Technical Note: 00128

FT-IR vs. Dispersive Infrared

Theory of Infrared Spectroscopy Instrumentation

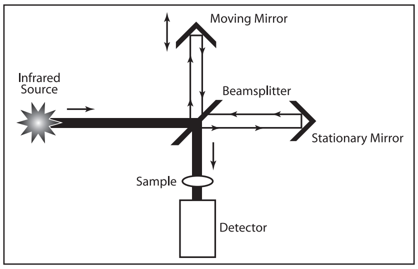
Key Words

- Dispersive
- Fourier transform
- Infrared
- Interferometer
- Spectroscopy

The dispersive infrared spectrometer emerged in the 1940's. This design helped to spread the use of infrared spectroscopy as a common analytical technique for organic compound characterization in laboratories. Fourier transform infrared (FT-IR) spectrometers were developed for commercial use in the 1960's, but at that time were mainly used for advanced research. This was due to the cost of the instrument components and the large computers required to run them. Gradually, technology advancements in computers and instruments have reduced the cost and enhanced the capabilities of an FT-IR. Today, an FT-IR instrument is the standard for organic compound identification work in modern analytical laboratories.

FT-IR: How Does It Work?

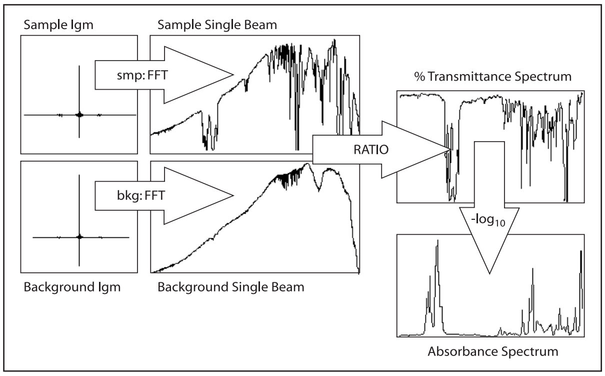
An FT-IR instrument uses a system called an interferometer to collect a spectrum. The interferometer consists of a source, beamsplitter, two mirrors, a laser and a detector. The energy goes from the source to the beamsplitter which splits the beam into two parts. One part is transmitted to a moving mirror; one part is reflected to a fixed mirror. The moving mirror moves back and forth at a constant velocity. This velocity is timed according to the very precise laser wavelength in the system which also acts as an internal wavelength calibration. The two beams are reflected from the mirrors and recombined at the beamsplitter. The beam from the moving mirror has traveled a different distance than the beam from the fixed mirror. When the beams are combined some of the wavelengths recombine constructively and some destructively, which creates an interference pattern. This interference pattern is called an interferogram. This interferogram then goes from the beamsplitter to the sample, where some energy is absorbed and some is transmitted. The transmitted portion reaches the detector. The detector reads information about every wavelength in the infrared range simultaneously.



Interferometer Diagram

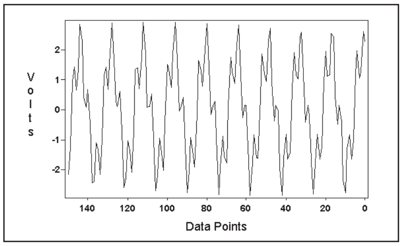
To obtain the infrared spectrum, the detector signal is sent to the computer, and an algorithm called a Fourier transform is performed on the interferogram to convert it into a single beam spectrum. A reference or "background" single beam is also collected without a sample and the sample single beam is ratio-ed to the background single beam to produce a transmittance or "%T" spectrum. This transmittance spectrum can be converted to absorbance by taking the negative $\log_{10}$ of the data points.

The x-axis of the FT-IR spectrum is typically displayed in "wavenumbers", or cm^{-1}. This unit of measure is a product of the Fourier transform algorithm operating on the interferogram and is the reciprocal of the actual wavelength of light measured in centimeters at a point in the infrared spectrum.

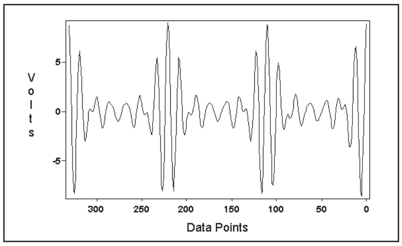


The process of collecting an infrared spectrum in an FT-IR spectrometer

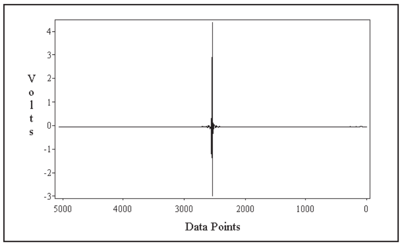
Interference Patterns



Two wavelengths



Multiple wavelengths



Infrared interferogram

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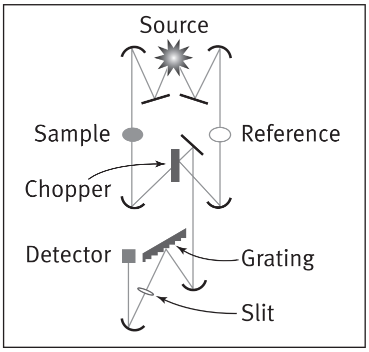
Dispersive Infrared Instruments

Dispersive infrared instruments are sometimes called grating or scanning spectrometers. A dispersive infrared instrument also has a source and mirrors, but the similarities to an FT-IR end there. The source energy is sent through both a sample and a reference path, through a chopper to moderate the energy reaching the detector, and directed to a diffraction grating. This grating is similar to a prism. It separates the wavelengths of light in the spectral range and directs each wavelength individually through a slit to the detector. Each wavelength is measured one at a time, with the slit monitoring the spectral bandwidth and the grating moving to select the wavelength being measured. The x-axis of a dispersive infrared spectrum is typically nanometers which can be converted to the FT-IR unit wavenumbers by dividing by 10 and taking the reciprocal. An external source of wavelength calibration is required, since there is no high-precision laser wavelength to reference in the system.



Dispersive spectrometer diagram

FT-IR Advantages

There are three major advantages in the performance of an FT-IR spectrometer over a dispersive infrared spectrometer. These advantages are the reason for the switch to the more modern FT-IR technique in the last decade by infrared spectroscopists.

Multiplex Advantage

An interferometer in an FT-IR instrument does not separate energy into individual frequencies for measurement of the infrared spectrum. Each point in the interferogram contains information from each wavelength of light being measured. Every stroke of the moving mirror in the interferometer equals one scan of the entire infrared spectrum, and individual scans can be combined to give better representation of the actual absorbance of the sample. In contrast, every wavelength across the spectrum must be measured individually in a dispersive spectrometer. This is a slow process, and typically only one measurement scan of the sample is made in a dispersive instrument. The FT-IR advantage is that many scans can be completed and combined on an FT-IR in a shorter time than one scan on a dispersive instrument. The multiplex advantage results in faster data collection of an FT-IR spectrum.

Throughput Advantage

An FT-IR instrument does not use a slit to limit the individual frequency reaching the sample and detector as a dispersive instrument does. There are also fewer mirror surfaces in an FT-IR spectrometer, so there are less reflection losses than in a dispersive spectrometer. Overall, more energy reaches the sample and hence the detector in an FT-IR spectrometer than in a dispersive spectrometer. This means that the signal-to-noise ratio of an infrared spectrum measured on an FT-IR is higher than the signal-to-noise ratio attained on a dispersive instrument. Higher signal-to-noise means that the sensitivity of small peaks will be greater, and details in a sample spectrum will be clearer and more distinguishable in the FT-IR spectrum than the dispersive spectrum of the same sample. In addition, high-resolution measurement of infrared spectra is of higher quality on an FT-IR system. The slit on a dispersive instrument must severely limit the amount of energy reaching the sample in order to measure data points spaced closely together on a high resolution spectrum, resulting in poor quality spectra. The process is also extremely slow due to the coordination of the grating and slit systems to collect the large number of data points required.

Precision Advantage

An FT-IR spectrometer requires the use of a laser to control the velocity of the moving mirror and to time the collection of data points throughout the mirror stroke length for each scan. This laser is also available as a source of wavelength calibration within the instrument. The laser wavelength is a constant value, and the x-axis data points of the FT-IR spectrum are automatically referenced to this known value to maintain internal precision and accuracy of the wavelength positions. Spectra collected with an FT-IR spectrometer can be compared with confidence whether they were collected five minutes or five years apart. This capability is not available on a dispersive infrared system. External calibration standards are required to control the accuracy of a dispersive instrument, making spectra less comparable due to instrumental unknowns during and between scans. Accuracy and precision in infrared spectra are much higher when collected on an FT-IR.

Summary

As discussed here, FT-IR spectrometers have numerous performance advantages over dispersive instrumentation. Virtually all infrared spectrometer manufacturers are using FT designs instead of dispersive today. The benefits of upgrading to an FT-IR from an existing dispersive infrared instrument will be immediately evident in spectral quality, data collection speed, reproducibility of data, and ease of maintenance and use.

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