



Standard Terminology Relating to Molecular Spectroscopy^{1, 2}

This standard is issued under the fixed designation E131; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ϵ) indicates an editorial change since the last revision or reapproval.

1. Scope

1.1 The values stated in SI units are to be regarded as standard. No other units of measurement are included in this standard.

2. Referenced Documents

2.1 ASTM Standards:³

[E135 Terminology Relating to Analytical Chemistry for Metals, Ores, and Related Materials](#)

[E168 Practices for General Techniques of Infrared Quantitative Analysis \(Withdrawn 2015\)⁴](#)

[E204 Practices for Identification of Material by Infrared Absorption Spectroscopy, Using the ASTM Coded Band and Chemical Classification Index \(Withdrawn 2014\)⁴](#)

[E284 Terminology of Appearance](#)

[E386 Practice for Data Presentation Relating to High-Resolution Nuclear Magnetic Resonance \(NMR\) Spectroscopy](#)

[E456 Terminology Relating to Quality and Statistics](#)

2.2 Other Documents:⁵

[ISO Guide 30–1981 \(E\) Terms and definitions used in connections with reference materials](#)

3. Terminology

absorbance, A —the logarithm to the base 10 of the reciprocal of the transmittance, (T).

$$A = \log_{10}(1/T) = -\log_{10}T \quad (1)$$

DISCUSSION—In practice the observed transmittance must be substituted for T . Absorbance expresses the excess absorption over that of a specified reference or standard. It is implied that compensation has

¹ This terminology is under the jurisdiction of ASTM Committee E13 on Molecular Spectroscopy and Separation Science and is the direct responsibility of Subcommittee E13.94 on Terminology.

Current edition approved May 1, 2015. Published June 2015. Originally approved in 1957. Last previous edition approved in 2010 as E131 – 10. DOI: 10.1520/E0131-10R15.

² For other definitions relating to nuclear magnetic resonance, see Practice E386.

³ For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

⁴ The last approved version of this historical standard is referenced on www.astm.org.

⁵ Available from American National Standards Institute (ANSI), 25 W. 43rd St., 4th Floor, New York, NY 10036, <http://www.ansi.org>.

been effected for reflectance losses, solvent absorption losses, and refractive effects, if present, and that attenuation by scattering is small compared with attenuation by absorption. Apparent deviations from the absorption laws (see **absorptivity**) are due to inability to measure exactly the true transmittance or to know the exact concentration of an absorbing substance.

absorption band—a region of the absorption spectrum in which the absorbance passes through a maximum.

absorption coefficient, α —a measure of absorption of radiant energy from an incident beam as it traverses an absorbing medium according to Bouguer's law, $P/P_o = e^{-\alpha b}$.

DISCUSSION—In IRS, α is a measure of the rate of absorption of energy from the evanescent wave.

absorption parameter, a —the relative reflection loss per reflection that results from the absorption of radiant energy at a reflecting surface: $a = 1 - R$, and R = the reflected fraction of incident radiant power.

absorption spectrum—a plot, or other representation, of absorbance, or any function of absorbance, against wavelength, or any function of wavelength.

absorptivity, a —the absorbance divided by the product of the concentration of the substance and the sample pathlength, $a = A/bc$. The units of b and c shall be specified.

DISCUSSION—1—The recommended unit for b is the centimetre. The recommended unit for c is kilogram per cubic metre. Equivalent units are g/dm^3 , g/L , or mg/cm^3 .

DISCUSSION—2—The equivalent IUPAC term is “specific absorption coefficient.”

absorptivity, molar, ϵ —the product of the absorptivity, a , and the molecular weight of the substance.

DISCUSSION—The equivalent IUPAC term is “molar absorption coefficient.”

acceptance angle, n —for an optical fiber, the maximum angle, measured from the longitudinal axis or centerline of the fiber to an incident ray, within which the ray will be accepted for transmission along the fiber by total internal reflection.

DISCUSSION—If the incidence angle exceeds the acceptance angle, optical power in the incident ray will be coupled into leaky modes or rays, or lost by scattering, diffusion, or absorption in the cladding. For a clad step-index fiber in the air, the sine of the acceptance angle is given by the square root of the difference of the squares of the refractive indexes of the fiber core and the cladding, that is, by the relation as follows:

$$\sin A = \sqrt{n_1^2 - n_2^2} \quad (2)$$

where A is the acceptance angle and n_1 and n_2 are the refractive indexes of the core and cladding, respectively. If the refractive index is a function of distance from the center of the core, as in the case of graded index fibers, then the acceptance angle depends on the distance from the core center. The acceptance angle is maximum at the center, and zero at the core-cladding boundary. At any radius, r , the sine of the acceptance angle of a graded index fiber is defined in compliance with that of a step-index fiber as follows:

$$\sin A_r = \sqrt{n_1^2 - n_2^2} \quad (3)$$

where A_r is the acceptance angle at a point on the entrance face at a distance, r , from the center, n_r is the refractive index of the core at a radius, r , and n_2 is the refractive index of the cladding. In air, $\sin A$ and $\sin A_r$ are the numerical apertures. Unless otherwise stated, acceptance angles and numerical apertures for fiber optics are those for the center of the endface of the fiber, that is, where the refractive index, and hence the numerical aperture, is the highest.

accuracy—the closeness of agreement between an observed value and an accepted reference value (see Terminology E456).

DISCUSSION—The term accuracy, when applied to a set of observed values, will be a combination of a random component and a common systematic error or bias component. Since in routine use, random components and bias components cannot be completely separated, the reported “accuracy” must be interpreted as a combination of these two components.

active fiber optic chemical sensor, n —a fiber optic chemical sensor in which a transduction mechanism other than the intrinsic spectroscopic properties of the analyte is used to modulate the optical signal.

DISCUSSION—Examples include a pH sensor composed of a chemical indicator substance whose color changes with pH, and an oxygen sensor coupled to an optical fiber bearing a chemical indicator whose fluorescence intensity depends on oxygen concentration.

aliasing—the appearance of features at wavenumbers other than their true value caused by using a sampling frequency less than twice the highest modulation frequency in the interferogram; also known as “folding.”

analytical curve—the graphical representation of a relation between some function of radiant power and the concentration or mass of the substance emitting or absorbing it.

analytical wavelength—any wavelength at which an absorbance measurement is made for the purpose of the determination of a constituent of a sample.

angle of incidence, θ —the angle between an incident radiant beam and a perpendicular to the interface between two media.

anti-Stokes line (band)—a Raman line (band) that has a frequency higher than that of the incident monochromatic beam.

aperture of an IRE, A' —that portion of the IRE surface that can be utilized to conduct light into the IRE at the desired angle of incidence.

apodization—modification of the ILS function by multiplying the interferogram by a weighting function the magnitude of which varies with retardation.

DISCUSSION—This term should strictly be used with reference to a weighting function whose magnitude is greatest at the centerburst and decreases with retardation.

attenuated total reflection (ATR)—reflection that occurs when an absorbing coupling mechanism acts in the process of total internal reflection to make the reflectance less than unity.

DISCUSSION—In this process, if an absorbing sample is placed in contact with the reflecting surface, the reflectance for total internal reflection will be attenuated to some value between zero and unity ($0 < R < 1$) in regions of the spectrum where absorption of the radiant power can take place.

attenuation index, κ —a measure of the absorption of radiant energy by an absorbing material. κ is related to the absorption coefficient by: $n\kappa = ac_o/4\pi v$, where c_o = the speed of light in vacuo, v = the frequency of radiant energy, and n = the refractive index of the absorbing medium.

background—apparent absorption caused by anything other than the substance for which the analysis is being made.

baseline—any line drawn on an absorption spectrum to establish a reference point representing a function of the radiant power incident on a sample at a given wavelength.

basic NMR frequency, ν_o —the frequency, measured in hertz (Hz), of the oscillating magnetic field applied to induce transitions between nuclear magnetic energy levels.

bathochromic shift, n —change of a spectral band to longer wavelength (lower frequency) because of structural modifications or environmental influence; also known as “red shift.”

beamsplitter—a semireflecting device used to create, and often to recombine, spatially separate beams.

DISCUSSION—Beamsplitters are often made by depositing a film of a high refractive index material onto a flat transmitting substrate with an identical compensator plate being held on the other side of the film.

beamsplitter efficiency—the product $4RT$, where R is the reflectance and T is the transmittance of the beamsplitter.

Beer’s law—the absorbance of a homogeneous sample containing an absorbing substance is directly proportional to the concentration of the absorbing substance (see also **absorptivity**)

bias—a systematic error that contributes to the difference between a population mean of the measurements or test results and an accepted or reference value (see Terminology E456).

DISCUSSION—Bias is determined by the following equation:

$$\text{bias} = \bar{e} = \frac{1}{n} \sum_{i=1}^n e_i \quad (4)$$

where:

n = the number of observations for which the accuracy is determined,

e_i = the difference between a measured value of a property and its accepted reference value, and

\bar{e} = the mean value of all the e_i .

Bouguer's law—the absorbance of a homogeneous sample is directly proportional to the thickness of the sample in the optical path.

DISCUSSION—Bouguer's law is sometimes also known as Lambert's law.

boxcar truncation—identical effective weighting of all points in the measured interferogram prior to the Fourier transform; all points outside of the range of the measured interferogram take a value of zero.

buffer—*in fiber optics*, see **fiber optic buffer**.

bulk reflection—reflection in which radiant energy is returned exclusively from within the specimen.

DISCUSSION—Bulk reflection may be diffuse or specular.

centerburst—the region of greatest amplitude in an interferogram.

DISCUSSION—For unchirped or only slightly chirped interferograms, this region includes the “zero path difference point” and the “zero retardation point.”

certified reference material, n —a reference material, the composition or properties of which are certified by a recognized standardizing agency or group.

DISCUSSION—A certified reference material produced by the National Institute of Standards and Technology (NIST) is designated a Standard Reference Material (SRM).

chemical shift (NMR), δ —the defining equation for δ is the following:

$$\delta = \frac{\Delta\nu}{\nu_R} \times 10^6 \quad (5)$$

where ν_R is the frequency with which the reference substance is in resonance at the magnetic field used in the experiment and $\Delta\nu$ is the frequency difference between the reference substance and the substance whose chemical shift is being determined, at constant field. The sign of $\Delta\nu$ is to be chosen such that shifts to the high frequency side of the reference shall be positive.

DISCUSSION—If the experiment is done at constant frequency (field sweep) the defining equation becomes

$$\delta = \frac{\Delta\nu}{\nu_R} \times \left(1 - \frac{\Delta\nu}{\nu_R}\right) \times 10^6 \quad (6)$$

chirping—the process of dispersing the zero phase difference points for different wavelengths across the interferogram, so that the magnitude of the signal is reduced in the short region of the interferogram where all wavelengths would otherwise constructively interfere.

clad—see **cladding**.

cladding, n —*of an optical fiber*, a layer of a optically transparent lower refractive index material in intimate contact with a core of higher refractive index material used to achieve total internal reflection.

DISCUSSION—The cladding confines electromagnetic waves to the core, provides some protection to the core, and also transmits evanescent waves that usually are bound to waves in the core.

concentration, c —the quantity of the substance contained in a unit quantity of sample.

DISCUSSION—For solution work, the recommended unit of concentration is grams of solute per litre of solution.

core, n —*of an optical fiber*, the center region of an optical waveguide through which radiant energy is transmitted.

DISCUSSION—In a dielectric waveguide such as an optical fiber, the refractive index of the core must be higher than that of the cladding. Most of the radiant energy is confined to the core.

correlation coefficient (r)—a measure of the strength of the linear relationship between X and Y , calculated by the equation:

$$r_{xy} = \frac{\left(\sum_{i=1}^n X_i Y_i\right)}{\left(\sum_{i=1}^n X_i^2\right)^{1/2} \left(\sum_{i=1}^n Y_i^2\right)^{1/2}} \quad (7)$$

where:

n = the number of observations in X and Y .

DISCUSSION— X_i and Y_i are any two mean corrected variables. For the simple linear regression only,

$$r_{xy} = R = (\text{sign of } b_1)(R^2)^{1/2} \quad (8)$$

where:

R^2 = the coefficient of multiple determination.

critical angle, θ_c —the angle whose sine is equal to the relative refractive index for light striking an interface from the greater to the lesser refractive medium: $\theta_c = \sin^{-1} n_{21}$, where n_{21} = the ratio of the refractive indices of the two media.

DISCUSSION—Total reflection occurs when light is reflected in the more refractive of two media from the interface between them at any angle of incidence exceeding the critical angle.

depth of penetration, d_p —in internal reflection spectroscopy, the distance into the less refractive medium at which the amplitude of the evanescent wave is e^{-1} (that is, 36.8 %) of its value at the surface:

$$d_p = \frac{\lambda_1}{2\pi(\sin^2\theta - n_{21}^2)^{1/2}} \quad (9)$$

where: $n_{21} = n_2/n_1$ = refractive index of sample divided by that of the IRE; $\lambda_1 = \lambda/n_1$ = wavelength of radiant energy in the sample; and θ = angle of incidence.

derivative absorption spectrum—a plot of rate of change of absorbance or of any function of absorbance with respect to wavelength or any function of wavelength, against wavelength or any function of wavelength.

difference absorption spectrum—a plot of the difference between two absorbances or between any function of two absorbances, against wavelength or any function of wavelength.

diffuse reflection—reflection in which the flux is scattered in many directions by diffusion at or below the surface (see Terminology E284).

digitization—the conversion of an analog signal to digital values using an analog-to-digital converter “sampling” or “digital sampling.”

digitization noise—the noise generated in an interferogram through the use of an analog-to-digital converter whose least