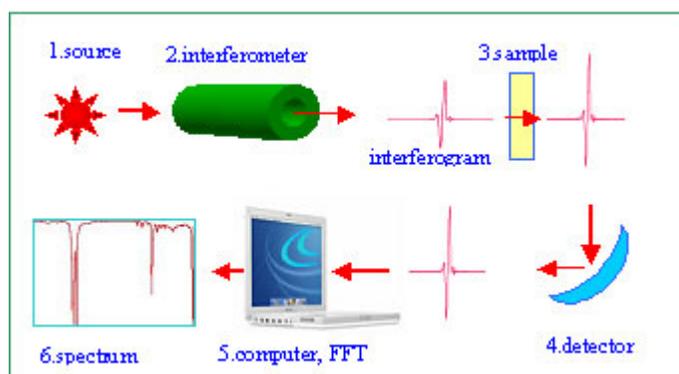


What is FT-IR?

Infrared (IR) spectroscopy is a chemical analytical technique, which measures the infrared intensity versus wavelength (wavenumber) of light. Based upon the wavenumber, infrared light can be categorized as far infrared ($4 \sim 400\text{cm}^{-1}$), mid infrared ($400 \sim 4,000\text{cm}^{-1}$) and near infrared ($4,000 \sim 14,000\text{cm}^{-1}$).

Infrared spectroscopy detects the vibration characteristics of chemical functional groups in a sample. When an infrared light interacts with the matter, chemical bonds will stretch, contract and bend. As a result, a chemical functional group tends to adsorb infrared radiation in a specific wavenumber range regardless of the structure of the rest of the molecule. For example, the C=O stretch of a carbonyl group appears at around 1700cm^{-1} in a variety of molecules. Hence, the correlation of the band wavenumber position with the chemical structure is used to identify a functional group in a sample. The wavenumber positions where functional groups adsorb are consistent, despite the effect of temperature, pressure, sampling, or change in the molecule structure in other parts of the molecules. Thus the presence of specific functional groups can be monitored by these types of infrared bands, which are called group wavenumbers.

The early-stage IR instrument is of the dispersive type, which uses a prism or a grating monochromator. The dispersive instrument is characteristic of a slow scanning. A Fourier Transform Infrared (FTIR) spectrometer obtains infrared spectra by first collecting an interferogram of a sample signal with an interferometer, which measures all of infrared frequencies simultaneously. An FTIR spectrometer acquires and digitizes the interferogram, performs the FT function, and outputs the spectrum.



Schematic illustration of FTIR system

An interferometer utilizes a beamsplitter to split the incoming infrared beam into two optical beams. One beam reflects off of a flat mirror which is fixed in place. Another beam reflects off of a flat mirror which travels 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 together at the beamsplitter. The re-combined signal results from the “interfering” with each other. Consequently, the resulting signal is called interferogram, which has every infrared frequency “encoded” into it. When the interferogram signal is transmitted through or reflected off of the sample surface, the specific frequencies of energy are adsorbed by the sample due to the excited vibration of function groups in molecules. The infrared signal after interaction with the sample is uniquely characteristic of the sample. The beam finally arrives at the detector and is measure by the detector. The detected interferogram can not be directly interpreted. It has to be “decoded” with a well-known mathematical technique in term of Fourier Transformation. The computer can perform the Fourier transformation calculation and present an infrared spectrum, which plots adsorbance (or transmittance) versus wavenumber.

When an interferogram is Fourier transformed, a single beam spectrum is generated. A single beam spectrum is a plot of raw detector response versus wavenumber. A single beam spectrum obtained without a sample is called a background spectrum, which is induced by the instrument and the environments. Characteristic bands around 3500cm^{-1} and 1630cm^{-1} are ascribed to atmospheric water vapor, and the bands at 2350cm^{-1} and 667cm^{-1} are attributed to carbon dioxide. A background spectrum must always be run when analyzing samples by FTIR. When an interferogram is measured with a sample and Fourier transformed, a sample single beam spectrum is obtained. It looks similar to the background spectrum except that the sample peaks are superimposed upon the instrumental and atmospheric contributions to the spectrum. To

eliminate these contributions, the sample single beam spectrum must be normalized against the background spectrum. Consequently, a transmittance spectrum is obtained as follows.

$$\%T = I/I_0$$

Where $\%T$ is transmittance; I is the intensity measured with a sample in the beam (from the sample single beam spectrum); I_0 is the intensity measured from the background spectrum

The absorbance spectrum can be calculated from the transmittance spectrum using the following equation.

$$A = -\log_{10} T$$

Where A is the absorbance.

The final transmittance/absorbance spectrum should be devoid of all instrumental and environmental contributions, and only present the features of the sample. If the concentrations of gases such as water vapor and carbon dioxide in the instrument are the same when the background and sample spectra are obtained, their contributions to the spectrum will ratio out exactly and their bands will not occur. If the concentrations of these gases are different when the background and sample spectra are obtained, their bands will appear in the sample spectrum.

Reference:

Brian C. Smith, Fundamentals of Fourier Transform Infrared spectroscopy, CRC press, Boca Raton, 1996.