

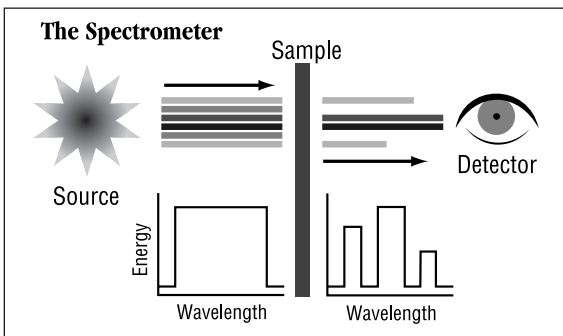
Introduction to Fourier Transform Infrared Spectroscopy



Introduction

What is FT-IR?

FT-IR stands for Fourier Transform InfraRed, the preferred method of infrared spectroscopy. In infrared spectroscopy, IR radiation is passed through a sample. Some of the infrared radiation is absorbed by the sample and some of it is passed through (transmitted). The resulting spectrum represents the molecular absorption and transmission, creating a molecular fingerprint of the sample. Like a fingerprint no two unique molecular structures produce the same infrared spectrum. This makes infrared spectroscopy useful for several types of analysis.



So, what information can FT-IR provide?

- It can identify unknown materials
- It can determine the quality or consistency of a sample
- It can determine the amount of components in a mixture

This booklet is an introduction to the concepts behind FT-IR spectroscopy. It covers both the basic theory of FT-IR and how it works as well as discussing some the practical aspects of FT-IR use. We hope that it gives you a good understanding of the importance and usefulness of this powerful technique.

Theory of FT-IR

Why Infrared Spectroscopy?

Infrared spectroscopy has been a workhorse technique for materials analysis in the laboratory for over seventy years. An infrared spectrum represents a fingerprint of a sample with absorption peaks which correspond to the frequencies of vibrations between the bonds of the atoms making up the material. Because each different material is a unique combination of atoms, no two compounds produce the exact same infrared spectrum. Therefore, infrared spectroscopy can result in a positive **identification** (qualitative analysis) of every different kind of material. In addition, the size of the peaks in the spectrum is a direct indication of the **amount** of material present. With modern software algorithms, infrared is an excellent tool for quantitative analysis.

Older Technology

The original infrared instruments were of the **dispersive** type. These instruments separated the individual frequencies of energy emitted from the infrared source. This was accomplished by the use of a prism or grating. An infrared prism works exactly the same as a visible prism which separates visible light into its colors (frequencies). A grating is a more modern dispersive element which better separates the frequencies of infrared energy. The detector measures the amount of energy at each frequency which has passed through the sample. This results in a **spectrum** which is a plot of intensity vs. frequency.

Fourier transform infrared spectroscopy is preferred over dispersive or filter methods of infrared spectral analysis for several reasons:

- It is a non-destructive technique
- It provides a precise measurement method which requires no external calibration
- It can increase speed, collecting a scan every second
- It can increase sensitivity – one second scans can be co-added together to ratio out random noise
- It has greater optical throughput
- It is mechanically simple with only one moving part

Why FT-IR?

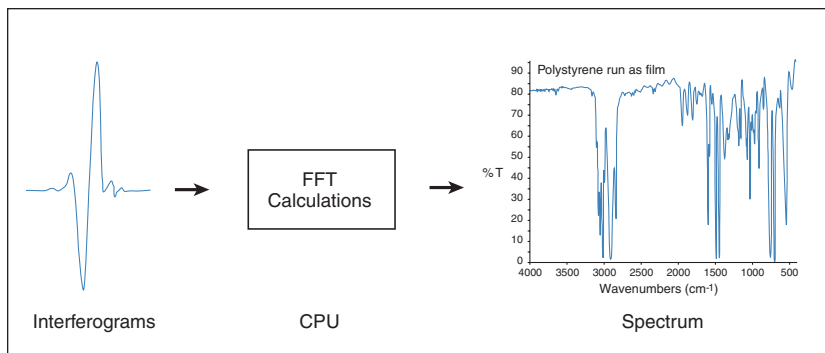
Fourier Transform Infrared (FT-IR) spectrometry was developed in order to overcome the limitations encountered with dispersive instruments. The main difficulty was the slow scanning process. A method for measuring all of the infrared frequencies **simultaneously**, rather than individually, was needed. A solution was developed which employed a very simple optical device called an interferometer. The **interferometer** produces a unique type of signal which has all of the infrared frequencies "encoded" into it. The signal can be measured very quickly, usually on the order of **one second** or so. Thus, the time element per sample is reduced to a matter of a few seconds rather than several minutes.

Most interferometers employ a **beamsplitter** which takes the incoming infrared beam and divides it into two optical beams. One beam reflects off of a flat mirror which is fixed in place. The other beam reflects off of a flat mirror which is on a mechanism which allows this mirror to move a very short distance (typically a few millimeters) away from the beamsplitter. The two beams reflect off of their respective mirrors and are recombined when they meet back at the beamsplitter. Because the path that one beam travels is a fixed length and the other is constantly changing as its mirror moves, the signal which exits the interferometer is the result of these two beams "interfering" with each other. The resulting signal is called an **interferogram** which has the unique property that every data point (a function of the moving mirror position) which makes up the signal has information about every infrared frequency which comes from the source.



This means that as the interferogram is measured, all frequencies are being measured simultaneously. Thus, the use of the interferometer results in extremely fast measurements.

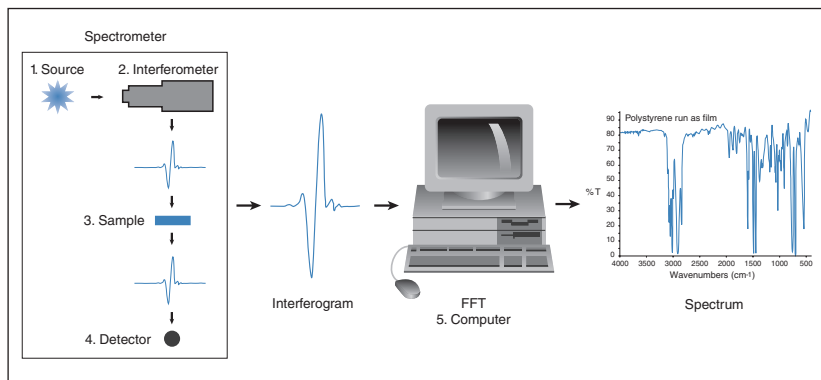
Because the analyst requires a **frequency spectrum** (a plot of the intensity at each individual frequency) in order to make an identification, the measured interferogram signal can not be interpreted directly. A means of "decoding" the individual frequencies is required. This can be accomplished via a well-known mathematical technique called the **Fourier transformation**. This transformation is performed by the computer which then presents the user with the desired spectral information for analysis.



The Sample Analysis Process

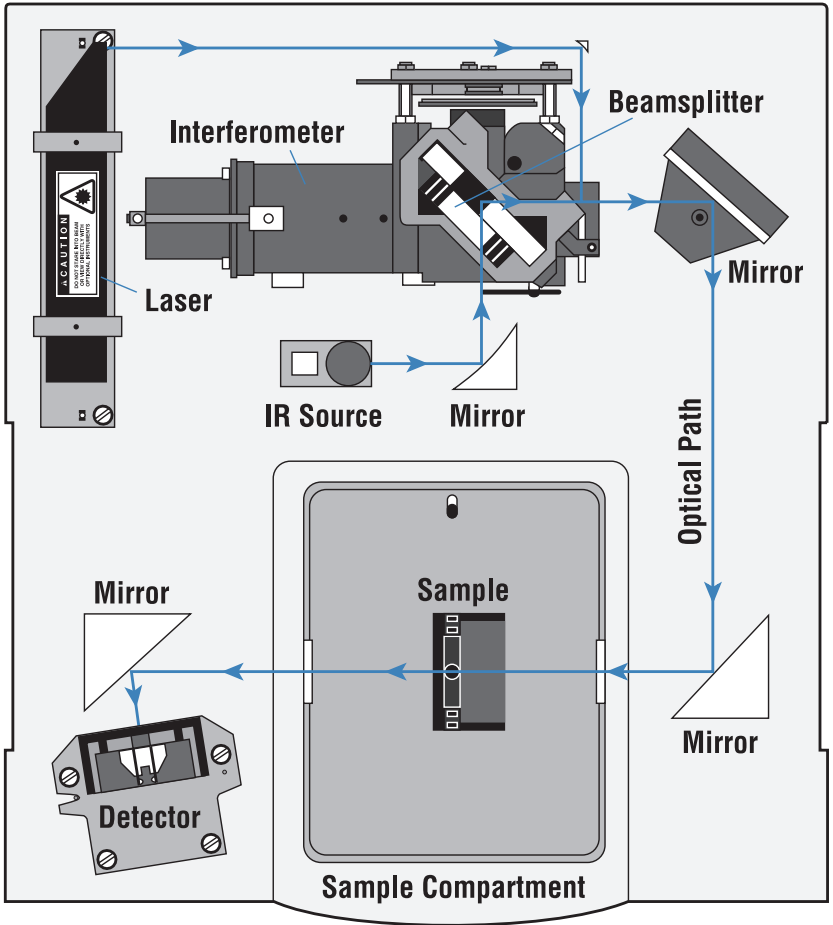
The normal instrumental process is as follows:

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 exits the interferometer.
3. **The Laser:** The Laser beam also passes through the interferometer. It is used for wavelength calibration, mirror position control and data collection triggering of the spectrometer
4. **The Sample:** The beam enters the sample compartment where it is transmitted through or reflected off of the surface of the sample, depending on the type of analysis being accomplished. This is where specific frequencies of energy, which are uniquely characteristic of the sample, are absorbed.
5. **The Detector:** The beam finally passes to the detector for final measurement. The detectors used are specially designed to measure the special interferogram signal.
6. **The Computer:** 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.



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 can be used for many sample measurements because this spectrum is characteristic of the **instrument** itself.

A Simple Spectrometer Layout



Advantages of FT-IR

Some of the major advantages of FT-IR over the dispersive technique include:

- **Speed:** Because all of the frequencies are measured simultaneously, most measurements by FT-IR are made in a matter of seconds rather than several minutes. This is sometimes referred to as the **Felgett Advantage**.
- **Sensitivity:** Sensitivity is dramatically improved with FT-IR for many reasons. The detectors employed are much more sensitive, the optical throughput is much higher (referred to as the **Jacquinot Advantage**) which results in much lower noise levels, and the fast scans enable the coaddition of several scans in order to reduce the random measurement noise to any desired level (referred to as signal averaging).
- **Mechanical Simplicity:** The moving mirror in the interferometer is the only continuously moving part in the instrument. Thus, there is very little possibility of mechanical breakdown.
- **Internally Calibrated:** These instruments employ a HeNe laser as an internal wavelength calibration standard (referred to as the **Connes Advantage**). These instruments are self-calibrating and never need to be calibrated by the user.

These advantages, along with several others, make measurements made by FT-IR extremely accurate and reproducible. Thus, it a very reliable technique for **positive identification** of virtually any sample. The sensitivity benefits enable identification of even the smallest of contaminants. This makes FT-IR an invaluable tool for **quality control** or quality assurance applications whether it be batch-to-batch comparisons to quality standards or analysis of an unknown contaminant. In addition, the sensitivity and accuracy of FT-IR detectors, along with a wide variety of software algorithms, have dramatically increased the practical use of infrared for **quantitative analysis**. Quantitative methods can be easily developed and calibrated and can be incorporated into simple procedures for routine analysis.

Thus, the Fourier Transform Infrared (FT-IR) technique has brought significant practical advantages to infrared spectroscopy. It has made possible the development of many new sampling techniques which were designed to tackle challenging problems which were impossible by older technology. It has made the use of infrared analysis virtually limitless.

Thermo Electron Corporation's Family of FT-IR Technology

Thermo Electron Corporation is the worldwide leader in FT-IR instrumentation, delivering powerful solutions to scientists since the 1970's.

Nicolet™ Series

- Easily upgradeable
- Superior optical throughput
- High resolution
- Multiple spectral ranges
- Rapid scanning/fast kinetics



Nicolet Avatar™ Series

- Easy sampling
- Easy purge
- Easy interface
- Easy identification
- Easy presentation



Nicolet IR Series

- Minimal training
- Suits basic sampling needs
- Flexibility of personal compute (PC)
- Compact, easy-to-use system



Nicolet Centaurus™ Infrared Microscope

- Simultaneous view and collect
- Flexible ATR
- Binocular and video view
- Easy to use



Nicolet Continuum™ Infrared Microscope

- Highest infrared resolving power
- DIC & fluorescence illumination
- Simultaneous view and collect
- Dual detectors
- View ATR contact
- Full automation



Sample Compartment Accessories

- Samples as small as 50 µm using ATR
- Fibers, pellets, paper, powdered samples
- Plug and play design for quick analysis



Australia
+61 2 8844 9500

Austria
+43 1 333 50340

Belgium
+32 2 482 30 30

Canada
+1 800 532 4752

China
+86 10 5850 3588

France
+33 1 60 92 48 00

Germany
+49 6103 4080

India
+91 22 2778 1101

Italy
+39 02 950 591

Japan
+81 45 453 9100

Netherlands
+31 76 587 98 88

Scandinavia
+46 8 556 468 00

South Africa
+27 11 570 1840

Spain
+34 91 657 4930

Switzerland
+41 61 48784 00

UK
+44 1442 233555

USA
+1 800 532 4752

www.thermo.com



Thermo Electron Scientific
Instruments LLC, Madison, WI
USA is ISO Certified.

©2005 Thermo Electron
Corporation. All rights
reserved. All trademarks are
the property of Thermo
Electron Corporation and
its subsidiaries.

Specifications, terms and
pricing are subject to
change. Not all products are
available in all countries.
Please consult your local
sales representative for
details.

BR50555_E 11/05M

Thermo
ELECTRON CORPORATION