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Review on Instrumentation of IR Spectroscopy

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Abstract: *Infrared (IR) spectroscopy is a versatile analytical technique that has revolutionized the way scientists analyze the molecular structure, composition, and behavior of substances. It is based on the principle that molecules absorb specific frequencies of infrared radiation, corresponding to the vibrational transitions of chemical bonds. The absorbed energy causes the molecules to vibrate in characteristic ways, and the resulting absorption pattern serves as a molecular fingerprint, allowing for qualitative and quantitative analysis. At the heart of this technique lies a suite of carefully designed and integrated instrumentation components, each playing a critical role in ensuring the accuracy, sensitivity, and reliability of the measurement process.*

The instrumentation of IR spectroscopy has evolved significantly over time, from early dispersive spectrometers to modern Fourier Transform Infrared (FTIR) systems. Regardless of the configuration, the fundamental components of an IR spectrometer typically include the radiation source, sample handling system, monochromator or interferometer, detector, and signal processing/output devices. Each of these elements contributes to the generation of precise and interpretable infrared spectra.

Keywords: Radiation Source, Sample Holder, Interferometer, Detector, Recorder

I. INTRODUCTION

Infrared (IR) spectroscopy is one of the most widely used analytical techniques in modern chemistry, biology, material science, environmental science, and pharmaceutical industries. It is a branch of vibrational spectroscopy that explores the interaction between infrared radiation and matter to provide valuable information about the molecular composition and structure of substances. By measuring the absorption of IR radiation by a molecule, infrared spectroscopy offers insights into the functional groups present and the vibrational transitions within a sample. The development of sophisticated IR spectroscopy instrumentation over the years has greatly enhanced the precision, versatility, and ease with which molecular analyses can be conducted.[1]

The fundamental principle of IR spectroscopy relies on the fact that molecules absorb specific frequencies of infrared light, which causes vibrational excitation of the bonds within the molecule. This spectrum acts like a molecular fingerprint, enabling qualitative identification and, in many cases, quantitative analysis.[2]

The infrared region of the electromagnetic spectrum lies between the visible and microwave regions, spanning wavelengths from approximately 0.78 micrometers (µm) to 1000 µm, or in terms of wavenumber (the reciprocal of wavelength in centimeters), from 12,800 to 10 cm^{-1}. This region is further divided into three sub-regions:

Near-infrared (NIR): 12,800–4000 cm^{-1}

Mid-infrared (MIR): 4000–400 cm^{-1}

Far-infrared (FIR): 400–10 cm^{-1}

Region of IR	Wave length(µm)	Wave Number(cm^{-1})
Near IR (overtone region)	0.8-2.5	12500-4000
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

TABLE NO. 1-REGION OF IR

Each of these regions provides different types of molecular information, with mid-IR being the most widely used for chemical analysis due to its direct correlation with fundamental vibrational modes of most functional groups.[3]

Instrumentation in IR spectroscopy has evolved significantly from early dispersive spectrometers to the advanced Fourier Transform Infrared (FTIR) spectrometers used today. Traditional dispersive IR instruments utilized a monochromator to scan individual frequencies of IR radiation, which required mechanical movement and offered relatively lower resolution and slower data collection. In contrast, FTIR instruments use a Michelson interferometer that allows simultaneous collection of all IR frequencies, followed by a mathematical process called Fourier transformation to generate the spectrum. This innovation revolutionized IR spectroscopy by improving signal-to-noise ratios, reducing scan times, and enhancing sensitivity and accuracy.[4]

An IR spectroscopic instrument typically consists of five major components: a radiation source, a sample handling system, a wavelength selector (monochromator or interferometer), a detector, and a signal processing unit. Each component plays a critical role in ensuring accurate spectral acquisition. The radiation source emits continuous IR radiation; the sample handling system ensures proper interaction between the IR beam and the sample, which may be in solid, liquid, or gaseous form; the wavelength selector isolates specific frequencies or records interferograms; the detector measures the intensity of transmitted or absorbed radiation; and the signal processor converts this information into a usable spectrum.[5]

In addition to the standard transmission mode, modern IR spectroscopy instruments are equipped with specialized sampling accessories that expand the technique's versatility. These include Attenuated Total Reflectance (ATR), Diffuse Reflectance Infrared Fourier Transform (DRIFT), and specular reflection accessories, each suitable for analyzing samples with specific characteristics or requirements. ATR, for instance, has become a standard method for analyzing solids and liquids with minimal or no sample preparation.

IR spectroscopy's applications are vast and span various disciplines. It is routinely used in the identification of organic and inorganic compounds, structural elucidation, monitoring chemical reactions, quality control, forensic investigations, environmental assessments, and even in the analysis of historical artifacts. Its non-destructive nature and the ability to analyze minute sample quantities add to its attractiveness in both research and industrial settings.

The continuous advancement of IR spectroscopy instrumentation, including miniaturization, automation, and integration with computer systems and hyphenated techniques (like GC-IR, TGA-IR), has expanded its reach and capabilities. Moreover, the development of portable and handheld IR spectrometers has opened new frontiers in field analysis, allowing for real-time monitoring and rapid decision-making in sectors such as agriculture, pharmaceuticals, homeland security, and environmental science.[6]

Principle of Infrared (IR) Spectroscopy

Infrared (IR) spectroscopy is based on the interaction of infrared radiation with matter, specifically on the absorption of this radiation by molecules. The fundamental principle of IR spectroscopy lies in the fact that molecules absorb specific frequencies of infrared light, which correspond to the vibrational energies of the chemical bonds within the molecule. This absorption leads to an increase in the vibrational energy of the bonds and is characteristic of the molecular structure.

When infrared radiation passes through a sample, certain frequencies of the IR radiation are absorbed by the sample while others are transmitted. The absorbed frequencies correspond to the natural vibrational frequencies of the bonds in the molecule. These absorbed frequencies cause a transition between vibrational energy levels of the molecule. As

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different bonds and functional groups within a molecule vibrate at specific frequencies, the IR spectrum produced is unique to that molecule and serves as a molecular fingerprint.[7]

Molecules can undergo several types of vibrational motions such as:

Stretching: A change in bond length between two atoms.

Symmetric stretching: Bonds stretch in unison.

Asymmetric stretching: One bond contracts while another stretches.

Bending: A change in bond angle between two bonds.

Types of bending include scissoring, rocking, wagging, and twisting.

For a vibrational mode to be IR-active (i.e., observable in an IR spectrum), there must be a change in the dipole moment of the molecule during the vibration. This is a key requirement. A dipole moment arises when there is an unequal distribution of charge between atoms in a bond, leading to partial positive and negative charges. When the dipole moment of the molecule changes as it vibrates, it can interact with the oscillating electric field of the infrared radiation, leading to absorption.

The energy of infrared radiation falls within the range required to excite these vibrational transitions. The corresponding wavenumbers of these vibrations typically fall in the mid-IR region (4000–400 cm^{-1}), which is commonly used for chemical analysis.

The IR spectrometer measures the amount of radiation absorbed at each wavenumber. The output is an IR spectrum, which plots either transmittance (%T) or absorbance (A) against wavenumber (cm^{-1}). Peaks in the spectrum represent frequencies where IR radiation was absorbed by the sample.

Each peak corresponds to a specific bond or functional group within the molecule. For example:

O–H stretching appears near 3200–3600 cm^{-1},

C=O stretching appears near 1650–1750 cm^{-1},

C–H stretching appears near 2800–3000 cm^{-1}.

Thus, by analyzing the position, shape, and intensity of the peaks in an IR spectrum, one can identify the functional groups and structural features of a compound.

Types of Infrared (IR) Spectroscopy

Infrared spectroscopy can be categorized into various types based on the technique employed to obtain the IR spectrum and the region of the IR spectrum being utilized. Each type has its own instrumentation approach, advantages, and application areas. The two most commonly used types of IR spectroscopy are Dispersive IR Spectroscopy and Fourier Transform Infrared (FTIR) Spectroscopy, but there are also subtypes and techniques based on sampling methods and spectral regions. Below is a detailed description of each:

1. Dispersive Infrared Spectroscopy

Dispersive IR was the traditional form of IR spectroscopy used before the development of FTIR. This technique involves:

A monochromator (usually a prism or grating) that disperses the IR radiation into its component frequencies.

A mechanical scanning system that passes one frequency at a time through the sample.

A detector that records the amount of radiation absorbed by the sample at each frequency.

The instrument works by gradually varying the frequency of the IR radiation and recording the absorption at each frequency to produce the full spectrum. Although effective, dispersive IR spectroscopy has limitations:

Slower data collection.

Lower signal-to-noise ratio.

Less sensitivity and resolution.

It has largely been replaced by FTIR, but it’s still used in some educational or older laboratory settings.

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2. Fourier Transform Infrared (FTIR) Spectroscopy

FTIR spectroscopy is the most advanced and widely used IR spectroscopy technique today. Rather than scanning through individual frequencies, FTIR uses an interferometer (typically a Michelson interferometer) to collect data for all IR frequencies simultaneously. The key components include:

- A broadband IR source.
- A beam splitter that divides the IR beam between two mirrors (one fixed, one movable).
- An interferogram that results from the recombination of beams after reflecting off the mirrors.
- A Fourier Transform algorithm applied by the computer to convert the time-domain interferogram into a frequency-domain IR spectrum.

Advantages of FTIR:

- High speed: Collects all wavelengths at once.
- High sensitivity and signal-to-noise ratio.
- Better wavelength precision and accuracy.
- Higher resolution and throughput.

FTIR has become the standard in modern laboratories due to its superior performance and data quality.

3. Near-Infrared (NIR) Spectroscopy

This technique uses the near-infrared region (12800–4000 cm^{-1}) and is commonly employed for quantitative analysis, particularly in the pharmaceutical, food, and agricultural industries. NIR spectra arise from overtone and combination vibrations, making them more complex and less specific than mid-IR spectra.

Advantages:

Minimal sample preparation.

Widely used for non-destructive testing and online process monitoring.

4. Mid-Infrared (MIR) Spectroscopy

Operating in the 4000–400 cm^{-1} region, this is the most informative and commonly used region in IR spectroscopy. It provides detailed information about the fundamental vibrations of molecular bonds and is highly specific for functional group identification.

5. Far-Infrared (FIR) Spectroscopy

FIR covers the 400–10 cm^{-1} range and is used for studying:

Lattice vibrations in inorganic and solid-state materials.

Low-frequency vibrations in large organic molecules or polymers.

It often requires specialized sources and detectors due to lower energy IR radiation.

6. Attenuated Total Reflectance (ATR) Spectroscopy

ATR is a sampling technique used with FTIR. It allows direct analysis of solid and liquid samples without complex preparation. An IR beam reflects internally within an ATR crystal (like ZnSe or diamond), interacting with the sample through the evanescent wave. This method is ideal for surface analysis and greatly simplifies the sampling process.

7. Reflectance Spectroscopy

Reflectance methods are used when transmission is impractical:

Diffuse Reflectance Infrared Fourier Transform (DRIFT): For powders and rough surfaces.

Reflection-Absorption IR Spectroscopy (RAIRS): Used in surface science, particularly for thin films on reflective substrates.[8]

Components of IR Spectroscopy Instrument

- Radiation Source
- Sample Handling System
- Monochromator/Interferometer
- Detector

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- Signal Processor and Output Devices

Fig No. 1- IR Spectroscopy Instrument

Radiation Source

The radiation source is a crucial component of an infrared (IR) spectrometer. It generates and emits continuous infrared radiation over the range of interest (near-, mid-, or far-infrared). The quality, intensity, and spectral distribution of the radiation source significantly affect the sensitivity and accuracy of the measurements. Therefore, the choice of source depends on the IR region being analyzed and the specific application.

An ideal IR radiation source should possess the following characteristics:

Emit a broad and continuous spectrum of IR radiation.

Provide stable and reproducible output over time.

Have sufficient intensity across the entire IR spectral region of interest.

Be durable and have a long operational lifespan.

Below are the main types of radiation sources used in IR spectroscopy, categorized by the spectral region they cover:[9]

1. Globar Source (Silicon Carbide Rod)

Fig No.2- Silicon Carbide Rod

Material: Sintered silicon carbide (SiC).

Operating Temperature: ~1200–1650°C.

Spectral Range: Mid-IR to Far-IR (approx. 4000 to 200 cm^{-1}).

Description: The Globar source is the most commonly used source in modern FTIR instruments. When heated electrically, it emits strong, continuous IR radiation over a wide range of wavelengths. It is highly effective for mid-IR applications and is relatively stable and robust.

Advantages: Broad spectral output, durability.

Limitations: Requires optical components to handle the heat, lower output in near-IR.[10]

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2. Nernst Glower

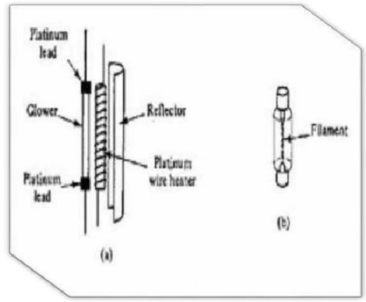

Fig No.3- Nernst Glower

Material: A mixture of rare-earth oxides such as zirconium oxide, yttrium oxide, and thorium oxide.

Operating Temperature: ~1500–2000°C.

Spectral Range: Mid-IR (approx. 4000–100 cm^{-1}).

Description: The Nernst glower becomes electrically conductive only after reaching a certain temperature. It emits IR radiation upon heating and is commonly used in older or specialized IR instruments.

Advantages: High intensity in mid-IR.

Limitations: Brittle, requires preheating to become conductive, more fragile than globar.[11]

3. Incandescent (Tungsten) Filament Lamp

Fig No.4-Incandescent wire

Material: Tungsten filament (similar to that used in visible light bulbs).

Operating Temperature: ~2000–3000°C.

Spectral Range: Near-IR (approx. 12,800 to 4000 cm^{-1}).

Description: This is the standard source for near-infrared spectroscopy. The filament emits both visible and near-IR radiation.

Advantages: Readily available, inexpensive.

Limitations: Ineffective for mid- and far-IR; intensity drops off at longer wavelengths.[12]

4. Mercury Arc Lamp

Fig No.5- Mercury Arc Lamp

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Material: Enclosed gas discharge lamp with mercury vapor.
Operating Principle: Electrical discharge excites mercury atoms, which emit radiation.
Spectral Range: Far-IR (approx. 100–10 cm^{-1}).
Description: Typically used for far-IR spectroscopy, where vibrational and rotational transitions of heavy atoms or lattices are observed.
Advantages: Strong output in far-IR.
Limitations: Emits discrete lines rather than a continuous spectrum, requires filters or monochromators. [13]

5. Carbon Dioxide (CO_2) Laser

Type: Coherent IR source.
Spectral Range: Narrow bands in mid-IR (~10.6 µm, or around 940 cm^{-1}).
Description: Used in high-resolution spectroscopy or specific gas analysis applications. Emits highly intense and monochromatic IR radiation.
Advantages: High intensity and selectivity.
Limitations: Limited to specific wavelengths, more expensive and complex. [14]

6. Blackbody Sources

Material: Heated metal surfaces or cavities that approximate ideal blackbody radiation.
Spectral Range: Broad, depending on temperature.
Description: Provide stable and continuous radiation across a wide IR range. Used in calibration or specialized measurements.
Advantages: Predictable emission spectrum.
Limitations: Lower intensity than other sources, requires careful temperature control.[15]

Monochromator/Interferometer

Monochromator and Interferometer in IR Spectroscopy Instrumentation

In infrared (IR) spectroscopy, one of the most critical steps is the selection and separation of specific wavelengths of IR radiation from a broad-spectrum source to analyze the sample. This process is accomplished using either a monochromator or an interferometer, depending on whether the system is a dispersive IR spectrometer or a Fourier Transform Infrared (FTIR) spectrometer, respectively.[16]

Both devices serve the essential purpose of resolving the IR radiation into individual wavelengths (or frequencies) to measure the sample's absorption characteristics. However, they operate on very different principles and technologies.

1. Monochromator (Used in Dispersive IR Spectroscopy)

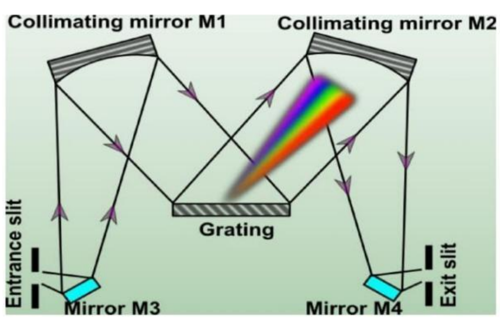

Fig No. 6- Monochromator

Definition:
A monochromator is an optical device used in dispersive IR spectrometers to isolate a narrow band of wavelengths from a broadband IR source by physically separating them based on their wavelength.[17]
Key Components:
Entrance Slit: Allows a narrow beam of IR radiation to enter.

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Collimating Mirror: Directs the light into parallel beams.

Dispersing Element: Usually a prism or a diffraction grating that separates the IR radiation into its component wavelengths.[18]

Focusing Mirror: Refocuses the dispersed light onto an exit slit.

Exit Slit: Selects a specific wavelength to be passed to the sample.

Working Principle:

The monochromator scans through a range of IR wavelengths one at a time by mechanically rotating the dispersing element (grating or prism). At each wavelength, the intensity of the IR radiation transmitted or absorbed by the sample is measured. The process continues step-by-step until the full spectrum is collected.[19]

Types of Dispersing Elements:

Prism:

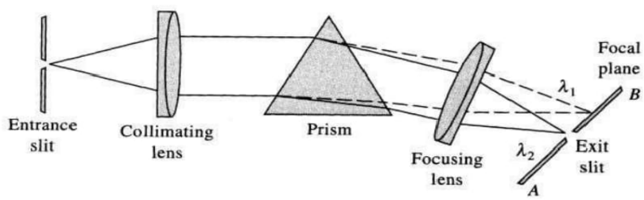

Fig No.7- Prism

Made of materials like KBr, NaCl, or CaF_2; separates IR light by refraction.[20]

Grating:

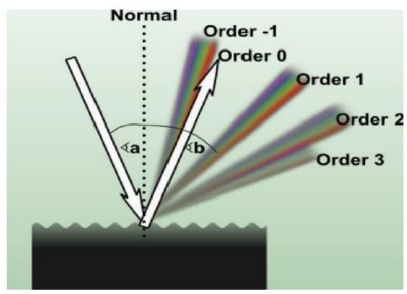

Fig No. 8-Grating

Made of a ruled reflective surface; separates IR light by diffraction.[21]

Advantages:

- Simple and historically well-established.
- Effective for narrow-band analysis.

Limitations:

- Slow scanning process.
- Low energy throughput (due to slit and component losses).
- Poor signal-to-noise ratio compared to interferometers.
- Mechanical parts prone to wear and alignment issues.[22]

2. Interferometer (Used in FTIR Spectroscopy)

Definition:

An interferometer is an optical device that modulates IR radiation by causing interference patterns and is used in FTIR spectrometers. It allows simultaneous measurement of all wavelengths of IR radiation, leading to faster and more accurate analysis.[23]

Most Common Type: Michelson Interferometer

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Components of a Michelson Interferometer:

1. Beam Splitter: Semi-reflective material (often KBr or CaF_2) that divides the incoming IR beam into two paths.
2. Fixed Mirror: Reflects one part of the beam back to the beam splitter.
3. Moving Mirror: Reflects the second part of the beam but is mounted on a precise linear actuator that moves back and forth.
4. Recombination at Beam Splitter: The two beams are recombined at the beam splitter, creating interference patterns depending on their path difference.
5. Detector: Measures the resulting modulated IR signal (interferogram).[24]

Working Principle:

As the moving mirror changes position, it creates a path difference between the two beams.

This leads to constructive and destructive interference at different wavelengths.

The interferogram (a signal that contains all the IR spectral information encoded in time-domain form) is generated.

The Fourier Transform (mathematical process) is applied to convert the interferogram into a conventional IR spectrum (intensity vs. wavelength).[25]

Advantages of Interferometer in FTIR:

Fellgett's Advantage (Multiplex Advantage): All wavelengths are measured simultaneously, increasing speed.

Jacquinot’s Advantage (Throughput Advantage): No slits are required, so more radiation reaches the detector, improving sensitivity.[26]

High Signal-to-Noise Ratio: Especially important for trace-level detection.

Precise Wavelength Accuracy: Due to use of a laser reference for calibration.

Fast Data Acquisition: Ideal for kinetic studies or automation.

Comparison: Monochromator vs. Interferometer

	Monochromator	*Filter*
Means of selection	Diffraction	Absorption
Wavelength width	Narrow	Wide
Cost	Expensive	Cheap
Portability	None	Very
Capable of recording spectra	Yes	No
Suitable for quantitative analysis	Yes	Yes

TABLE NO.2- COMPARISON TABLE

Detector

Certainly! Here's a detailed section on detectors used in IR spectroscopy instrumentation, perfect for including in your IR spectroscopy write-up:

Detectors in IR Spectroscopy Instrumentation

In infrared (IR) spectroscopy, detectors play a crucial role in converting the transmitted or reflected IR radiation—after interaction with the sample—into an electrical signal that can be processed and displayed as a spectrum. The performance, sensitivity, and speed of an IR spectrometer depend significantly on the type and quality of the detector used.[27]

The choice of detector is primarily determined by:

The IR spectral region (near, mid, or far IR),

Signal strength,Required sensitivity and response time, and Type of spectrometer (dispersive vs FTIR).

IR detectors can be broadly classified into two categories:

1. Thermal Detectors

Respond to the heating effect of IR radiation.

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The incident IR radiation increases the temperature of the detector material, which leads to a measurable change in some physical property (resistance, voltage, or current).

Used for a broad spectral range (often used in FTIR spectrometers).[28]

a) Thermocouple

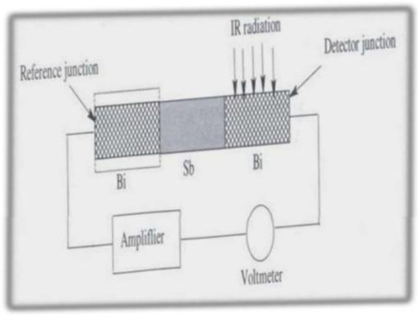

Fig No.9- Thermocouple

Working Principle: IR radiation heats the junction of two dissimilar metals, producing a voltage proportional to the temperature difference.

Spectral Range: 5000–200 cm^{-1} (mid to far-IR).

Advantages: Simple, rugged, inexpensive.

Limitations: Low sensitivity, slow response time.

b) Bolometer

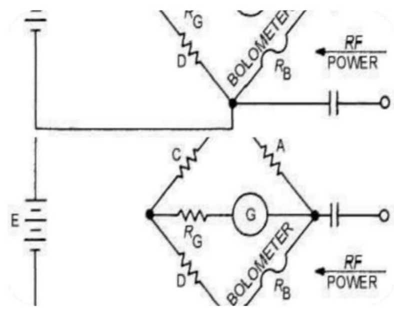

Fig No.10- Bolometer

Working Principle: Absorbs IR radiation, causing a change in electrical resistance due to heating.

Spectral Range: Broad (depends on design).

Advantages: High sensitivity.

Limitations: Sensitive to ambient temperature fluctuations; slow response.

c) Golay Cell

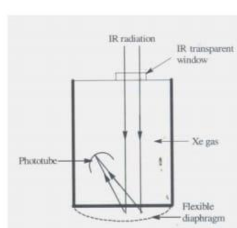

Fig No.11- Golay Cell

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Working Principle: IR radiation heats an enclosed gas cell, causing expansion that deflects a flexible membrane, changing reflected light intensity detected by a photodetector.

Spectral Range: Far-IR (below 400 cm^{-1}).

Advantages: High sensitivity in the far-IR region.

Limitations: Mechanically delicate, expensive, slow.

Selection Criteria for Detectors

Cost and Maintenance: Thermal detectors are more affordable and easier to maintain, while quantum detectors offer better performance at a higher cost.

Spectral Range: Choice of detector must match the IR region of interest.

Speed of Analysis: For dynamic or real-time studies, fast detectors like MCT are preferred.

Sample Type and Sensitivity Needs: Trace analysis or weak absorbers require high-sensitivity detectors.

Signal Processor and Output Devices

Signal Processor and Output Devices in IR Spectroscopy Instrumentation

In IR spectroscopy, after infrared radiation interacts with a sample and is captured by a detector, the resulting electrical signal must be interpreted and displayed in a meaningful format. This is where the signal processor and output devices come into play. These components are essential for converting raw data into a usable infrared spectrum, providing insights into molecular vibrations, chemical bonds, and functional groups present in the sample.[29]

1. Signal Processor

The signal processor is a critical component of IR spectroscopy instrumentation that handles the conversion, processing, and analysis of signals received from the detector.

Functions of the Signal Processor:

Signal Amplification: The electrical signal from the detector is usually very weak. The signal processor amplifies it without introducing significant noise.

Analog-to-Digital Conversion (ADC): The amplified analog signal is converted into a digital signal for further analysis, especially in FTIR systems.

Filtering: The processor may include filters to remove background noise and enhance the signal-to-noise ratio.

Fourier Transform (in FTIR): For FTIR spectrometers, the raw output is an interferogram (a time-domain signal). A Fourier Transform algorithm is applied to convert this into a frequency-domain spectrum.

Baseline Correction and Smoothing: Digital algorithms help correct baseline drifts and smooth the spectrum for easier interpretation.

Data Storage and Management: Modern processors include data acquisition systems to store spectra, reference files, calibration curves, and analysis results.

2. Output Devices

The output devices in IR spectroscopy are used to display or present the final processed spectrum in a readable and interpretable form. Over time, these have evolved from simple analog recorders to advanced digital systems.

a) Graphical Output (IR Spectra)

The most common form of output is an IR spectrum, a graph of absorbance (or transmittance) versus wavenumber (cm^{-1}).

The peaks in the spectrum correspond to specific molecular vibrations and are used for qualitative and quantitative analysis.

b) Types of Output Devices

i. Analog Recorders (Historical)

Early IR instruments used pen-and-paper chart recorders that physically plotted the spectrum as the monochromator scanned through wavelengths.

These devices have largely been replaced by digital systems but are still found in basic teaching setups.

ii. Digital Displays

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Modern instruments feature LCD or LED display panels that show numerical data or simplified spectra in real-time.
Useful for immediate feedback and quick checks during analysis.
iii. Computer Systems and Monitors
Most modern IR and FTIR instruments are controlled by dedicated computer systems with User interfaces for setting parameters and running scans.
Graphical software to display and analyze spectra.
Zoom, peak pick, integration, and overlay tools for detailed spectral interpretation.

Fourier Transform Infrared Spectroscopy (FTIR)

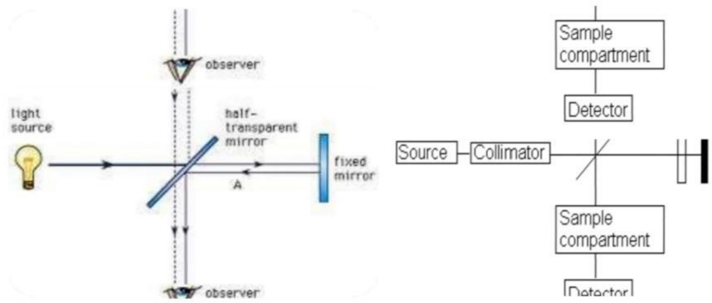

Fig No.12-FTIR

1. Introduction to FTIR
Fourier Transform Infrared Spectroscopy (FTIR) is a powerful analytical technique that identifies and quantifies materials by measuring how infrared radiation is absorbed, transmitted, or emitted by a sample. Unlike traditional dispersive IR spectroscopy, which measures one wavelength at a time, FTIR measures all wavelengths simultaneously and applies a mathematical algorithm called the Fourier Transform to produce the spectrum.
FTIR has largely replaced dispersive IR methods due to its superior speed, resolution, sensitivity, and data handling capabilities. It is widely used in organic and inorganic chemistry, pharmaceuticals, materials science, environmental science, forensic analysis, and polymers.
2. Basic Principle of FTIR
The fundamental principle behind FTIR is that molecules absorb specific frequencies of IR radiation, which cause vibrations (stretching, bending, twisting) of chemical bonds. These absorption frequencies are characteristic of particular functional groups and molecular structures.[30]
In FTIR:
1.The entire IR spectrum is passed through the sample at once.
2.The interferometer modulates the IR signal into an interferogram.
3.The Fourier Transform is applied to the interferogram to extract the spectrum.
4.This simultaneous measurement of all frequencies is known as the Multiplex (Fellgett's) Advantage.
3. Components of an FTIR Spectrometer
a) IR Source
Typically a Globar (silicon carbide rod) or Nernst glower, providing a continuous broadband IR spectrum.
b) Interferometer (Michelson Interferometer)
1.Key component that modulates the IR beam by splitting it into two paths (fixed and moving mirror).
2.The recombined beam creates an interference pattern (interferogram), which contains all IR frequencies encoded in time-domain format.
c) Sample Compartment
Where the IR beam interacts with the sample. Sample forms may include solid, liquid, gas, thin film, or powder.

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d) Detector
Converts the modulated IR beam into an electrical signal.
Common detectors:
DTGS (Deuterated Triglycine Sulfate) – room temperature, general use.
MCT (Mercury Cadmium Telluride) – high sensitivity, needs cooling.
e) Computer & Fourier Transform Processor
Performs the Fourier Transform to convert the interferogram into a usable IR spectrum.
Displays, stores, and analyzes the final data.

4. Working of FTIR

1. IR source emits broadband radiation.
2. Interferometer modulates the light, generating an interferogram.
3. IR beam passes through the sample and reaches the detector.
4. The detector signal (still an interferogram) is digitized.
5. Fourier Transform is applied to convert it into a spectrum.
6. The output is a plot of intensity vs. wavenumber (cm^{-1}).

5. Sample Handling Techniques in FTIR

Transmission: Thin films, KBr pellets (solids), or liquid films between salt plates.
Attenuated Total Reflectance (ATR): Most common for solids and liquids; minimal prep.
Diffuse Reflectance (DRIFTS): For powders.
Specular Reflectance: For reflective surfaces or thin films.

6. Applications of FTIR

a) Qualitative Analysis
Identification of functional groups.
Compound identification by spectral matching with reference libraries.
b) Quantitative Analysis
Concentration determination using Beer-Lambert Law.
c) Material Characterization
Polymer structure and degradation.
Coating analysis, plastic additives.
d) Pharmaceuticals
API (Active Pharmaceutical Ingredient) verification.
Drug stability and formulation studies.
e) Environmental Analysis
Detection of pollutants (e.g., CO_2, NOx, hydrocarbons).
f) Forensics
Identification of residues, fibers, and unknown substances.

7. Limitations of FTIR

Water and CO_2 Interference: Must be minimized by purging or drying the sample chamber.
Complex Spectra: Overlapping peaks can complicate interpretation.
Sample Preparation: Some samples still require prep (e.g., pellets or films).
Cost: FTIR instruments are more expensive than simple dispersive spectrometers.

8. Advances in FTIR

Micro-FTIR: Combines FTIR with microscopy for spatially resolved analysis.
Portable FTIR: Used for field analysis and on-site testing.
2D-FTIR: Provides time-resolved and multi-dimensional spectral data.
Quantum Cascade Lasers (QCL): Used for tunable, high-resolution IR sources.

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Applications of Infrared (IR) Spectroscopy

1. Pharmaceutical and Biomedical Applications

a) Drug Identification and Purity Testing

Used to verify the identity of Active Pharmaceutical Ingredients (APIs).

IR spectra can confirm the presence of functional groups and overall molecular structure.

Assists in checking the purity and composition of drugs.

b) Formulation Analysis

Helps in studying interactions between drug substances and excipients.

Ensures compatibility and stability in pharmaceutical formulations.

c) Quantitative Analysis of Drugs

FTIR can be used for concentration measurements in tablets, creams, or solutions.

d) Disease Diagnosis

FTIR is being investigated for diagnosing diseases by analyzing biological fluids like blood, saliva, or urine.

Identification of disease markers, such as proteins or lipids.

2. Polymer and Material Science

a) Polymer Characterization

Identifies functional groups, monomeric units, and additives.

Used to track polymerization and degradation processes.

b) Coating and Surface Analysis

Determines the chemical composition of paints, coatings, and laminates.

Specular reflectance FTIR is used for thin film and surface studies.

c) Failure Analysis

Investigates contaminants, degradation, and cracking in materials.

3. Environmental Analysis

a) Pollutant Detection

Measures air pollutants, including CO, NOx, SOx, and hydrocarbons, using gas-phase IR cells.

Detection of volatile organic compounds (VOCs) in industrial emissions.

b) Water Quality Monitoring

Identifies contaminants in water such as organic solvents, chlorinated compounds, and detergents.

c) Soil and Sediment Analysis

Analysis of organic matter and contaminants in soil samples.

4. Food and Agriculture

a) Food Quality and Adulteration

Detects adulterants in milk, oil, honey, and other foods.

Analyzes nutritional content (proteins, fats, carbohydrates).

b) Shelf-Life and Spoilage

Monitors oxidation, moisture content, and spoilage markers.

Evaluates food packaging and migration of substances.

c) Pesticide Residue Detection

Identifies and quantifies trace levels of pesticides in crops and produce.

5. Forensic Science

a) Substance Identification

Identifies unknown materials such as drugs, explosives, and toxins.

Common in forensic labs for trace evidence analysis (e.g., fibers, hair, paint).

b) Crime Scene Investigation

Non-destructive technique used on-site using portable IR spectrometers.

Analysis of inks, documents, and counterfeit items.
6. Petrochemical and Chemical Industry
a) Hydrocarbon Analysis
Identification of functional groups in fuels, lubricants, and oils.
Tracks the oxidation or contamination of oils.
b) Process Monitoring
In-situ analysis of chemical reactions in real-time using online FTIR probes.
Ensures process control and safety in manufacturing plants.
7. Academic and Research Applications
a) Structural Elucidation
Confirms the presence of functional groups in organic and inorganic compounds.
Complementary to NMR and mass spectrometry for full molecular analysis.
b) Spectral Library Building
IR spectra are collected and cataloged for comparison and automated identification.
c) Kinetic Studies
Real-time monitoring of reaction kinetics and catalytic processes.
8. Nanotechnology and Material Development
a) Surface Modification
IR helps track changes in surface chemistry of nanomaterials.
b) Nanocomposite Characterization
Monitors the interaction between polymers and nanoparticles.
Detects functional group modifications on nanocarriers (e.g., drug-loaded nanoparticles).
9. Textile and Fiber Analysis
Determines fiber type (e.g., cotton, polyester, nylon).
Analyzes dyes, finishes, and surface treatments.
Identifies synthetic vs. natural fiber compositions in fabrics.
10. Art and Archaeology
Non-destructive testing of ancient pigments, binders, and varnishes.
Authenticates artifacts and distinguishes originals from forgeries.
Investigates degradation and restoration materials in artworks.
11. Semiconductor and Electronics Industry
Analyzes wafer surfaces, residues, and contaminants.
Used in cleanroom environments for process validation and failure analysis.[31]

REFERENCES

1. Elliot and E. Ambrose, Nature, Structure of Synthetic Polypeptides, 1950; 165: 921; D.L. Woernley, Infrared Absorption Curves for Normal and Neoplastic Tissues and Related Biological Substances, Current Research, 1950; 12: 516p.

2. Theophanides T, editor. Introduction to Infrared Spectroscopy-Materials Science, Engineering and Technology.Rijeka, Croatia: InTech; 2012. Available from:http://www.intechopen.com/books/ infrared-spectroscopy-materials science engineering and-technology/introduction-to-infrared-spectroscopy

3. Hesse M, Meier HBZ. Spectroscopic Methods in Organic Chemistry. 2nd ed. Stuttgart: Georg Thieme Verlag, 2008.

4. Pavia D, Lampman GGK. Introduction to Spectroscopy: A Guide for Students of Organic
Chemistry. 3rd ed. Fort Worth, TX: Harcourt College Publishers, 2001.

5. Monnier GF. A review of infrared spectroscopy in microarchaeology: Methods, applications, and recent trends. Journal of Archaeological Science: Reports, 2018; 18:806-823

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6. J. Anastasopoulou and Th. Theophanides, Chemistry and Symmetry‖, In Greek National Technical University of Athens, NTUA, 1997; 94.
7. G.Herzberg, Atomic spectra and atomic structure, Dover Books, New York, Academic press, 1969; 472.
8. Maas, J.H. van der, Basic Infrared Spectroscopy. 2nd edition. London: Heyden & Son Ltd, 1972;105.
9. Banwell CN, McCash EM. Fundamentals of Molecular Spectroscopy. 4th ed. Berkshire, England:McGraw Hill, 1994.
10. Sherman HC. Handbook of Instrumental Techniques for Analytical Chemistry. New Jersey: Prentice Hall, 1997.
11. Koenig JL. Infrared and Raman Spectroscopy of Polymers. Smithers Rapra Technology, 2001.
12. Griffiths PR, de Haseth JA. Fourier Transform Infrared Spectrometry. 2nd ed. Hoboken, New Jersey: John Wiley & Sons, 2007.
13. Smith BC. Fundamentals of Fourier Transform Infrared Spectroscopy. 2nd ed. Boca Raton, FL: CRC Press, 2011.
14. Gomez, M.A., Perez, M.A.B., Gil, F.J.M., Identification of species of Brucella using Fourier transform infrared spectroscopy‖, Journal of Microbiological Methods, 2003; 55: 121-131.
15. Sacksteder, C., Barry, B.A., Fourier Transform Infrared Spectroscopy: A Molecular Approach to an Organismal Question‖, Journal of Phycology, 2001; 37: 197-199.
16. R. R. Willey. Fourier Transform Infrared Spectrophotometer for Transmittance and Diffuse Reflectance Measurements‖ Applied Spectroscopy, 1976; 30(6): 593-601.
17. Peter J. Larkin. ―Infrared and Raman Spectroscopy. Principles and Spectral Interpretation Chapters 1 to 6. Radarweg 29, PO Box 211, 1000 AE Amsterdam, The Netherlands. Elsevier, 2011.
18. John A. Dean. ―Lange's Handbook of Chemistry‖ Section 7.5. Fifteenth Edition. United States of America. McGraw Hill, 1999.
19. Authors: John McMurry, Professor Emeritus Publisher/website: OpenStax Book title: Organic Chemistry Publication date: Sep 20, 2023.
20. Melissa A. Page and W. Tandy Grubbs, J. Educ, 1999; 76(5): 666.
21. Modern Spectroscopy, 2nd Edition, J.Michael Hollas, ISBN: 471-93076-8.
22. Schuster, K.C., Mertens, F., Gapes, J.R., ―FT-IR spectroscopy applied to bacterial cells as a novel method for monitoring complex biotechnological processes‖, Vibrational Spectroscopy, 1999; 19: 467-477.
23. Wikipedia, the free encyclopedia. Infrared spectroscopy http://en.wikipedia.org, July 28, 2007.
24. Mount Holyoke College, South Hadley, Massachusetts. Forensic applications of IR http://www.mtholyoke.edu July 28, 2007.
25. T. Theophanides, Infrared and Raman Spectra of Biological Molecules, NATO Advanced Study Institute, D. Reidel Publishing Co. Dodrecht, 1978; 372.
26. T. Theophanides, C. Sandorfy) Spectroscopy of Biological Molecules, NATO Advanced Study Institute, D. Reidel Publishing Co. Dodrecht, 1984, 646.
27. T. Theophanides Fourier Transform Infrared Spectroscopy, D. Reidel Publishing Co. Dodrecht, 1984.
28. T. Theophanides, Inorganic Bioactivators, NATO Advanced Study Institute, D. Reidel Publishing Co. Dodrecht, 1989; 415.
29. G. Vergoten and T. Theophanides, Biomolecular Structure and Dynamics: Recent experimental and Theoretical Advances, NATO Advanced Study Institute, Kluwer Academic Publishers, The Netherlands, 1997; 327.
30. C. Conti, P. Ferraris, E. Giorgini, C. Rubini, S. Sabbatini, G. Tosi, J. Anastassopoulou, P. rapantoni, E. Boukaki, S FT-IR, T. Theophanides, C. Valavanis, FT-IR Microimaging Spectroscopy: Discrimination between healthy and neoplastic human colon tissues , J. Mol Struc, 2008; 881: 46-51.
31. M. Petra, J. Anastassopoulou, T. Theologis & T. Theophanides, Synchrotron micro-FTIR spectroscopic evaluation of normal paediatric human bone, J. Mol Structure, 2005; 78: 101