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Review Article on FTIR Spectroscopy

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***Abstract*— Fourier Transform Infrared (FTIR) spectroscopy, which is used to examine molecule rotations and vibrations. Through the simultaneous measurement of infrared light absorption over a broad frequency range, it generates distinct spectral fingerprints for various substances. Molecular structures, functional groups, and molecular interactions in solids, liquids, and gases can all be quickly and nondestructively analysed with this method. A broadspectrum infrared beam is passed through a sample using a Michelson interferometer in an FTIR spectrometer, which simultaneously gathers data on all frequencies. An absorption spectrum that offers a distinct molecular "fingerprint" of the sample is then produced by a Fourier transformation of the resultant signal, or interferogram. Advanced techniques like ATR-FTIR enhance its applicability for surface thin layer analysis. FTIR extensively used in pharmaceuticals, polymers, food, environmental science.**

***Index Terms*— FTIR Spectroscopy, Radiation source, Sample preparation, Interferometer, Detectors, fingerprint region.**

I. INTRODUCTION

Fourier transform infrared (FTIR) spectroscopy has diverse applications, including the analysis of small molecules and tissue imaging. This technique leverages light waves that can interfere constructively or destructively, with its functionality rooted in the Michelson-Morley experiment. FTIR is particularly useful for mapping cellular components and identifying abnormal cells. Its growing application in protein studies focuses on analyzing protein conformation, folding, and details at active sites during enzyme reactions using reaction-induced FTIR. In FTIR spectroscopy, a molecule absorbs energy to transition to a vibrational excited state, revealing its absorption spectrum and rotational movements, particularly through vibrational modes affecting the molecular dipole moment. Different types of molecular vibrations arise from various binding forces and angles, affecting absorption bands in a spectrum. Complex molecules show more absorption options with stronger bindings and lighter atoms. The wavenumber, the reciprocal of the wavelength, indicates the position of these bands, which is directly proportional to the absorbed energy. Functional groups absorb between 4000-1500 cm-1, with double and triple bonds having higher wavenumbers. The 1500 cm-1 range is important for identifying substances and is known as the fingerprint region. FTIR spectroscopy records radiation over a full wavelength range through interferometric modulation, resulting in an interferogram that reflects the sample's data. Unlike traditional methods, Fourier transform spectroscopy uses a beam of multiple frequencies, capturing data rapidly before processing it with algorithms to determine absorption wavelengths, all facilitated by a Michelson interferometer setup.

II. PRINCIPLE

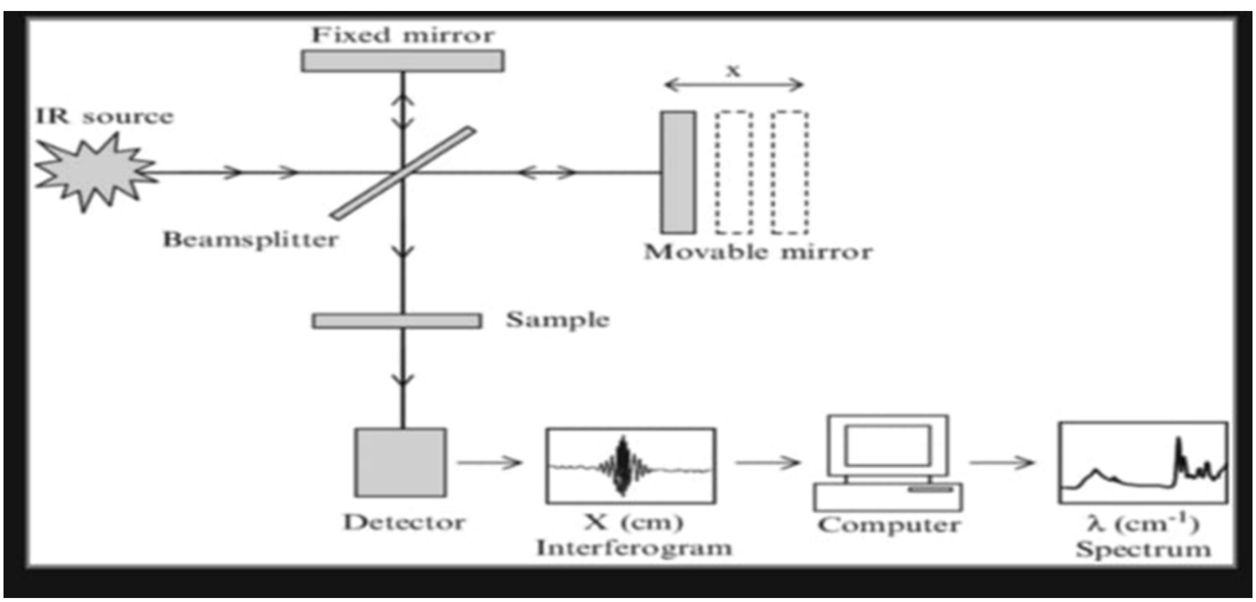
Infrared spectroscopy is a crucial tool in organic chemistry for identifying functional groups and assessing compound purity by analyzing unique absorption bands. It operates on the principle that molecules vibrate at specific frequencies within the infrared region of the electromagnetic spectrum. When infrared radiation hits a sample, it is absorbed at frequencies corresponding to the molecule's vibrational frequencies, creating an infrared spectrum. Nonlinear molecules demonstrate 3N-6 vibrational motions, but only those that induce a change in dipole moment are IR active and appear in the spectrum. This method effectively detects asymmetric vibrations and identifies various chemical groups, including amino acids and water, which are challenging to analyze with other techniques. Proteins show distinct absorption peaks in their IR spectra due to the carbonyl groups in polypeptide chains. Stretching vibrations involve bond length changes, while bending vibrations involve bond angle changes. FTIR overcomes slow scanning in dispersive IR by using a Michelson interferometer (beam splitter, moving mirror, fixed mirror) to generate an interferogram where all IR frequencies are embedded; each data point contains information of all frequencies, recorded rapidly through interference of recombined light beams with varying optical path difference.

III. MATERIALS AND METHODS

1.Transmission mode: Widely used method; sample on IR-transparent material, aqueous suspension, dried films, or KBr pellets. Spectrum quality depends on homogeneity, particle size, thickness. Requires fine grinding to avoid Christiansen effect.
2.Attenuated Total Reflection (ATR): Direct investigation of smooth surfaces, minimal sample preparation, biofilm studied in native state, analysis of thin films, membranes, polymers. Allows aqueous media, in situ, non-destructive, real-time measurements at substratum/liquid interface.
3.Diffuse reflectance spectroscopy is an analytical technique effective in various fields, particularly when traditional methods are ineffective, such as in biofilm research where sample removal from surfaces is problematic. Scattering light measures diffuse reflectance spectrum.
4. Equivalent for FTIR spectroscopy. FTIR spectroscopy used Burker IFS 66, custom optics. Zinc selenide and germanium served as IRE crystals, while the DRIFT optics, sourced from Harrick Scientific, functioned off-axis to mainly capture diffusely reflected components.
5. Membrane test the membrane fouling investigations utilized a reverse osmosis membrane test cell operating at 40 bar with a crossflow velocity of 20 h^{-1}, producing a sheer force of 3 Nm^{-2}. The cell processed drinking water with a performance rate of 80 l m^{-2}h-2 featuring a polyamide composite membrane for separation and poly sulfone for mechanical support.

IV. INSTRUMENTATION

in FTIR systems involves an IR source, typically a silica ceramic heated to around 1550 Kelvin, which emits a broad spectrum of IR radiation. Instead of a monochromator, a Michelson interferometer is used to analyze the infrared beam after it passes through a sample. The interferometer modulates the IR radiation by applying an optical inverse Fourier transform. As the modulated IR beam passes through a gas sample, different molecules absorb it at varying wavelengths. A detector then measures the intensity of the IR radiation, while a computer digitizes the signal and performs a Fourier transform to generate the IR spectrum of the gas sample. The FTIR (Fourier transform infrared) method uses an interferometer to split a light beam into two paths, with one beam transmitted to a fixed mirror and the other reflected to a moving mirror. The interferogram, collected from the sample signal, is then digitized and analyze through a Fourier transform to produce the spectrum. A key component of this system is the IR source, which emits broad-band radiation across various wavelengths.



1.The source
A glowing black body emits infrared (IR) radiation, which is directed through an aperture that regulates the energy incident on the sample.

2.The interferometer
FTIR spectrometers use an interferometer with mirrors, a beam splitter, and detectors to analyze infrared radiation through interference patterns.

3. FT-IR sample preparation
Involves different processes for liquids and solids. For liquids, a drop of the compound is placed between KBr plates, turned to create a thin film, and a spectrum is run. If too concentrated, one plate is cleaned before reassembling. After use, plates must be thoroughly cleaned with solvents like methylene chloride and ethanol. For solids, a concentrated solution is prepared, being cautious of water content which can affect KBr plates. Alternatively, solids can be prepared as Nujol mulls by grinding them down to 1-2 microns and mixing with mineral oil before placing between KBr plates. If the resultant spectrum is distorted, it indicates the particle size is too large. Common issues leading to cloudy disks include inadequate grinding of KBr, excess moisture in the sample, incorrect sample-KBr ratio, and insufficiently tightened bolts causing thick pellets.

4. Detectors [10]

- Photon detectors

FTIR spectrophotometers convert thermal or light energy into electrical signals, primarily categorized as thermal and photodetectors. Semiconductor IR detectors are the most sensitive, utilizing the internal photoelectric effect to convert photon energy into electrical charge. HgCdTe operates within 8 to 13µm, PbS and PbSe range from 1 to 3µm and 1 to 6µm, respectively, whereas InSb and InAs cover 1 to 5.5µm and 1 to 3.5µm respectively

- Thermal Detectors:

This type of detector measures a change in temperature of a material by absorbing the incident electromagnetic radiations. Thermal detectors transformed thermal Fourier Transform Infrared Spectroscopy. Fundamentals and Application. energy to electrical signals. Bolometers, thermopiles, thermocouples, pyroelectric, photoacoustic, and pneumatic detectors are some of the most common thermal detectors. Thermal detectors usually used a broad spectral radiation.

- Pyroelectric Detectors

Pyroelectric effect is the variation in the spontaneous polarization of a piezoelectric crystal with change in temperature. As compared to the other thermal detectors, the pyroelectric detectors are robust and inexpensive and have comparatively constant sensitivity range through the whole spectral range. TGS and DTGS detectors measure the voltage due to the change in temperature by changing their capacitance; however, less sensitivity makes them less efficient.

- Bolometers

Bolometers detect temperature changes via resistance variations, are sensitive but slow, needing liquid He. Photodiodes convert light to electrical signals and have different IR radiation sources for various wavelengths

V. FACTORS INFLUENCING VIBRATIONAL FREQUENCIES

Factors influencing vibrational frequencies include the application of Hooke's law, which provides calculations for wave numbers of absorption, though discrepancies exist due to surrounding molecular influences. Infrared absorption spectra reveal shifts in vibrational frequencies in different states, affected by coupled vibrations and Fermi resonance. Methylene (-CH-) groups show distinct symmetric and asymmetric stretching vibrations, which differ from isolated C-H bonds, causing frequency variations. Electronic effects, such as inductive and mesomeric effects, also lead to frequency shifts. For example, alkyl groups cause the lengthening of bonds, lowering absorption frequency, while electronegative atoms amplify it. Hydrogen bonding significantly impacts absorption, with stronger interactions shifting bands toward lower wave numbers and being concentration-dependent. Selection rules dictate which vibrations are effective in infrared spectroscopy based on changes in molecular dipole moments during vibrations. The position and intensity of absorption bands reflect bond types, confirming or ruling out structural components. The infrared spectrum has defined regions, with those from 2.5 to 8 µm linked to vibrational changes and the fingerprint region (below 1500 cm) being critical for molecular identity, despite similar compounds showing distinct absorption characteristics in this region.

VI. APPLICATIONS

1. Biomedical and protein analysis

FTIR spectroscopic imaging is crucial for analyzing biological samples, enabling characterization without dyes. It's applied in medical imaging, including colorectal adenocarcinoma and Alzheimer's disease studies, along with protein analysis.

2. Biological studies

FT-IR spectroscopy provides specific fingerprint-like signatures for identifying microbial species and strains, detecting CO_2, characterising cell-drug interactions, and ensuring food safety. It's also a non-destructive method for geochemical analysis of minerals. Additionally, FTIR is crucial in evaluating herbal medicines for quality, enhancing analytical capabilities with mathematical tools and reducing costs

3. Pharmaceutical analysis

FTIR is crucial for identifying chemical compounds and analyzing pharmaceuticals for composition, consistency, and impurity detection. It aids in materials science by assessing polymers and coatings. In environmental monitoring, FTIR detects pollutants, assesses air and water quality, and studies gas concentrations and biological processes across various states

4. Organic and inorganic compounds

FTIR spectroscopy is vital for identifying various samples, including resins, paints, polymers, and drugs. It analyses solids, liquids, and solutions, enabling the detection of organic and inorganic compounds, trace contaminants, and the characterization of polymers. In life science, FTIR assesses protein structure and stability, even in water. It identifies organic compounds through unique infrared spectrums, ensuring identical spectra under consistent conditions. Differences in spectra arise from variations in physical states or environmental factors. Spectral analysis of inorganic complexes is challenging due to high vibrational modes, which can complicate IR spectra interpretation, making them composite in nature

5. Food analysis

Analysis of 70 wheat flours revealed significant physicochemical differences among species, with ancient varieties showing higher protein and fat. FT-IR spectroscopy promises rapid disease diagnosis but faces adoption challenges due to clinician awareness and training.

6. FTIR combined with chemometrics

It effectively detects dairy adulteration. It identifies various adulterants in milk, with neural networks achieving over 76.6% classification accuracy. Models for sugar analysis in milk also demonstrate high predictive accuracy (95%) and robust determination coefficients

VII. ADVANTAGES

FTIR offers high speed, sensitivity, accuracy, and reproducibility, with self-calibration. It captures data from small samples and has high throughput. ATR-FTIR is non-destructive, fast, and also highly sensitive

VIII. DISADVANTAGES

- Infrared water absorbs strongly in the IR regio, making FTIR analysis of aqueous solution challenging.
- It is cost effective, surface sensitive.

IX. LIMITATIONS

- ATR-FTIR limitations include surface sensitivity, sample compatibility requirements, spectral artefacts, challenges detecting trace components, and reduced effectiveness for some inorganic compounds.

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