Republic of Iraq
Ministry of Higher Education & Scientific research
Al-Mustaqbal University
Science College
Biochemistry Department

Analytical Chemistry Instrumental Analysis

For

Second Year Student/course 1

Lecture 5

By

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2025-2026

Infrared Spectroscopy

- Infrared spectroscopy is used in identification of functional groups in pure compounds.

- Infra-red (IR) does not have sufficient energy to induce electronic transition as seen in UV spectroscopy. When molecule absorbed electromagnetic radiation in IR region, undergoes vibrational or a rotational transitions which causes net change in the dipole moment in the molecule (IR active, for example HCl, CO etc), if dipole moment does not change in molecules then they are IR inactive (for example: O_2, H_2, N_2 etc.) means they does not absorb IR radiation. IR region ranges from 4000-400 cm^{-1}

- If the frequency of IR radiation matched with the vibrational frequency of molecule, then molecule absorb radiation.

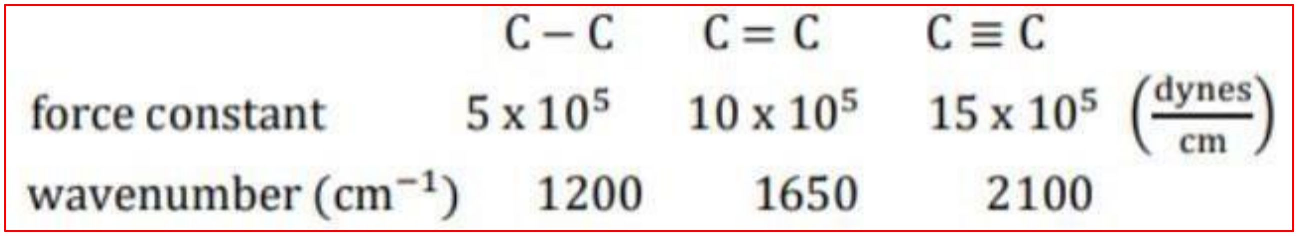
- IR spectroscopy based on Hooke's law, suppose two atoms or masses are connected through spring (bond), then frequency of vibration can be represented by following equation:

$$\boxed{\nu = \frac{1}{2\pi}\sqrt{\frac{\kappa}{\mu}} \quad \text{or} \quad \bar{\upsilon} = \frac{1}{2\pi c}\sqrt{\frac{\kappa}{\mu}}}$$

- Where, κ is force constant of the bond, $\bar{\upsilon}$ is wave-number (cm^{-1}), ν is the frequency, c is speed of light and μ is reduce mass (m1 and m2 are the masses of atoms)

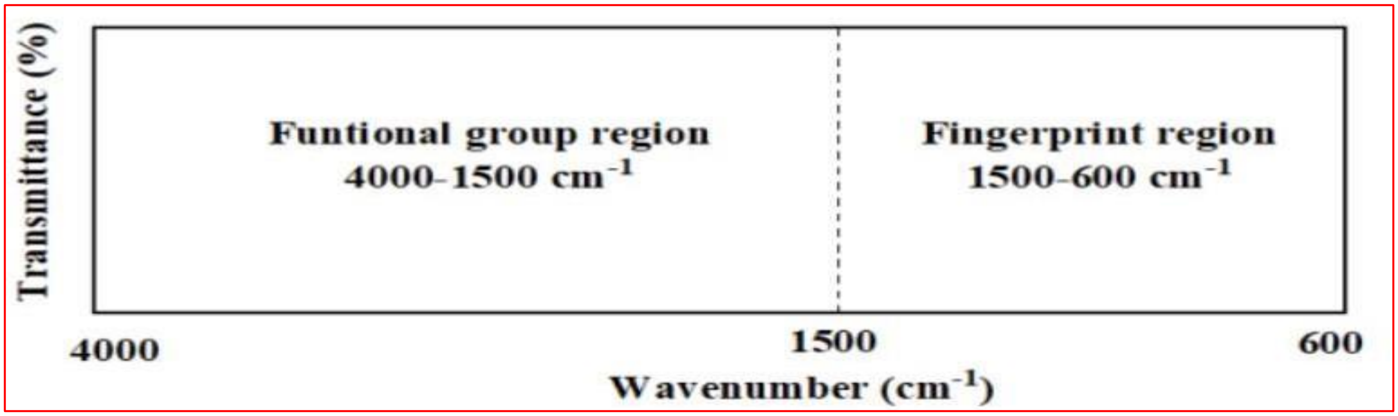
$$\boxed{\mu = \frac{m_1 \times m_2}{(m_1 + m_2)}}$$

- Stronger the bond, greater the value of force constant (κ), higher the frequency vibration or wave-number (cm^{-1}). For example,



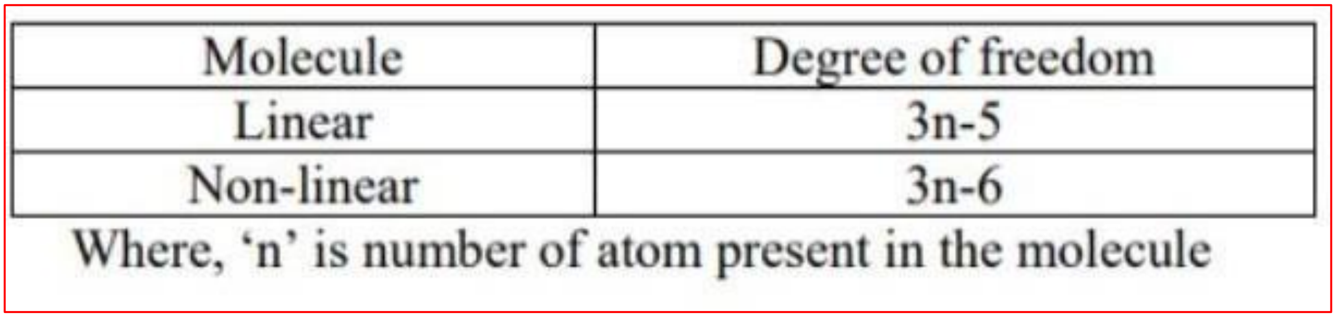
	$C-C$	$C=C$	$C\equiv C$	
force constant	5×10^5	10×10^5	15×10^5	$\left(\frac{dynes}{cm}\right)$
wavenumber (cm^{-1})	1200	1650	2100	

IR spectrum is divided mainly into two region as follows;



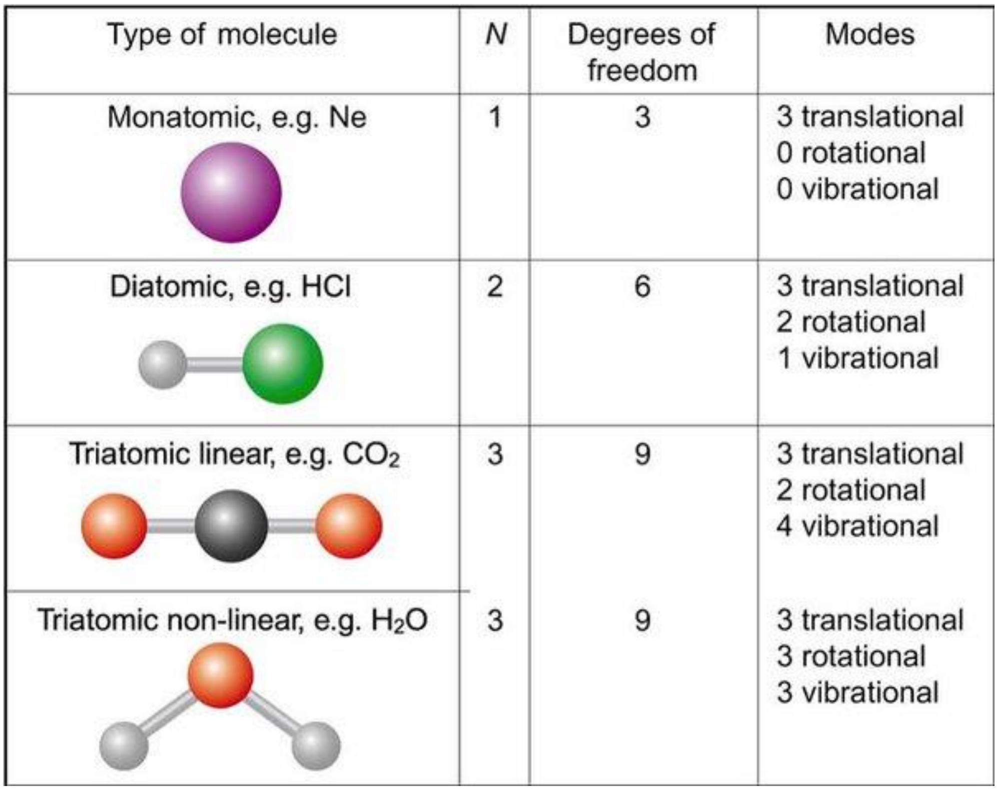
Fundamental Vibration

These vibrations are arising when molecule promoted from ground state to lower excited state. The fundamental vibrations for linear and non-linear molecules are determined by following way:



Molecule	Degree of freedom
Linear	3n-5
Non-linear	3n-6

Where, ‘n’ is number of atom present in the molecule

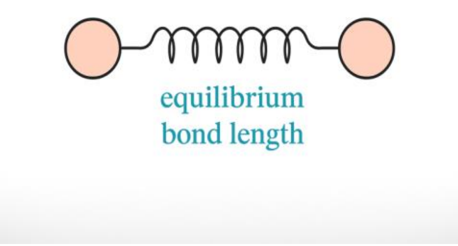


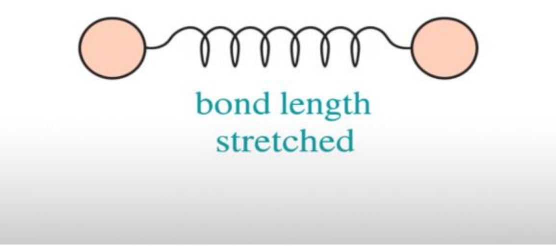
Type of molecule	N	Degrees of freedom	Modes
Monatomic, e.g. Ne	1	3	3 translational 0 rotational 0 vibrational
Diatomic, e.g. HCl	2	6	3 translational 2 rotational 1 vibrational
Triatomic linear, e.g. CO_2	3	9	3 translational 2 rotational 4 vibrational
Triatomic non-linear, e.g. H_2O	3	9	3 translational 3 rotational 3 vibrational

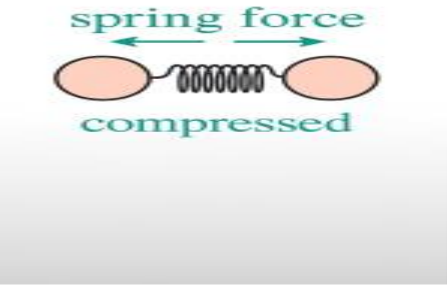
Fundamental Vibration

- ✓ IR Region: Wavelength from 2.5 to 15 μm& Wavenumber(600 -4000 cm^{-1}.
- ✓ **Wavenumber = vibrational frequency**
- ✓ **Stretching Vibrations:** Stretching vibration is a type of molecular vibration where the length of a chemical bond changes periodically, similar to the stretching and compressing of a spring.
- ✓ his type of vibration requires higher energy compared to bending vibrations.
- ✓ **Bending Vibrations:** Bending vibration is a type of molecular vibration where the angle between bonds changes periodically.

- ✓ his type of vibration **requires lower energy** compared to stretching vibrations.

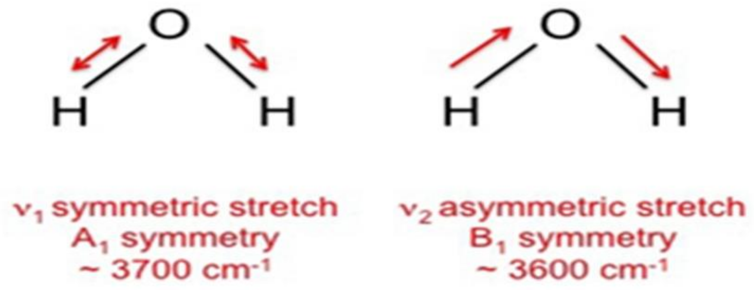




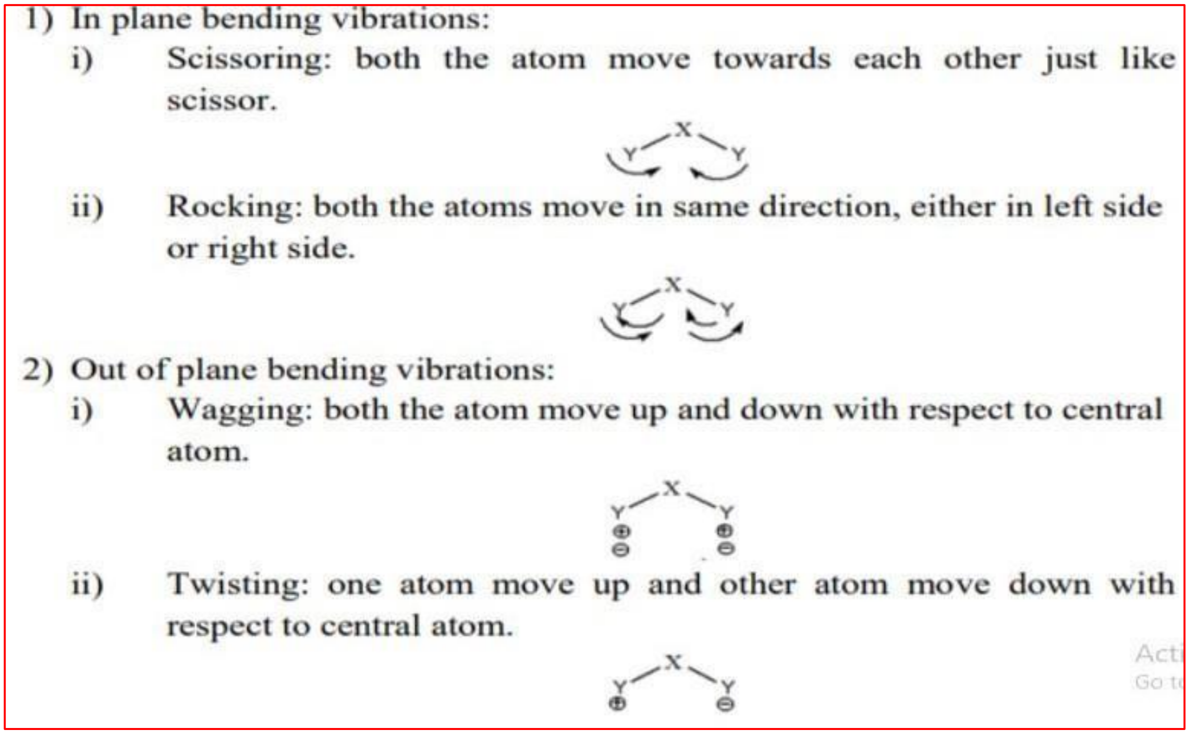


Types of stretching vibrations

- ✓ **Symmetric stretching vibration**: In this case both the atoms stretched or compressed in same direction.
- ✓ **Asymmetric stretching vibration**: In this vibration one atom undergoes stretching and other atom undergoes compression and vice versa.



Bending vibrations: Distance between two atom remains constant but bond angle changes. These vibrations can occur either in plane or out of plane



1) In plane bending vibrations:

   i) Scissoring: both the atom move towards each other just like scissor.

   ii) Rocking: both the atoms move in same direction, either in left side or right side.

2) Out of plane bending vibrations:

   i) Wagging: both the atom move up and down with respect to central atom.

   ii) Twisting: one atom move up and other atom move down with respect to central atom.

Function groups

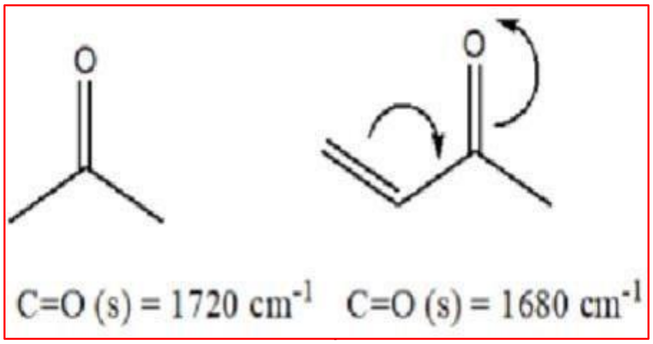
- ✓ Number of molecules contains same functional group & show similar peak above 1500 cm^{-1} but they show different peak in finger print region. Therefore we can say that each and every molecule have unique peak or band which is observed in finger print region, it is just like the finger print of human.

Functional Group	Type of Vibration	Wavenumber (cm^{-1})	Notes
O–H (alcohol)	Stretch	3200–3600	Broad, strong
O–H (carboxylic acid)	Stretch	2500–3300	Very broad
N–H (amine/amides)	Stretch	3300–3500	Medium, may show two peaks (primary amines)
C–H (alkane)	Stretch	2850–2960	Sharp, medium
C–H (alkene)	Stretch	3010–3100	Weak
C–H (alkyne)	Stretch	3300	Sharp
C≡C (alkyne)	Stretch	2100–2260	Weak to medium
C≡N (nitrile)	Stretch	2220–2260	Medium to strong
C=O (carbonyl)	Stretch	1650–1750	Strong, sharp; shifts depending on compound type
— Aldehyde	C=O stretch	1720–1740	Also has C–H stretch near 2720, 2820
— Ketone	C=O stretch	1705–1725	Strong
— Carboxylic acid	C=O stretch	1700–1725	Strong
— Ester	C=O stretch	1735–1750	Strong
— Amide	C=O stretch	1630–1690	Medium
C=C (alkene)	Stretch	1600–1680	Medium
Aromatic ring	C=C stretch	1450–1600	Multiple medium bands
C–O (alcohol, ether, ester)	Stretch	1000–1300	Strong
NO_2 (nitro group)	Asymmetric + symmetric stretch	1500–1600, 1300–1360	Two strong bands

Factor affecting vibrational frequency

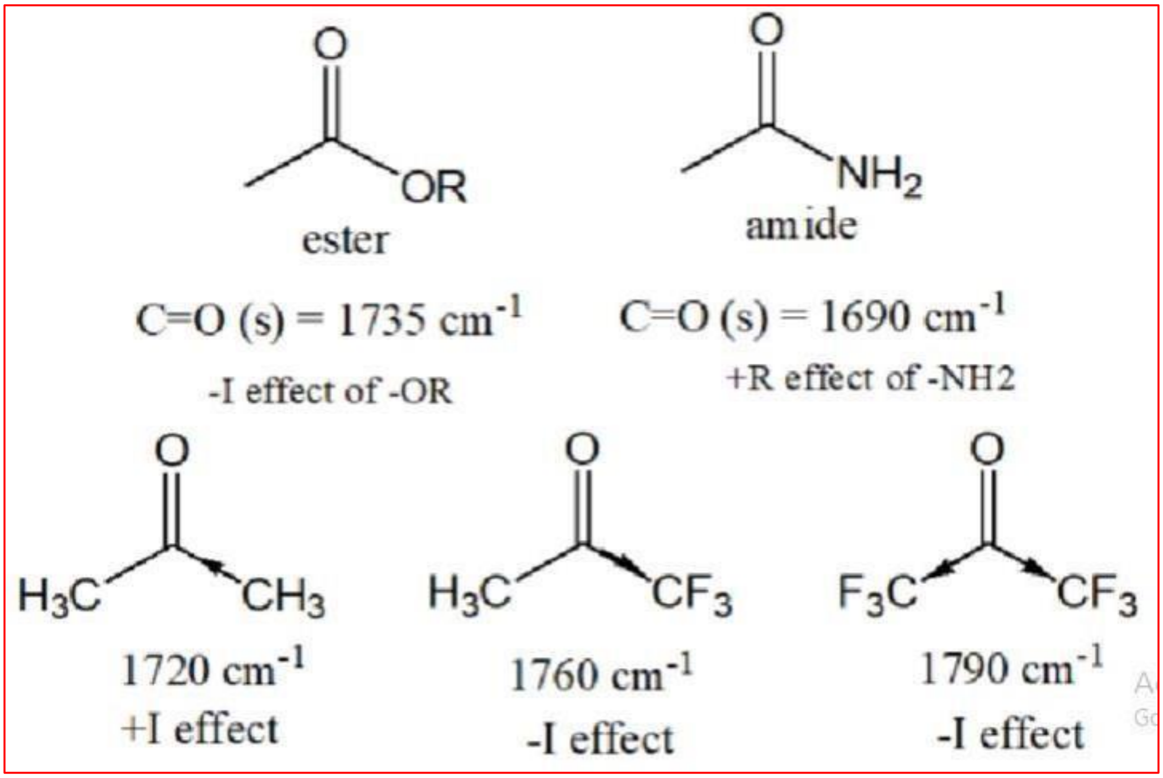
1-Conjugation:

As the conjugation increase, stretching frequency decreases , because force content decrease due to conjugation.



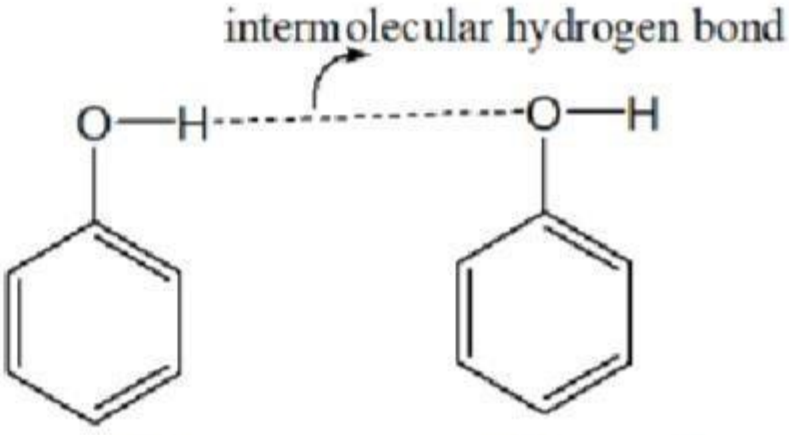
2-Inductive effect and resonance effect:

Oxygen is more electronegative than nitrogen, therefore nitrogen easily donate electron or lone pair of nitrogen undergoes delocalization with C=O bond. Due to delocalization double bond of C=O changes into partial double bond therefore force constant decreases which decrease the C=O stretching frequency.



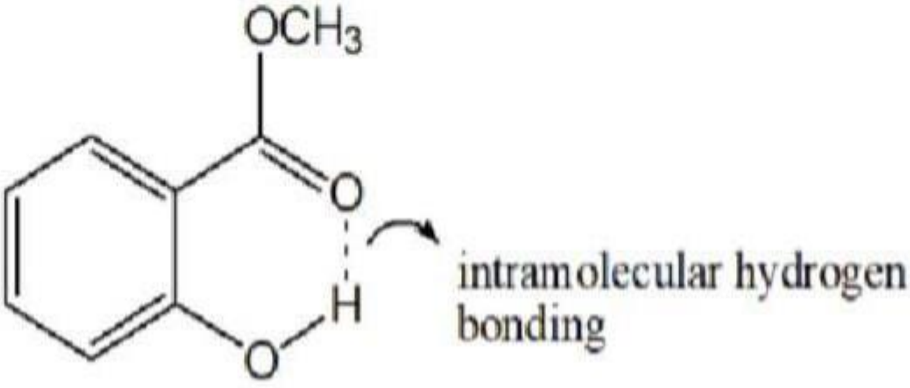
3-Hydrogen bonding:

Intermolecular hydrogen bonding weakens the O- H bond, thereby shifting the band to lower frequency. For example, in neat solution O-H stretching vibration of phenol observed in the range from 3400- 3300 cm^{-1}. When solution is dilute then O-H frequency shifted towards higher frequency at 3600 cm^{-1}.



O-H frequency = 3400-3300cm^{-1}

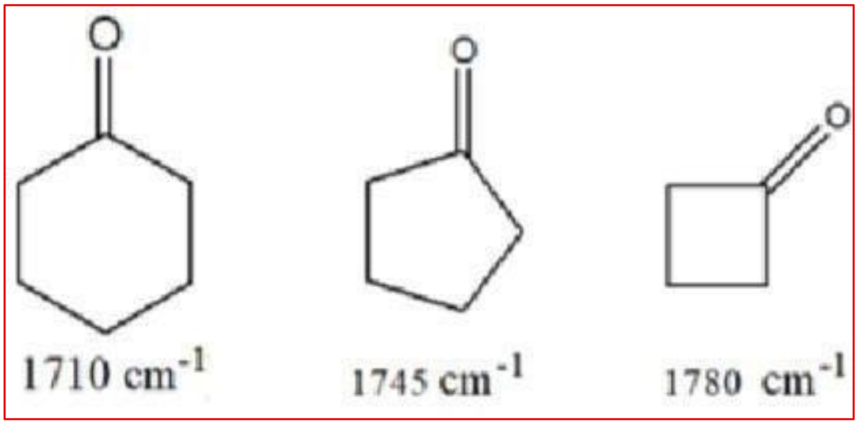
- Whereas in case of methyl salisilate, intramolecular hydrogen bonding lower down the stretching frequency of O-H at 3200 cm^{-1} . Intramolecular hydrogen bonding does not change its frequency even in very dilute solution because upon dilution structure of compound does not change.



O-H frequency centered at 3200 cm^{-1}

4-Ring strain:

As the size of the ring decrease, vibrational frequency of C=O increase. For example.



IR Spectroscopy Instrumentation

1. Source:

Emits infrared radiation — usually a Nernst glower or Globar (silicon carbide).

2. Sample Cell / Sample Holder:

Holds the sample in solid, liquid, or gaseous form.

3. Monochromator / Interferometer:

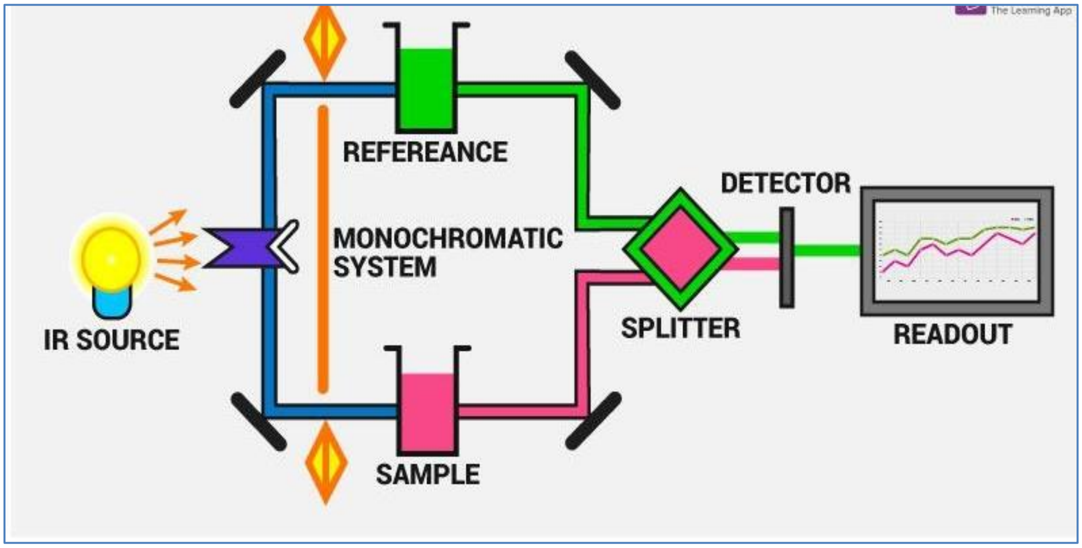
Separates the IR radiation into its component frequencies.

4. Detector:

Detects the transmitted or absorbed IR radiation — e.g., Thermocouple, Pyroelectric detector, or Photoconductive cell.

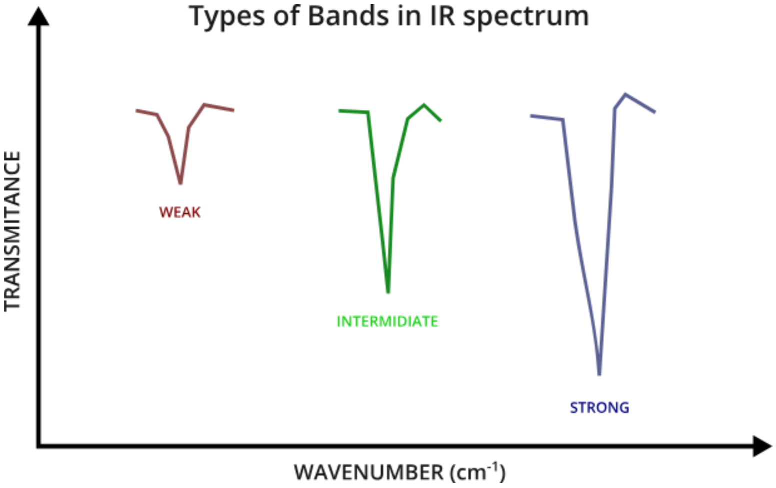
5. Recorder / Computer:

Converts the detected signal into a spectrum — a graph of **Transmittance (%) vs. Wavenumber (cm^{-1})**.



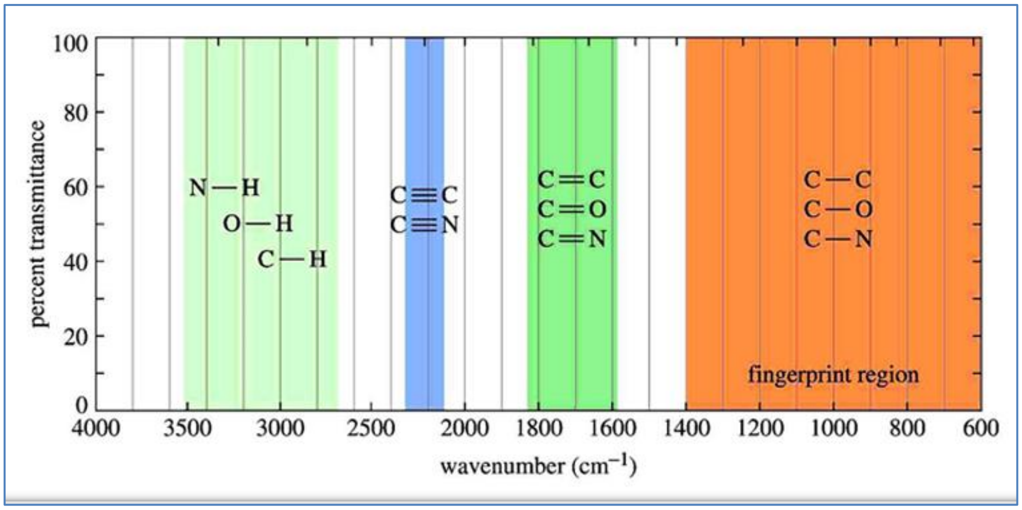
Uses and applications

- Infrared spectroscopy is a simple and reliable technique widely used in both organic and inorganic chemistry, in research and industry..
- It is used in quality control, used to analyze the insect repellent, Food and Drug Administration.
- Scientist uses portable near infrared spectroscopy device to detect potentially illegal substances.
- It is also used in forensic analysis in both criminal and civil cases, for example in identifying the blood alcohol content of a suspected drunk driver.

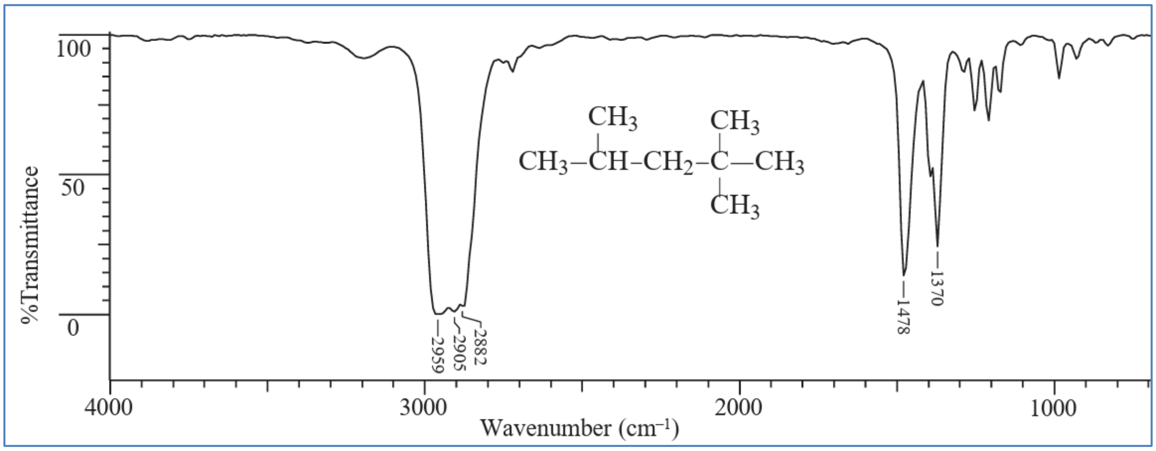


IR Absorption Range

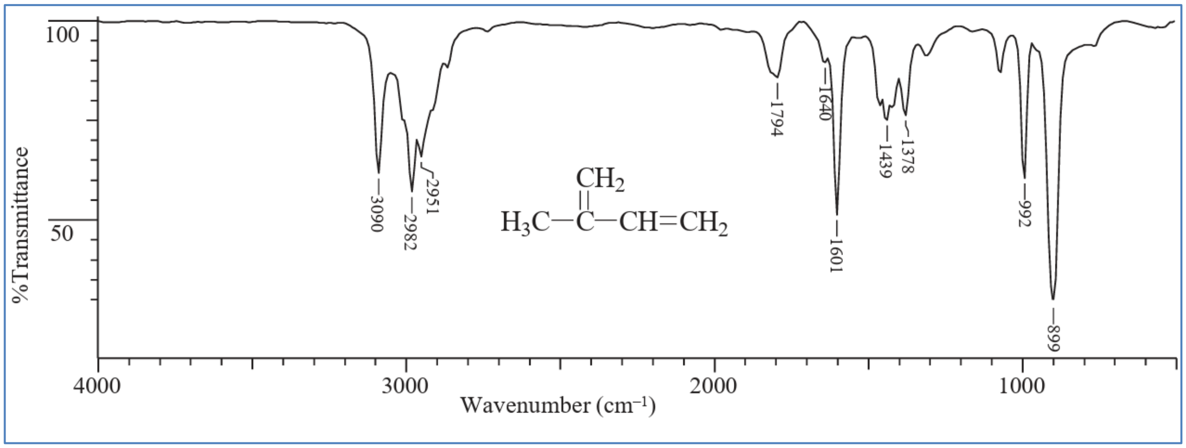
The typical IR absorption range for covalent bonds is 600 -4000 cm-1. The graph shows the regions of the spectrum where the following types of bonds normally absorb. For example a sharp band around 2200-2400 cm-1would indicate the possible presence of a C-N or a C-C triple bond.



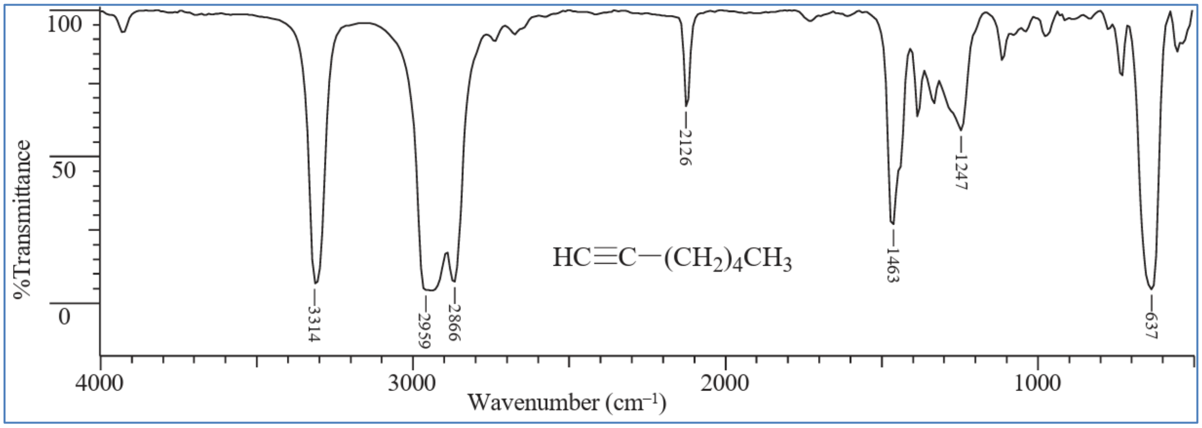
Alkanes



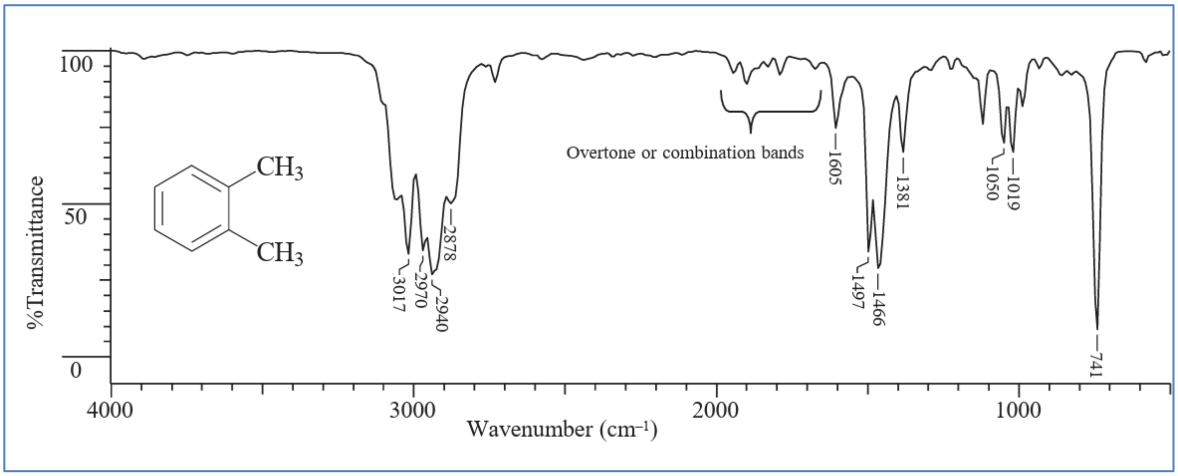
Alkenes



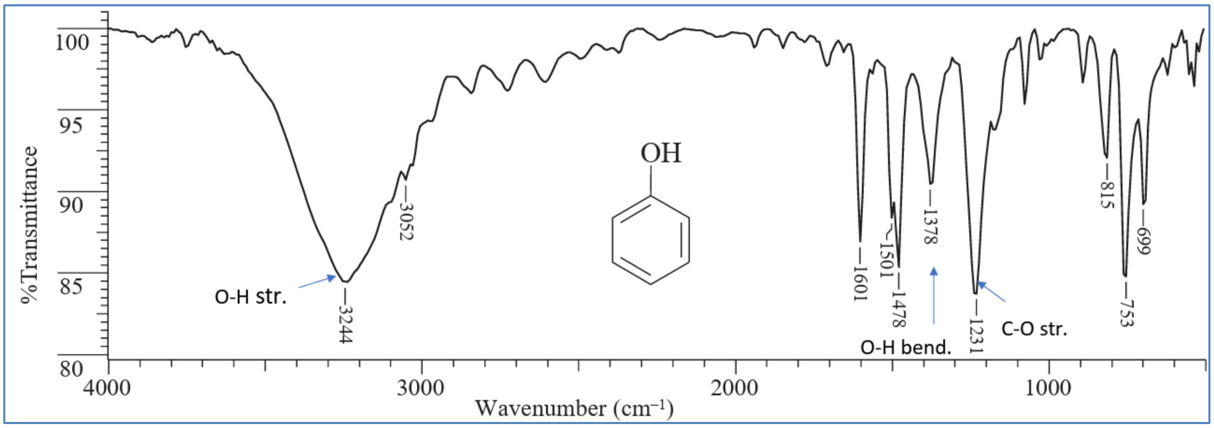
Alkynes



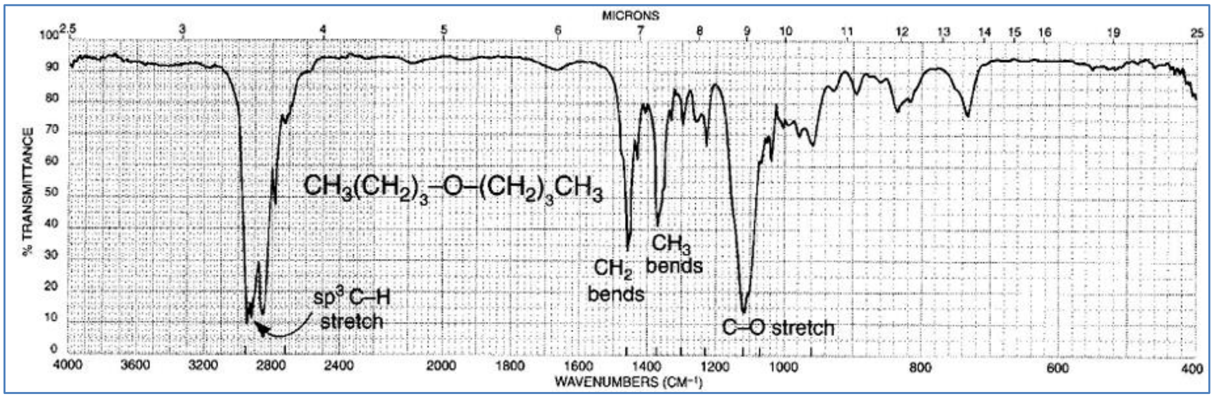
Aromatic Hydrocarbon



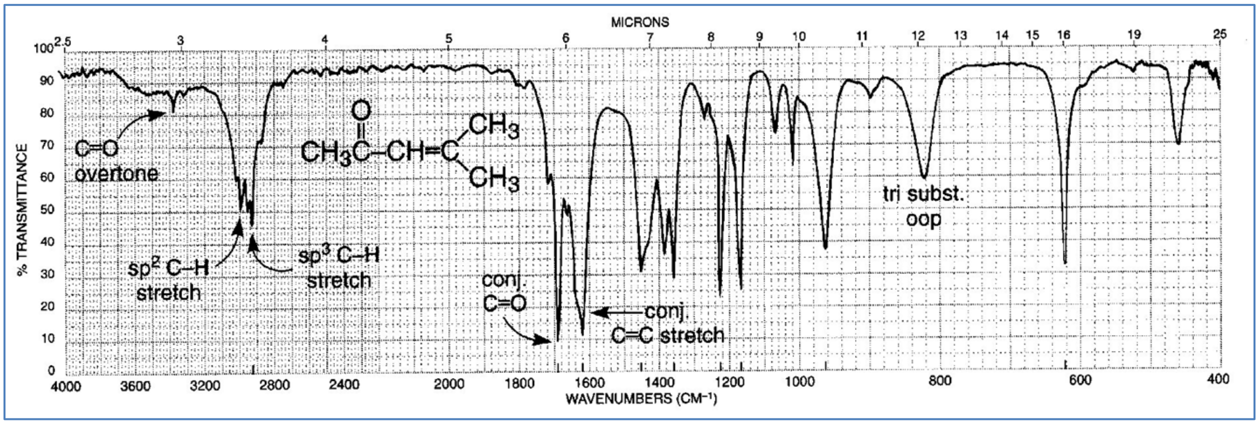
AlcoholsandPhenols



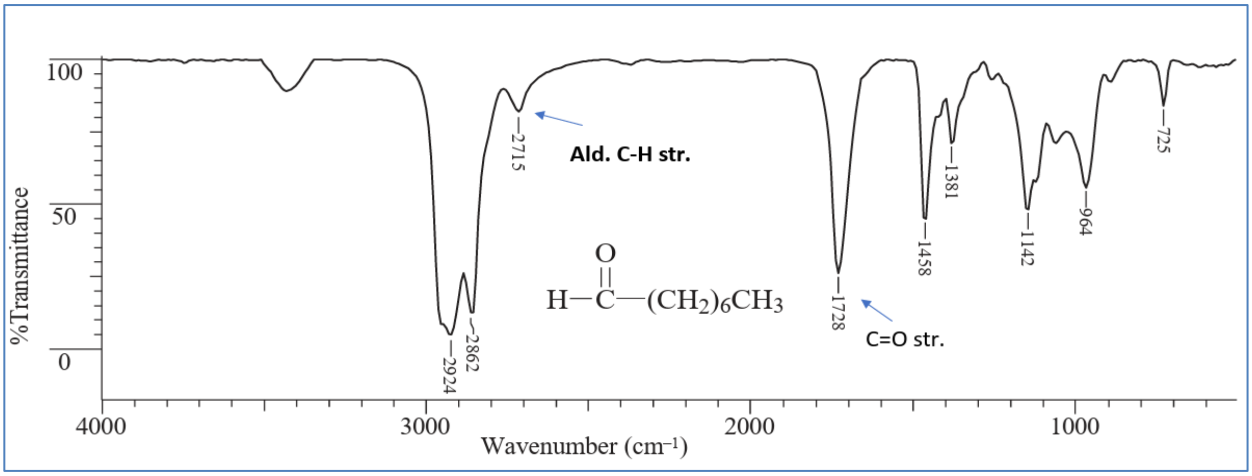
Ethers



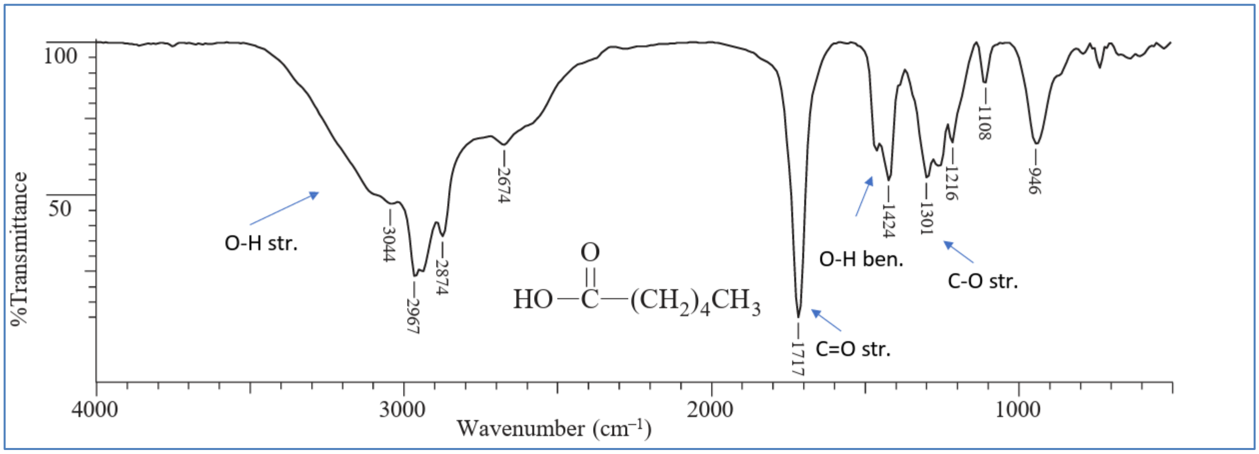
Ketone



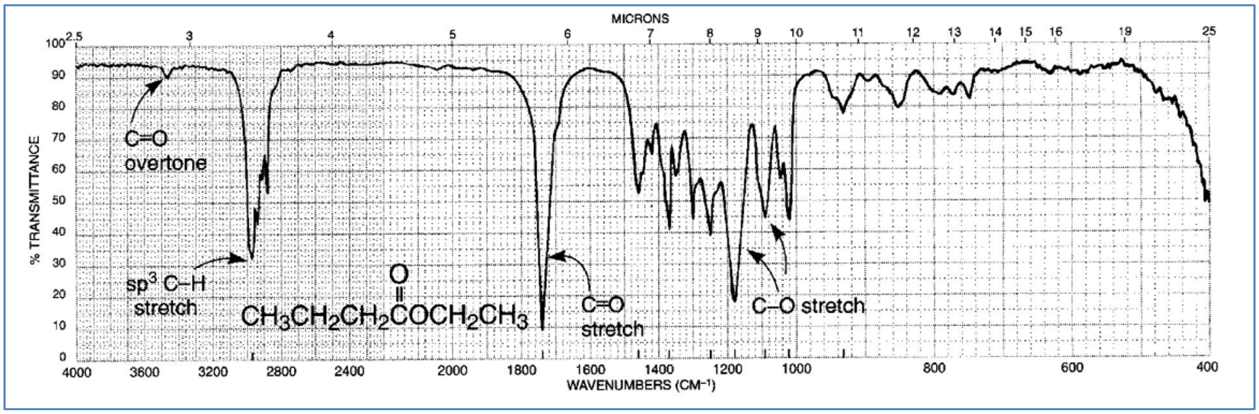
Aldehydes



Carboxylic Acids



Esters



Amines