STUDY OF INFRARED SPECTROSCOPY METHOD AND APPLICATION

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ABSTRACT:

Spectroscopy is the chief experimental technique of atomic and molecular physics and involves determining the energy states of atoms or molecules by looking at the light absorbed or emitted when they change states. Measuring the frequency of light absorbed or emitted which is determined by the energy difference between the two states, can provide a sensitive probe of interactions which perturb those energy states. Based on the principle and the range of electromagnetic radiation spectroscopy is classified into several types. Among those in this review we revealed that the principle, instrumentation and applications of Near Infrared spectroscopy.

Authenticity and adulteration detection are primary concerns of various stakeholders, such as researchers, consumers, manufacturers, traders, and regulatory agencies. Traditional approaches for authenticity and adulteration detection in edible oils are time-consuming, complicated, laborious, and expensive; they require technical skills when interpreting the data. Over the last several years, much effort has been spent in academia and industry on developing vibrational spectroscopic techniques for quality, authenticity, and adulteration detection in edible oils. Among them, Fourier transforms infrared (FT-IR) spectroscopy has gained enormous attention as a green analytical technique for the rapid monitoring quality of edible oils at all stages of production and for detecting and quantifying adulteration and authenticity in edible oils.

keywords: *Infrared Spectroscopy (IR),Molecular Vibrations, Functional Groups, Pharmaceutical Applications, Sample Preparation Techniques, Instrumentation*

INTRODUCTION:

Infrared spectrum is an important record which gives sufficient information about the structure of a compound. In recent years, NIR spectroscopy has become so widespread in process analysis and within pharmaceutical industry for raw material testing, product quality control and process monitoring(1). Not only in the pharmaceutical industry it has gained wide acceptance in biotechnology, genomics analysis, proteomic analysis, interactomics research, inline textile monitoring, food analysis, plastics, textiles, insect detection, forensic lab application, crime detection, various military applications, and is a major branch of astronomical spectroscopy and so on(2). NIR absorption bands are typically broad, overlapping and 10–100 times weaker than their corresponding fundamental mid-IR absorption bands.

Infrared (IR) radiation was firstly recognized by Sir William Herschel in 1800 by the observation of sunlight decomposition through a prism. In his experiments, Herschel measured the temperature of each rainbow colour noticing that the temperature increased from the blue to the red part of the spectrum. He also realized that immediately after the red part of the spectrum, the temperature was even higher and hypothesized that it should be another type of light that could not be seen. These findings were the first recognition of the existence of the IR radiation.

PRINCIPLE :

IR spectroscopy is based on the interaction of an IR beam with a sample. The nature of the IR radiation (near, mid, or far infrared) and/or the processing methods define the technique designation. Near infrared spectroscopy (NIRS) refers to the use of near infrared radiation. Similar designations are used for mid and far IR radiation. Dispersive instruments using some type of wavelength decomposition are intrinsically different from Fourier-transform instruments. The latter make use of an interferometer and the Fourier-transform algorithm. These spectroscopic techniques can be used to characterize solids, liquids, or gaseous samples with the aid of different accessories depending on the physical state.

The increasing demand for product quality improvement and production rationalization in the chemical, petrochemical, polymer, pharmaceutical, cosmetic, food, and agricultural industries has led to the gradual substitution of time-consuming conservative analytical techniques (GC, HPLC, NMR, MS) and nonspecific control procedures (temperature, pressure, pH, dosing weight) by more specific and environmentally compatible analytical tools

INSTRUMENTATION :

Sampling Cells and Sampling of Substances. As infrared spectroscopy has been used for the characterization of solid, liquid or gas samples, it is evident that samples of different phases have to be handled. But these samples have to be treated differently. However, the only common point to the sampling of different phases is that the material containing the sample must be transparent to IR radiation.

Introduction The usual optical materials (glass or quartz) absorb strongly in the IR region, and thus the apparatus for measuring IR spectra is different from that for the visible and UV regions. The main components of are IR spectrometer are:

1) Sources of radiation,
2) Monochromators,
3) Sample cells
4) Detectors

1 SOURCES OF RADIATION:

IR spectroscopy is the study of how molecules absorb infrared radiation, which causes them to vibrate. This process is also known as vibrational spectroscopy.

IR spectroscopy is used to identify chemical compounds and determine the functional groups and bonding patterns in molecules. The region of the IR spectrum below 1500 cm-1 is known as the "fingerprint region" because it provides characteristic information about the entire molecule.

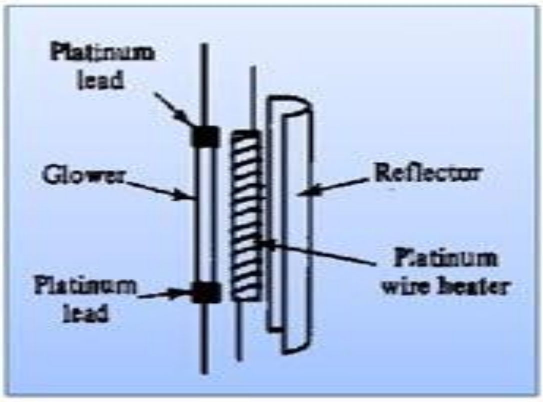
In infrared (IR) spectroscopy, light sources are crucial for producing the infrared radiation needed for analysis. Here are the primary types of light sources used in IR spectroscopy:

1. GLOBAR SOURCE

Description: A globar source is a ceramic rod made of silicon carbide that emits IR radiation when heated. It produces a continuous spectrum in the mid-infrared range (around 4000 to 400 cm^{-1}).: It consists of a rod or hollow tube (2cm long and 1mm in diameter) made by sintering a mixture of cerium, zirconium, thorium and yttrium oxides. It is heated between 1000-1800°C temperature. It provides maximum radiation at 7100 cm- region.

2. NERNST GLOWER

Description: This is a solid-state source made of a mixture of rare earth oxides (like zirconium oxide) that emits IR radiation when electrically heated.



3. QUARTZ INFRARED LAMP

Description: These lamps produce IR radiation through the thermal excitation of a filament and are usually used for specific applications requiring high-intensity IR light.

4. LASER SOURCES

Description: Lasers such as CO_2 lasers and other tuneable diode lasers can produce specific wavelengths of IR radiation.

5. BLACKBODY RADIATION SOURCES

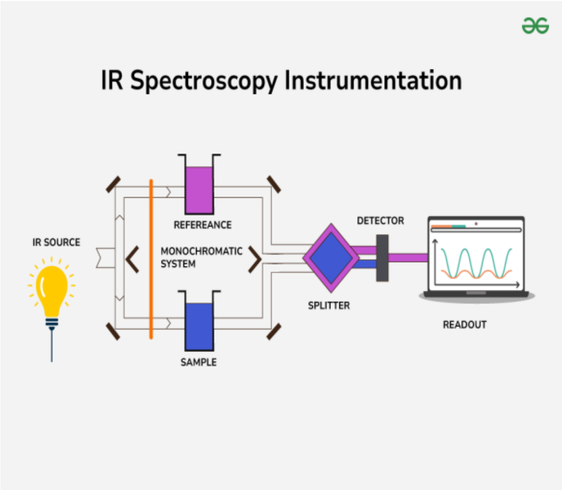
Description: These sources emit IR radiation across a wide range of wavelengths and are based on the principle of blackbody radiation. Examples include heated metal bodies.

6. HEATED FILAMENT SOURCES

Description: Similar to incandescent light bulbs, these sources use heated filaments to emit IR radiation.

5. RHODIUM WIRE:

This wire is sealed in a cylinder. Since the sample in IR spectroscopy absorbs at certain frequencies, desired frequencies from the radiation source should be selected and the radiations of other frequencies should be rejected.

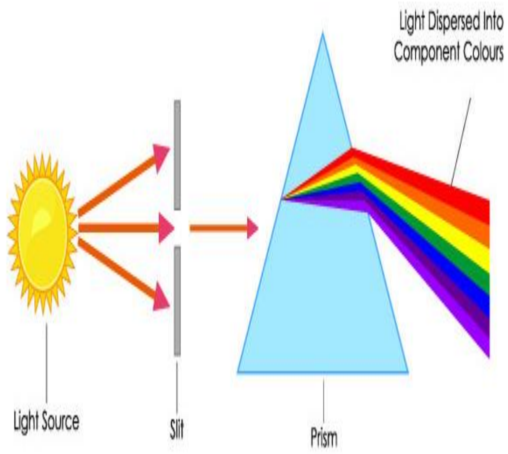


This selection is achieved using monochromators of the following two types:

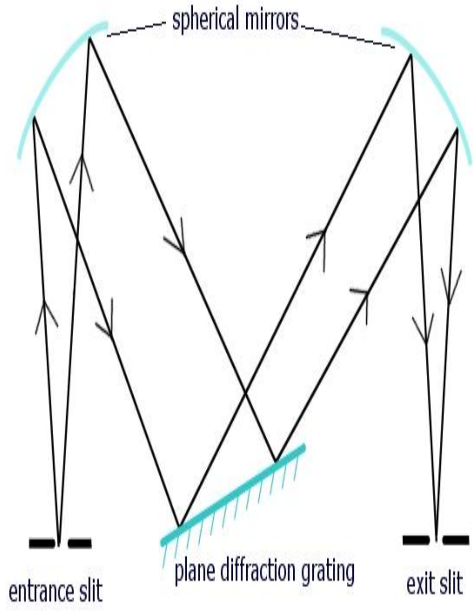
1) Prism monochromator, and 2) Grating monochromator

PRISM MONOCHROMATOR:

A prism to be used as a dispersive element should be made up of materials that transmit in the infrared region (e.g., various metal halide salts). Sodium chloride is the most common prism salt. " Sodium chloride is the most common prism salt due to its high dispersion in the 4 -15um region (a region significantly important in the study of functional groups).



GRATINGS MONOCHROMATORS: Same as UV radiation, the dispersion of the IR radiation can be brought about either by transmission grating or reflection gratings. For isolation UV-visible radiation, gratings having grooves of the order of 2000-6000 per mm of its length are used, whereas for an IR region, gratings having only 10-100 grooves per mm of its length are used. Where, nà = d(sin i t sin 0) n= The order (a whole number). A= Wavelength of the radiation. d= Distance between grooves. i= Angle of incidence of IR radiation beam. 0= Angle of dispersion of light of a particular wavelength. Incident beam radiation Vertical radiation Grating Diffracted radiation Path of IR radiation diffracted by a grating monochromator O Detectors These give responses for all frequencies. If the radiant power for IR region is low, detector signal will also be low. 4) The various types of detectors are as follows: 1) Golay cell, 2) Bolometer, 3) Thermocouple, Thermistor, and 5) Pyroelectric used in FTIR spectrometers.



APPLICATIONS:

Pharmaceutical applications. Infrared spectroscopy has been extensively used in both qualitative and quantitative pharmaceutical analysis. certain functional groups. This technique is important for the evaluation of the raw materials used in production the active ingredients and the excipients. For the identification of drug substances, impurities in drug substances. Provide valuable additional structural information.

Biological applications. Used to study ratio of isomers in a mixture of compounds. > Biological systems, including lipids, proteins, peptides, bio membranes, nucleic acids, animal tissues, microbial cells, plants and clinical samples, have all been successfully studied by using infrared spectroscopy. PENORUNCE termed dysplasia.

Agriculture applications:. The major constituents of grains are water, protein, oil, fibre, minerals and carbohydrates and it is commercially LEADNG pHi1 20.5C MBAR 1010 SMART Agriculture Water 32% UV 72% 15 MPH important to quantitate the composition. O Pulp and paper industries. Infrared spectroscopy plays an important role in quality control in the pulp and paper industries.

Paint Industry. Infrared spectroscopy is used in the paint industry for quality control, product improvement and failure analysis, and for forensic identification purposes

Environmental applications. Infrared spectroscopy has been applied to a broad range of environmental sampling problems, including air, water and soil analysis. Common applications include industrial gas emissions, emissions from fires, and astronomical applications. Determination of the compositions of atmospheric gases is important for an understanding of global climate changes.

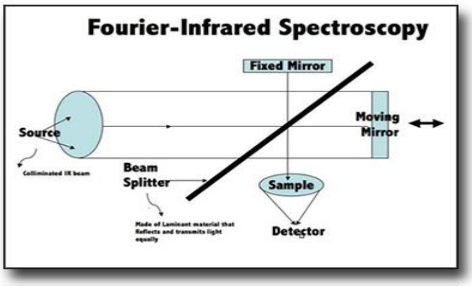
TYPES OF IR SPECTOSCOPY:

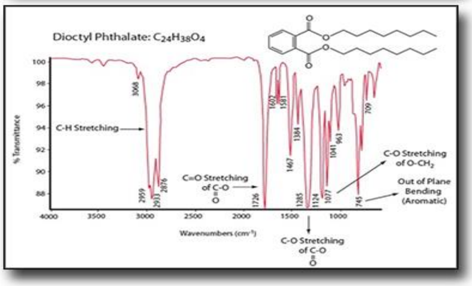
compounds based on their molecular vibrations. There are several types of IR spectroscopy, each serving different purposes and employing various techniques:

1. Fourier Transform Infrared (FTIR) Spectroscopy

Principle: FTIR uses a Michelson interferometer to obtain spectra. The sample is exposed to a broad range of IR frequencies simultaneously, and a Fourier transform is applied to convert the data from the time domain to the frequency domain.

Applications: Characterization of organic compounds, polymer analysis, identification of functional groups, and more.





. 2. Attenuated Total Reflectance (ATR) Spectroscopy

Principle: ATR involves measuring the IR spectrum of a sample in contact with a crystal (often diamond or ZnSe). The IR light is directed into the crystal, reflecting at the interface, which penetrates a short distance into the sample.

Applications: Surface analysis, coatings, and biological samples.

3. Near-Infrared (NIR) Spectroscopy

Principle: NIR spectroscopy operates in the 780–2500 nm wavelength range. It primarily measures overtones and combinations of molecular vibrations.

Applications: Food and agriculture analysis, pharmaceutical formulations, and quality control.

4. Diffuse Reflectance Infrared Fourier Transform (DRIFT) Spectroscopy

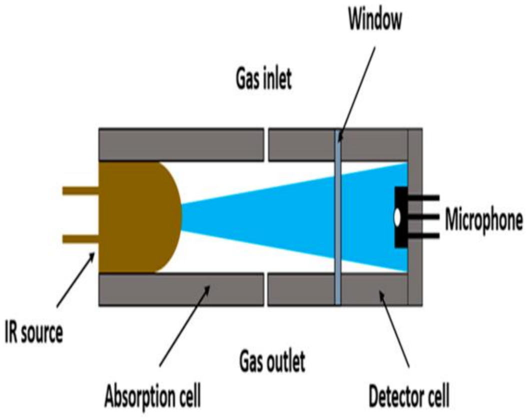
Principle: DRIFT is a variation of FTIR used for powdered samples. It measures the light scattered off the surface of the sample rather than transmitted through it..

Applications: Solid-state materials, catalysts, and minerals.

5. Photoacoustic Infrared Spectroscopy

Principle: In photoacoustic spectroscopy, IR radiation is absorbed by a sample, leading to localized heating and the generation of acoustic waves, which are then measured.

Applications: Environmental monitoring and biological samples.



6. Transmission IR Spectroscopy

Principle: The IR light passes through a thin film or solution of the sample, and the transmitted light is analyzed to obtain the spectrum..

Applications: Identification of organic compounds, studying molecular interactions, and more.

7. Microscopic Infrared Spectroscopy (IR Micro-spectroscopy)

Principle: This technique couples IR spectroscopy with microscopy to obtain spectra from small sample areas (micron or sub-micron scale).

Applications: Biological tissues, microplastics, and forensic analysis.

8. Spectral Imaging

Principle: Combines imaging and spectroscopy to obtain both spatial and spectral information from a sample.

Applications: Materials science, biomedical research, and environmental studies.

9. Raman-IR Spectroscopy

Principle: Combines Raman spectroscopy with IR spectroscopy to enhance molecular characterization by utilizing complementary techniques.

Applications: Complex mixtures, pharmaceuticals, and polymer characterization.

HISTORY OF IR SPECTOSCOPY:

The history of infrared (IR) spectroscopy is a fascinating journey that spans several centuries and involves significant scientific advancements. Here's a brief overview:

Early Discoveries

1. **1820s – Infrared Radiation**:
   - **William Herschel**: In 1800, the astronomer discovered infrared radiation while studying sunlight. He used a prism to separate light into its components and noticed that the temperature increased beyond the visible spectrum, leading to the identification of infrared light.
2. **19th Century – Theoretical Foundations**:
   - Theoretical work in the field of molecular vibrations began to develop, laying the groundwork for understanding how molecules interact with IR radiation.

Development of IR Spectroscopy

3. **1930s – Early Instruments**:
   - The first IR spectrometers were developed during this decade. These instruments utilized prisms and gratings to disperse IR light, allowing scientists to measure absorption spectra.
4. **1940s – Fourier Transform Spectroscopy**:

   - The introduction of Fourier Transform (FT) techniques revolutionized the field. Researchers like **Richard A. H. Smith** began exploring the application of FT methods, improving speed and resolution in IR spectroscopy.
5. **1950s – Commercialization**:
   - The first commercial FTIR spectrometers became available, making IR spectroscopy more accessible to chemists and researchers.

Advances in Technology

6. **1970s – Computerization**:
   - The integration of computers into spectroscopic analysis allowed for more complex data processing and interpretation, significantly enhancing the capabilities of IR spectroscopy.
7. **1980s – ATR and NIR Techniques**:
   - The development of Attenuated Total Reflectance (ATR) spectroscopy provided a simple and effective way to analyze samples without extensive preparation.
   - Near-infrared (NIR) spectroscopy gained prominence, particularly in agricultural and pharmaceutical applications.

Modern Era

8. **1990s to Present**:
   - Continuous advancements in detector technology, sampling techniques, and data analysis have refined IR spectroscopy.
   - The rise of hyperspectral imaging and the combination of IR with other techniques, such as Raman spectroscopy, have expanded its applications in various fields, including materials science, biology, and forensics.

Current Applications:

Today, IR spectroscopy is an essential tool in organic chemistry, pharmaceuticals, environmental science, and many other disciplines, providing critical insights into molecular structure, functional groups, and material properties.

The evolution of IR spectroscopy reflects a broader trend in science towards increased precision, accessibility, and interdisciplinary collaboration.

Vibration work in IR spectroscopy:

In infrared (IR) spectroscopy, molecular vibrations are key to understanding how molecules interact with IR radiation. There are several types of vibrational motions that can be observed, typically categorized into two main types:

1)stretching vibrations.

2) bending vibrations.

1. Stretching Vibrations

These involve changes in the length of a bond between atoms. Stretching vibrations can be further classified into:

- **Symmetric Stretching**:
  - **Description**: Involves two bonds expanding and contracting in unison. For example, in a molecule like

ethylene (C_2H_4), both C-H bonds move in the same direction simultaneously.

- **Asymmetric Stretching**:
  - **Description**: Involves one bond lengthening while another shortens. This type of vibration can occur in molecules with multiple similar bonds, leading to different frequency shifts.

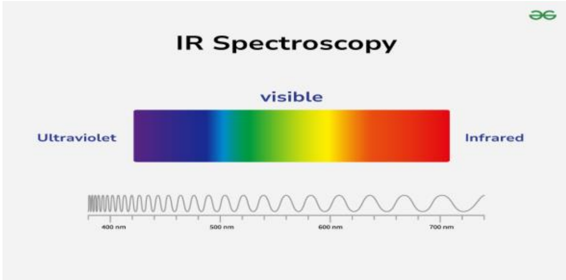
2. Bending Vibrations

These involve changes in the angle between bonds and can also be classified into different types:

- **Scissoring**:
  - **Description**: Involves two atoms moving toward and away from each other in a scissors-like motion. For example, in a molecule like water (H_2O), the H-O-H angle changes during this vibration.
- **Rocking**:
  - **Description**: The entire group of atoms moves as a unit, rocking back and forth without significant change in bond lengths. This is often seen in larger organic molecules.
- **Wagging**:
  - **Description**: Involves a motion where the atoms move in and out of the plane of the molecule. This type of vibration typically involves atoms that are not in the same plane.
- **Twisting**:
  - **Description**: Involves rotation of atoms around a bond, changing the angle between them while remaining within the same plane.

3. Overtones and Combination Bands

In addition to fundamental vibrations, higher-energy transitions known as **overtones** (multiples of fundamental frequencies) and **combination bands** (simultaneous excitations of two or more modes) can also be observed in IR spectra.



IR-Region: 12,800 - 10 cm^{-1}

REGION	WAVE LENGTH λ (µm)	WAVE NUMBER ν (cm⁻¹)	FREQUENCY RANGE Hz
NEAR	0.78 - 2.5	12800 - 4000	3.8×10^{14}-1.2×10^{14}
MIDDLE	2.5 - 50	4000 - 200	1.2×10^{14} - 6×1^{12}
FAR	50 - 1000	200 -10	6×10^{12}- 30×10^{11}
MOST USED	2.5 - 15	4000 - 670	1.2×10^{14}-2×10^{13}

1.Near IR----Carbohydrates and Proteins
2.Middle IR-----Organic molecules—functional groups
3.Far IR—in-organic –co-ordination bonds & quaternary ammonium compounds

CLASSIFY IR SPECTROSCOPY ON THE BASIS OF RANGE:

Infrared (IR) spectroscopy is typically divided into different regions based on the wavelengths or frequencies of the IR radiation used. Each region corresponds to specific types of molecular vibrations and is suited for different applications. Here's a breakdown of the IR spectrum range according to its type:

1. Near-Infrared (NIR) Region

- **Wavelength Range**: Approximately 750 nm to 2500 nm (13,333 to 4000 cm^{-1})Near-infrared (NIR) spectroscopy has an established pedigree. When Herschel studied NIR energy in 1800, it was the first region of the electromagnetic spectrum to be discovered (after the visible region). Almost a hundred years later the Michelson interferometer is often given as the historical beginning of Fourier Transform (FT) spectroscopy. Almost a hundred years ago William Coblentz measured infrared (IR) spectra of organics. Almost 50 years ago, Karl Norris used NIR to characterize agricultural products using the new field of chemometrics. Over 25 years ago, the advent of minicomputers allowed Fourier Transform Infrared (FTIR) spectroscopy to dominate IR identification, but the chemometrics techniques were slow to be adopted in FTIR
- **Applications**: Commonly used in agriculture, food analysis, and pharmaceuticals. NIR spectroscopy often involves overtones and combination bands of fundamental vibrations and is useful for quantitative analysis.

2. Mid-Infrared (Mid-IR) Region

- **Wavelength Range**: Approximately 2500 nm to 25,000 nm (4000 to 400 cm^{-1})
- **Applications**: The most commonly used region in IR spectroscopy for organic and inorganic compound analysis. It provides fundamental vibrations and is particularly useful for identifying functional groups in molecules.

3. Far-Infrared (Far-IR) Region

- **Wavelength Range**: Approximately 25,000 nm to 100,000 nm (400 cm^{-1} to 10 cm^{-1})
- **Applications**: Less commonly used, but important for studying low-frequency vibrations and molecular rotations. Far-IR spectroscopy can provide information on lattice vibrations in solids and is useful in solid-state chemistry and material science.

SAMPLE PREPRATION:

Sample preparation is a critical step in IR spectroscopy that significantly influences the quality and accuracy of the spectra obtained. Here's a detailed overview of sample preparation methods for different types of IR spectroscopy:

1. Solid Samples

a. **Pellet Method**

Procedure:

- Mix the solid sample (typically a few milligrams) with a non-absorbing matrix (usually potassium bromide, KBr).
- Grind the mixture in a mortar and pestle to achieve a homogeneous powder.
- Press the powder into a transparent pellet using a hydraulic press.

- **Advantages**: Provides a uniform sample for analysis and minimizes scattering.

b. **Thin Films**

- **Procedure**:
  - Dissolve the sample in a suitable solvent.

- Deposit a small amount on a clean, IR-transparent substrate (like a glass slide or NaCl plate).
- Allow the solvent to evaporate, leaving a thin film of the sample.

- **Advantages**: Useful for liquids and solids; enables transmission measurements.

c. **Micro sampling Techniques**

- **Procedure**: Use techniques like microtomy to prepare thin sections of solid samples for analysis under a microscope (e.g., IR microspectroscopy).
- **Advantages**: Allows for analysis of small or heterogeneous samples.

2. Liquid Samples

a. **Thin Film Technique**

- **Procedure**: Place a few drops of the liquid sample between two IR-transparent plates (e.g., NaCl or KBr) to form a thin film.
- **Advantages**: Simple and effective for low-concentration samples.

b. **Liquid Cells**

- **Procedure**: Use a dedicated liquid cell with IR-transparent windows. Fill the cell with the liquid sample and seal it.
- **Advantages**: Allows for quantitative measurements and can handle a range of sample volumes.

3. Powdered Samples

a. **Diffuse Reflectance Method**

Procedure: Directly analyze powdered samples by placing them in a diffuse reflectance accessory.

- **Advantages**: Requires minimal sample preparation and is suitable for solid materials.

4. Gaseous Samples

a. **Gas Cells**

- **Procedure**: Use gas cells with IR-transparent windows and appropriate path lengths (usually several meters for low-concentration gases). Inject the gas sample into the cell.
- **Advantages**: Effective for measuring gas-phase spectra and concentration.

5. Biological Samples

a. **Tissue Samples**

- **Procedure**: Cut tissues into thin sections using a microtome or cryostat. Mount on IR-transparent slides.
- **Advantages**: Enables the study of biological samples while preserving structural integrity.

b. **Cell Cultures**

- **Procedure**: Culture cells in a suitable medium, then prepare as a thin film or in a liquid cell for analysis.
- **Advantages**: Allows for real-time monitoring of biochemical changes.

General Considerations

- **Purity**: Ensure samples are free from contaminants that could interfere with the spectrum.
- **Homogeneity**: Aim for a uniform sample to avoid scattering and absorption inconsistencies.
- **Handling**: Use gloves and proper handling techniques to prevent contamination from oils or moisture.
- **Solvent Selection**: Choose solvents that do not absorb in the IR range of interest, as they can interfere with the analysis.

INTERPRETATION OF SPECTRA:

Interpreting IR (infrared) spectra involves understanding the information conveyed by the absorption bands and peaks in the spectrum. Here's a detailed guide on how to interpret IR spectra effectively:

1. Understanding the Spectrum

- **X-Axis**: Typically represents the wave number (cm^{-1}) or wavelength (µm) of the IR radiation. Wave number is the reciprocal of the wavelength and is commonly used in IR spectroscopy.
- **Y-Axis**: Represents transmittance (%T) or absorbance (A). In most spectra, absorbance is plotted, indicating how much light is absorbed by the sample at various wavelengths.

2. Identifying Key Regions

IR spectra can be divided into different regions, each associated with specific types of molecular vibrations:

- **Near-Infrared Region (NIR)**: 4000–12500 cm^{-1}
- **Mid-Infrared Region (MIR)**: 400–4000 cm^{-1} (most commonly analyzed)
- **Far-Infrared Region**: Below 400 cm^{-1}

3. Common Absorption Bands

Certain functional groups have characteristic absorption bands in specific regions:

a. **Functional Group Regions**

- **O-H Stretching**: 3200–3600 cm^{-1} (broad for alcohols, sharp for phenols)
- **N-H Stretching**: 3300–3500 cm^{-1} (primary amines show two peaks)
- **C-H Stretching**:
  - Alkanes: 2850–2950 cm^{-1}
  - Alkenes: 3020–3100 cm^{-1}
  - Aromatics: 3030 cm^{-1}
- **C=O Stretching**: 1650–1750 cm^{-1} (strong, sharp peak)
- **C=C Stretching**: 1600–1680 cm^{-1} (weak to moderate)
- **C-O Stretching**: 1000–1300 cm^{-1}

b. **Fingerprint Region**

- **600–1500 cm^{-1}**: This area contains complex absorption patterns unique to specific molecules, making it useful for compound identification. It's called the "fingerprint region" because it provides a unique spectral signature for each substance.

4. Analyzing Peak Characteristics

- **Position of Peaks**: The wave number of peaks indicates the type of bond and functional group present. Higher wave number peaks generally indicate stronger bonds (e.g., triple bonds) or lighter atoms (e.g., C-H vs. C-O).
- **Intensity of Peaks**: The strength of the peaks reflects the concentration of the absorbing species and the type of bond. Stronger bonds (e.g., C=O) produce more intense peaks than weaker bonds (e.g., C-H).
- **Width of Peaks**: Broader peaks may indicate hydrogen bonding or other intermolecular interactions.

5. Identifying Functional Groups

1. **Look for Major Peaks**: Identify significant peaks in the spectrum and correlate them with known functional group absorption ranges.
2. **Check for Overlapping Bands**: Some functional groups can exhibit overlapping bands; consider the overall context of the molecule.
3. **Use Reference Spectra**: Compare your spectrum to reference spectra

in databases to identify compounds or functional groups.

6. Examples of Interpretation

- **Alcohols**: A broad O-H stretch around 3200–3600 cm^{-1} and C-O stretch around 1000–1300 cm^{-1}.
- **Carboxylic Acids**: Similar to alcohols but with a sharp C=O peak near 1700 cm^{-1} and a broad O-H peak.
- **Amines**: N-H stretches appear around 3300–3500 cm^{-1}, often showing two peaks for primary amines.

7. Complex Mixtures

For samples with multiple components:

- Identify major components first and then analyze for additional peaks that may correspond to minor components.
- Consider using techniques like ATR or DRIFT for solid samples to minimize interference.

8. Challenges in Interpretation

- **Noise and Baseline Corrections**: Ensure proper baseline correction to avoid misinterpretation of noise as peaks.
- **Overlapping Peaks**: Use de convolution techniques or software to resolve overlapping peaks.
- **Matrix Effects**: Be aware that the presence of other materials can alter the observed spectrum.

ADVANTAGES OF IR: Infrared (IR) spectroscopy is a powerful analytical technique with several advantages, including:

1. **Non-destructive Analysis**: IR spectroscopy typically does not alter or destroy the sample, allowing for further testing or analysis.
2. **Rapid Results**: The technique provides quick data acquisition, enabling faster decision-making in research and quality control.
3. **Chemical Information**: IR spectroscopy can provide detailed information about molecular structure, functional groups, and chemical bonds.
4. **Sensitivity**: It can detect low concentrations of compounds, making it useful for trace analysis.
5. **Versatility**: Applicable to a wide range of samples, including solids, liquids, and gases, across various fields such as chemistry, biology, and materials science.
6. **Minimal Sample Preparation**: Many samples require little to no preparation, saving time and resources.
7. **Quantitative Analysis**: IR spectroscopy can be used for quantitative measurements, helping to determine concentrations of specific components in a mixture.
8. **Identifying Functional Groups**: It is particularly effective in identifying organic compounds based on characteristic absorption bands.
9. **Automation and Integration**: Modern IR spectrometers can be automated and integrated with other analytical techniques, enhancing efficiency.
10. **Real-Time Monitoring**: It can be used for real-time analysis in processes such as chemical reactions or monitoring environmental changes.

DISADVANTAGES:

While IR spectroscopy has many advantages, it also has several disadvantages:

1. **Limited Structural Information**: IR spectroscopy mainly identifies functional groups but may not provide comprehensive structural details about complex molecules.
2. **Interference**: Water VAPOUR and other atmospheric gases can absorb IR radiation, which may interfere with the analysis, especially in samples containing moisture.
3. **Sample Preparation Issues**: Some samples may require specific preparation techniques (e.g., pellets, thin films) that can complicate the analysis.
4. **Overlapping Peaks**: In complex mixtures, overlapping absorption bands can make it difficult to identify individual components accurately.
5. **Quantitative Limitations**: While IR can be used for quantitative analysis, its accuracy can be affected by factors like sample thickness and scattering.
6. **Sensitivity to Sample State**: The state of the sample (solid, liquid, or gas) can influence the spectra, potentially complicating comparisons.
7. **Cost of Equipment**: High-quality IR spectrometers can be expensive to purchase and maintain, which may limit access for some labs.
8. **Skill Required**: Proper interpretation of IR spectra requires expertise and experience, which can be a barrier for less experienced users.
9. **Range Limitations**: IR spectroscopy is limited to a certain range of wavelengths (typically 4000 to 400 cm^{-1}), which may not cover all types of analyses needed.
10. **Non-Universal Applicability**: Certain materials, such as very low molecular weight compounds or highly symmetrical molecules, may not produce distinct IR spectra.

Factor affecting IR spectroscopy :

Several factors can affect the results and interpretation of IR spectroscopy. Here are some key factors to consider:

1. Sample Preparation

- **Thickness**: The thickness of solid samples or the path length of liquid samples can influence absorbance. Too thick samples may lead to saturation and distortion of peaks.
- **Homogeneity**: Inhomogeneous samples can produce variable results. Proper mixing and preparation are crucial for consistent spectra.

2. Concentration

- **Concentration of Analyte**: The amount of substance present in the sample affects peak intensity. Low concentrations can lead to weak signals, while very high concentrations may cause overlapping peaks.

3. Temperature

- **Temperature Variations**: Changes in temperature can affect molecular vibrations and, consequently, the position and intensity of peaks. Heating can also lead to changes in sample state (e.g., evaporation of solvents).

4. Moisture and Contaminants

- **Water Absorption**: Water vapour can interfere with the analysis, especially in organic samples, by producing broad absorption bands in the spectrum.
- **Contaminants**: Presence of impurities or contaminants can lead to additional peaks or interfere with the interpretation of the spectrum.

5. Chemical Environment

- **Interactions with Other Molecules**: Hydrogen bonding, dipole-dipole interactions, or solvation effects can shift peak positions or alter intensities.
- **pH and Ionic Strength**: In biological samples, changes in pH or ionic strength can affect the molecular structure and vibrational modes.

6. Type of IR Spectroscopy

- **ATR vs. Transmission**: Different methods of sample analysis (e.g., Attenuated Total Reflectance vs. traditional transmission) may yield different spectral characteristics.

7. Instrument Calibration

- **Calibration**: Proper calibration of the spectrometer is essential for accurate wavelength and intensity measurements. Poor calibration can lead to incorrect interpretations.

8. Spectral Resolution

- **Resolution of the Instrument**: Higher resolution instruments can resolve closely spaced peaks better, leading to more accurate interpretations.

9. Spectral Range

- **Range of Detection**: The selected range of wavelengths can limit the information obtained. Not all functional groups are detectable in all ranges of IR.

10. Molecular Symmetry

- **Symmetry of Molecules**: Highly symmetrical molecules may exhibit fewer absorption bands, making it difficult to detect certain functional groups

Conclusion :

Infrared (IR) spectroscopy is a vital analytical technique that plays a significant role in various scientific fields, including chemistry, biology, pharmaceuticals, materials science, and environmental science. Its ability to provide detailed information about molecular structure and functional groups makes it an essential tool for both qualitative and quantitative analysis. This review describes some of the numerous possibilities of NIR spectroscopy in the pharmaceutical environment: ranging from the identification of raw materials to the 100% on-line quality control.

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