INSTRUMENTATION

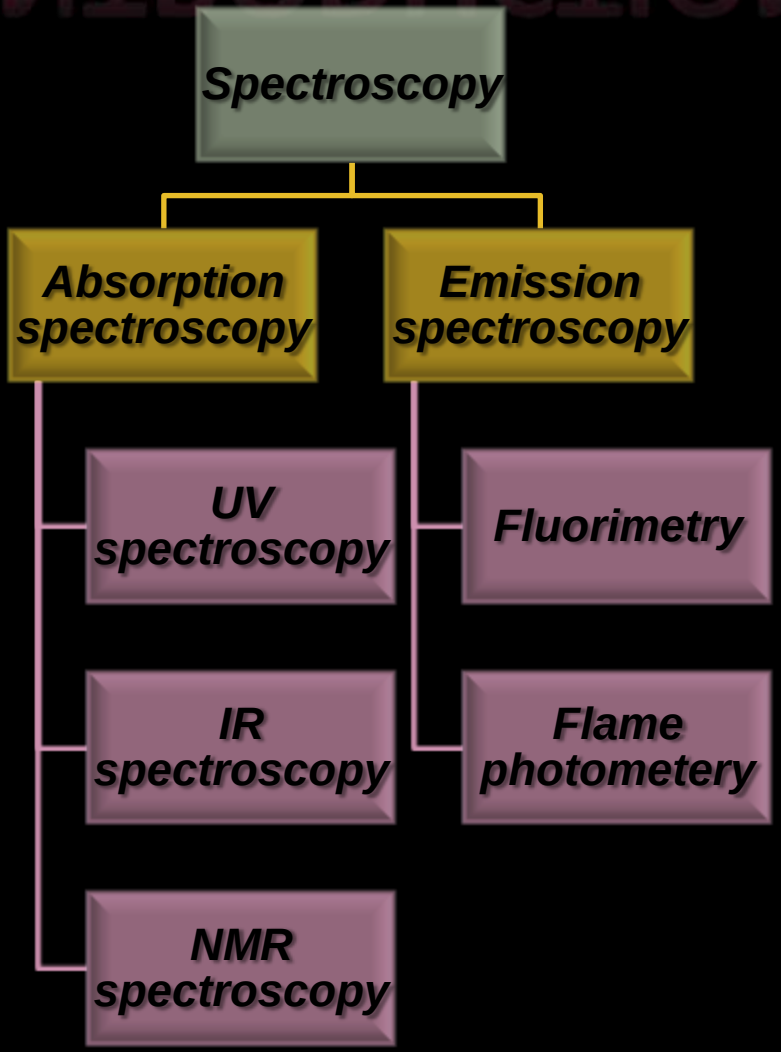
“INFRARED ABSORPTION SPECTROSCOPY”

“Introduction To IR Spectroscopy”

ANUM ASLAM

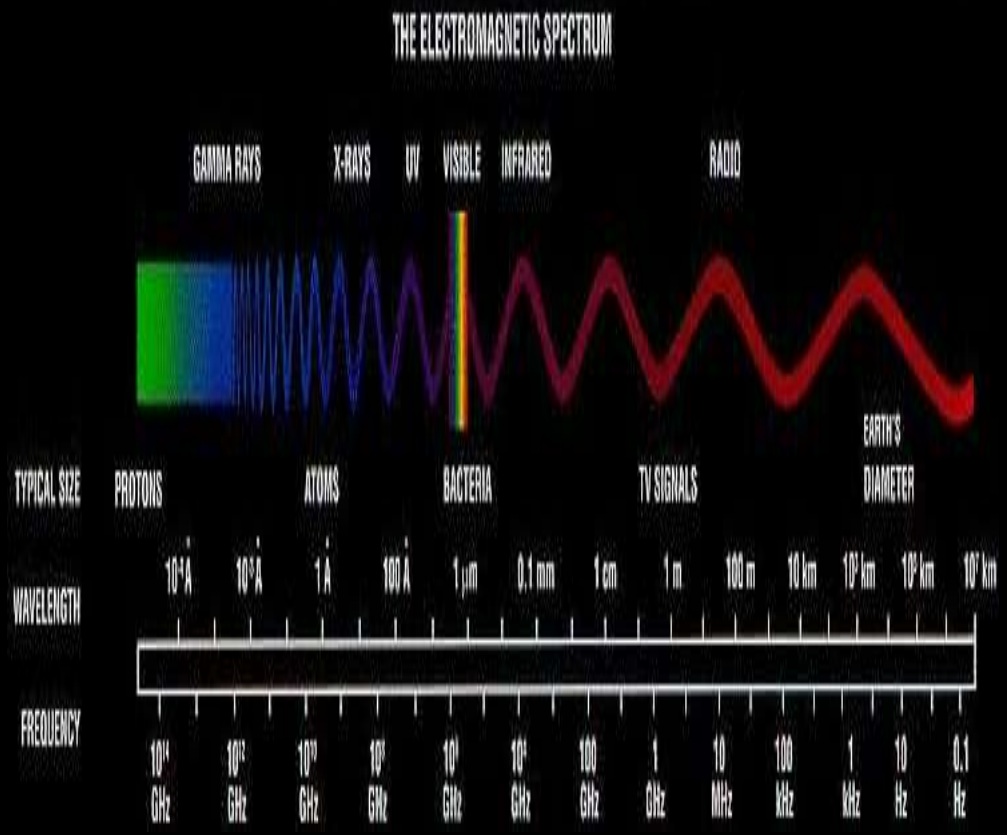
ROLL NO: 1214180

INTRODUCTION

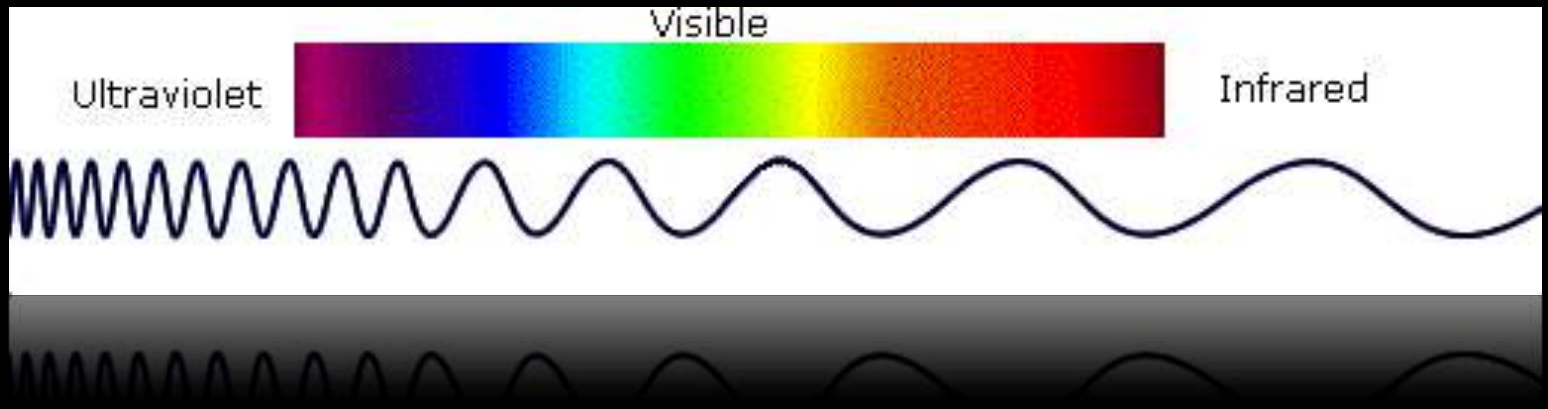


INFRARED SPECTROSCOPY

- **Infrared spectroscopy** (IR spectroscopy) is the spectroscopy that deals with the infrared region of the electromagnetic spectrum, that is light with a longer wavelength and lower frequency than visible light
- Infrared Spectroscopy is the analysis of infrared light interacting with a molecule.
- It is based on absorption spectroscopy



INFRARED REGIONS

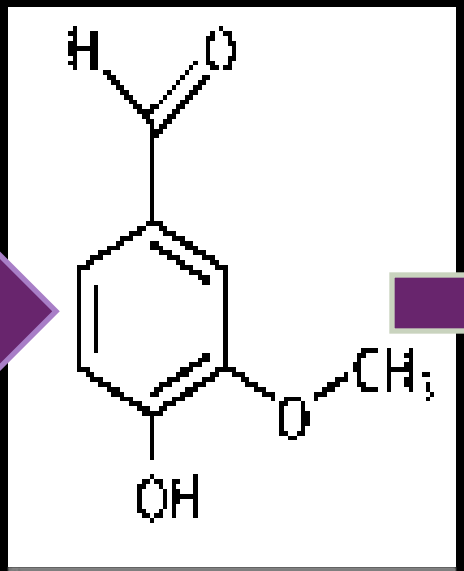


INFRARED REGIONS	RANGE
Near infrared region	*0.8-2.5 μ(12,500-4000 cm-1)*
Main infrared region	*2.5-15 μ(4000-667cm-1)*
Far infrared region	*15-200 m μ(667-100 cm-1)*

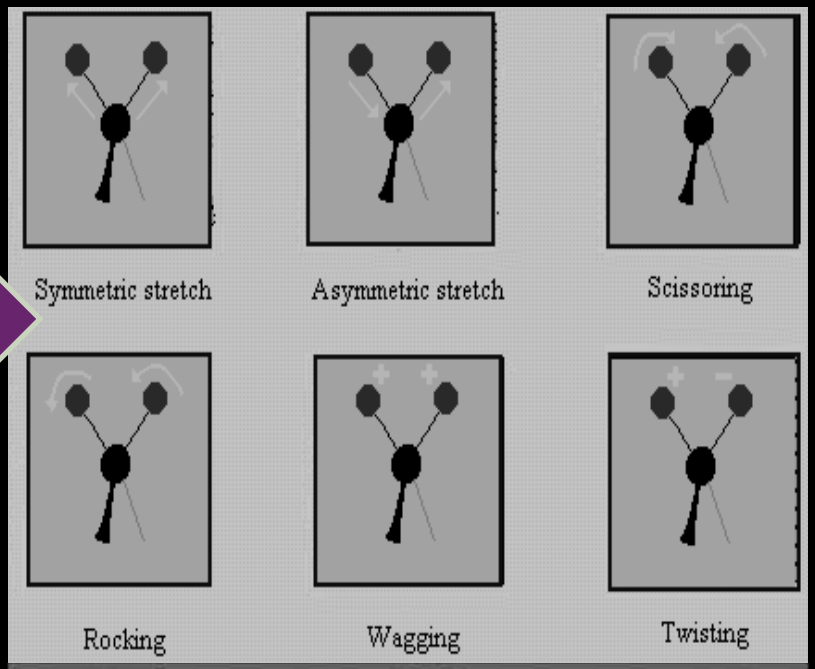
PRINCIPLE

- When infrared 'light' or radiation hits a molecule, the bonds in the molecule absorb the energy of the infrared and respond by vibrating.

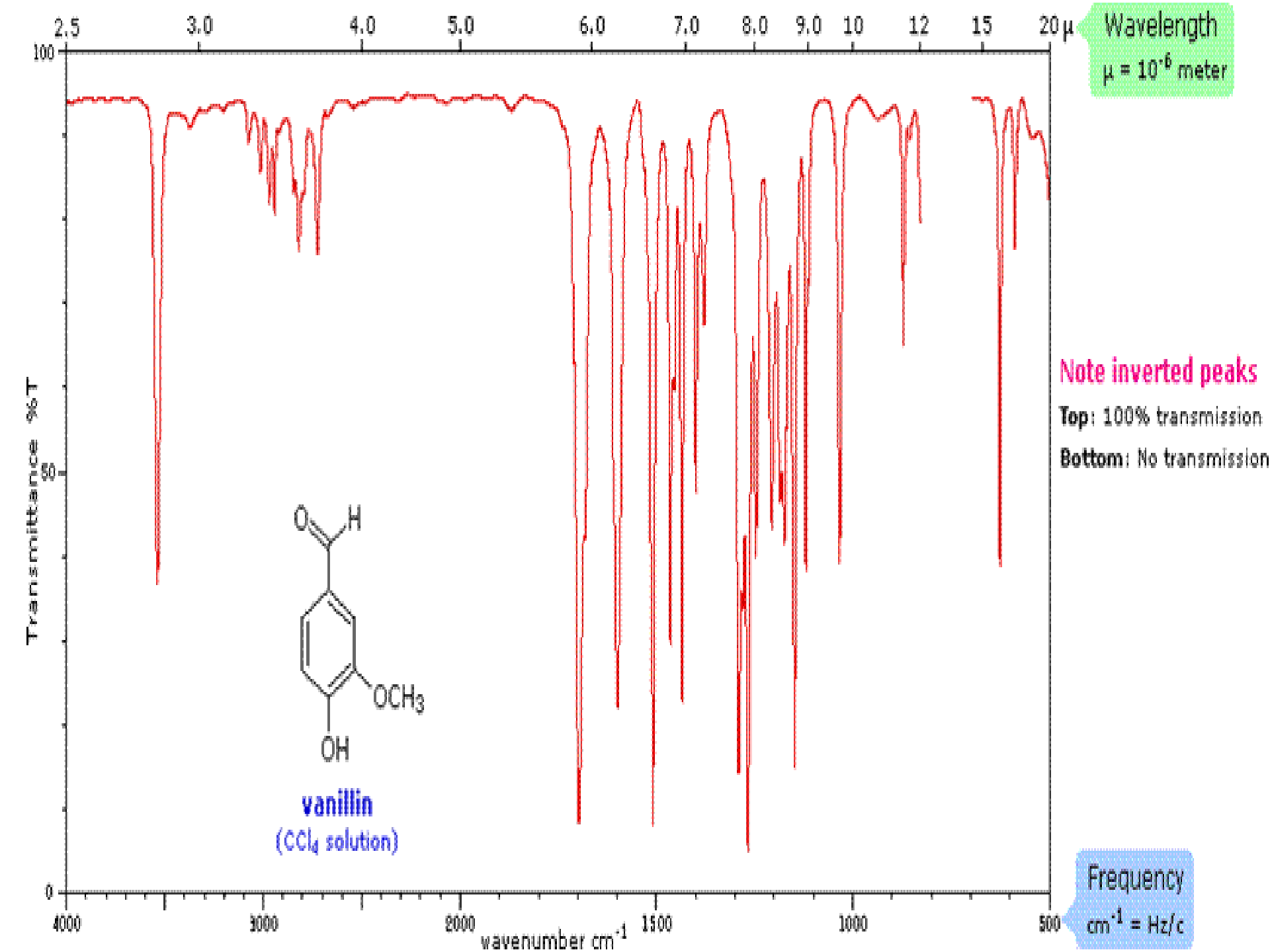
IR radiation



vanllin



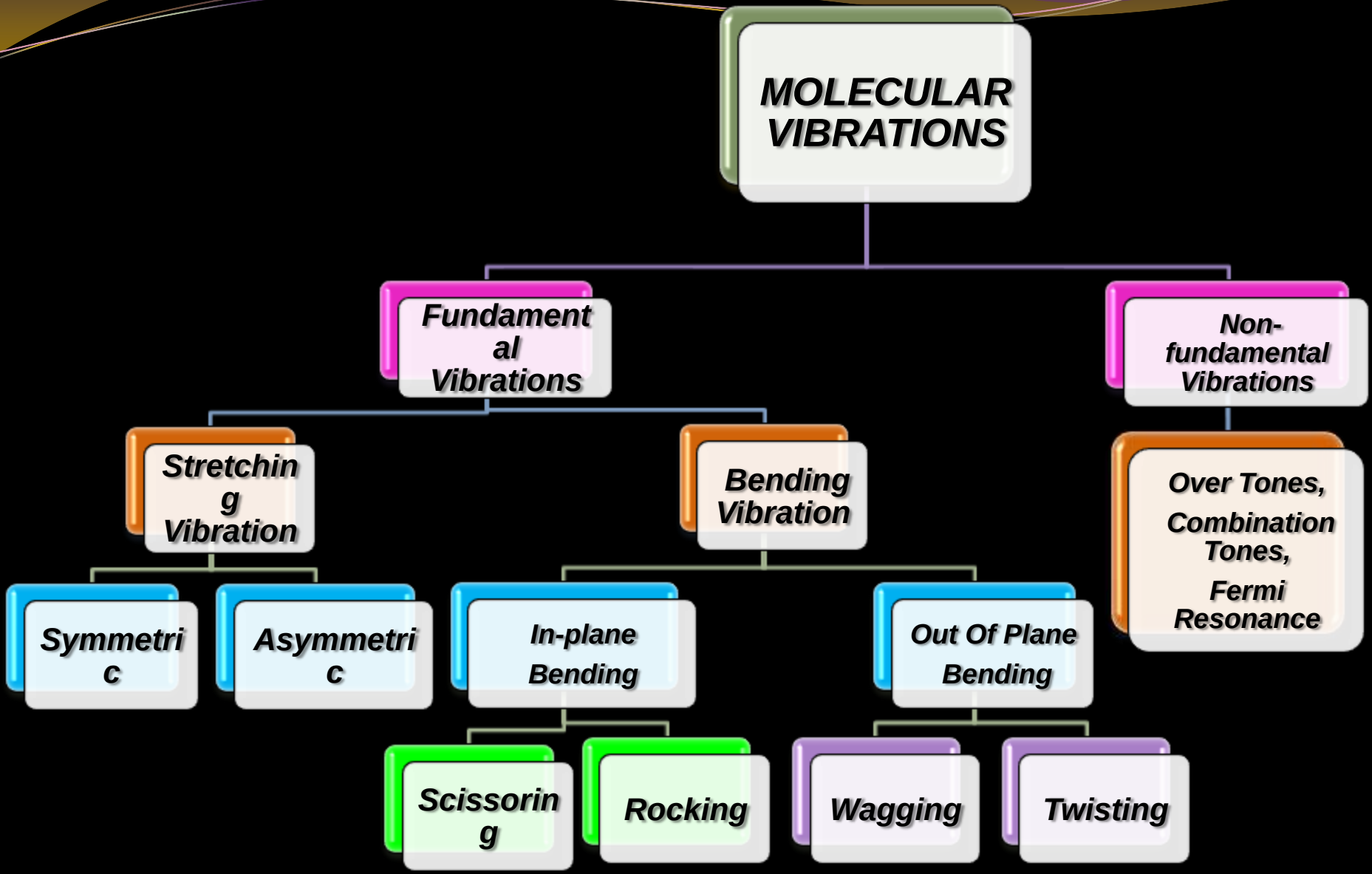
Molecular vibrations


2.5
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10
12
15
20 μ
Wavelength
μ = 10-6 meter
100
50
0
Transmittance %T
Note inverted peaks
Top: 100% transmission
Bottom: No transmission
O
H
OCH3
OH
vanillin
(CCl4 solution)
4000
3000
2000
1500
1000
500
wavenumber cm-1
Frequency
cm-1 = Hz/c

“Molecular Vibrations”

NAMEERA AHMED

ROLL NO. 1214230


MOLECULAR VIBRATIONS
Fundamental Vibrations
Non-fundamental Vibrations
Stretching Vibration
Bending Vibration
Over Tones, Combination Tones, Fermi Resonance
Symmetric
Asymmetric
In-plane Bending
Out Of Plane Bending
Scissoring
Rocking
Wagging
Twisting

“MOLECULAR VIBRATIONS”

What is a vibration in a molecule?

“*Any change in shape of the molecule- stretching of bonds, bending of bonds, or internal rotation around single bonds*”.

Why we study the molecular vibration?

Because whenever the interaction b/w electromagnetic waves & matter occur so change appears in these vibrations.

Mol. vibration divided into 2 main types:

FUNDAMENTAL VIBRATIONS

- *Vibrations which appear as band in the spectra.*

NON-FUNDAMENTAL VIBRATIONS

- *Vibrations which appears as a result of fundamental vib.*

FUNDAMENTAL VIBRATIONS

Fundamental vibration is also divided into types:

STRETCHING VIB.

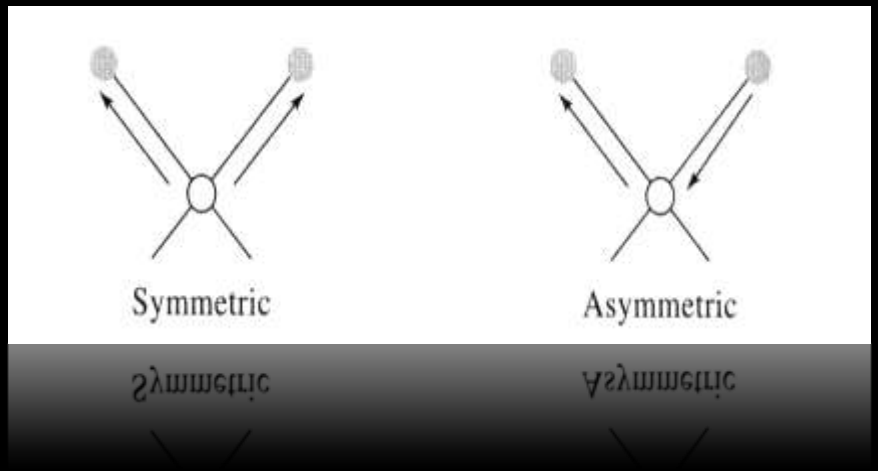
1. *Streching vibration Involves a continuous change in the inter atomic distance along the axis of the bond b/w 2 atoms.*
2. *It requires more energy so appear at shorter wavelength.*

BENDING VIB.

1. *Bending vibrations are characterized by a change in the angle b/w two bonds.*
2. *It requires less energy so appear at longer wavelength.*

Now, streching vibration is further divided into :

SYMMETRIC VIB.	ASYMMETRIC VIB.
• *Inter atomic distance b/w 2 atoms increases/decreases.*	• *Inter atomic distance b/w 2 atoms is alternate/opposite.*



Bending vibration is divided into:

IN PLANE BENDING

- *If all the atoms are on same plane*.

OUT OF PLANE BENDING

- *If 2 atoms are on same plane while the 1 atom is on opposite plane*.

In-plane bending further divided into:

SCISSORING:

When 2 atoms move away or close towards each other.

ROCKING:

Change in angle b/w a group of atoms.

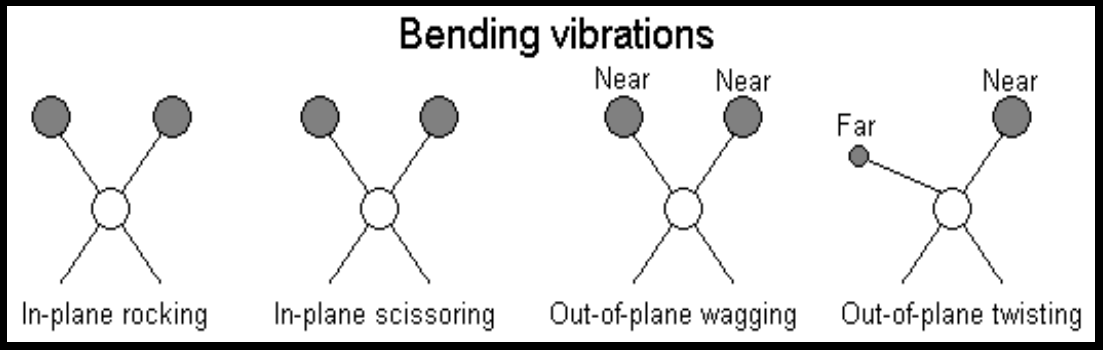
Out plane bending is further divided into:

- *Change in angle b/w the plane of a group of atom*

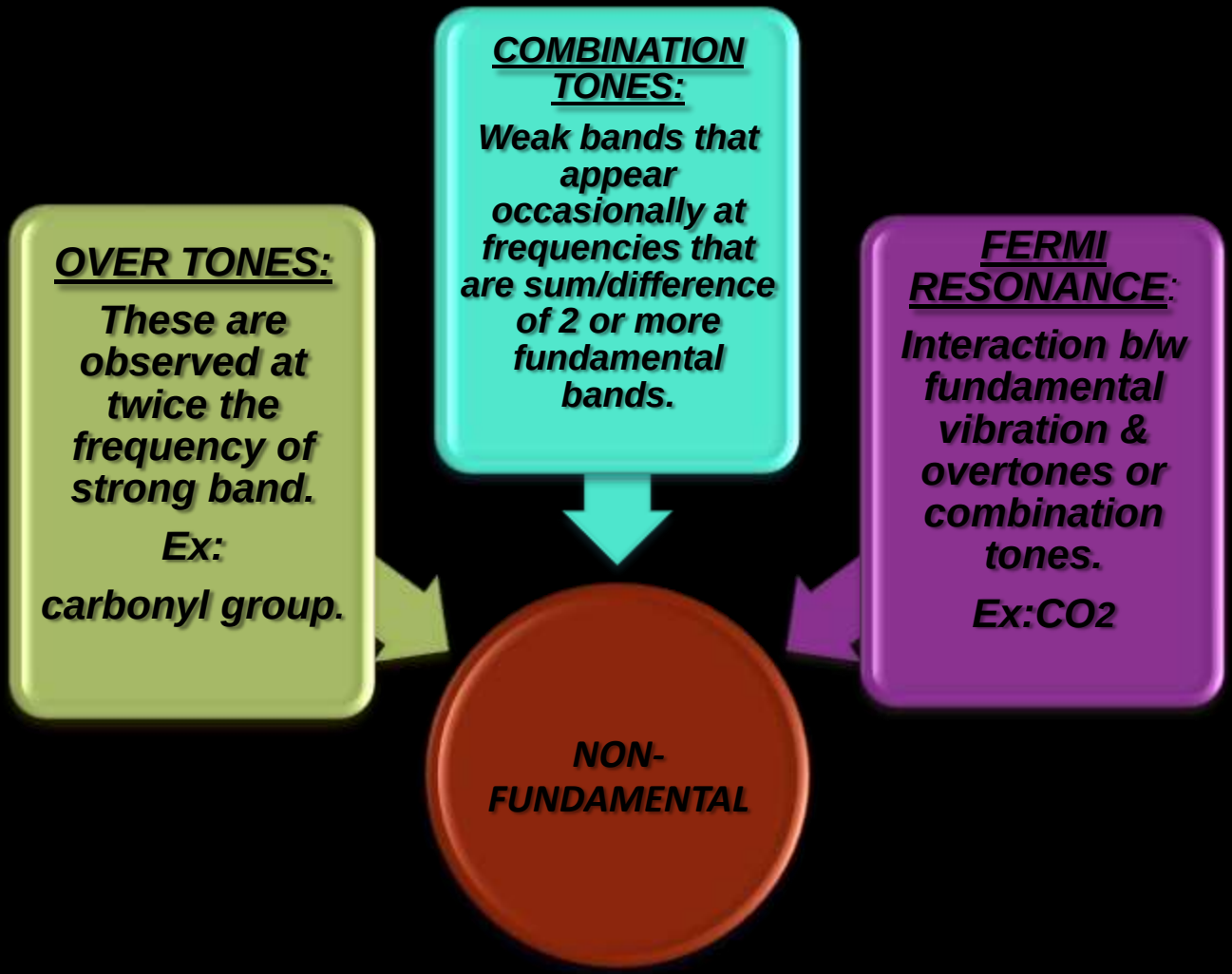
WAGGING

TWISTING

- *Change in angle b/w the plane of 2 groups of atoms.*



NON-FUNDAMENTAL VIBRATIONS



“Coupled Interactions And Factors”

NAJAF FAROOQ

ROLL NO. 1214229

COUPLED INTERACTIONS

Interactions between vibrations can occur (Coupling) if the vibrating bonds are joined to a single, central atom.

This is because there is mechanical coupling interaction between the oscillators.

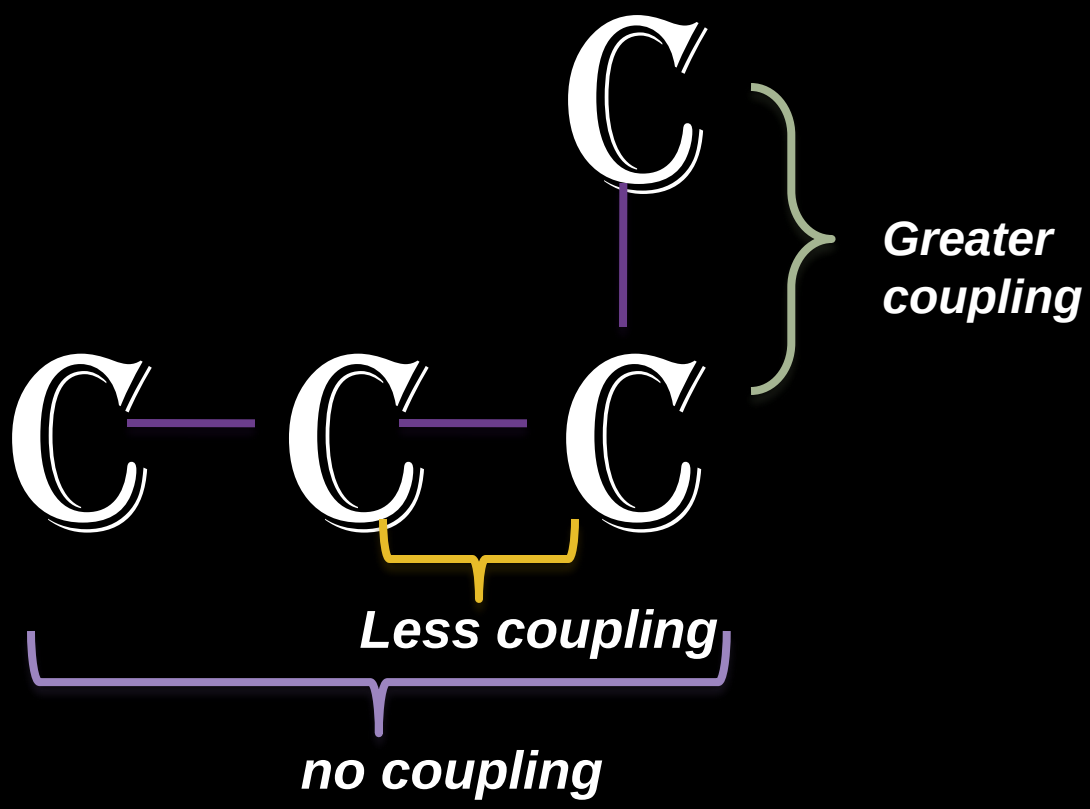
Example:

C=O (both symmetric and asymmetric stretching vibrations)

REQUIREMENTS FOR COUPLING

- The vibrations must be of the same symmetry species if interaction is to occur
- Strong coupling of stretching vibrations occurs when there is a common atom between the two vibrating bonds.
- Coupling of bending vibrations occurs when there is a common bond between vibrating groups.

- Coupling is greatest when the coupled groups have approximately equal energies
- Coupling between a stretching vibration and a bending vibration occurs if the stretching bond is one side of an angle varied by bending vibration.
- No coupling is seen between groups separated by two or more bonds


Greater coupling
Less coupling
no coupling

FACTORS AFFECTING THE FREQUENCY OF THE IR ABSORPTION :

- *Relative mass of the atom*
- *Force constant of the bonds*
- *Geometry of the atom*

THE RELATIVE MASS OF THE ATOMS: *heavier the atoms lower is the vibration frequency of the bond between them.*

THE FORCE CONSTANT OF THE BONDS*: Stronger the bond higher is the vibration frequency.*

Stronger bonds O-H, N-H & C-H weaker bonds C-C & C-O bond.

EFFECTS OF BONDS: *C=C stretching is expected to absorb at a higher frequency than C-C stretching.*

Example: C≡C 2200cm^{-1}

C=C 1650cm^{-1}

C-C 1200cm^{-1}

“Degree Of Freedom”

BUSHRA RUBAB

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Fundamental vibration of molecule depend on degree of freedom

Each atom has 3 degree of freedom depend on x , y ,z

For a molecule containing n number of atom s has 3n degree of freedom

For non linear molecule 3 degree of freedom represent rotational & transational motion

For non linear (3n-6)degree of freedom represent fundamental vibrations

For linear (3n-5)degree of freedom represent fundamental vibrations

All vibrational changes don't appear as band

Only those vibrational changes that result in change in dipole movement appear as band

HOOKES LAW

- It gives the relation between frequency of oscillation , atomic mass , force constant of the bond .
- Thus vibrational frequency is

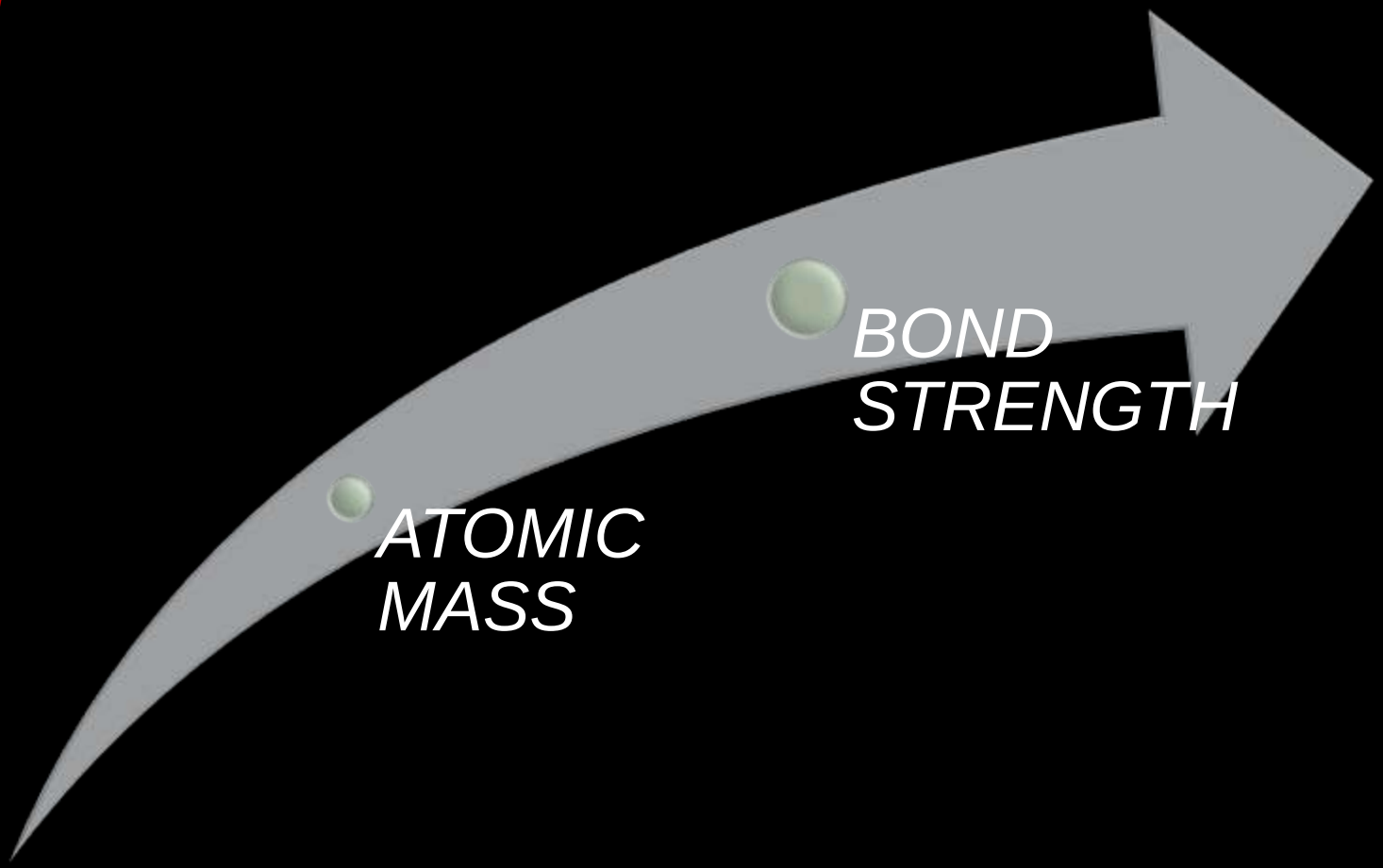
$$= \frac{1}{2} \pi c \sqrt{f/(MxMy)/(Mx+My)}$$

- C = velocity of light
- F = force constant
- Mx= mass of atom x
- My = mass of atom y

- Since force constant measures the strength of bond, value of f is

FOR SINGLE BOND	• 5×10^5 dynes/cm
FOR DOUBLE BOND	• 10×10^5 dynes /cm
FOR TRIPLE BOND	• 15×10^5 dynes/cm

Factors On Which Vibrational Frequency Depends:



“Hydrogen Bonding”

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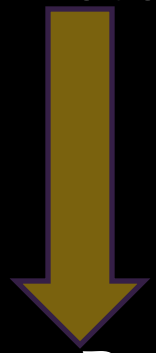
EFFECT OF HYDROGEN BONDING ON IR

Proton Donor Group (S-Orbital)

Proton Acceptor Group (P-Orbital)



Hydrogen Bonding

EXAMPLES OF PROTON DONOR AND PROTON ACCEPTOR GROUP

Proton Donor Group

Carboxyl, Hydroxyl, Amine Or Amide Group

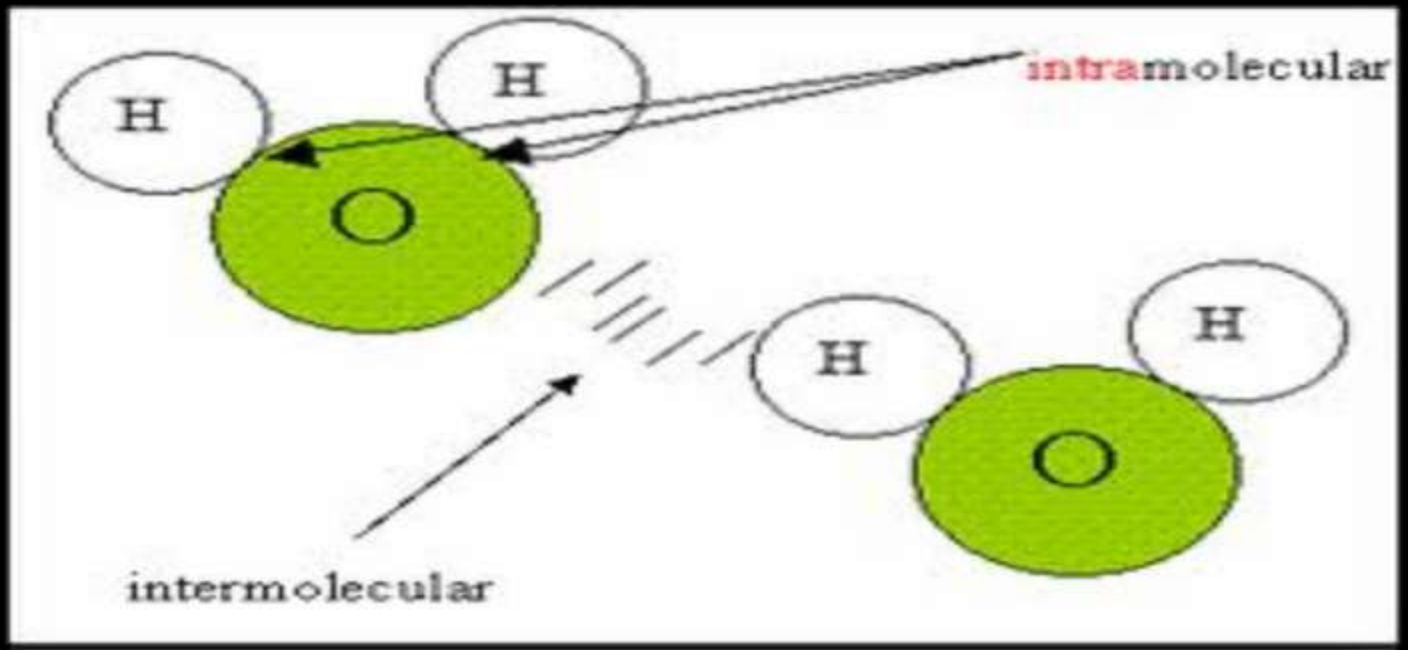
Proton Acceptor Group

Oxygen, Nitrogen, Halogens And Unsaturated Group

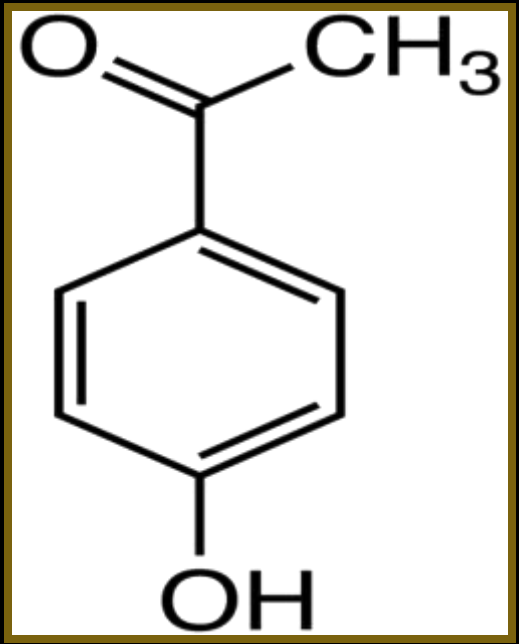
TYPES OF HYDROGEN BONDING

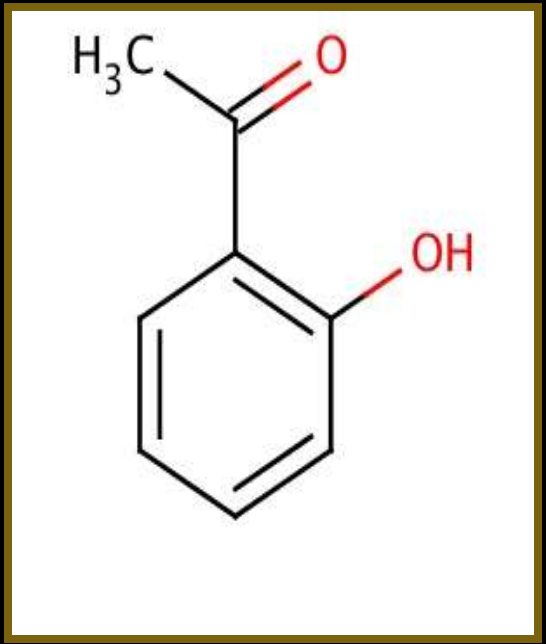
1-Intermolecular Hydrogen Bonding

2-Intramolecular Hydrogen Bonding



STRENGTH OF HYDROGEN BONDING



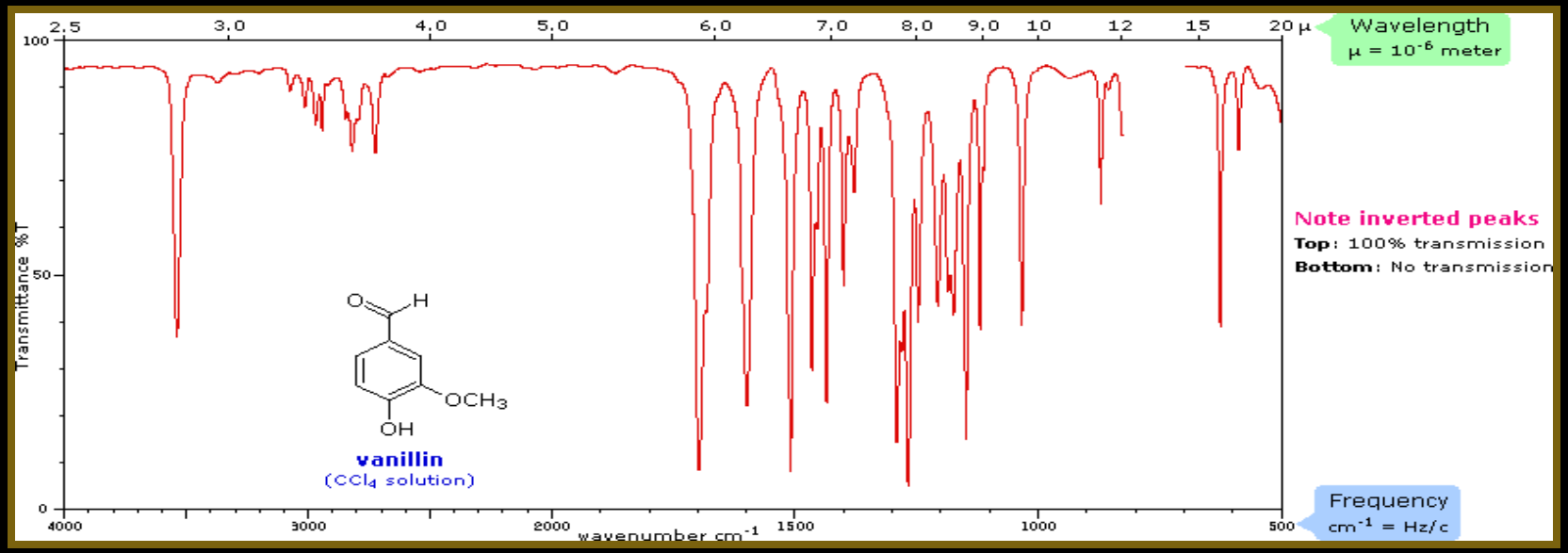


P-Hydroxyacetophenone

o-Hydroxyacetophenone

WHY HYDROGEN BOND ALTERS THE FORCE CONSTANT???

Stretching bands move towards longer wavelength or lower frequencies And Bending vibrations shift towards Shorter wavelength or Higher frequencies.



Bending vibrations

Stretching vibrations

FACTORS AFFECTING ON HYDROGEN BONDING

- ✓ *Temperature*
- ✓ *Concentration*
- ✓ *Molecular Geometry*
- ✓ *Relative Acidity*
- ✓ *Basicity*

“Instrumentation”

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INSTRUMENTATION

The main parts of IR spectrometer are as follows:

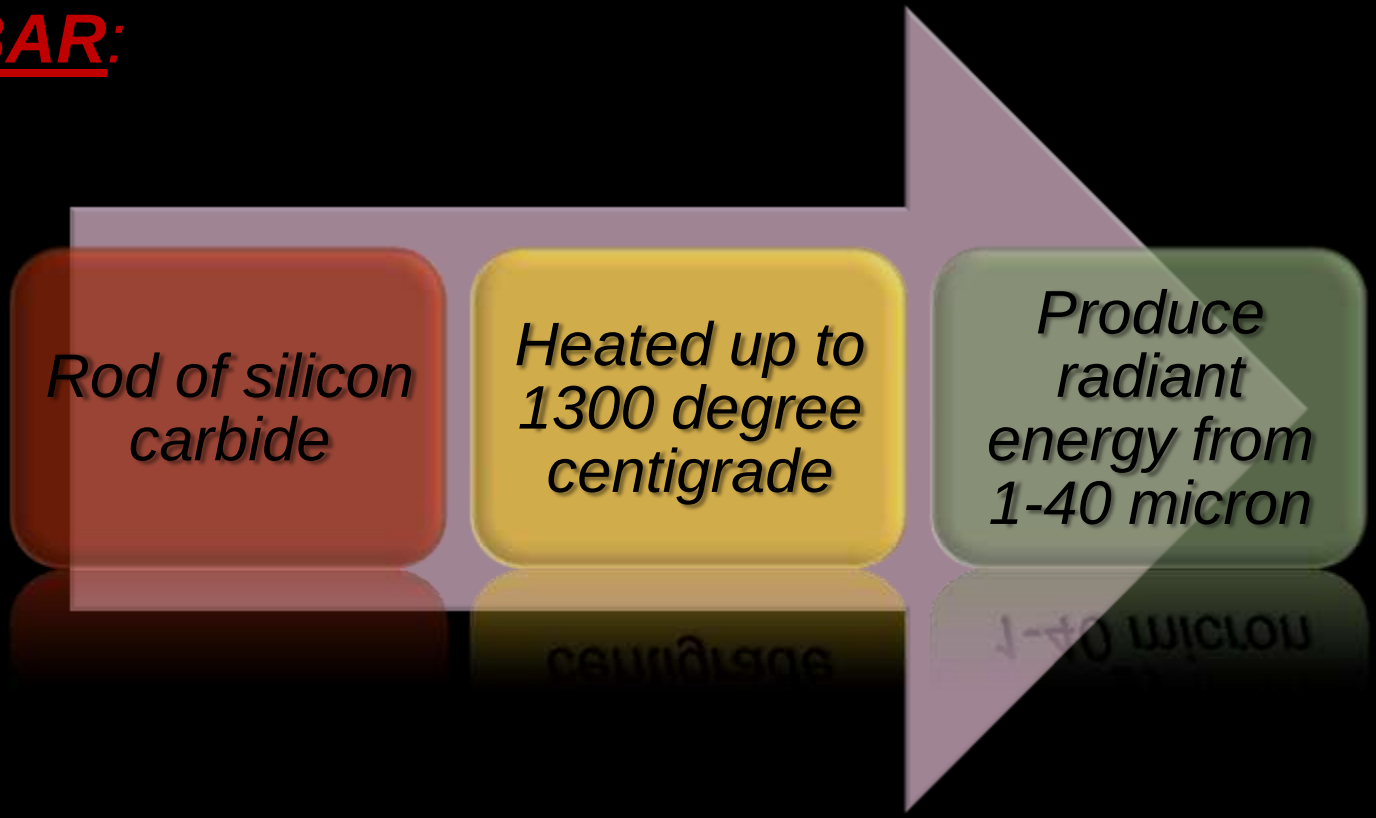
- *radiation source*
- *sample cells and sampling of substances*
- *monochromators*
- *detectors*
- *recorder*

INFRARED SOURCES

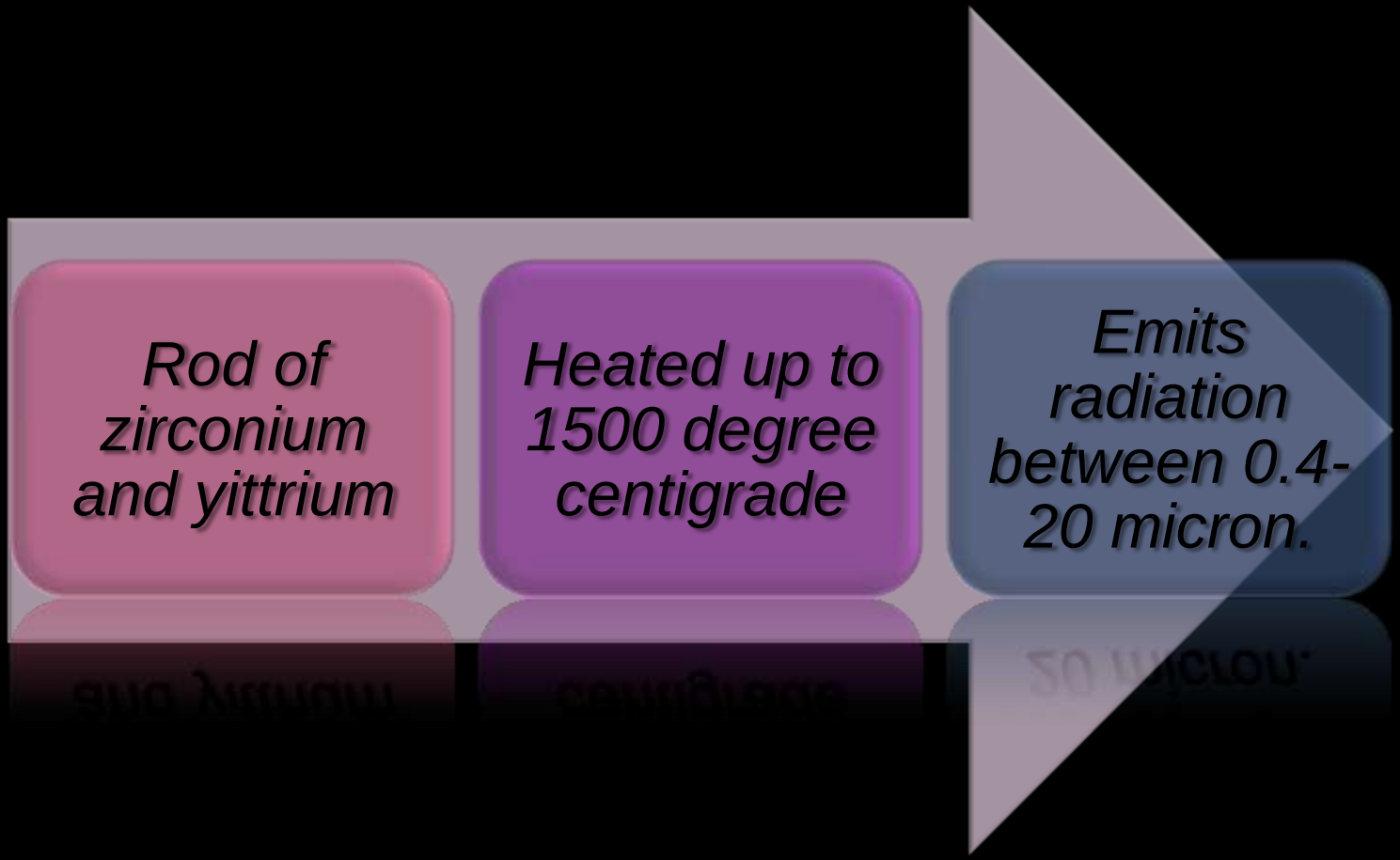
IR instruments require a source of radiant energy which emit IR radiation which must be:

Sources of IR radiations are as follows:

GLOBAR:



- ***NERNST GLOWER:***



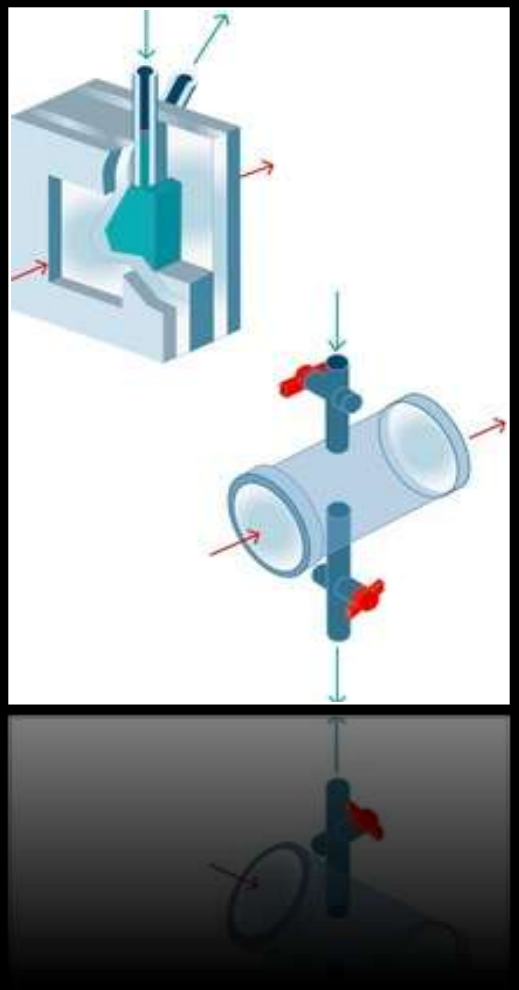
SAMPLE CELL

- **For gas samples:**

The spectrum of a gas can be obtained by permitting the sample to expand into an evacuated cell, also called a cuvette.

- **For solution sample:**

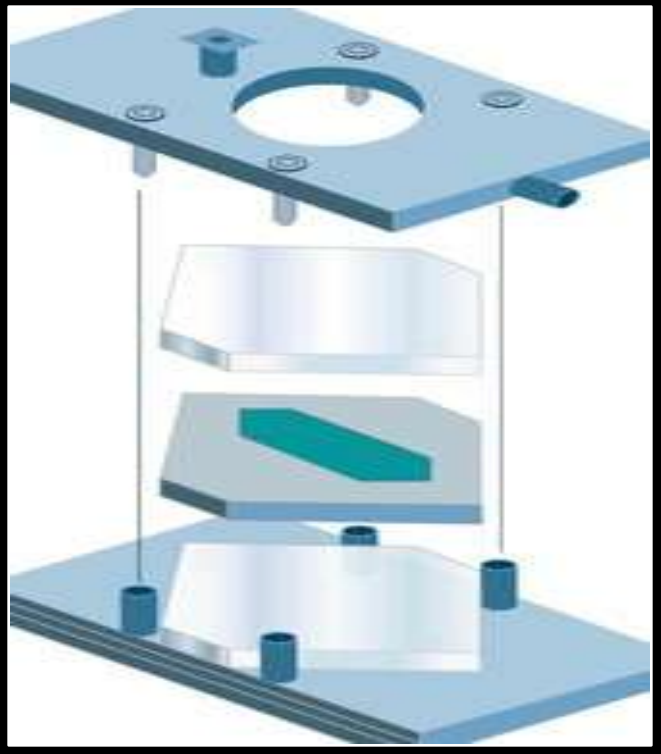
Infrared solution cells consists of two windows of pressed salt sealed. Samples that are liquid at room temperature are usually analyzed in pure form or in solution. The most common solvents are Carbon Tetrachloride (CCl4) and Carbon Disulfide (CS2).



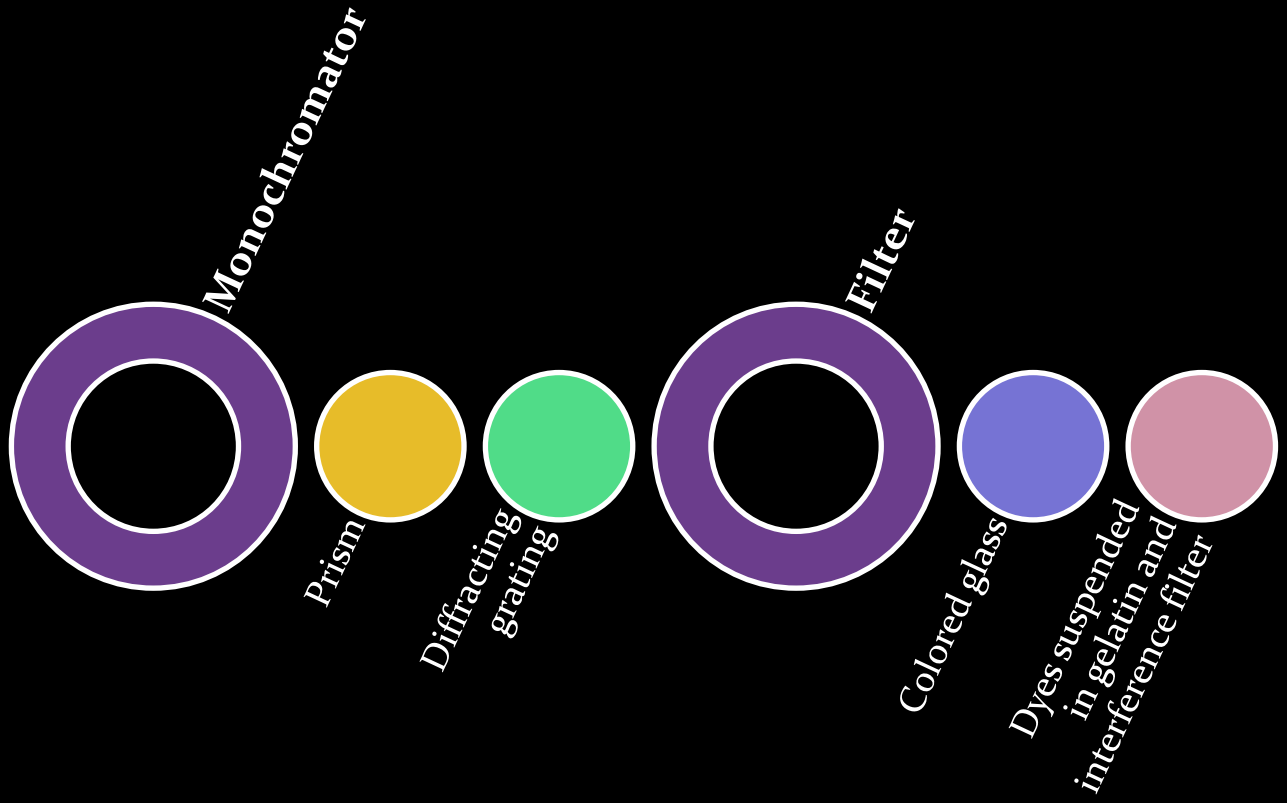
- **For solid sample:**

Solids reduced to small particles (less than 2 micron) can be examined as a thin paste or mull. The mull is formed by grinding a 2-5 milligrams of the sample in the presence of one or two drops of a hydrocarbon oil (nujol oil). The resulting mull is then examined as a film between flat salt plates.

Another technique is to ground a milligram or less of the sample with about 100 milligram potassium bromide. The mixture is then pressed in an evaluable die to produce a transparent disk.



MONOCHROMATORS



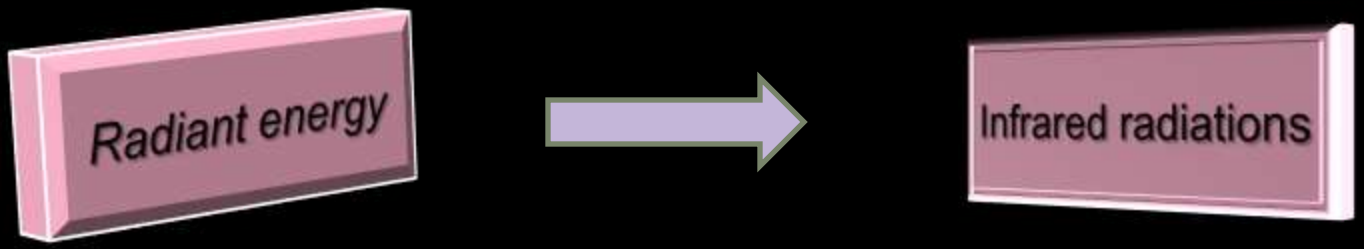
“Detectors”

NIDA ASHRAF

ROLL NO. 1214232

RADIATION DETECTOR

- *An infrared detector is a detector that reacts to infrared (IR) radiation.*
- *It is simply a transducer of radiant energy.*

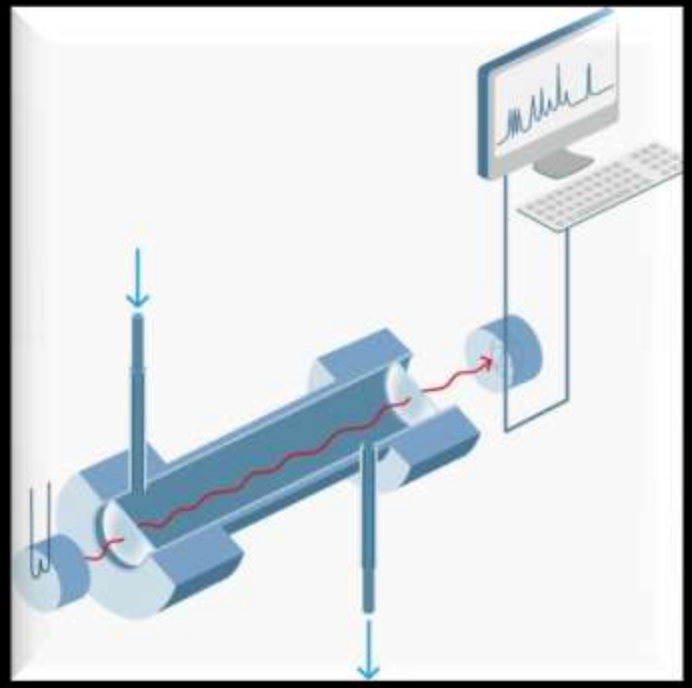


TYPES OF DETECTOR

Detector

Thermal

Non-thermal



THERMAL DETECTOR

Thermal detectors can be used over a wide range of wavelengths and they operate at room temperature.

Disadvantages:

slow response time and lower sensivity relative to other types of detectors.

TYPES OF THERMAL DETECTOR

There are four types of thermal detector.

- *Bolometers*
- *Thermocouple and thermopile*
- *Pyro electric detector*
- *Golay cell*

BOLOMETERS

Bolometer is derived from a Greek word (bolometron)

Bolo = for something thrown

Metron = measure

Construction

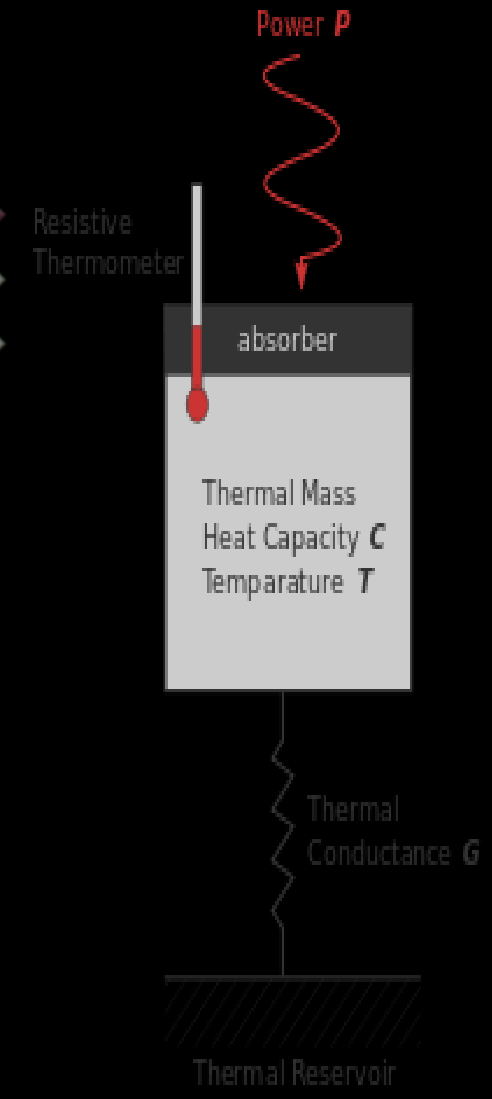
- A bolometer consists of an absorptive element, such as a thin layer of metal.
- Most bolometers use semiconductor or superconductor absorptive elements rather than metals.

Working

Thin layer of metal connected to a reservoir

Any radiation on the absorptive element raises its temperature above that of the reservoir.

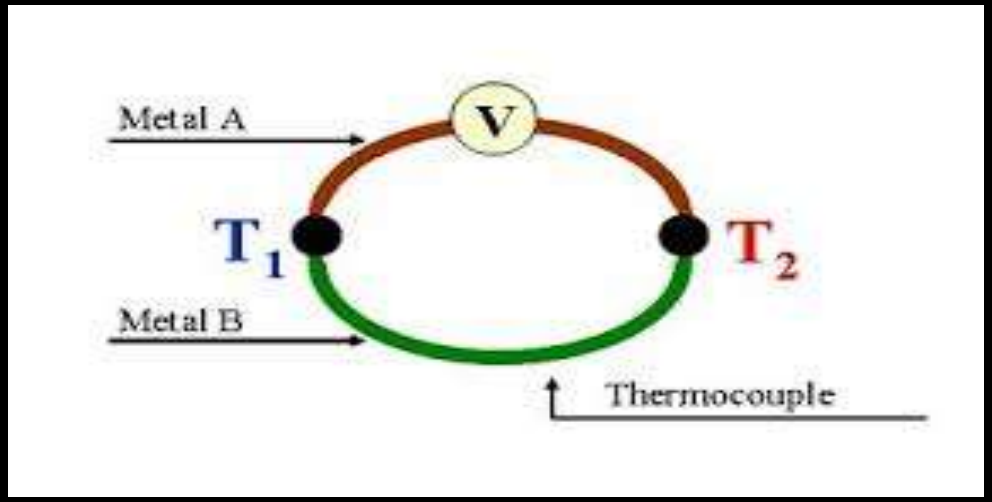
The temperature change can be measured directly with an attached thermometer.



THERMOCOUPLE AND THERMOPILE

Thermocouples consist of a pair of junctions of different metals; for example, two pieces of bismuth fused to either end of a piece of antimony.

Temperature changes → *Potential difference changes*

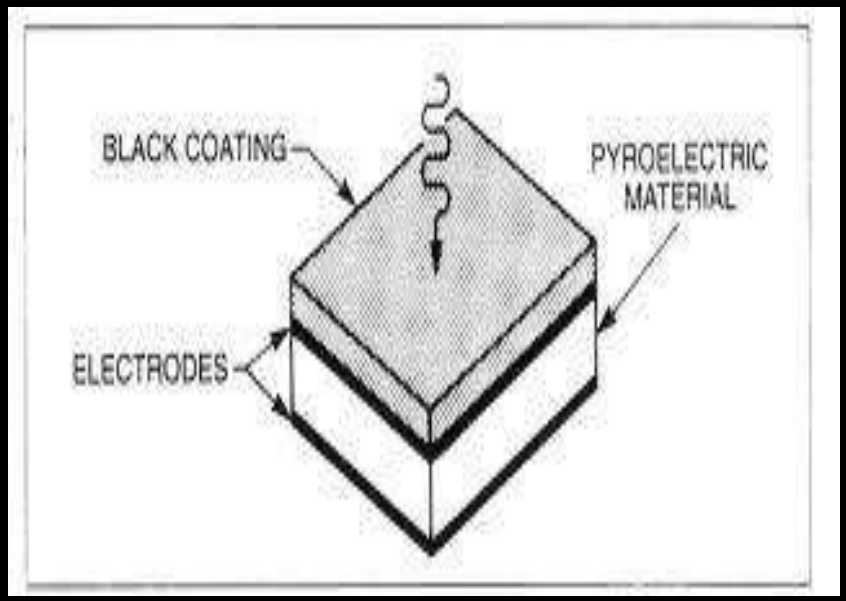


Thermopile detectors are voltage-generating devices, which can be thought of as miniature arrays of thermocouple junctions.

PYRO ELECTRIC DETECTOR

Construction:

- Single crystalline wafer of a pyro electric material, such as triglycerine sulphate.
- Pyro electric Infrared Detectors (PIR) convert the changes in incoming infrared light to electric signals.



Below curie temperature

Pyro electric materials exhibit electrical polarization.

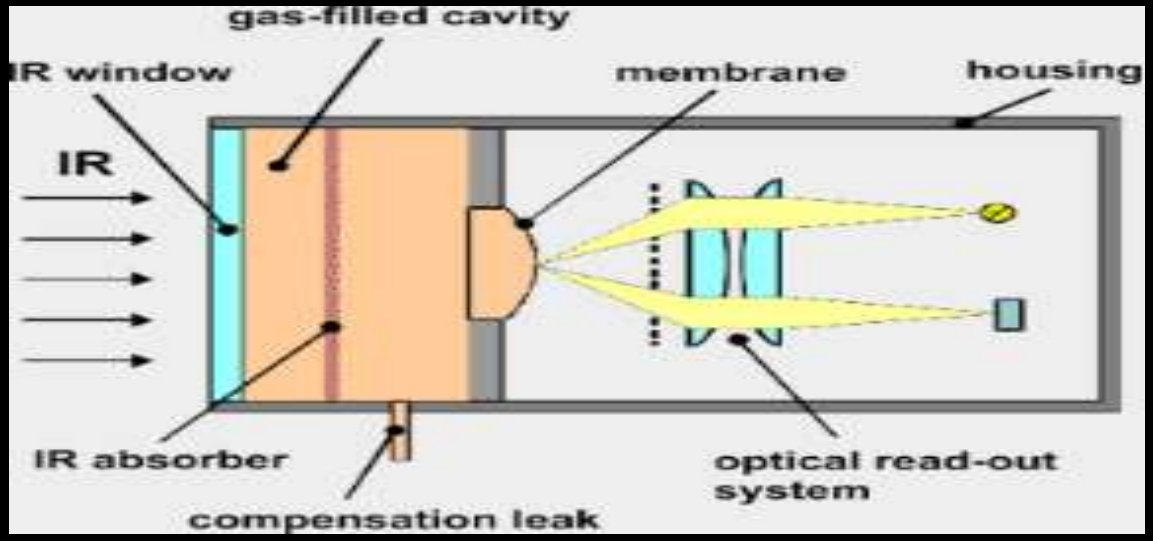
Temperature is altered, the polarization changes.

Observed as an electrical signal
(if electrodes are placed on opposite faces of a thin slice of the material to form a capacitor)

GOLAY CELL

Construction:

- *Small metal cylinder*
- *Flexible silvered diaphragm*
- *Whole chamber is filled with xenon gas.*



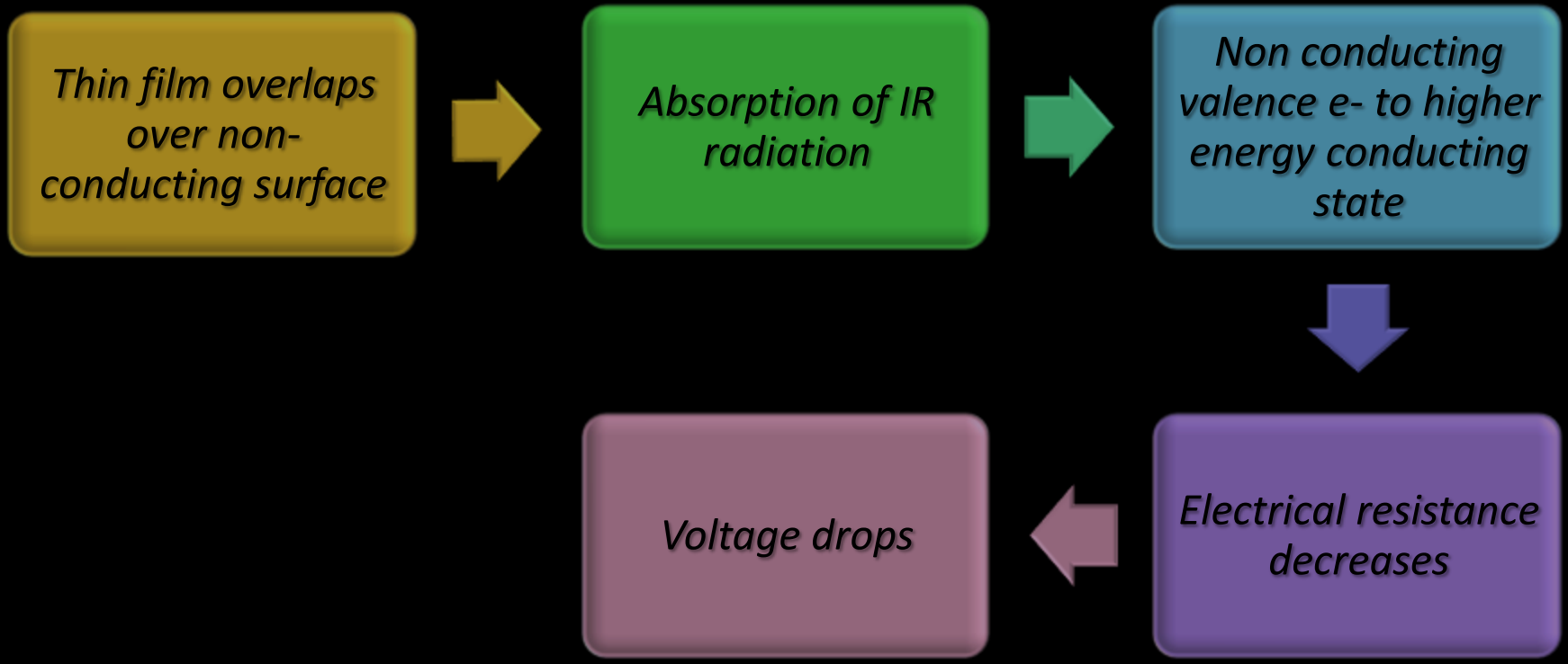
Metal cylinder and flexible diaphragm

Temperature increases

Gas is expended and diaphragm deforms

detect as a signal

NON-THERMAL DETECTORS



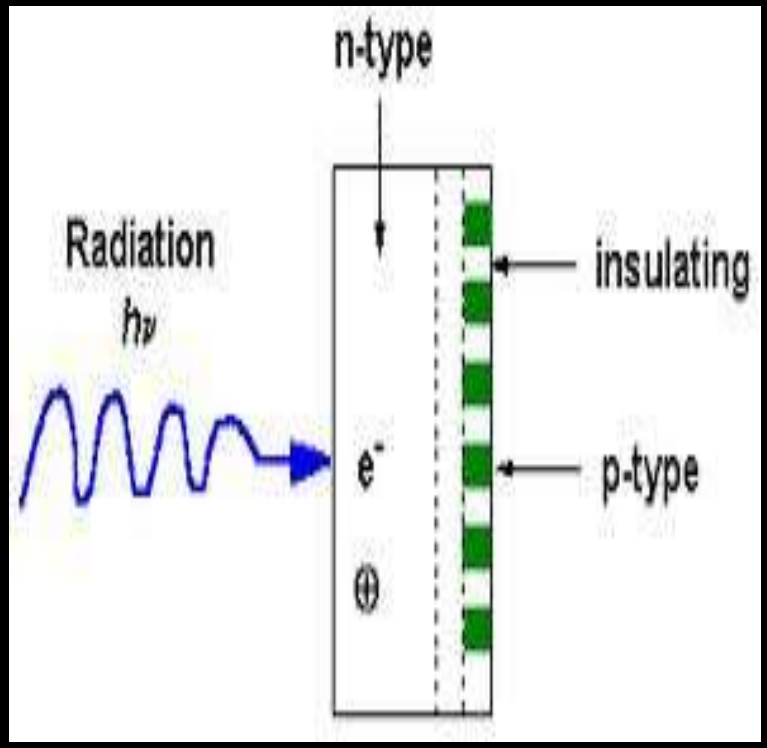
PHOTOVOLTAIC DETECTOR

Infrared radiations

Photovoltaic detector

Generates a small voltage

Detected as a signal



"Single/Double Beam IR Absorption Spectrophotometers"

UROOBA IQBAL

ROLL NO. 1214265

IR ABSORPTION SPECTROPHOTOMETERS

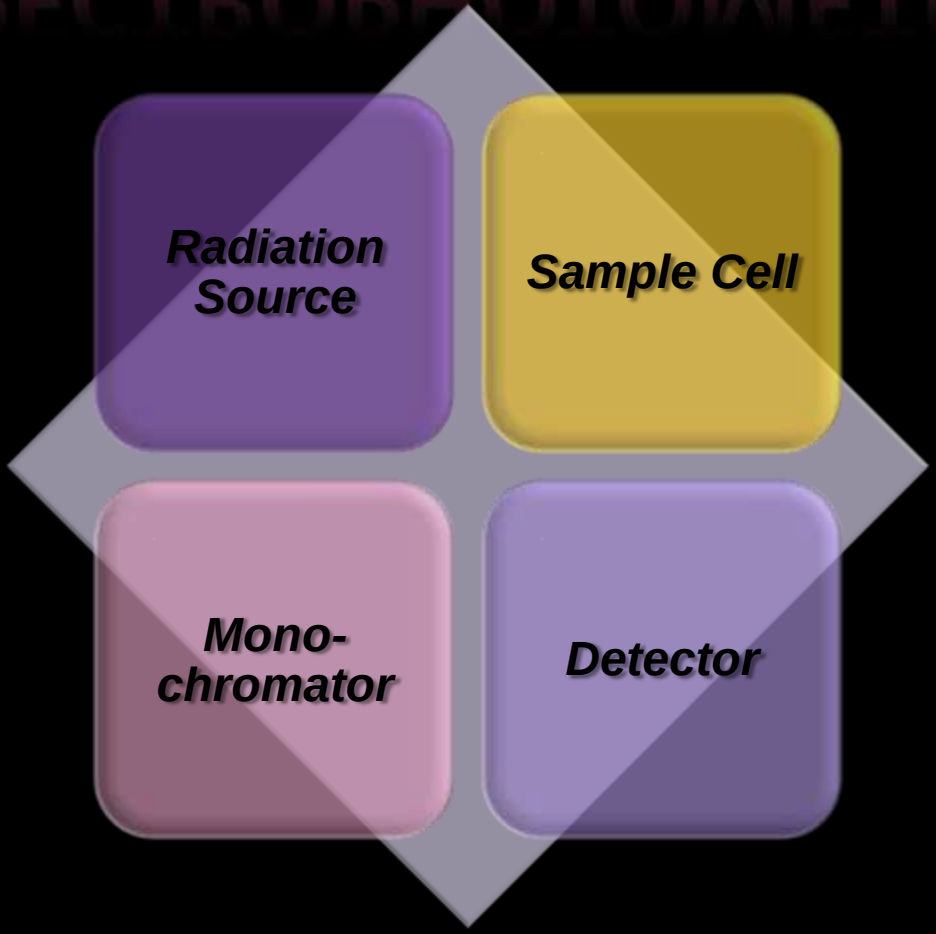
SINGLE BEAM SPCETROPHOTOMETER

- A single beam of light , which can pass through one solution at a time (sample *or* reference).

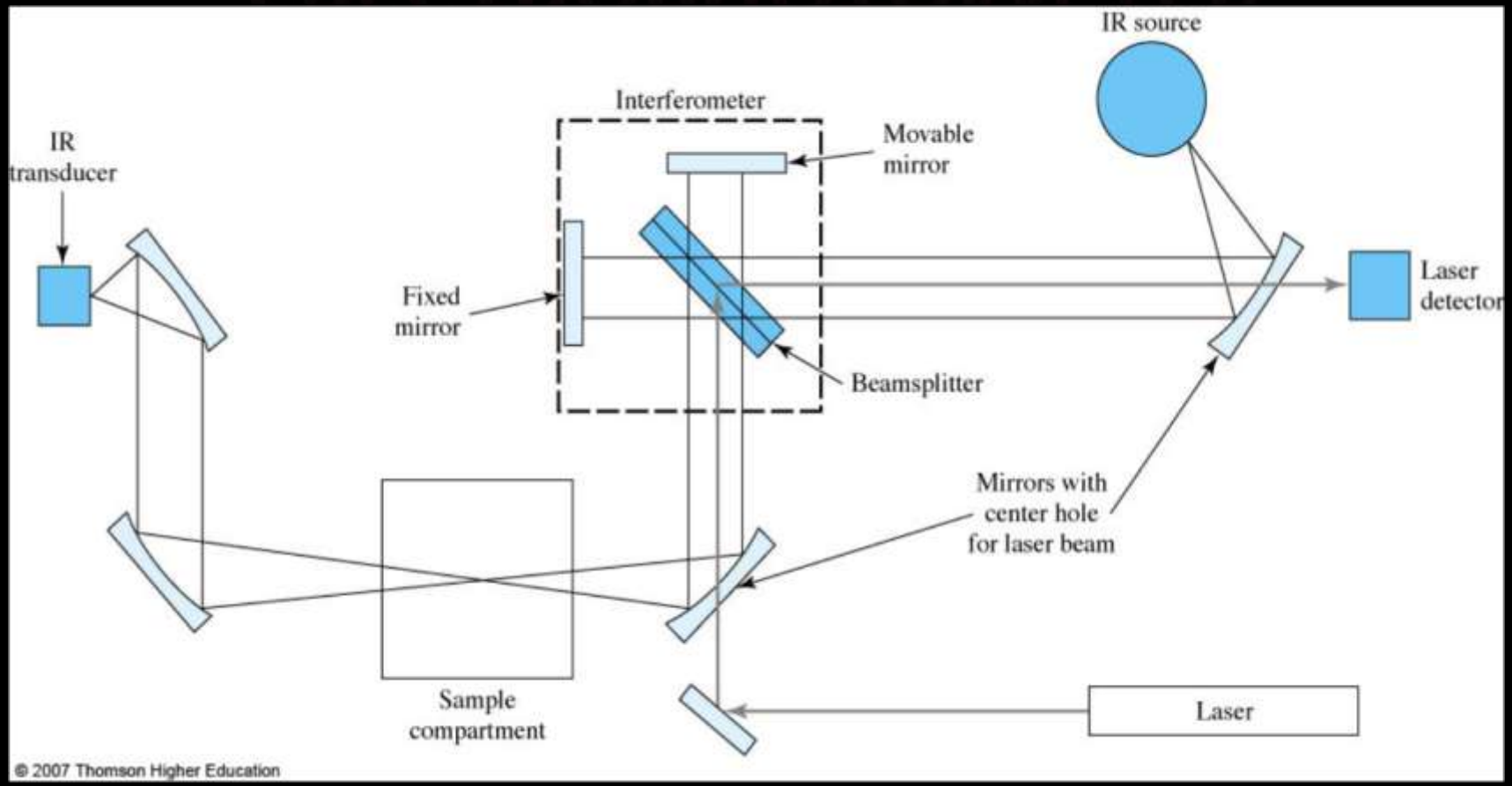
DOUBLE BEAM SPECTROPHOTOMETER

- A single beam of light splits into two separate beams. One passes through the sample, another passes through the reference.

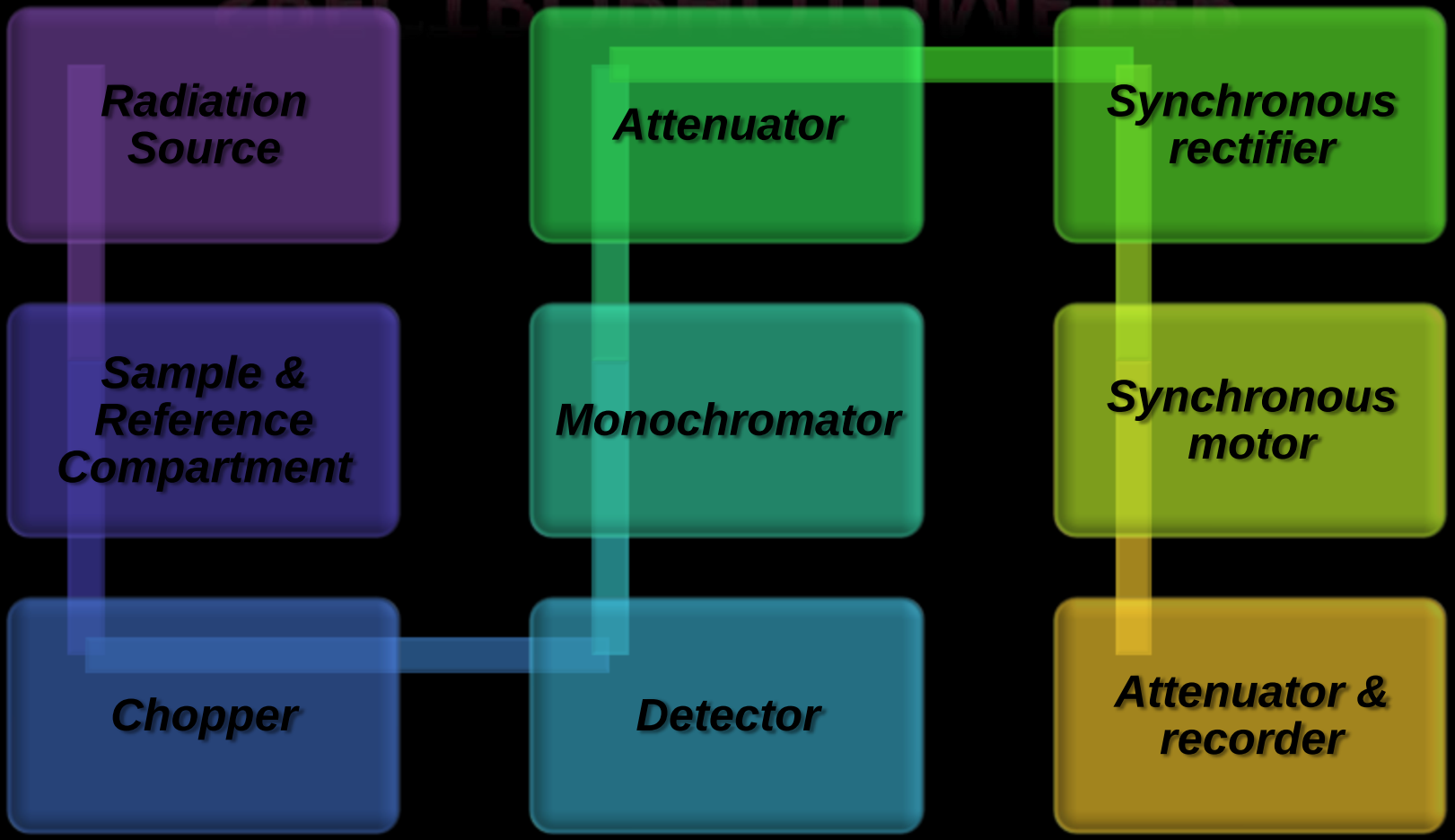
SINGLE BEAM IR SPECTROPHOTOMETER



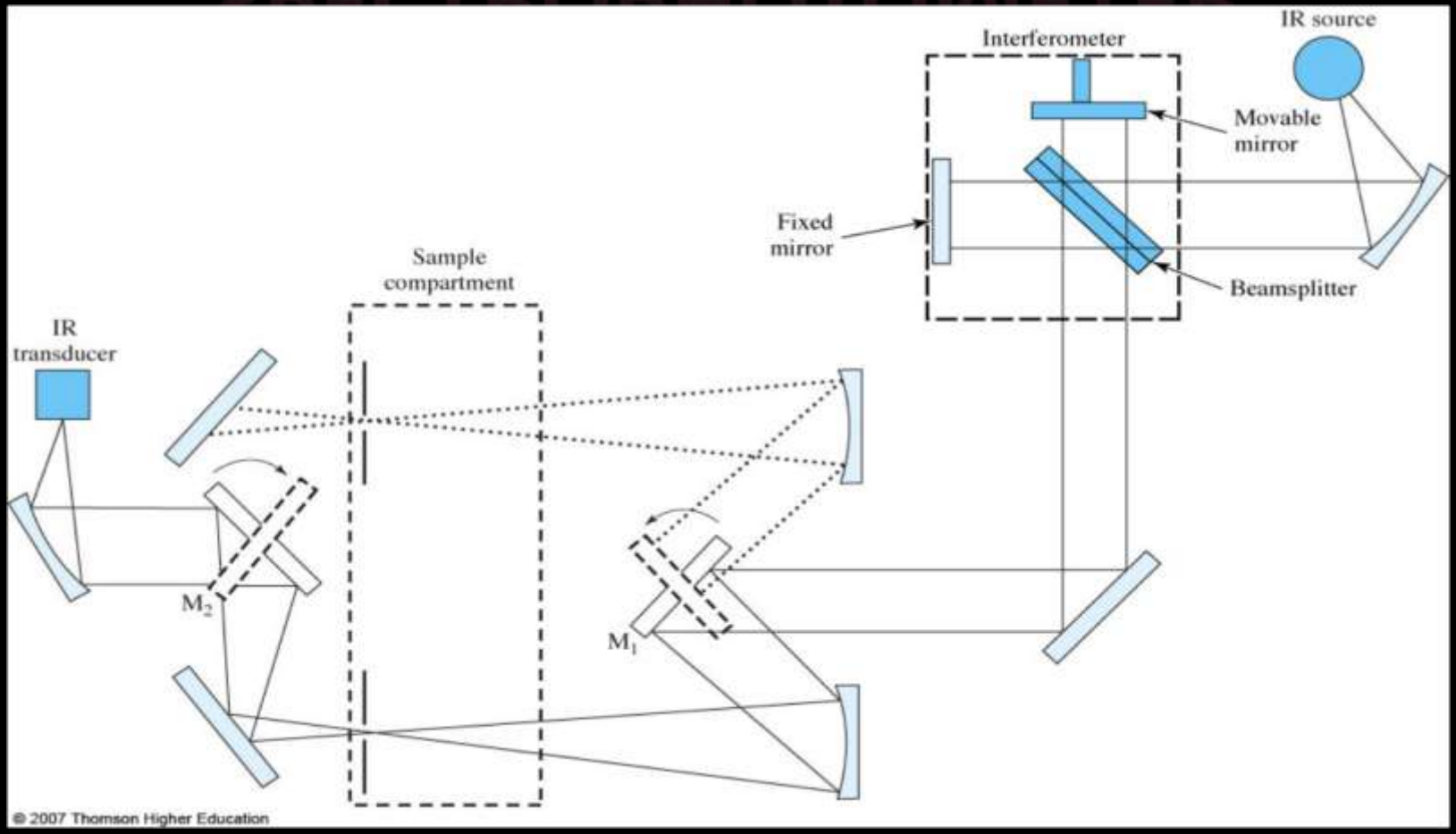
SINGLE BEAM IR ABSORPTION SPECTROPHOTOMETER



DOUBLE BEAM IR ABSORPTION SPECTROPHOTOMETER

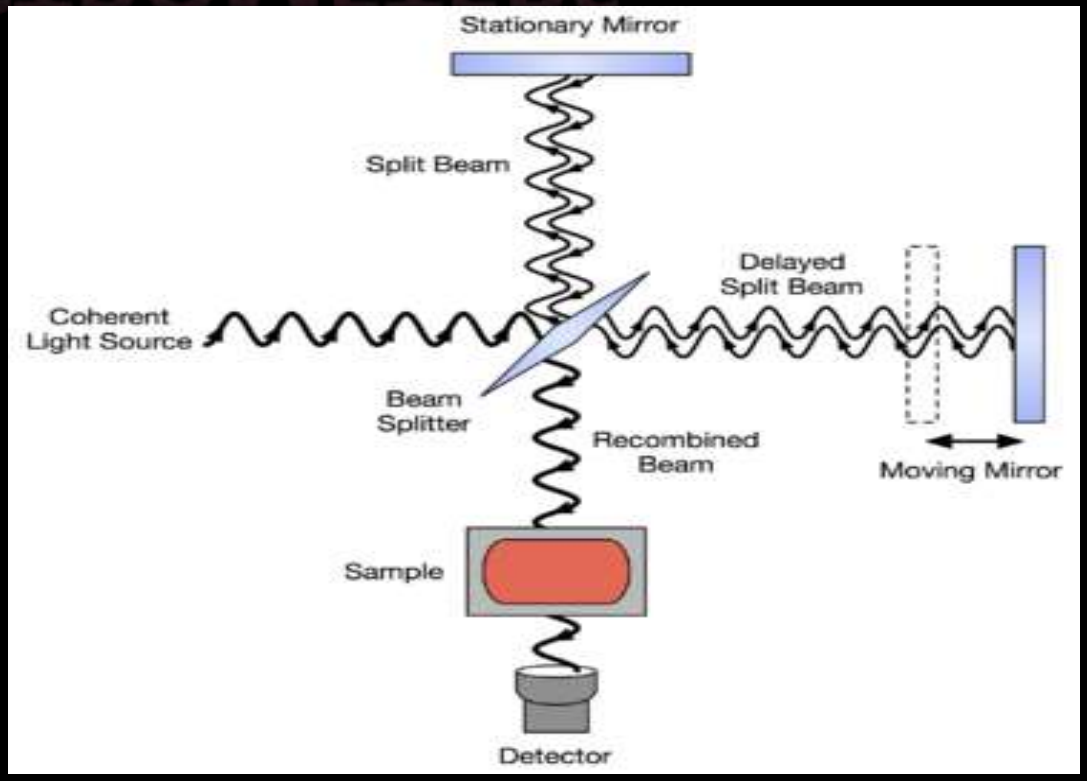


DOUBLE BEAM IR ABSORPTION SPECTROPHOTOMETER



FOURIER TRANSFORM SPECTROMETERS

- *All frequencies are examined simultaneously in Fourier transform infrared (FTIR) spectroscopy.*



“Applications Of IR Absorption Spectrocopy”

RABIA KHALID NADEEM

ROLL NO. 1214265

*Since different molecules with different combination of atoms produce their unique spectra, infrared spectroscopy can be used to **qualitatively** identify substances.*

QUALITATIVE ANALYSIS

FUNDAMENTAL REGION (ROCK SALT REGION)

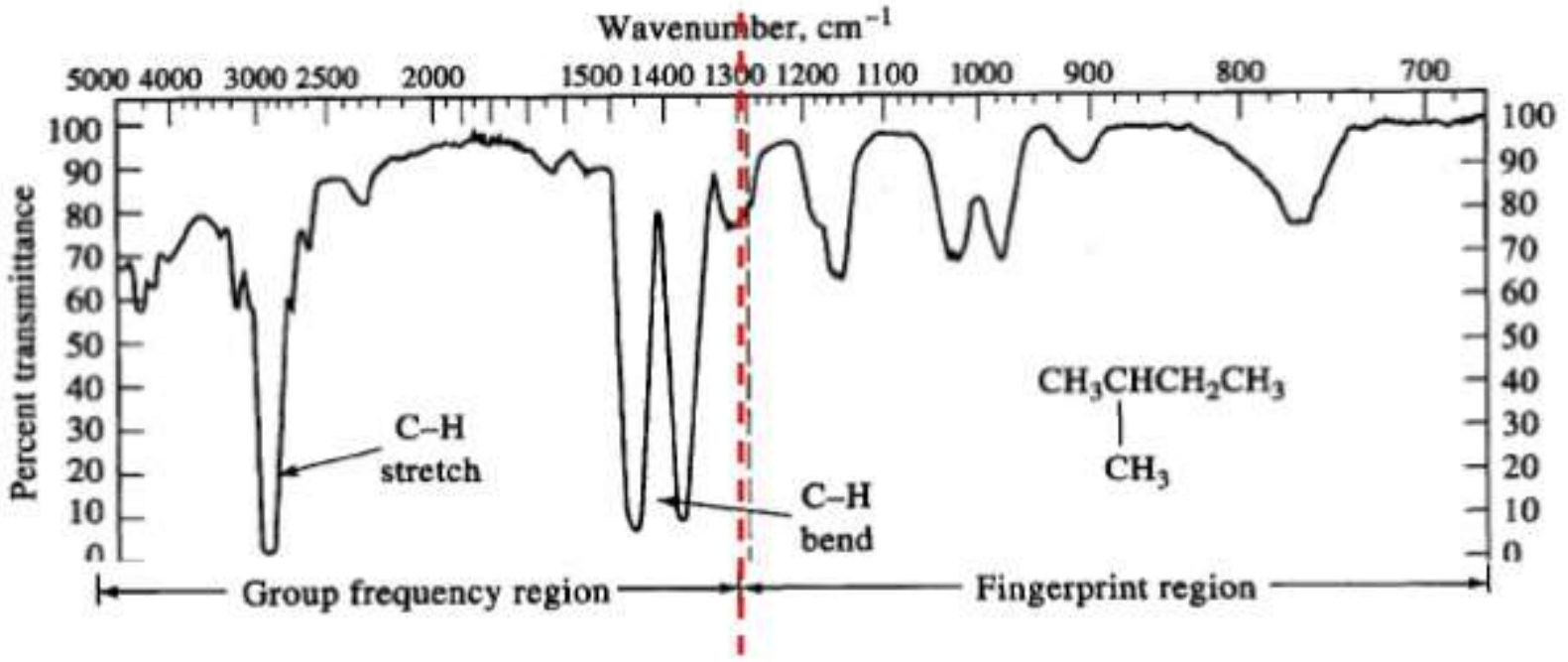
Group Frequency Region

- *consisting of the absorption bands of the functional groups.*
- *frequency = 4000-1300cm-^{1}*
- *wavelength = 2.5-8*

Fingerprint Region

- *IR spectra is called "fingerprints" because no other chemical species will have similar IR spectrum.*
- *Single bonds give their absorption bands in this region.*
- *Frequency=1300-650cm-1*
- *Wavelength=8-15.4*

Infrared Spectra



APPLICATION OF IR SPECTROSCOPOY TO ORGANIC MOLECULES:

- Organic groups differ from one another both in the strength of the bond and the masses of the atom involved.

THREE REGIONS OF IR SPECTRUM:

- *4000 and 1300 cm-1*
- *Alcohols and amines*

- *1300 and 909 cm-1*
- *Complex interactions*

- *909 and 65o cm-1*
- *Benzene rings*

STUDYING PROGRESS OF REACTIONS

- Observing rate of disappearance of characteristic absorption band in reactants; or
- Rate of increasing absorption bands in products of a particular product.
- *E.g.: O—H = 3600-3650 cm-^{1}*

  C=O = 1680-1760 cm-^{1}

HOPE YOU LIKE OUR PRESENTATION

THANK YOU! ☺