

APPLIED SPECTROSCOPY

Spectroscopic Nomenclature

Transmittance T , τ	Ratio of the radiant power transmitted by the sample to the radiant power incident on the sample. The incident radiant power is usually obtained as that transmitted by a non-absorbing reference material. (Not used: transmittancy or transmission). (Footnotes 1 to 3).	Molar absorptivity or Molar (decadic) absorption coefficient ϵ	Internal absorbance divided by the product of sample path length, λ , and mole concentration, c , of the absorbing material. $\epsilon = A_i/c\ell$. SI unit: $\text{m}^2 \text{mol}^{-1}$. Common unit: $\text{L mol}^{-1} \text{cm}^{-1}$; $\text{cm}^2 \text{mol}^{-1}$. (Not used: molar absorbancy index or molar extinction coefficient.)
Percent transmission	Transmittance $\times 100$.		
Absorptance α	Ratio of the radiant power absorbed by the sample to the incident radiant power. (Footnotes 1 to 3).	Naperian absorbance, A^e	The absorbance calculated in base e , i.e., $\ln(1/T)$
Reflectance ρ	Ratio of the radiant power reflected by the sample to the incident radiant power. (Footnotes 1 to 3).	Linear absorption coefficient, α	The Naperian absorbance divided by the path length, $\alpha = A_e/l$
Emittance ϵ	Ratio of the radiant flux emitted by the sample to that emitted by a black body at the same temperature. (Footnotes 3 and 5).	Beer-Lambert law	Absorptivity of a substance is constant with respect to changes in path length and concentration of the absorber. Often called Beer's law when only changes in concentration are of interest.
Internal transmittance T_i , τ_i	Ratio of the radiant power transmitted by the sample to the incident radiant power, fully corrected for reflection losses and any window absorption. (Footnotes 6 and 7).	Net absorption cross-section σ_{net}	The absorptivity per molecule, i.e., the molar absorptivity, ϵ , divided by Avogadro's number, usually corrected to base e through $\sigma_{\text{net}} = 2.303 \epsilon/N_A$. SI unit: m^2 .
Internal absorptance α_i	Ratio of the radiant power absorbed by the sample to the incident radiant power, fully corrected for reflection losses and any window absorption. (Footnotes 6 and 7).	Mass concentration ρ , γ	Mass of sample divided by volume of solution or mixture. SI unit: kg/m^3 . Common unit: g/L ; mg/L .
Absorbance A	Negative logarithm to the base 10 of the transmittance: $A = -\log_{10}(T)$. (Not used: absorbancy, extinction, or optical density). (Footnote 3).	Amount concentration or mole concentration or molarity c	Amount of sample divided by volume of solution or mixture. SI unit: mol/m^3 . Common unit: mol/L .
Internal absorbance A_i	Negative logarithm to the base 10 of the internal transmittance: $A_i = -\log_{10}(T_i)$.	Mole fraction x_B	The number of moles of component B divided by the total number of moles in the mixture. Frequently given as parts-per-million or billion, ppm or ppb (Footnote 8).
Absorptivity α	Internal absorbance divided by the product of sample path length, ℓ , and mass concentration, ρ , of the absorbing material. $\alpha = A_i/\rho\ell$. SI unit: $\text{m}^2 \text{kg}^{-1}$. Common unit: $\text{cm}^2 \text{g}^{-1}$; $\text{L g}^{-1} \text{cm}^{-1}$. (Not used: absorbancy index, extinction coefficient, or specific extinction.)	Mass fraction w_B	The mass of component B divided by the total mass of the sample. Frequently given as ppm or ppb (Footnotes 8 and 9).
		Volume fraction ϕ_B	The volume of component B divided by the total volume of the sample. Frequently given as ppm or ppb. (Footnotes 8 and 9).
		Pressure fraction	The partial pressure of component divided by the total pressure of the sample. Frequently given as ppm or ppb. (Footnotes 8, 9, and 10).

Wavelength λ	Smallest distance in the direction of propagation between equivalent points on a wave at constant time. SI unit: m. Common unit: μm ; nm.	Remission	The process by which radiation that is incident on one side of a scattering sample is redirected to leave the sample on the same side; often called diffuse reflection (Footnote 3).
Frequency f , ν	Number of cycles in unit time. SI unit: Hertz ($1 \text{ Hz} = 1 \text{ s}^{-1}$).	Diffuse transmission	The process in which radiation is transmitted by a scattering sample and leaves the sample in directions other than that required by Snell's law of refraction. The process is complicated and involves transmission, reflection, and scattering (Footnote 3).
Wavenumber σ or $\tilde{\nu}$	Number of waves in unit length, i.e., $\sigma = 1/\lambda$. σ is used for wavenumber in medium of refractive index n ; $\tilde{\nu}$ is used for wavenumber in vacuum, i.e., $\tilde{\nu} = 1/n\lambda$. When used to characterize radiation, the wavenumber is defined as the reciprocal of the wavelength in vacuum and the symbol $\tilde{\nu}$ is used. SI unit: m^{-1} . Common unit: cm^{-1} .	Diffuse reflectance	The ratio of the spectral intensity reflected by a scattering sample to that reflected by an equivalent non-absorbing reference that replaces the sample; sometimes refers to a measurement where specularly reflected radiation has been prevented from reaching the detector. The term "Remittance" may be used in place of "Diffuse reflectance" to emphasize inclusion of the specularly reflected radiation. SI unit: none, a dimensionless quantity.
Raman wavenumber shift $\Delta\tilde{\nu}$	The vacuum wavenumber of the exciting light minus the vacuum wavenumber of the Raman scattered light. SI unit: m^{-1} . Common unit: cm^{-1} .	Remission fraction remittance, R	The fraction of the incident radiation that undergoes remission. The sum of the remission fraction (R), the transmission fraction (T), and the absorption fraction (A) equals one. SI unit: none, a dimensionless quantity.
Sample path length λ , b	The length of sample through which the radiation passes. SI unit: m. Common unit: μm ; mm; cm.	Transmission fraction Total transmittance Total transmission fraction T	The fraction of the spectral intensity incident upon a scattering sample that leaves the opposite side of the sample. SI unit: none, a dimensionless quantity.
Intensity I	The radiant power that crosses unit area. Intensity and irradiance are formally the same quantity, but the term intensity is usually used for collimated beams of radiation. SI unit: W m^{-2} .	Kubelka–Munk function Remission function $f(R_\infty)$	This function is defined as: $f(R_\infty) = (1 - R_\infty)^2/2R_\infty$ where R_∞ is the diffuse reflectance from a sample of infinite depth. Theoretically, $f(R_\infty)$ equals the ratio of the linear absorption coefficient to the scattering coefficient. Under the assumptions of the Kubelka–Munk theory, if the scattering coefficient at a given wavenumber is a constant for a given set of samples, then $f(R_\infty)$ is directly proportional to the product of the absorptivities and concentrations of the components of a mixture, analogous to the behavior of absorbance under Beer's law.
Irradiance I	The radiant power received on unit area. SI unit: W m^{-2} .	Volume reflection	The process by which light enters a scattering sample, is refracted and reflected by the particles, and ultimately emerges from the surface at which it entered the sample. The combined process of volume reflection and specular reflection is known as diffuse reflection or remission. (Also known as Kubelka–Munk reflection.)
Diffuse reflection	The process in which radiation is incident on a scattering sample at a certain angle and is returned (or remitted) over all angles. Diffuse reflection is a complicated process and involves transmission, reflection, and scattering (Footnote 3).	Linear remission coefficient b	The negative napierian logarithm of the fraction of light remitted by a non-absorbing scattering sample, divided by the path length ℓ . $b = -\ln_e(I_R/I_0)/\ell$. SI unit: m^{-1} .
Kubelka–Munk reflection	The process of light penetrating into a powdered sample and re-emerging from the surface of incidence; sometimes incorrectly called diffuse reflection (Footnote 3).		

Penetration depth d_p	<p>In attenuated total reflection, the distance from the boundary with the internal reflection element at which the mean square electric field intensity of the evanescent wave, i.e., the intensity of a collimated radiation beam, is reduced to $1/e$ of its value at the boundary.</p> <p>In photoacoustic (PA) spectroscopy, an analogous definition may be cited for strongly absorbing samples. For weakly absorbing PA samples, the depth of penetration is given by the thermal diffusion depth. In practice, the depth below the surface that gives rise to most of the measured PA spectrum is the smaller of the thermal diffusion depth and the optical absorption depth.</p> <p>SI unit: m. Common unit: μm.</p>	Reflection-absorption	<p>A sampling technique used to investigate films on flat metallic surfaces in which radiation is passed onto the surface of the sample at grazing incidence. Usually applied to the case where the thickness of the film is much less than the wavelength of the radiation. (Footnote 3.)</p>
Optical absorption depth μ_β	<p>The depth in a sample at which the radiant intensity is reduced to $1/e$ of its value at the surface of the sample. It equals the reciprocal of the linear absorption coefficient.</p> <p>SI unit: m. Common unit: μm.</p>	<p>Reflection-absorption at grazing incidence Infrared reflection-absorption spectroscopy, IRRAS Reflection-absorption infrared spectroscopy, RAIRS</p>	<p>Reflection-absorption with very thin layers of an absorbing material on a metallic surface and the angle of incidence between 70° and 90°; i.e., with the incident radiation beam traveling nearly parallel to the surface. The electric vector of the radiation is then either parallel or nearly perpendicular to the surface, which allows improved discrimination between species at the surface and those in the bulk.</p>
Attenuated total reflection, ATR	<p>A sampling technique in which the evanescent wave of a beam that has been internally reflected from the internal surface of a material of high refractive index at an angle greater than the critical angle is absorbed by a sample that is held very close to the surface. (Footnote 3.)</p>	Transflection	<p>A sampling technique used to investigate relatively thick films on a reflecting surface of either a metal or "low-e" glass substrate (for mid-infrared measurements) or a diffusely reflecting substrate such as a ceramic disk for near-infrared measurements. The thickness of the film is large enough to yield an interpretable spectrum. (Footnote 3.)</p>
Attenuated total reflectance	<p>The ratio of the spectral intensity of the beam in an ATR measurement measured with and without a sample present at the surface of the internal reflection element. (Footnote 3.)</p>	Transflectance	<p>The ratio of the spectral intensity of the transflected beam to the spectral intensity of the incident beam in a transflection experiment. 'Transflectance' has also been used to mean 'transflection'; this is clearly confusing and is strongly discouraged (Footnote 3).</p>
Internal reflection element, IRE	<p>A transparent material of high refractive index that is used for ATR measurements. Note: These materials are often not crystalline and so should not be called ATR crystals.</p>	Circular birefringence	<p>$n^L - n^R$, the difference between the refractive index of a medium for left, n^L, and right, n^R, circularly polarized radiation. Like the refractive indices, circular birefringence changes with wavenumber.</p> <p>SI unit: none, a dimensionless quantity.</p>
Low-emissivity ("low-e") glass slides	<p>Slides that are made of glass coated with a thin Ag/SnO₂ layer. They are chemically inert and nearly transparent to visible light. However, they reflect mid-infrared radiation almost completely and thus are ideal and inexpensive substrates for transflection infrared microspectroscopy, as they allow both visual and infrared images to be collected from the same sample.</p>	Circular dichroism	<p>In general, the property of different absorption of left and right circularly polarized radiation by an optically active material. Specifically, the circular dichroism is $k^L - k^R$, where k^L and k^R are the absorption indices (imaginary refractive indices) of the sample for left and right circularly polarized radiation, respectively. Note that some authors use the absorptivity or molar absorptivity instead of the absorption index. Like absorption of radiation, circular dichroism changes with wavenumber.</p>

Vibrational circular dichroism, VCD	Specifically, circular dichroism, $k^L - k^R$, for vibrational transitions.	2D correlation spectrum	A three-dimensional surface in which two of the dimensions show wavenumber $\tilde{\nu}_1$ and wavenumber $\tilde{\nu}_2$ and the third axis shows a correlation function of the spectral intensities observed at $\tilde{\nu}_1$ and $\tilde{\nu}_2$. The shape of the surface shows whether the bands at the two wavenumbers are or are not correlated, and hence allows deductions to be made about the extent to which the different parts of the molecule are linked in their response to the applied external perturbation.
2D correlation spectroscopy	A form of spectroscopy in which spectra are recorded at different levels of an applied external perturbation of the sample and are processed to yield a 2D correlation spectrum. The applied external perturbation may be cyclic or non-cyclic, and for vibrational spectroscopy changes of temperature, pressure, or mechanical strain have been used. The technique is applicable to all forms of vibrational spectroscopy.	Fourier transform infrared spectroscopy, FT-IR	A form of spectroscopy in which an interference pattern is recorded that, on Fourier transformation, is subsequently converted to the spectrum. The abbreviation should be FT-IR to distinguish it from frustrated total internal reflection. (See Footnote 4).

Notes

1. For collimated beams, the *radiant power* can be replaced by *intensity*. It is usually measured as the unratiod spectrum obtained from a Fourier transform spectrometer or a single-beam spectrum from a dispersive spectrometer.
2. If scattering and luminescence can be neglected, $T + \alpha + \rho = 1$.
3. A spectrum should generally be termed a *transmission spectrum*, an *absorption spectrum*, a *reflection spectrum*, a *diffuse reflection spectrum*, an *attenuated total reflection spectrum*, or an *emission spectrum*. The same adjectives should be used with *spectra* when more than one spectrum is meant. The terms *transmittance spectrum*, *absorbance spectrum*, *reflectance spectrum*, *diffuse reflectance spectrum*, *attenuated total reflectance spectrum*, or *emittance spectrum*, should only be used when the ordinate explicitly presents the transmittance, absorbance, reflectance, diffuse reflectance, attenuated total reflectance, or emittance spectrum.
4. Once the instrument on which the spectrum has been measured has been defined as a FT-IR spectrometer (e.g., in the Experimental section), spectra should subsequently be referred to as "infrared spectra", or simply "spectra", not "FT-IR spectra".
5. The *radiant flux* can be replaced by *radiant power* if the sample and the black body have the same area, and by *intensity* if in addition the emission is measured as a collimated light beam.
6. In optical spectroscopy, internal properties such as the internal transmittance, T_i and internal absorptance α_i are defined to exclude surface effects and effects of the sample cell such as reflection losses or vignetting. Thus, $T_i + \alpha_i = 1$ if scattering and luminescence can be neglected. This leads to the usual form of the Beer Lambert law, $I_{tr}/I_0 = T_i = 1 - \alpha_i = \exp(-\epsilon c l)$.
7. In gas-phase spectroscopy in which the sample cell remains in the light beam between spectra, the ratio of the spectrum of the cell full of sample to the spectrum of the empty cell gives the internal transmittance without correction. This is usually the case in GC/FT-IR, for example. Similarly, the spectrum of a cell full of a solution of a dilute solute divided by the spectrum of the same cell full of solvent gives the internal transmittance of the solute directly, provided that the position of the cell in the beam is unchanged. In both cases, the internal absorptance is obtained directly as $\alpha_i = 1 - T_i$. However, to obtain the internal transmittance of a cell full of a neat liquid, or of the solvent of a solution, the transmittance spectrum obtained with a suitable reference requires correction for reflection effects.
8. Authors should use the American billion, 10^9 , in preference to the European billion, 10^{12} , and the American trillion, 10^{12} , in preference to the European trillion, 10^{18} . Thus 1 part per billion (ppb) is one part in 10^9 and 1 part per trillion (ppt) is one part in 10^{12} . Parts per thousand should be abbreviated as ppth to distinguish it from parts per trillion.
9. Fractions are dimensionless quantities. Terms like ppm and ppb should only be used to describe dimensionless quantities. The frequently used terms ppmg, ppbv, etc., to mean parts-per-million grams, parts-per-million volume, etc., are ambiguous because they are used to describe sometimes mass fractions or volume fractions and sometimes ratios of mass to volume. Thus, their use should be avoided unless their meaning is clearly defined in the paper. In particular the use of ppmv to conveniently describe a ratio of mass to volume in the units mg/L should be avoided unless it is clearly stated that ppmv describes the mass concentration in mg/L.
10. The pressure fraction is usually essentially equal to the mole fraction through Dalton's Law of partial pressures.