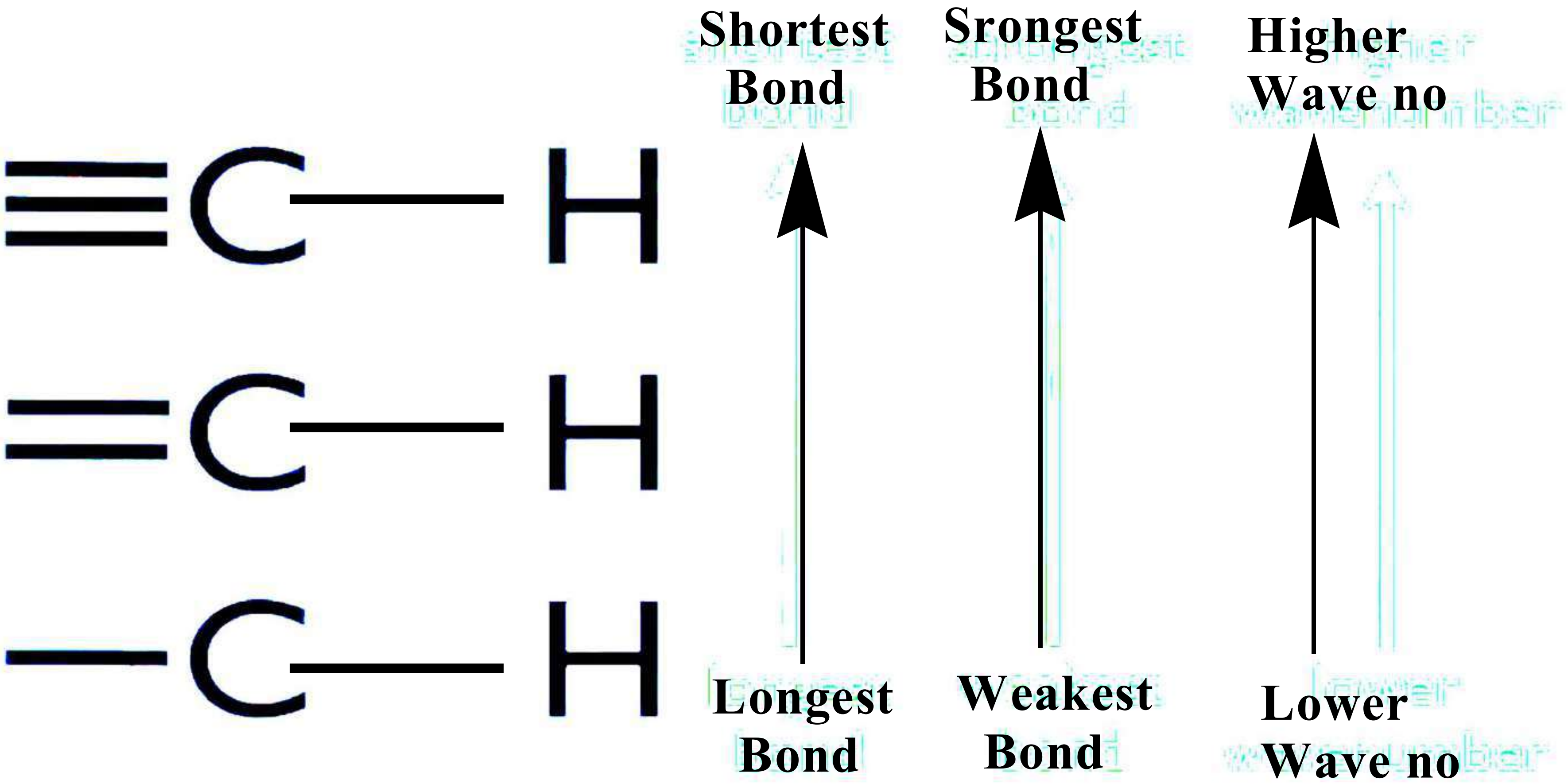
increasing s character in bond

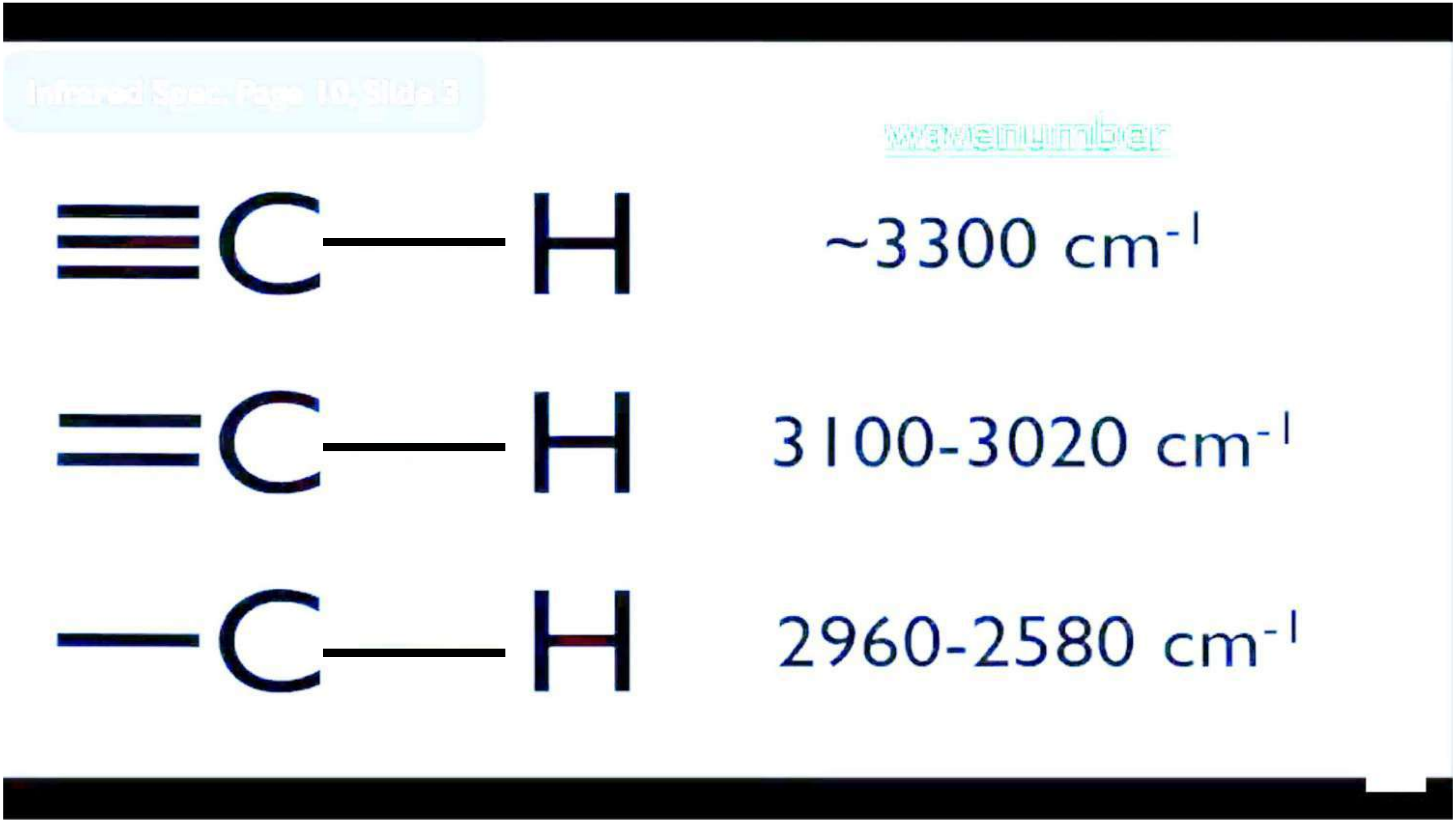
increasing CH Bond Strength

# C-H STRETCH

# Hybridization and S-character affect bond length; consequently the bond strength



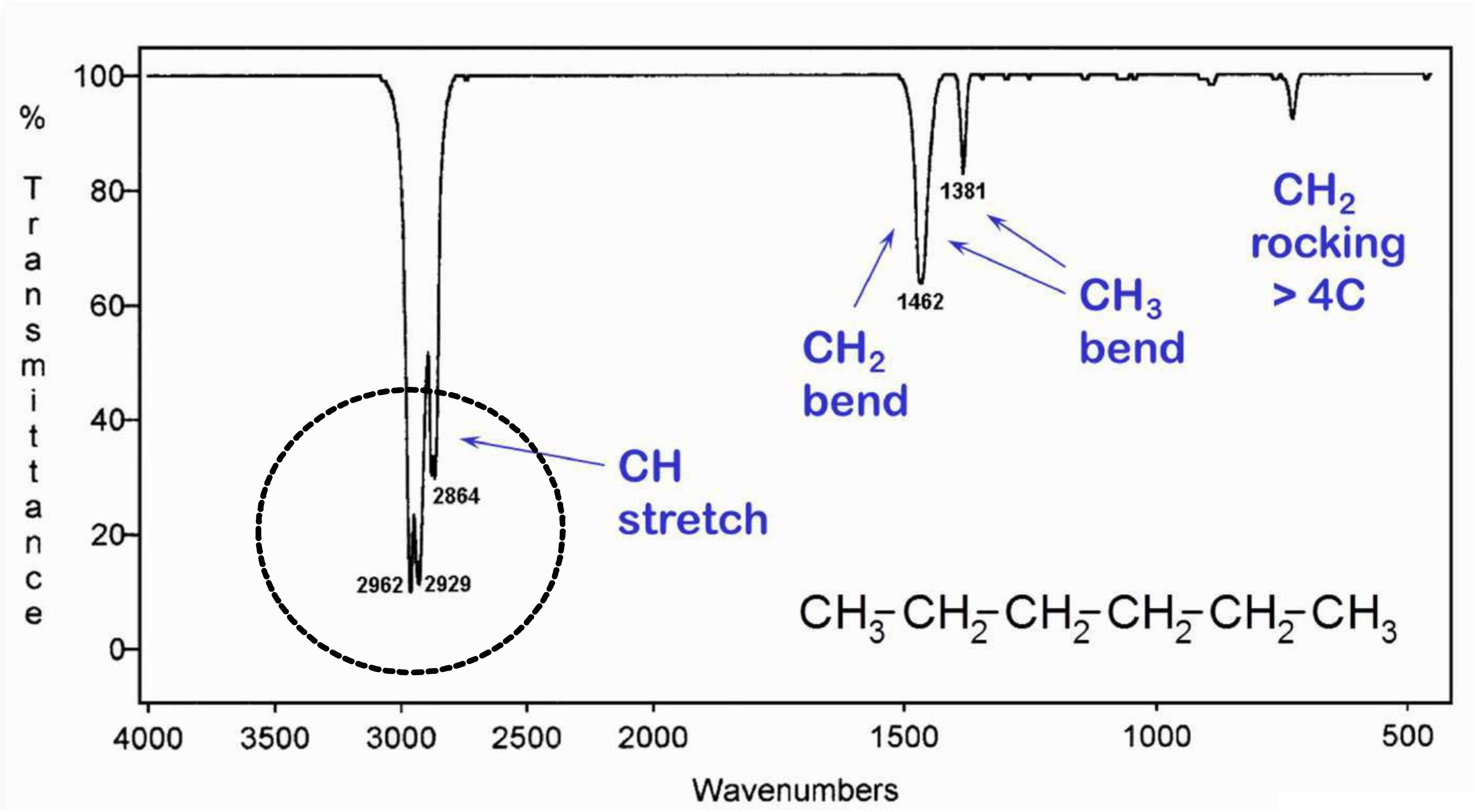

Shortest
Bond
Srongest
Bond
Higher
Wave no
Longest
Bond
Weakest
Bond
Lower
Wave no



| | wavenumber |
|---|---|
| $\equiv C-H$ | ~3300 cm$^{-1}$ |
| $=C-H$ | 3100-3020 cm$^{-1}$ |
| $-C-H$ | 2960-2580 cm$^{-1}$ |

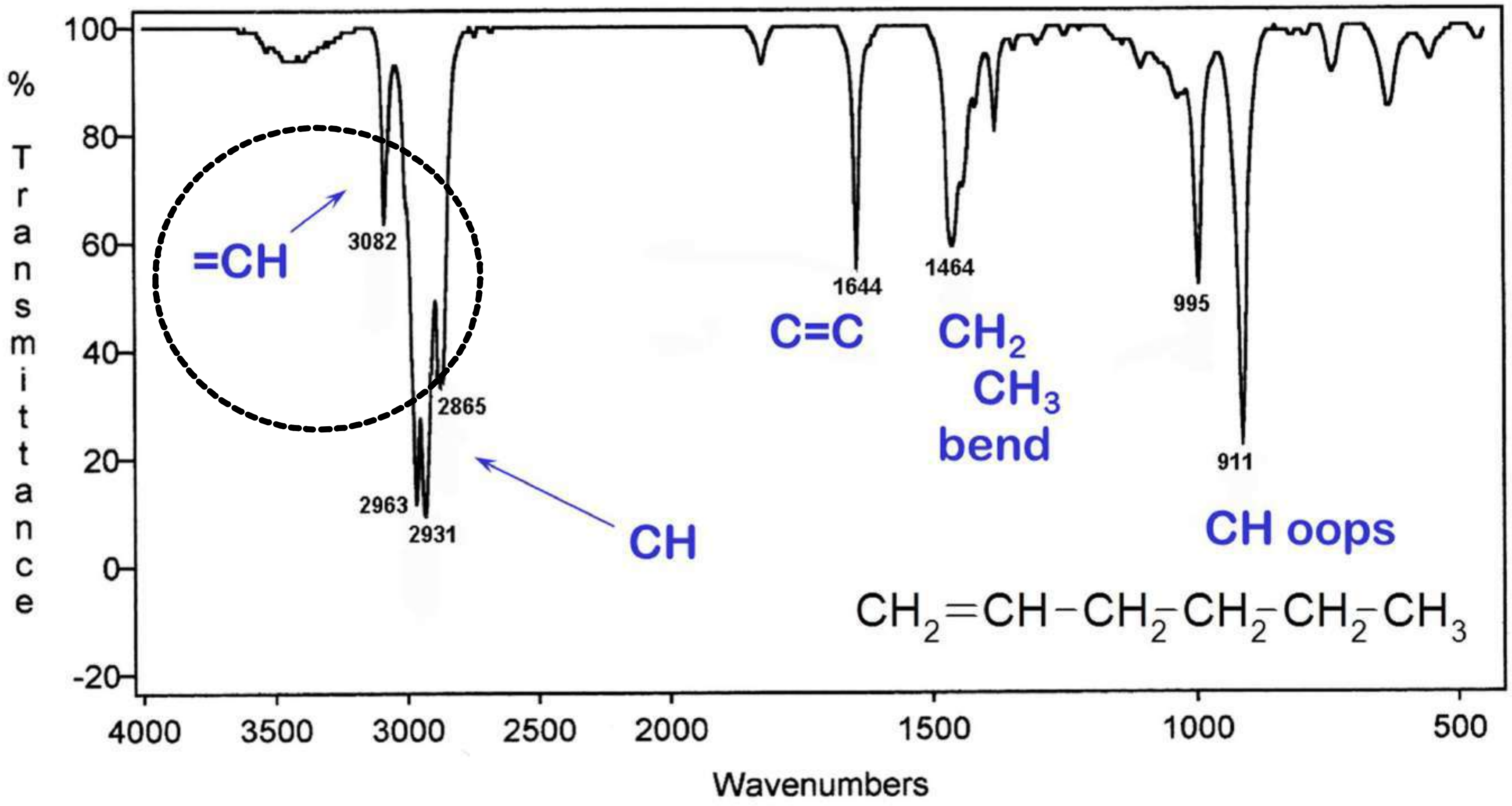
# Alkane

## Hexane



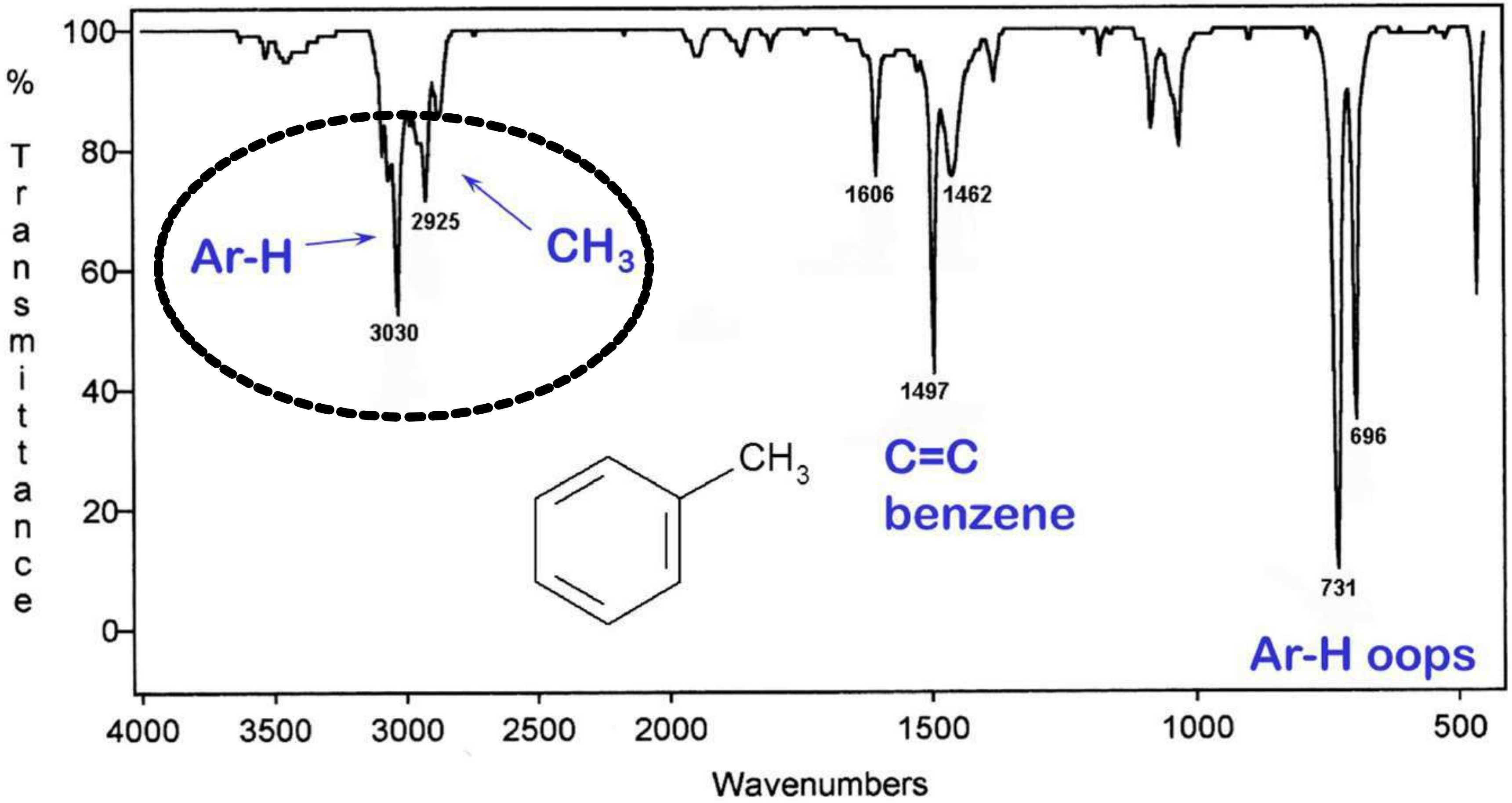
# Alkene

## 1-Hexene



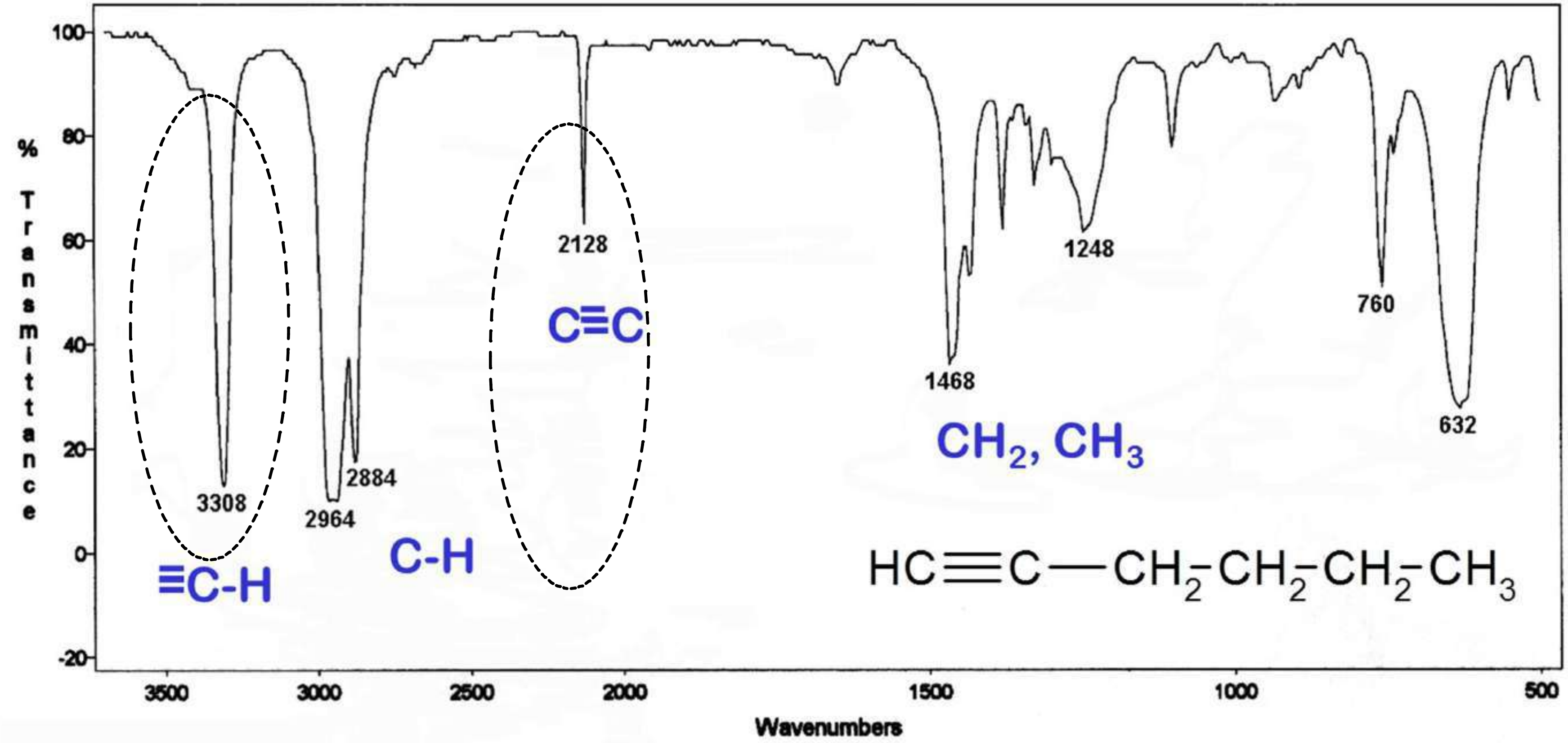
# Aromatic

## Toluene



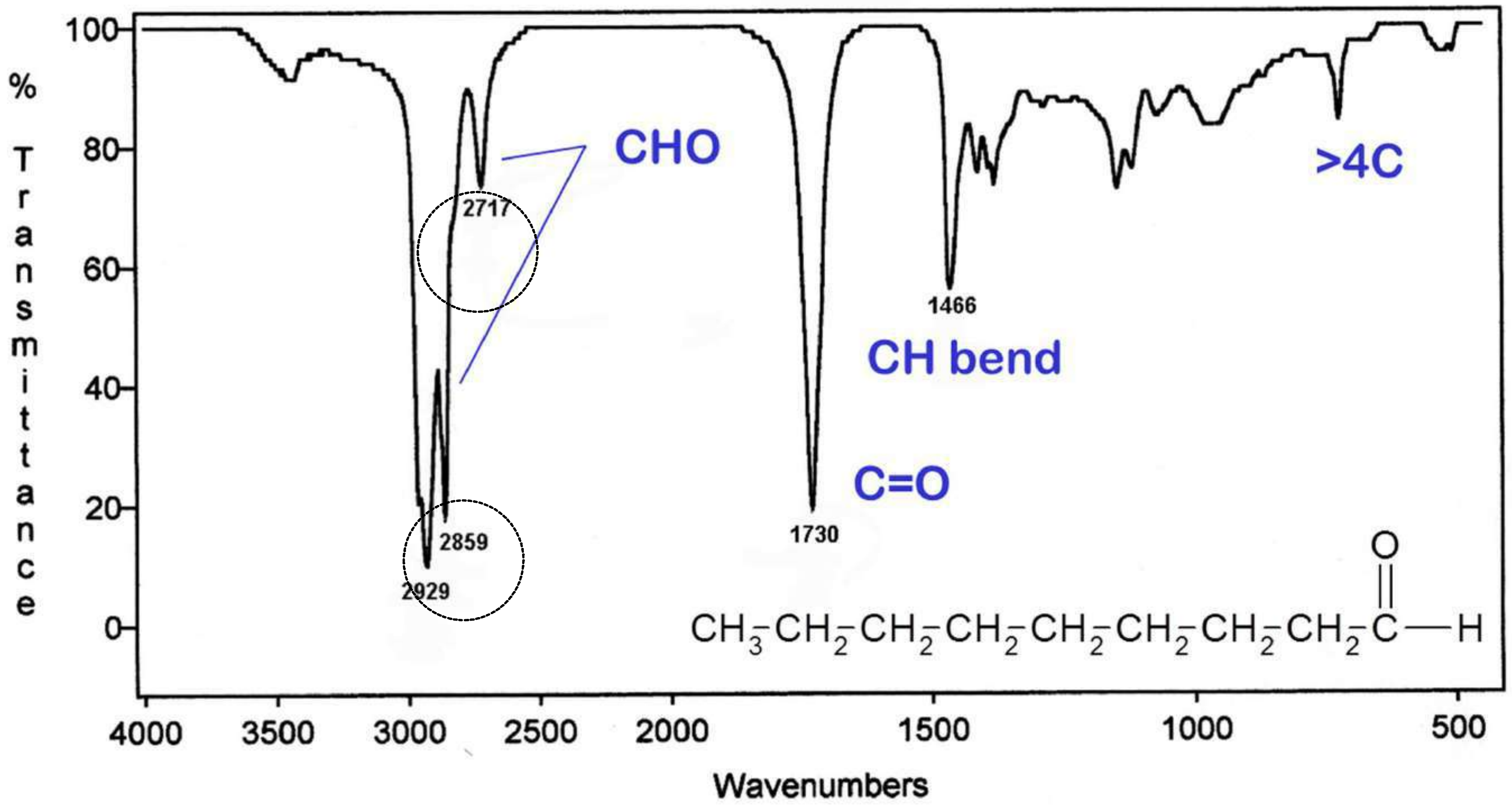
# Alkyne

## 1-Hexyne



# Aldehyde

## Nonanal



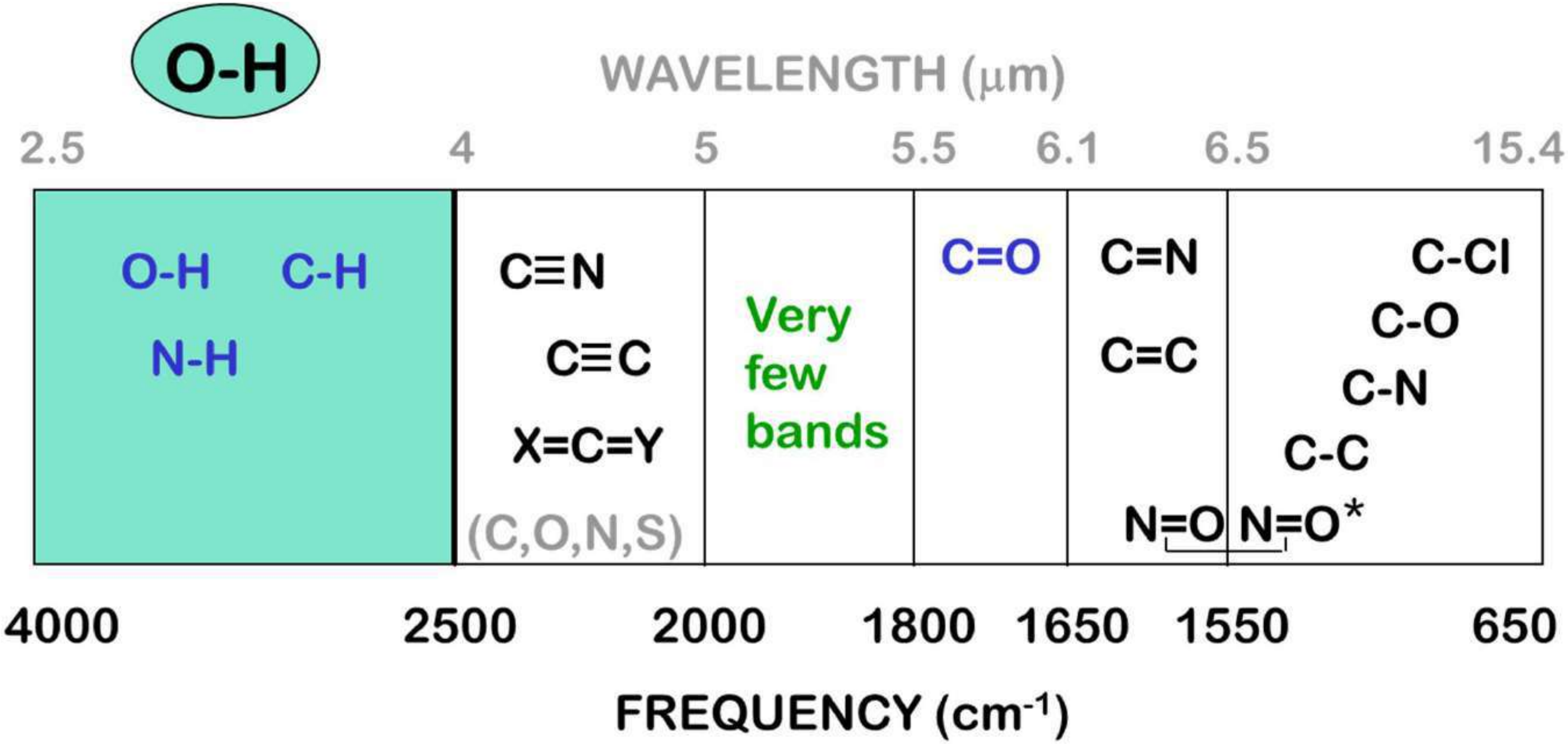
# Infrared Spectroscopy

## Absorption regions

## O–H

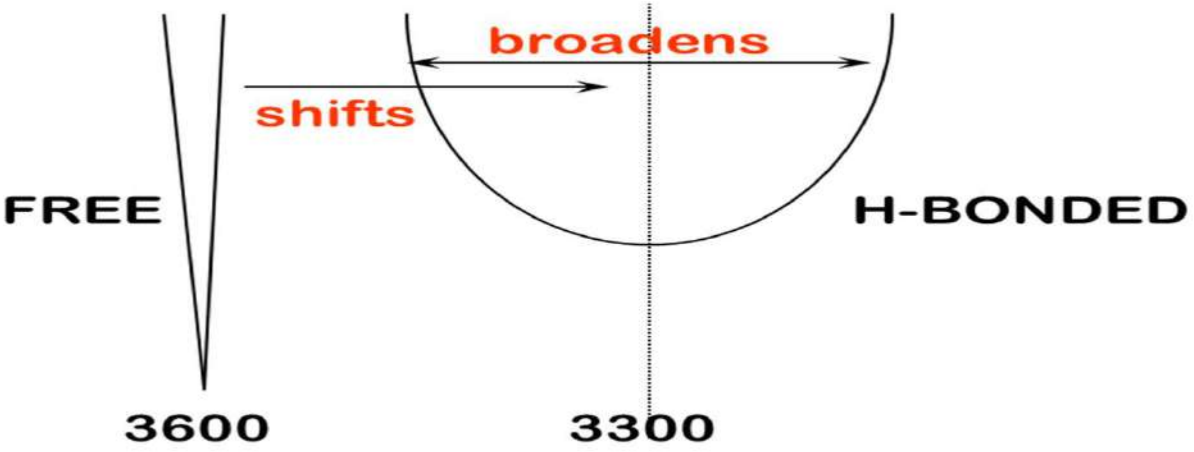
## (2a & 2b)

# The O-H Stretching Region

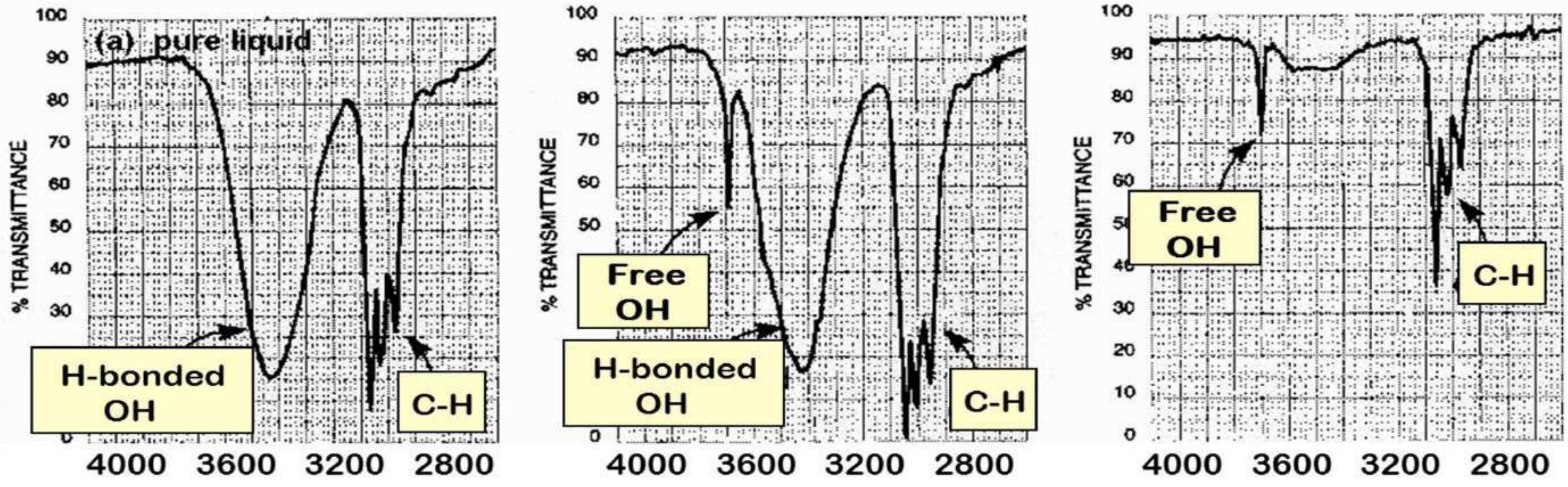


- **O-H** 3600 cm$^{-1}$ (alcohol, free)
- **O-H** 3300 cm$^{-1}$ (alcohols & acids, H-bonding)

# Effect of Hydrogen-Bonding on O-H Stretching



## 1-Butanol

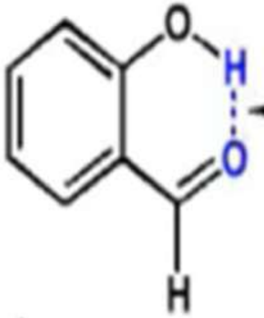


(a) Pure Liquid

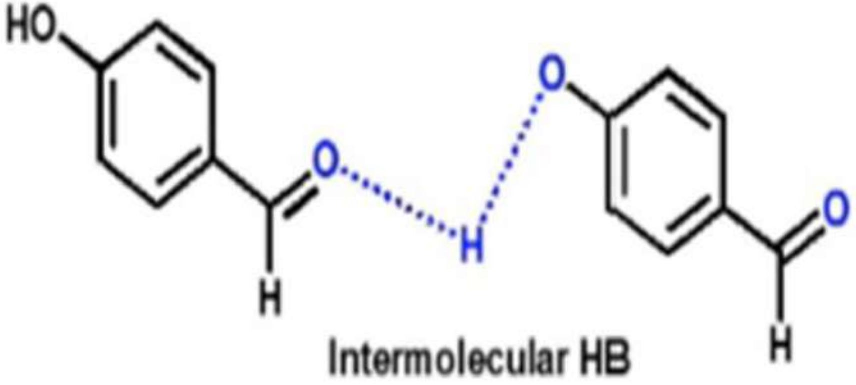
(b) Dilute Solution

(c) Very Dilute Solution

- Hydrogen bonding brings about <u>remarkable downward frequency shifts</u>.
- Stronger the hydrogen bonding, greater is the absorption shift towards lower wave length than the normal value! Why??
- There is 2 types of hydrogen bonding
  - a) intermolecular →broad bands
  - b) intramolecular → sharp bands



Intramolecular HB



Intermolecular HB

- hydrogen bonding in O-H and N-H compounds deserve special attention.

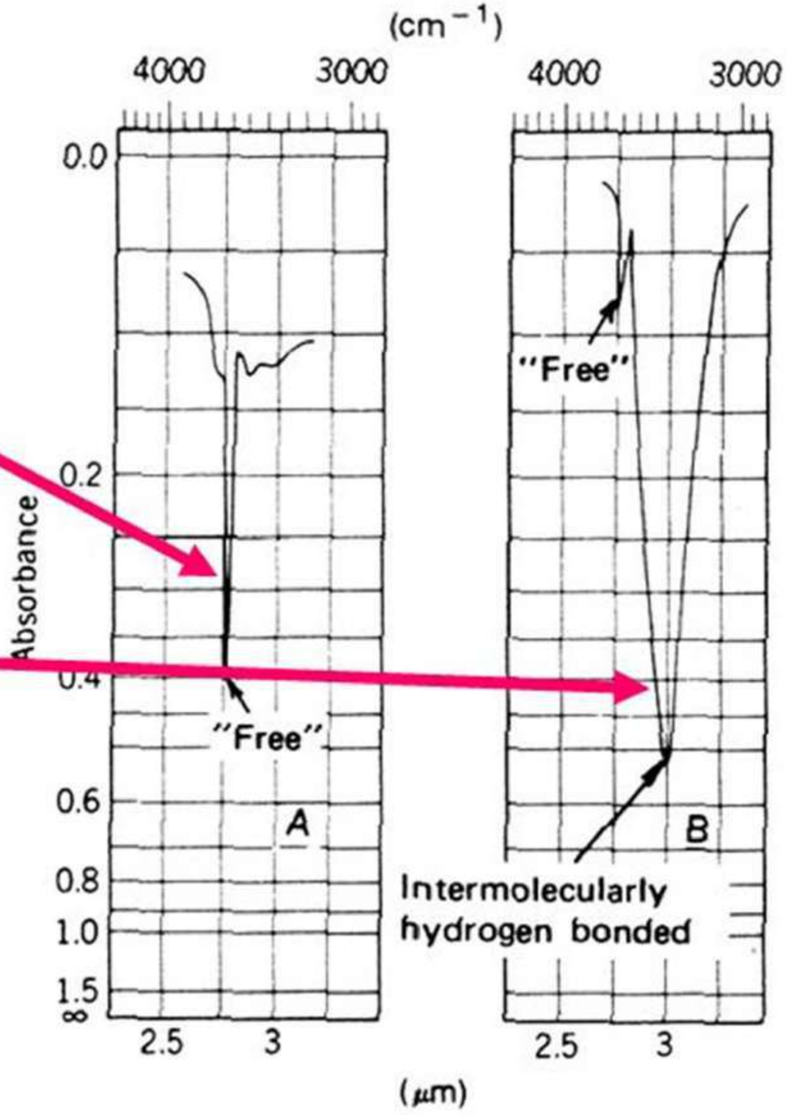
- Eg: alcohols&phenols .......enols & chelates

# IR of Alcohols

O-H non-hydrogen bonded
or free OH 3650-3584
(sharp bands in gas phase)

Intermolecular H-Bonding
in solution increase with
concentration gives bands
at 3550-3200 (broader)

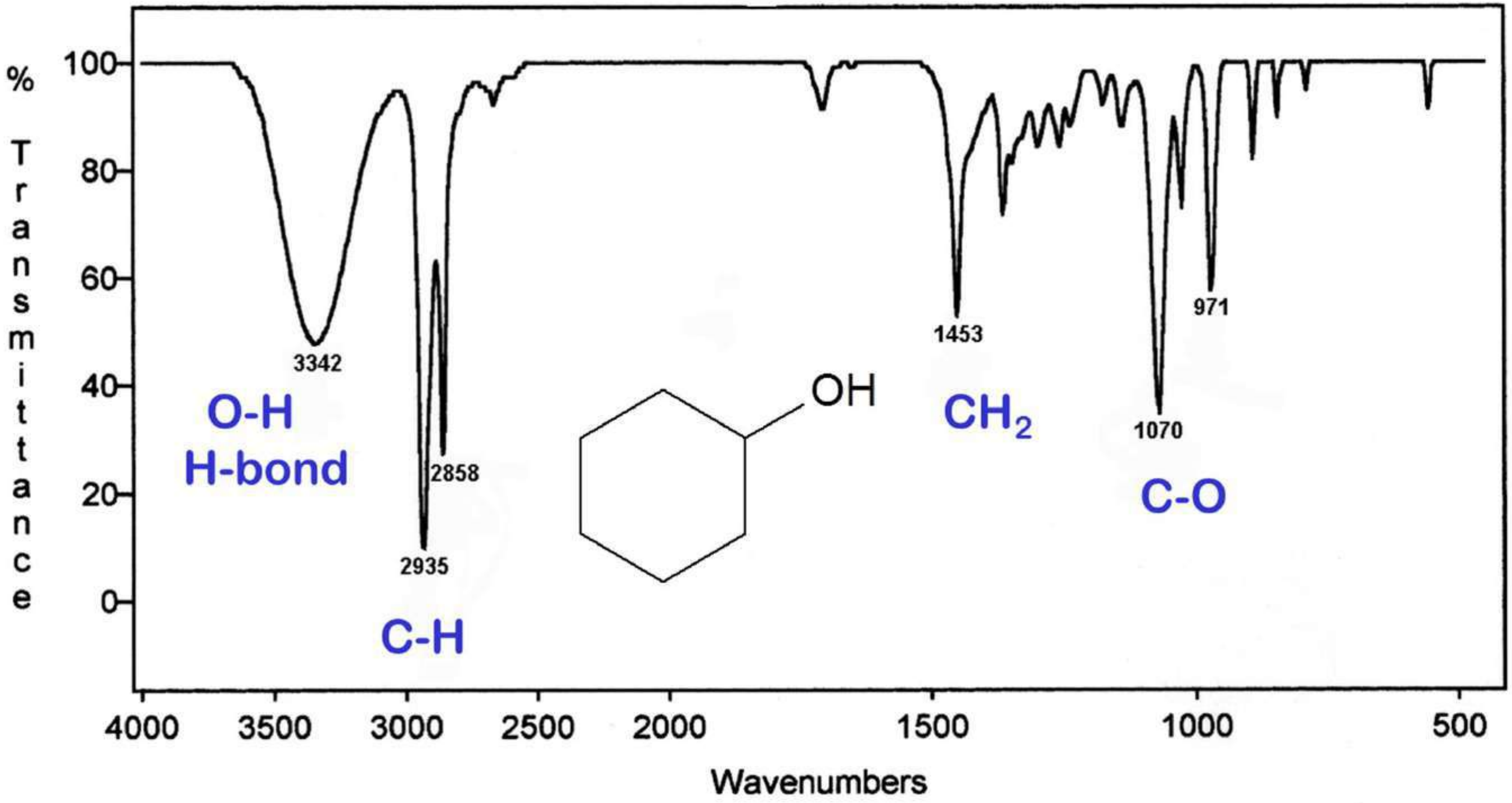
cyclohexylcarbinol



# Alcohol

## Cyclohexanol

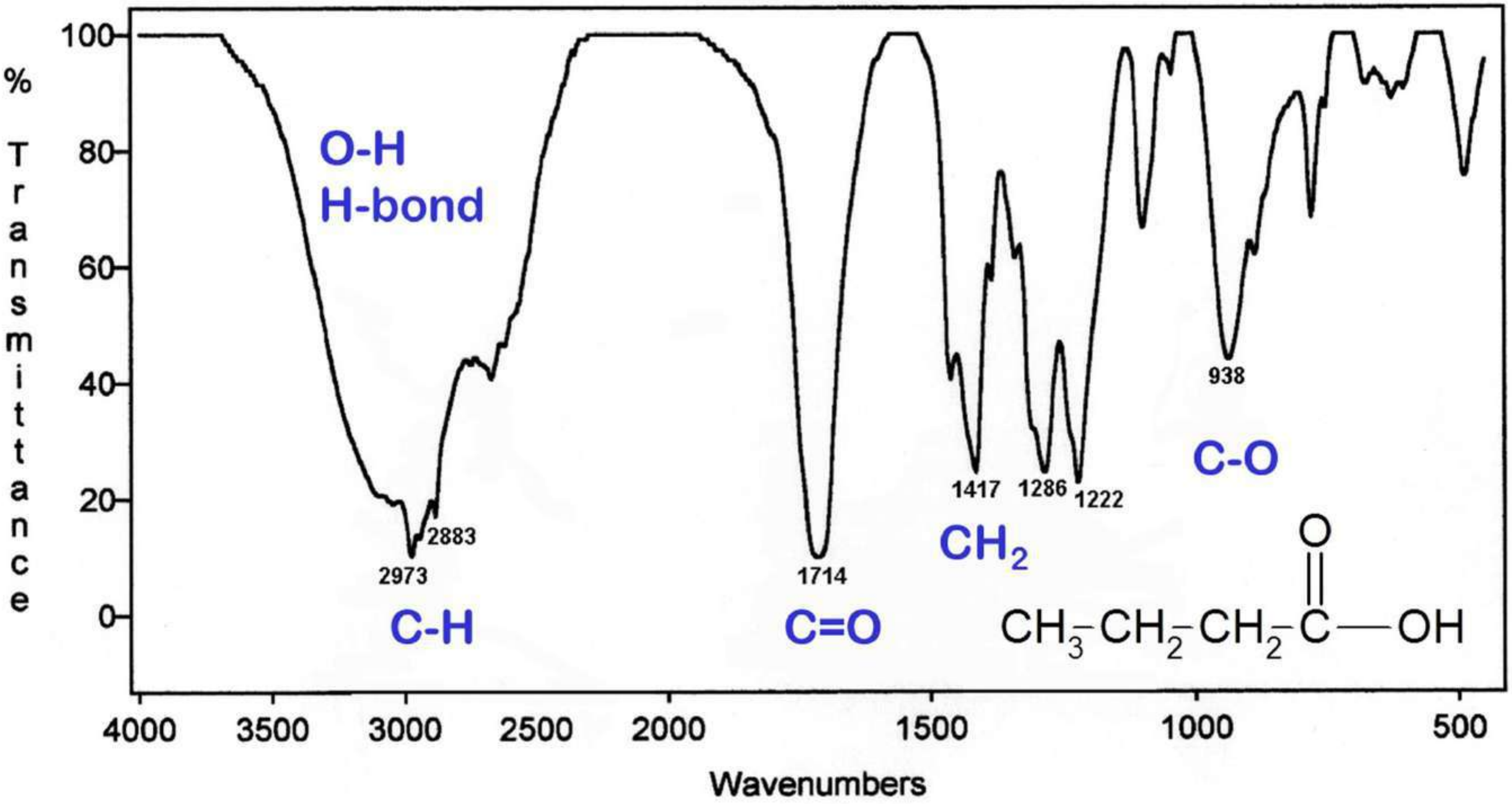
pure solution

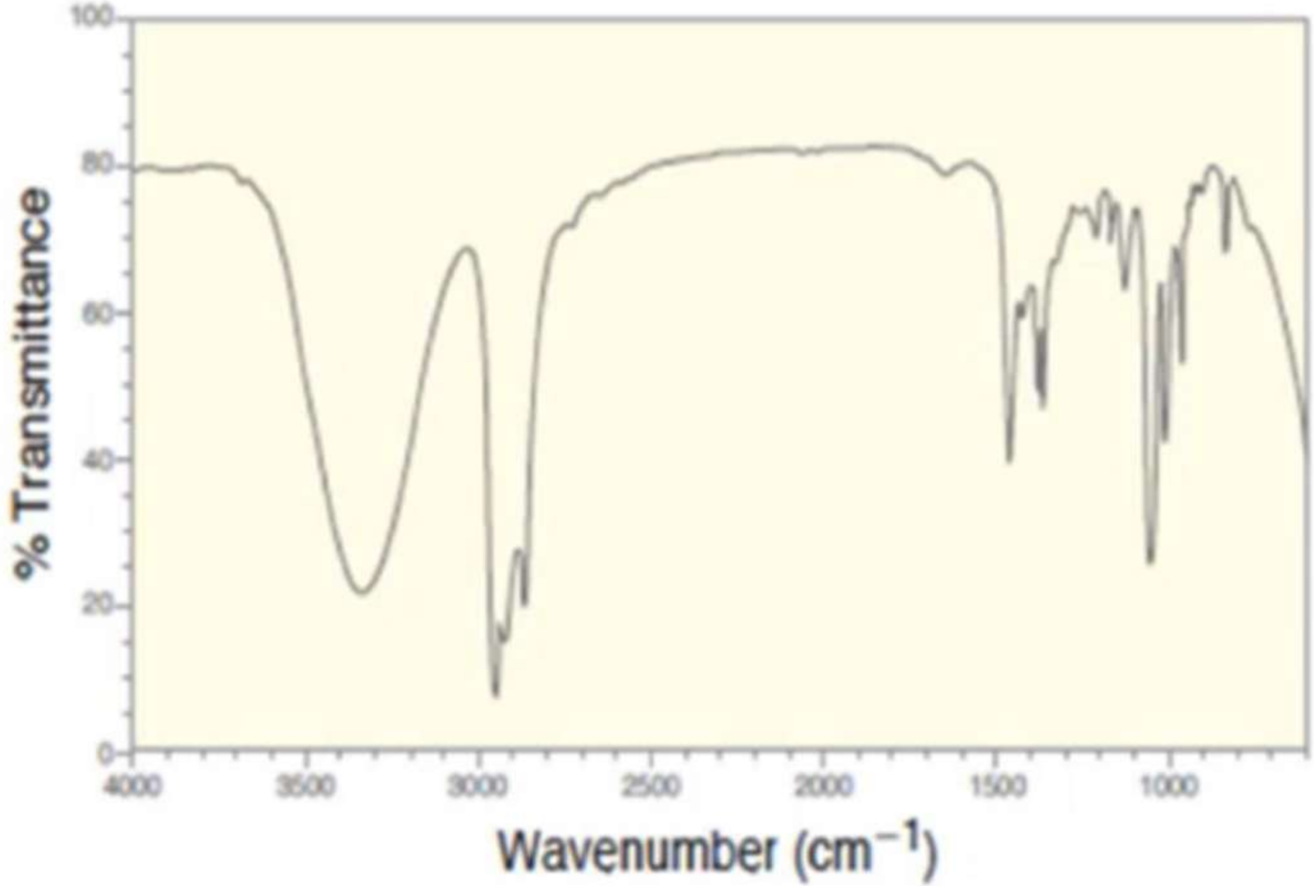


# Carboxylic acid

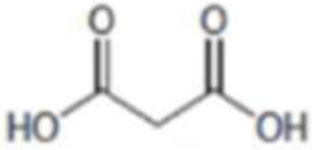
## Butanoic Acid

pure solution

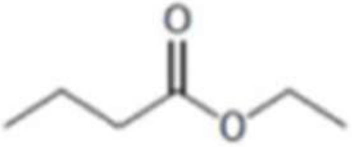



% Transmittance
100
80
60
40
20
0
4000
3500
3000
2500
2000
1500
1000
Wavenumber (cm$^{-1}$)


OH


O
O
HO
OH


NH$_2$

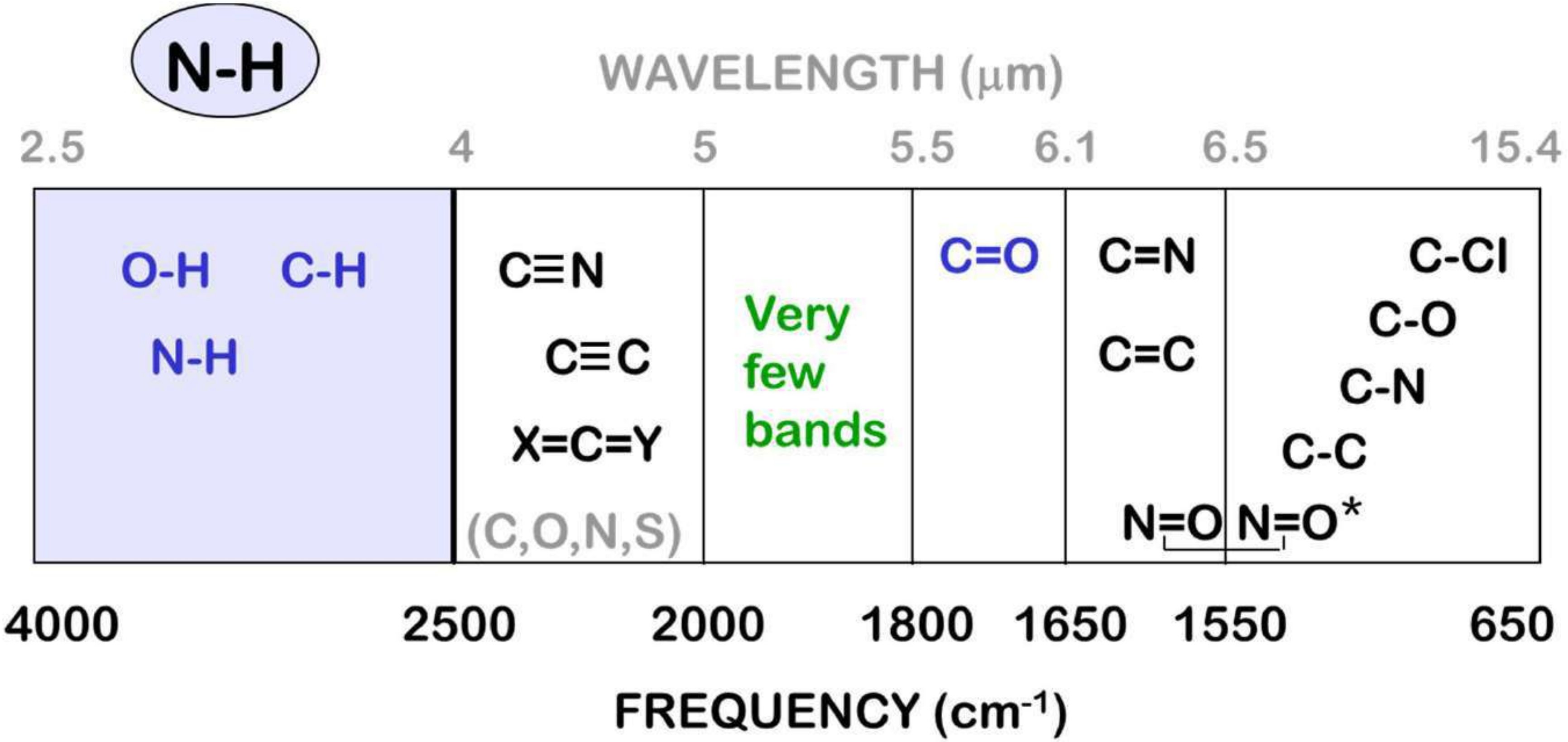

O
O

# Infrared Spectroscopy

## Absorption regions

## (3)

# The N-H Stretching Region



- N-H 3300 - 3400 cm$^{-1}$

- Primary amines give <u>two</u> peaks
- Secondary amines give <u>one</u> peak
- Tertiary amines give <u>no peak</u>

# Primary amine

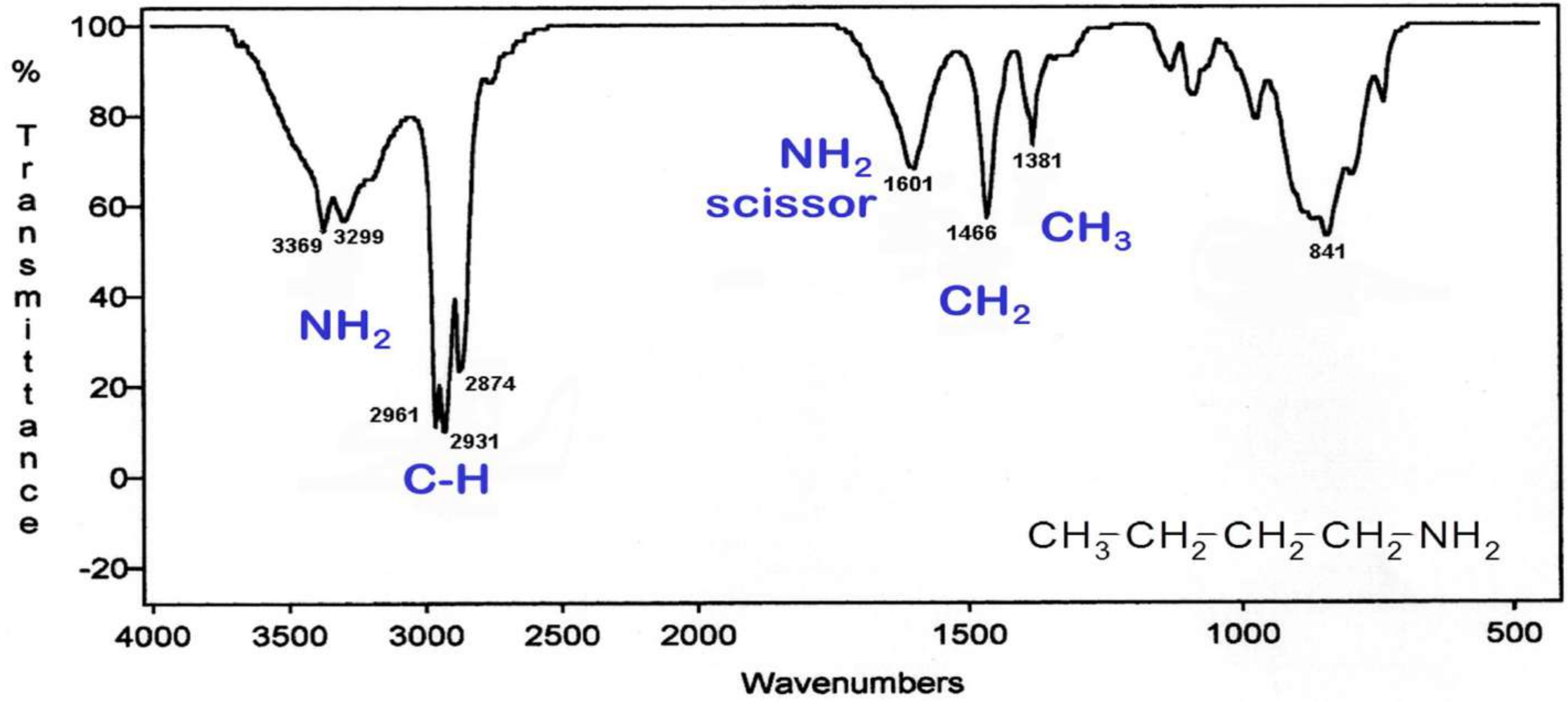
## 1-Butanamine

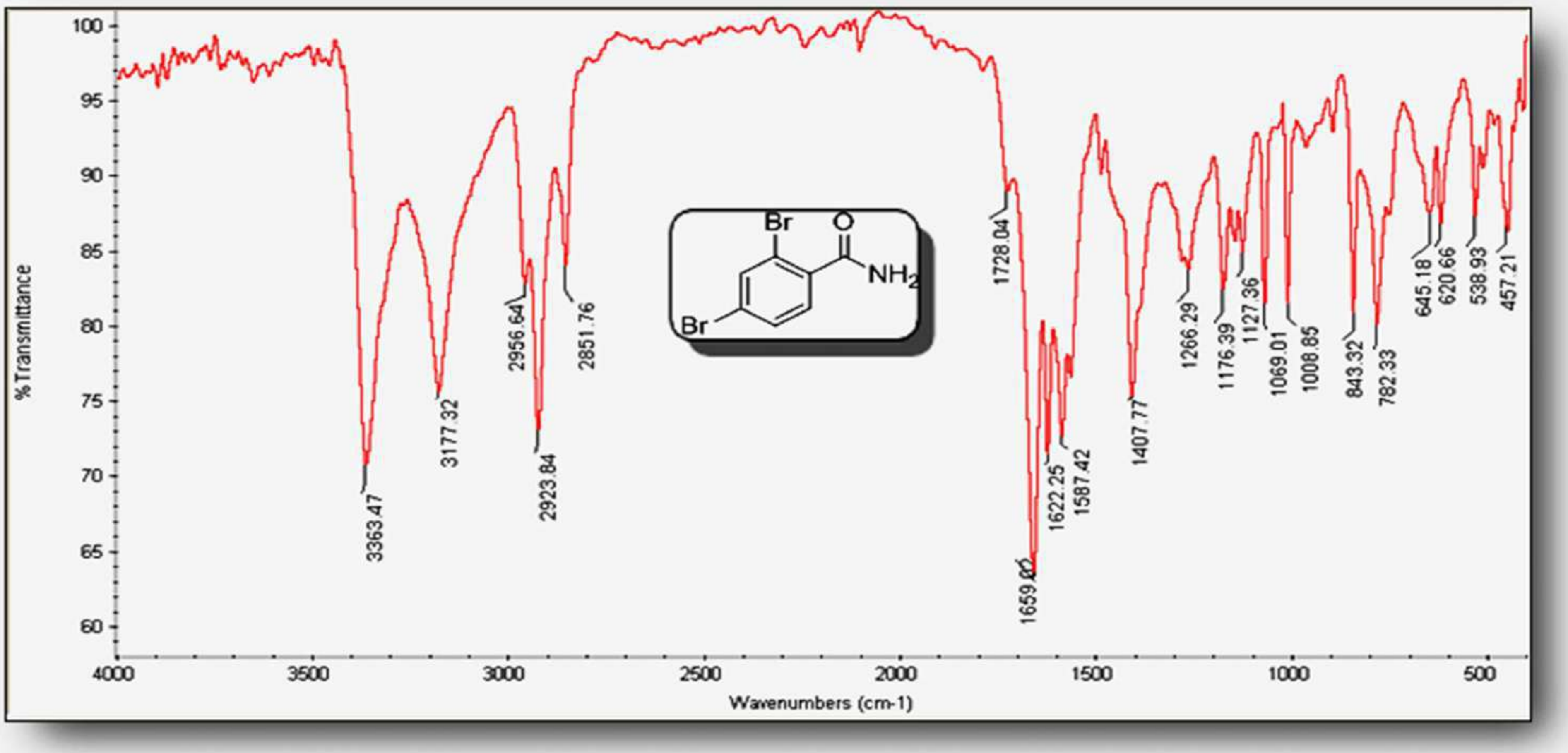
## The N-H stretching region

N-H 3300 - 3400 $cm^{-1}$

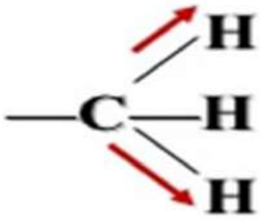
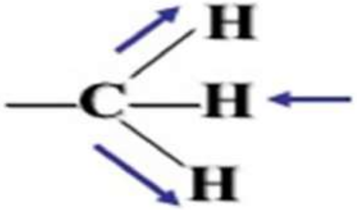
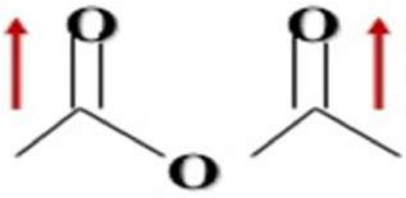
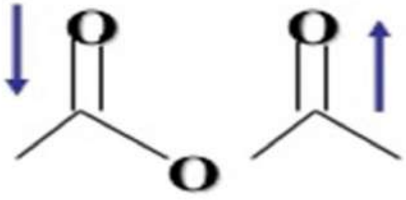
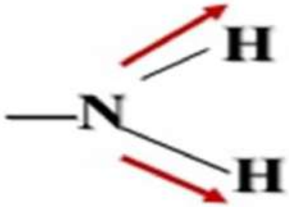
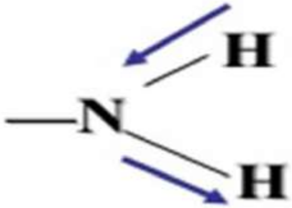
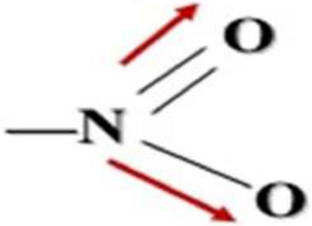
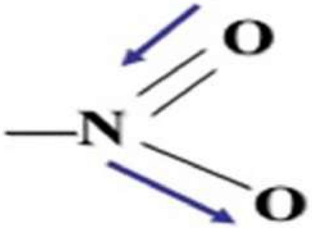
- ☐ **Primary amines give <u>two</u> peaks**

- ☐ **Secondary amines give <u>one</u> peak**
- ☐ **Tertiary amines give <u>no peak</u>**



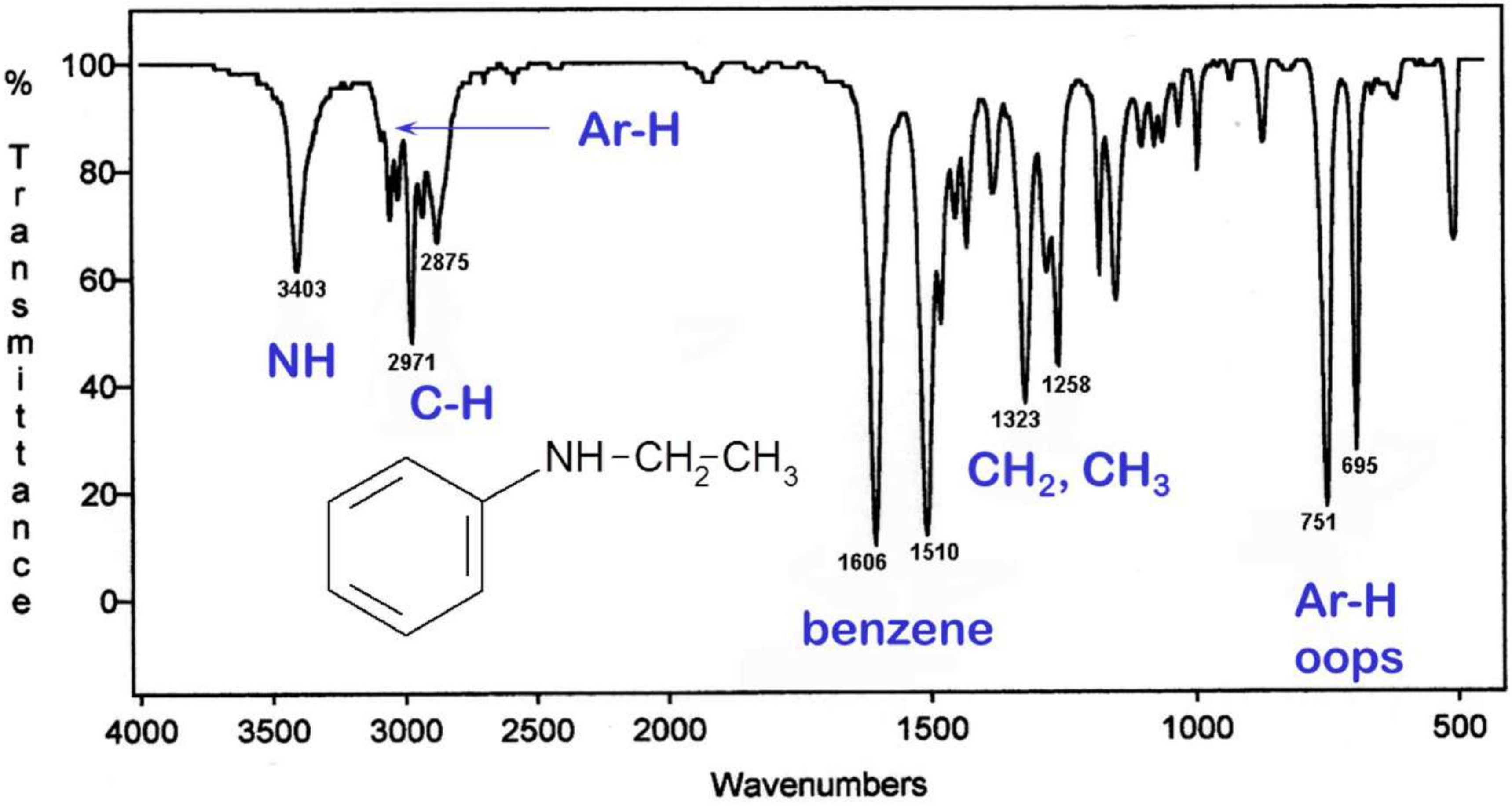

%Transmittance
100
95
90
85
80
75
70
65
60
4000
3500
3000
2500
2000
1500
1000
500
Wavenumbers (cm-1)
3363.47
3177.32
2956.64
2923.84
2851.76
1728.04
1659.02
1622.25
1587.42
1407.77
1266.29
1176.39
1127.36
1069.01
1008.85
843.32
782.33
645.18
620.66
538.93
457.21
Br
O
NH2
Br

# Symmetrical and asymmetrical stretch

| | Symmetrical Stretch | | Asymmetrical Stret | |
|---|---|---|---|---|
| **Methyl** |  | 2872 $cm^{-1}$ |  | 2962 c |
| **Anhydride** |  | 1760 $cm^{-1}$ |  | 1800 c |
| **Amino** |  | 3300 $cm^{-1}$ |  | 3400 c |
| **Nitro** |  | 1350 $cm^{-1}$ |  | 1550 c |

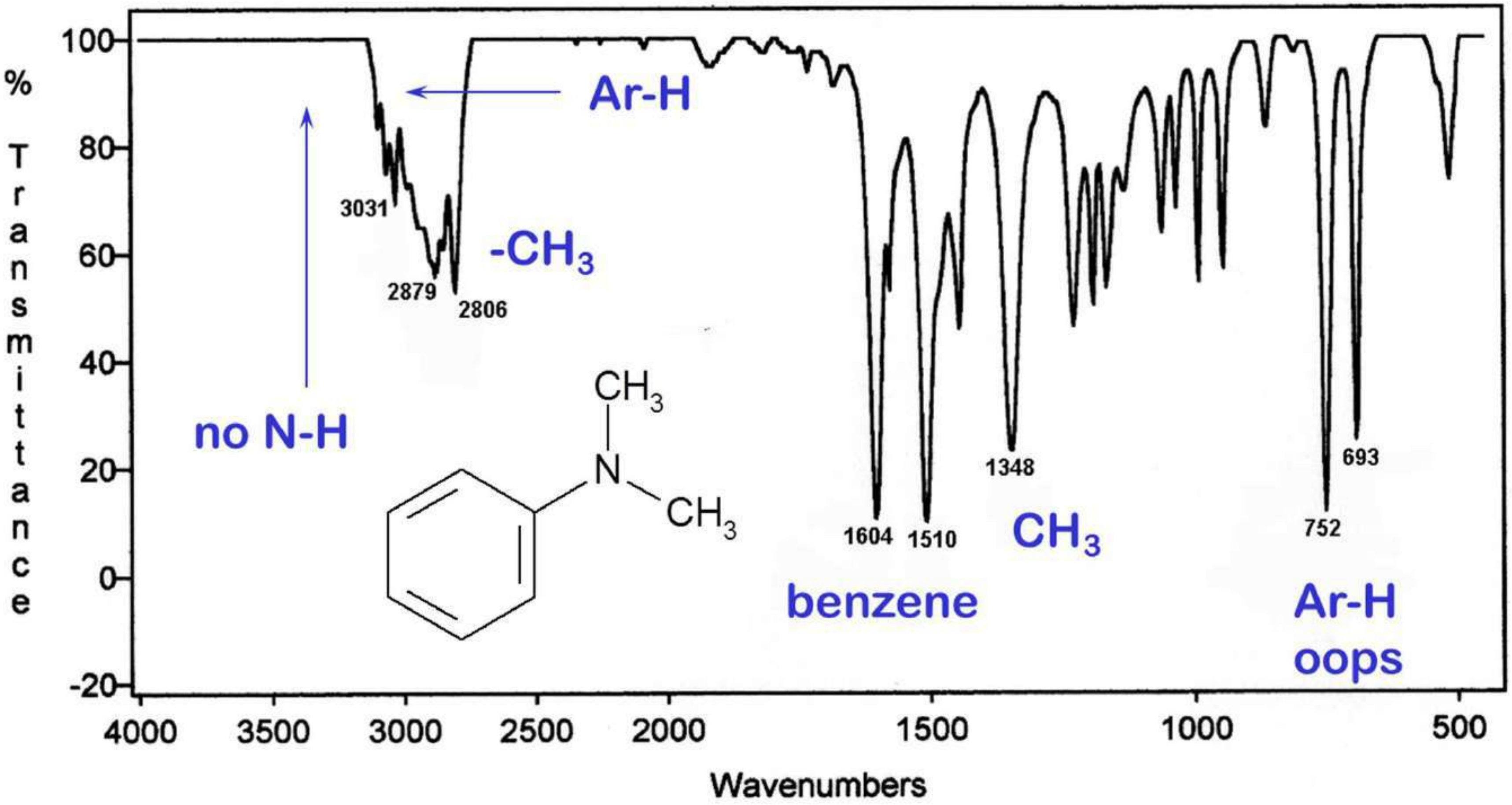
# Secondary amine

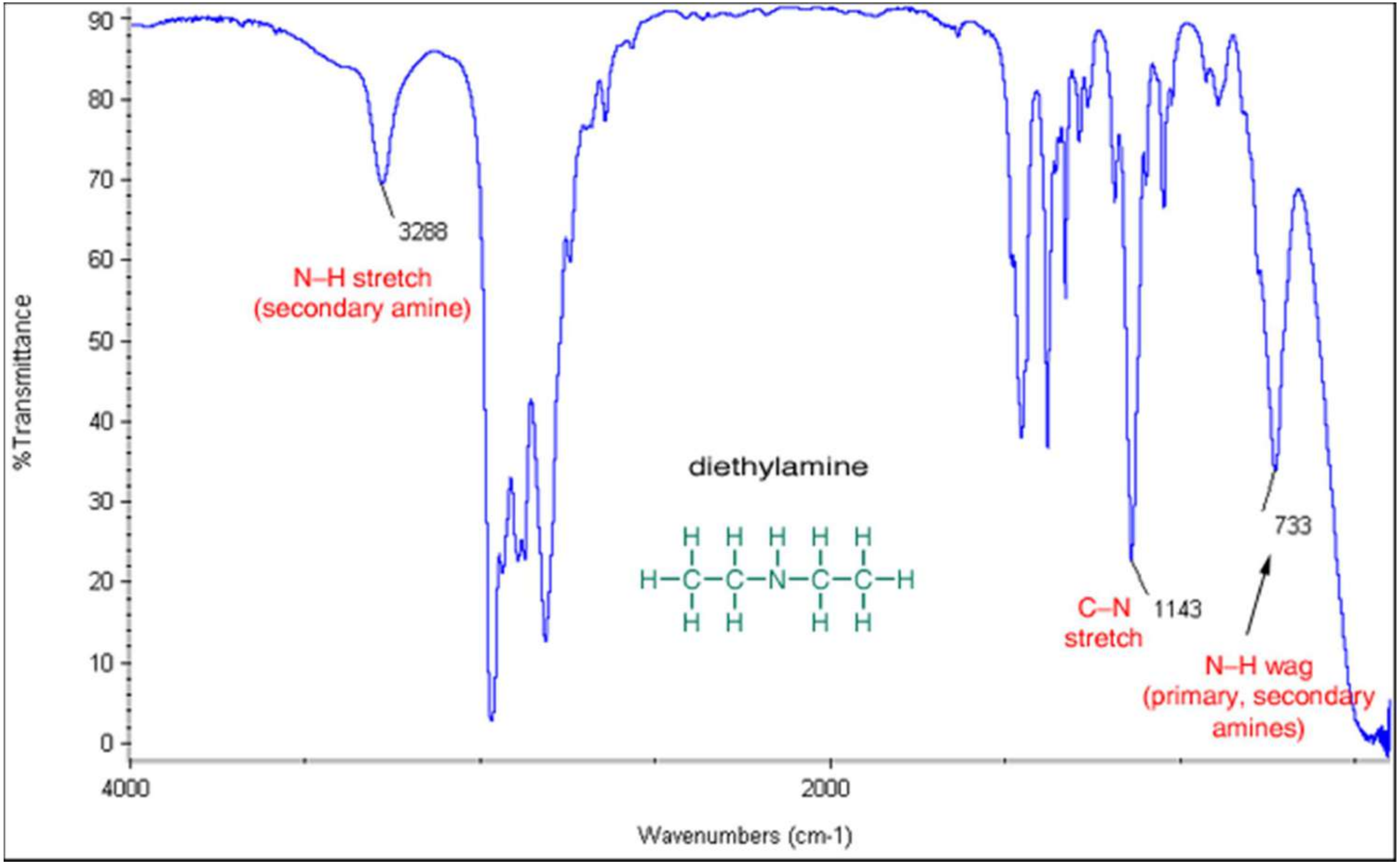
## *N*-Ethylbenzenamine



# Tertiary amine

## *N,N*-Dimethylaniline




90
80
70
60
50
40
30
20
10
0
%Transmittance
4000
2000
Wavenumbers (cm-1)
3288
N–H stretch
(secondary amine)
diethylamine
C–N
stretch
1143
733
N–H wag
(primary, secondary
amines)

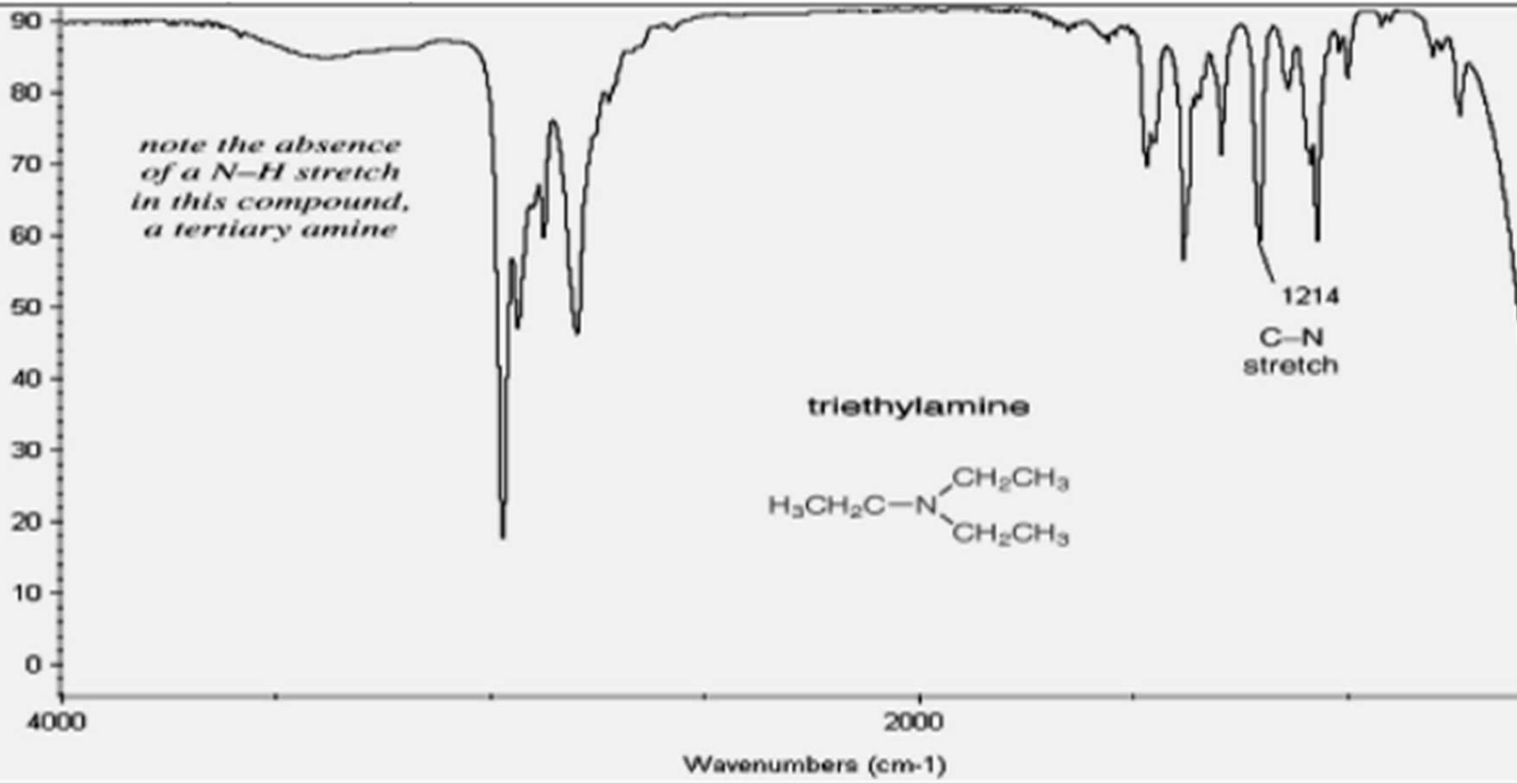


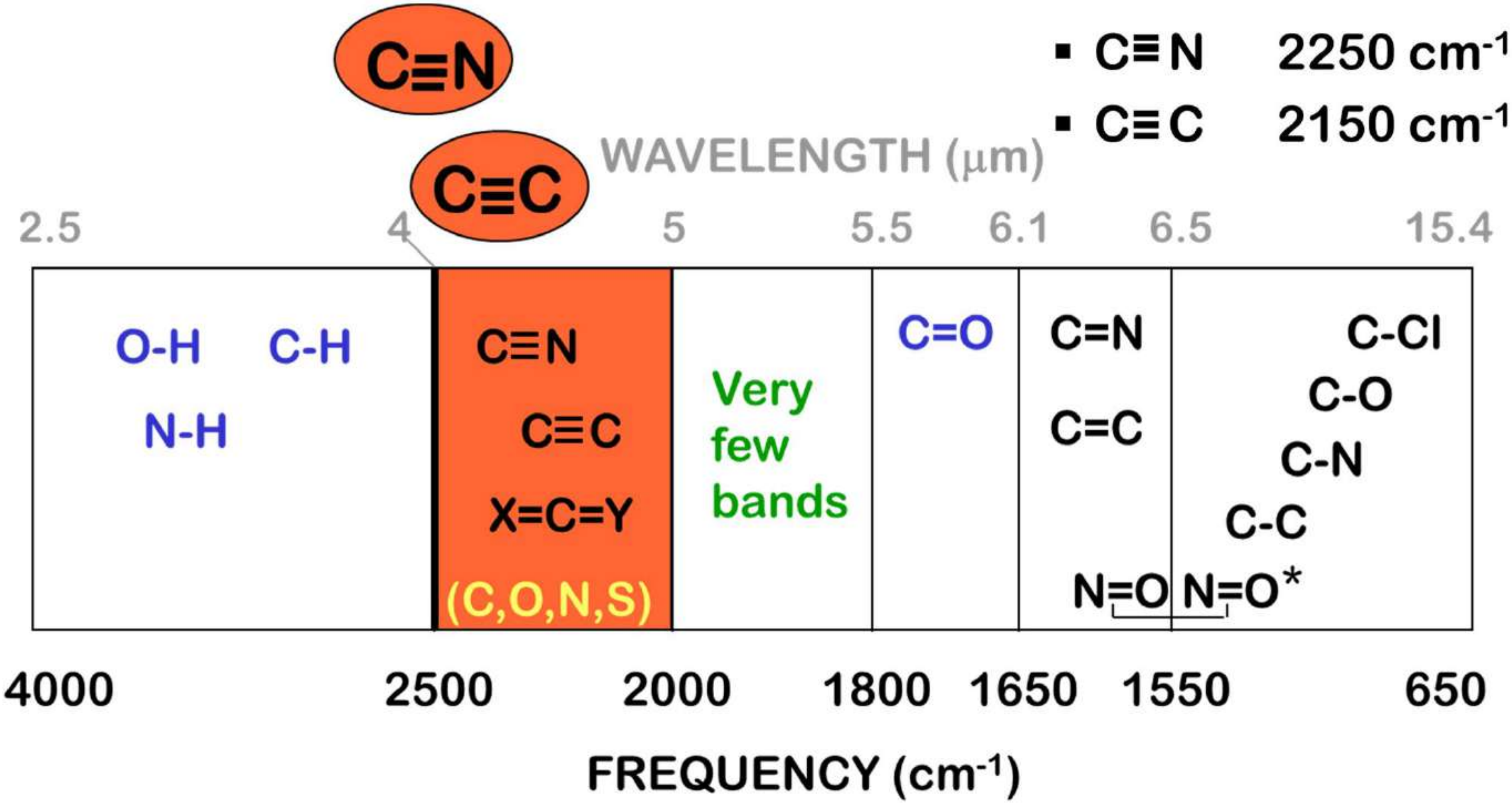
Figure 1.7 Tertiary Amine (triethylamine)

# Infrared Spectroscopy

## Part “4”

## Absorption regions

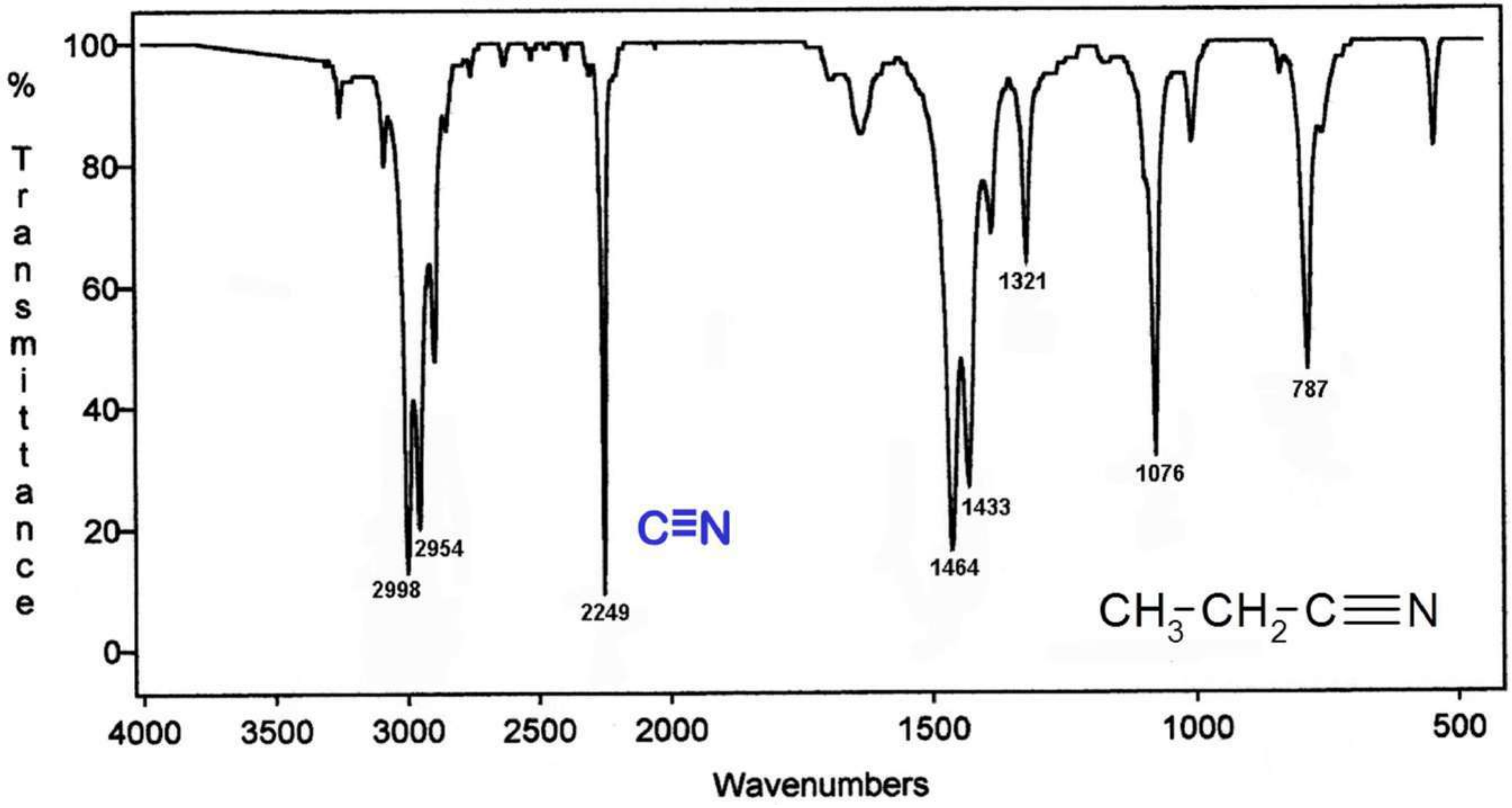
# The Triple Bond Stretching Region



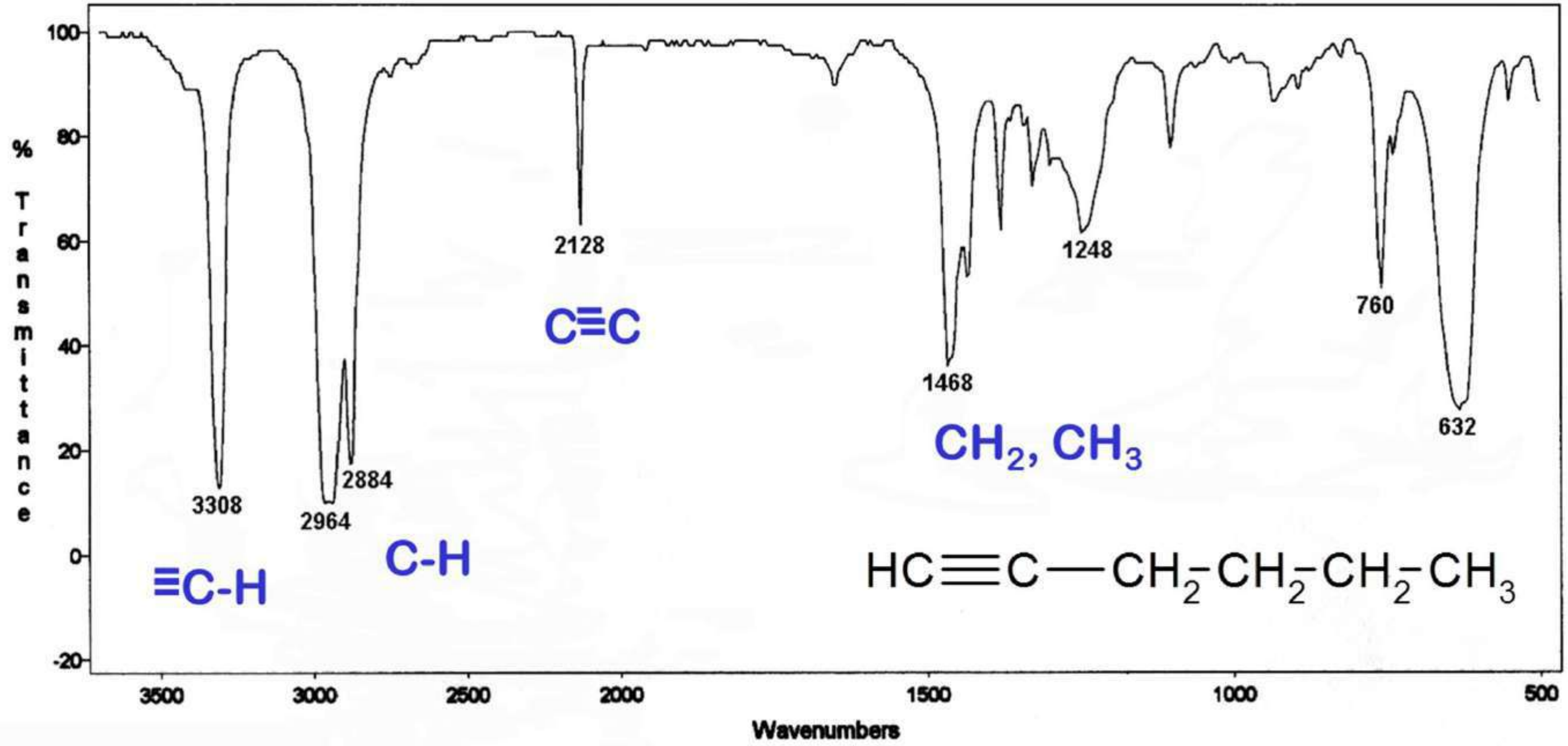
- C≡N $2250\ cm^{-1}$
- C≡C $2150\ cm^{-1}$

- The cyano group often gives a strong, sharp peak due to its large dipole moment.
- The carbon-carbon triple bond gives a sharp peak, but it is often weak due to a lack of a dipole.

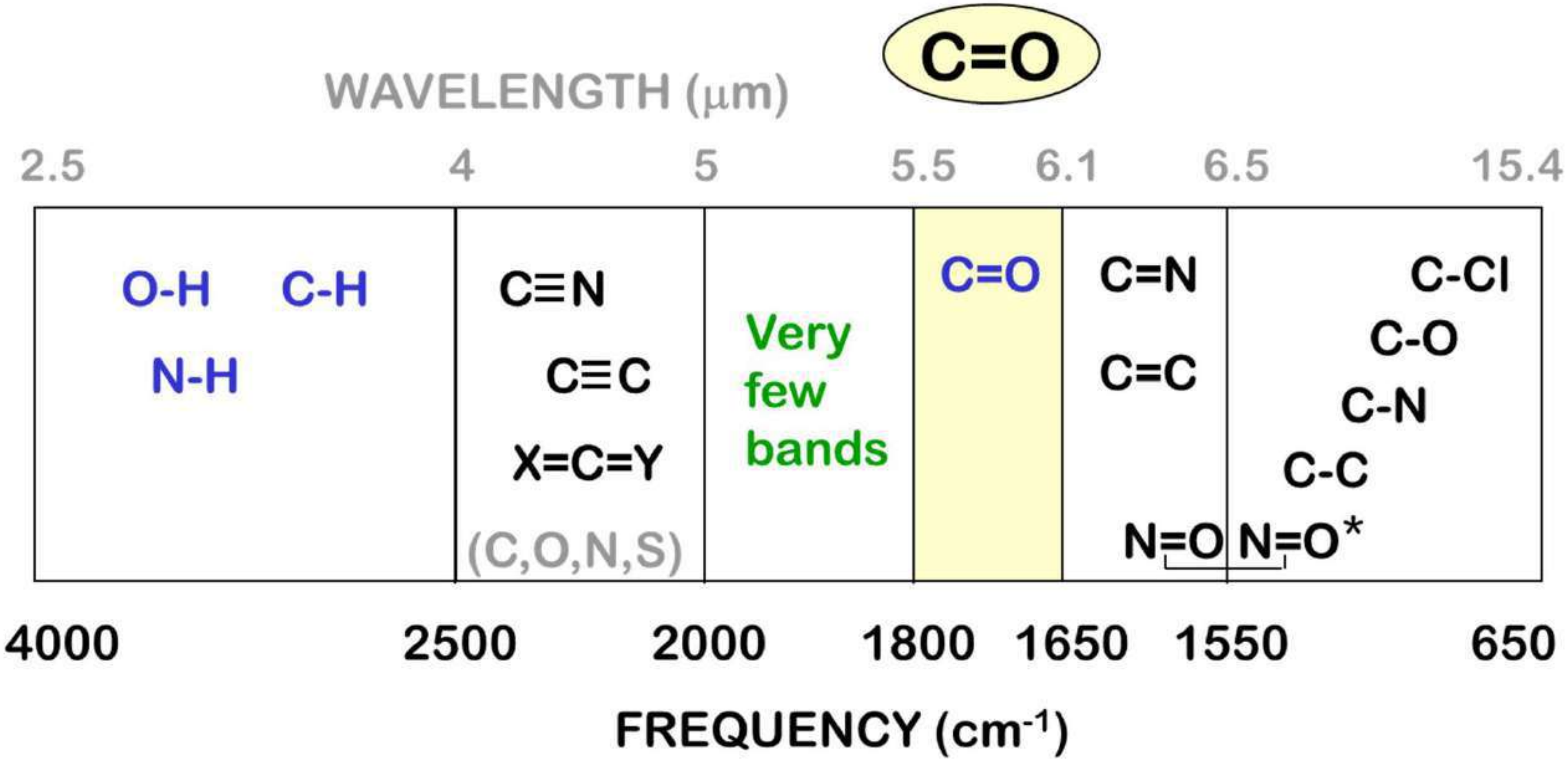
# Propanenitrile



# 1-Hexyne


% Transmittance
100
80
60
40
20
0
-20
3500
3000
2500
2000
1500
1000
500
Wavenumbers
3308
2964
2884
2128
1468
1248
760
632
≡C-H
C-H
C≡C
$CH_2$, $CH_3$
HC≡C—$CH_2$-$CH_2$-$CH_2$-$CH_3$

# The Carbonyl Stretching Region

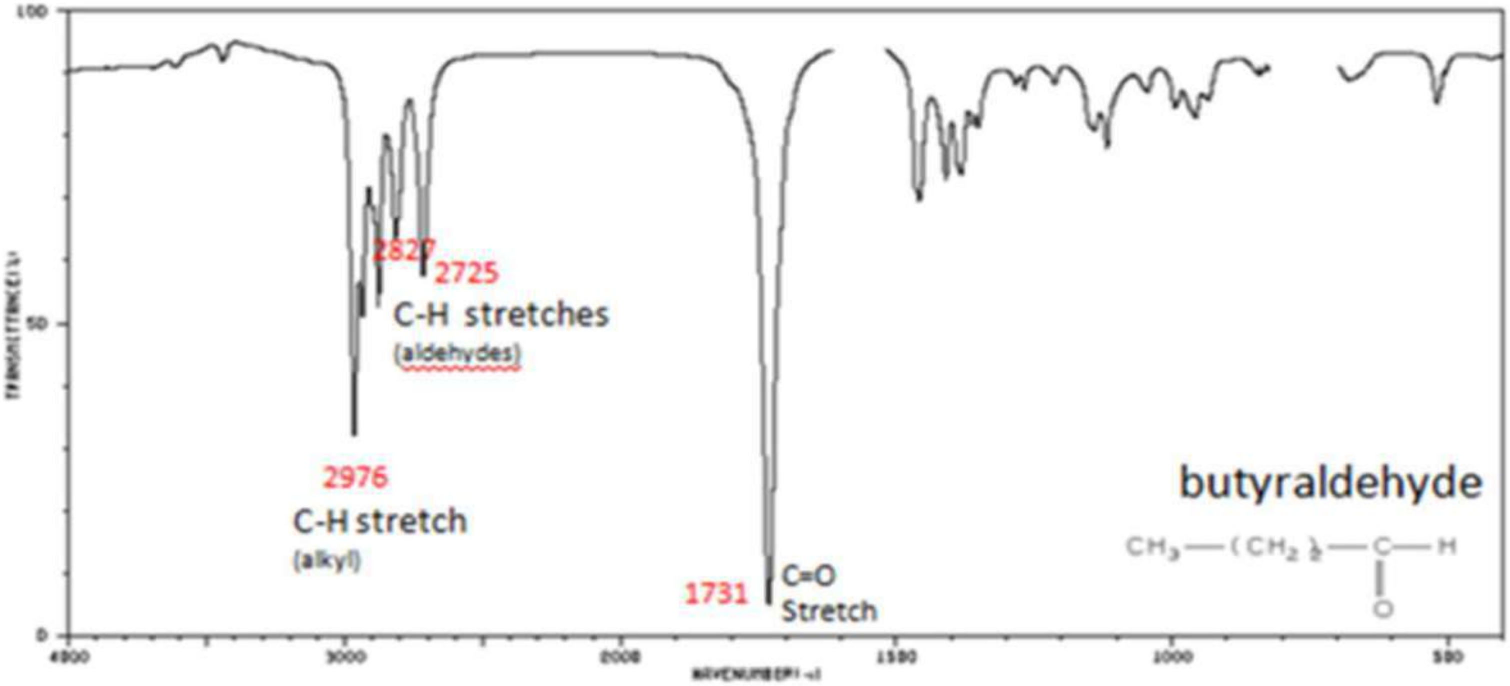


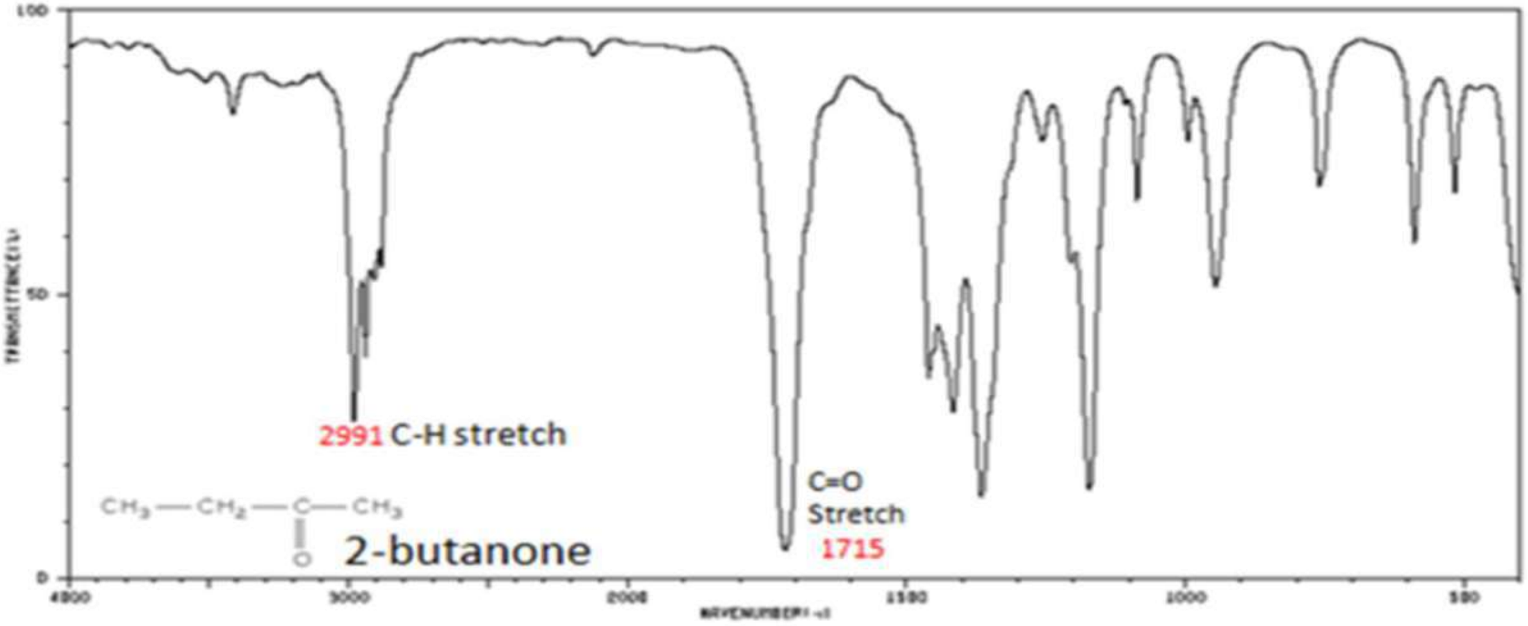
- This region stretches from about 1800 to 1650 cm$^{-1}$ .
- The base value is 1715 cm$^{-1}$ (ketone).
- The bands are very strong !!! due to the large C=O dipole moment.
- C=O is often one of the strongest peaks in the spectrum.

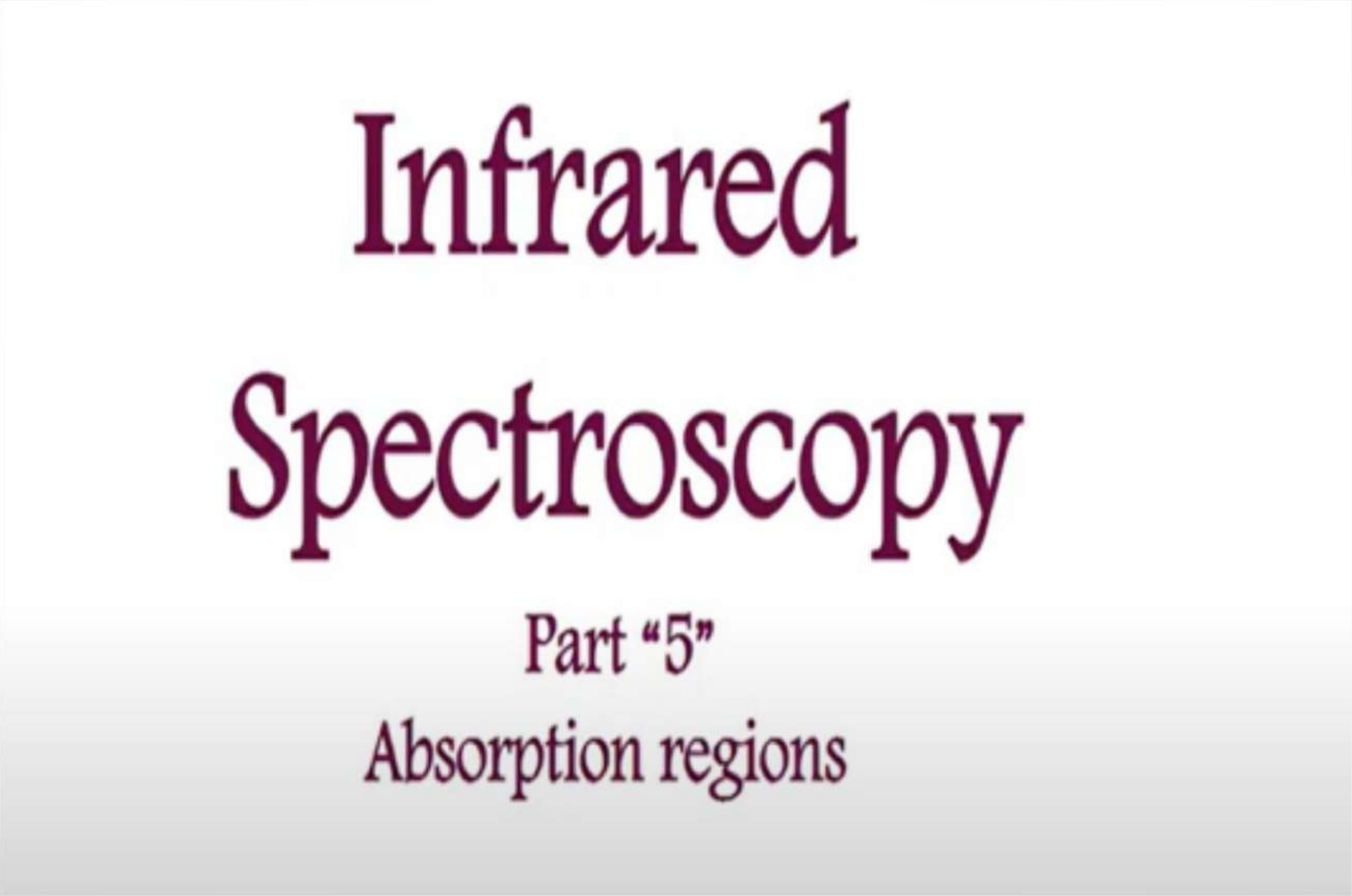
# How to distinguish between aldehyde and ketone?

# IR SPECTRUM OF ALDEHYDES AND KETONES

- In aldehydes, **C=O functional group** is at the end of a carbon chain, whereas in ketones it's in the middle of the chain. As a result, the carbon in the C=O bond of aldehydes is also bonded to another carbon and a hydrogen, whereas the same carbon in a ketone is bonded to two other carbons.
- Aldehydes and ketones show a strong, prominent, stake-shaped band around **1710 - 1720 $cm^{-1}$**. This band is due to the **highly polar C=O bond.**
- Because aldehydes also contain a C-H bond to the $sp^2$ carbon of the C=O bond, they also show a pair of medium strength bands positioned about **2700** and **2800 $cm^{-1}$**. These bands are missing in the spectrum of a ketone because the $sp^2$ carbon of the ketone lacks the C-H bond.


100
50
0
TRANSMITTANCE(%)
4000
3000
2000
1500
1000
500
WAVENUMBER(-1)
2827
2725
C-H stretches
(aldehydes)
2976
C-H stretch
(alkyl)
1731
C=O
Stretch
butyraldehyde
CH₃—(CH₂)₂—C—H
O


100
50
0
TRANSMITTANCE(%)
4000
3000
2000
1500
1000
500
WAVENUMBER(-1)
2991 C-H stretch
C=O
Stretch
1715
CH₃—CH₂—C—CH₃
O
2-butanone

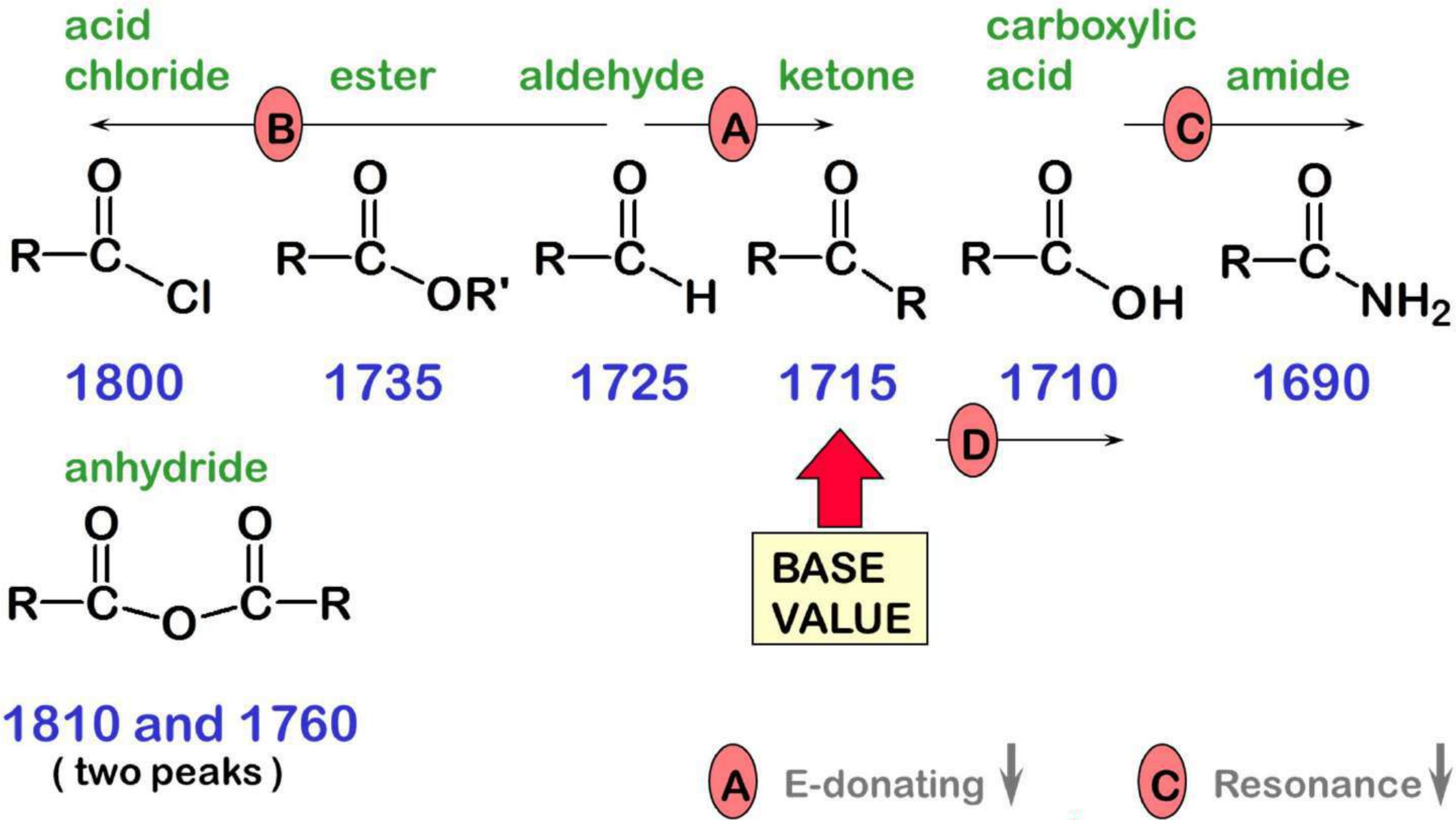


# Infrared Spectroscopy

## Part “5”

## Absorption regions

# How the Factors affect C=O



A E-donating ↓

B E-withdrawing ↑

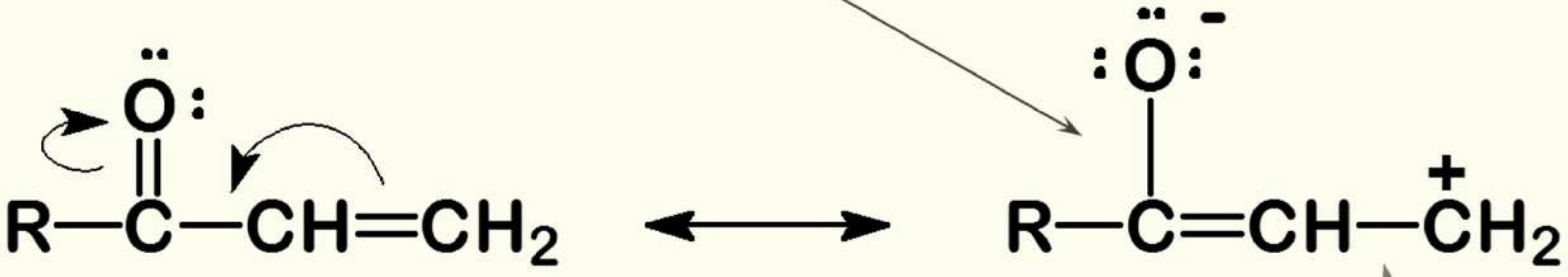
C Resonance ↓

D H-bonding ↓

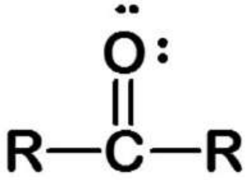
# Carbonyl stretching is affected by

1. Conjugation and Inductive effect
2. Angle strain
3. Hydrogen bonding

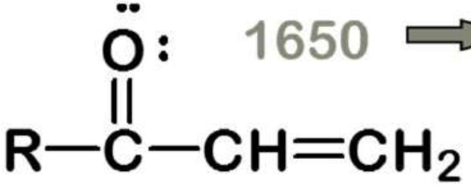
resonance lengthens
(weakens) C=O



$$R-\overset{\ddot{O}:}{\overset{\|}{C}}-CH=CH_2 \longleftrightarrow R-\overset{:\ddot{O}:^-}{\overset{|}{C}}=CH-\overset{+}{C}H_2$$



$$R-\overset{\ddot{O}:}{\overset{\|}{C}}-R$$



$$R-\overset{\ddot{O}:}{\overset{\|}{C}}-CH=CH_2$$

1650 → 1625 $cm^{-1}$

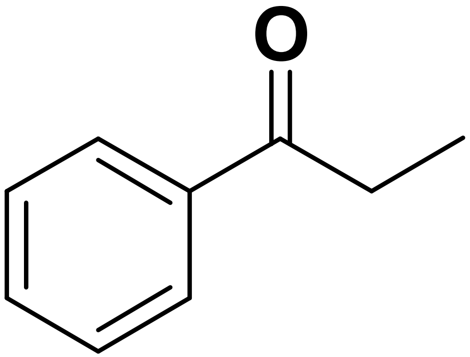
1715 → 1690 $cm^{-1}$

lowered

C=C is also
lengthened
(weakened)
….. and
polarized !

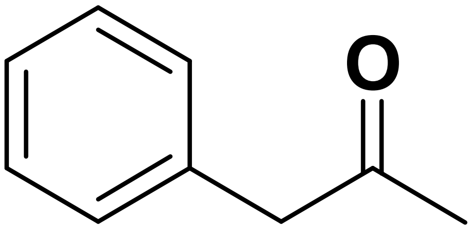
# 1] Conjugation

by resonance, conjugation lowers the energy of a double or triple bond. The effect of this is readily observed in the IR spectrum:



**1684 cm$^{-1}$**

**C=O**



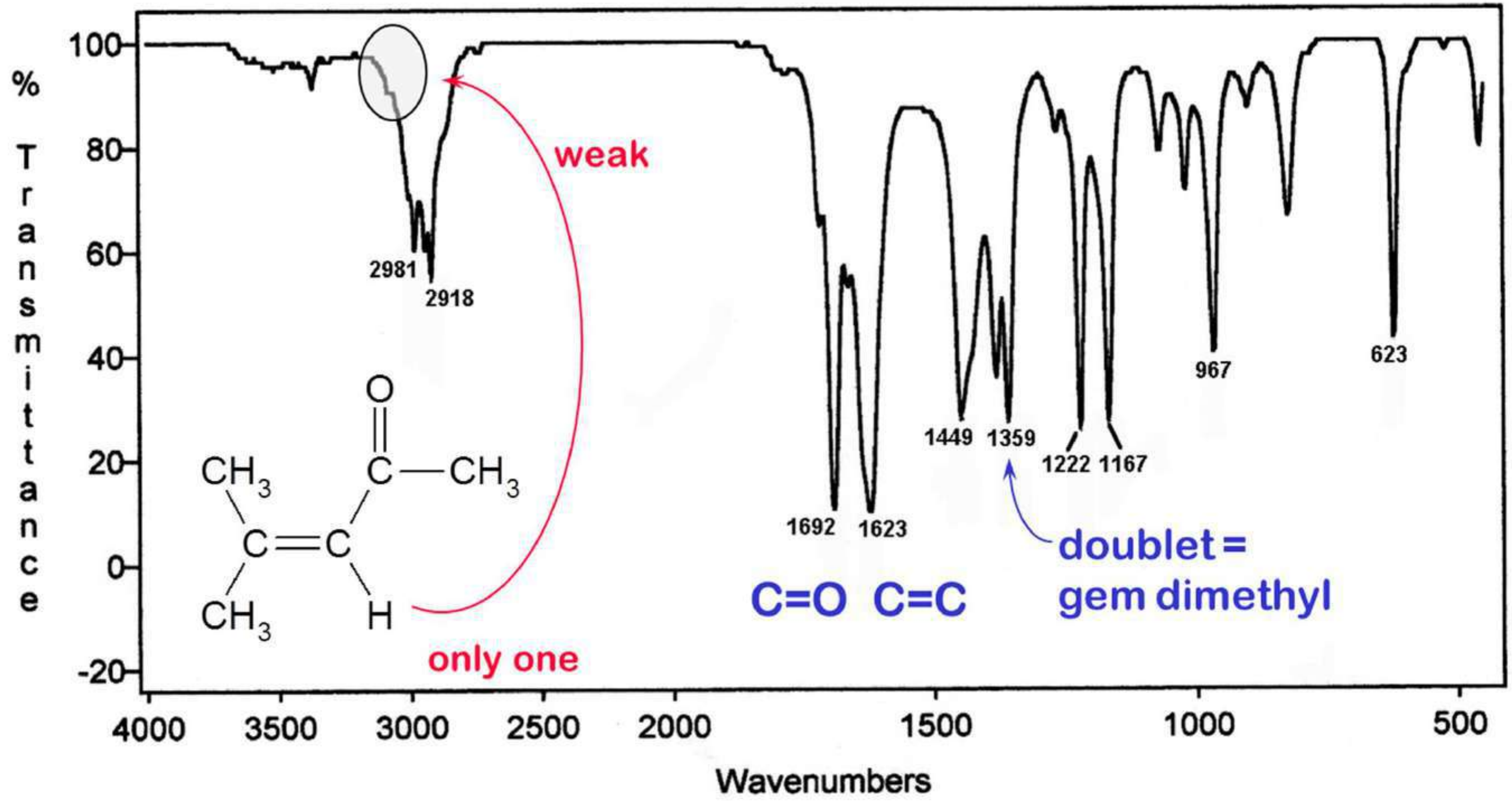
**1715 cm$^{-1}$**

**C=O**

C=O : 1715 - 30 = 1685
C=C : 1650 - 25 = 1625

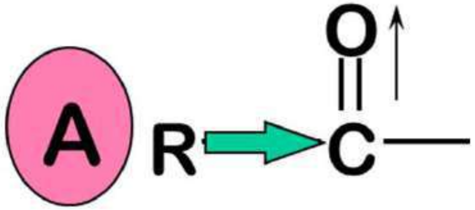
# Ketone conjugated

## 4-Methyl-3-penten-2-one



# Factors that influence the C=O absorption

## Inductive and Resonance effects on the Carbonyl Frequency

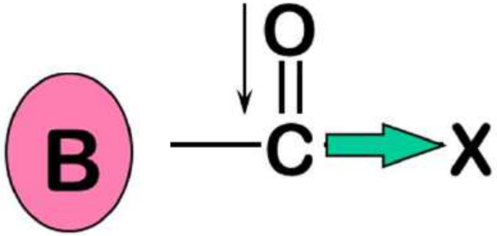


R = Me, Et, etc.

Electron-donating groups

weaken the carbonyl and

↓ lower its absorption frequency

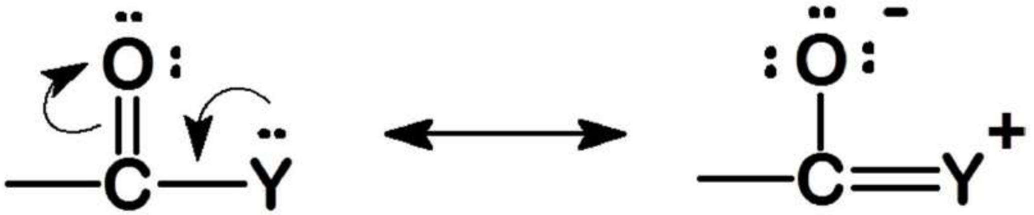


X = F, Cl, Br, O

Electron-withdrawing groups

strengthen the carbonyl and

↑ raise its absorption frequency



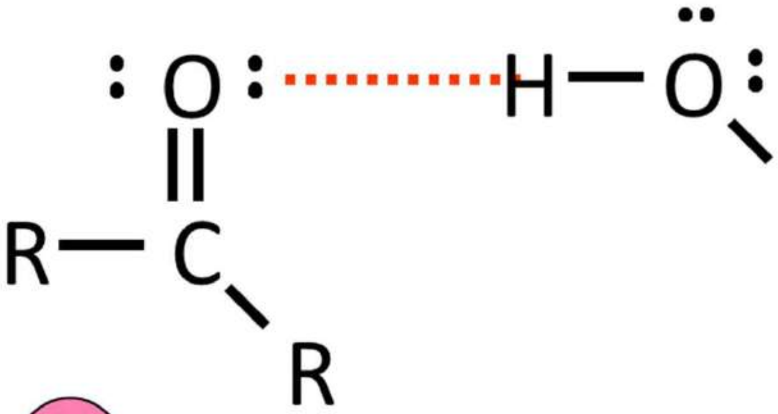
**C**

Y = N, O, or C=C

**Resonance**

weakens the carbonyl and

↓ lowers its absorption frequency

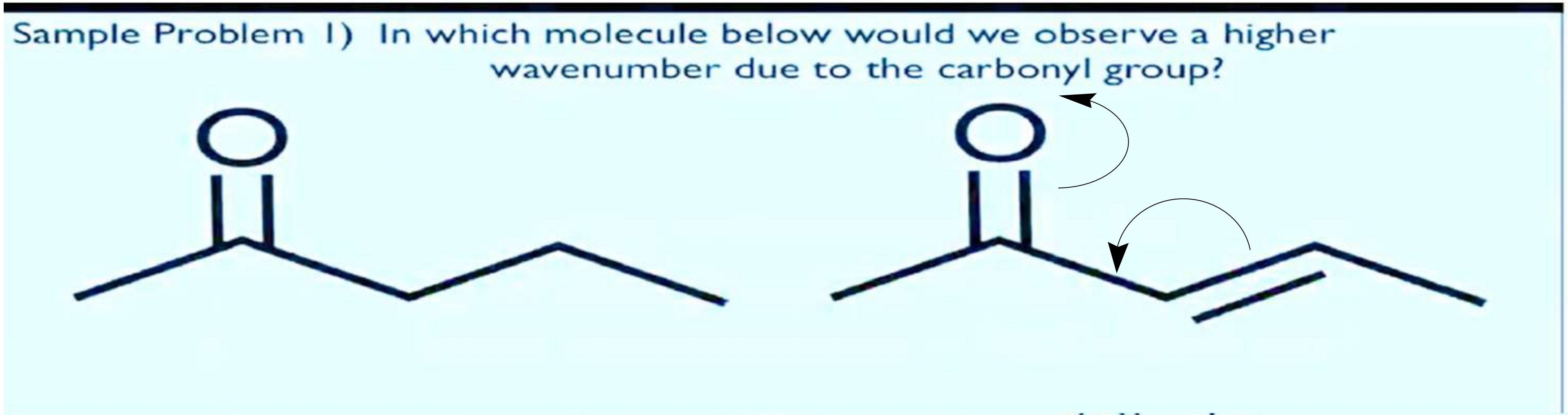


**D**

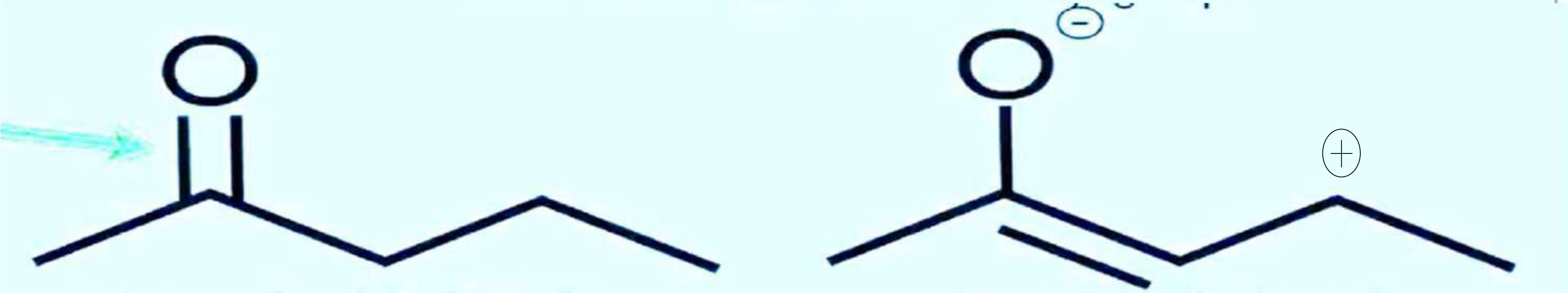
**Hydrogen bonding**

lengthens and weakens the C=O bond and

↓ lowers its absorption frequency

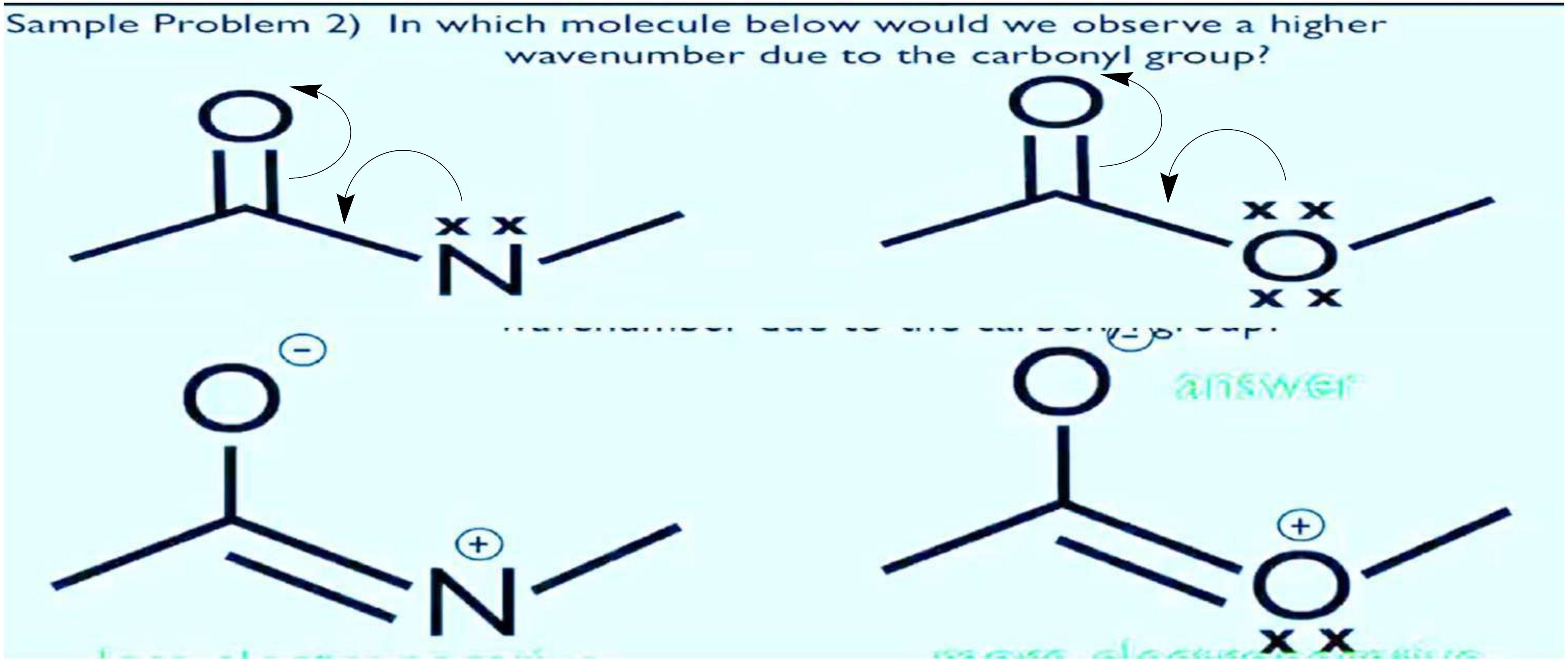


Sample Problem 1) In which molecule below would we observe a higher wavenumber due to the carbonyl group?



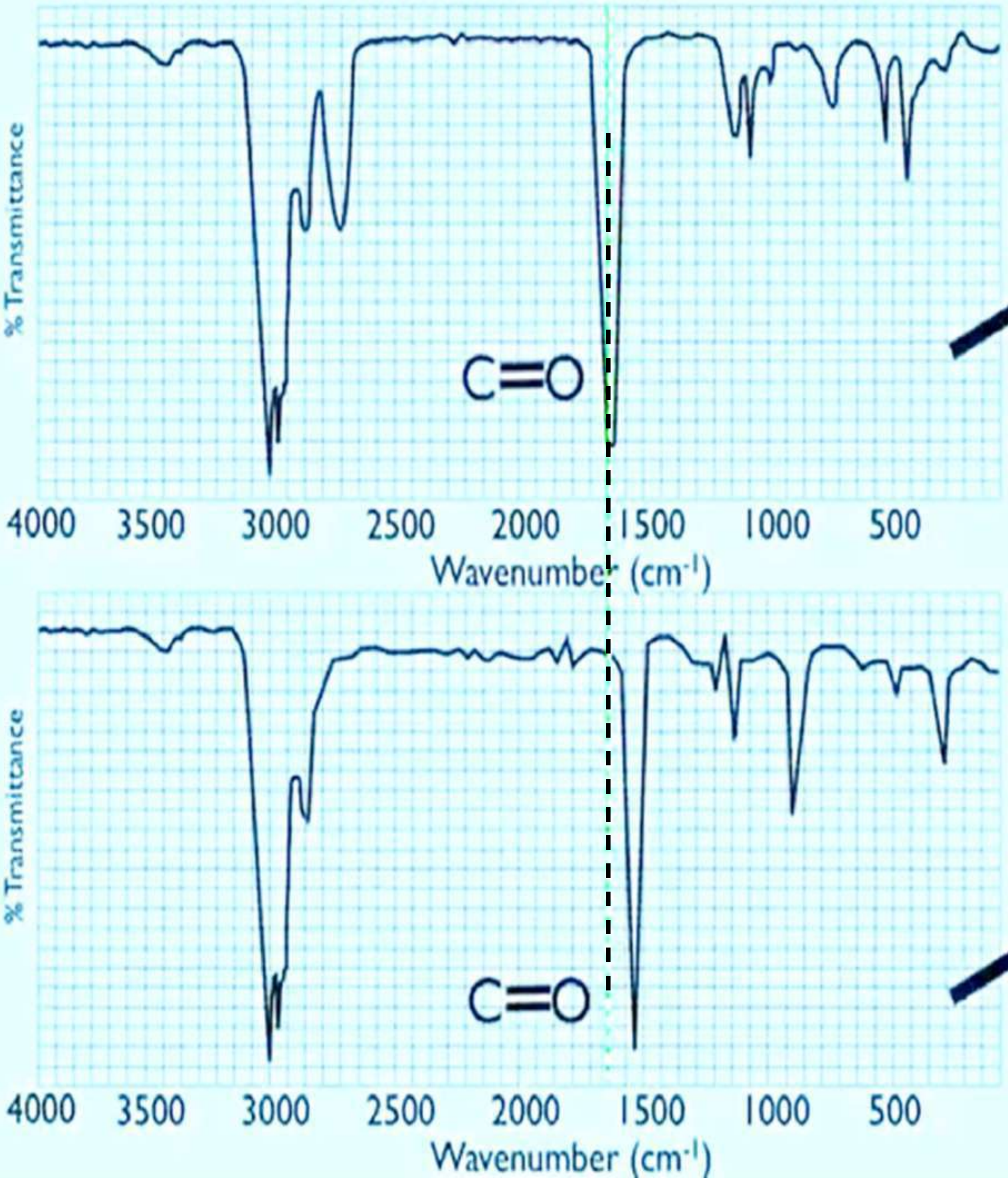
- More Double bond character
- Shorter bond
- Stronger bond
- Higher Wavenumber

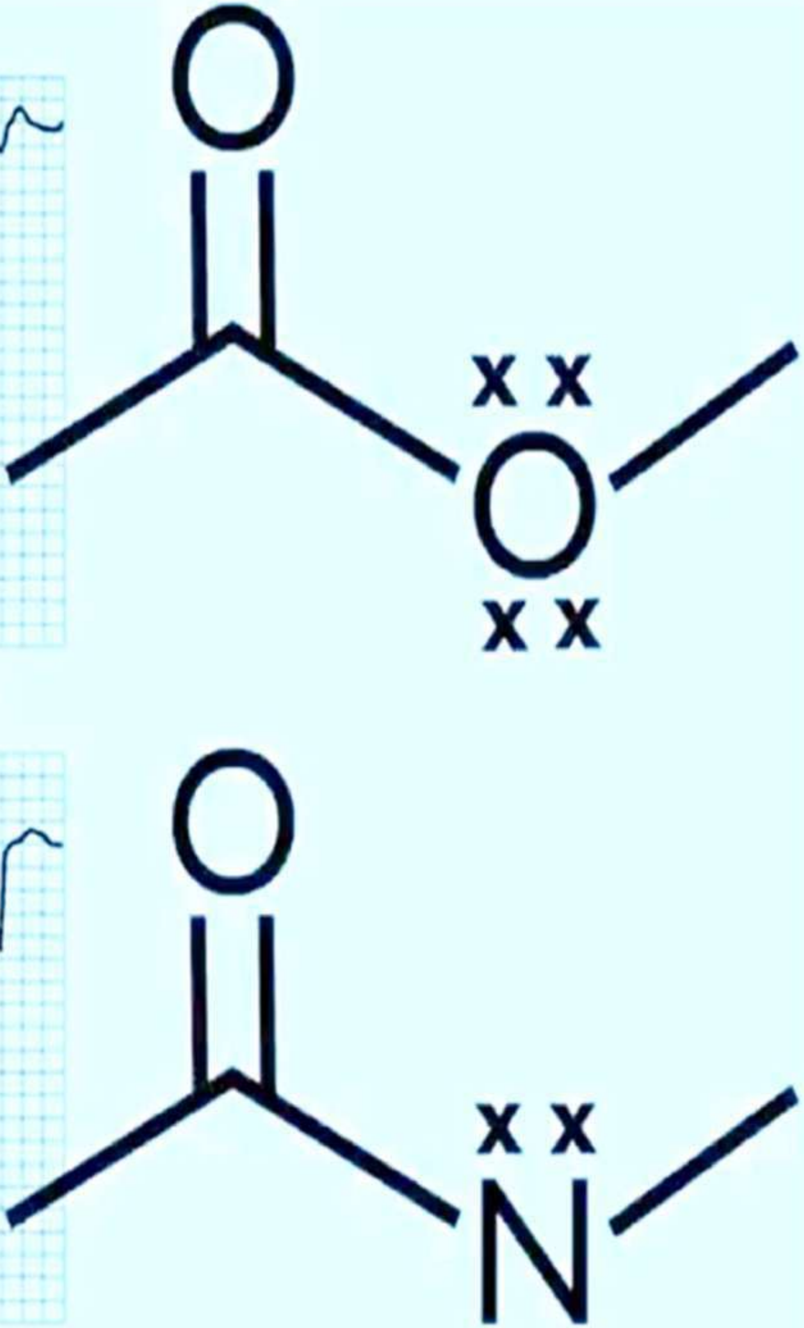
- Less Double bond character
- Longer bond
- Weaker bond
- Lower Wavenumber

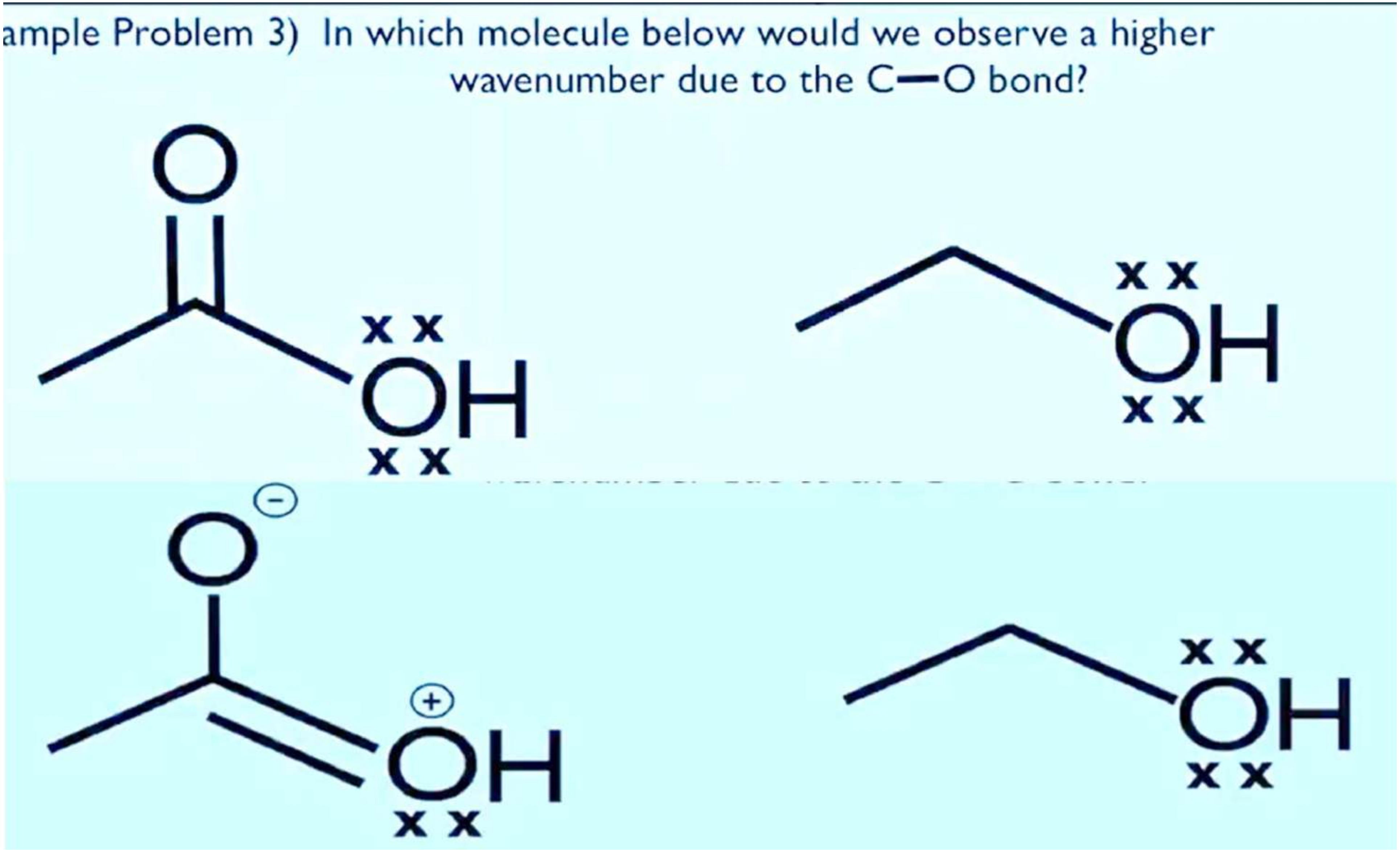


Sample Problem 2) In which molecule below would we observe a higher wavenumber due to the carbonyl group?

| | |
|---|---|
| Less electronegative | More electronegative |
| More donating | Less donating |
| Greater resonance | Less resonance |
| More single bond character | Less single bond character |
| Lower Wavenumber | Higher Wavenumber |


% Transmittance
C=O
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber (cm⁻¹)
% Transmittance
C=O
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber (cm⁻¹)


O
x x
O
x x
O
x x
N

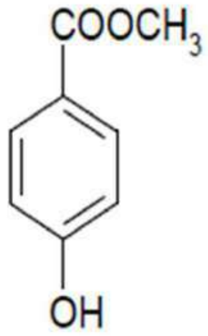


ample Problem 3) In which molecule below would we observe a higher wavenumber due to the C—O bond?

**Less single bond character**
**Higher Wavenumber**

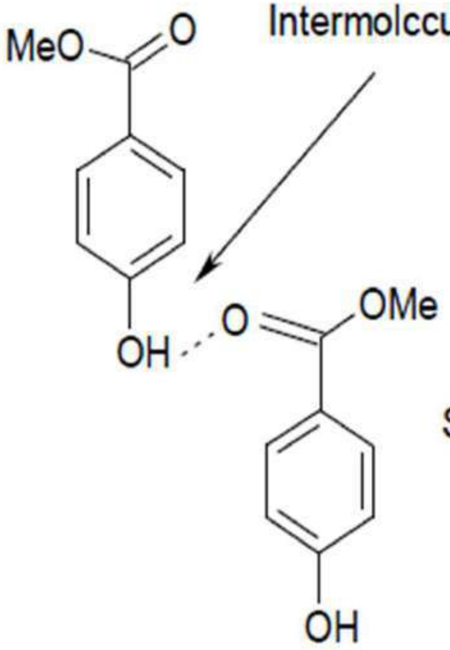
**More single bond character**
**Lower Wavenumber**

# 2] Effect of HB on carbonyl stretching



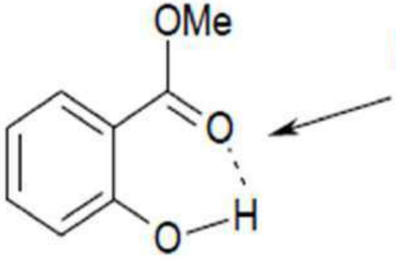
P- hydroxy methyl benzoate

Stretching 1740-1780 cm-1



Intermolccular hydrogen bonding

Stretching 1710cm-1



Intramolecular hydrogen bonding

Stretching 1680 cm-1

# Infrared Spectroscopy

## Part “6”

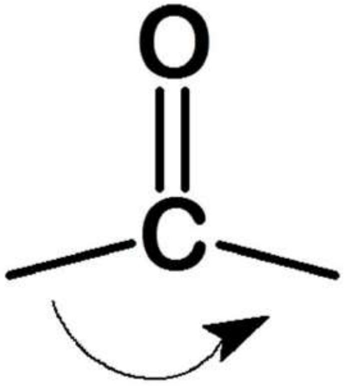
## Absorption regions

# Conjugation of C=O with C=C

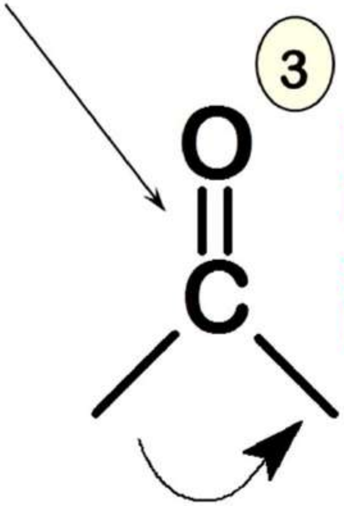
- Conjugation of a carbonyl with a C=C bond shifts values to lower frequencies.

- For aldehydes, ketones and esters, subtract about 25-30 $cm^{-1}$ for conjugation with C=O.

# 3] Angle Strain raises The Carbonyl Frequency



120° angle is normal

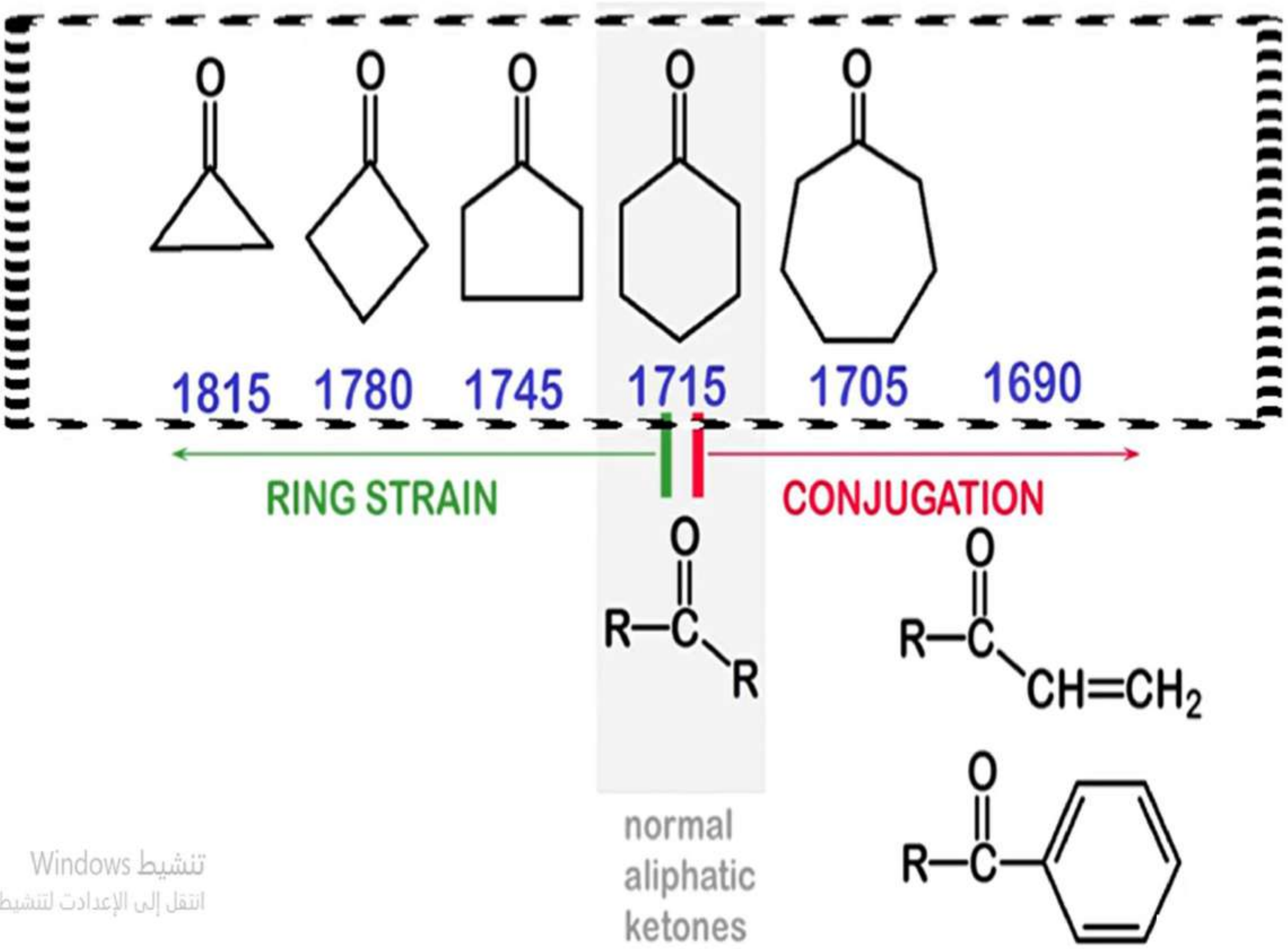


① A smaller angle requires more p character in the hybrids forming the ring.

② In response to more p character in the ring bonds, there is more s character in the bonds to C=O.

③ More s character leads to a shorter and stronger bond and a higher frequency.

# Conjugation and Ring Size Effects

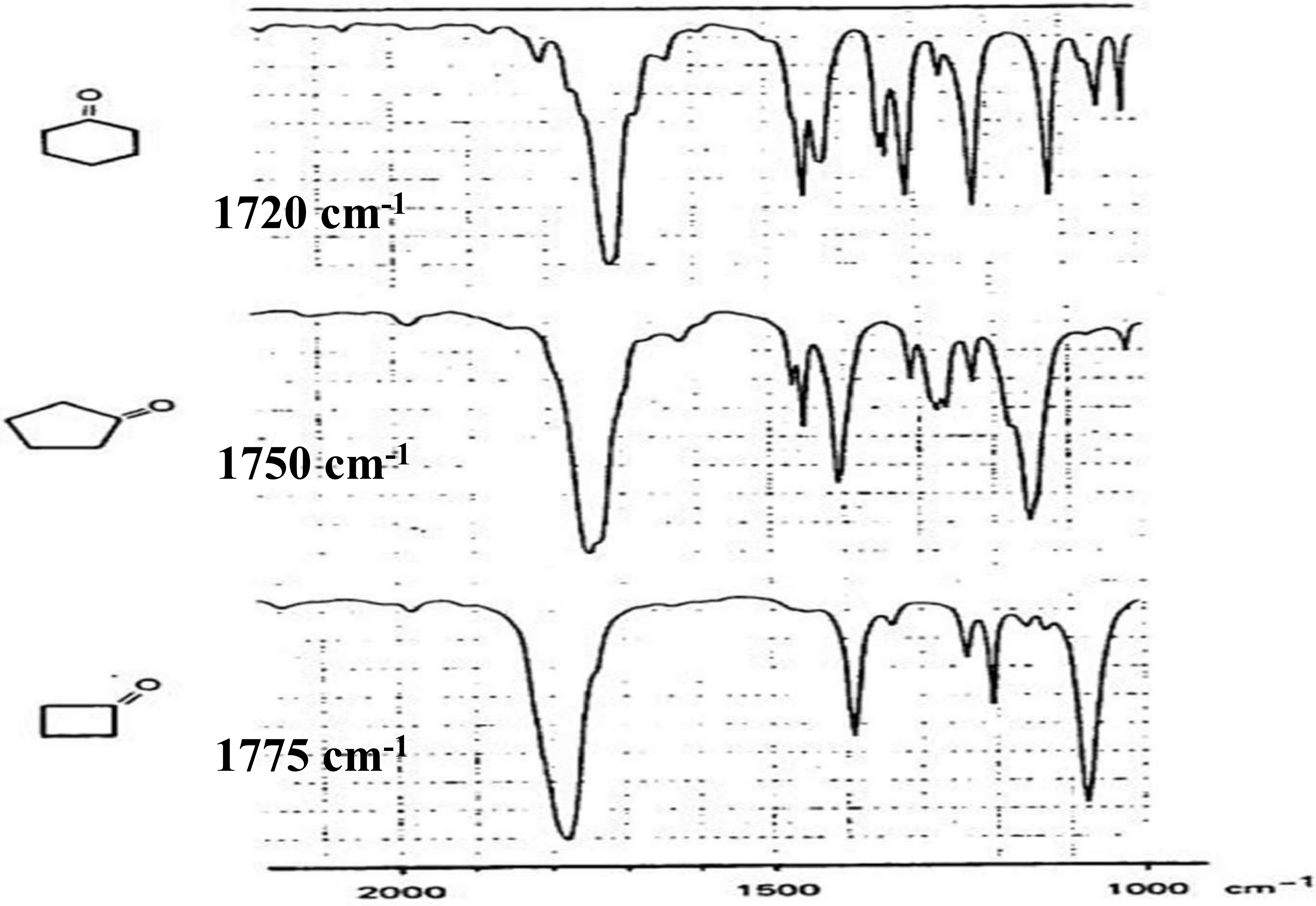


1815 1780 1745 1715 1705 1690

RING STRAIN

CONJUGATION

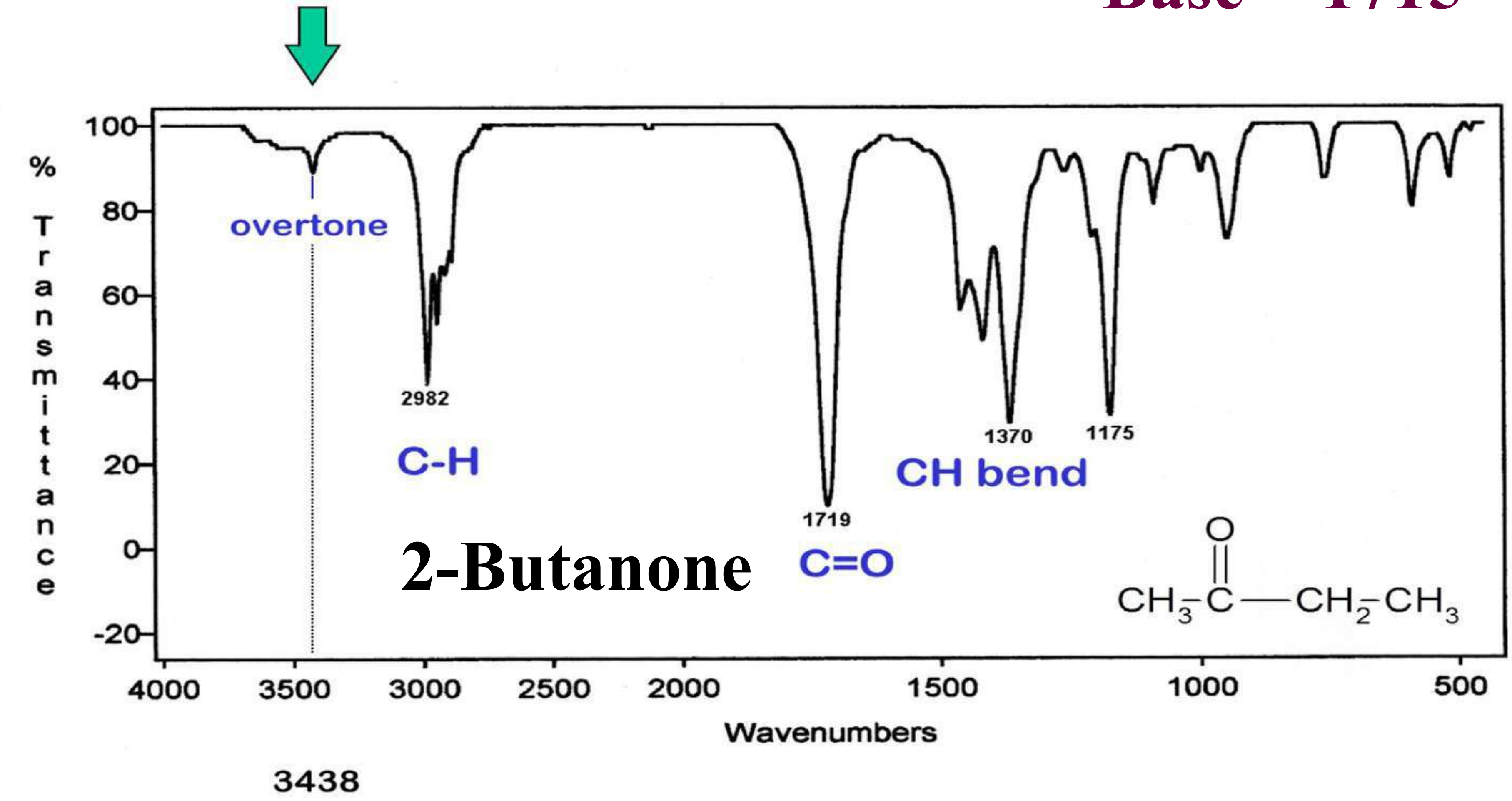
normal
aliphatic
ketones


1720 cm$^{-1}$
1750 cm$^{-1}$
1775 cm$^{-1}$
2000
1500
1000
cm$^{-1}$

# Carbonyl containing compound

**Ketone**
**Base = 1715**

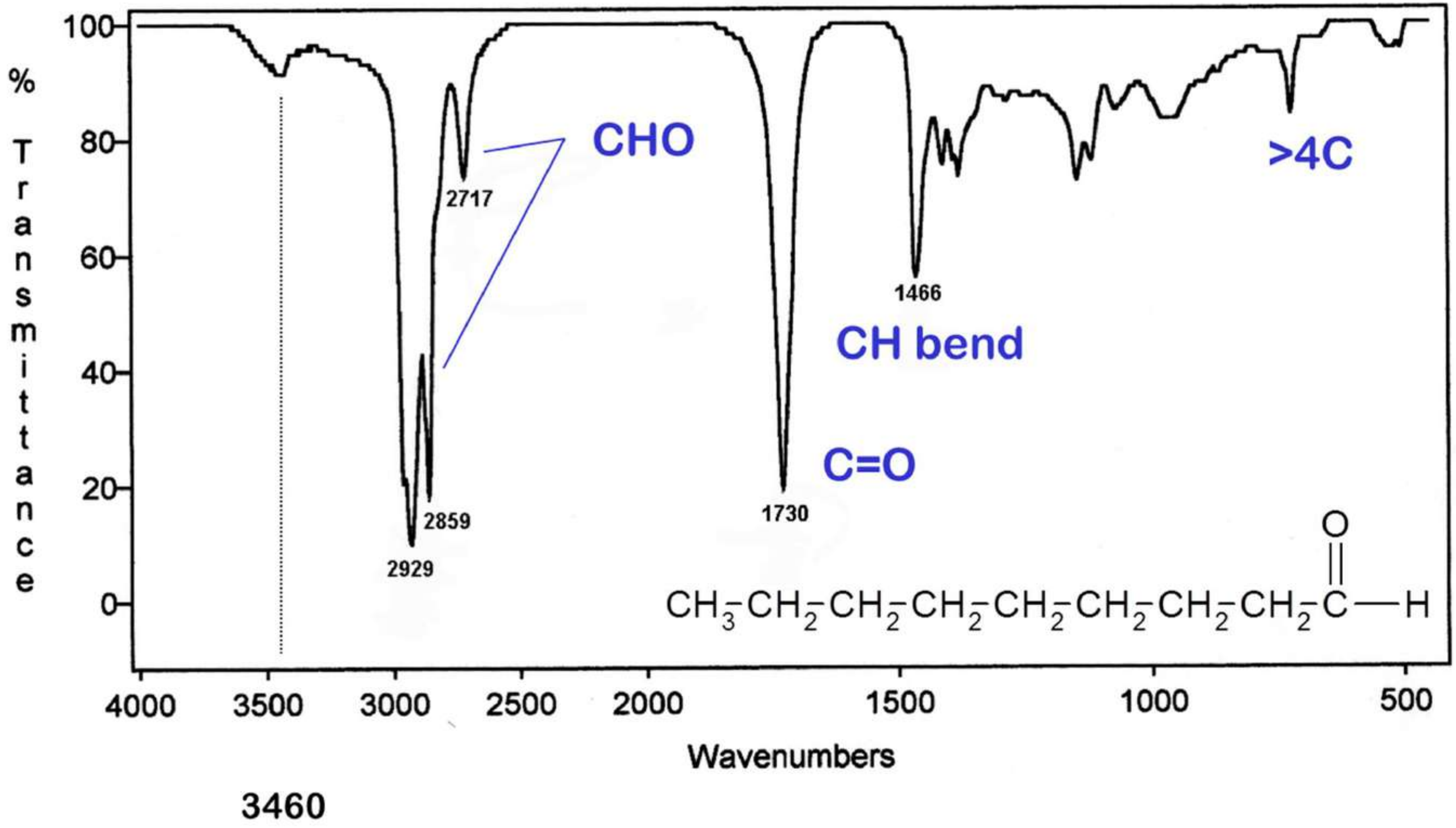
overtone of strong C=O peak
1719 x 2 = 3438



**2-Butanone**

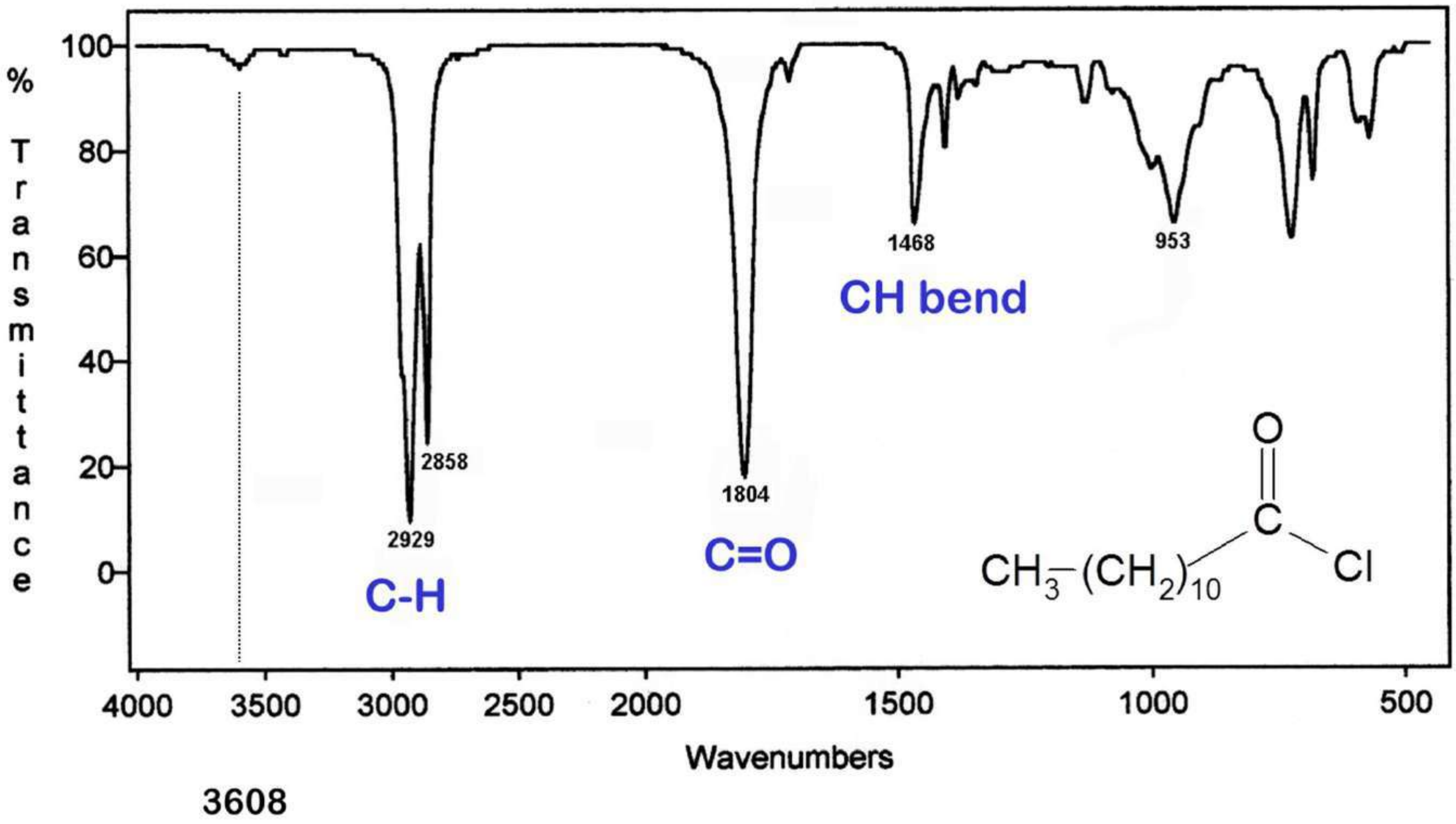
# Aldehyde
# Base = 1725

## Nonanal



# Acid Chloride
# Base = 1800

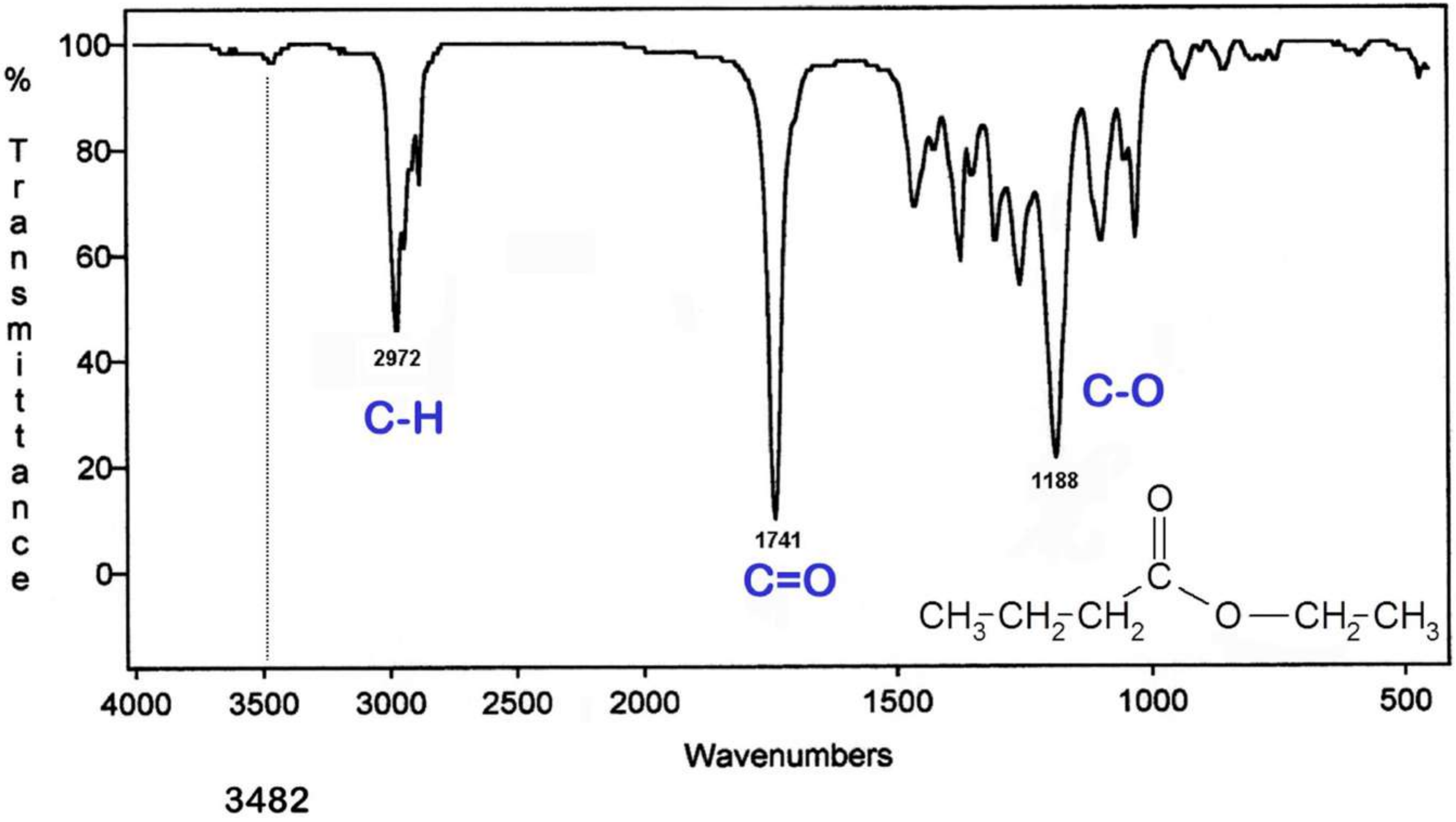
## Dodecanoyl Chloride



# Ester

# Base = 1735

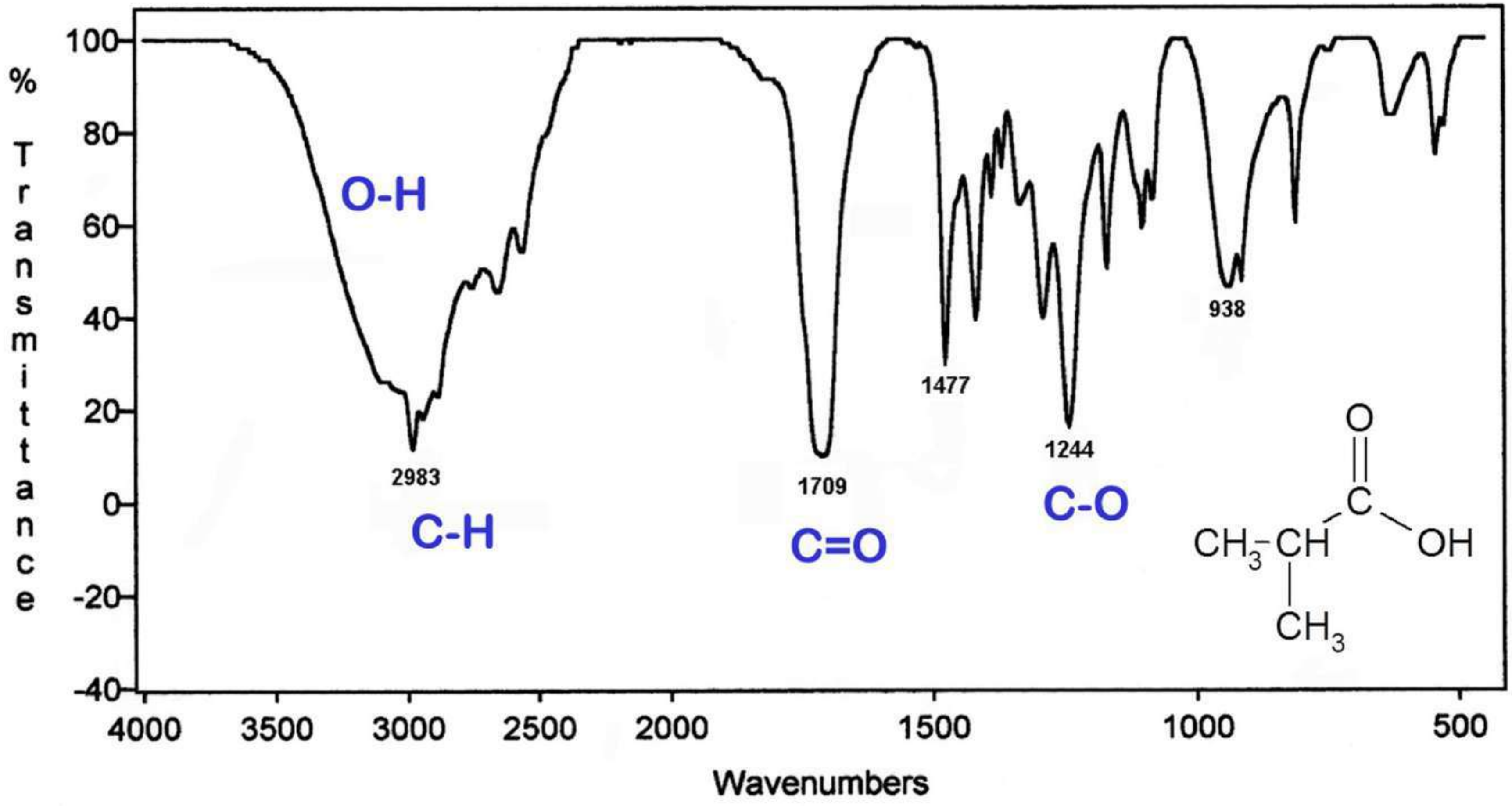
## Ethyl Butanoate



# Carboxylic acid

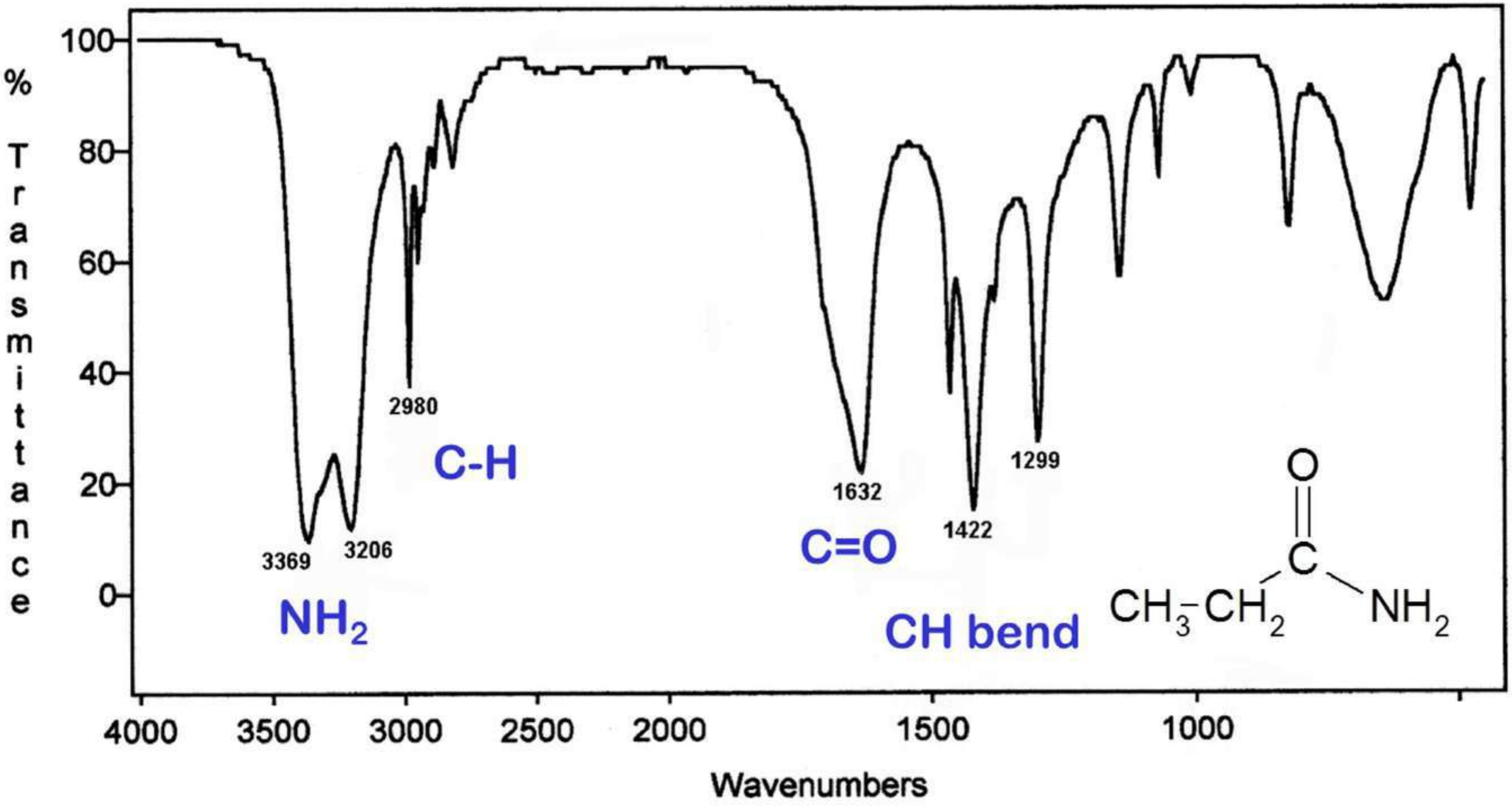
## Base = 1710

## 2-Methylpropanoic Acid



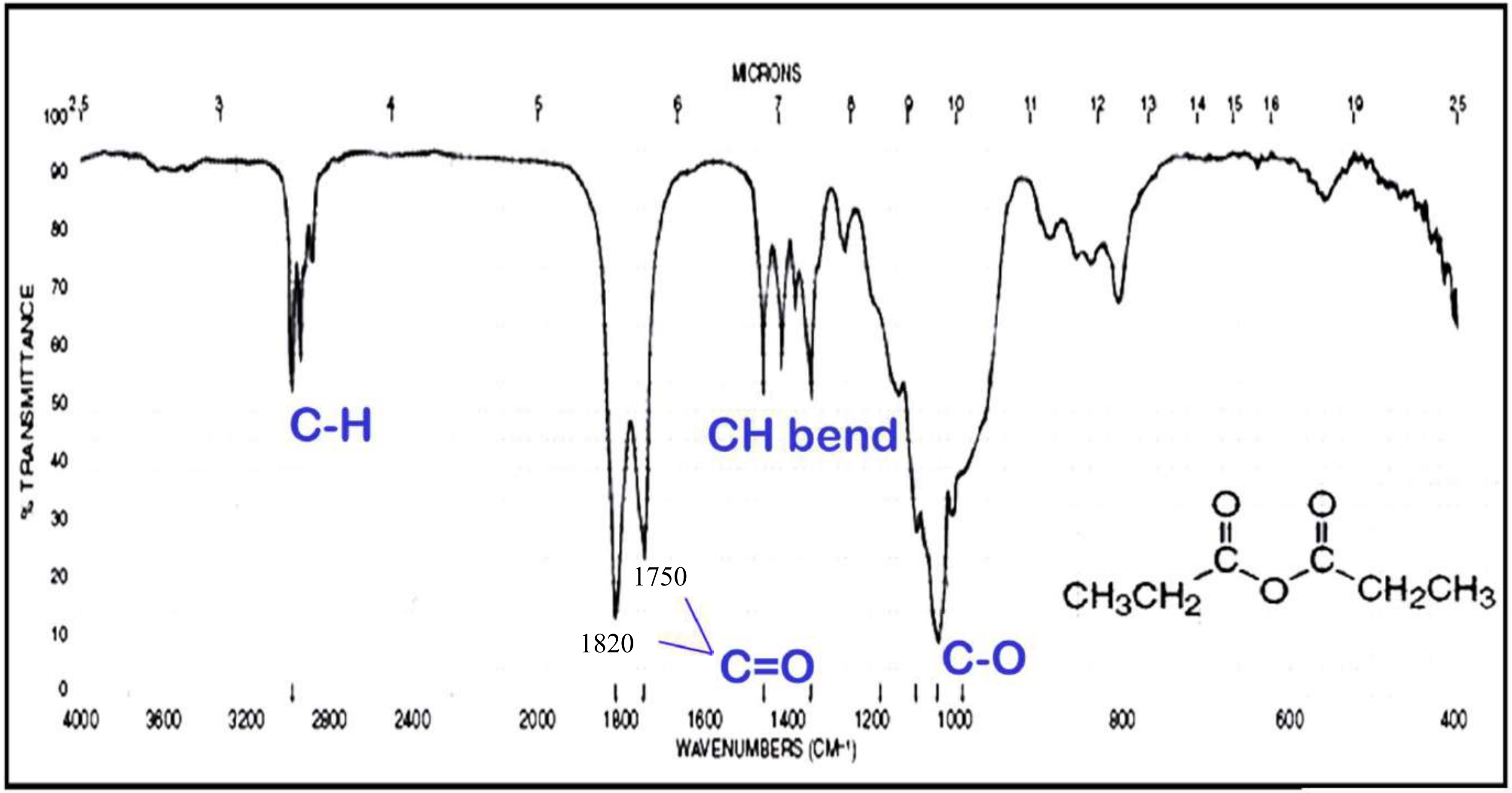
# Amide
# Base = 1690

## Propanamide



# Anhydride
## Base = 1810 and 1760

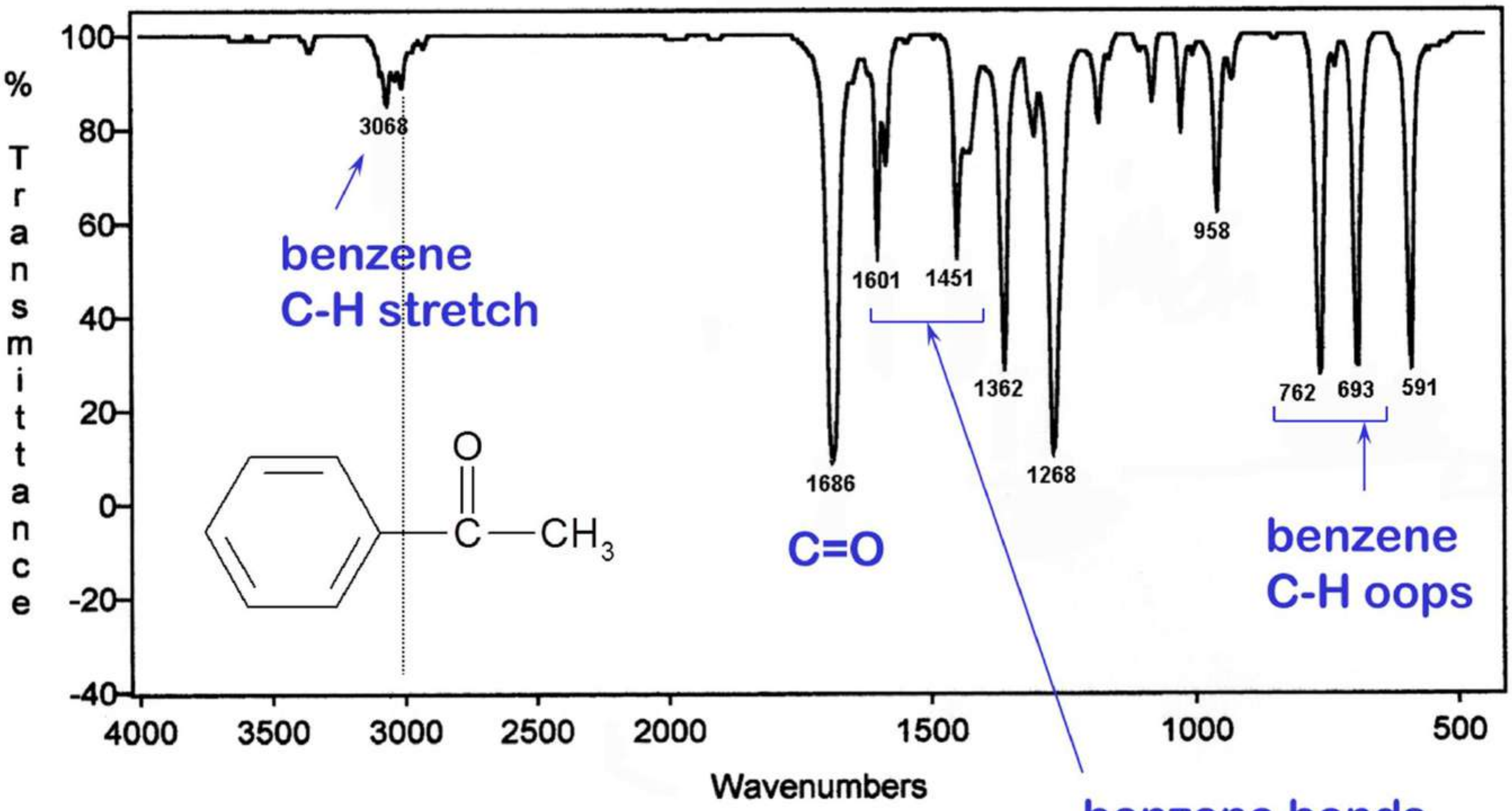
## Propionic anhydride



# Aromatic Ketone conjugated

C=O : 1715 - 30 = 1685

## Acetophenone

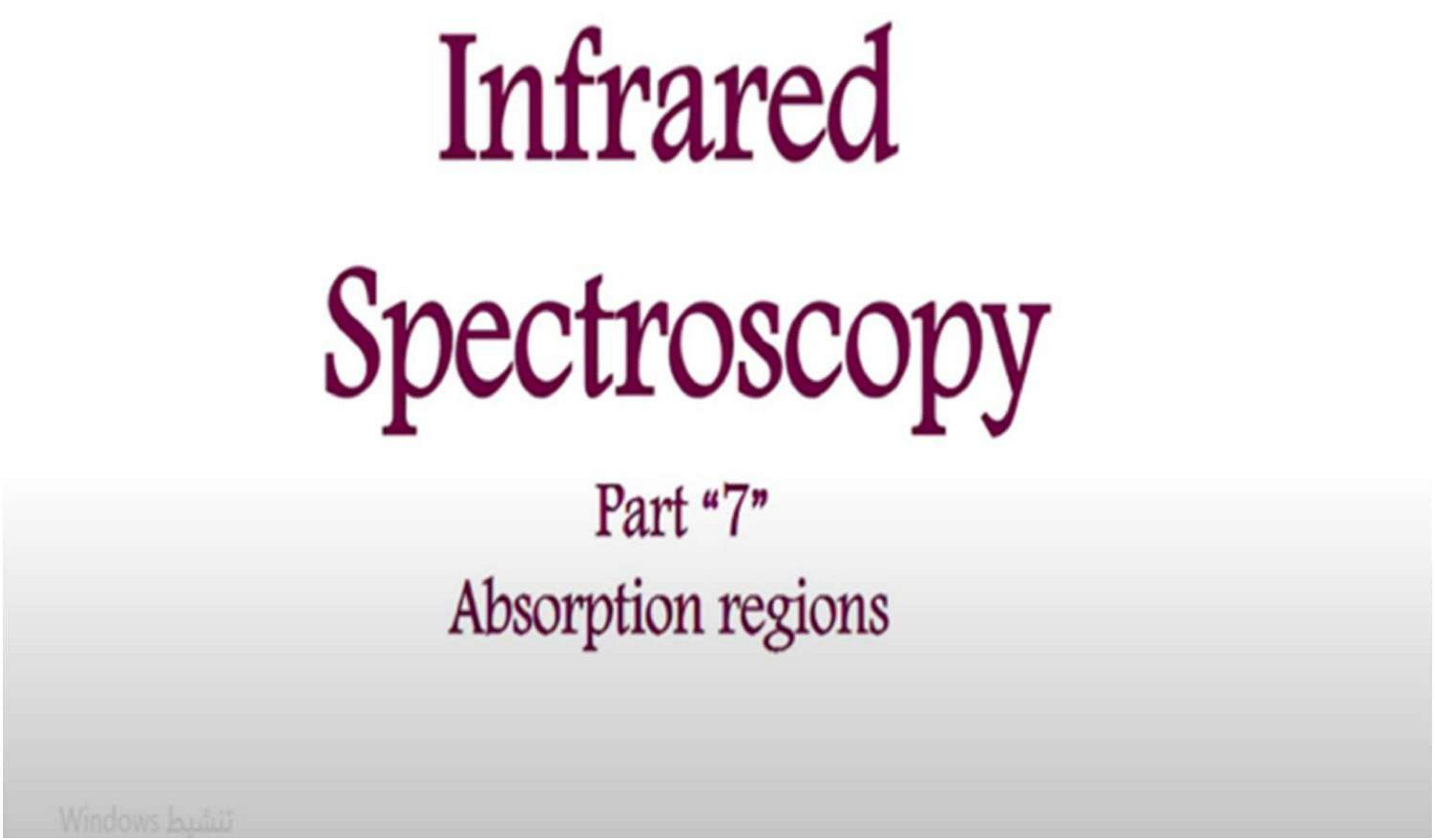


benzene
C-H stretch

C=O

benzene
C-H oops

benzene bonds
1400 - 1600

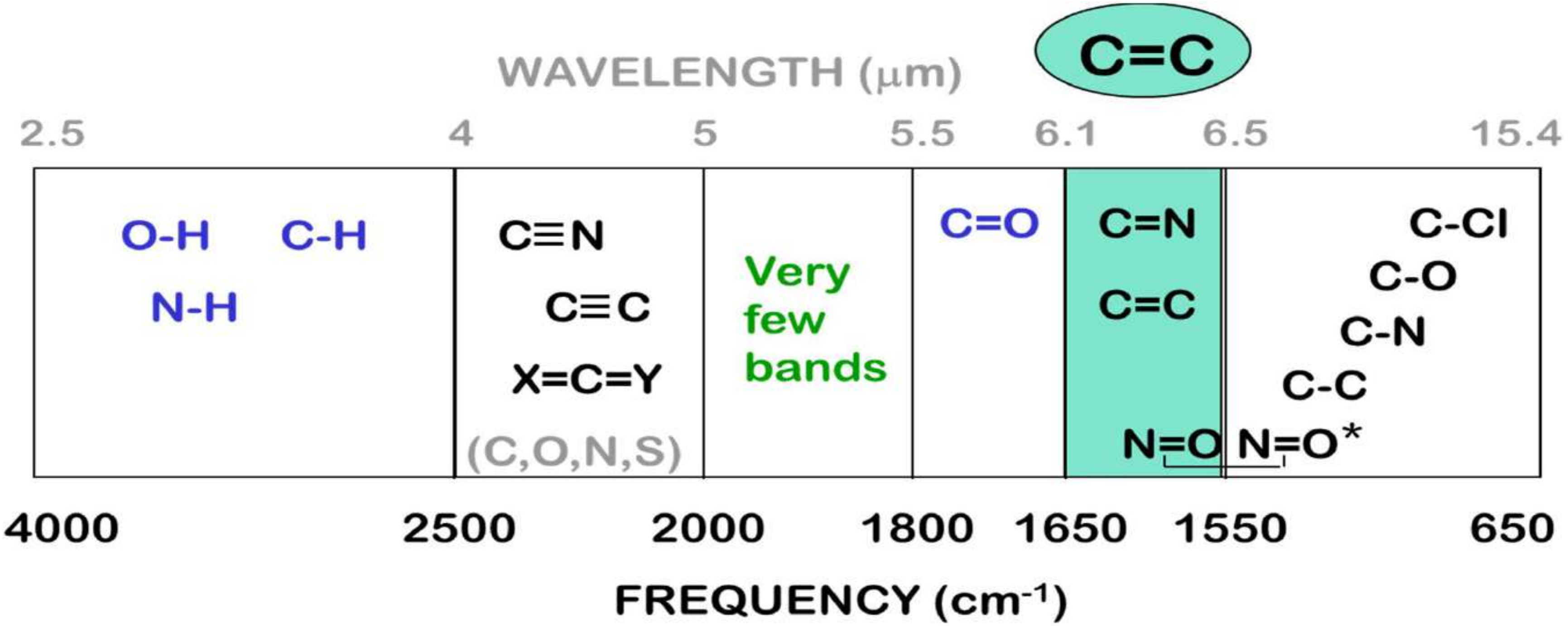


# Infrared Spectroscopy

## Part "7"

## Absorption regions

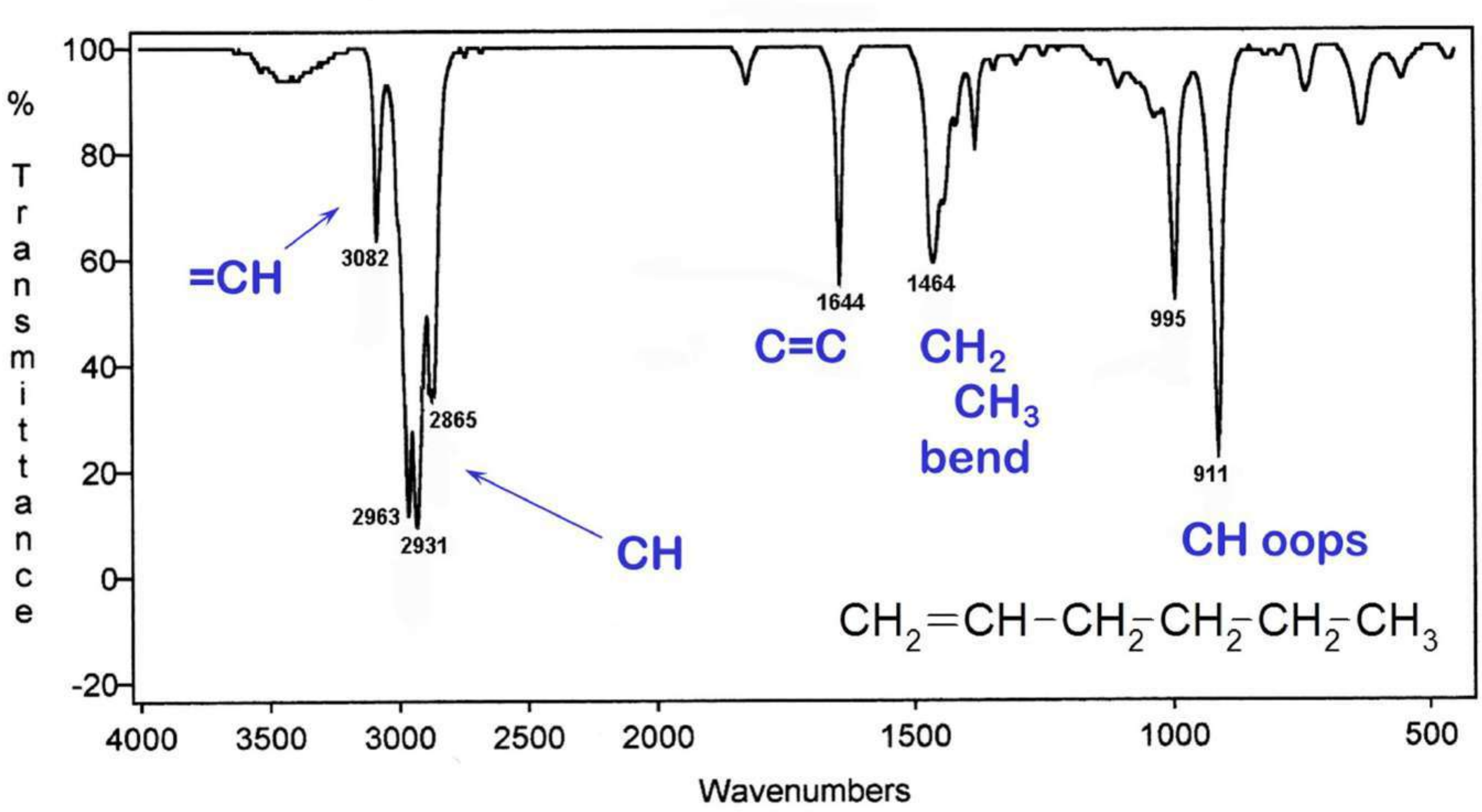
# The C=C stretching region



- C=C double bond at 1650 $cm^{-1}$ is often weak or not even seen.
- C=C benzene ring shows peak(s) near 1600 and 1475 $cm^{-1}$ , one or two at each value - Conjugation lowers the value.
- When C=C is conjugated with C=O it is stronger and comes at a lower frequency.

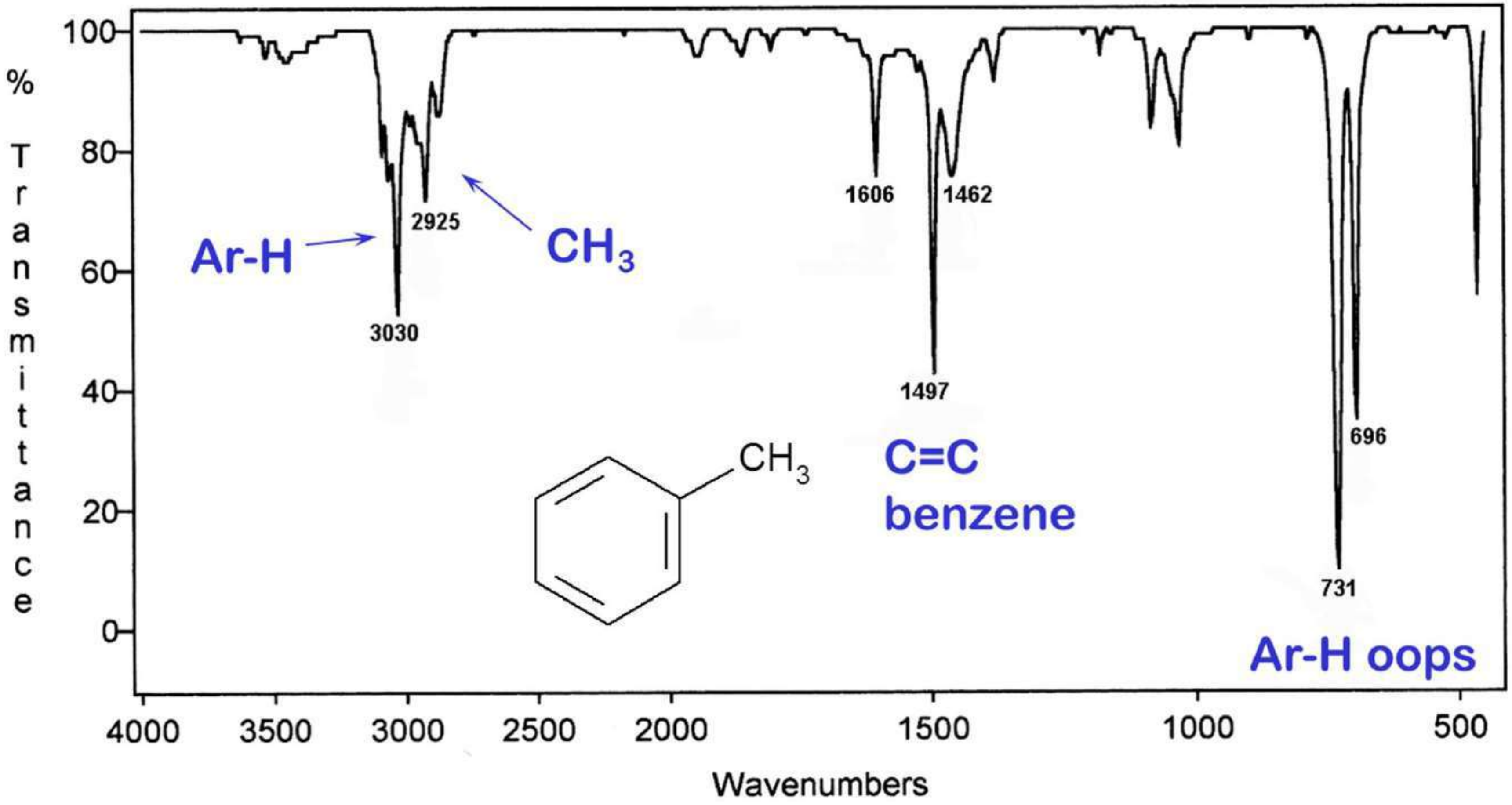
# Alkene

## 1-Hexene

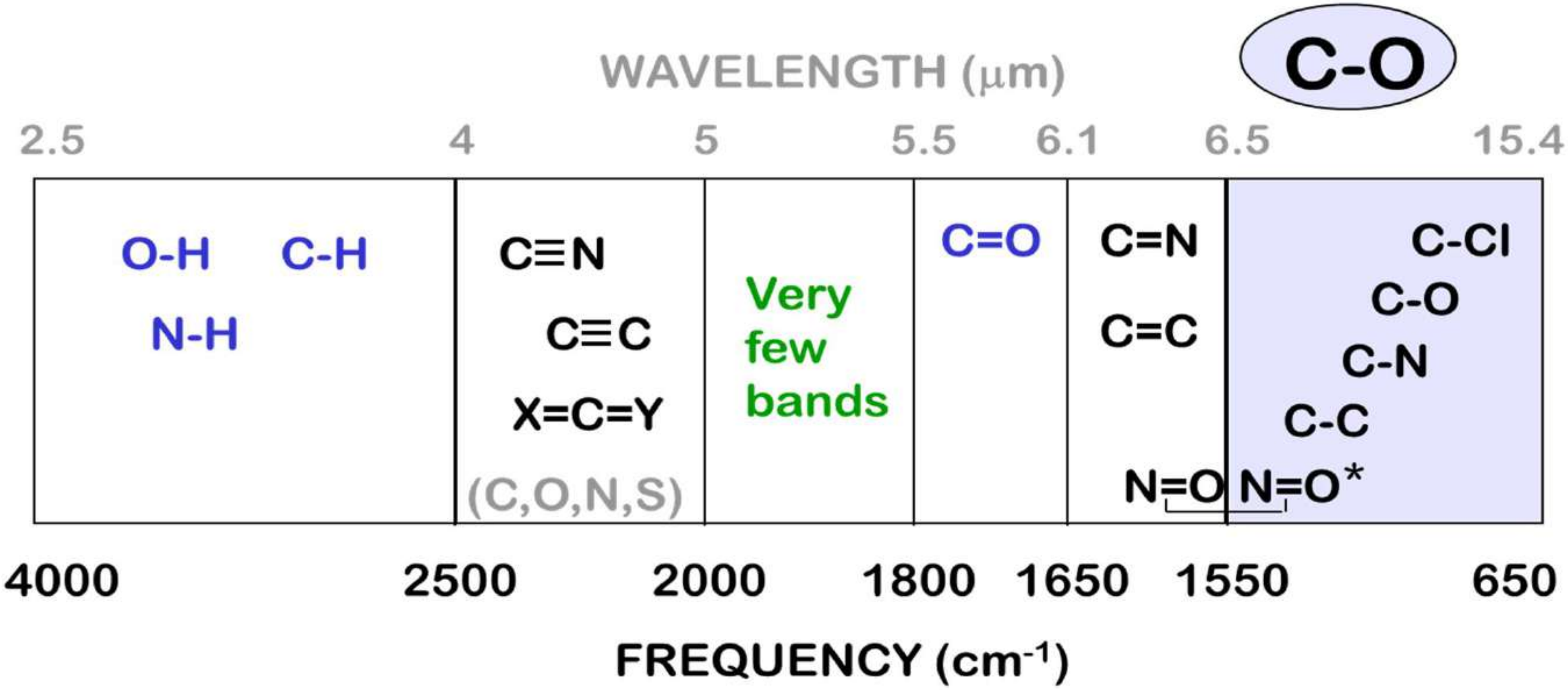


# Aromatic

## Toluene



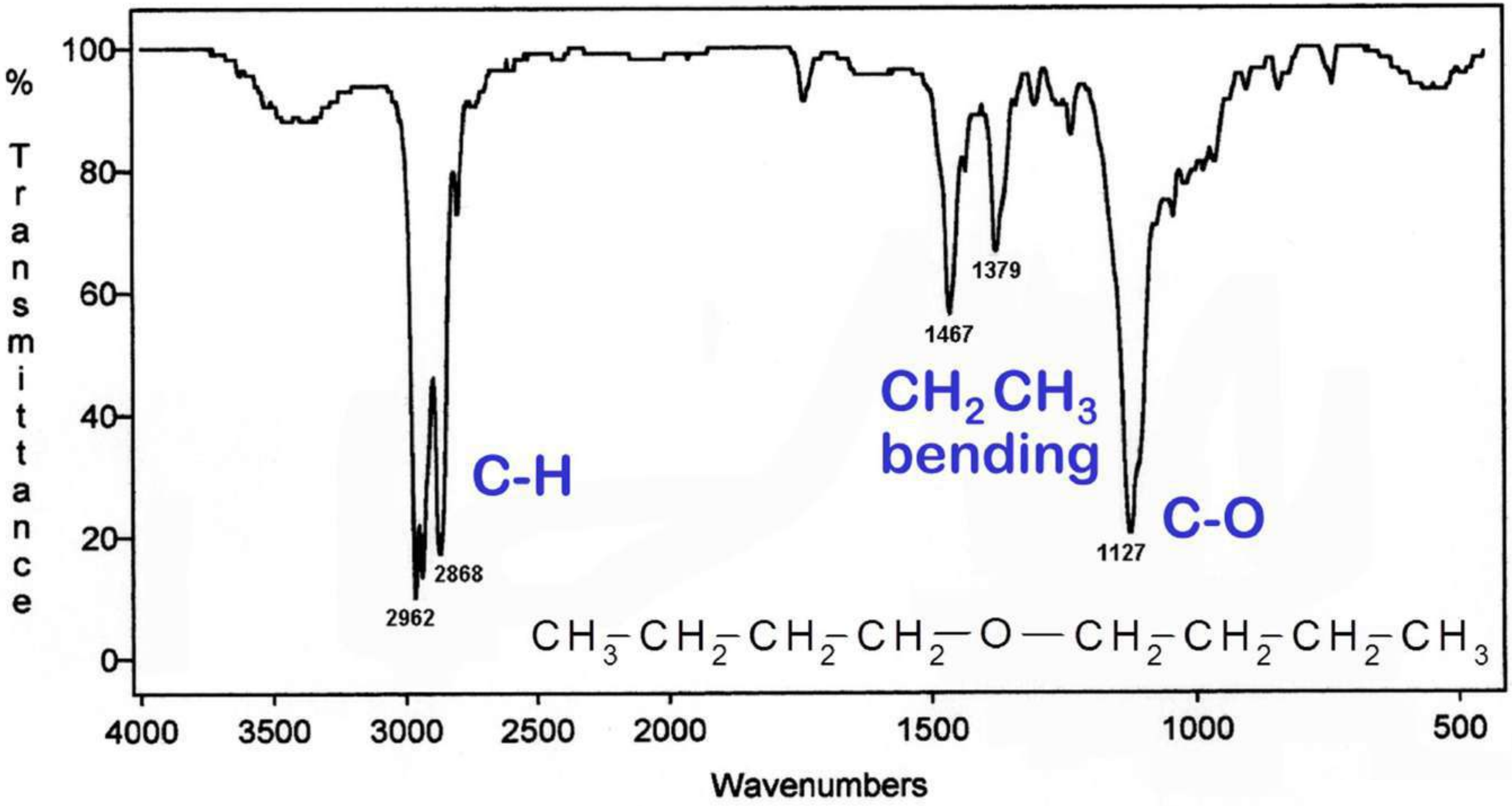
# The C-O stretching region



- The C-O band appears in the range of 1300 to 1000 cm$^{-1}$.
- Look for one or more strong bands appearing in this range!
- Ethers, alcohols, esters and carboxylic acids have C-O bands.

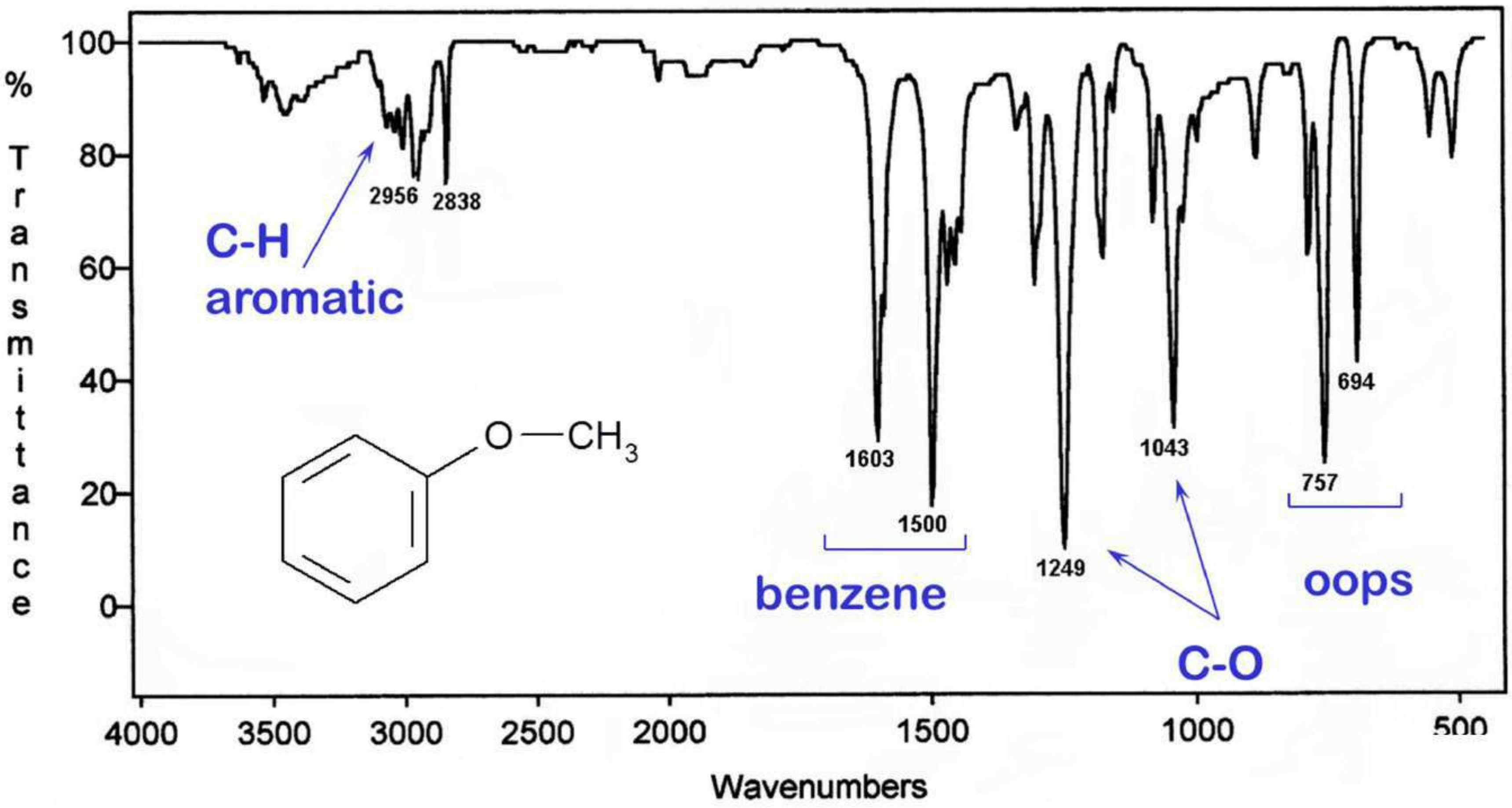
# Ether
# Base = 1100

## Dibutyl Ether



# Aromatic Ether
# Base = 1100

## Anisole


C-H aromatic

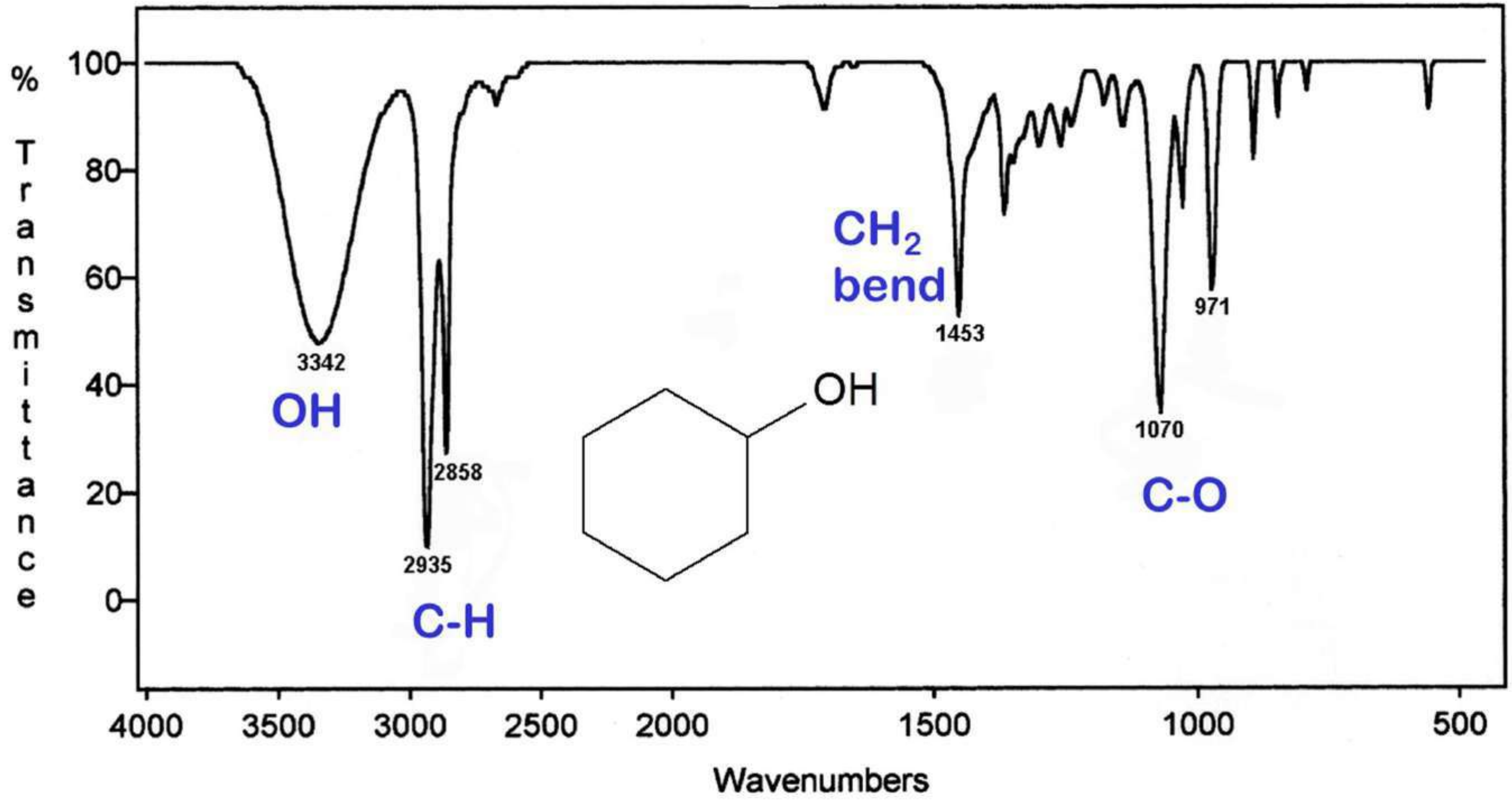
benzene

C-O

oops

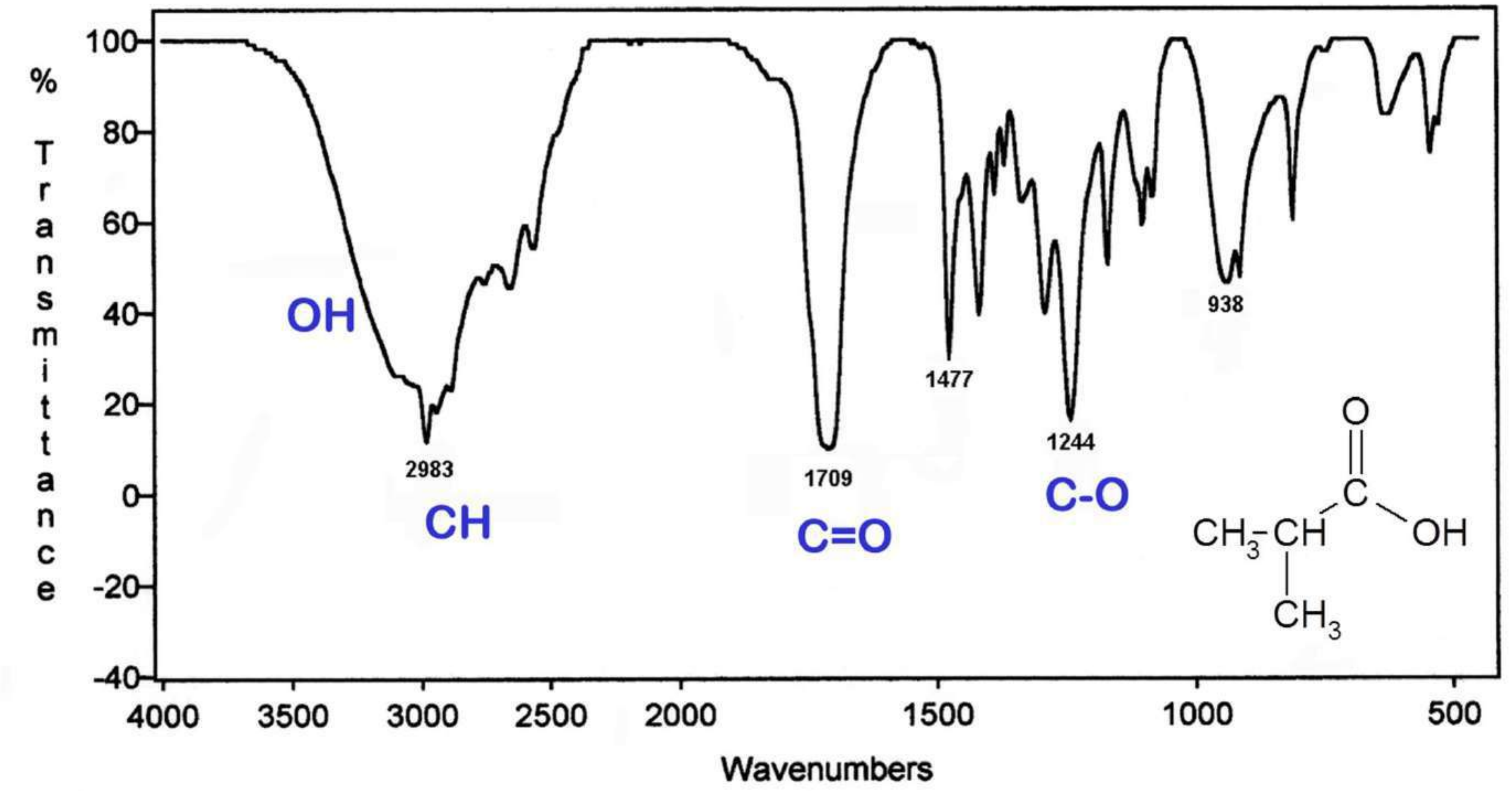
## Alcohol
## Base = 3600
## Base = 1100

Cyclohexanol



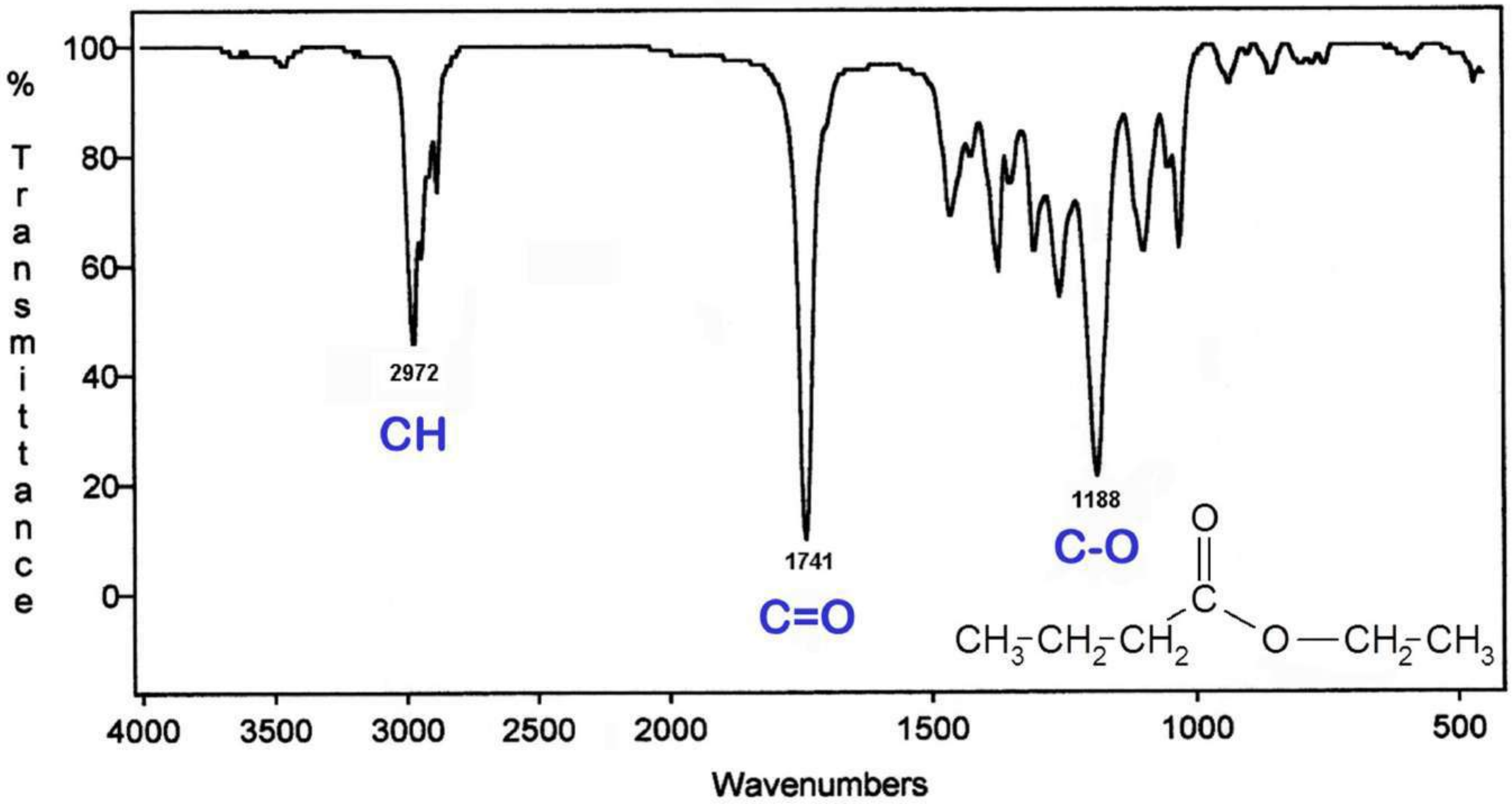
# Carboxylic acid

## 2-Methylpropanoic Acid

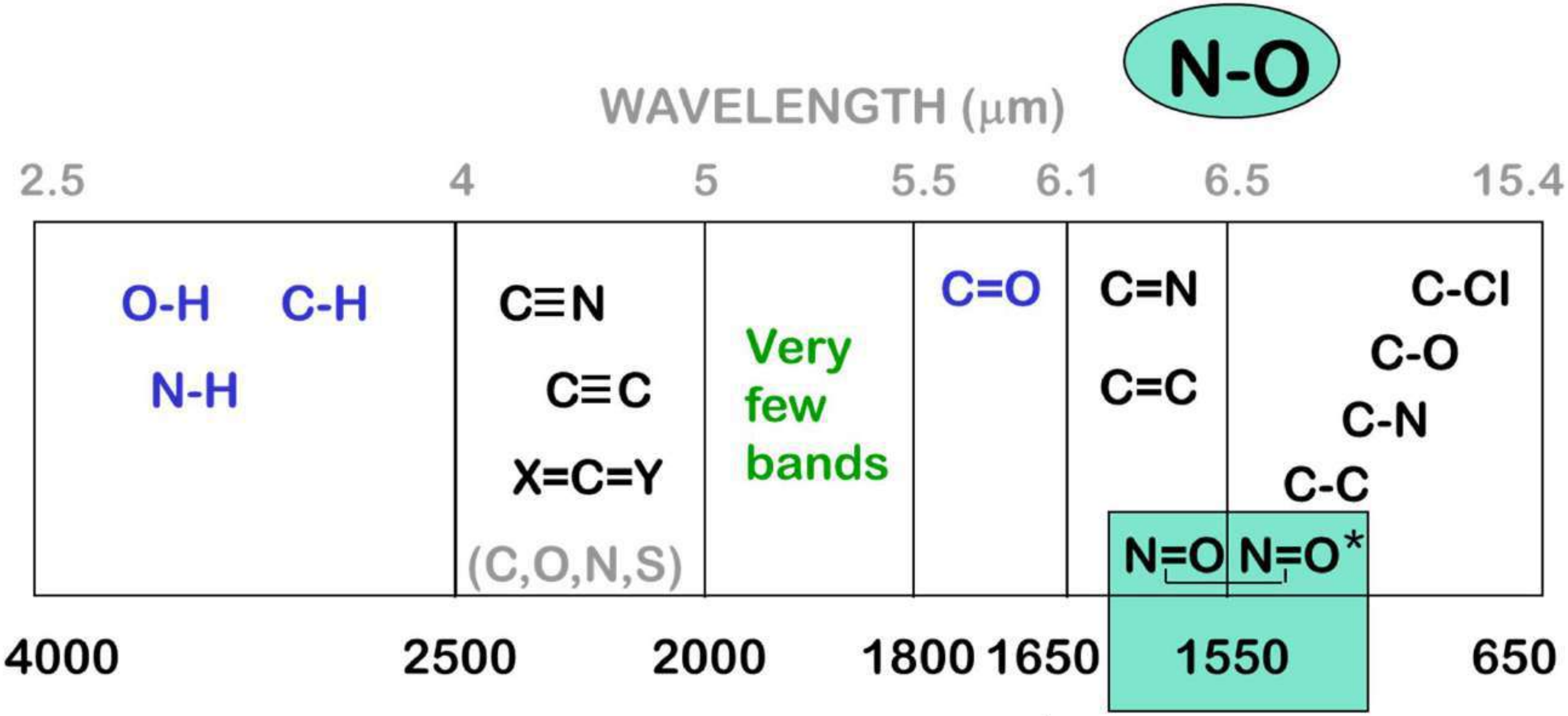


# Ester

## Ethyl Butanoate



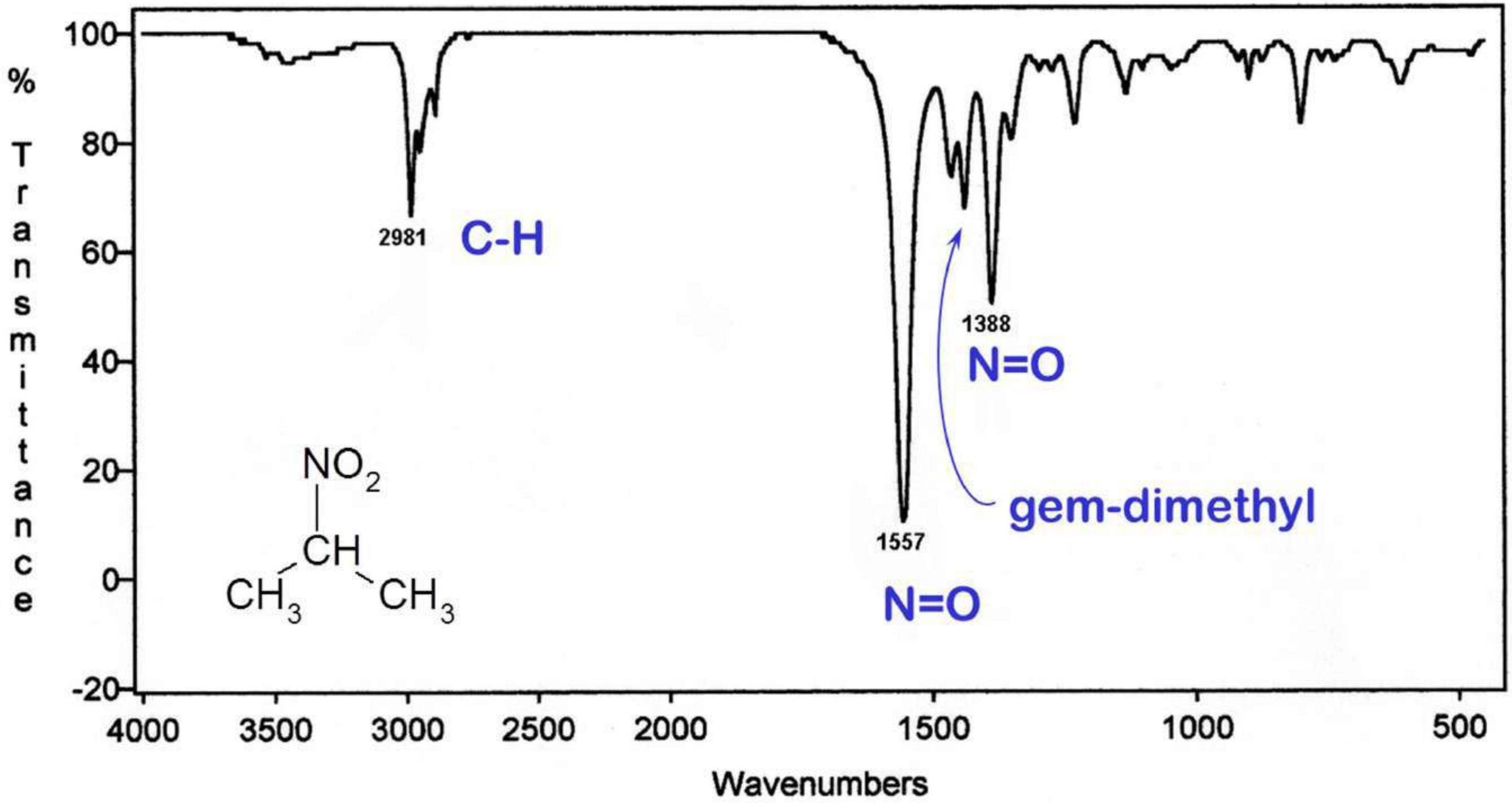
# The N=O stretching region



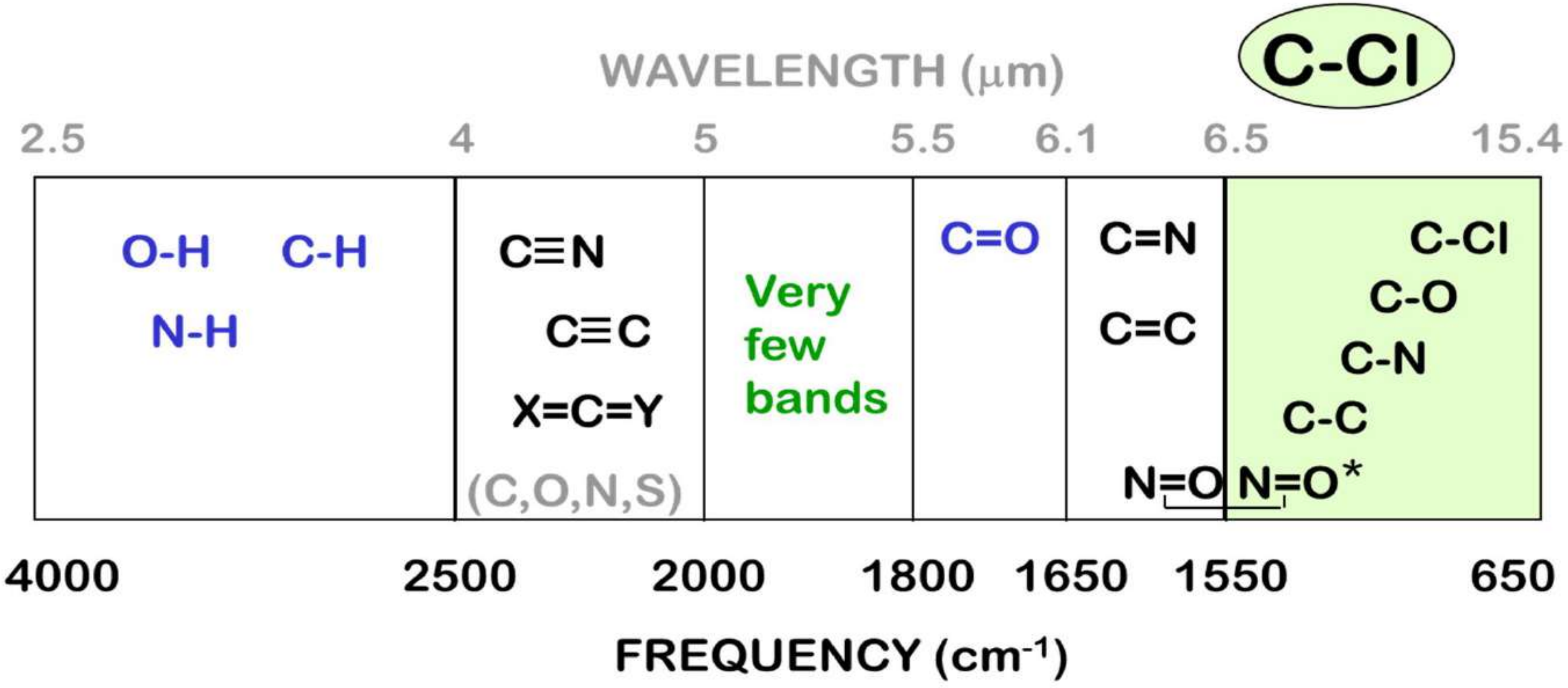
- N=O stretching : 1550 and 1350 cm$^{-1}$ asymmetric and symmetric stretching.
- Often the 1550 cm$^{-1}$ peak is stronger than the other one.

# Nitroalkane

## 2-Nitropropane

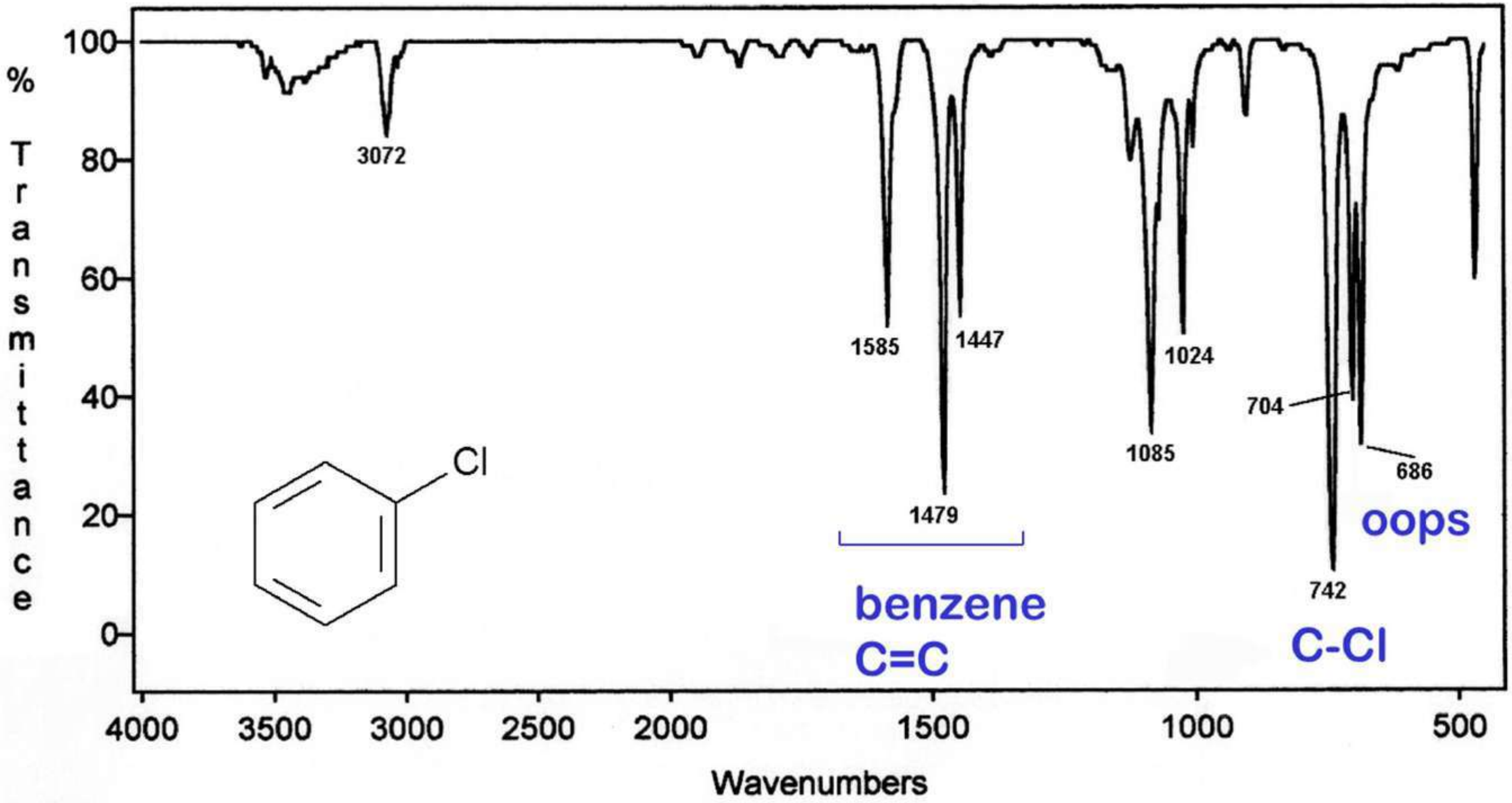


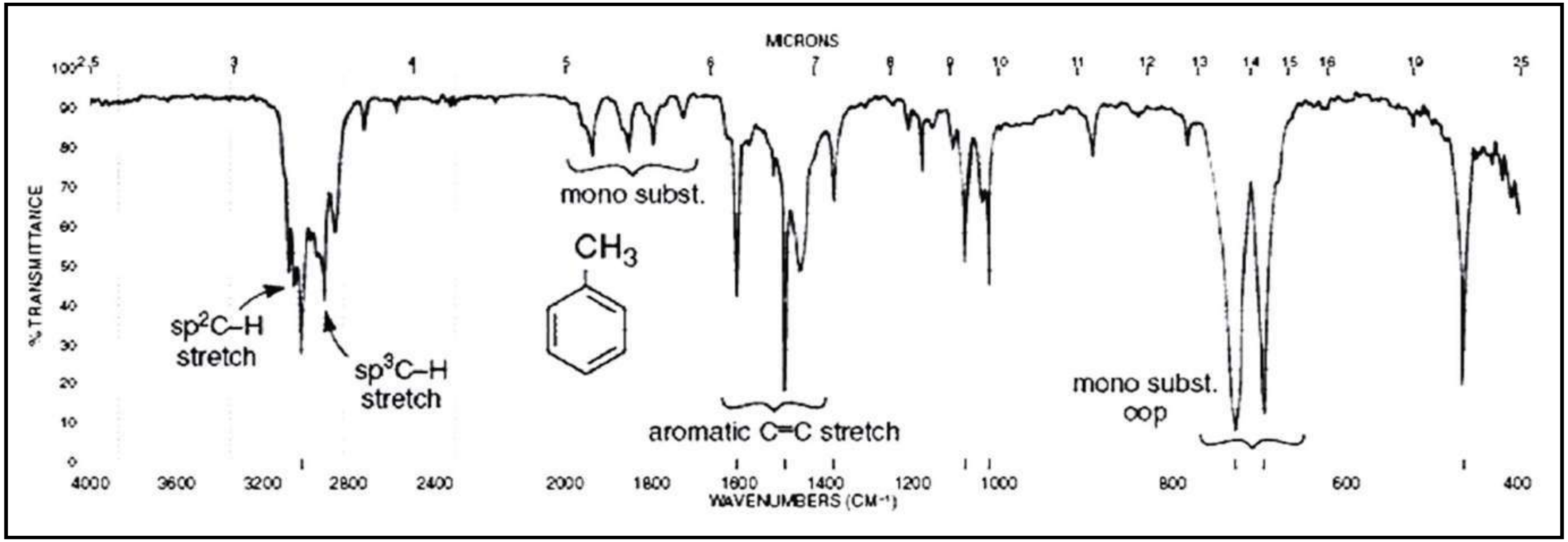
# The C-X stretching region



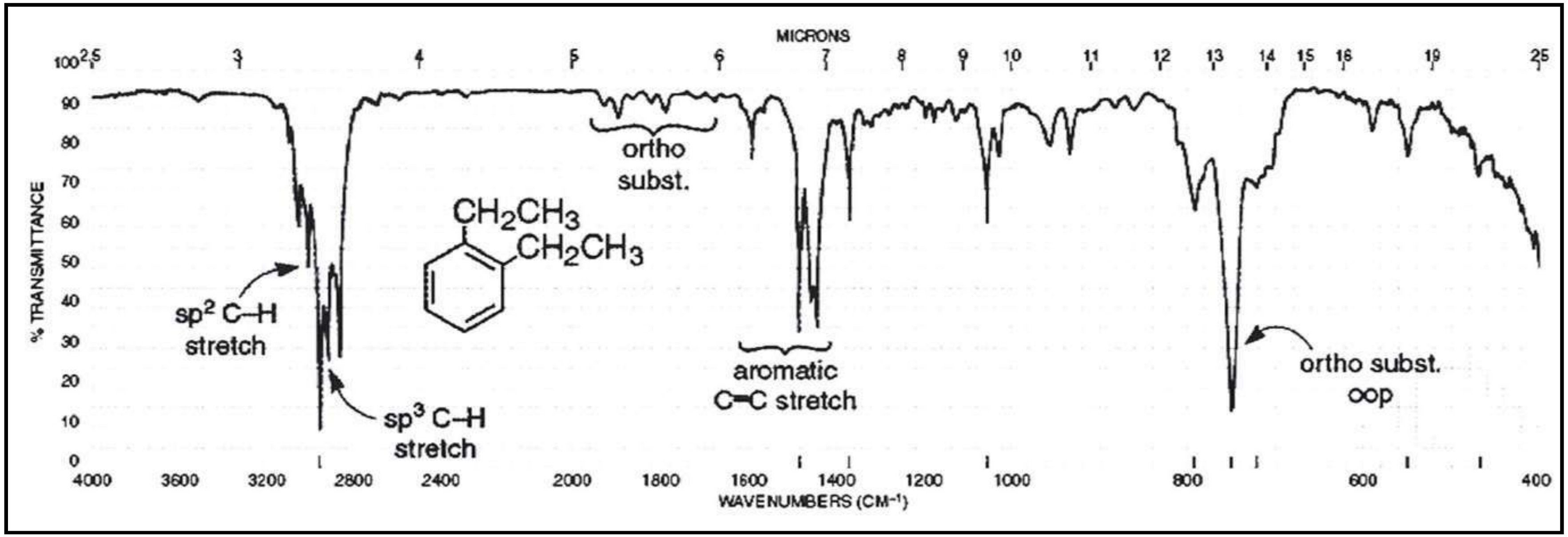
- C-Cl 785 to 540 $\mathrm{cm}^{-1}$,
  often hard to find amongst the fingerprint bands!!
- C-Br and C-I
  appear outside the useful range of infrared spectroscopy.
- C-F bonds can be found easily, but are not that common.

# Chlorobenzene

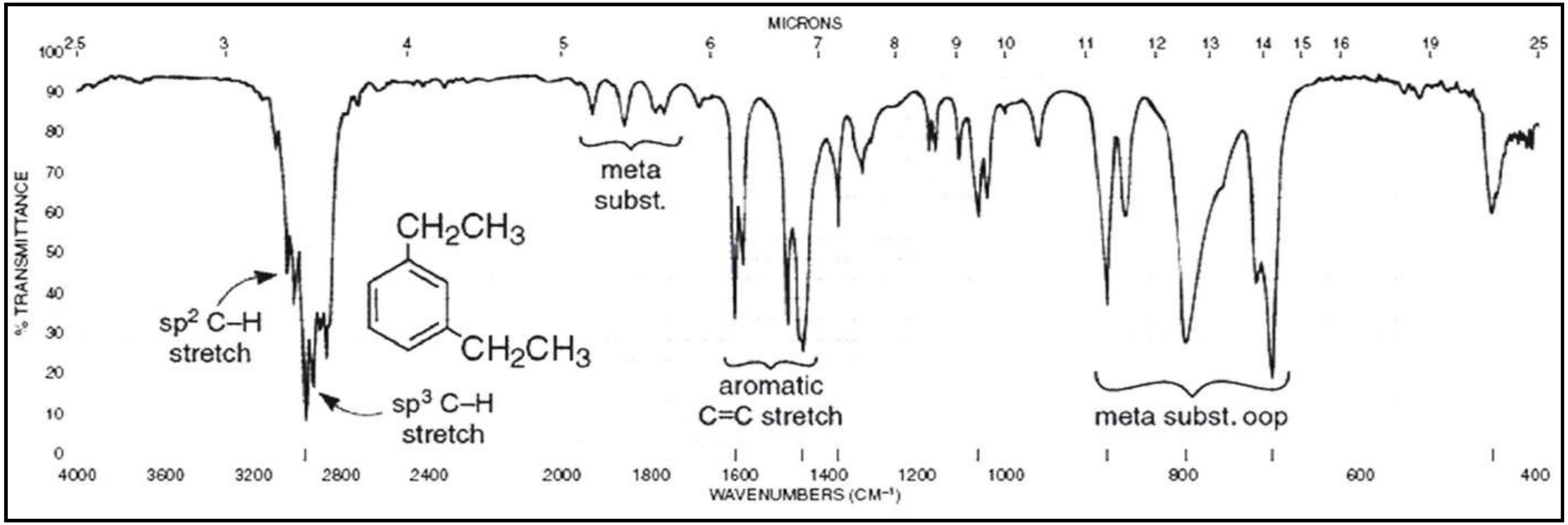


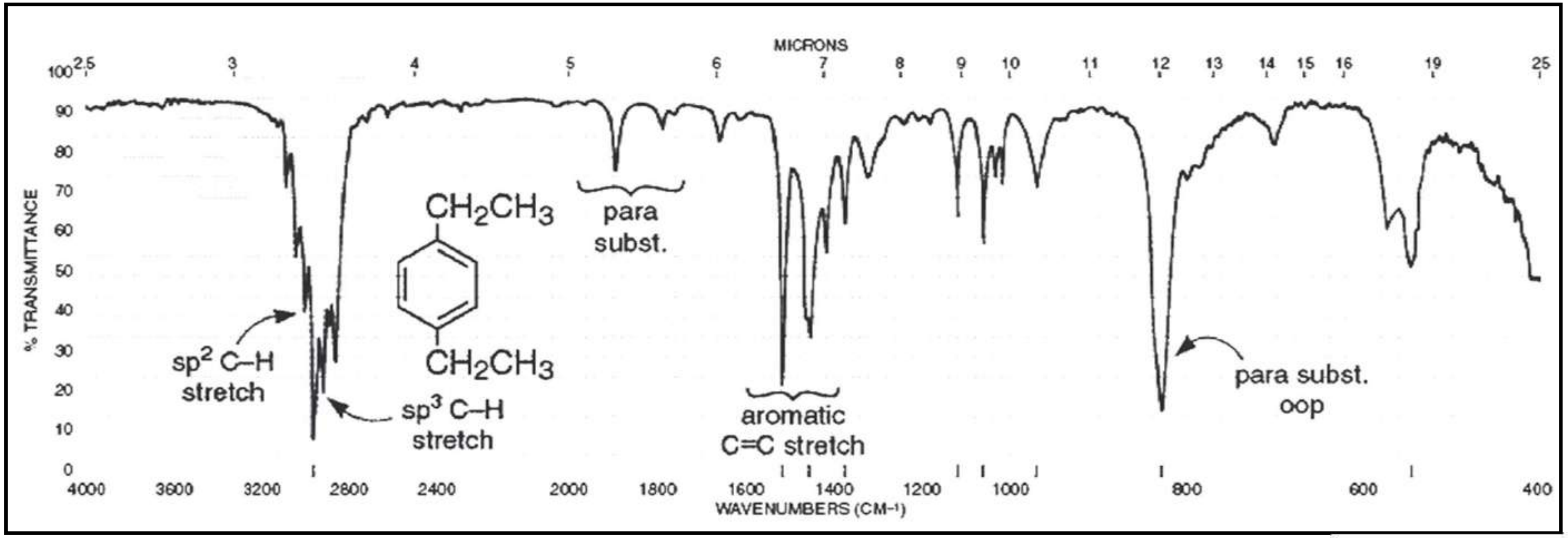


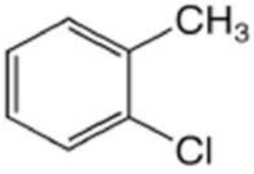
MICRONS
2.5
3
4
5
6
7
8
9
10
11
12
13
14
15
16
19
25
% TRANSMITTANCE
100
90
80
70
60
50
40
30
20
10
0
mono subst.
$CH_3$
$sp^2C–H$ stretch
$sp^3C–H$ stretch
aromatic C=C stretch
mono subst. oop
4000
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
600
400
WAVENUMBERS (CM⁻¹)



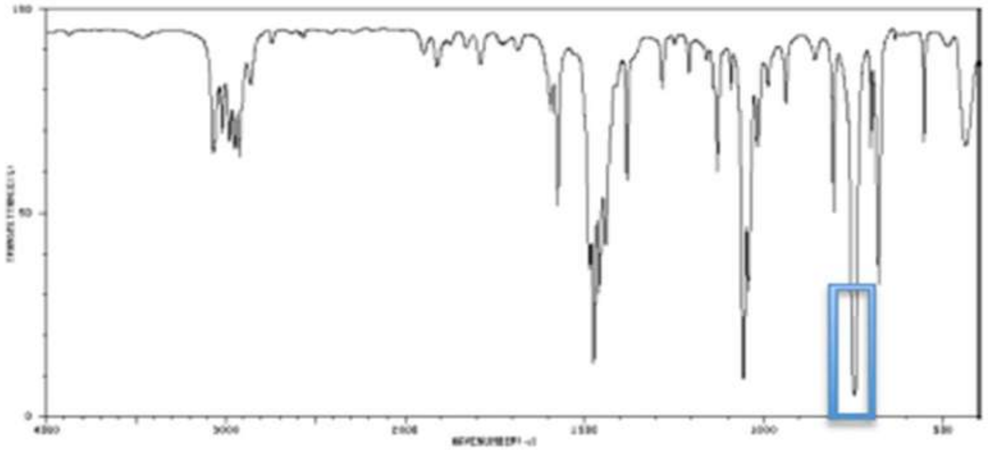
MICRONS
2.5
3
4
5
6
7
8
9
10
11
12
13
14
15
16
19
25
% TRANSMITTANCE
100
90
80
70
60
50
40
30
20
10
0
ortho subst.
$CH_2CH_3$
$CH_2CH_3$
$sp^2$ C–H stretch
$sp^3$ C–H stretch
aromatic C=C stretch
ortho subst. oop
4000
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
600
400
WAVENUMBERS (CM⁻¹)

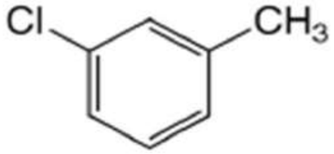

MICRONS
2.5
3
4
5
6
7
8
9
10
11
12
13
14
15
16
19
25
100
90
80
70
60
50
40
30
20
10
0
% TRANSMITTANCE
$CH_2CH_3$
$CH_2CH_3$
meta
subst.
$sp^2$ C–H
stretch
$sp^3$ C–H
stretch
aromatic
C=C stretch
meta subst. oop
4000
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
600
400
WAVENUMBERS (CM⁻¹)


MICRONS
2.5
3
4
5
6
7
8
9
10
11
12
13
14
15
16
19
25
100
90
80
70
60
50
40
30
20
10
0
% TRANSMITTANCE
$CH_2CH_3$
$CH_2CH_3$
para
subst.
$sp^2$ C–H
stretch
$sp^3$ C–H
stretch
aromatic
C=C stretch
para subst.
oop
4000
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
600
400
WAVENUMBERS (CM⁻¹)

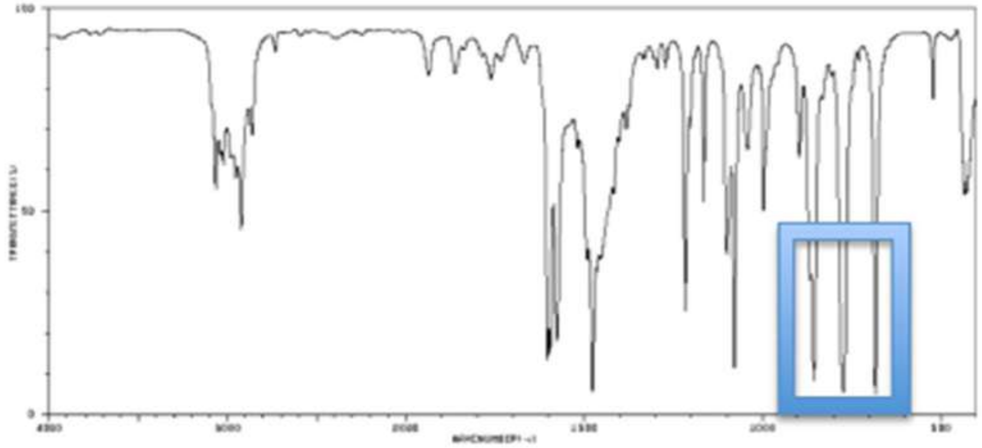


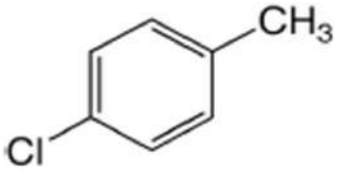
strong peak 747 cm-1





strong peaks 866, 773, 682 cm-1





strong peak 806 cm-1