

Fourier Transform Infrared Spectroscopy in Modern Analytical Chemistry: A Comprehensive Review

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Abstract:

Fourier Transform Infrared (FTIR) spectroscopy is an advanced analytical technique used for both qualitative and quantitative analysis of chemical substances. It works on the principle that molecules absorb infrared radiation at specific wavelengths corresponding to their vibrational movements. These absorption patterns create unique spectra that act as molecular fingerprints, allowing accurate identification and structural characterisation of compounds. Modern FTIR instruments use a Michelson interferometer to collect spectral data as an interferogram, which is then converted into a standard infrared spectrum using the Fourier transformation. This method enables simultaneous measurement of multiple wavelengths, resulting in faster data acquisition, higher sensitivity, and improved spectral resolution compared to conventional dispersive infrared spectroscopy. Fourier Transform Infrared spectroscopy is widely used in many scientific fields due to its reliability, versatility, and minimal sample preparation. In pharmaceutical sciences, it plays an important role in drug identification, compatibility studies, impurity detection, and quality control of active pharmaceutical ingredients and formulations. It is also applied in polymer analysis, materials science, nanotechnology, and environmental monitoring. Additionally, Fourier Transform Infrared Spectroscopy helps in soil analysis, pollution monitoring, microplastic detection, and nanoparticle characterisation by providing detailed information about molecular structures and chemical interactions. Although limitations such as spectral overlap and water absorption interference exist, FTIR remains a powerful and essential technique in modern analytical chemistry.

Keywords: Fourier Transform Infrared Spectroscopy; Vibrational Spectroscopy; Michelson Interferometer; Functional Group Analysis; Molecular Characterisation.

I. Introduction:

Fourier transform infrared (FTIR) spectroscopy has undergone remarkable technological and methodological advancements over the past decade, significantly enhancing its diagnostic potential by enabling rapid, non-destructive, and highly objective analytical assessments with improved accuracy and reproducibility [1,2]. The absorption of infrared radiation causes an excitation of a molecule from a lower to a higher vibrational level. We know that each vibrational level is associated with a number of closely spaced rotational levels. Clearly, the infrared spectra are considered vibrational spectra. Not all the bonds in a molecule are capable of absorbing infrared energy, but only those bonds that are accompanied by a change in dipole moment will absorb in the infrared region. Such vibrational transitions, which are accompanied by a change in the dipole-moment of the molecule, are called infrared active transitions. On the other hand, those that are not accompanied by a change in dipole-moment of the molecule are not directly observed, and these are infrared inactive. For example, vibrational transitions of C = O, N – H, O – H, etc. bonds are accompanied by a change in dipole-moment and thus absorb strongly in the infra-red region. But transitions in Carbon–Carbon bonds in symmetrical alkenes and alkynes are not accompanied by the change in dipole-moment and hence do not absorb in the infra-red region. It is important to note that since the absorption in infra-red region is quantized, a molecule of the organic compound will show a number of peaks in the infra-red region[3]. FTIR spectroscopy analyzes the interaction of matter with infrared electromagnetic radiation, producing distinct spectral signatures that correspond to molecular vibrational transitions. These unique spectral fingerprints are intrinsic to each molecular structure, allowing accurate identification, characterization, and discrimination of substances at the molecular level [4]. Fourier

Transform Spectroscopy (FTS) is a method used to study how a sample absorbs light. Unlike traditional methods that use one wavelength at a time, FTS uses many wavelengths together in a single, broad beam of light. When this light passes through the sample, the instrument measures the total absorption from all wavelengths at once. Instead of directly measuring each wavelength, the absorption information is collected as a signal that changes with time, called an interferogram. This signal contains information from all wavelengths mixed together. A mathematical process called Fourier transformation is then used to separate this information and convert it into a normal absorption spectrum showing absorption versus wavelength. The broad light used in FTS is produced using a device called a Michelson interferometer. It has one fixed mirror and one moving mirror. As the moving mirror goes back and forth, the light waves interfere with each other, creating patterns of constructive and destructive interference. Each

wavelength changes in a unique way as the mirror moves, so every wavelength is encoded differently in the signal. Because all wavelengths are measured at the same time, Fourier transform spectroscopy is fast, sensitive, and accurate, and it gives high-quality spectra with good resolution [5]. FTIR spectroscopy enables the differentiation and comprehensive characterization of cells and tissues through detailed analysis of individual spectral bands and band groupings. This approach allows precise elucidation of molecular conformations, bonding environments, functional groups, and intermolecular interactions that collectively define the biochemical composition and structural organization of the specimen [2,6].

Instrumentation:

Source of FTIR Radiation: Infrared energy is emitted from a glowing black-body source. This radiation is broadband, covering a wide range of IR wavelengths [7].

Table 01: Sources of radiation for FTIR

Source Type	Material /Type	Temperature	Spectral Range	Typical use
Globar	Silicon Carbide rod	1000-1800	Mid IR	General FTIR
Nernst glower	Oxide mixture	1900	Mid IR to near IR	Research Instruments
Mercury Arc lamp	Mercury discharge	-	Far IR	Far IR studies
Tungsten Halogen	Tungsten filament	~3000	Near IR to visible	Near IR FTIR
Synchrotron source	Particle accelerator Beam	-	Wide (Far IR to UV)	Advanced microscopy

Basic components of Interferometer: The beam enters the interferometer where the “spectral encoding” takes place. The resulting interferogram signal then exits the interferometer[7]. The interferometer, which consists of a beamsplitter, a stationary mirror, and a moving mirror, is the heart of an FTIR spectrometer. The beamsplitter is a semi-transparent mirror that divides a collimated light beam into two optical channels. Half of the light is transferred to the moving mirror and half is reflected to the stationary mirror. The moving and stationary mirrors reflect the two light beams, which are recombined at the beamsplitter before going through the sample chamber and onto the detector[8]. Almost all FTIR instruments use a Michelson Interferometer design.

a) Beam splitter: Divides the incoming IR beam into two parts:

- One beam goes to the **fixed mirror**.
- The other goes to the **moving mirror**.
- Coated partially with a reflective film (e.g., germanium or aluminum).

b) Fixed Mirror: Reflects one portion of the split beam back to the beamsplitter.

c) Moving Mirror: Moves back and forth at a controlled speed, changing the optical path difference (OPD) between the two beams.

Recombination of the two reflected beams recombine at the beamsplitter. Depending on their relative phase (due to OPD), they interfere constructively or destructively. The detector measures the interferogram, a signal showing intensity vs. mirror position.

Sample holder: The infrared beam enters the sample compartment, where it interacts with the sample. Depending on the type of analysis being performed, the beam is either transmitted through the sample or reflected from its surface (e.g., ATR analysis). During this interaction, specific infrared

frequencies that are uniquely characteristic of the sample are absorbed, resulting in a wavelength-dependent reduction in beam intensity. This absorption provides molecular information related to the sample's chemical structure.

Table 02: Types of Sample holders [9]

Accessory	Sample type	Common applications	Advantages	Disadvantages
Transmission	. Liquids .solids .gases	Universal	.strong spectrum .Economical .Well, established	.sample preparation not always reproducible .cannot measure highly absorbent samples
ATR(Attenuated Total Reflectance)	. Liquids .solids	Universal	.Minimal to no sample preparation .Reproducible .Easy to use	.Requires contact .careful cleaning
Specular Reflectance	.smooth surfaces	Polymers,water analysis	.Minimal to no sample preparation .No contact	.sample type limited
Transflectance	.Films on reflective substances	Polymer films	.Minimal to no sample preparation .No contact	.sample type limited
DRIFITS (Diffuse Reflectance Infrared Fourier Transform Spectroscopy)	Rough surfaces	Geology, pharmaceuticals	.Minimal to no sample preparation .No contact	.sample type limited
FT-PL (Fourier Transform Photoluminescence)	. Liquids .solids	Materials	.Faster data collection compared to dispersive instrument	.Limited to MIR measurements

Detector: After passing through the interferometer, the beam reaches the detector for final measurement. FTIR instruments use specially designed detectors to measure the interferogram signal. These detectors capture the transmitted or reflected radiation from the sample and convert it into an electrical signal that can be processed by the computer. The detector's sensitivity and usable wavelength range depend on its type and construction material.

When radiation reaches the detector, it is converted into an electrical response proportional to the intensity of the incident light, enabling accurate spectral analysis. Commonly used FTIR detectors include:

- **DLATGS (Deuterated L-alanine-doped triglycine sulfate)** detectors, which operate

at room temperature and are widely used for routine analysis.

- **Liquid-nitrogen-cooled detectors**, which provide enhanced sensitivity for low-signal or high-precision applications.
- **Silicon photodiodes**, commonly used in near-infrared and visible spectral regions
- **Silicon far-infrared bolometers**, which are suitable for far-infrared measurements.

Computer/ Read out device: The measured signal is digitized and sent to the computer where the Fourier transformation takes place. The final infrared spectrum is then presented to the user for interpretation and any further manipulation.

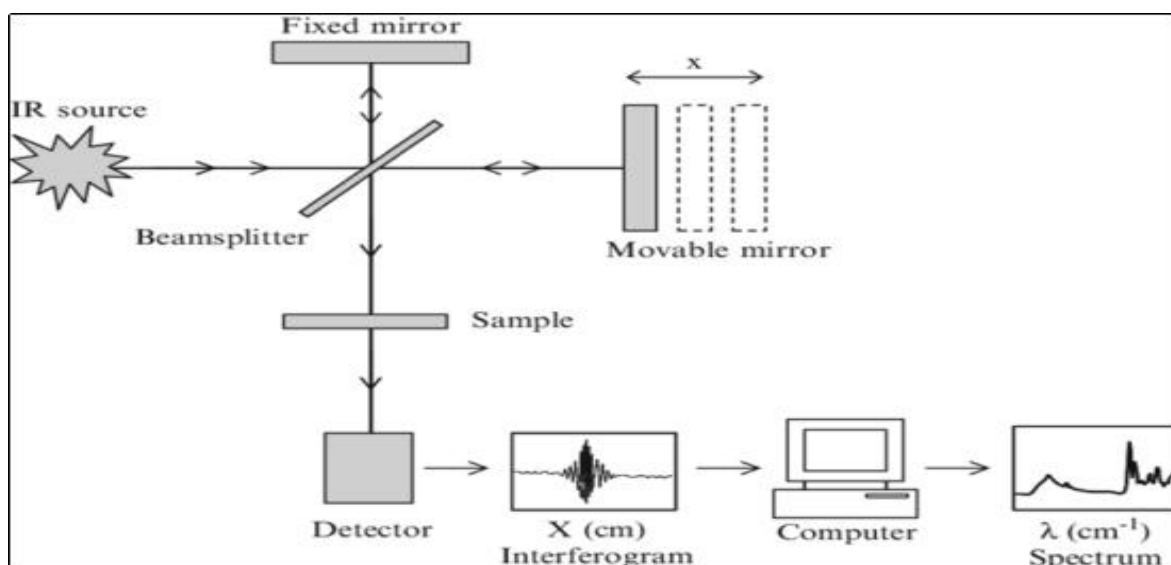


Figure 1: Schematic sketch of the essential features of a FTIR instrument

Applications:

- i. Identification of Unknown Compounds:** Determine the molecular structure or identity of an unknown sample and each functional group (–OH, –COOH, –C=O, –NH₂, etc.) absorbs IR radiation at specific wavenumbers.

Example: Identifying organic compounds such as alcohols, aldehydes, ketones, or esters based on their unique absorption peaks. Used in the organic synthesis, pharmaceuticals, polymers, and petrochemicals.

- ii. Determination of Functional Groups:** Detect and confirm the presence of specific chemical bonds in molecules and the spectrum shows absorption bands corresponding to stretching or bending vibrations. Used in Structural characterization of molecules and reaction intermediates.

Example:

- Broad band around 3200–3600 cm⁻¹ → O–H stretch (alcohols, carboxylic acids)
- Sharp peak near 1700 cm⁻¹ → C=O stretch (carbonyl groups)

- iii. Purity and Quality Control :** Assess sample purity and detect impurities or contaminants and even small impurities can introduce new peaks or alter band intensities in the spectrum.

Example: Detecting residual solvents, unreacted monomers, or degradation products in chemical manufacturing.

- iv. Quantitative Analysis:** Determine concentration of components in mixtures and Follows Beer–Lambert law — absorbance is proportional to concentration.

Example: Measuring water content, carbonyl index, or additive concentration in polymers or lubricants.

- v. Reaction Monitoring and Kinetics :** Track chemical changes in real-time and Successive FTIR scans during a reaction reveal changes in characteristic peaks also used in Studying reaction mechanisms and optimizing synthesis conditions.

Example:

- Disappearance of reactant peaks (e.g., C=O of anhydride)
- Appearance of product peaks (e.g., C–O–C of ester)

- vi. Characterization of Mixtures and Blends :** Identify individual components within a chemical mixture and deconvolution of overlapping peaks or use of FTIR with chemometric analysis (PCA, PLS).

Example: Analyzing complex petrochemical or polymer mixtures.

- vii. Study of Chemical Bonding and Molecular Interactions:** Understand hydrogen bonding, coordination, or charge transfer interactions and shifts in peak

position or intensity indicate bond strength or environment changes.

Example: Studying metal-ligand interactions in coordination compounds.

viii. **Polymers:**

a) **Polymer characterization:** Polymer products are not singular species, but rather, they are population of polymer molecules varying in composition and configuration. James L. Dwyer et al., carried out polymer characterization by combined chromatography-infrared spectroscopy that provides benefits of resolving polymer population into discrete entities that can be identified. No other technique has the potential to provide as much information about polymer characterization as FTIR can provide. Characterization of distributed composition and structural properties is essential to optimize physical properties of polymer. The combination of LC-FTIR instrumentation coupled with the interpretative capabilities of infrared software greatly assist in interpretation of IR spectra and renders hyphenated LC-FTIR a practical working technique for polymer scientists and synthesis chemists. [10].

b) **Degree of conversion in dental composites:** Moreas L.P.G et al. used FTIR as a tool for determining the degree of conversion (DC) in dental composites composed of at least two dimethacrylate monomers. The DC is determined by the proportion of the remaining concentration of the aliphatic C=C double bonds in a cured sample relative to the total number of C=C bonds in the uncured material. To determine DC two spectral infrared regions can be used; NIR or MIR. In the MIR region, DC is determined by measuring the intensity (or area) decrease of the methacrylate (C=C) stretch absorption band at 1,638 cm^{-1} as the methacrylate monomer is converted to polymer. In the NIR region, there are two aliphatic bands that can be used, one at 6,165 cm^{-1} (overtone=CH₂) and the other at 4,743 cm^{-1} . Hence, the study of conversion degree in dental composites by FTIR technique provides a better understanding of these materials, which is expected to optimize the polymerization process. This will result in improved dental restorations with aggregated higher quality and durability.

ix. **Nanoparticles:** FTIR spectroscopy is exceptionally versatile, with applications spanning multiple domains, including materials science, biology and environmental studies. Its ability to analyze complex mixtures without extensive sample preparation makes it particularly valuable for studying nanoparticles and their interactions with

biological systems. Key applications include identification of functional groups and molecular structures in nanoparticles, aiding in the understanding of their chemical properties and potential applications in fields like drug delivery (including characterization of drug-polymer interactions [11,12], monitoring of drug loading and release, interaction of nanoparticles with biological tissues and cells [11,13,14] and quality control and process validation [15], environmental remediation and degradation of pollutants [16,17,18,19,20] and interactions between nanoparticles and biological entities, such as bacteria [20,21]. FTIR spectroscopy has emerged as a pivotal technique in the field of nanoparticle science, providing detailed insights into the molecular composition and interactions of materials at the nanoscale. The employment of FTIR in the analysis of green synthesized NPs is driven by numerous crucial factors associated with their synthesis, stabilization and application. FTIR analysis has the capability to discern specific absorption peaks corresponding to various functional groups, thereby signifying their involvement in the reduction of metal ions, or the formation of metal oxide NPs and their subsequent stabilization. The presence of characteristic peaks in the FTIR spectrum serves to substantiate the efficacious synthesis of nanoparticles by indicating the existence of biomolecules that contribute to nanoparticle formation. Furthermore, the interactions between the synthesized nanoparticles and the capping agents can be studied through FTIR, which provides insights into how these interactions influence particle stability. This understanding is essential for ensuring that the NPs maintain their desired properties over time, making them suitable for various applications such as drug delivery and bioremediation.

x. **Pharmaceutical and Molecular Docking Analysis:** The hybrid correlation method was applied to analyze the spectra of 2-Hydroxy-5-nitrobenzaldehyde (2H5NB) across FT-IR, FT-Raman, UV-vis, and nuclear magnetic resonance (NMR) analysis techniques. Using density functional theory (DFT) with B3LYP and the 6-311++G(d,p) basis set, the study focused on determining the optimum molecular shape, vibrational wavenumbers, IR intensities, and Raman spectra. MOLEcular VIBrations (MOLVIB) software provided detailed interpretations of the vibrational spectra, revealing that intermolecular charge transfer results from bonding orbitals functioning as donors and acceptors in all phases of natural bond orbital

(NBO) analysis, thereby stabilizing the molecules [22].

xi. Environmental science :

a) Soil Analysis:

i. Characterization of Soil Organic Matter (SOM):

- FTIR spectroscopy enables the identification of functional groups present in soil organic matter, such as –OH, –COOH, –C=O, and –CH₃.
- It distinguishes among major organic components including humic substances, lignin, carbohydrates, and proteins.
- This information is valuable for evaluating soil fertility, carbon sequestration potential, and overall organic matter content [23].

ii. Determination of Soil Contaminants:

- FTIR is used to detect organic pollutants in soils, including hydrocarbons, pesticides, and phenolic compounds.
- Interactions between heavy metals and soil organic matter can be inferred from shifts or changes in characteristic absorption bands [24].

iii. Mineralogical Composition:

- FTIR spectroscopy identifies inorganic mineral components such as silicates, carbonates, phosphates, and metal oxides.
- It can also differentiate clay minerals including kaolinite, montmorillonite, and illite based on their diagnostic vibrational bands [25].

b) Pollution Monitoring

I. Air Pollution:

- FTIR gas analyzers are employed to monitor atmospheric pollutants such as CO₂, CO, SO₂, NO_x, CH₄, and volatile organic compounds (VOCs).
- The technique is widely used for real-time emission monitoring in industrial and environmental settings [26].

ii. Water Pollution:

- FTIR spectroscopy detects organic contaminants in water samples, including oil residues, surfactants, and microplastics.

- Microplastics are identified by comparing their spectra with polymer reference libraries, such as polyethylene and polystyrene [27].

iii. Microplastic Pollution:

- FTIR is extensively used for the identification and quantification of microplastics in soils, sediments, and aquatic environments.
- Techniques such as ATR-FTIR and FTIR microscopy enable polymer identification at the microscale with high specificity [28].

Data interpretation:

FTIR spectroscopy is an analytical technique used to identify functional groups and molecular structures based on the absorption of infrared radiation at characteristic wavenumbers (cm⁻¹). Each chemical bond vibrates at a specific frequency, producing a unique infrared spectrum that serves as a molecular fingerprint.

Principle Behind FTIR Interpretation

When a molecule is exposed to infrared radiation:

- Specific chemical bonds absorb energy at characteristic frequencies.
- This absorption induces molecular vibrations in the form of stretching or bending modes.
- The detector records absorption peaks at specific wavenumbers corresponding to these vibrations.

The resulting spectrum is interpreted by comparing the observed peaks with standard reference spectra to elucidate the chemical structure of the sample [29].

Major Regions of an FTIR Spectrum

(a) Functional Group Region (4000–1500 cm⁻¹):

- The most informative region for functional group identification.
- Characterized by sharp and well-defined absorption bands.

(b) Fingerprint Region (1500–500 cm⁻¹):

- Exhibits complex absorption patterns resulting from coupled vibrational modes.
- Used to confirm compound identity due to its uniqueness for each molecule [30].

Table 03: Interpretation of Common FTIR Peaks [31].

Wavenumber (cm ⁻¹)	Functional Group	Type of Vibration
3200–3600	O–H (alcohol, phenol)	Stretching
3300–3500	N–H (amine, amide)	Stretching
2850–3000	C–H (alkanes)	Stretching
3000–3100	=C–H (alkenes/aromatics)	Stretching
1700–1750	C=O (carbonyl)	Stretching

1650–1690	C=C (alkenes)	Stretching
1600–1450	Aromatic C=C	Stretching
1300–1000	C–O	Stretching
900–650	C–H (aromatic)	Bending

Steps in FTIR Data Interpretation

Step 1: Identify Broad Peaks

- Broad peak around 3400 cm^{-1} → O–H group
- Sharp peak near 3300 cm^{-1} → N–H group

Step 2: Locate Carbonyl Region

- Strong peak near 1700 cm^{-1} → presence of C=O group

Step 3: Analyse Fingerprint Region

- Match peaks with reference standards
- Confirms compound identity

Step 4: Compare with Reference Spectrum

- Overlay sample spectrum with standard
- Check peak position, intensity, and shape[32]

Important Tips for Interpreting an Infra-red Spectrum

The following are some useful tips for interpreting an infrared spectrum.

(1) Always place more reliance upon the negative evidence. The absence of a band in a particular region is a sure indication of the absence of group/groups absorbing in that region. For example, if there is no absorption in the region $1900\text{--}1600\text{ cm}^{-1}$, the carbonyl group

($> \text{C} = \text{O}$) must be absent from the compound.

(ii) Always start from the higher frequency end of the spectrum. Mostly stretching vibrations occur in the region above 1500 cm^{-1} and are most informative. cm^{-1}

(iii) To distinguish between intermolecular and intramolecular hydrogen bonding, the spectra of the sample are scanned at two different concentrations. Various solvents may be used to study association effects.

(iv) For easy detection of the various groups present in the compound, the infra-red region ($4000\text{ to }667\text{ cm}^{-1}$) may be visualised as consisting of the following portions:

Table 04: Characteristic absorption frequencies of functional groups

Type of vibration	Class of compound	Frequency	Intensity
C-H Str	(1) Alkanes	2960-2850	(s)
C-H Str	(2) Alkenes	3100-3010	(s)
C-H Str	(3) Alkynes	~3300	(s)
C-H Str	(4) Aromatics	3150-3020	(s)
C-H Str	(5) Aldehydes	~2820	(W)
		2775-2720	(W)
C=C Str	(1) Alkenes	1675-1600	(m, w)
C=C Str	(2) Aromatics	1600-1450	(m, w)
C-C-C Str	(3) Alkynes	2260-2100	(s)
C=O Str	(4) Aldehydes	1740-1720	(s)
C=O Str	(5) Ketones	1725-1705	(s)
C=O Str	(6) Carboxylic acid	1725-1705	(s)
C=O Str	(7) Esters	1725-1700	(s)
C=O Str	(8) Amide	1750-1730	(s)
C=O Str	(9) Anhydrides	1680-1630	(s)
C=O Str	(10) Acid chlorides	1850-1800	(s)
		1790-1740	(s)
		~1790	(s)
O-H Str	(1) Alcohols and Phenols (dilute solution)	3650-3580	(sharp, v)
	(2) Alcohols, Phenols (Hydrogen bond)		
	(3) Carboxylic acid		
O-H Str		3550-3200	(b, s)

O-H Str		2700-2500	(b)
N-H Str	(1) Primary amines, amides (Free) (Two bands)	~3500	(m)
N-H Str	(2) Primary amines, amides (H-bonded)	~3400	(m)
N-H Str	(3) Secondary amines, amides(one bonded)	3500-3300	(m)
N-H Str	(4) Secondary amines, amides(Hydrogen bonded) Nitriles Nitro Compounds	3310-3140	(m)
N-H Str	(5) Asymmetric (6) Symmetric	2260-2220	(m)
C=N Str		1620-1535	(s)
N=O		1375-1275	(v)

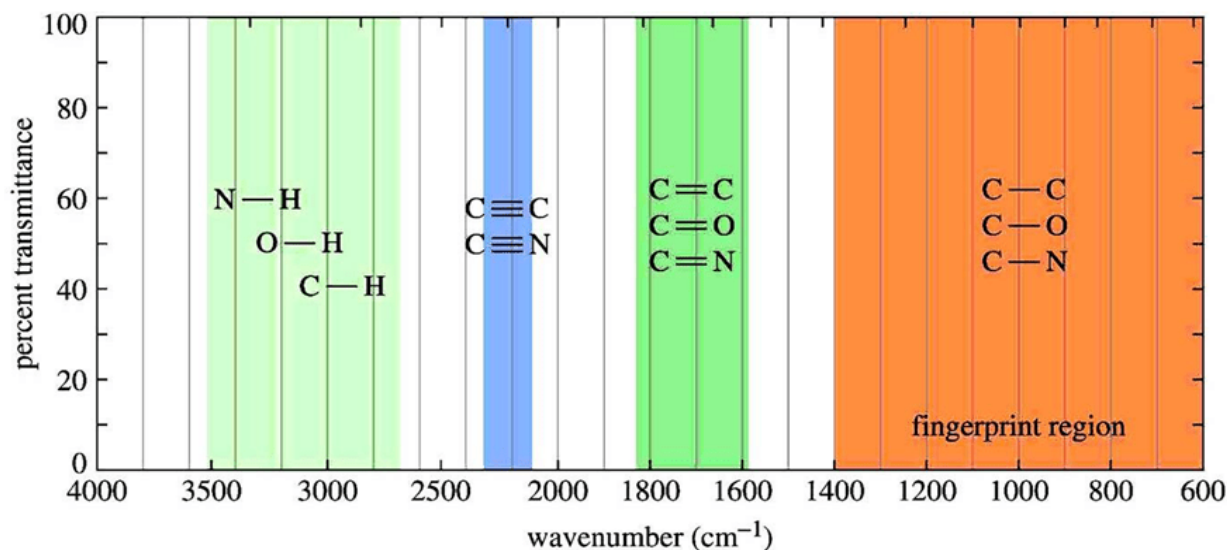


Figure 2: The characteristic absorption ranges for various functional groups in infrared (IR) spectroscopy,

(a) 3600-1200 cm^{-1} . The appearance of the bands in this region shows the presence of the OH-NH, NH group in the compound. The position, intensity and the breadth of the bands tell whether the group is free, intramolecularly bonded or exhibits intermolecular hydrogen bonding. C-H stretching also shows a medium band near 3300 cm^{-1} .

(b) 3200-3000 cm^{-1} . Absorptions due to C-H stretching and Aromatic C-H stretching occur in this region. The sharp bands of weak to medium intensities are observed.

(c) 3000-2500 cm^{-1} . The absorptions due to C-H stretching from methyl or methylene groups occur in this region. The asymmetric C-H stretching occurs at a slightly higher wave number than that of the

symmetric C-H stretching. A very broad band between groups. Two weak bands, at 2720 cm^{-1} and the other near 2820 cm^{-1} are most characteristic of C-H stretching. The higher frequency band is seldom observed.

(d) 2300-2100 cm^{-1} . This is the region in which alkynes, cyanides, cyanates, and isocyanates absorb. The bands observed are weak and variable. C=C stretching occurs between 2140-2100 cm^{-1} . CN stretching shows a variable band between 2260-2200 cm^{-1} . Isocyanates show a strong band between 2280-2250 cm^{-1} .

(e) 1900-1650 cm^{-1} . Strong bands due to C=O stretching occur in this region.

Anhydrides show two strong bands in the region 1850-1740 cm. Esters, aldehydes, ketones, lactones, carboxylic acids, and amides show strong bands due to C = O stretching in this region. Imides are also recognised by two strong bands (doublet) in the region around 1700 cm⁻¹. The following points regarding C = O stretching may be helpful.

B-unsaturation lowers the frequency of absorption by 15-40 cm. But in amides, a small absorption shift towards lower frequency is observed.

(I) An increase in the ring strain in the case of cyclic ketones raises C = O absorption.

(ii) Hydrogen bonding to the carbonyl compound lowers C = O absorption by 40 – 60 cm⁻¹ and 1600-1000 cm. This region is very important for identifying nitro compounds and also confirming the presence of ethers, esters, primary, secondary and tertiary alcohols. The appearance of strong bands due to C-O stretching at 1300-1050 indicates (1) an ester, provided C = O stretching is observed in the region 1750-1735 cm and (ii) an alcohol if O-H stretching free and/or bonded occurs between 3600-3200 cm⁻¹. Ethers show a strong band in the region 1150-1070cm⁻¹ due to C-O stretching in-O-C-. This region also helps identify aromatic compounds. For aromatic rings, medium bands around 1600 cm⁻¹, 1580 cm⁻¹, and 1500 cm are observed.

(g) Below 1000 cm⁻¹. This region is very useful in identifying the type of substitution on the aromatic ring:

- i. A strong band at 770-730 cm⁻¹ (s) shows mono substitution.
- ii. Ortho and para disubstituted compounds show one band each. The latter absorbs at a higher wavenumber.
- iii. Meta-disubstituted compounds are usually recognised by two medium bands in the region 850-710 cm⁻¹[3].

Advantages:

Non-destructive and Sample-Preserving Analysis
Fourier Transform Infrared (FTIR) spectroscopy is inherently non-destructive, enabling molecular characterization without altering the chemical integrity of the sample. This attribute is particularly critical in pharmaceutical quality assurance, forensic investigations, and stability studies, where preservation of the original sample is mandatory for confirmatory or longitudinal analyses [33].

High Throughput and Rapid Spectral Acquisition

FTIR operates on the multiplex (Follett) and throughput (Jacquinot) advantages, allowing simultaneous acquisition of all spectral frequencies. This significantly enhances signal-to-noise ratio and

reduces analysis time when compared with dispersive infrared spectroscopic techniques, thereby enabling rapid screening and high-throughput analytical workflows [34].

Minimal and Versatile Sample Preparation

FTIR accommodates a wide range of physical states—solids, liquids, semi-solids, and gases—often requiring minimal or no sample preparation. The availability of accessories such as ATR, DRIFT, and transmission cells further enhances analytical versatility while minimizing sample handling errors and improving reproducibility in routine pharmaceutical analysis [35].

Broad and Critical Pharmaceutical Applications

FTIR spectroscopy is extensively employed for qualitative and semi-quantitative pharmaceutical analysis, including active pharmaceutical ingredient (API) identification, excipient compatibility assessment, polymorphic and solid-state characterization, impurity profiling, and stability monitoring. It also plays a pivotal role in process analytical technology (PAT) and quality-by-design (QIBs) frameworks for real-time process monitoring [36,37].

Limitations:

Insufficient Sensitivity for Ultra-Trace Analysis

Despite its analytical robustness, FTIR lacks the sensitivity required for trace-level and ultra-trace detection when compared with hyphenated techniques such as GC-MS or LC-MS. This limitation restricts its applicability in impurity quantification at parts-per-billion (ppb) or lower concentration levels [38].

Spectral Interference from Water Absorption

Water exhibits intense and broad absorption bands in the infrared region, particularly around 3400 cm⁻¹ and 1640 cm⁻¹. These absorptions can obscure diagnostically important functional group vibrations, complicating spectral interpretation in aqueous and hygroscopic pharmaceutical samples [34].

Band Overlap in Multicomponent Systems

Complex formulations and multi-component mixtures often produce overlapping vibrational bands, reducing spectral resolution and interpretability. Advanced chemometric techniques such as principal component analysis (PCA) or partial least squares (PLS) regression are frequently required to resolve such overlaps and extract meaningful analytical information [35].

Constraints in Quantitative Accuracy

While FTIR can be applied to quantitative analysis based on Beer-Lambert law principles, achieving high accuracy and precision necessitates rigorous

calibration models, validated reference standards, and strict control of experimental variables such as path length, particle size, and sample homogeneity [37].

Limited Structural Insight for Inorganic Materials

FTIR spectroscopy is predominantly effective for organic and organometallic compounds due to their characteristic vibrational modes. Purely inorganic substances, particularly those lacking IR-active functional groups, yield limited structural information, thereby reducing FTIR's utility in comprehensive inorganic analysis [33].

II. Conclusion:

Fourier Transform Infrared (FTIR) spectroscopy is one of the most important and widely used analytical techniques for the characterization of chemical substances and molecular structures. It is based on the absorption of infrared radiation by molecules, which produces unique spectral patterns corresponding to specific functional groups and vibrational modes. These spectra act as molecular fingerprints, enabling accurate identification and structural analysis of a wide range of organic and inorganic compounds. FTIR spectroscopy is highly valued for its rapid analysis, high reproducibility, and non-destructive nature, making it an essential tool in modern analytical laboratories. A key advantage of this technique is its ability to analyse samples in different physical states, including solids, liquids, and gases, with minimal or no sample preparation. The use of advanced components such as the Michelson interferometer and modern detectors improves spectral resolution, sensitivity, and data acquisition speed. FTIR has extensive applications in fields such as pharmaceutical quality control, polymer science, environmental monitoring, nanotechnology, and materials research. It is commonly used for functional group identification, reaction monitoring, impurity detection, and studying molecular interactions. Although limitations such as spectral overlap, water absorption interference, and lower sensitivity for trace analysis exist, advancements in chemometric analysis and modern sampling techniques like ATR and DRIFT have significantly enhanced its analytical performance.

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