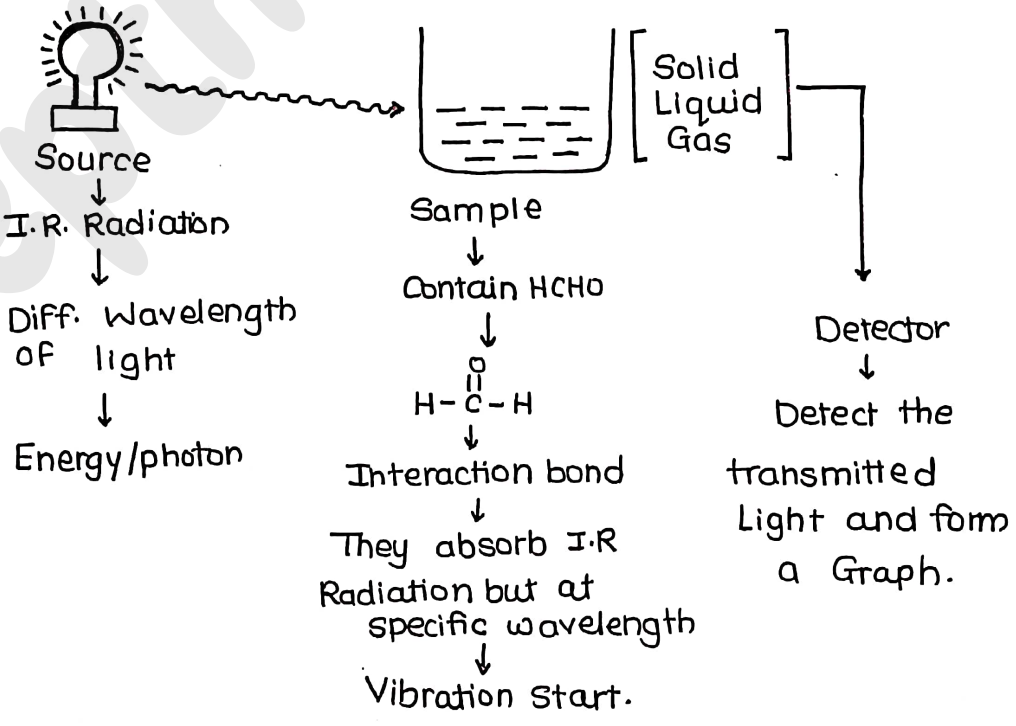
IR Spectroscopy

- IR spectroscopy is used to detect the presence of functional group or which type of functional group present in molecule or chemical compound
- To perform IR spectroscopy we use a specific range of EM Spectrum called IR (Infrared Radiation).
- Application of IR radiation called IR Spectroscopy.
- Instrument which is used in IR spectroscopy is called IR Spectrophotometer.
- IR radiation are lights of different wavelength.



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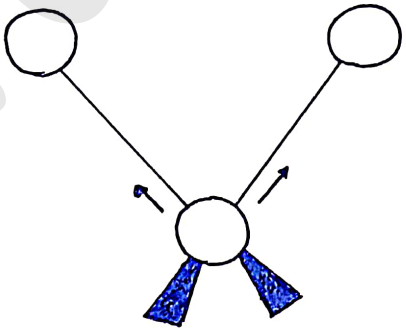
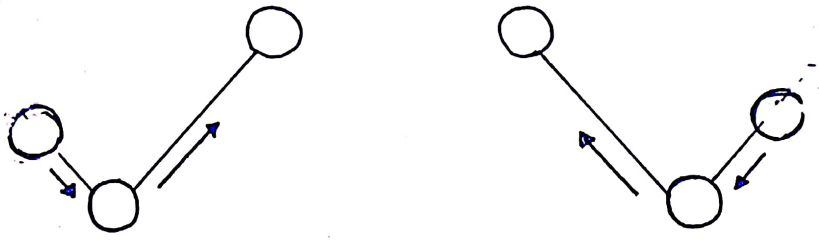
- Vibrations are of two types
  - Streching
    - Symmetric stretching
    - Assymetric Streching
  - Bending
    - Scissoring
    - Wagging
    - Rocking
    - Twisting



Symmetric Streching.



Asymmetric Streching .

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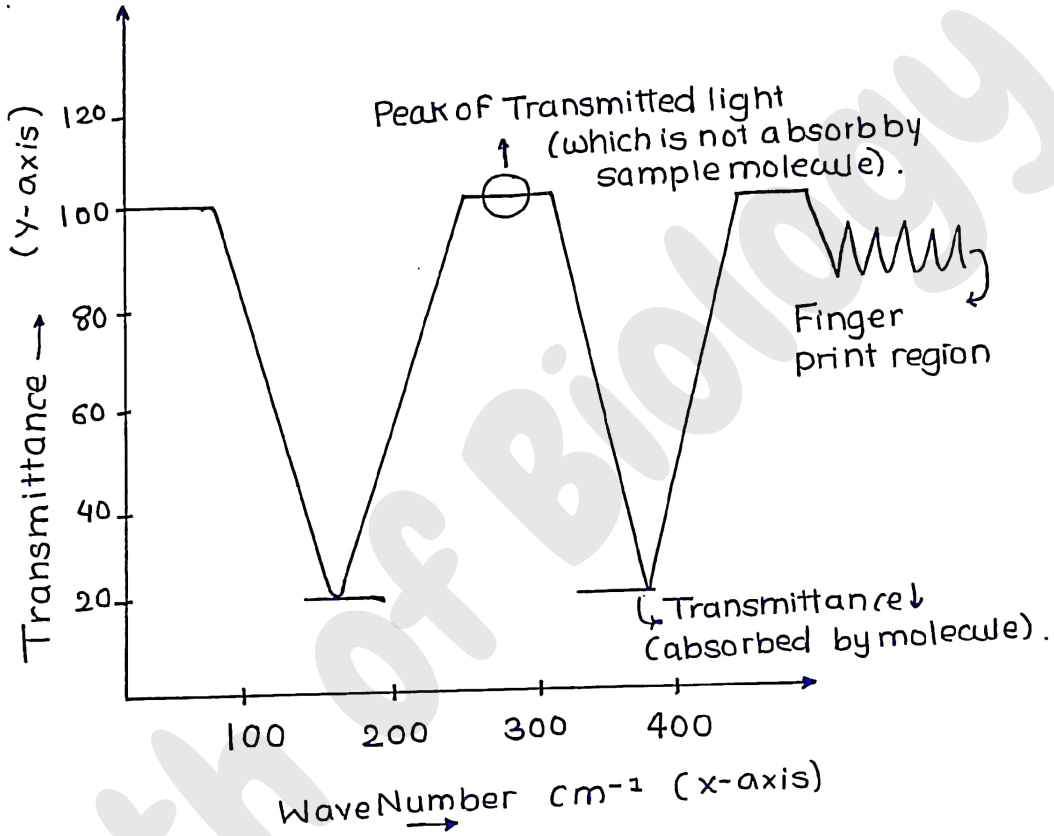


- Bonds show different types of Vibrations at different wavelength of light.
- One molecule are able to show different types of Vibration. For calculate the vibration we have

Formula. → For linear → 3N-5
→ For non-linear → 3N-6

eg. Linear molecule → CO_2
↳ N (No. of atoms) = 3
= 3 (3) - 5
= 4 Vibrations.

- On the basis of wavenumber we can easily identify functional group in compound.

$$\bar{\nu} = \frac{1}{\lambda}$$

$\bar{\nu}$ = wave number

λ = Wave length

- **Principle of IR Spectroscopy**

- When I.R radiation pass through sample / IR Active compound, then the sample Absorbs I.R. radiation and sample only absorb the I.R radiation when the frequency of I.R is same as the Vibrational frequency of compound.

- Selection of Sample → a. Frequency must be match.
  b. Dipole moments not be 0.

- **Fundamental Vibrations**

Vibrations are of two types → i. Stretching
ii. Bending

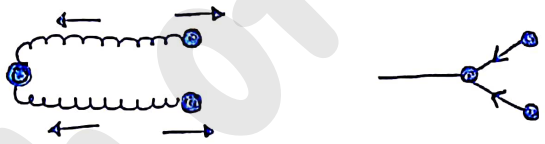
1. Streching

In this type of vibration the distance between two atom increases or decreases but in the same directions.

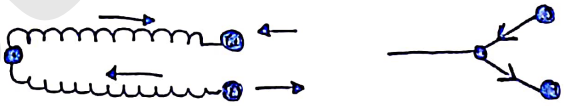
- Stretching are of two types
  - a. Symmetric
  - b. Asymmetric

a. Symmetric

Movements of atoms are in same direction.



b. Asymmetric



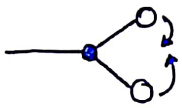
2. Bending

In bending position of atom changes with respect to the original bond axis.

- Bending are of four types
  - i. Scissoring.
  - ii. Rocking.
  - iii. Wagging.
  - iv. Twisting.

i) Scissoring

Two atoms approaches each other.



ii) Rocking

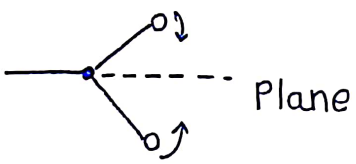
Movement of atom in same direction

iii) Wagging

In wagging two atoms move up and down the plane with respect to central atom.

iv) Twisting

In twisting one atom move up the plane and they moves down with respect to the central atom.



Factors affecting Vibrations

1. Coupled vibrations.
2. Resonance.
3. Electronic effect.
4. Hydrogen Bonding.

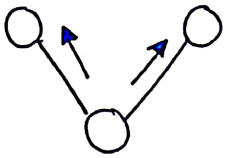
1. Coupled Vibration

- An isolate C-H bond has only one stretching vibrational frequency whereas Methylene (CH_2) group show two stretching vibrations, symmetrical and Asymmetrical.

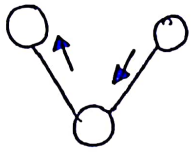
Example :

Group	Assymmetrical	symmetrical
$-CH_2$	3400 cm^{-1}	2900cm^{-1}

- Asymmetric vibration occurs at higher frequency or wave number then symmetric Stretching vibration.
- These are known as Coupled Vibration because this vibrations occurs at different frequency.



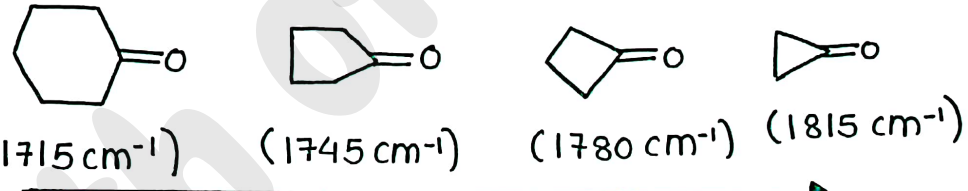
Symmetric stretch



Asymmetric Stretch.

2. Bond Angle

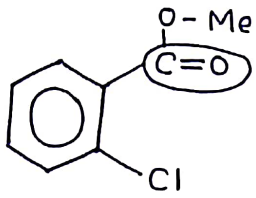
Bond Angle ↓ ⟶ Strain ↑ (Ringstrain) ⟶ Vibrational frequency ↓

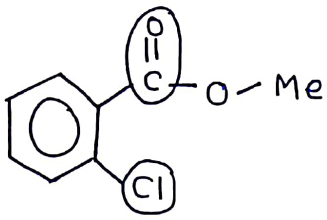


3. Field effect

- Two functional group often influence each other Vibrational frequency.

eg.





- Distance between two functional group in spatial arrangement also affect vibration.

4. Hydrogen bonding

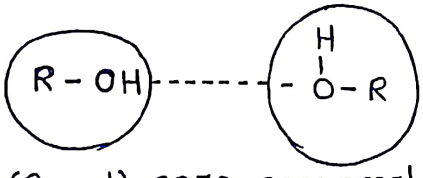
- H-bonding changes the position and shape of an I.R absorption band.

- 2 types of H-bonding → Intermolecular H-bonding
  → Intramolecular H-bonding.

- **Intermolecular H-bonding**
- Gives rise to broad band.
- Concentration dependent.

- **Intramolecular H-bonding**
- Gives rise to sharp band.
- Concentration independent.

- Example



(Broad) 3350-3200 cm^{-1}

R-O-H
(diluted solution).
3650-3590 cm^{-1}
(sharp).

5. Electronic effect → a. Inductive effect.
b. Mesomeric effect.
c. Conjugation effect.

a. Inductive effect → (I)

+ I effect → ↓IR frequency.

- I effect → ↑ IR frequency.

(More - I) effect (Less - I) effect.

V.F ⇒ 1790 cm^{-1} 1720 cm^{-1}

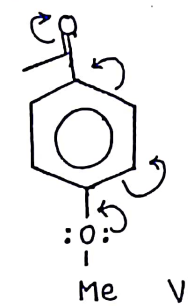
b. Mesomeric effect → (M)

+ M effect → ↓ Vibration frequency.

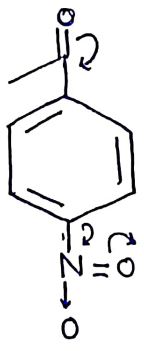
- M effect → ↑ vibration frequency.

Methoxy group

- OMe → ERG
- NO_2 → EWG

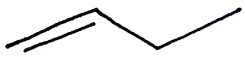


V.F↓



V.F↑

c. Conjugation effect → Conjugation ↑ I.R frequency ↓
(=, ≡)

eg.  1650 cm^{-1}

 1610 cm^{-1}

- **Sample Handling Technique**
- For IR spectroscopy, there are four techniques bywhich we can put the sample in sample holder in IR Spectroscopy.

1. Solid Sampling technique.
2. Liquid sampling technique.
3. Gas sampling technique.
4. Solution sampling technique.

1. **Solid Sampling Technique**

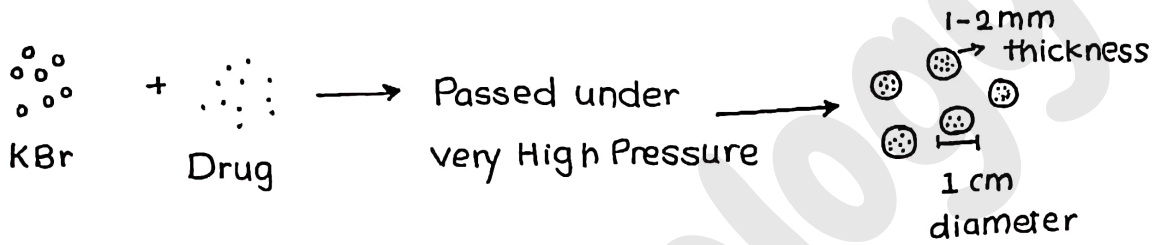
- Here we prepare solid samples.

i. Direct sampling → Here solid sample is directly placed in a sample holder.

ii. Pelletization Technique → Here, we mixed solid sample with KBr, Then passed under very high pressure and press to

form a small 1-2 mm thick pellets (10m diameter).

- These pellets are transparent to IR radiation.



- KBr or NaCl is used because it is Transparent so, it is useddue to Transparency light (IR) is easily passed from them.

iii. Mulling technique → (Mulling Agent example → (FC, Nujol)

- Mulling is the process of grinding up a sample into fine powder through mortar and Pestle& then dispersing into a liquid or solid matrix. to form a Mull.
- Liquid mulls have been formed by combining the powdered analyte with Nujol.
- Nujol is a mulling agent and then thick paste is formed.

iv. As Solid film

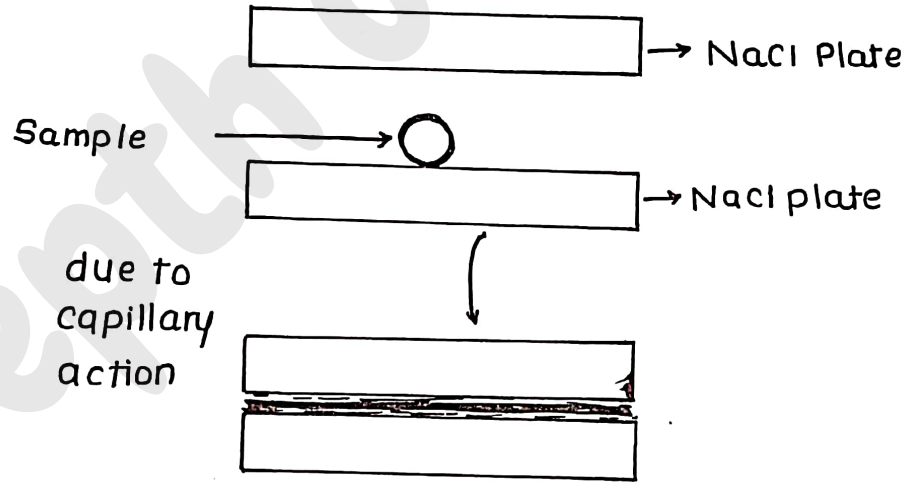
- In which we placed our sample solution on NaCl or KBr Surface and then solvent is evaporated.
- Due to evaporation solid sample leave behind and a thin film left on the cell surface.

* (Here we use volatile liquid, so liquid evaporates and solid film is formed and then we analyze this via IR).

2. **Liquid Sampling Technique**

- In this sample the liquid sample is squeezed between two NaCl plates produces thin film of sample about (0.01-0.1mm) thickness.

* Plates are immediately cleaned via using $CHCl_3$, Toluene, etc.



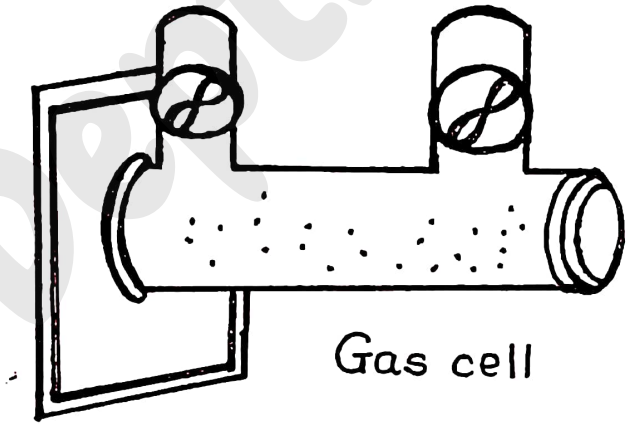
3. **Sampling of Gases**

- Gas sample are introduced into Gas cell and Transparent cell which allow the cell to pass the Beam. (NaCl cell is also present here).

- The beam falls on sample and then detector detect or Analyze.

* Usually sample cell / Gas cell with long path length of 5- 10 cm is needed. because the gases show relatively weak absorbance.

Gas cell → 5-10 cm → Path length ↑ → Light Travel in more time ↓ Absorbance via Gas ↑



Gas cell

UNIT –II

IR spectroscopy

Introduction, fundamental modes of vibrations in poly atomic molecules, sample handling, factors affecting vibrations

Instrumentation - Sources of radiation, wavelength selectors, detectors - Golay cell, Bolometer, Thermocouple, Thermister, Pyroelectric detector and applications

Instrumentation

Instrumentation - Sources of radiation, wavelength selectors, detectors - Golay cell, Bolometer, Thermocouple, Thermister, Pyroelectric detector and applications.

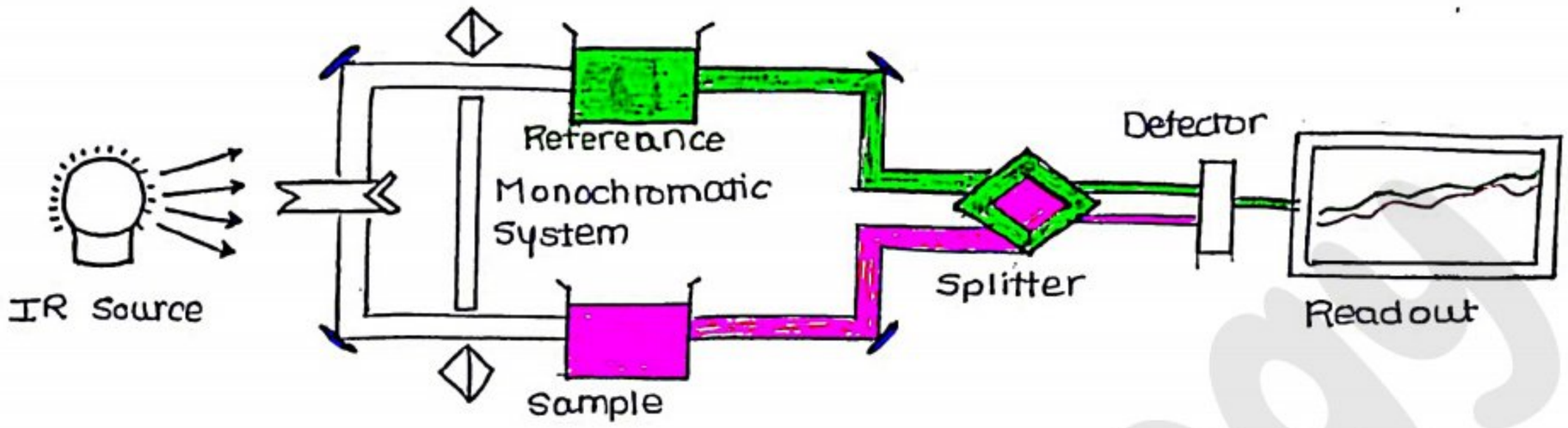
IR spectroscopy

- IR spectroscopy deals with the interaction of infrared radiation with matter by absorption, emission or reflection.
- It [1] used to study and identify chemical substances or functional groups in solid, liquid or gaseous forms.
- The method or technique of infrared spectroscopy is conducted with an [2] instrument called an infrared spectrometer.
- Infra-red spectrometer produces an [3] infrared spectrum.

IR Spectroscopy Instrumentation

The main parts of IR spectrometer are as follows:

- Radiation source
- Monochromators
- Sample cells and sampling of substances
- Detectors
- Recorders



IR Radiation Sources.

- IR instruments require a source of radiant energy which emit IR radiation which must be steady, (stable). intense enough for detection and extend over the desired wavelength. Various sources of IR radiations are as follows:
  - Nernst glower
  - Incandescent wire
  - Glober source.

Nernst Glower

- At, Starting → T↓ & Resistance for flow of Current↑
- After Sometime → T↑ & Resistance↓ (IR-Produced).

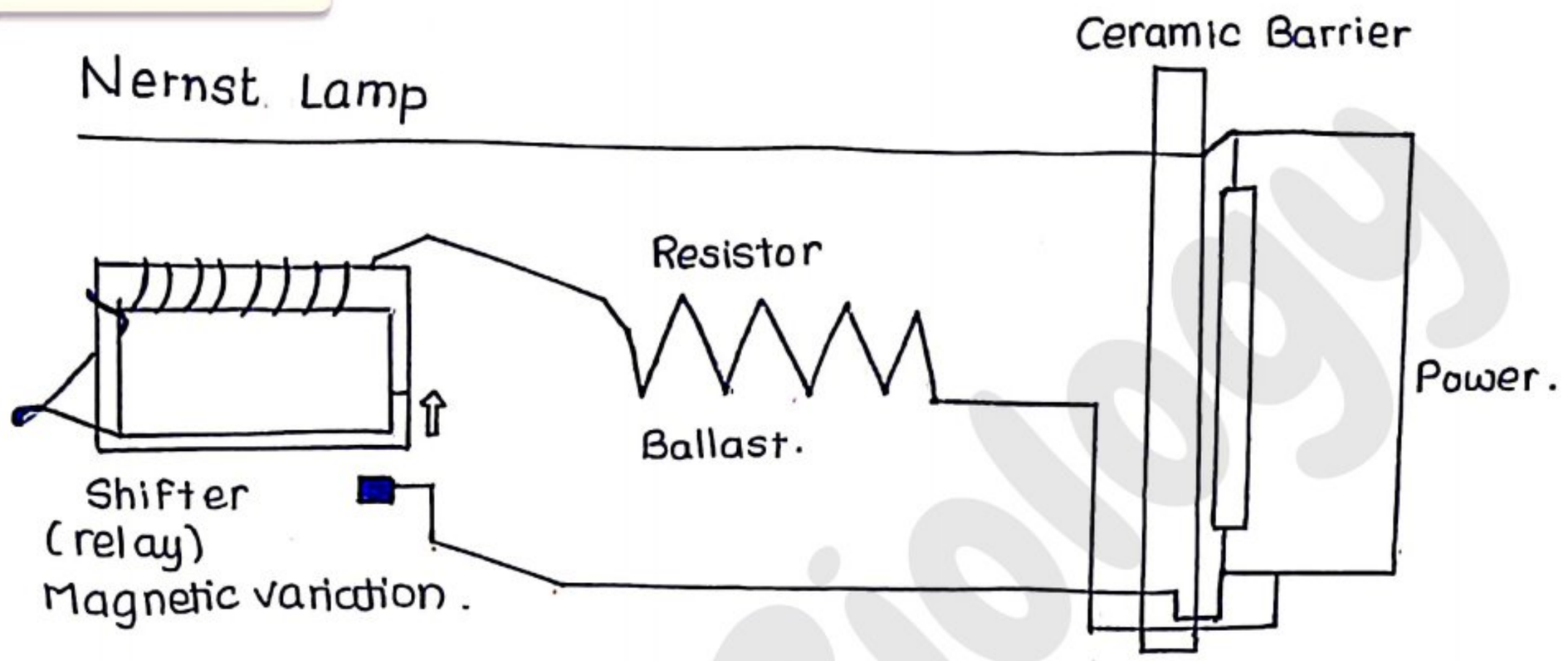
2. Mostly Used in IR Spectroscopy.

Consist of a

1. The Nernst Glower is ↑ cylinder (1-2 mm diameter, approximately 20 mm long) of rare earth oxides. (Oxide of Cerium). (Metal).
   - Platinum wires are sealed to the ends, and a current passed through the cylinder.
   - The Nernst glower can reach temperatures of 2200 K. → Then large amount of Current flow through it.

The platinum wires are connected at two ends of this cylinder for the passage of current. When sufficient amount of current is alowed to flow through the cylinder, it gets heated up and produces radiation in the IR region.

1. It emits IR radiations over a wide range of wavelength.
2. Intensity of radiation remains steady and constant over a long period of time.

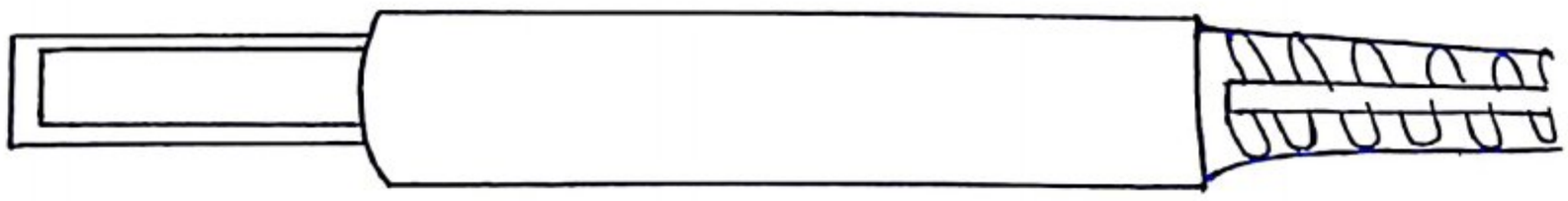


Globar Source

→ At, Starting → T↓ & Resistance↓ & Current flow↑ → More & More Current flow So, Cylinder T↑ & I·R produce

→ After Sometime → T↑ & R↑ & Current flow↓

- The Globar source is a silicon carbide rod (5mm diameter, 50 mm long) which is electrically heated to about 1500 K.
- Water cooling (→ To Prevent Overheating.) of the electrical contacts is needed to prevent arcing. (Type of Electrical Discharge).
- The spectral output is comparable with the Nernst glower, except at short wavelengths (less than 5 μm) where it's output becomes larger.

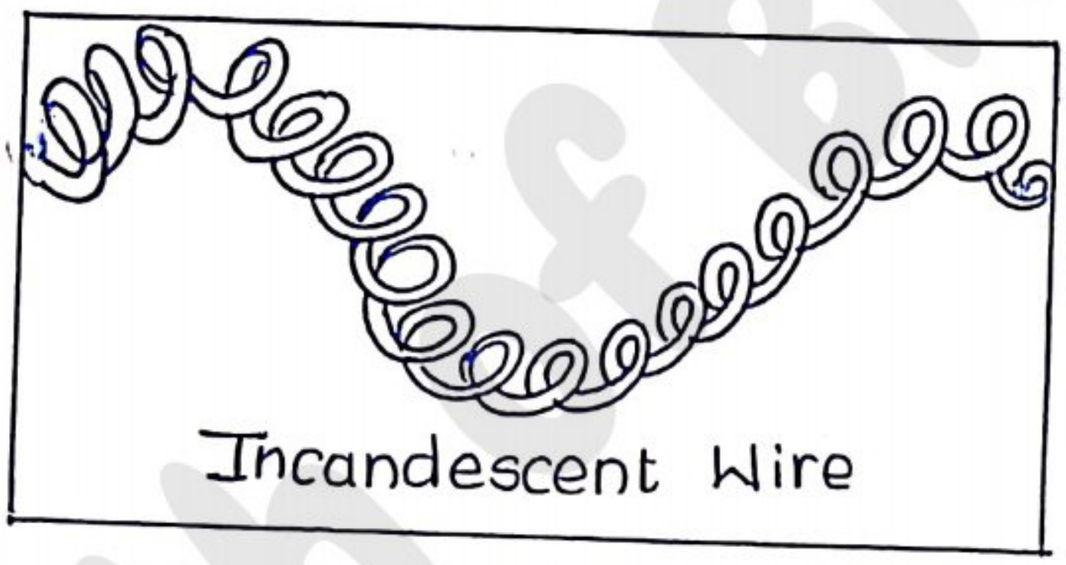


Globar Source

Incandescent Wire

- The incandescent wire source is a tightly woundcoil of nichrome wire, electrically heated to 1100K. → Restrict Current flow in Circuit.

- It produces a lower intensity of radiation than the Nernst or Globar sources, but has a longer working life.



Monochromators

- A monochromator is an optical instrument which measures the light spectrum.

- Light is focused in the input slit and diffracted by a grating.

- Only one colour is transmitted through the output slit at a given time.

- Spectra are then recorder wavelength by wavelength, rotating the grating.

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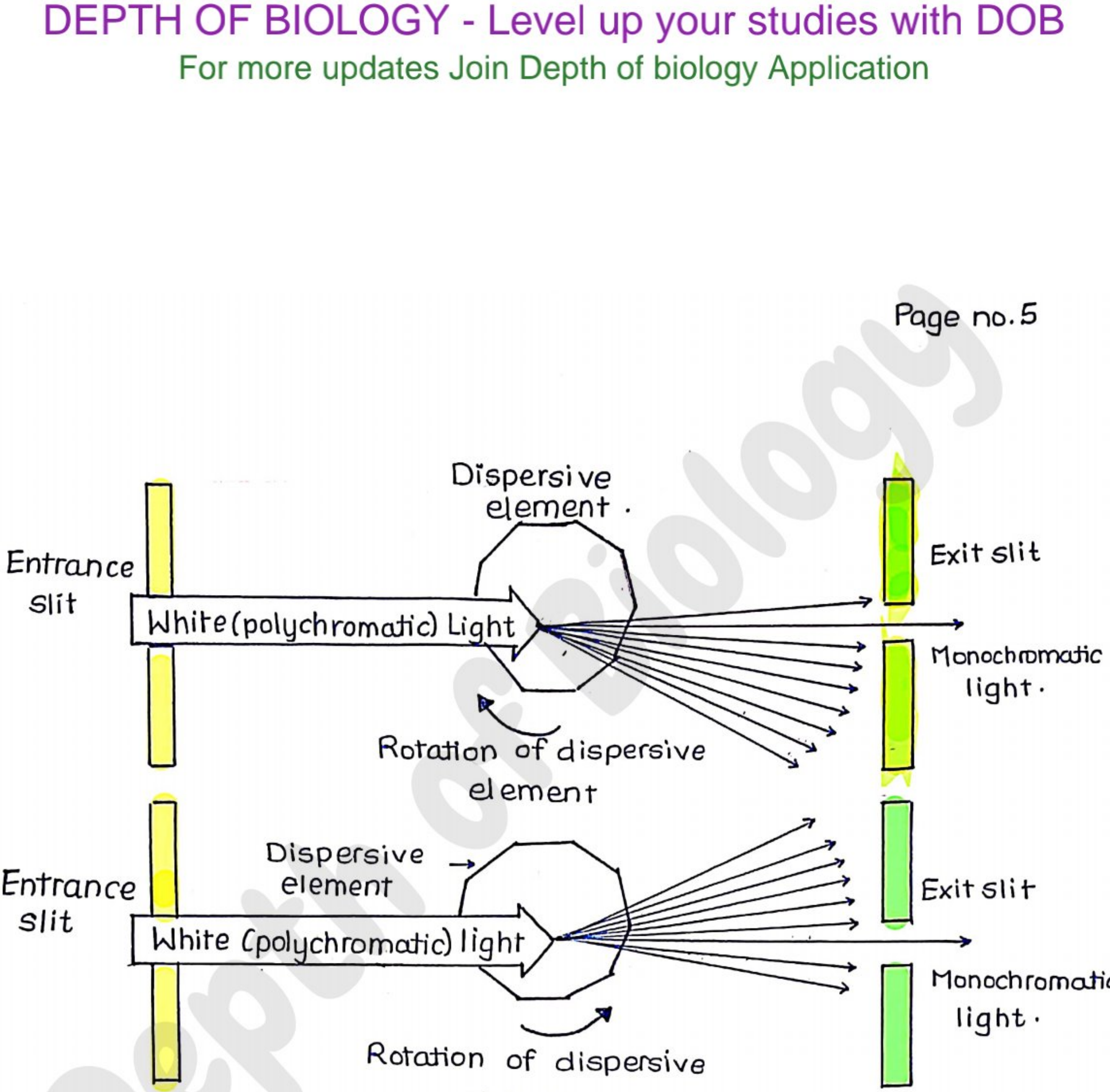
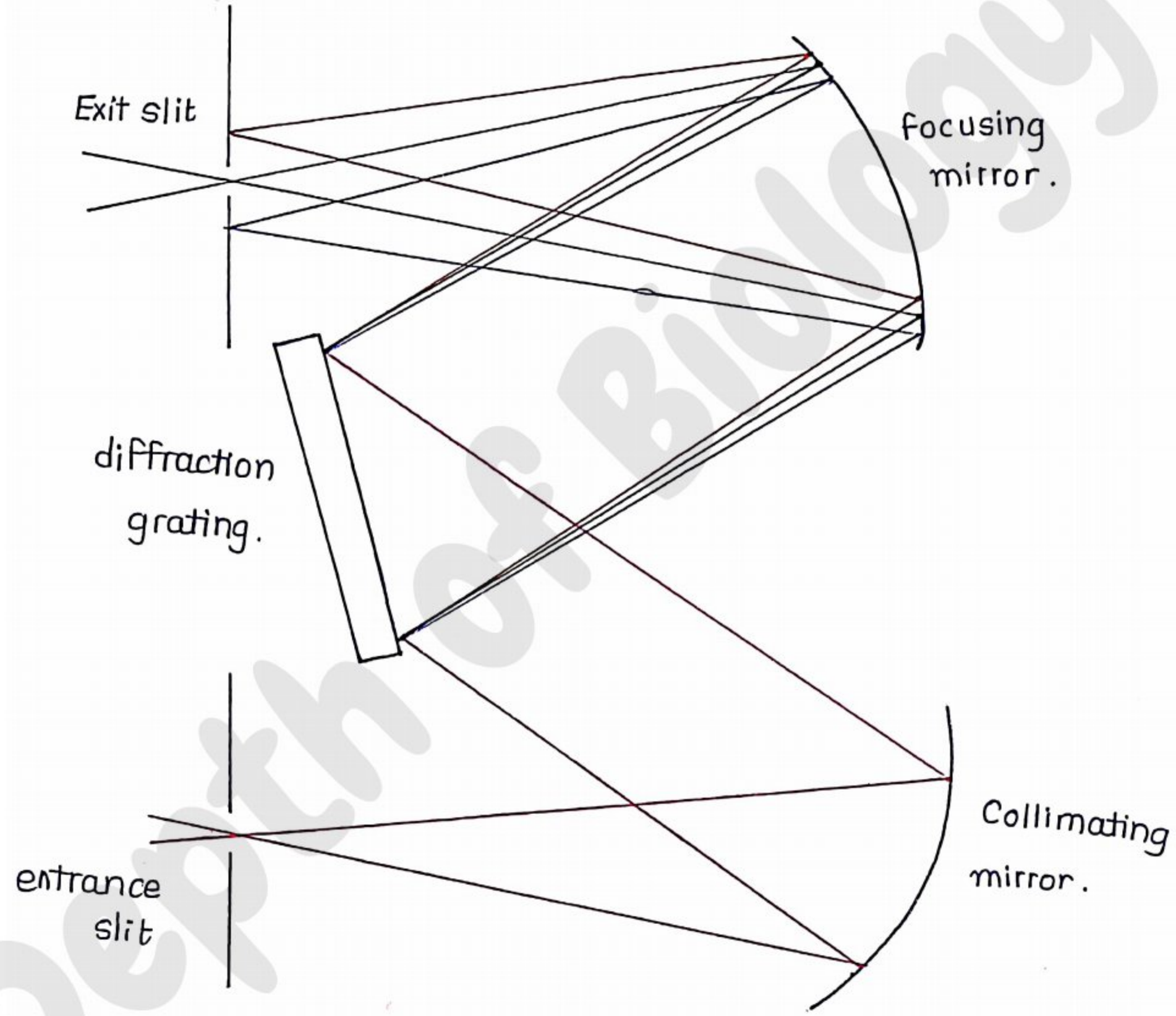


Monochromator.

diffraction gratings are often used in modern instruments.

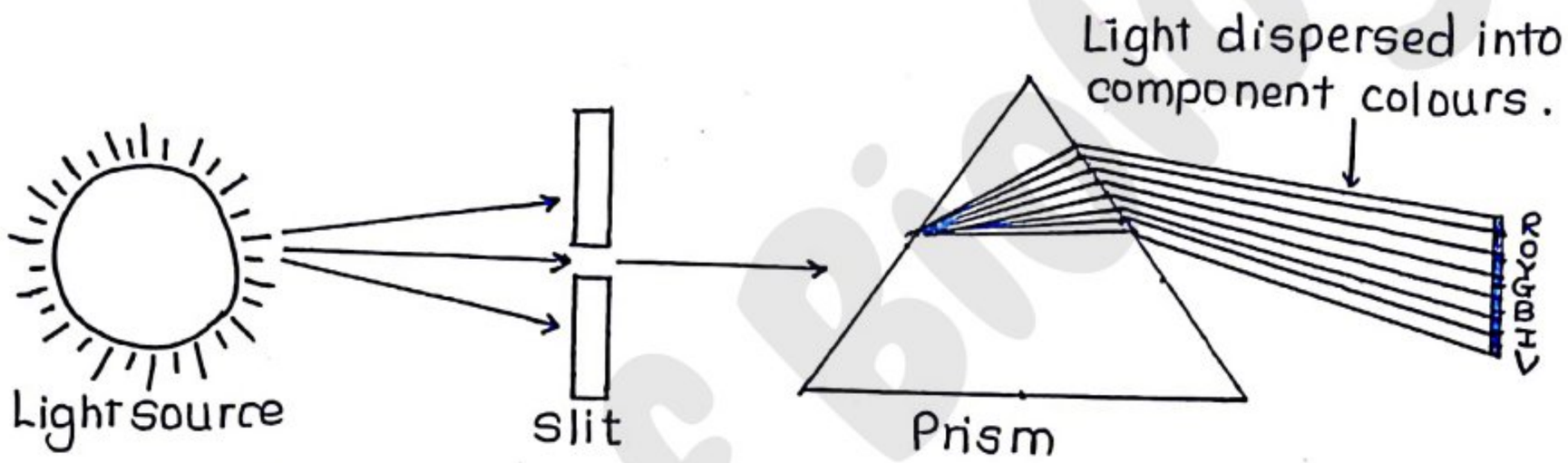


2. **Prisms**

- The dispersive element in prism monochromators is a prism. Prisms have a high light utilization efficiency

and do not produce higher order light and very little stray light.

- However, dispersion is dependent on wavelength (high for UV, low for IR) and temperature.

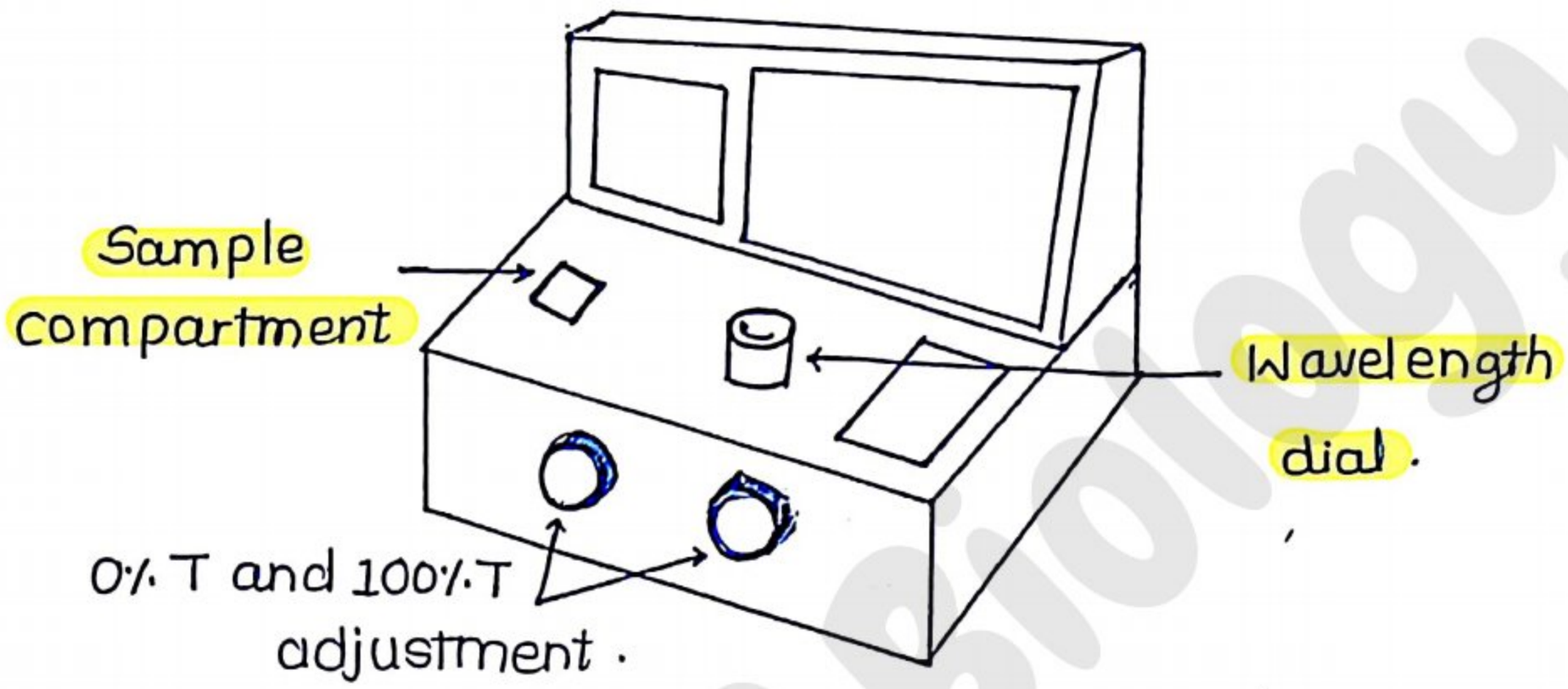


Dispersion of light through Prism

Sample cells

- Infrared spectroscopy routinely is used to analyze gas, liquid, and solid samples.
- Sample cells are made from materials, such as NaCl and KBr, that are transparent to infrared radiation.
- Gases are analyzed using a cell with a pathlength of approximately 10 cm.
- Longer pathlengths are obtained by using mirrors to pass the beam of radiation through the sample several times.

Sample cells.



Sampling of Substances

- IR spectroscopy has been used for the characterization of solid, Liquid or gas samples.
- **Solid :** Various techniques are used for preparing solid samples such as pressed pellet technique, mull technique, etc.
- **Liquid :** Samples can be held using a liquid sample cell made of alkali halides. Aqueous solvents cannot be used as they will dissolve alkali halides. only organic solvents like chloroform can be used.
- **Gas :** Sampling of gas is similar to the sampling of liquids.

Sampling of Solids

Various techniques used for preparing solid samples are as follows:

Mull technique: In this technique, the finely crushed sample is mixed with Nujol (mulling agent) in a marble or agate mortar, with a pestle to make a thick paste. A thin film is applied onto the salt plates. This is then mounted in a path of IR beam and the spectrum is recorded.

- **Pressed pellet technique:** In this technique, a small amount of finely ground solid sample is mixed with 100 times its weight of potassium bromide and compressed into a thin transparent pellet using a hydraulic press. These pellets are transparent to IR radiation and it is used for analysis.

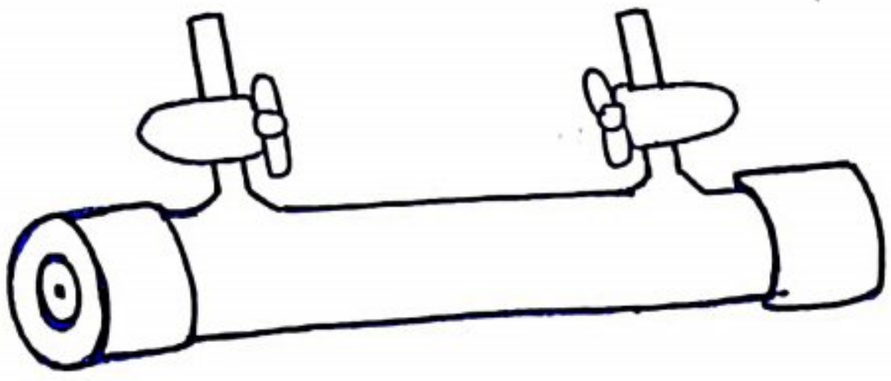
Sampling of liquids

- Liquid sample cells can be sandwiched using liquid sample cells of highly purified alkali halides, normally NaCl.

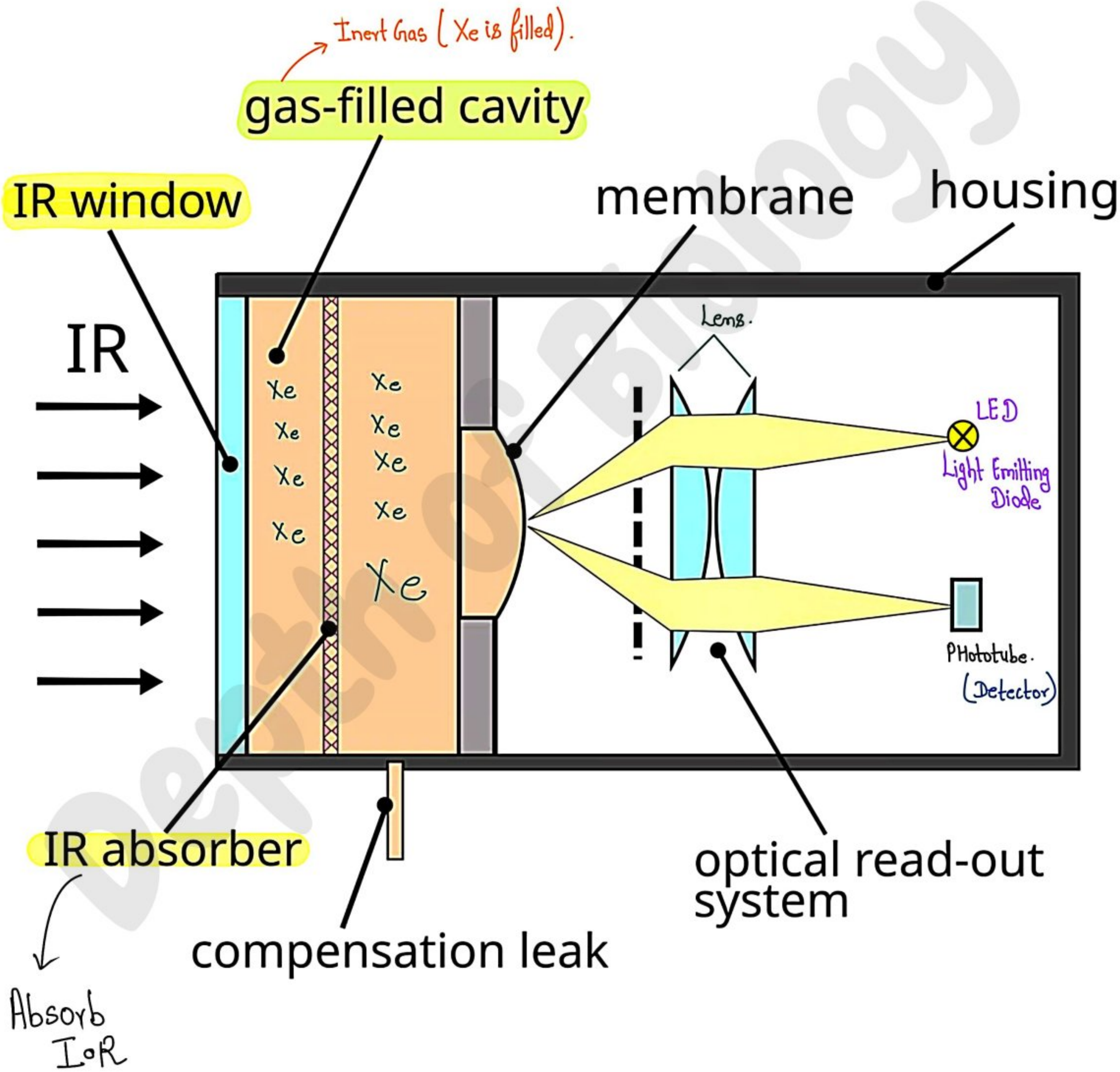
- Other salts such as KBr and CaF_2 can also be used. Aqueous solvents cannot be used because they cannot dissolve alkali halides.
- The sample thickness should be selected so that the transmittance lies between 15-20%. Solvents like chloroform can be used.
- For most liquids, the sample cell thicknessis 0.01 - 0.05 mm. Some salt plates are highly soluble in water, so the sample and washing reagents must be anhydrous.

Sampling of gases

- The sample cell is made up of NaCl, KBr, etc. and it is similar to the liquid sample cell.
- A sample cell with a long path length (5 - 10cm) is needed.
- Because the gases show relatively weak absorbance.



Gas cell



Construction of Golay Cell.

1. It is Consist of IR Window which allow to pass the I.R radiation.

2. IR Absorber Road → This Rod Absorb I.R Radiation & after absorbtion of I.R Radiation Temprature of Rod is Increased.

3. A Diaphram or Membrane is Movable which reflect the I.R radiation.

4. LED → Light Emitting Diode which emits light.

5. A phototube (Detector) → which detect Visible Light.

Working of Golay Cell

- I.R radiation produces by different radiation sources like Nernst Glower, Globar source & this I.R radiation are passed from I.R Window & fallson I.R Absorber / I.R Absorber Road. This Absorber Absorb the I.R radiation.

& due to this Temprature of Rod increases. Due to this Xe gas Temprature also (↑)ses, & as we know very well in Case of Gas (Temp. ∝ Volume) it means due to (↑)se in Temprature of Gas, Volume of Gas also (↑)sed.

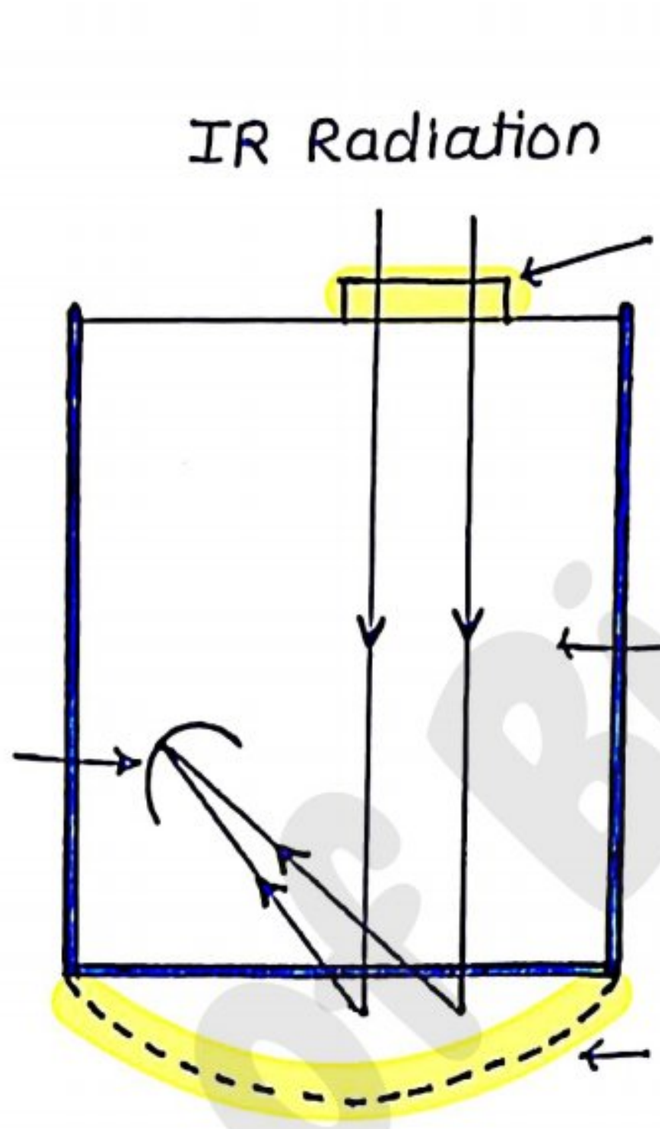
- As the Volume of Gas (↑)sed the Diaphragm become deforms or Expand or Move away.
- Due to this the Light of LED not go towards Phototube or Detector. Properly.
- So, With the help of this we can easily detect I.R radiation

✡ Fraction of Beam reaching to Photodiode depends on Curve of diaphragm/membrane → which depends on I.R absorbed by gas → which depends on I.R reaches to Detector.

✡ This Changes detect by Photocell & then we can Compare the Changes & easily detect the I.R radiation absorb by Gas.

Golay cell

→ Also known as Pneumatic Detector.

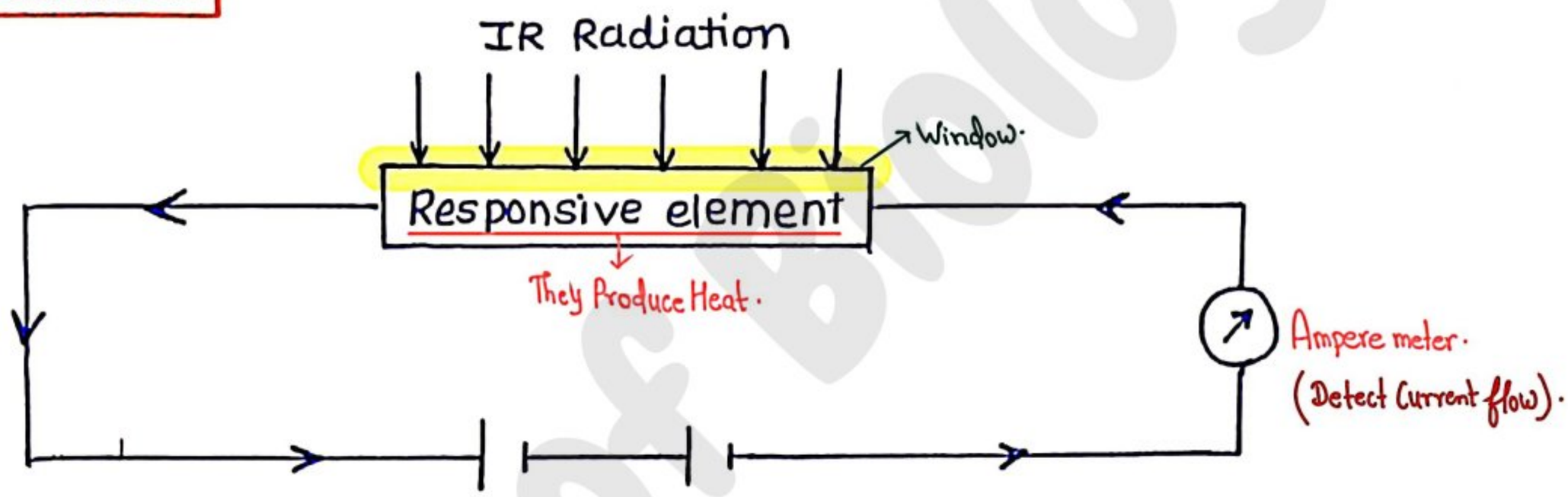


- Consists of a gas-filled enclosure with an infrared absorbing material and a flexible diaphragm or membrane.
- When infrared radiation is absorbed, it heats the gas, causing it to expand.

by IR Absorber Rod → Temp. (↑) sed.

- The resulting increase in pressure deforms the membrane. Light reflected off the membrane is detected by a photo-diode, and motion of the membrane produces a change in the signal on the photodiode.

- **Bolometer**



- Made from strips of metals like platinum or nickel or semiconductor (Germanium). The metals have the high-temperature coefficient, i.e their temperature increases with the increase in temperature. Exhibit large change in resistance with temperature.
- The resistance of metal is directly proportional to the temperature.

Bolometer

Principle ↴

- Work on the principle of Change in Current & Resistance in the Circuit Caused by the Responsive element when I.R falls on the Element.

Working ↴

Detector Contain responsive element whose work is to absorb Radiations.

I.R radiation falls on Responsive Element
& Heat is generated.

↓

Increase in Heat leads to (↑)se in Resistance

↓

(↑)se in Resistance leads to (↓)se in Current flow.

↓

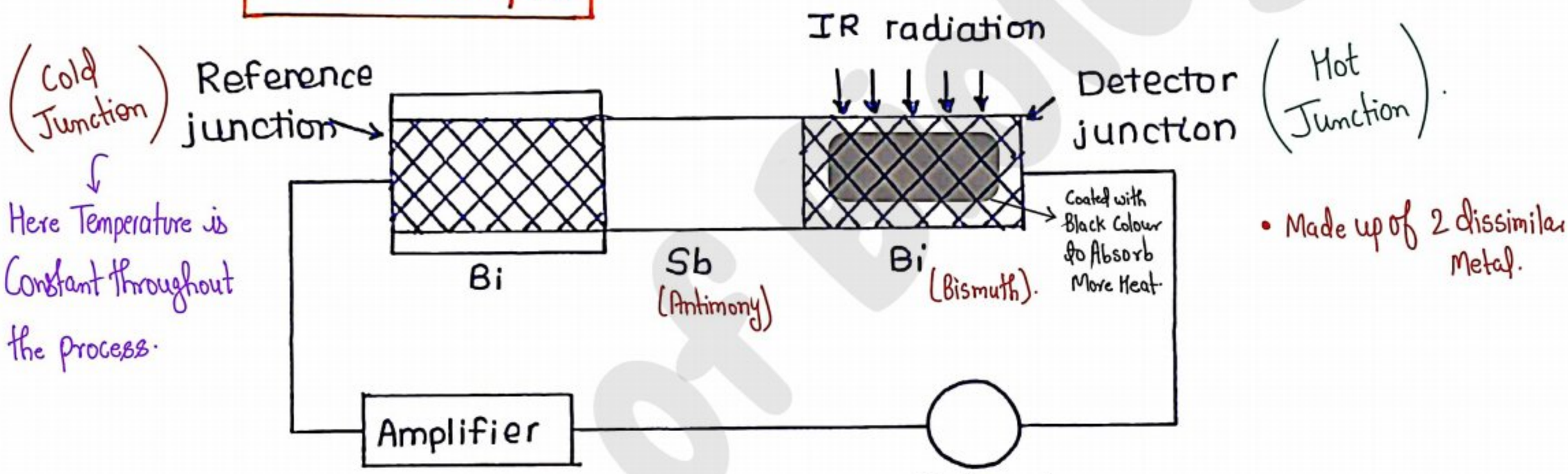
Change in Current is detected by Amperemeter.

- Lesser the Current passes through Circuit More the Response by detector

☆ Response time of Bolometer is few Mili Seconds

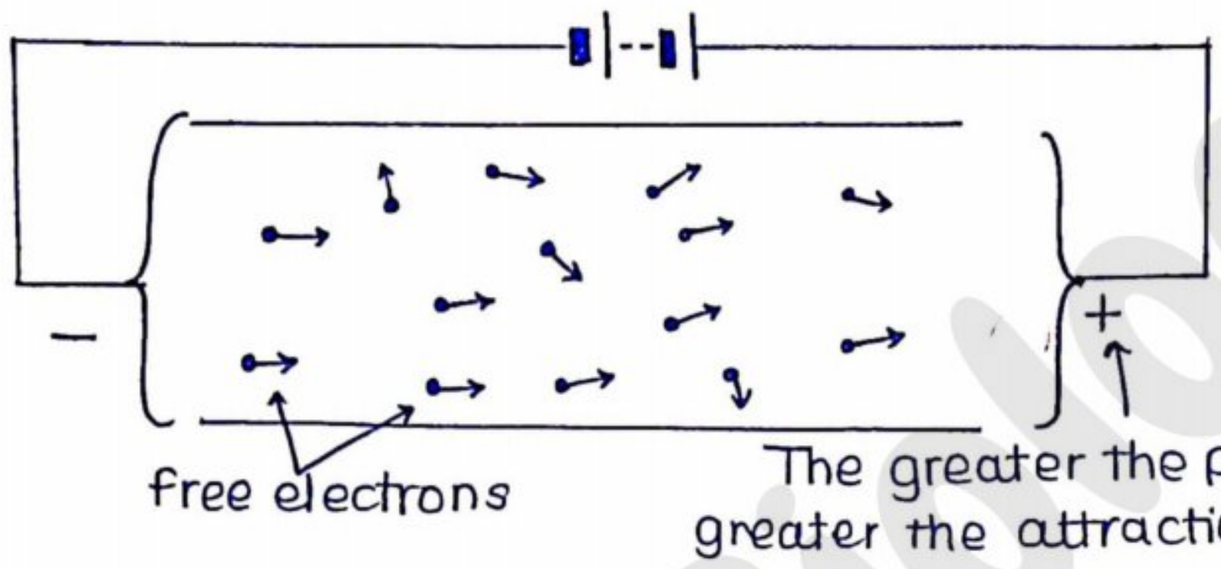
☆ Detector has Limited Sensitivity.

Thermocouple



- Made up of 2 dissimilar Metal.
- Has two junctions
- Difference in the temperature of two junctions, creates a voltage due to thermoelectric effect which provides a signal.
- Several thermocouples in series is called thermopile (increased sensitivity).

- Voltage can be considered as the pressure that forces the charged electrons to flow in an electrical circuit.



- The flow of charge carriers between the hot and cold regions in turn creates a voltage difference.

- Made up of 2 metal like bismuth and antimony coated by metal oxides.

- If wires of 2 dissimilar metals joined head to tail, then a difference in temperature between head and tail causes a current to flow in the wire.

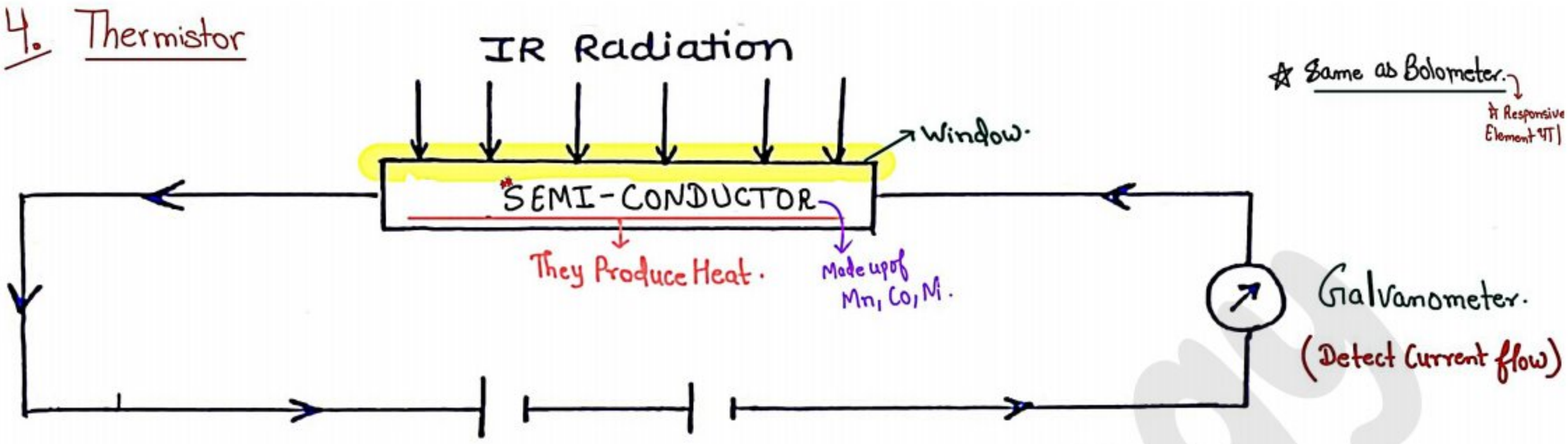
- This current is proportional to the intensity of radiation. → Detected by Galvanometer.

- These are also called as thermopile detectors.

- Materials should be thermally active and these are used in dispersive instruments.

- Response time is 30 milliseconds and they give response for all frequencies.

4. Thermistor



☆ Same as Bolometer.
☆ Responsive Element ΔT

- Thermistors work on the principle that the resistance of the semiconductor material changes in response to temperature changes, allowing for accurate temperature measurement.

IR radiation falls on SemiConductor -
↓
Temperature of Semi-Conductor (↑)ses.
↓
Resistance (↓)se & Current flow (↑)sed.
↓
(↑)sed in Current detected by Galvanometer.

Semi-Conductor show ⊖ve Coefficient of Resistivity
(
*It Means (↑)se in Temperature leads to (↓)se in Resistance.

1. Sensing element → usually a metal oxide (NiO, FeO, etc).
2. Electrodes → Typically made up of (Au, Ag, Pt).
3. Lead wires → connects electrodes to external circuitry.
4. Encapsulation → Sensing element & electrodes are protected.
5. Housing → Some thermistors are mounted in a metal or plastic housing for added protection.

- Thermistors help ensure the quality, safety and efficacy of pharmaceutical products by providing accurate temperature control and monitoring.

- It includes,

1. Temperature control in storage:
   For Storing sensitive medications & vaccines.

2. Freezer temperature monitoring:
   For storing vaccines and biologicals.

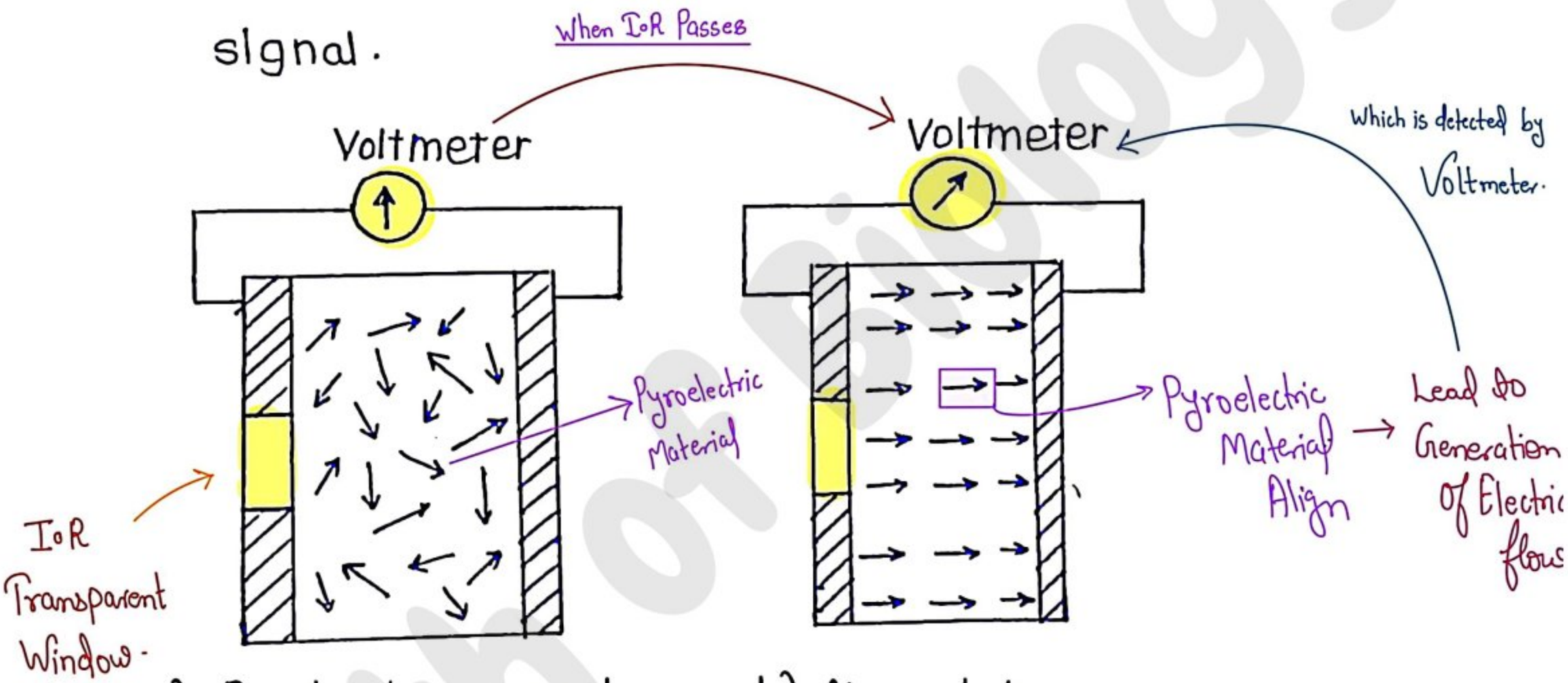
3. Incubator temperature control:
   For cell cultures, microbiological testing and other laboratory applications.

4. Autoclave temperature monitoring:
   For sterilization processes.

5. Quality Control:
   During manufacturing processes, such as lyophilization and granulation.

6. Stability testing:
   Monitoring temperatures during stability testing of pharmaceutical products.

- **Pyroelectric detector**



a) Randomly oriented dipoles (At room temperature).

b) Aligned dipoles (above room temperature and below Curie temperature).

- Pyroelectric material is sandwiched in the form of single crystalline wafers between two electrodes, one of which is IR transparent, a temperature dependent capacitor is formed.

Pyroelectric Detector

- It is Made up of Temprature sensitive ferroelectric Material (Deuterium Triglycerin Sulfate) & it is Sandwiched b/w two I.R Transparent electrodes Connected With Voltameter

✡ At room Temprature Dipoles are randomly oriented

↓

As, you Know Pyroelectric Material are Temprature Sensitive

↓

I.R radiation falls on Pyroelectric Material

↓

Dipoles (of Pyroelectric Material) get aligned.

↓

This Changes in polarization produce Electric Signal that depends of Heat. & Current flow is Measured by Voltmeter.

✡ Pyroelectric Substance loses it polarization above Curie Temprature.

Applications of IR Spectroscopy

1. Identification of Organic Compound

- The identity of an organic compound can be established from its fingerprint region (1400-900cm^{-1}).
- The identity of an organic compound is conformed of its fingerprint region exactly matches with the known spectrum of the compound.
- The compounds containing same functional group may have similar absorption above 1500cm^{-1} but they differ in the fingerprint region.

2. Structural Determination

- This technique helps to establish the structure of an unknown compound.
- All major functional groups absorbs at their characteristic wave numbers.

Example:

I. This IR spectra of amino acids exhibits bands for ionised carboxylic acids and amine salts ($-^{+}NH_3$). No band for free $-NH_2$ and –COOH groups is observed.

$$^{+}NH_3\text{-}CH\text{-}COO^{-}$$

I. From the IR bands of sulphanilic acid, it is solid that the compound contains $^{+}NH_3$ and SO_3^{-} and not free groups as $-NH_2$ and $-SO_3H$.

3. Qualitative Analysis of Functional Groups

- The presence or absence of absorption bands help in predicting the presence of certain functional groups in the compound.

Example:

I. The presence of oxygen reveals that the groups maybe –OH, C=O, -COOR, -COOH, anhydride, etc. But the absorption band is in between 3600-3200cm^{-1}. The band in this region maybe due to -O-H.

II. In case of $–NH_2$, -NH groups , all this can be seen. $–NH_2$ shows two absorption bands while –NH shows only one band.

III. Its distinction from –OH structure can be made from the extent of H-bonding which is stronger in –OH compounds and causes lowering in wave number.

4. Distinction Between Two Types of Hydrogen Bonding

- It is known that in H-bonding the electron clouds transfer from a hydrogen atom to the neighbouring electronegative atom.
- The strength of H-bond is maximum when the proton donor group and the axis of lone pair orbital are collinear and varies inversely to the distance to the distance between hydrogen and oxygen.

Example:

- The hydroxyl compounds in the solid or liquid state exist as polymeric aggregates.
- The absorption in aggregate form occurs at lower frequencies and bands formed are relatively broad.
- But when such a substance is dissolved in non-polar solvent such as CCl_4, the aggregates or polymers break in dimers and monomers.
- Due to this, the O-H structure absorption shifts to higher frequencies and the peaks below become sharp.
- This technique helps to distinguish between intra-molecular H-bonding.
- Ortho nitro phenol exhibits intra-molecular H-bonding. Intra-molecular H-bonded compound doesn't show any shift in absorption or dilution whereas intermolecular H-bonded does.

5. Quantitative Analysis

The estimation of the compound of the mixture can be done by:-

- Measuring the intensities of absorption bands characteristic of each compound.
- Knowing the optical density of the absorption band for a pure component.

Example:

- Xylene exists as a mixture of three isomers, i.e. ortho, meta and para xylenes.
- The percentage composition of mixture can be determined by IR spectrum of the mixture.
- Bands are formed at:

a) $740cm^{-1}$ for ortho isomers
b) $880cm^{-1}$ for meta isomers
c) $830cm^{-1}$ for para isomers

- Mixtures of known composition are recorded and the working curves are drawn for the bands.

6. Study of a Chemical Reaction

- Reduction of a standard aliphatic ketone to form a stronger bond at about 1710cm^{-1} when it is subjected to reduction, it forms butan-2-ol which absorbs at 3300cm^{-1}due to –O-H.
- IR spectroscopy is also used to predict the products formed in a photochemical reaction.

Example:

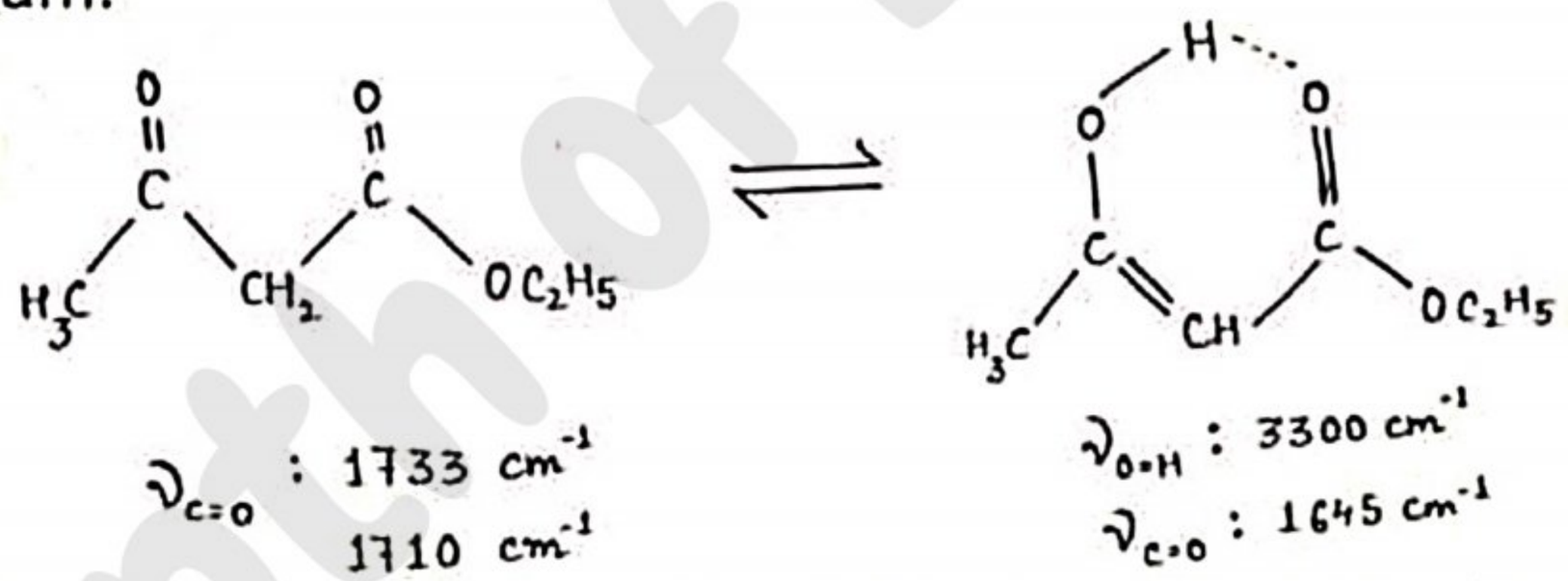
When verbenone is irradiated in ethanol solution, the UV absorption maximum due to verbenone disappears and the IR spectrum of crude verbenone appears at 1787, 1740, 1715 and 1685cm^{-1}.

- By chromatographic separation we get chrysanthenone, ethyl geraniate,ethyl-3,7- dimethyl octa-3,6-dienoate.

7. Study of Keto- enol Tautomerism

- Diketones and keto esters exhibit keto-enol tautomerism.
- They have α-H atom in them. The IR spectrum of such compound contains bands due to C=O, O-H, C=C bonds.

Example: Ethyl aceto acetic ester- It exists in keto-enol isomers in equilibrium.



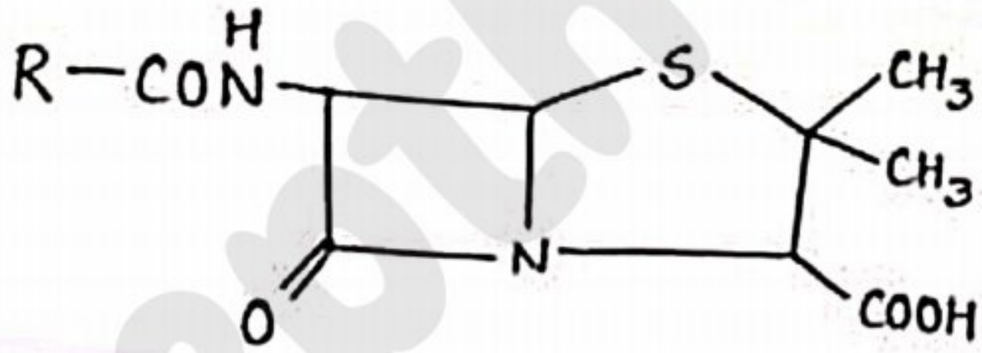
- The lowering of $\nu_{C=O}$ absorption in the enolic bonding form is due intra-molecular H-bonding which is stabilised by resonance.
- The appearance of bands clearly confirms keto-enol tautomerism in aceto acetic ester.

8. Study of Complex Molecules

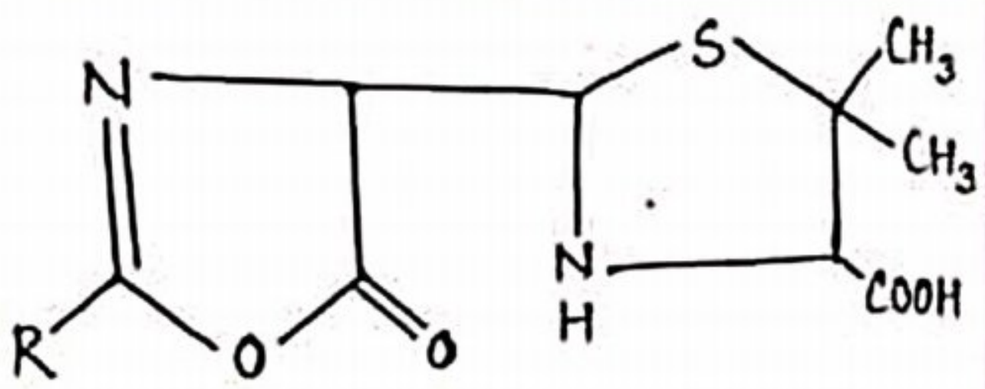
- This technique is also useful to establish the structure of complex molecules.

Example:

Two structures of penicillin were prepared on the basis of IR spectral.



β-lactam



Oxazolone

The IR structure of oxazolone shows two characteristic bands:

a) 1825cm^{-1} due to $\nu_{C=O}$
b) $\nu_{C=N}$ due to 1675cm^{-1}

- It is found that no such band appear in the spectrum of penicillin. Thus, oxazolone structure for penicillin is ruled out.
- It is known that β- lactams do not absorb near 1770cm^{-1} whereas β- lactam fused to thiazolidine ring exhibits a band at 1770cm^{-1}. Thus, the β- lactam structure of penicillin is confirmed.

9. Conformational Analysis

- Useful for conformations of cyclic compounds cyclohexane exists in boat form and chair form.

Chair Form

Boat Form

- There are 18 IR active C-C structure and CH_2 rocking and twisting vibration for boat form (II) whereas there are only five for the chair form (I).

- The spectral examination of cyclohexane in the region 1350-700cm^{-1} reveals five bands expected for chair form.
- This shows the greater stability for chair conformation over boat conformation.
- By IR spectroscopy, axial and equatorial substituents in cyclohexane substituents in cyclohexane can be distinguished.
- The equatorial substituent usually absorbs at a higher frequency than does the same substituent at axial position.
- This is due to steric hindrance of C-X bond with adjacent H-atoms.

10. Detection of Impurity in a Compound

- IR spectroscopy is also useful in the detection of impurity in a compound by comparing its spectrum with the spectrum of the authentic sample of the compound.
- Pure sample always consists of poor bands and also some additional bands.

Dispersive and Fourier transform IR spectrophotometer

Dispersive IR Spectrometer:

—Uses prism or grating to break IR light into individual wavelengths.

-Scans one wavelength at a time.

-Like moving a flashlight one step at a time.

📘 Definition:

A Dispersive IR Spectrometer is a type of infrared spectrophotometer that uses a monochromator (like a prism or grating) to separate infrared (IR) light into individual wavelengths and then passes them one by one through the sample.

How It Works (Step by Step):

1. IR light source emits a broad range of IR wavelengths.
2. The monochromator (a prism or grating) disperses the light into separate wavelengths (like a rainbow).
3. Only one wavelength at a time is allowed to pass through using slits.
4. This single wavelength passes through the sample.
5. The detector measures how much light is absorbed by the sample.
6. The instrument scans all wavelengths one by one to build the full IR spectrum.

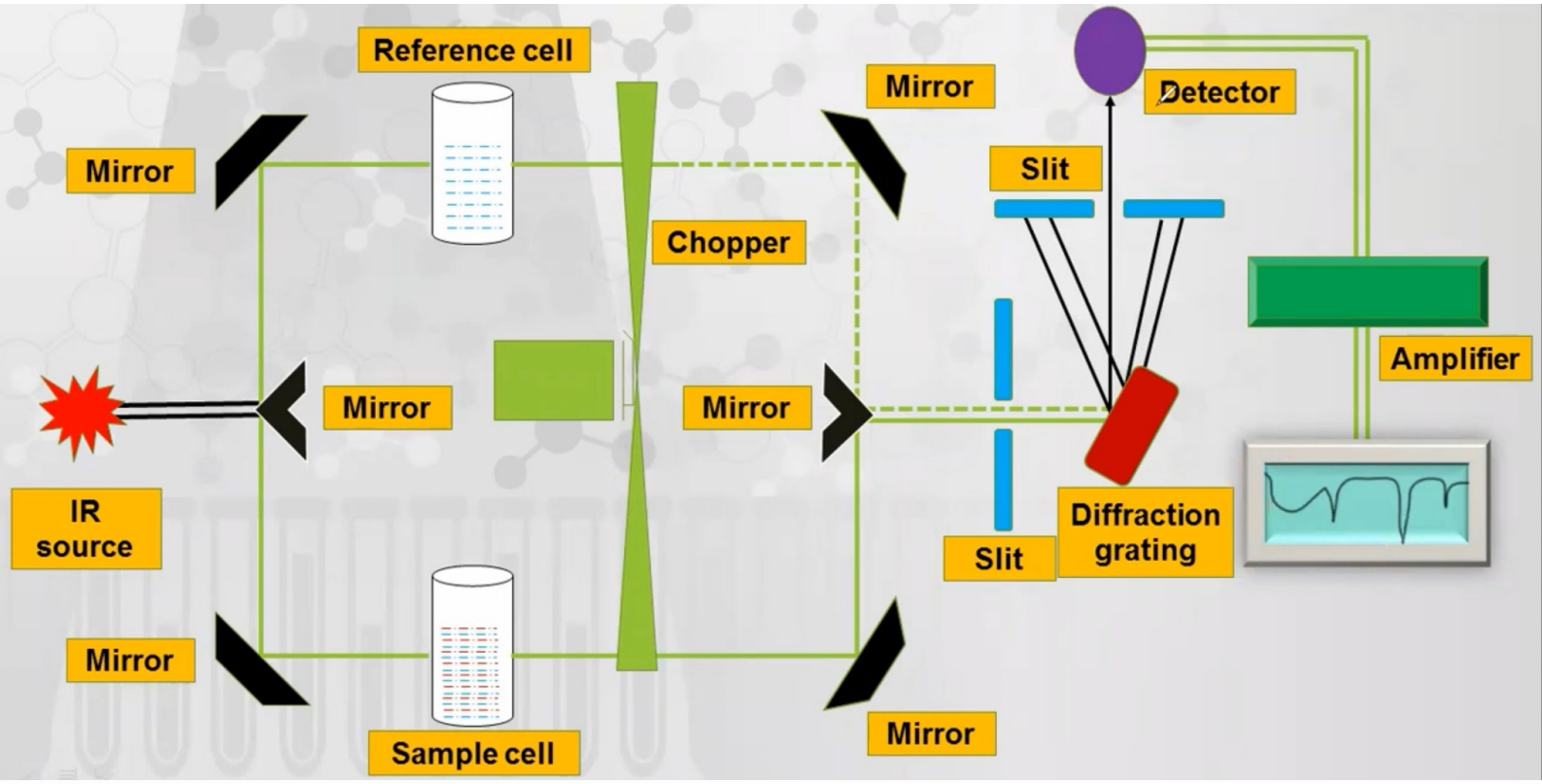
Spectrum Output:

You get a graph of:

-Wavelength (or wavenumber) on X-axis

-Absorbance or transmittance on Y-axis

-It helps identify functional groups in molecules.



Key Features-

Scans one wavelength at a time → makes it slow

Lower sensitivity than modern FT-IR

Was commonly used before FT-IR was invented

Still used in teaching labs or where cost is a concern

Fourier transform IR spectrophotometer

📘 Definition -

An FT-IR (Fourier Transform Infrared) Spectrometer is an advanced type of IR instrument that collects all infrared wavelengths at once, then uses a mathematical process (Fourier Transform) to produce the spectrum quickly and accurately.

🧩 Main Components:

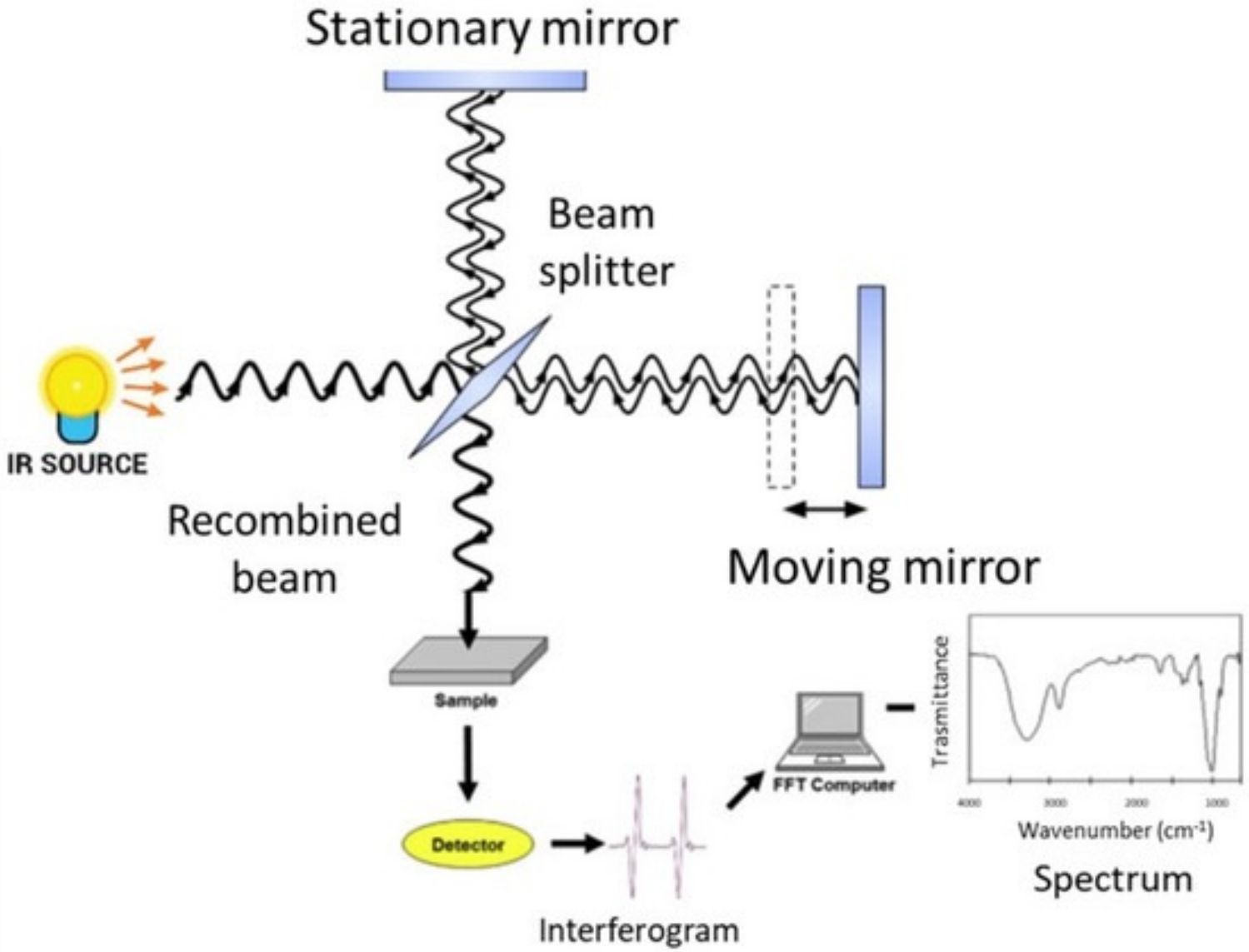
🔧 Part	📝 Function
IR Source	Emits broad-range IR radiation
Michelson Interferometer	Modulates IR light to produce all wavelengths at once
Sample Holder	Holds the sample (solid, liquid, gas)
Detector	Measures absorption of IR light
Computer	Applies **Fourier Transform** to create the spectrum

How It Works (Step by Step) -

1. IR light from the source goes into a device called a Michelson interferometer.
2. This device modifies the IR light by splitting and recombining it (produces a signal called an interferogram).
3. The interferogram passes through the sample.
4. The detector measures how the IR light is absorbed by the sample.
5. A computer applies Fourier Transform to convert the raw data into a normal IR spectrum.

Spectrum Output:
Graph of:

Wavenumber (cm^{-1}) on X-axis
Absorbance or Transmittance on Y-axis
Used to identify functional groups in molecules



🎯 *Key Features:*

Very fast (all wavelengths measured at once)
High resolution and high sensitivity
Requires less sample
Better for detecting mixtures and weak peaks
Most commonly used modern IR technique