

FT-IR Glossary

Absorption The transfer of energy from an infrared beam to the molecules present in the path of the radiation.

Absorbance Spectrum Absorbance is related to Transmittance as follows: $A = \log 1/T$ where A is absorbance and T is transmittance. Transmittance spectra are calculated by ratioing a sample single beam spectrum to a background spectrum. Absorbance is linearly proportional to concentration (see Beer's Law), and should be used for quantitative analysis.

Absorption Image An image wherein contrast results from differences in radiant energy absorption. A drop of dye in water is an example of an absorption image.

Absorption Spectrum A spectrum that shows how the absorptivity of a sample varies with frequency or wavelength.

Absorptivity The value represented by the letter a in the formula of Beer's Law: $A(n) = a(n)bc$ where A(n) is the absorbance at wavenumber n, a(n) is the absorptivity at wavenumber n, b is the pathlength, and c is the concentration. Also known as absorptive power or molar absorptivity.

Alignment Adjustment of spectrometer components to maximize the detector signal.

Analyzer In a polarization experiment, an optical device, such as a Nicol prism, capable of producing plane-polarized light, and used for detecting the effect of the object on plane-polarized light produced by the polarizer.

Angle of Incidence The angle at which the initial ray of light strikes a surface. The angle of incidence is measured from the ray to the normal to the surface.

Angular Aperture (A.A.) The maximum angle of light rays that pass through an optical element, lens, aperture, etc.

Aperture An opening or hole through which radiation or matter may pass.

Apodization A mathematical function applied to the interferogram prior to Fourier Transform. Apodization compensates for the fact that the interferogram is a finite set of data points.

Attenuated Total Reflection (ATR) Infrared radiation entering a prism made from a high-refractive index, infrared transmitting material can be totally internally reflected. This internal reflection creates an effect called the evanescent wave that extends beyond the surface of the crystal into the sample that is in contact with the crystal. In regions of the infrared spectrum where the sample absorbs energy, the evanescent wave will interact with the sample and a spectrum can be obtained. Attenuated Total Reflection produces a very short pathlength for the infrared light in the sample. This makes this technique ideal for highly absorbing materials such as aqueous solutions, rubbers, and polymers.

Attenuation The decrease in amplitude of a signal that occurs during its transmission.

Background The characteristics of the environment of the spectrometer, including the detector and atmospheric conditions. A reference spectrum that accounts for the unique optics of a sampling accessory and an instrument. The background spectrum is the result of the output of the source, the response of the beamsplitter optics, sampling module or sample holder, and detector and any atmospheric absorptions inside the analyzer. Sample spectra are ratioed against a background spectrum so that the final spectrum is free of those features.

Background Spectrum A single beam spectrum obtained without a sample in place. The background spectrum is the result of the output of the source; the response of the beamsplitter, optics, sampling accessory or holder, and detector; and any atmospheric absorptions inside the spectrometer.

Band An infrared absorption in a spectrum; that is, a region containing a peak. See also Peak.

Baseline The portion of spectrum or chromatogram that contains no bands or peaks. The baseline represents those regions where the sample absorbs little or no infrared energy.

Baseline Correction Removal of an offset, slope or curvature from the baseline of a spectrum.

Beam The stream of infrared light emitted by the source that travels to the detector.

Beam Path The route followed by the infrared beam as it travels from the source to the detector. Using an accessory such as a GC interface or an infrared microscope changes the beam path, since the beam must pass through the accessory before reaching the detector.

Beamsplitter Any optical device for dividing a beam into two or more separate beams. Beamsplitters are used in Michelson interferometers to send infrared radiation to the moving mirror and fixed mirror respectively.

Beer's Law The equation that relates absorbance to concentration. Its form is $A = elc$ where A is absorbance, e is molar absorptivity (a proportionality constant), l is the pathlength of the sample, and c is the concentration.

Birefringence Optically anisotropic substances are double refracting. In birefringent crystals, light is resolved into two components that are polarized at right angles to each other and that travel at different velocities through the substance. Thus, the crystal exhibits two refractive indices (one for each ray). This phenomenon is called birefringence. Numerically, it is the difference in index between the greater and lesser index values of any anisotropic material.

Bright-field Illumination The common form of microscope illumination. The image of the sample appears on a bright, well-lit field.

Cassegrain Lens A reflecting element optical system that uses two spherical mirrors (a primary concave mirror and a secondary convex mirror) to focus light energy. In a true Cassegrain system the slower beam is incident on the primary mirror.

Chamber Refers to an enclosed, usually airtight, vessel (as in the diffuse reflectance chamber) where a sample is contained.

Coaxial Optical System An optical assembly wherein the optical axes of the elements fall on a common line. (a.k.a. **Colinear System**)

Condensate A liquid obtained by condensation of a gas or vapor.

Condenser In a microscope, the optical element that focuses light onto the sample.

Corrected Peak Area The area that is below a peak, above the baseline and between two vertical lines that define the left and right limits of the area.

Corrected Peak Height The difference in the Y axis unit value between the maximum of a peak and the baseline.

CPC (Compound Parabolic Concentrator) Diffuse An optical element that both directs energy to the sample and collects the reflected energy.

Critical Angle (θ_c) $\theta_c = \sin^{-1}(n_2/n_1)$, where n_2 and n_1 are the refractive indices of two materials at an interface (n_2 being the index of the more optically dense material).

Current Background The background spectrum that is in active computer memory and will be used when the next collected sample spectrum is ratioed. When you collect a background spectrum, it becomes the current background regardless of whether you place it into a spectral window following collection.

Darkfield Illumination Any method of illumination that illuminates the sample but does not admit light directly into the objective.

Data Spacing The number of wavenumbers between consecutive data points.

Depth of Field The distance above and below the plane where a distinct image is observed. Depth of field decreases with an increase in numerical aperture or with an increase in magnification.

Desiccator A chamber containing a water trap or absorbing material that keeps beamsplitters and other spectrometer parts dry.

Detector A device inside the spectrometer (or in another location such as in an auxiliary experiment module) that produces an electrical signal in response to the infrared beam striking it.

DIC (Differential Interference Contrast) Technique A microanalysis technique used in the Thermo Scientific™ Nicolet™ Continuum™ microscope, developed and patented by Nomarski, which enables visualizing and defining samples with poor contrast for IR data collection.

Diffraction A modification that light undergoes when passing by the edges of opaque bodies, through narrow slits or apertures, which results in light intensity appearing in the geometrical shadow of a high-contrast edge.

Diffuse Reflection The energy that penetrates one or more particles of a sample and emerges at angles other than the specular reflection angle. The diffuse reflection technique can be used for most solids that can be put into a powder or crystalline state. It can also be used for cloth, fibers, and coatings that can be abraded.

Dispersion Variation in the refractive index of a sample at different wavenumber values of the incident energy.

Dynamic Alignment A method of continuous, automatic alignment of the interferometer.

Emittance A measure of the infrared radiation emitted by a sample.

European Pharmacopoeia Published under the direction of the Council of Europe, the European Pharmacopoeia (EP) is an official text of drug standards in seventeen countries throughout Europe. Where national standards differ from those of the EP, they must be brought into alignment with it. The Single European Act enhances the importance of the EP as the Pan-European standard for pharmaceuticals and certain medical device products.

Experiment (1) A file containing parameter settings that are appropriate for a particular application. Selecting or opening an experiment sets features in the Experiment Setup dialog box, Library Setup dialog box and Series Setup dialog box (if present) in one step. (2) A procedure in which sample spectra are collected.

External Beam A beam of radiation, usually collimated, that is deflected from the normal beam path and travels through an opening in the spectrometer cover to an external accessory.

f-number A measure of the relative aperture of a lens. It is the ratio of the focal length to the diameter of the exit pupil of the lens.

Far-IR (Far Infrared) The region of infrared radiation from 400 to 10 wavenumbers.

Fiber Optic Cable A bundle of thin, glass or plastic transparent fibers that are enclosed by a less refractive material. The fibers transmit light by internal reflection.

Field The area of the sample that is seen when the image is observed.

Field of View The maximum area that can be seen through a lens or an optical instrument.

Fluorescence Emission of light caused by absorption of energy into the emitting body usually from a short wavelength light source.

Fourier Transform (1) To convert an interferogram (data in the time domain) to a single-beam spectrum (data in the frequency domain) to reveal the response at all frequencies within the spectral range. (2) The mathematical operation used to convert an interferogram to a single-beam spectrum.

Frequency The number of light wave cycles that occur per unit time or space. Infrared frequency is typically expressed in wavenumbers (cm^{-1}).

FT-IR (Fourier Transform Infrared) An infrared spectroscopic technique that uses an interferometer for data collection and a digital Fourier transformation to process the data.

FT-NIR (Fourier Transform Near Infrared) A near infrared spectroscopic technique that uses an interferometer for data collection and digital Fourier transformation to process the data.

FT-Raman (Fourier Transform Raman) Raman spectroscopy in which an interferometer is used as the dispersing element to achieve spectral resolution. Typically performed with a 1064 nm laser and either Ge or InGaAs detectors.

Full-Field Aperture A sample-defining aperture used in microspectroscopy enabling the viewer to visibly see the entire field of view while also defining the sample data collection area.

Gain The increase in the detector signal amplitude that is due to electronic amplification. Gain is used to increase the intensity of weak detector signals.

Ge Detector Liquid nitrogen-cooled detector for FT-Raman applications with very low Raman emission.

Gimbal A mounting mechanism that provides a means for maintaining a level surface regardless of any motion of its support.

Grazing Angle Reflection Occurs when light strikes a surface at an angle almost perpendicular to the normal. The absorption spectra of very thin films (between 20 Å and 0.5 µm) on a metal can be measured this way.

Index of Refraction The ratio of the velocity of radiation in a vacuum to its velocity in the medium through which it passes.

Infrared Radiation Electromagnetic radiation found between 10 and 14000 cm⁻¹. The Far Infrared is found between 400 and 10 cm⁻¹, the Mid Infrared is between 400 and 4000 cm⁻¹, and the Near Infrared is between 4000 and 14000 cm⁻¹.

InGaAs Detector The room temperature detector used for most FT-Raman and FT-NIR applications. This is the detector recommended for all but the most challenging measurements when the highest sensitivity is required.

Integrating Sphere A device used in diffuse-reflectance spectroscopy. When using an integrating sphere, the light beam is angled into the sphere and travels directly through the center of the sphere, through the optical window (if used), and into the sample. Reflected light from the sample re-enters the sphere. An internal detector measures the reflection and sends the information to the computer.

Interferogram A photographic or electronic recording of an optical interference pattern. The interferograms recorded by an infrared spectrometer are plots of infrared intensity versus optical path difference. Interferograms are Fourier transformed to obtain single beam spectra.

Interferogram Peak The point in an interferogram where the optical path difference between the moving and fix mirror is zero signal at its maximum intensity. Sometimes called the "centerburst".

Interferometer A device that splits and then recombines a beam of radiation. The output signal is an interferogram. Usually one beam passes through the interferometer's beamsplitter, is reflected from the moving mirror and returns to the beamsplitter. The other beam is reflected from the beamsplitter and then is reflected from the fixed mirror and returns to the beamsplitter. The recombined beam exits the interferometer, passes through the sample and travels to the detector.

Japanese Pharmacopeia (JP) Pharmaceutical manufacturing and quality standards used in Japan.

Koehler Illumination An illumination method that uses an auxiliary condenser to image the source onto the focal plane of the condenser. This renders the rays from any point on the source as a parallel beam at the sample and makes the illumination at the sample highly uniform.

Kubelka-Munk Units The appropriate units to use when performing quantitative analysis by diffuse reflectance. Kubelka-Munk units are calculated from the Kubelka-Munk equation.

Log An automatically recorded list that shows some of the collection and processing operations that have been performed, along with the results of the operations.

Magnification The number of times by which the linear size of an optical image exceeds the size of the original object.

Matrix A surrounding substance within which something else originates, develops, or is contained

Micrometer (Micron) An X axis unit used for wavelength. One micrometer equals 0.000001 meter.

Mid-IR (Mid-Infrared) The region of infrared radiation from 4,000 to 400 wavenumbers (2.5 to 25 micrometers).

Mirror Velocity The linear speed of the moving mirror.

Moving Mirror The mirror in the interferometer that reflects the infrared beam back to the beamsplitter while moving toward and away from the beamsplitter in a repeating cycle

Nanometer An X axis unit used for wavelength. One nanometer equals 0.000000001 meter.

NIR (Near Infrared) A region of the electromagnetic spectrum extending from approximately 12000 cm⁻¹ to 4000 cm⁻¹.

Noise Random signals produced by a number of components in a spectrometer, including the detector and signal-processing electronics.

Numerical Aperture (N.A.) A mathematical formula for the direct comparison of objectives for resolving power and optical throughput.

$N.A. = n \sin(A.A. / 2)$

N.A. is the numerical aperture

A.A. is the angular aperture

n is the refractive index of the medium in contact with the sample.

Objective The lens closest to the sample in an image-forming system.

On-axis For each optical element in a device, the axis of the element lies on the axis of the device as a whole.

Optical Alignment The arrangement of optical parts – lenses and diaphragms – so that all of their axes are coincident.

Optical Bench The component of a spectrometer that contains the optics, generally including the source, interferometer or monochromator, and detector.

Optical Density A measure of the efficiency of a filter, which filters a given wavelength of light. The higher the optical density at a given wavelength, the more photons of that wavelength that can be collected.

Parameter A setting within the software that affects how data are collected or processed.

Parfocal Objectives Objectives that are positioned so that, when changing from one objective to another, the microscope image is at or near focus. (Small adjustment of the fine focus may be required.)

Pathlength The distance that the infrared beam travels within a sample. A longer pathlength increases the absorption of infrared energy by the sample. If the pathlength is too great, totally absorbing bands will result.

Peak A point within a region of a spectrum, Gram-Schmidt reconstruction or Chemigram where the sample absorbs maximum radiation. In an absorption spectrum, the peak is the maximum, or highest point, of the region; in a % transmittance spectrum, the peak is the minimum, or lowest point, of the region

Peak Height The Y axis unit value at the maximum of a peak. See also Corrected Peak Height.

Peak to Peak Noise The difference in intensity between the highest point and lowest point in a spectral region containing no spectral features.

Phase Image An image wherein contrast results only from differences in refractive index at interfaces. Glass in air is an example of a phase image.

Phase-contrast Microscopy An optical configuration of a microscope's objective and condenser that amplifies visible contrast by enhancing small differences in refractive index.

Photoacoustic When modulated infrared radiation is absorbed by a sample, the substance heats and cools in response the energy impinging on it. The heating and cooling is converted into a pressure wave that can be communicated to a surrounding gas and detected by an acoustic detector (essentially a sensitive microphone in the enclosed sample chamber). The acoustic detector replaces the infrared detector of the spectrometer. Carbon black is commonly used as a reference material.

Photomicrograph A photograph of a small object, the image of which has been magnified. (Not to be confused with a microphotograph, which is an extremely small photograph.)

Pixel The individual light sensitive elements on a CCD array. Each pixel can be considered an independent detector element.

Platen A flat plate that exerts or receives pressure.

Polarization For linear polarization, the manipulation of light to preferentially filter those waves with a path orthogonal to the desired angle of propagation. Typically this involves working at 0 or 90 degree polarization either in the incident laser beam or the collected Raman scatter in a Raman experiment. Polarization is important in Raman, since the Raman tensor is a vector that can exhibit strong polarized responses for solids and liquids, unlike FT-IR where polarization is typically limited to solid crystals.

Polarizer A device (or film) into which ordinary light passes and from which polarized light emerges.

Polymorphs Different crystalline forms of the same compound. This is an important distinction, particularly for pharmaceutical synthesis, since the different forms can affect dissolution, reactivity or other characteristics of drug delivery. The different forms are also recognized as different chemical entities that can be independently covered by patent.

Precision (a.k.a. Reproducibility) Amount of variance observed in multiple measurements of the same sample.

Purge A flow of air that purifies the environment in the spectrometer. Can significantly decrease the spectral interference from water, carbon dioxide and other air impurities. Also used to protect internal components.

Quantitative Analysis The use of peak heights, band ratios, or peak areas to calculate the amount of a substance in an unknown sample.

Raleigh Scatter The dominant scattering event when electrons in a molecule are excited to a virtual state by a laser. This scatter is exactly the same wavelength as the laser, therefore provides no vibrational information about the sample. It is 104 to 106 more intense than Stokes or Anti-Stokes scatter so must be efficiently filtered.

Ratio %T is calculated by dividing the intensity with sample in the beam by the intensity with no sample in the beam (background). This ratio also eliminates any spectral features common to both single beam spectra such as water and CO₂ peaks.

Redundant Aperturing™ Our patented design for masking the infrared energy going (a.k.a. Confocal Dual to and emerging from a sample in an infrared microscope system. One aperture Remote Masking) is located at a sample plane between the source and the sample and another aperture is located at a sample plane between the sample and the detector.

Reference Spectrum An FT-IR spectrum of a known substance. As an example, a reference spectrum of a pure component may be subtracted from a sample spectrum to remove peaks due to the component.

Reflachromat Our design for Schwarzschild-type objectives with adjustable compensation for spherical aberration caused by window thickness.

Reflection/Absorption A method for measuring the absorption spectrum of an absorbing layer on a reflective substrate. The radiation passes through the absorber, reflects from the substrate and passes back through the absorber.

Refractive Index The ratio of the velocity of radiation in a vacuum to its velocity in the medium through which it passes.

Remote Aperture A patented Thermo Scientific optical beam splitting design for Image Beamsplitter microspectroscopy. The infrared beam coming from a radiant energy source is physically split in half with a mirror at an aperture plane before the sample. Radiant energy reflected from the sample returning to the aperture plane is reflected from the mirror to a detector. The beamsplitter provides the highest infrared reflection performance without compromising transmission throughput.

Reprocess To Fourier transform the interferogram data for a spectrum using different transform parameter settings or a different background to improve the final data.

Resolution A measure of how well closely spaced peaks in a spectrum are differentiated. The higher the resolution, the more peaks that can be revealed. Increasing the resolution requires that the distance traveled by the moving mirror be increased. The resolution is approximately twice the data spacing value. May also refer to size of sample in a microscope; see spatial resolution and spectral resolution.

RMS (Root Mean Square) Noise A statistical measurement of the variation in an analytical signal. Most often used to characterize baseline noise.

Sample Compartment A compartment inside a spectrometer or accessory where a sample can be mounted for analysis.

Sampling Spectrum The spectrum of a substance being analyzed.

Scan (1) To collect data with an interferometer. (2) One movement of the moving mirror from the point closest to the beamsplitter to the farthest point or vice versa.

Schwarzschild Objective A specific two mirror design of a reflecting optic used as a microscope objective.

Sensitivity

(1) The ability of an instrument to detect small amounts of a substance as distinguished from noise.

(2) The ability to detect shoulders on peaks and small peaks surrounded by noise features in the baseline using the Find Peaks command.

(3) The ability to select shoulders on peaks and small peaks surrounded by noise features for automatic peak processing.

(4) The ability to detect data collection problems using the spectral quality checks on the Quality tab in the Experiment Setup dialog box.

Shoulder A small hump or variation in curvature on the side of a peak. A shoulder may indicate the presence of a small peak that is obscured by the larger peak.

Signal-to-Noise Ratio (SNR) The ratio of signal in a spectrum to the noise in a spectrum. Signal is often measured as the intensity of a peak, noise is measured as the random fluctuations of the baseline.

Single-Beam Spectrum A spectrum (data in the frequency domain) obtained by Fourier transforming an interferogram (data in the time domain). A single-beam spectrum shows the response at all frequencies in the spectral range. A sample single-beam spectrum can be ratioed against a background single-beam spectrum to produce a sample spectrum with the background information removed.

Smooth To improve the appearance of a spectrum by reducing the fluctuations caused by noise. Smoothing always results in a reduction in resolution.

Source A component inside the spectrometer that emits the infrared radiation that travels to the detector.

Spatial Definition The ability to define a given sampling area in FT-IR microscopy.

Spatial Resolution The fineness of detail that is revealed by the microscope. Usually specified as the minimum distance by which two lines or points in an object must be separated before they can be revealed as separate lines or points in the image.

Spectral Range The range of frequencies included in a spectrum.

Spectral Resolution The ability of an instrument to distinguish between two spectral features that are close to each other in wavenumber. Resolution is measured in terms of the closest two features that can be distinguished. In FT-IR, high resolution is denoted by small numbers, e.g. 0.01 cm⁻¹. Low resolution is denoted by large numbers, e.g. 64 cm⁻¹.

Spectrum A graphical representation of the intensity of the infrared radiation reaching the detector at each frequency or wavelength measured. The intensity at a given frequency or wavelength is determined by the characteristics of the spectrometer and the sample, if one is present. See also Beer's Law.

Spectrum Title A useful description of a spectrum that is saved with the spectrum. The title of a spectrum appears in the title box when the spectrum is selected.

Specular Reflection Specular reflection is the Fresnel reflection from the exterior surface of a material, without the beam penetrating the sample. Specular reflection obeys the law of reflection, where the angle of reflection equals the angle of incidence.

Spherical Aberration When a ray of a single color passing through the outer periphery of a lens does not come to the same focus as the rays passing through the center. The image is more or less blurred.

Stokes Scatter The low energy Raman event resulting from a molecule in the ground vibrational level, being excited to a virtual state and then relaxing back to an upper vibrational level. This is stronger than Anti-Stokes Raman signal because the Boltzmann distribution predicts most molecules will reside in the ground vibrational level prior to excitation. The Stokes spectrum will be identical in band positions to the Anti-Stokes but on the opposite side of the laser line.

Targeting The placement of a defining aperture at a sample plane between the source and the sample in an infrared microscope.

Throughput The intensity of the infrared energy that reaches the detector. This intensity value is shown above the live display on the Bench tab in the Experiment Setup dialog box. Often used to express the relative intensity of energy remaining when a sampling accessory is used.

Transflectance Also known as reflection-absorption. A spectroscopy technique in which a beam enters the sample, reflects off a reflective surface, and passes through the sample layer a second time. Under many conditions, particularly when studying liquids, the resulting spectrum resembles a transmission spectrum.

Transmission The fraction of the incident radiation that passes completely through an object or sample.

Transmission Spectrum A spectrum that shows how the transmittance of a sample varies with frequency or wavelength.

Transmittance Spectrum The fraction of radiation at each wavelength that passes through a sample expressed as where:

I_0 is the incident radiation intensity

I is the intensity of radiation leaving the sample

Transmittance is frequently expressed as a percentage. In the infrared, transmittance spectra are usually plotted as %T vs. wavenumber.

USP (United States Pharmacopeia) A private, voluntary, not-for-profit organization established in 1820. USP encourages and promotes the science and art of medicine and pharmacy by selecting research and experiment and other proper methods and by naming such materials as may be properly used as medicines and drugs with formulas for the preparations, by establishing one uniform standard and guide for the use of those engaged in the practice of medicine and pharmacy in the United States of America whereby the identity, strength and purity of all such medicines and drugs may be accurately determined. USP also prints and distributes at suitable intervals such formulas; the results of research and experiment methods; and a listing of members, pharmacists, and physicians generally in the United States.

Validation A high-level review to determine the conformity of a system, process, or product to internally established standards and the appropriateness of those standards. User validation determines the conformity of a system, process, or product to internally established standards relating to its use in a specific (user site) environment; and the appropriateness of those standards to that specific site. Vendor validation refers to the determination of the conformity of a system, process, or product to those internally established standards in use by the vendor and the appropriateness of those standards.

Validation Wheel A wheel inside an instrument that contains standards used to verify performance results.

View-Thru™ An arrangement that allows viewing both the aperture and the entire sample field at the same time.

Wavelength The distance between corresponding points in consecutive light waves. Wavelength is measured in micrometers or nanometers.

Wavenumber The number of waves per centimeter. Wavenumber is the inverse of wavelength. Often used as the X-axis unit of an FT-IR spectrum.

Working Distance The distance between the sample and the first mechanical obstruction of the objective, (a.k.a. Free Working Distance) when the objective is focused on the sample.

Zero Filling A method of improving the line shape of a spectrum by adding interpolated data points.