Technical Note 50674

Advantages of a Fourier Transform Infrared Spectrometer

Key Words
Dispersive, Fourier Transform, Infrared, Interferometer, Spectroscopy

The Thermo Scientific™ Nicolet™ iS™10 FT-IR spectrometer is an excellent example of what can be achieved with FT-IR, giving a 10,000:1 signal-to-noise ratio in 5 seconds. The Nicolet iS10 spectrometer can collect spectra with better than 0.4 cm^{-1} resolution and acquire high quality ATR spectra, all in a compact, yet robust package.

Introduction

Infrared spectroscopy grew out of the need for a simple, reliable analytical technique for organic materials. The first generations of infrared spectrometers emerged in the 1940's, based on dispersive technology. In spite of the power of infrared for the task, there were several short-comings, including the slow scanning speeds, low throughput and manual operations. Fourier transform infrared (FT-IR) spectrometers were developed for commercial use in the 1960's, mainly for advanced research due to the instrument costs and the large computers required to run them. Gradually, technology advancements have reduced the cost and enhanced the capabilities of an FT-IR. Today, FT-IR is the standard for organic compound identification work in academic, analytical, QC/QA and forensics laboratories.

Dispersive Infrared Instruments

Dispersive infrared instruments are sometimes referred to as grating or scanning spectrometers. The key components are the source, entrance slit, grating (monochromator) and detector, as shown in Figure 1. The source energy is directed along both a sample and a reference path and then into the monochromator. The diffraction grating disperses the light, as water vapor does to make the visible rainbow. The now spatially separated wavelengths of light are directed, by moving the grating, through a narrow slit, which chooses which frequencies are being detected, and then onto the detector.

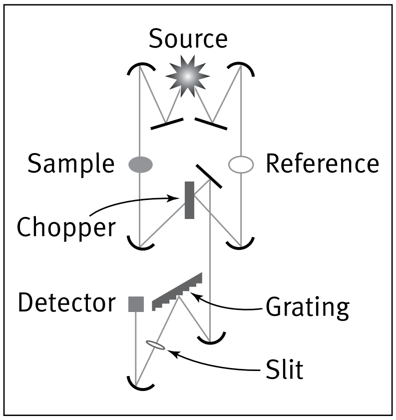

Figure 1: Dispersive spectrometer diagram

The wavelengths are measured one at a time, with the slit controlling the spectral bandwidth (how wide a range of frequencies are permitted to strike the detector). The grating-slit combination selects the wavelengths being measured. The x-axis of a dispersive infrared spectrum is typically recorded in nanometers (= 10^{-9} meters, as gratings act linearly in wavelength). The most common presentation of infrared uses wavenumbers (cm^{-1}), which are linear in energy ($cm^{-1} = 1/(nm * 10^{-7})$, such that 500 nm = 20,000 cm^{-1} and 5000 nm = 5 microns = 2000 cm^{-1}). Dispersive spectrometers require an external wavelength calibration source, since there is no internal reference.

Fourier Transform Instruments (FT-IR)

An FT-IR instrument relies upon interference of various frequencies of light to collect a spectrum. The spectrometer consists of a source, beamsplitter, two mirrors, a laser and a detector; the beamsplitter and mirrors are collectively called the interferometer. The assembled whole is shown in Figure 2. The IR light from the source strikes the beamsplitter, which produces two beams of roughly the same intensity. One beam strikes a fixed mirror and returns, while the second strikes a moving mirror. A laser parallels the IR light, and also goes through the interferometer.

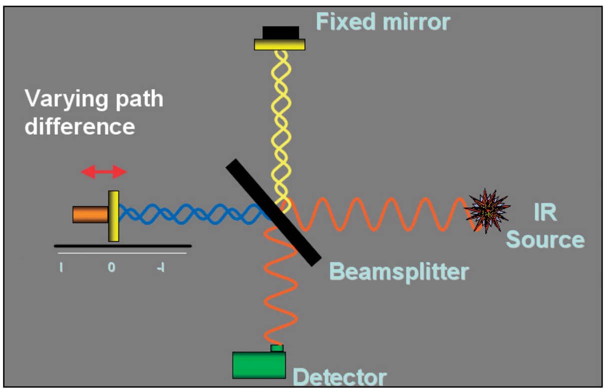

Figure 2: Interferometer Diagram

The moving mirror oscillates at a constant velocity, timed using the laser frequency. The two beams are reflected from the mirrors and are recombined at the beamsplitter. If the distance the two beams travel is the same, then they will recombine constructively. However, if the beam from the moving mirror has traveled a different distance (further or shorter) than the beam from the fixed mirror, then recombination will result in some destructive interference. The movement of the mirror thus generates an interference pattern during the motion.

The IR beam next passes through the sample, where some energy is absorbed and some is transmitted. The transmitted portion reaches the detector, which records the total intensity. The raw detector response yields an interferogram. The interference pattern contains information about all wavelengths being transmitted at once, which is a function of the source, beamsplitter, mirrors and sample. This signal is digitized and processed using a computer. The untangling of the frequencies into a spectrum is done by the Fourier transform algorithm, which gives the name to the entire spectrometer. This produces a “single beam” spectrum. A reference or “background” single beam is collected without a sample; the sample single beam is collected with the only change being the presence of the sample. The ratio of these two leads to the spectrum.

The entire process is shown in Figure 3. The final spectrum can be presented as transmittance (%T) or absorbance; the computer easily performs this conversion. Figure 3 shows results as transmittance. The interested reader is directed to the references for more details about the instrumentation.

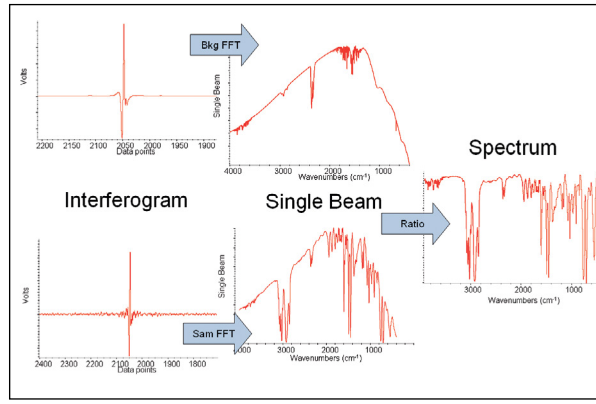

Figure 3: The process of collecting an infrared spectrum in an FT-IR spectrometer

FT-IR Advantages

The modern FT-IR spectrometer has three major advantages over a typical dispersive infrared spectrometer. These advantages are the reason FT-IR is now the standard tool, having largely displaced dispersive instruments by the mid-1980’s.

Multiplex Advantage

As seen from the operations description above, the interferometer does not separate energy into individual frequencies for measurement. Each point in the interferogram contains information from each wavelength of light being measured. Every stroke of the moving mirror equals one scan of the entire infrared spectrum, and individual scans can be combined to allow signal averaging. In the dispersive instrument, every wavelength across the spectrum must be measured individually as the grating scans. This can be a slow process, and typically only one spectral scan of the sample is made in a dispersive instrument. The multiplex advantage means many scans can be completed and averaged on an FT-IR in a shorter time than one scan on most dispersive instruments.

Throughput Advantage

The FT-IR instrument does not limit the amount of light reaching the detector using a slit. The Thermo Scientific FT-IR spectrometers also use the fewest number of mirrors necessary, which means less reflective losses occur. Overall, these mean more energy reaches the sample and hence the detector in an FT-IR spectrometer than in a dispersive spectrometer. The higher signal leads to an improved signal-to-noise ratio of the FT-IR. Higher signal-to-noise means that the sensitivity of the instrument for small absorptions will be greater, and details in a sample spectrum will be clearer and more distinguishable. The IR analysis of proteins is a good example – this is almost impossible in a classical dispersive instrument, while it is a fairly routine measurement for FT-IR.

The slit in a dispersive instrument becomes even more of a limitation as the spectral resolution desired increases. To see a narrower range, the slit closes down, choking the amount of light passing the instrument, resulting in poor quality spectra for all except ideal samples. Further, high resolution also implies a very slow scan speed, so it can take long times to collect a high resolution dispersive spectrum. To attain ultra-high resolution, the IR also uses an aperture, but the limitation of the light is not nearly so severe, and the multiplex advantage quickly gains back the loss.

Precision Advantage

An FT-IR spectrometer uses a laser to control the velocity of the moving mirror and to time the collection of data points throughout the mirror stroke. This laser is also used as a reference signal within the instrument. The interferogram of the laser is a constant sine-wave, which provides the reference for both precision and accuracy of the infrared spectrometer. Well-designed FT-IR spectrometers rely exclusively on this reference laser, rather than any external reference sample. In this case, 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, or any system requiring external calibration standards.

Summary

FT-IR spectrometers have numerous performance advantages over traditional dispersive infrared instrumentation. Virtually all infrared spectrometer manufacturers are now using FT designs instead of dispersive. 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.

Africa +43 1 333 50 34 0
Australia +61 3 9757 4300
Austria +43 810 282 206
Belgium +32 53 73 42 41
Canada +1 800 530 8447
China +86 21 6865 4588
Denmark +45 70 23 62 60
Europe-Other +43 1 333 50 34 0
Finland/Norway/Sweden +46 8 556 468 00
France +33 1 60 92 48 00
Germany +49 6103 408 1014
India +91 22 6742 9494
Italy +39 02 950 591
Japan +81 45 453 9100
Latin America +1 561 688 8700
Middle East +43 1 333 50 34 0
Netherlands +31 76 579 55 55
New Zealand +64 9 980 6700
Russia/CIS +43 1 333 50 34 0
Spain +34 914 845 965
Switzerland +41 61 716 77 00
UK +44 1442 233555
USA +1 800 532 4752

Thermo SCIENTIFIC
A Thermo Fisher Scientific Brand

TN50674_E 02/15M