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REVIEW ARTICLE ON FTIR SPECTROSCOPY

Dr.Namratha Sunkara[1] G.Anvitha[2] G. Yamini[3] G.Deepika[4] G.Indupriya[5] G.Srikanth[6]
Bharat Institute of Technology, Mangalpally, Hyderabad, 501510.

ABSTRACT:
Qualitative Fourier transform infrared (FTIR) spectroscopy has long been established and implemented in a wide variety of fields including pharmaceutical, bio-medical, and clinical fields. While the quantitative applications are yet to reach their full potential, this technique
is flourishing. It is tempting to shed light on modern engaging and the applicability of analytical quantitative FTIR spectroscopy in the aforementioned fields. More importantly, the credibility, validity, and generality of the application will be thoroughly demonstrated by reviewing the latest published work in the scientific literature. Utilizing FTIR spectroscopy in a quantitative approach in pharmaceutical, biomedical, and interdisciplinary fields has many
undeniable advantages over traditional procedures. An insightful account will be undertaken in this regard. The technique will be introduced as an appealing alternative to common methods such as high performance liquid chromatography. It is anticipated that the review will offer researchers an update of the current status and prospection the subject among the pharmacy and biomedical sciences both in academic and industrial fields.

INTRODUCTION:

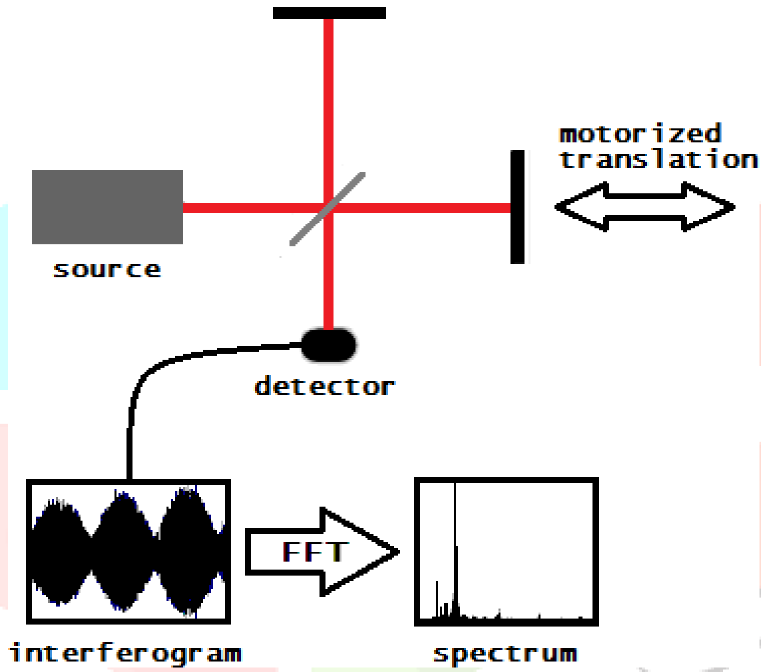
The measurement of infrared light absorption (or transmission) by a material as a function of wavelength is known as infrared (IR) spectroscopy (or frequency). The IR spectrum is produced as a plot of absorption (or transmission) versus wavelength (or frequency). The fundamental heat spectrum of materials, which is principally caused by molecular vibrations and their corresponding rotating absorption bands, is examined using infrared spectroscopy. [1]The IR spectroscopy was the first structural spectroscopic technique and is an analytical method which is used to characterize the bonding structure of atoms based on the interaction of the IR radiation at which the substance absorbs and lead to the production of vibration in molecules. It gives the techniques for identification and characterization of chemical structures to obtain information from biological to composite materials, from liquids to gases. [3]The basic principle of IR is measurement of amount of IR radiation by absorption, emission or reflection. It is also called asvibrational spectroscopy. It is widely used for structural elucidation of molecules. The spectral regions can be divided into further 3 regions; the FAR Infrared (400-10 cm-1), MID Infrared (4000-400 cm-1), NIR
(13000-4000 cm-1). It is based on the absorption pattern of other compounds including isomers. When reference spectra available, most compound can be obvious identified on the basis of spectra of IR. [2]
Most widely used IR is MIR, but remaining both can also provide important information. FTIR is real time measurement analytical method and
non-destructive technique, which is unable to identify the unknown compounds (quantitative determination) and their corresponding concentration (qualitative determination) from liquid, gas or solid samples. During vibrations, there is change in the dipole moment. In this case we can called as IR active substances and a radiation corresponds to a change in dipole moment. For
IR inactive substances, the dipole moment is zero, there is no matter how long the bond is in the molecule (IR -active; polar bonds, asymmetric molecules. IRinactive; non-polar bond, symmetrical molecule).In IR each chemical bond hasa very specific vibrational frequency which is corresponding to an energy level.

E=hν=hc/λWhere,
h=planks constant ν =frequency,
c=speed of light, λ= wavelength. [3]

Principles of FTIR Spectroscopy:

In FTIR analyses, Infrared light from the light source passes through a Michelson interferometer along the optical path. The Michelson interferometer comprises a beam splitter, moving mirror, and fixed mirror. The light beam split into two by the beam splitter is reflected from the moving mirror and fixed mirror, before being recombined by the beam splitter.

As the moving mirror makes reciprocating movements, the optical path difference to the fixed mirror changes, such that the phase difference changes with time. The light beams are recombined in the Michelson interferometer to produce interference light. The intensity of the interference light is recorded in an interferogram, with the optical path difference recorded along the horizontal axis. $f = 2vm\ c\ \upsilon$ interferogram frequency $vm = \delta\ 2t$ mirror velocity



Instrumentation:

The normal instrumental process is as follows:

1. The Source: Infrared energy is emitted from a glowing black-body source. This beam passes through an aperture which controls the amount of energy presented to the sample (and, ultimately, to the detector).
2. The Interferometer: The beam enters the interferometer where the “spectral encoding” takes place. The resulting interferogram signal then exitsthe interferometer.
3. The Sample: The beam enters the sample compartment where it is transmitted through or reflected off of the surface of the sample, depending onthe type of analysis being accomplished. This is where specific frequencies of energy, which are uniquely characteristic of the sample, are absorbed.
4. The Detector: The beam finally passes to the detector for final measurement. The detectors used are specially designed to measure thespecial interferogram signal.

5. The Computer: The measured signal is digitized and sent to the computerwhere the Fourier transformation takes place. The final infrared spectrum is then presented to the user for interpretation and any further manipulation.

Because there needs to be a relative scale for the absorption intensity, a background spectrum must also be measured. This is normally a measurement with no sample in the beam. This can be compared to the measurement with the sample in the beam to determine the "percent transmittance." This technique results in a spectrum which has all of the instrumental characteristics removed. Thus, all spectral features which are present are strictly due to the sample. A single background measurement canbe used for many sample measurements because this spectrum is characteristic of the instrument itself.

General Applications of FTIR Spectroscopy:

The areas where FTIR is applicable are listed below:

1. Agricultural / Food
2. Polymer
3. Petroleum and fuel industry
4. Environmental
5. Textiles
6. Biomedical / Clinical

7. Pharmaceutical and cosmetics

Agriculture / Food:

a) Prediction of soil macronutrients:

Phosphorous (P), Potassium (P), Organic Matter (OM)

and pH content in a loamy mixed soil. The spectral features of soil materials inthe NIR spectral region are associated with vibration modes of functional groups that are overtones or the combination of vibration bands of light atoms that have strong molecular bonds. Hence it is possible to measure soil contents such as moisture, organic C and N using NIR technique. To correlate wavelength information with each constituent concentration, principal component analysis / partial least square (PCA / PLS) was used as multivariate analysis technique. Observing the regression coefficient results obtained we can say that, NIR spectroscopy is emerging technique that could be considered to have good potential for assessing soil N, OM and pH. NIRS could be useful in site as a rapid technique that could be combined with geographic information system (GIS) and precision forming principles application.[16] Also Madari B. E et al., analyzed soil samples for total C, N, sand, silt and clay composition. [17]

b) Characterizing edible oils & fats:

N. Vlachos et al., have extended the use of FTIR to the field of food research especially to study edible oils and fats. They have used FTIR for mainly 2 purpose:

i) to determine adulteration of extra virgin olive oil and

ii) to monitor oxidation process of corn oil samples.

Here as mid-IR spectra are able to differentiate the intensity and exact frequency at which the maximum absorption of the bands appear according to nature and composition of sample, they are used to characterize edible oils and fats. A band shift observed due to C-H stretching vibration of the cis-double bond allows the determination of extra virgin oil adulteration and FTIR combined with discriminant analysis (DA) and PLSused to quantify this adulteration. The oxidation of oil occurs when it is exposed to air, heating, light or catalyzers and this will facilitate the degradation process. Hence FTIR is used to measure the carbonyl compounds produced due to oxidation. [18]

Polymer:

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 coupledwith the interpretative capabilities of infrared software greatly assists in interpretation of IR spectra and renders hyphenated LC-FTIR a practical working technique for polymer scientists and synthesis chemists. [19]

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 conversiondegree 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.

Petroleum & fuel industry:

Michael D. Judge, investigated the viability of NIR spectroscopy technique for the quality control analysis of ingredient concentrations in rocket propellent fuel liquid pre-mix. The propellent pre-mix comprised of polybutadiene pre-polymer, a plasticizer and 2 antioxidants. Formerly, the pre-mix was tested for viscosity as a quality control test. So ameliorated method for monitoring correct ingredient ratios in the slurry was needed.

Watching at the results of this study, it was ascertained that NIR spectroscopy offered a fast and convenient method of validating the % level of all 4 constituents while requiring no sample preparation. The NIR technique demoed a high level of accuracy and precision with an added advantage ofallowing monitoring of antioxidants depletion in the pre-mix on ageing.

Environmental:

Andreas Beil et al. used passive FTIR spectrometry for remote sensing of atmospheric pollution. It permits detection and identification of pollutant cloudsin the atmosphere. In this study, the measurement technique and a data analysis method does not require a previously measured background spectrum are described. Here the ambient infrared radiation is detected.

Passive remote sensing is the only detection method, which allows mobile,fast, man-held and stand-off detection of hazardous chemical agents.

Textile:

Angela Allen et al. conducted analysis of cotton trash using FTIR. Botanical cotton trash including leaf, stem, hull, bark etc. poses a problem in processingefficiency and quality of cotton throughout ginning and textile processing. Here FTIR spectroscopy is utilized to develop a database for classifying different trash found in cotton. The evaluation of cotton trash in mid-IR region of 4000 to 650 cm-1 has provided the means for development ofa spectral database that distinguishes the type of cotton trash based on chemical composition. During ginning and textile processing, cotton trash undergoes different physical modifications that affect the FTIR spectroscopic properties. The application of reduction in particle size of trash and heat treatment led to changes in FTIR spectra revealing the complex arrangementswithin each trash and the irreversible loss of volatile components associated with water respectively.

Biomedical / Clinical:

FTIR spectroscopic imaging in ATR mode is a powerful tool for studyingbiomedical samples.

Kazarian S. G. et al., described recent advances in the application of ATR-FTIR imaging to dissolution of pharmaceutical formulation and drugrelease. Here two different ATR accessories to obtain chemical images of formulations in contact with water as a function of time are presented. The innovative use of diamond ATR accessory permitted in situimaging of tablet compaction and dissolution. This was applied to obtain images of skin surface and spatial distribution of protein and lipid richdomains. The preliminary result of this study demoed the possibility of studying the skin surface in contact with topical formulations to probe the mechanism of transdermal delivery. This is for the first time that it has been possible to acquire FTIR images of arterial tissue in contact with solutions containing drug molecule. This approach may help in understanding the mechanism of treatment of atherosclerosis

Pharmaceutical & cosmetics:

a) Blend homogeneity:

Lyon R. C et al., conducted a study to evaluate NIR spectroscopic imaging asa tool to access a pharmaceutical quality assurance problem – blend uniformity in the final dosage product. NIR spectroscopic imaging is a unification of digital imaging and molecular spectroscopy which helps providing a visual distribution of components within formulation. Contrastingly, traditional spectroscopy cannot directly determine the spatial distribution of components in final product. This study was carried out on the blend uniformity of furosemide and microcrystalline cellulose tablets prepared by deliberately varying the homogeneity of the components by NIR imaging and by traditional NIR spectroscopy. As a result, each grades of tablets were clearly distinguished quantitatively by NIR spectral imaging and traditional NIR spectroscopy demonstrating the power of this new imaging toolfor assessing pharmaceutical quality assurance.

b) Analysis of lard in cream cosmetics:

Abdul Rohman et al., carried out analysis of lard in cream cosmetic formulations using FTIR spectroscopy and chemometrics. Lard rendered from fatty porcine tissue is the most powerful choice as viscosity enhancing agent in several cosmetic products which is prohibited for use by followers ofsome religions. So the authors developed FTIR spectroscopy combined withPLS and discriminant analysis (DA) for the quantification and classification of lard in creams. Hence FTIR emerged as a potential analyticaltechnique for quantitation and classification of lard in cream cosmetics with total analysis time of about 3 min/one sample measurement.

CONCLUSIONS:

The present review expresses that FTIR technique analyses differentbiomedicals, food, and counterfeit drug with high output, zero
impurity, rapid cost analysis. It also applicable for API quality control. Thisreview on FTIR technique will be useful for herbal analysis which helps in understanding in available application.

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