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Ftir advantages and disadvantages

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FTIR spectroscopy is a highly sought-after technique in science, renowned for its unique blend of sensitivity, flexibility, specificity, and robustness. This method can analyze solid, liquid, or gaseous substances, making it one of the most widely used analytical tools across various industries like food, chemicals, engineering, environmental, pharmaceuticals, and clinical settings. Despite some limitations, such as intolerance to water and sensitivity to matrix properties, FTIR remains extremely popular. FTIR instruments now come in different forms, including benchtop, handheld, and online real-time devices. The human eye can only perceive a narrow range of the electromagnetic spectrum, which includes ultraviolet (UV) and infrared (IR) regions. IR spectroscopy specifically focuses on the interaction between IR light and matter, with wavelengths typically ranging from 2,500 to 16,000 nanometers. Historically, IR has been described in terms of wavenumber, where a shorter wavelength corresponds to a larger wavenumber. There are three main categories of IR: far-IR (500-20 cm⁻¹), mid-IR (4,000-500 cm⁻¹), and near-IR (10,000-4,000 cm⁻¹). When IR light interacts with molecules, it absorbs energy at specific frequencies depending on the molecular bonds between atoms. This absorption causes vibrational excitation of covalently bonded atoms, which can stretch, bend, rotate, or scissor. Mid-IR radiation excites fundamental vibrations when energy is absorbed by molecules, raising them from their ground state to the first vibrational state. NIR spectroscopy, on the other hand, consists of combination bands, or "overtones," produced from those fundamental vibrations. The key difference between IR and FTIR spectroscopy lies in the raw signal acquisition. FTIR employs an interferogram, which represents light intensity as a function of mirror position within the interferometer, rather than wavelength. This requires Fourier-transforming the signal to produce a wavenumber-intensity spectrum. Conventionally, FTIR is associated with the mid-IR region, but FT instrumentation is available for UV and NIR spectral forms as well. While FTIR and FT-NIR can be complementary techniques, analysts often must choose between them depending on their specific application requirements. One significant advantage of FTIR over IR spectroscopy is its faster acquisition speed and superior signal-to-noise ratio. Additionally, the wavelength scale calibration with a precise reference laser provides higher accuracy than traditional IR methods. The development of infrared spectrophotometers began in the mid-1940s, primarily for research purposes on organic compounds and petrochemical applications. Initially, dispersive scanning instruments were used, but they were slow and limited to laboratory settings. In recent years, miniaturized and affordable dispersive instruments have found new life in various novel applications. Most modern mid-IR instruments are now of the FT type, with their history dating back to Albert Michelson's invention of the interferometer in the 1890s. Today's FTIR instruments employ an interferometer consisting of a source, beam splitter, mirrors, laser, and detector. The energy is split into two parts, one transmitted through a moving mirror and another reflected onto a fixed mirror. The resulting interference pattern encodes all wavelength information, which must be subjected to the Fourier transform mathematical function to generate an interpretable spectrum. ##### The Coey-Tukey algorithm introduced the "fast Fourier transform" or FFT, which revolutionized the calculation process. This breakthrough, combined with the advent of commercial computing systems, led to the launch of the first commercial FTIR, the FTS-14, in 19698 (Figure 5). The analysis process involves several steps. The source emits IR energy, which passes through an aperture controlling the amount of energy. The interferometer uses spectral encoding and a reference laser for precise wavelength calibration. The sample compartment transmits or reflects the IR beam, allowing specific frequencies to be absorbed by the sample. The detector measures the signal, which is then digitized and calculated using FFT. The final infrared spectrum is presented to the user. FTIR instruments have evolved, offering interchangeable accessories for analyzing gaseous, liquid, and solid samples of varying sizes and forms. Notably, normal glass is not mid-IR transmissible, so all instrument optics and sampling accessories must be constructed from IR-compatible materials. Early techniques required grinding and mixing samples with IR-transmissible substrates under high pressure. Liquid samples were formed as thin films between two such discs with a small spacer. However, time and reproducibility were issues with this method. In recent years, alternatives have emerged, notably the ubiquitous technique of attenuated total reflectance (ATR). This device allows for quick and easy analysis without sample preparation, making it suitable for various applications. Other devices include reflective hemispheres for diffuse reflectance or gas sample sealed cells for specific uses. Even microtiter format plates made from IR-compatible materials are available for high-throughput screening using specialized FTIR accessory units (Figure 6). To obtain FTIR-ATR data, first collect a blank spectrum to account for light beam path and atmospheric absorbance. Then, analyze the sample and subtract the blank spectrum to isolate its unique spectral responses. Optimize wavenumber resolution (typically 4-16 cm⁻¹) and co-added scans (typically 8-64) to balance signal-to-noise. Individual scans are rapid, taking less than a second on modern instruments. This allows for efficient analysis of hundreds or thousands of samples in manufacturing or screening applications. FTIR spectra can be complex and challenging to interpret. Even simple single-component samples have multi-peak spectra that require library matching approaches to identify compounds. However, FTIR data is often used in combination with statistical modeling techniques like multivariate analysis (MVA) or chemometrics to address these challenges. To apply MVA, collect multiple spectra from each sample and construct a data matrix where each row represents an individual sample's complete spectrum and each column represents the aligned absorbance for consecutive wavenumbers. Techniques like principal components analysis (PCA) can then be used to explore class-based relationships between sample groups' spectral responses, providing immediate interpretability of sample differences. The text discusses the processing of green material using FTIR (Fourier Transform Infrared) spectroscopy. The goal can be either qualitative or quantitative, where the latter involves building models that predict properties like chemical concentrations based on previously gathered data. This approach has been shown to effectively replace wet chemistry assays for unknown samples, saving time and money. The output table from MVA modeling allows identifying the most important wavelengths used in building the model, which can provide direct chemical insights. FTIR is typically considered "mid"-FTIR, as non-FT mid-IR dispersive instruments cannot produce the same broad spectrum. However, NIR (Near Infrared) instruments with high energy can produce similar spectra to mid-FTIR instruments, but at a slower scan rate and lower resolution. The text highlights the importance of the fingerprint region in the mid-IR range, which provides unique molecular fingerprints specific to each compound. Mid-IR spectra contain sharper absorption bands for organic species, making them suitable for structural elucidation and compound identification. Organic molecules strongly absorb mid-IR radiation, allowing good spectra to be obtained from small sample amounts. However, FTIR also has some disadvantages, including intolerance of water and limited penetration depth due to strong absorption by organics. On the other hand, NIR's advantages include its strong response to both chemical and physical attributes of the sample, making it useful for overall analysis. NIR radiation provides more sample penetration due to weak absorption, allowing for increased sampling volume, better homogeneity, and reduced preparation requirements. However, NIR's chemical specificity is limited by signal overlap, potentially reducing discriminatory power. The choice between mid-IR and NIR instruments depends on the application. Figure 11: Typical NIR (left) vs mid-IR (right) spectra of dried mosquito samples used to identify vertebrate blood meals in *Anopheles arabiensis*. FTIR occupies a unique position with regards to equipment costs, ease of use, and information production. Its flexibility has led to its application in various areas, including pharmaceuticals and medicine. The development of chemical imaging based on FTIR video chips (focal plane array, "FPA") for microscopy use is particularly noteworthy. In the past two decades, the evolution of mid-infrared imaging chips has enabled spatially resolved applications, such as forensics, archeological artifacts, physical contaminants like microplastics, pharmaceutical pressed tablet testing, and tissue biopsy screening. These advancements allow chemical signals to be interpreted within a broad spatial context. Quantitative screening of pharmaceutical ingredients for the rapid identification of substandard and falsified medicines using reflectance infrared spectroscopy is crucial. PLoS One publishes studies on this topic, including one by Lawson et al., who used reflectance infrared spectroscopy to identify substandard and falsified medicines. Fourier-transform infrared (FTIR) spectroscopy is a valuable tool in the field of medicine, enabling the rapid analysis of complex biological samples. Bioresour Technol has published research on FTIR spectroscopy's application in analyzing hydroxycinnamic acids and lignin in perennial forage and energy grasses. The use of vibrational spectroscopy fingerprinting in medicine is a growing area of research, as demonstrated by Balan et al.'s study in Materials. This technique can be used to identify various biomarkers and diagnose diseases more accurately. FTIR spectroscopy has also been used in the analysis of biopharmaceuticals, as shown in Spectrochim Acta A Mol Biomol Spectrosc. The rapid detection of brain structure and tumour margins on whole frozen tissue sections is another area where FTIR spectroscopy has been applied, as demonstrated by Kümmel et al.'s study. The use of infrared spectroscopy in medicine is not new, with the first commercial FT-IR spectrometers appearing in the late 1960s. Griffiths PR provided a personal perspective on this early history in Appl Spectrosc. FTIR spectroscopy has also been used in high-throughput screening applications, as demonstrated by Sasmaz et al.'s study in Engineering. This technique can be used to quickly identify potential drug candidates and analyze their mechanisms of action. In conclusion, FTIR spectroscopy is a valuable tool in the field of medicine, enabling the rapid analysis of complex biological samples and the detection of various biomarkers and diseases. FTIR spectroscopy, a powerful analytical technique in chemistry and materials science, excels at identifying and quantifying chemical compounds. This blog delves into the benefits and drawbacks of this method. High sensitivity: FTIR spectroscopy can detect tiny amounts of compounds, making it an excellent tool for analyzing complex mixtures. Wide range of applications: From solid to gas samples, FTIR spectroscopy is versatile and suitable for various substances. Non-destructive: The analysis process doesn't alter the sample, making it perfect for fragile or valuable materials. Rapid analysis: Results are typically available within seconds to minutes, allowing for swift decision-making. Quantitative analysis: Concentration of compounds can be accurately determined. However, FTIR spectroscopy has some limitations: Limited to functional groups: It can only identify specific chemical groups rather than individual molecules. Difficulty in complex samples: Analyzing mixtures or overlapping spectra requires expertise and may lead to inaccurate results. Sensitivity to water: Water presence can interfere with the analysis process. Sample preparation: Thin film preparation is time-consuming and demands some knowledge. In summary, FTIR spectroscopy offers many advantages but also has limitations. It's essential to consider these factors when choosing a spectroscopy technique for your project.