

***SHREE H. N. SHUKLA INSTITUTE OF PHARMACEUTICAL EDUCATION
AND RESEARCH***



B.PHRAM

(SEMESTER –VII)

SUBJECT NAME: INSTRUMENTAL METHOD OF ANALYSIS

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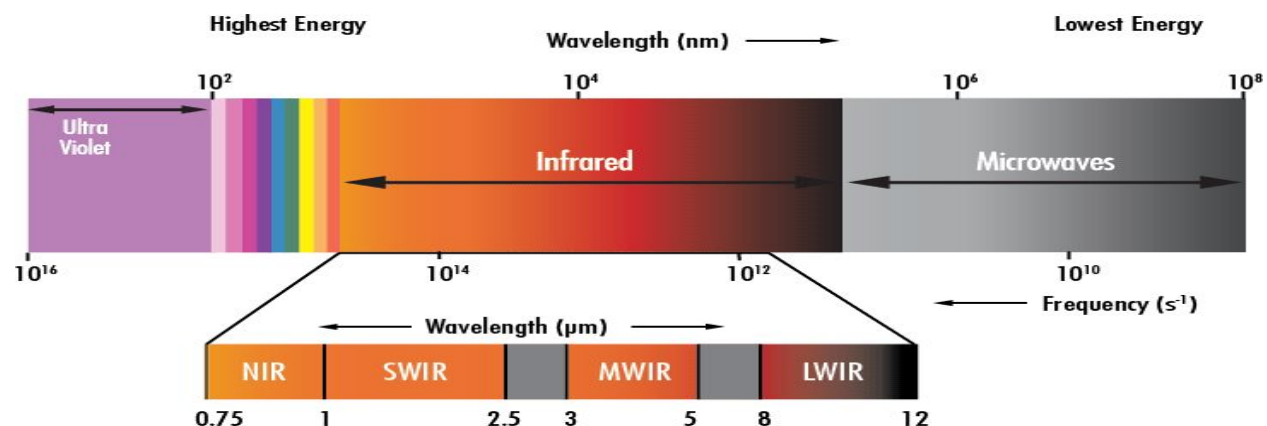
CHAPTER 2 : INFRARED SPECTROSCOPY

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. It covers a range of techniques, mostly based on absorption spectroscopy. As with all spectroscopic techniques, it can be used to identify and study chemicals. A common laboratory instrument that uses this technique is a Fourier transform infrared (FTIR) spectrometer.

The infrared portion of the electromagnetic spectrum is usually divided into three regions; the near-, mid- and far- infrared, named for their relation to the visible spectrum. The higher energy near-IR, approximately 14000-4000 cm^{-1} (0.8-2.5 μm wavelength) can excite overtone or harmonic vibrations. The mid-infrared, approximately 4000-400 cm^{-1} (2.5-25 μm) may be used to study the fundamental vibrations and associated rotational-vibrational structure. The far-infrared, approximately 400-10 cm^{-1} (25-1000 μm), lying adjacent to the microwave region, has low energy and may be used for rotational spectroscopy. The names and classifications of these subregions are conventions, and are only loosely based on

the relative molecular or electromagnetic properties.



IR Region

Region of IR	Wave length (μm)	Wave number (cm ⁻¹)
Near IR (Overtone region)	0.8-2.5	12,500-4000
Mid IR (Vibration-rotation region)	2.5-50	4000-200
Far IR (Rotation region)	50-1000	200-10
Most used	2.5-25	4000-400

Theory

Infrared spectroscopy exploits the fact that molecules absorb specific frequencies that are characteristic of their structure. These absorptions are resonant frequencies, i.e. the frequency of the absorbed radiation matches the frequency of the bond or group that vibrates. The energies are determined by the shape of the molecular

potential energy surfaces, the masses of the atoms, and the associated vibronic coupling.

In particular, in the Born-Oppenheimer and harmonic approximations, i.e. when the molecular Hamiltonian corresponding to the electronic ground state can be approximated by a harmonic oscillator in the neighborhood of the equilibrium molecular geometry, the resonant frequencies are determined by the normal modes corresponding to the molecular electronic ground state potential energy surface. Nevertheless, the resonant frequencies can be in a first approach related to the strength of the bond, and the mass of the atoms at either end of it. Thus, the frequency of the vibrations can be associated with a particular bond type.

In order for a vibrational mode in a molecule to be "IR active," it must be associated with changes in the permanent dipole. A molecule can vibrate in many ways, and each way is called a vibrational mode. Linear molecules have $3N - 5$ degrees of vibrational modes whereas nonlinear molecules have $3N - 6$ degrees of vibrational modes (also called vibrational degrees of freedom). As an example H₂O, a non-linear molecule, will have $3 \times 3 - 6 = 3$ degrees of vibrational freedom, or modes.

Simple diatomic molecules have only one bond and only one vibrational band. If the molecule is symmetrical, e.g. N₂, the band is not observed in the IR spectrum, but only in the Raman spectrum. Unsymmetrical diatomic molecules, e.g. CO, absorb in the IR spectrum. More complex molecules have many bonds, and their

vibrational spectra are correspondingly more complex, i.e. big molecules have many peaks in their IR spectra.

The atoms in a CH₂ group, commonly found in organic compounds, can vibrate in six different ways: symmetric and antisymmetric stretching, scissoring, rocking, wagging and twisting:

The **Heisenberg uncertainty principle** argues that all atoms in a molecule are constantly in motion (otherwise we would know position and momentum accurately). For molecules, they exhibit three general types of motions: translations (external), rotations (internal) and vibrations (internal). A diatomic molecule contains only a single motion., while polyatomic molecules exhibit more complex vibrations, known as **normal modes**.

Principle of IR Spectroscopy

- When IR light is passed through a sample of organic compound some of the frequencies are absorbed while others are transmitted. Plot of Absorbance or Transmittance Vs Wave no. gives an IR spectrum But conventionally Wave No. Vs % Transmittance is plotted (because the numbers are more manageable)

Requirements of IR radiation Absorption

1. Correct wavelength of radiation

If a molecule absorbs radiation only when the natural frequency of vibration of some part of the molecule is the same as the frequency of incident radiation.

2. Electric Dipole:

- If a frequency of vibration of HCl molecule exactly matches with that coming from the source NET TRANSFER of energy takes place change in amplitude of molecular vibration absorption of radiation
- In case of O₂, N₂, Cl₂ NO NET change in dipole moment occurs thus they cannot absorb IR radiations & do not show IR spectra

Two types changes occur in molecule :

- **Molecular vibrations**

The positions of atoms in a molecules are not fixed; they are subject to a number of different vibrations • **Molecular rotations:**

Rotational transitions are of little use to the spectroscopist.

Molecular Vibrations

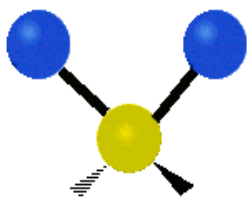
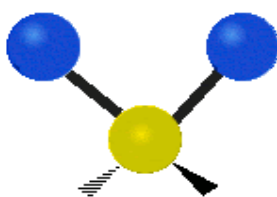
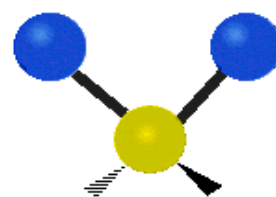
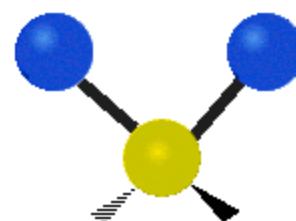
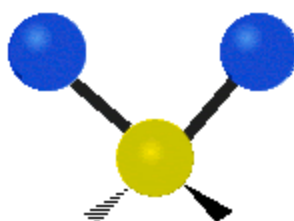
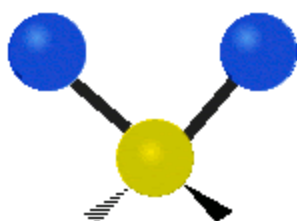
A molecule has translational and rotational motion as a whole while each atom has its own motion. The vibrational modes can be IR or Raman active. For a mode to be observed in the IR spectrum, changes must occur in the permanent dipole (i.e. not diatomic molecules). Diatomic molecules are observed in the Raman spectra but not in the IR spectra. This is due to the fact that diatomic molecules have one band and no permanent dipole, and therefore one single vibration. An example of this would be O₂ or N₂. However, unsymmetric diatomic molecules (i.e. CN) do absorb in the IR spectra. Polyatomic molecules undergo more complex vibrations that can be summed or resolved into normal modes of vibration.

The normal modes of vibration are: asymmetric, symmetric, wagging, twisting, scissoring, and rocking for polyatomic molecules.

Symmetric Stretching

Asymmetric Stretching

Wagging

**Twisting****Scissoring****Rocking**

Factors affecting vibrational frequencies in IR

The value of absorption frequency is shifted if the force constant of a bond changes with its electronic structure. Frequency shifts also take place on working with the same substance in different states (solids, liquids & vapour). A substance usually absorbs at higher frequency in a vapour state as compared to liquid and solid states.

Factors responsible for shifting the vibrational frequencies from their normal values

- 1. Coupled vibrations**
- 2. Fermi resonance**
- 3. Electronic effects**
- 4. Hydrogen bonding**

1.COUPLED VIBRATIONS

An isolated C-H bond has only one stretching vibrational frequency where as methylene group shows two stretching vibrations, **symmetrical and asymmetrical**.

Because of mechanical coupling or interaction between C-H stretching vibrations in the CH₂ group. Assymmetric vibrations occur at higher frequencies or wave numbers than symmetric stretching vibrations.

These are known as coupled vibrations because these vibrations occur at different frequencies than that required for an isolated C- H stretching. A strong vibrational coupling is present in carboxylic acid anhydrides in which symmetrical and asymmetrical stretching vibrations appear in the region 1720 – 1825 cm⁻¹.

The interaction is very effective probably because of the partial double bond character in the carbonyl oxygen bonds due to resonance which also keeps the system planar for effective coupling.

- Asymmetrical stretching band in acyclic anhydride is more intense where as symmetrical stretching band is more intense in cyclic anhydrides.

Requirements For interaction to occur,

- the vibrations must be of same symmetry species.
- There must be a common atom between the groups for strong coupling between stretching vibrations.
- For coupling of bending vibrations , a common bond is necessary.
- Interaction is greatest when coupled groups absorb, individually, near the same frequency.
- Coupling is negligible when groups are separated by one or more carbon atoms and the vibrations are mutually perpendicular.

2.FERMI RESONANCE

Resonance -A vibration of large amplitude produced by a relatively small vibration. Coupling of two fundamental vibration modes produces two new modes of vibration ,with frequencies higher and lower than that observed in absence of interaction. Interaction can also take place between fundamental vibrations and overtones or combination tone vibrations and such interactions are known as Fermi Resonance.

If two different vibrational levels, belonging to the same species, have nearly the same energy. A mutual perturbation of energy may occur. Shifting of one towards lower and other towards higher frequency occur. A substantial increase in the intensity of the respective bands occur.

In this , a molecule transfers its energy from fundamental vibrational level to overtone or combination tone level and back. Resonance pushes the two levels apart and mixes their character, consequently each level has partly fundamental and partly overtone or combination tone character.

For eg. symmetrical stretching vibration of CO₂ in Raman spectrum shows band at 1337 cm⁻¹. The two bending vibrations are equivalent and absorb at the same frequency of 667.3 cm⁻¹. The first overtone of this is $2 \times 667.3 = 1334.6$ cm⁻¹.

Fermi resonance occurs There is mixing of 1337 cm⁻¹ and 1334.6 cm⁻¹ to give two bands at 1285.5 cm⁻¹ and at 1388.3 cm⁻¹ with intensity ratio 1 : 0.9 respectively.

Asymmetric stretching Symmetric stretching

4. HYDROGEN BONDING

It occurs in any system containing a proton donor group (X-H) and a proton acceptor. if the s-orbital of the proton can effectively overlap the P or π orbital of the acceptor group.

The stronger the hydrogen bond, the longer the O-H bond, the lower the vibration frequency and broader and more intense will be the absorption band.

The N-H stretching frequencies of amines are also affected by hydrogen bonding as that of the hydroxyl group but frequency shifts for amines are lesser than that for hydroxyl compounds. Because nitrogen is less electronegative than oxygen so the hydrogen bonding in amines is weaker than that in hydroxy compounds.

Intermolecular hydrogen bonds gives rise to broad bands, while intramolecular hydrogen bonds give sharp and well defined bands. The inter and intramolecular hydrogen bonding can be distinguished by dilution. Intramolecular hydrogen bonding remains unaffected on dilution and as a result the absorption band also remains unaffected where as in intermolecular, bonds are broken on dilution and as a result there is a decrease in the bonded O-H absorption .

The strength of hydrogen bonding is also affected by :

- ❖ Ring strain
- ❖ Molecular geometry
- ❖ Relative acidity and basicity of the proton donor and acceptor groups

ELECTRONIC EFFECT:

Changes in the absorption frequencies for a particular group take place when the substituents in the neighbourhood of that particular group are changed.

It includes :

- Inductive effect
- Mesomeric effect
- Field effect

INDUCTIVE EFFECT :

The introduction of alkyl group causes +I effect which results in the lengthening or the weakening of the bond. Hence the force constant is lowered and wave number of absorption decreases. Let us compare the wave numbers of ν (C=O) absorptions for the following compounds : Formaldehyde (HCHO) 1750 cm^{-1} . Acetaldehyde (CH_3CHO) 1745 cm^{-1} . Acetone (CH_3COCH_3) 1715 cm^{-1} . Introduction of an electronegative atom or group causes -I effect which results in the bond order to increase. Hence the force constant increases and the wave number of absorption rises.

MESOMERIC EFFECT:

It causes lengthening or the weakening of a bond leading in the lowering of absorption frequency. As nitrogen atom is less electronegative than oxygen atom, the electron pair on nitrogen atom in amide is more labile and participates more in conjugation. Due to this greater degree of conjugation, the C=O absorption frequency is much less in amides as compared to that in esters.

FIELD EFFECT:

In ortho substituted compounds, the lone pair of electrons on two atoms influence each other through space interactions and change the vibrational frequencies of both the groups. This effect is called field effect.

Instrumentation

IR radiation source

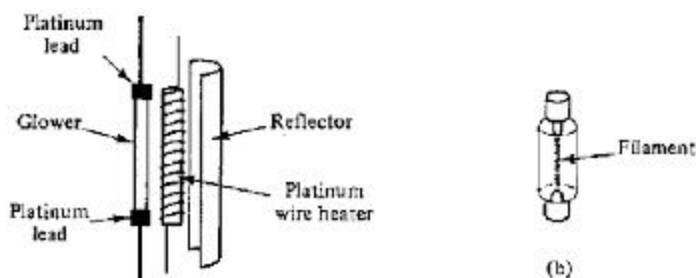
Wavelength selector (Monochromator)

Sample Holder or cell

Detector

Recorder

Sources: Inert solids heated electrically to temp of 1500- 2000K



1. Nernst Glower:

- Consists of cylinder of rare earth oxides formed into a cylinder of diameter 1-2mm length approx. 20mm.
- Platinum discs are attached at the ends of cylinder to permit electrical connection.
 - They are heated to a temp of 1200-2200K where IR radiations are emitted.
- Rare earth metals have large -ve temperature coefficient of electrical resistance. (A negative temperature coefficient (NTC) occurs when a physical property (such as thermal conductivity or electrical resistivity) of a material lowers with increasing temperature, typically in a defined temperature range.)
 - Temp is inversely related to resistance
 - At low temp, they provide high resistance to flow current and as cylinder gets heated resistance gets reduced allowing conduction of current.
 - If large amount of current flows through cylinder it can destroy the source.
 - To avoid this source circuit should be designed to limit the current.

2. The Globar source



- Similar to nernst glower it is also made up of cylinder
- Material used is silicon carbide
- Length of cylinder is 50mm & diameter is 5mm
- It has positive temperature coefficient of electrical resistance
- At low temp, they provide low resistance to flow current and as cylinder gets heated resistance increases allowing conduction of current.
- To avoid excessive heating water cooling is necessary
- At high temp source emits IR radiations.

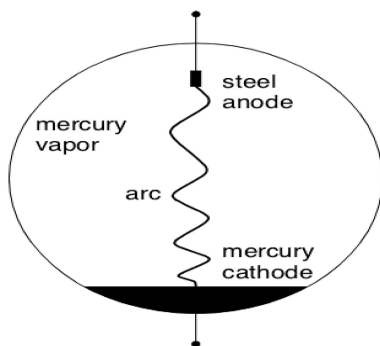
3. Incandescent wire source (nichrome wire)



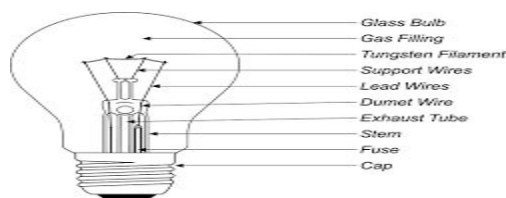
- Cylinder in the above sources is tightly wound by spiral wire of nichrome / rhodium
- It is electrically heated at 1100 k

4. Mercury arc:

- Quartz jacketed tube Hg vapors • Electricity passed through Hg vapour provides radiations



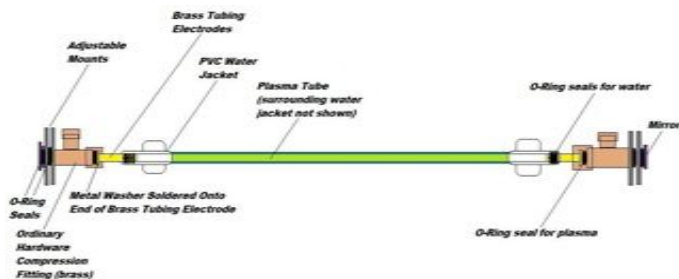
5. Tungsten filament : used in Near IR



6. CO₂ laser source:

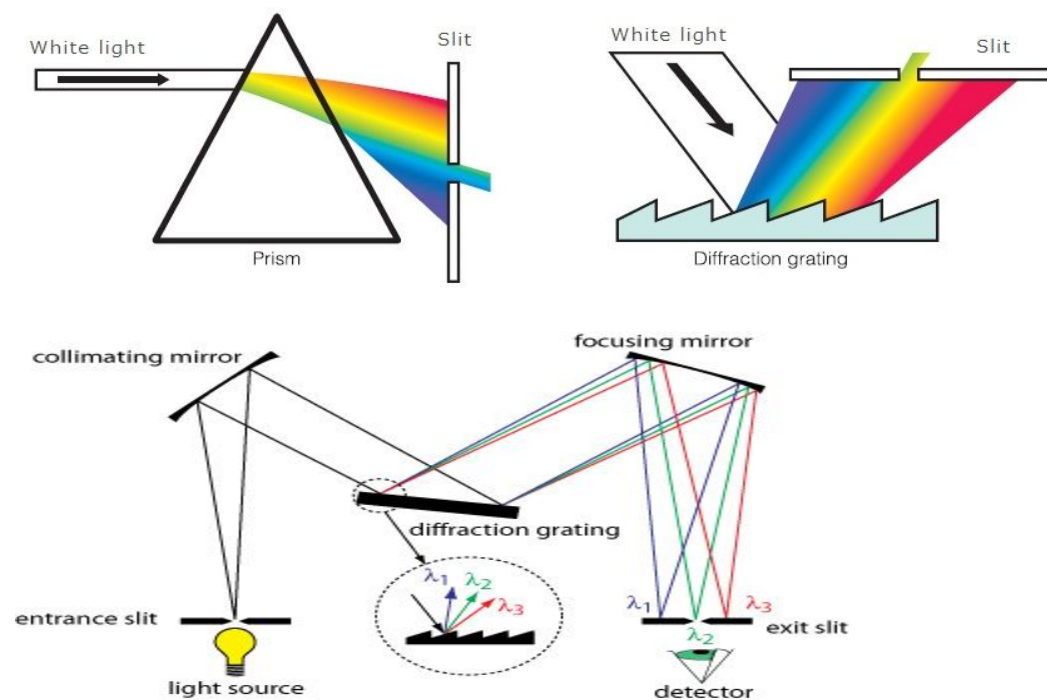
- A tunable IR source
- Detection of pollutants in air.
- Used to monitor atmospheric and aqueous solutions pollutants.
- Band of radiation consists of 100 closely spaced discrete lines in the range of 900-1100 cm^{-1} .
- Some of these lines coincide with the narrow vibrational– rotational lines of gas phase analytes.
- This makes the laser an excellent source for measuring gases in the atmosphere or gases in a production process Open path environmental measurements

- This source used in quantitative determination of many species such as ammonia, butadiene, benzene, ethanol, nitrogendioxide and trichloroethylene hydrogen sulfide, nitrogen dioxide, chlorinated hydrocarbons, and other pollutants.
- The radiant power is strong comparing of blackbody sources
- Tunable gas phase lasers are expensive.



Wavelength Selectors

- ❖ Filters
- ❖ Monochromators
- Entrance slit
- Collimating lens or mirror
- Dispersion element (prism or grating)
- Focusing lens or mirror
- Exit slit Output from a wavelength selector is a band of wavelengths.



Difference between Monochromator & Filter

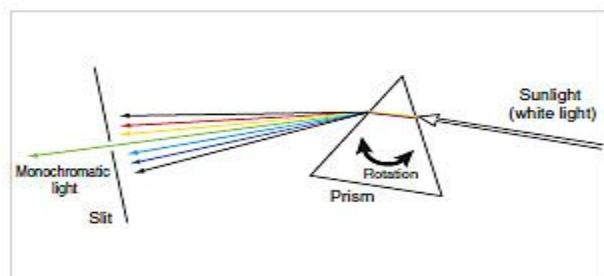
Filters

- Filters are very simple: they are sheets of plastic or glass that simply absorb wavelengths other than those required for the analysis.
- Generally, the range of wavelengths allowed by a filter is relatively wide

Monochromators

- are far more complicated, and comprise a series of optics inside a lightproof box, which has entry and exit slits which allows the radiation of all wavelengths in and a narrow range of wavelengths out.

Prism



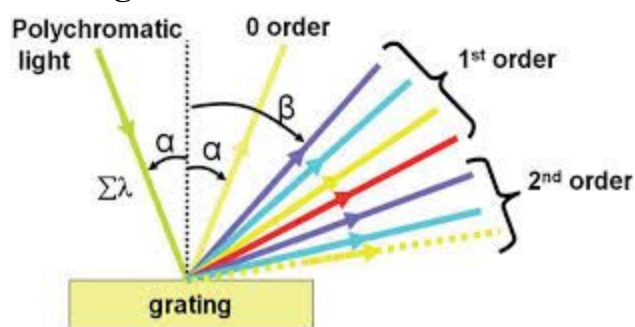
- The white light pass through a piece of glass and be divided into a rainbow spectrum.
- The problems with a prism include relatively poor throughput (the total amount of light passes through is significantly less than the amount that went in) and the difficulty in finding materials that diffract different wavelength ranges.

Entrance slit allows source radiation to illuminate the first lens which collimates the light spreading it across the face of the prism.

- Prism disperses radiation into component wavelengths and the second lens focuses the spectrum at the focal plane.

- **An exit slit** selects the band of radiation to reach the detector.

Gratings



- It is a device which consists of a series of parallel & closely spaced grooves rules on glass or any reflecting surface
- Gratings are of two types Transmission Gratings Reflection Gratings
- UV gratings have 2000-6000 grooves per mm
- IR gratings have 10-100 grooves per mm
- Materials used for construction are Quartz, NaCl, KBr..

Sample Preparation

IR spectroscopy is used for the characterization of solid, liquid or gas samples. Material containing sample must be transparent to the IR radiation. So, the salts like NaCl, KBr are only used.

1. Sampling of solids

Various techniques used for preparing solid samples are as follows

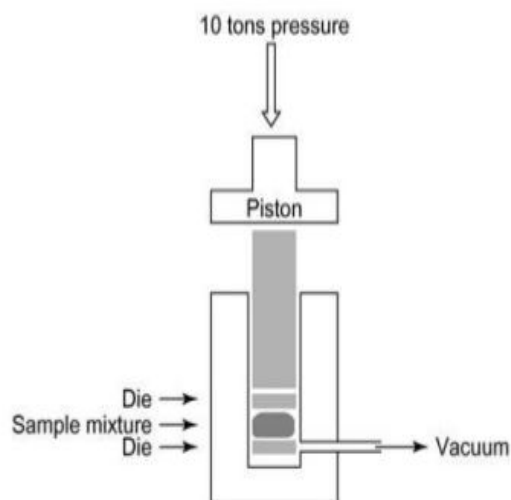
a) Mull technique: In this technique, the finely crushed sample is mixed with Nujol (mulling agent) in a marble or agate mortar, with a pestle to make a thick paste. A thin film is applied onto the salt plates. This is then mounted in a path of IR beam and the spectrum is recorded.

Disadvantages : 1.It shows absorption of maximum at 2915 cm^{-1} , 1462 cm^{-1} , 1376 cm^{-1} , 719 cm^{-1} 2.Polymorphic changes, degradation, and other changes may occur during grinding.

b) Solid run in Solution – In this technique, solid sample may be dissolved in a non-aqueous solvent provided that there is no chemical interaction with the solvent and the solvent is not absorbed in the range to be studied. A drop of solution is placed on the surface of alkali metal disc and solvent is evaporated to dryness leaving a thin film of the solute.

c) Case film technique – If the solid is amorphous in nature then the sample is deposited on the surface of a KBr or NaCl cell by evaporation of a solution of the solid and ensured that the film is not too thick to pass the radiation.

d) 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



Advantage :

- 1.The KBr pellet can be stored for longer time.
- 2.As the concentration of the sample can be suitably adjusted in the pellet, it can be used for quantitative analysis.
- 3.The resolution of the spectrum in KBr is superior to that obtained with Nujol mull technique.

Disadvantage :

- 1.It always has band at 3450cm^{-1} from the OH group of the moisture present in the sample.
- 2.The high pressure involved in the formation of pellet may bring about polymorphic changes in crystallinity in the sample(specially for inorganic complexes) which causes complication in IR spectrum. In some cases even substitution of the ligand by bromide may be possible in inorganic complexes.
- 3.This method is not successful for some polymers which are difficult to grind with KBr.

2. 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. Organic solvents like chloroform can be used. The sample thickness should be selected so that the transmittance lies between 15-20%. For most liquids, the sample cell thickness is 0.01-0.05 mm. Some salt plates are highly soluble in water, so the sample and washing reagents must be anhydrous

3. Sampling of gases:

Sampling of gases: Gas samples are examined in the IR spectrometer after removal of water vapour. The simplest gas cell consists of metal/gas cylinder of 10cm long and closed with a appropriate window. The gaseous sample is passed through a stopcock via a suitable gas handling apparatus and partial pressure of 5 to 15mmHG

gives a reasonable level of absorption in most cases. The end wall of gas cell is made of NaCl and for low concentrated gases long path lengths are required. Multi reflection can be used to make effective path length as long as 40cm so that constituent of gas can be determined.

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 – 10 cm) is needed because the gases show relatively weak absorbance.

Detectors:

TYPES OF TEMPERATURE SENSORS:

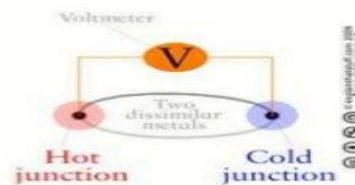
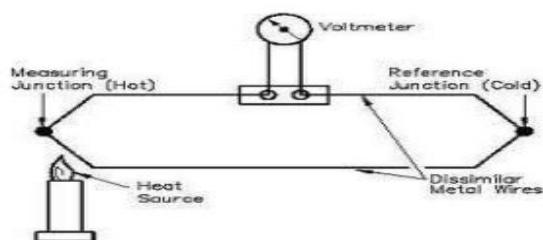
1. Thermocouples
2. Thermistors
3. Pneumatic devices : Golay cell.
4. Pyroelectric Infrared Detector

1. THERMOCOUPLE:

Two dissimilar metals like bismuth and antimony. Two ends are called Hot junction, Cold junction.

The surface at the junction of the wires is coated with black metallic oxide. IR radiation falls on hot junction. By heat source change in temperature at the junction between the metallic wires causes an electric potential to develop between the wires. The potential difference between the unjoined ends of the wires is amplified and measured. Cold junction is not exposed to IR. Response time is 60 m/sec.

Thermocouple:



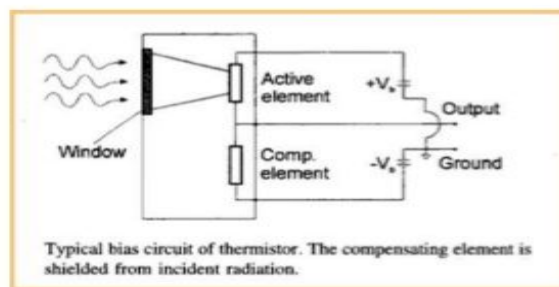
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2. THERMISTORS:

- Thermistors are the devices that have an electric resistance that is higher temperature dependent.
- The materials used in thermistors are sintered oxide of Cobalt, Manganese , Nickel.
- A constant potential is applied across the thermistor and the difference in current flow between an illuminated thermistor and a non-illuminated thermistor is measured using a differential operational amplifier.
- As the temperature of mixture increases, its electrical resistance decreases.
- Response time is 80 m/sec.
- It should be operate at a frequency of less than 12Hz.

d) Thermistors

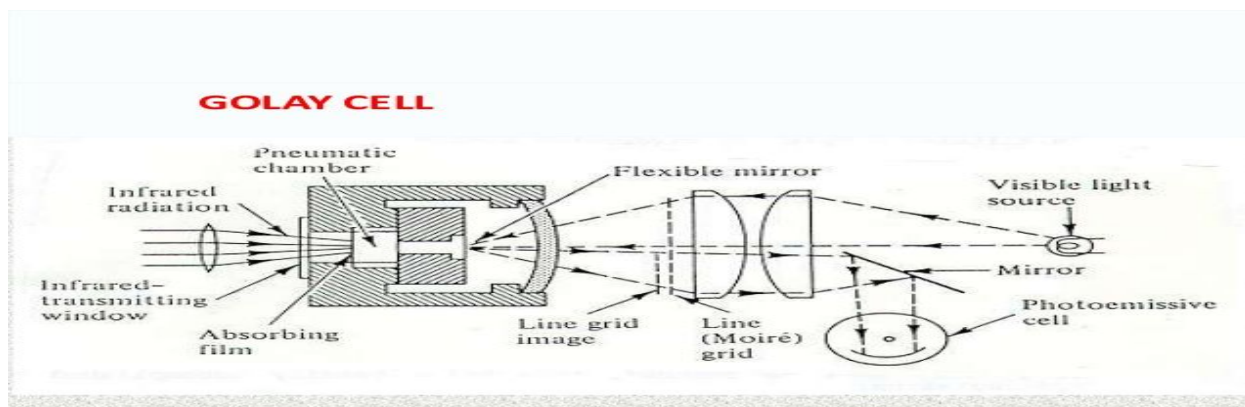
- It is made up of metal oxides.
- It functions by changing resistance when heated.
- It consists of two closely placed thermistor flakes, one of the 10 um is an active detector, while the other acts as the compensating / reference detector.
- A steady voltage is applied, due to the temperature increase there is change in resistance which is measured and this gives the intensity of the IR radiation



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23

3. GOLAY CELL



A Golay Cell is a "photo-acoustic" device that is sensitive, works at ambient temperatures and has a broad spectral response. Golay Cell is one of the most efficient devices detecting THz radiation.

- Terahertz radiation is considered as the electromagnetic spectrum whose frequency ranges from 0.1 to 10THz, lying between the microwave and infrared regions.
- THz waves can penetrate many materials and generate images with high spatial resolution such as THz radar, scattering, security detection, tomography, biology and medicine.
- Some other features of terahertz radiation are: All warm bodies naturally emit THz radiation. High frequency implies broad bandwidth and very high wireless data transmission rates. THz radiation enables imaging through clothing, bandages, and packaging materials.

PRINCIPLE OF OPERATION

Golay cell consists of a small metal cylindrical closed by a rigid blackened metal plate. Pneumatic chamber is filled with xenon gas.

At one end of cylinder a flexible silvered diaphragm and at the other end Infra red transmitting window is present.

When infra red radiation is passed through infrared transmitting window the blackened plate absorbs the heat. By this heat the xenon gas causes expand.

The resulting pressure of gas will cause deformation of diaphragm. This motion of the diaphragm detects how much IR radiation falls on metal plate.

Light is made to fall on diaphragm which reflects light on photocell.

4. Pyroelectric Infrared Detectors

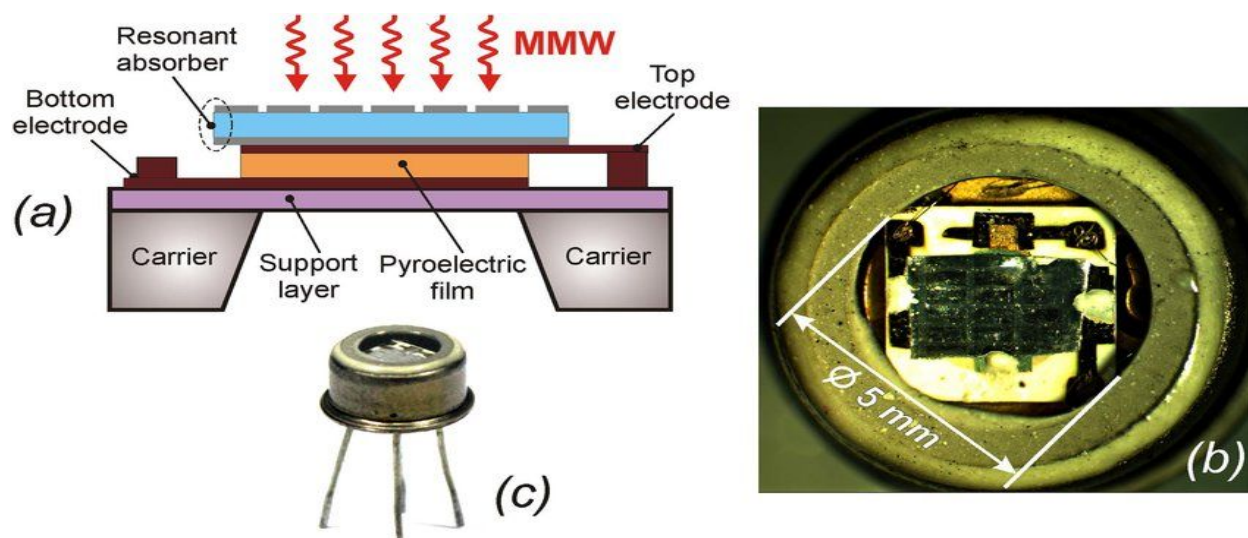
1. Principal set-up Figure 1 shows the principle set-up of a pyroelectric infrared detector. Components are the responsive element and the preamplifier whose essential elements are integrated in the detector. The sensitive element consists of a pyroelectric chip which is thin and covered with electrodes. In some cases an absorption layer is applied to the front of the responsive element to improve its absorption behavior. top electrode bottom electrode pyroelectric material amplifier sensitive element $d p \Phi S(t) A S u'(t) R u'(t) S$ Figure 1:

The incident radiation flux $\Phi S(t)$ hits the radiation-sensitive element with the area AS and absorption coefficient α .

The absorption of radiation flux results in a temperature change $\Delta T(t)$ within the pyroelectric material.

The pyroelectric effect generates charges $\Delta Q(t)$ on the electrodes. These charges are transformed into a signal voltage $uS'(t)$.

Various noise sources in the pyroelectric chip and the preamplifier generate a noise voltage $uR'(t)$ at the detector output. This voltage limits the radiation flux, which can be detected in the minimum. A bolometer is a device for measuring the power of incident electromagnetic radiation via the heating of a material with a temperature-dependent electrical resistance. It was invented in 1878 by the American astronomer Samuel Pierpont Langley.

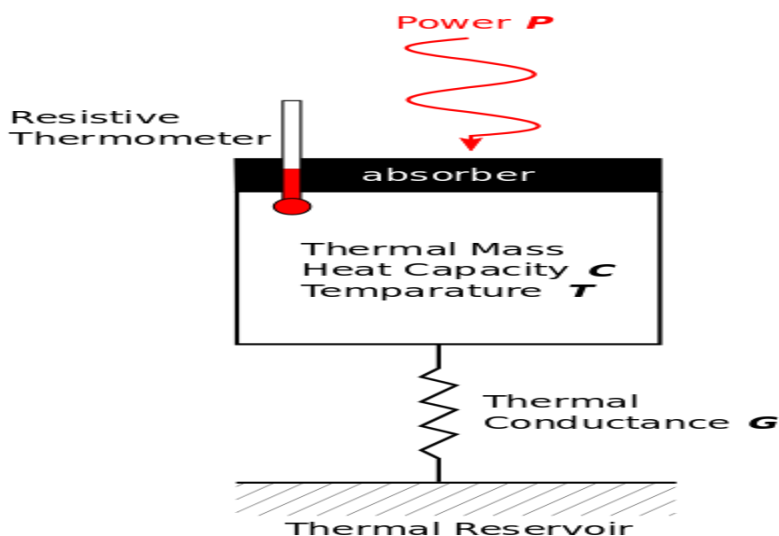


5. Bolometer

Principle of operation

Conceptual schematic of a bolometer. **Power, P**, from an incident signal is absorbed and heats up a thermal mass with **heat capacity, C**, and **temperature, T**. The thermal mass is connected to a reservoir of constant temperature through a link with thermal **conductance, G**. The temperature increase is $\Delta T = P/G$ and is measured with a resistive thermometer, allowing the determination of P. The intrinsic ther

A bolometer consists of an absorptive element, such as a thin layer of metal, connected to a thermal reservoir (a body of constant temperature) through a thermal link. The result is that any radiation impinging on the absorptive element raises its temperature above that of the reservoir – the greater the absorbed power, the higher the temperature. The intrinsic thermal time constant, which sets the speed of the detector, is equal to the ratio of the heat capacity of the absorptive element to the thermal conductance between the absorptive element and the reservoir.



The temperature change can be measured directly with an attached resistive thermometer, or the resistance of the absorptive element itself can be used as a thermometer. Metal bolometers usually work without cooling. They are produced from thin foils or metal films. Today, most bolometers use semiconductor or superconductor absorptive elements rather than metals. These devices can be operated at cryogenic temperatures, enabling significantly greater sensitivity.

Bolometers are directly sensitive to the energy left inside the absorber. For this reason they can be used not only for ionizing particles and photons, but also for non-ionizing particles, any sort of radiation, and even to search for unknown forms of mass or energy (like dark matter); this lack of discrimination can also be a shortcoming. The most sensitive bolometers are very slow to reset (i.e., return to thermal equilibrium with the environment). On the other hand, compared to more conventional particle detectors, they are extremely efficient in energy resolution and in sensitivity. They are also known as thermal detectors.

APPLICATIONS OF IR SPECTROSCOPY

Infrared spectroscopy is widely used in industry as well as in research. It is a simple and reliable technique for measurement, quality control and dynamic measurement. It is also employed in forensic analysis in civil and criminal analysis.

Some of the major applications of IR spectroscopy are as follows:

1. Identification of functional group and structure elucidation

Entire IR region is divided into group frequency region and fingerprint region. Range of group frequency is 4000-1500 cm^{-1} while that of finger print region is 1500-400 cm^{-1} .

In group frequency region, the peaks corresponding to different functional groups can be observed. According to corresponding peaks, functional group can be determined.

Each atom of the molecule is connected by bond and each bond requires different IR region so characteristic peaks are observed. This region of IR spectrum is called as finger print region of the molecule. It can be determined by characteristic peaks.

2. Identification of substances

IR spectroscopy is used to establish whether a given sample of an organic substance is identical with another or not. This is because large number of absorption bands is observed in the IR spectra of organic molecules and the probability that any two compounds will produce identical spectra is almost zero. So if two compounds have identical IR spectra then both of them must be samples of the same substances.

IR spectra of two enantiomeric compound are identical. So IR spectroscopy fails to distinguish between enantiomers.

For example, an IR spectrum of benzaldehyde is observed as follows.

C-H stretching of aromatic ring-	3080 cm^{-1}
C-H stretching of aldehyde-	2860 cm^{-1} and 2775 cm^{-1}
C=O stretching of an aromatic aldehyde-	1700 cm^{-1}
C=C stretching of an aromatic ring-	1595 cm^{-1}
C-H bending-	745 cm^{-1} and 685 cm^{-1}

No other compound then benzaldehyde produces same IR spectra as shown above.

3. Studying the progress of the reaction

Progress of chemical reaction can be determined by examining the small portion of the reaction mixture withdrawn from time to time. The rate of disappearance of a characteristic absorption band of the reactant group and/or the rate of appearance of the characteristic absorption band of the product group due to formation of product is observed.

4. Detection of impurities

IR spectrum of the test sample to be determined is compared with the standard compound. If any additional peaks are observed in the IR spectrum, then it is due to impurities present in the compound.

5. Quantitative analysis

The quantity of the substance can be determined either in pure form or as a mixture of two or more compounds. In this, characteristic peak corresponding to the drug substance is chosen and $\log I_0/I_t$ of peaks for standard and test sample is compared. This is called base line technique to determine the quantity of the substance.

NON-INVASIVE BLOOD GLUCOSE MONITORING

Near Infrared spectroscopy is used across the ear lobe to measure glucose. Amount of near infrared light passing through the ear lobe depends on the amount of blood glucose in that region. The ear lobe was chosen due to the absence of bone tissues and also because of its relatively small thickness.

OTHER APPLICATIONS OTHER APPLICATIONS

1. Determination of unknown contaminants in industry using FTIR.
2. Determination of cell walls of mutant & wild type plant varieties using FTIR.
3. Biomedical studies of human hair to identify disease states (recent approach).
4. Identify odor & taste components of food.
5. Determine atmospheric pollutants from atmosphere itself.

6. Examination of old paintings

7. It is also used in forensic analysis in both criminal and civil cases, example in identifying polymer degradation, in determining the blood alcohol content etc.

8. Chemical Analysis: Testing Pill Quality. According to "Medical News Today," scientists at the University of Maryland have been successful in using the method of near-infrared spectroscopy (NIR) to make a prediction regarding quick dissolution of pills inside the body.

Measurement of Paints & Varnishes

- Measured by 'reflectance analysis'
- Advt: Measure IR absorbance of paints on appliances or automobiles without destroying the surface.
- Make and year of car can be determined from IR spectral analysis

Examination of Old Paintings & Artifacts

- Help to determine fake "masterpieces".
- Varnish & paints from old items (statues, canvas, etc.) are analysed by IR spectroscopy.
- Presence of new paint traces implies the "masterpiece" is fake

In Industry

Determine impurities in raw materials (to ensure quality products).

2. For Quality Control checks; to determine the % of required product.

3. Identification of materials made in industrial research labs, or materials of competitors.

E.g.: Impurity in bees wax (with petroleum wax)

Analysis of Petroleum HCs, Oil & Grease contents

- These contain C-H bonds. Absorption at 3100-2700 cm^{-1} .
- 'Freons'—Fluorocarbon-113; do not contain C-H bond.

- Thus, quantity of HCs, oil & grease in freons is determined by measuring C–H absorption at 2930 cm^{-1} .