Glossary of Terms used in Vibrational Spectroscopy

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Quantity	Symbol	Meaning
$1/f$ noise		Noise for which the amplitude increases as the modulation frequency decreases.
2-D 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 2-D correlation spectrum. The applied external perturbation may be cyclic or non-cyclic, and for vibrational spectroscopy has been, for example, changes of temperature, pressure, or mechanical strain. The technique is applicable to all forms of vibrational spectroscopy. See also "2-D correlation spectrum" and "Dynamic spectrum".
2-D correlation spectrum		A three-dimensional surface in which two of the dimensions show wavenumber $\tilde{v}_1$ and wavenumber $\tilde{v}_2$ and the third axis shows a correlation function of the spectral intensities observed at $\tilde{v}_1$ and $\tilde{v}_2$. 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. See also "2-D correlation spectroscopy" and "Dynamic spectrum".
Absorbance	A	Widely used term for decadic absorbance (see below), napierian absorbance (see below) and other quantities. Chemists usually mean the decadic absorbance, frequently uncorrected for reflection and other non-absorption effects that must be removed before the absorbance has absolute numerical significance. See also "Experimental absorbance" and "Internal absorbance".

Quantity	Symbol	Meaning
Absorbance (continued)		SI unit: none, a dimensionless quantity. Confusingly, the term absorbance is also widely used for the negative log of the ratio of the final to the incident intensities of processes other than transmission, such as attenuated total reflection and diffuse reflection.
Absorptance	α	In spectroscopy, the ratio of the spectral intensity (see below) at wavenumber $\tilde{v}$ absorbed by the sample to that incident on the sample. For non-scattering and non-luminescent samples the sum of absorptance (α) transmittance (T) and reflectance (ρ) equals one. SI unit: none, a dimensionless quantity.
Absorption fraction	A	A term used instead of absorptance (see above) for scattering samples. It is the fraction of the spectral intensity absorbed by a scattering sample to that incident on the sample. The sum of the absorption fraction A, the transmission fraction T (see below), and the remission fraction R (see below) equals one.
Absorption index	k	The imaginary part of the refractive index. Sometimes called the extinction index by physicists. SI unit: none, a dimensionless quantity.
Absorption spectrum		A general term for the spectrum of radiation absorbed by a sample. If the ordinate quantity is the absorbance, but not otherwise, the spectrum may be called an absorbance spectrum.
Absorptivity	α, a	The decadic absorbance (see below) divided by the product of sample path-length, l, and mass concentration, ρ, of the absorbing material: $\alpha = A_{10}/\rho l$ SI unit: $m^2\,kg^{-1}$. Common unit: $cm^2\,g^{-1} = 0.1\,m^2\,kg^{-1}$; $L\,g^{-1}\,cm^{-1} = 100\,m^2\,kg^{-1}$. The absorptivity is a Beer–Lambert absorption coefficient. Note that this use of absorptivity continues, in spite of international agreement with non-chemical societies that absorptivity be reserved for absorptance per unit length.
Accidental degeneracy		The condition that different states have the same energy by coincidence, not because symmetry requires it. See also "degenerate" and "degeneracy".
Acoustic vibration Acoustic branch		In three of the branches of the dispersion curves of crystal vibrations, the frequency tends to zero as the wavelength tends to infinity, i.e. as the wavevector tends to zero. The vibrations with zero-wave-vector in these branches are the three translations of the crystal. These three branches are the acoustic branches and the vibrations in them are the acoustic vibrations. See also "Crystal vibrations", "Longitudinal vibration", "Transverse vibration" and "Optic vibration".
Acousto-optical tunable filter	AOTF	A solid-state electronically tunable spectral bandpass filter, which relies on the acoustic diffraction of light in an anisotropic medium. An AOTF provides fast discrete wavelength selection over a broad range. It consists of a birefringent crystal such as TeO_2 bonded to a piezoelectric detector. When a radio-frequency is applied to the transducer, the propagating acoustic wave

Quantity	Symbol	Meaning
		produces a periodic modulation of the index of refraction within the crystal. This creates a moving phase grating that diffracts portions of the incident radiation. AOTFs are available for the wavelength range from about 200 to 4500 nm, although individual filters only cover ranges of between 150 and 1500 nm. They offer resolutions between 2 nm at low wavelengths to about 20 nm at high wavelengths.
Aliasing		See "Folding".
Amount concentration	c	Amount (number of moles), n, of component divided by the volume of the mixture, e.g. for solute j, $c_j = n_j/V$. Frequently called molar concentration or mole concentration (see below). SI unit: $\mathrm{mol\,m^{-3}}$. Common unit: $\mathrm{mol\,dm^{-3} = mol\,L^{-1} = 1000\,mol\,m^{-3}}$. N.B. In polymer science c is often used for mass concentration.
Amplifier-readout noise		The noise that is observed, due to the processes of reading an amplifier, in the absence of analytical, background and dark current signals.
Amplitude modulation		Modulation of the amplitude of the radiation beam; by the movement of the moving mirror in a rapid scan Fourier transform spectrometer or by a mechanical chopper in other spectrometers.
AMTIR		The name AMTIR™ is an acronym for amorphous material transmitting infrared radiation. The materials are glasses made from elements of groups 4, 5 and 6. The AMTIRs are hard but can be brittle. Two examples are AMTIR-1 which is $\mathrm{Ge_{33}As_{12}Se_{55}}$ and AMTIR-3 which is $\mathrm{Ge_{28}Sb_{12}Se_{60}}$.
Angle of incidence		The angle in the plane of incidence between the incident radiation beam and the normal to the surface.
Angular frequency Angular velocity	ω	The rate of change of angle; $\omega = 2\pi v$, where v is frequency. SI unit: $\mathrm{rad\,s^{-1}}$.
Anharmonic constants	X_{ii}, X_{ij}	The X_{ij} constants in the vibrational term value (see below). SI unit: $\mathrm{m^{-1}}$. Common unit: $\mathrm{cm^{-1} = 100\,m^{-1}}$.
Anharmonicity		Commonly used abbreviation of "mechanical anharmonicity" (see below) but may also mean "electrical anharmonicity" (see below).
Anisotropic		Having properties that differ in different directions.
Anisotropic Raman scattering		Raman scattering by the anisotropic part of the derived polarizability tensor (see below). See also "Polarizability invariant".
Anomalous dispersion		In contrast to normal dispersion (see below), a material's real refractive index decreases markedly with decreasing wavenumber on the high wavenumber side of an absorption band, then increases rapidly through the band center and decreases markedly on the low wavenumber side of the band, before resuming normal dispersion at wavenumbers far from the band. This behavior in the vicinity of an absorption band is called anomalous dispersion of the refractive index.

Quantity	Symbol	Meaning
Anomalously polarized Raman band		A Raman band with a depolarization ratio (see below) greater than 0.75, as is frequently observed in resonance Raman spectroscopy.
Anti-Stokes scattering		Light scattering in which the molecules lose energy and the scattered radiation has higher wavenumber than the exciting radiation.
Antisymmetric		An entity is antisymmetric with respect to a symmetry element if the corresponding symmetry operation inverts it. In spectroscopy the term "asymmetric" is sometimes used when antisymmetric is meant, and this is not correct.
Apodization		Originally the procedure by which FT-IR spectra are corrected for the side lobes that appear in the wings of spectral bands when the interferogram is not zero at its limits, by multiplying the interferogram prior to Fourier transformation by a weighting function that is zero at its limits. Its use has broadened in recent years to include weighting functions that are not zero at their limits but yield spectral lineshapes with desired properties.
Apodization function		The weighting function discussed under "Apodization".
Array detector		A photoelectric detector in which a large number of pixels are distributed, usually in regularly spaced lines, over a usually rectangular area.
Asymmetric		An adjective that technically means without symmetry. Thus, spectral bands are often said to be asymmetric if they are not symmetric (see below). In general usage it often means of low symmetry. It is sometimes used incorrectly in vibrational spectroscopy to mean antisymmetric.
Asymmetric Fourier transform spectrometry		See "Dispersive Fourier transform spectrometry".
Asymmetric top		A rotor whose three principal moments of inertia are all different.
Atomic mass unit		See "Unified atomic mass unit".
Atomic polar tensor	APT	The 3×3 tensor that gives the change in the x, y and z components of the molecular dipole moment when the atom is displaced in the x, y and z directions, where x, y and z are space-fixed axes. The rows correspond to different components of the dipole moment and the columns to x, y and z displacements. APTs have been widely used in the analysis of infrared (IR) absorption intensities. SI unit: C. Common unit: $D\,\text{Å}^{-1} = 3.33564 \times 10^{-20}$ C; electronic charge, $e = 1.60218 \times 10^{-19}$ C.
Attenuated total reflection	ATR	Internal reflection (see below) from the interface between an internal reflection element and an absorbing material at angles of incidence at or above the critical angle. The reflection is total internal reflection at wavenumbers where the reflecting material does not absorb, but is attenuated total reflection where it does absorb. The resulting spectrum resembles an absorption spectrum of the reflecting material. ATR spectroscopy has also been called internal reflection spectroscopy, IRS, and frustrated total internal reflection, FTIR, spectroscopy.

Quantity	Symbol	Meaning
Attenuated total reflectance	R	The reflectance (see below) when radiation undergoes attenuated total reflection. SI unit: none, a dimensionless quantity.
Bandpass filter		Either: An optical filter that passes a band of wavelengths in a certain range and centered at a certain wavelength and rejects radiation of wavelength outside of the range. Or: An electrical filter that passes a band of electrical signals with a certain frequency range centered at a certain frequency and rejects signals at frequencies outside of the range.
Bandshape		The shape of a band. For a given band, the bandshape is independent of the band height in Raman spectra, IR absorbance spectra and IR pATR (see below) spectra. The bandshape changes if the band height changes in IR transmittance spectra or IR attenuated total reflectance spectra.
Baseline, tangential		See "Tangential baseline".
Beamsplitter Beam splitter		A device to split a beam of light into two parts. In an ideal two-beam Fourier transform spectrometer the beam splitter would transmit half of the light and reflect half of it to create the two beams.
Beer–Lambert absorption coefficient	$\varepsilon, a, \alpha, \kappa$	The absorbance divided by the path-length and concentration of absorber. Due to the possibility of decadic or napierian absorbance and the possibility of amount concentration or mass concentration, several different quantities are all Beer–Lambert absorption coefficients. SI unit: α, a, $m^2\,kg^{-1}$; ε, κ, $m^2\,mol^{-1}$. Common unit: α, a, $cm^2\,g^{-1} = 0.1\,m^2\,kg^{-1}$; ε, κ, $cm^2\,mol^{-1}$ $= 10^{-4}\,m^2\,mol^{-1}$ or $L\,mol^{-1}\,cm^{-1} = 0.1\,m^2\,mol^{-1}$.
Beer–Lambert law		The absorbance of a sample is the product of the Beer–Lambert absorption coefficient, the concentration and the path-length of the absorber $$A_{10} = \alpha \rho l \text{ or } A_{10} = \varepsilon c l \text{ or } A_e = \kappa c l.$$
Branch		See "Rotational branch".
Brewster angle		In external reflection, the angle of incidence at which the reflectance of the p-polarized radiation is zero. The angle is given by $\theta = \tan^{-1} n$, where n is the ratio of the refractive index of the reflecting medium to that of the incident medium.
Brightness		See "Radiance". Some distinguish between radiance as watt $sr^{-1}\,m^{-2}$ and brightness as photons $s^{-1}\,sr^{-1}\,m^{-2}$. The synchrotron community also uses brightness for photons $s^{-1}\,sr^{-1}\,m^{-2}$ $(0.1\%$ bandwidth$)^{-1}$, although this is really a measure of the spectral brightness (see "Spectral radiance").
Brilliance		The same as "brightness". In Europe "brilliance" is used and in North America "brightness" is used.

Quantity	Symbol	Meaning
CARS		Coherent anti-Stokes Raman spectroscopy uses the third order susceptibility and is one of several 4-wave mixing spectroscopies. The excitation is through lasers of wavenumber $\tilde{v}_1$ and $\tilde{v}_2$ which coincide spatially and temporally in the sample and produce a coherent, highly collimated output beam of wavenumber $\tilde{v}_3 = 2\tilde{v}_1 - \tilde{v}_2$. Experimentally, $\tilde{v}_1$ is kept constant and $\tilde{v}_2$ is scanned. A coherent, highly collimated beam output is observed at the anti-Stokes wavenumber $\tilde{v}_1 + \tilde{v}_M$ when $\tilde{v}_1 - \tilde{v}_2 = \tilde{v}_M$, where $\tilde{v}_M$ is the wavenumber of an active vibration in the sample. The Raman scattered radiation emerges as a laser beam instead of being scattered into three dimensions, thus greatly enhancing the sensitivity over that in normal Raman scattering.
Cauchy function		The function $y = a/(b^2 + x^2)$ where a and b are constants. If x is replaced by $\tilde{v} - \tilde{v}_o$ this function yields a Lorentzian band centered at $\tilde{v}_o$.
Centerburst		The region of an interferogram around zero-path-difference where the signal has its largest value.
Chalcogenides		Compounds that contains a group 6 element, but usually not oxygen. Several II–VI chalcogenides are useful infrared transmitting materials. Examples are ZnS (sphalerite, IRTRAN-2™, Cleartran™), ZnSe (IRTRAN-4™) CdS, CdSe and CdTe (IRTRAN-6™).
Channel fringes		A term sometimes used for interference fringes.
Channel spectrum		A term sometimes used for a spectrum of interference fringes.
Charge-coupled device	CCD	Charge-coupled devices store information in the form of charge packets in an array of closely spaced capacitors; the packets can be transferred from one capacitor to the next sequentially by electronic manipulation, so that the information contained in the array can be sequentially read electronically. In spectroscopy the charge packets are created by radiation and the devices are extremely sensitive detectors for near-infrared and visible radiation.
Christiansen effect		Collections of solid particles that are transparent to the radiation and are slightly larger than the wavelength of the radiation transmit poorly due to reflection and scattering from the interfaces. The transmission increases markedly at wavenumbers at which the refractive index of the particles is close to that of the surrounding medium. This phenomenon is known as the Christiansen effect. It frequently causes strong absorption bands from coarsely ground crystals to be distorted due to the change in refractive index associated with the anomalous dispersion of the refractive index through the absorption region.
Christiansen filter		A filter based on the Christiansen effect. Such filters have been made from quartz particles in air, immersed in CCl_4, or immersed in mixtures of CCl_4 and CS_2.

Quantity	Symbol	Meaning
Circular birefringence		$n^L - n^R$, 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. SI unit: none, a dimensionless quantity.
Circular dichroism		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.
Circular frequency		The same as "angular frequency" (see above).
Collimated beam		A radiation beam of approximately constant diameter.
Collinear		In the same straight line or following the same straight path. The IR and visible radiation beams are collinear in IR microscopes.
Collision broadening		The same as "pressure broadening" (see below).
Combination band Combination transition		A combination band results from a combination transition. A combination transition is a transition in which more than one vibration changes its degree of excitation; i.e. in which more than one vibrational quantum number changes. Combination transitions or bands are either sum or difference transitions or bands, although some authors restrict them to sum transitions or bands.
(Complex) refractive index	$\hat{n}$	$\hat{n} = n + ik$. The real part, n, is usually called the refractive index, and is the entire refractive index when no radiation is absorbed. The imaginary part, k, describes absorption. SI unit: none, a dimensionless quantity. The older literature, and some physics literature today, uses $\hat{n} = n(1 + i\kappa)$ where κ is called the attenuation index. For simplicity, this usage is discouraged.
Concentration		Amount or mass of component divided by the volume of the mixture. See "Mass concentration" and "Amount concentration".
Confocal		In optics, having the same focus or foci. In a confocal resonator, two identical spherical mirrors are separated by their radius of curvature, thus sharing the same focus. In a microscope, the sample is at the common focus of the objective and the condenser optical systems; in a confocal microscope, the measured area of the sample is defined by either one or two apertures. These apertures are typically placed at the rear focal plane of the objective or the rear focal plane of the condenser. The best spatial definition of the sample can be achieved by placing an aperture at both positions.

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Continuous scan interferometers		Interferometers (typically used for FT-IR spectroscopy) in which the optical path difference (OPD) is continually changed. In slow scan interferometers, the rate of change of OPD is $<0.05 \, \text{cm s}^{-1}$ and a mechanical chopper or some other ancillary modulation is frequently used to provide an adequate modulation frequency. In rapid-scan interferometers, the rate of change of OPD is $\geq 0.05 \, \text{cm s}^{-1}$, high enough that no additional modulation is needed. See also "Step-scan interferometers" and "Rapid-scan FT-IR"
Cooley–Tukey Algorithm		An algorithm described by J.W. Cooley and J.W. Tukey in 1965 which makes use of the symmetry inherent in the discrete Fourier transform to factor the computation in such a way that the number of required mathematical operations is drastically reduced. In its application to FT-IR the number of points is set to $N = 2^\alpha$ and the number of complex multiplications is reduced from N^2 to $N\alpha/2$. In the early days of FT-IR computers were sufficiently small and slow that this reduction made the technique generally useful instead of being restricted to experts.
Coriolis force		In vibrational theory, the motion of a polyatomic molecule is usually initially regarded as the independent superposition of a rotation and a vibration, with the vibration considered in a coordinate system that rotates with the molecule. This initial treatment must be corrected for centrifugal forces and for Coriolis forces. The Coriolis force on an atom is given by $F_{\text{Coriolis}} = 2m \, v_a \omega \sin \phi$, where m is the mass of the atom, v_a is its apparent velocity in the rotating coordinate system, ω is the angular velocity of the coordinate system, and ϕ is the angle between the velocity vector and the axis of rotation. SI unit: N.
Coriolis coupling		Coupling between rotational and vibrational molecular motion caused by Coriolis forces.
Correlation splitting		The same as "Davydov splitting" (see below).
Critical angle		The smallest angle of incidence, θ_c, at which total internal reflection occurs. If $n_2 > n_1$ are the refractive indices at the boundary, $\sin \theta_c = n_1/n_2$.
Crystal Field Splitting		In general the same as "site splitting" (see below), but usually refers to the reduction of the degeneracy of a state by the static crystal field.
Crystal vibrations		In the approximation of mechanical harmonicity crystal vibrations are described by the elastic wave $F(\boldsymbol{x}, t) = F_o(\boldsymbol{k}) \exp[i(\boldsymbol{k} \cdot \boldsymbol{x} - \omega t)]$, where $i = \sqrt{(-1)}$, $\boldsymbol{x}$ is the position vector, t is the time, $\omega = 2\pi f$, and $\boldsymbol{k} = \boldsymbol{j} 2\pi/\lambda$ is the wavevector, where f is the frequency, $\boldsymbol{j}$ is a unit vector in the direction of propagation, and λ is the wavelength of the crystal

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		vibration. $F_o(\boldsymbol{k})$ describes the relative displacements of the atoms in the primitive unit cell, which necessarily change slightly with $\boldsymbol{k}$. If there are A atoms in the unit cell there are $3A \times 6.02 \times 10^{23}$ vibrations per mole of unit cells, and $3A$ different $F_o(\boldsymbol{k})$s. Each $F_o(\boldsymbol{k})$ leads to a branch of dispersion curves, in which frequency is plotted against wavevector. Crystal vibrations may be longitudinal or transverse, optic or acoustic, intramolecular or intermolecular (lattice).
Darling–Dennison resonance		In general, anharmonic interaction between two or more overtone or combination states through quartic terms in the vibrational potential energy. Some use the following more restrictive definition based on Darling and Dennison's original treatment: anharmonic resonance between overtone states of two fundamentals, v_j and v_k, where the differences between quantum numbers v_j and v_k in the two states obey $\Delta v_j = -\Delta v_k = \pm 2$.
Davydov splitting		The appearance of more than one band in the spectrum of the crystal, when only one is seen in that of the gas, owing to intermolecular vibrational coupling. Davydov splitting arises from the dynamic intermolecular forces in the crystal.
Decadic		Relating to the base 10, e.g. 10^x or $\log x = \log x = \log_{10} x$
Decadic absorbance	A, A_{10}	$A_{10} = -\log_{10}(1 - \alpha_i)$, whence $A_{10} = -\log_{10}(T_i)$ for a sample that does not scatter or luminesce. Here the internal absorptance, α_i (see below) or internal transmittance, T_i (see below) are the absorptance or transmittance corrected for reflection and other non-absorption effects, and must be used if the decadic absorbance is to have absolute numerical significance. SI unit: none, a dimensionless quantity. Usually simply called "absorbance" by chemists (see above). Care must be taken to avoid confusion with the napierian absorbance $A_e = -\ln(1 - \alpha_i)$.
Deformation vibration		A vibration in which the dominant change from equilibrium is in one or more valence angles.
Degeneracy		"Degeneracy" is used in molecular spectroscopy to refer to the existence of degenerate states. Thus, the degeneracy of a vibration or vibrational state is the number of vibrations or states that have the same energy. See also "Degenerate" and "Accidental degeneracy".
Degenerate		Molecular states are said to be degenerate if they have the same energy. Thus vibrational states are said to be degenerate if they have the same energy above the ground state. This leads us to say, in the language of classical mechanics, that vibrations are degenerate if they have the same wavenumber. States may be degenerate by accident or because symmetry requires it. See also "Accidental degeneracy" and "Degeneracy".

Quantity	Symbol	Meaning
Dephasing		The term "dephasing" arises from the density matrix formalism that is used in a phenomenological approach to simplify the description of the relaxation dynamics of a molecule coupled to its surroundings. Dephasing is also called phase relaxation, and describes the loss of coherence between the upper and lower states of a transition. Dephasing leads to either homogeneous broadening or inhomogeneous broadening depending on the system. The continually changing intermolecular interactions cause a shift of the frequency of the intramolecular vibration. If these interactions change much more slowly than the amplitude of this shift, heterogeneous broadening results and causes a Gaussian band. If these interactions change much faster than the amplitude of this shift, homogeneous broadening occurs and the observed band is a motionally narrowed Lorentzian. In the general case the broadening due to dephasing is neither homogeneous nor heterogeneous and the line shape is neither Gaussian nor Lorentzian.
Depolarization ratio	ρ	The ratio of the Raman intensity with the electric vector of the scattered radiation perpendicular to that of the incident radiation to the Raman intensity with the electric vectors parallel to each other. In normal Raman scattering with linearly polarized exciting radiation, $\rho \leq 0.75$ for totally symmetric vibrations and $\rho = 0.75$ for all other vibrations. SI unit: none, a dimensionless quantity.
Depolarized Raman band		In normal Raman spectroscopy a depolarized band has depolarization ratio $\rho = 0.75$ for linear polarized incident radiation.
Depth of penetration	d_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. 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 (see below). 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 (see below). SI unit: m. Common unit: μm.
Derivative spectroscopy		A technique in which the absorbance, or other spectral ordinate, is differentiated n times with respect to wavenumber to give the nth derivative spectrum, i.e. the spectrum of the nth derivative of the original spectrum. The technique is used to transform changes of slope in the original spectrum into more prominent features in the derivative spectra, and is extensively used in the near-infrared to flatten spectral baselines to improve subsequent chemometric study.

Quantity	Symbol	Meaning
Derived polarizability tensor		The tensor formed by the derivatives of the polarizability with respect to the kth normal coordinate, i.e. by the $\partial\alpha_{ij}/\partial Q_k$, where i and j refer to principal axes of the equilibrium molecular polarizability tensor. SI unit: $J^{-1}\,C^2\,m\,kg^{-1/2}$. Common unit: $cm^3\,\text{Å}^{-1}u^{-1/2}$, as an abbreviation of $4\pi\varepsilon_o\,cm^3\,\text{Å}^{-1}\,u^{-1/2}$, where u = unified atomic mass unit; $cm^3\,\text{Å}^{-1}\,u^{-1/2} = 2.7304 \times 10^7\,J^{-1}\,C^2\,m\,kg^{-1/2}$. See also "Unified atomic mass unit".
Diagonal force constant	F_{ii}	The second derivative of the potential energy with respect to a single displacement coordinate; e.g. the F_{ii} in the vibrational potential energy (see below) in terms of internal coordinates.
Dichroic ratio		The ratio of the optical properties when the incident light is polarized parallel and perpendicular to some direction of significance. The optical property is frequently the absorbance or integrated absorbance. The direction of significance may be the fiber axis for a polymeric fiber (see "Magic angle") or a crystal axis for a crystal, or any other direction that is believed to have significance.
Dichroism		The phenomenon of different optical absorption in different directions in the sample and, consequently, different optical behavior under different polarizations of the radiation.
Dielectric constant Relative permittivity	ε	Formally, the 3×3 tensor that gives to first order the electric displacement, D, in a material in terms of the applied electric field, E, through $D = \varepsilon\varepsilon_o E$, where ε_o is the permittivity of vacuum. For isotropic materials the tensor is diagonal with the three diagonal elements equal, so a single quantity ε suffices. The equation $D = \varepsilon\varepsilon_o E$ is valid at all frequencies, and ε is a complex quantity, $\hat{\varepsilon} = \varepsilon' + i\varepsilon''$, where ε'' describes absorption. The dielectric constant is the square of the refractive index, thus $\hat{\varepsilon} = \hat{n}^2$ or, for a non-absorbing isotropic material, $\varepsilon = n^2$. SI unit: none, a dimensionless quantity. See also "Real dielectric constant", "Dielectric loss" and "Permittivity of vacuum".
Dielectric loss Imaginary relative permittivity	ε''	The imaginary part of the dielectric constant. Of importance to physicists in the interpretation of spectroscopic data on condensed phases. Related to the real, n, and imaginary, k, refractive indices through $\varepsilon'' = 2nk$. SI unit: none, a dimensionless quantity.
Difference band Difference transition		A difference band results from a difference transition. A difference transition is a combination transition (see above) which does not start on the ground state and in which at least one vibration decreases and at least one vibration increases its degree of excitation; i.e. a transition in which more than one vibrational quantum number changes and at least one becomes smaller.
Diffraction limit		The best spatial resolution allowed by the laws of diffraction.

Quantity	Symbol	Meaning
Difference spectroscopy		A technique in which spectral subtraction is used to help the study and identification of individual species in a mixture
Difference tone		Synonymous with difference band or transition (see above).
Diffuse reflectance		The ratio of the spectral intensity (see below) 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.
Diffuse reflection		The process in which radiation is incident on a scattering sample at a certain angle and is reflected (or remitted) over all angles. Diffuse reflection is a complicated process and involves transmission, reflection and scattering. See also "Remission".
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 (see below). The process is complicated and involves transmission, reflection and scattering. See also "Transmission".
Digitization noise		See "Quantization noise".
Dipole coupling		In general the coupling of different motions through dipole–dipole forces. In vibrational spectroscopy of crystals, intermolecular vibrational coupling through interaction of resonant transition dipoles throughout the whole crystal. Also called transition-dipole transition dipole coupling.
Dipole moment	$\boldsymbol{\mu}, \boldsymbol{p}$	In vibrational spectroscopy, almost always means the electric dipole moment, which is a vector quantity whose magnitude is the size of equal separated charges of opposite sign times the distance between them, and whose direction is taken from the negative to the positive charge. It is usually expanded as: $$\boldsymbol{\mu} = \boldsymbol{\mu}_\mathrm{o} + \sum_k \left(\frac{\partial \boldsymbol{\mu}}{\partial Q_k}\right) Q_k + \sum_k \left(\frac{\partial^2 \boldsymbol{\mu}}{\partial Q_k^2}\right) Q_k^2$$ $$+ \sum_{i<j} \left(\frac{\partial \boldsymbol{\mu}}{\partial Q_i}\right) \left(\frac{\partial \boldsymbol{\mu}}{\partial Q_j}\right) Q_i Q_j + \text{higher order terms}$$ where the Q_k, etc. are the normal coordinates and $\boldsymbol{\mu}_\mathrm{o}$ is the equilibrium dipole moment of the molecule. SI unit: C m. Common unit: Debye, D $= 3.33564 \times 10^{-30}$ C m.
Dipole moment derivative	$\partial \boldsymbol{\mu}/\partial Q_k$	The change in the dipole moment of a molecule during a normal vibration. SI unit: C kg$^{-1/2}$. Common unit: D Å^{-1} u$^{-1/2}$ $= 8.18568 \times 10^{-7}$ C kg$^{-1/2}$.
Dipole moment matrix element		The same as the transition dipole moment (see below).

Quantity	Symbol	Meaning
Dipole transition moment		The same as the transition dipole moment (see below).
Direct transmission		The process in which radiation is transmitted by a scattering sample and emerges at the angle required by Snell's law of refraction (see below). See also "Transmission".
Dispersive Fourier transform spectrometry		Fourier transform spectroscopy using a Michelson or other two-beam interferometer with the sample placed in one arm of the interferometer. This method provides information about the phase change as well as the amplitude change at the sample. Also called asymmetric Fourier transform spectrometry.
Dispersive spectrometer		A spectrometer in which radiation is separated spatially into its component wavenumbers by a dispersive element such as a prism or a diffraction grating.
Divided spinning cell		A dish-like cell that is divided by a vertical partition through its middle to allow different liquids in its two halves. It is rotated about a vertical axis through its center and the Raman scattered radiation from the different halves is measured alternately. With a standard liquid in one half it is used to determine Raman scattering intensities relative to the standard.
Doppler broadening		Inhomogeneous broadening caused by the Doppler effect (see below). For a stationary gas the distribution of velocities is random and Doppler broadening yields a Gaussian line of full width at half height $\gamma_D = 2[2\ln(2)RT/M]^{1/2}\tilde{v}$, where $\tilde{v}$ is the transition wavenumber, R is the ideal gas constant, T is the absolute temperature and M is the molar mass. Stated more conveniently, $\gamma_D/\tilde{v} = 7.16 \times 10^{-7}(T/M)^{1/2}$ if M is in $\mathrm{g\,mol^{-1}}$. At 295 K $\gamma_D \approx 10^{-6}\tilde{v}$ for a molecular weight of 100.
Doppler effect		The Doppler effect causes the observed wavenumber $\tilde{v}'$ of a molecule of natural wavenumber $\tilde{v}$ that moves relative to the observer with speed u to be $\tilde{v}' = \tilde{v}(1 \pm u/c)$, where c is the velocity of light in vacuum.
Doppler limit Doppler limited		A spectrum is Doppler limited when the measured line width equals that due to the Doppler broadening.
Double-beam		Double-beam spectrometer or double-beam spectrum. In a double-beam spectrometer beams of radiation from the source reach the detector via two paths alternately, the sample beam and the reference beam. The radiant power in each beam is measured at each wavenumber. A double-beam spectrum shows the radiant power that reaches the detector in the sample beam divided by that in the reference beam at each wavenumber, in order to show a flat baseline where the sample does not absorb.
Dynamic spectrum	$y(\tilde{v}, \tau)$	The spectrum of a material under the influence of an applied external perturbation represented by a variable τ, relative to a reference spectrum. The reference spectrum may be chosen in many ways; e.g. it may be the average over τ of the observed spectrum, or it may be zero. See also "2-D correlation spectroscopy" and "2-D correlation spectrum".

Quantity	Symbol	Meaning
Eigenvector		Mathematically, part of the solution of the matrix equation $AY = Y\Lambda$ where A is the matrix whose solution is sought, Λ is a diagonal matrix that contains the eigenvalues λ_k, and Y contains the eigenvectors Y_{ik}. For a specific eigenvalue this equation is often written $AY_k = \lambda_k Y_k$, where λ_k is the kth eigenvalue, a scalar, and Y_k is the column vector of the kth eigenvector. Eigenvectors occur in vibrational spectroscopy through the Schrödinger equation, through the solution of the normal coordinate problem $GFL = L\lambda$, and through solutions of problems in Factor Analysis. See "Vibrational eigenvector".
Einstein transition probability (or coefficient) of induced emission and absorption	B_{ij}	The probability that one molecule will emit energy and change from state i to state j, or will absorb energy and change from state j to state i, in unit time under the influence of unit spectral radiant energy density (see below) at average wavenumber $\tilde{v}_{ij}$. SI unit: $s\,kg^{-1}$.
Einstein transition probability (or coefficient) of spontaneous emission	A_{ij}	The probability that one molecule will spontaneously emit energy and change from state i to state j in one unit of time. SI unit: s^{-1}.
Electrical anharmonicity		The influence of the terms that are of 2nd and higher order in Q in the expansion of the dipole moment.
Electrical harmonicity		The influence of the linear term, $\Sigma_k(\partial\mu/\partial Q_k)Q_k$, in the expansion of the dipole moment.
Electromagnetic radiation		The flow of energy through space, usually called simply "radiation". In its propagation through vacuum, radiation behaves like synchronized sinusoidal waves of the electric field, E, and the magnetic field H, with frequency v, wavelength λ_o, and velocity c_o, where $v\lambda_o = c_o$. The wavelength and velocity decrease when radiation enters a medium. In its interaction with atoms and molecules, radiation behaves like particles, called photons, with zero mass, energy hv, and momentum h/λ.
Electron energy loss spectroscopy	EELS	A form of spectroscopy in which a constant-energy beam of electrons passes through or is reflected from a sample, and the energy distribution in the transmitted or reflected beam is analyzed to give a spectrum of number of electrons against electron energy loss. The method is used for the study of electronic states and the energy resolution is 0.25 eV or better ($0.25\,eV \approx 2000\,cm^{-1}$).
Electro-optic parameters	EOPs	Electro-optic parameters have been used in the analysis of absolute IR intensity data, and are based on the assumption that the molecular dipole moment can be described as the vector sum of bond dipole moments. The original EOPs were μ_k^o, the equilibrium bond moment, and $\partial\mu_k/\partial R_t$, the change in the dipole moment of bond k with change in internal displacement coordinate t. A later and completely equivalent formulation uses equilibrium atomic charges, q_α^o, and charge fluxes, $\partial q_\alpha/\partial R_t$, which are also called EOPs as well as ECCF for equilibrium charge, charge flux.

Quantity	Symbol	Meaning
Ellipsometry		Radiation that is linearly polarized oblique to the surface becomes elliptically polarized after reflection at non-normal incidence. Ellipsometry is the determination of the refractive indices of the reflecting material from the ellipticity of the reflected radiation. The ellipticity is obtained from measurements of the intensity and polarization of the incident and reflected radiation.
Ellipticity	ψ	The measure of the degree to which linearly polarized incident radiation becomes elliptically polarized in an absorbing optically active medium. Ellipticity, ψ, is defined by $$\tan \psi = \frac{E_R - E_L}{E_R + E_L} = \tanh \left[(k^L - k^R)\frac{\pi l}{\lambda} \right]$$ Here E_R and E_L are the electric vectors of right and left circularly polarized radiation, k^L and k^R are the imaginary refractive indices of the sample for left and right circularly polarized radiation, λ is the wavelength of the radiation and l is the path length through the medium.
Emission (of radiation)		The production of radiation from matter. The transfer of energy from matter to radiation.
Emissivity		A traditional name for emittance.
Emittance	ε	Ratio of the radiant flux emitted by the sample to that emitted by a black body at the same temperature. SI unit: none, a dimensionless quantity. The term "flux" can be replaced by "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 radiation beam.
Étendue	Θ	A measure of the light-gathering power of an optical instrument, i.e. of the radiant power transmitted per radiance of the source. In practice $\Theta = n\Omega A$, where n is the refractive index of the medium in the instrument through which the light travels, Ω is the solid angle accepted from the source by the limiting aperture and A is the area of the limiting aperture. SI unit: m^2 sr. Common unit: cm^2 sr. See also "Throughput".
Evanescent wave		The part of the wave that extends beyond the reflecting surface when an electromagnetic wave undergoes total internal reflection.
Evans hole		An unexpected minimum or hole in a broad absorption band due to a gap being created in a broad distribution of states by Fermi resonance with a sharp state. See also "Fermi resonance".
Excess dark current noise		The noise in the dark current of a photomultiplier tube or focal plane array that is due to non-thermal sources.
Excitation profile		The graph of Raman intensity at the desired Raman shift against the wavenumber of the excitation.
Excitation wavenumber	$\tilde{\nu}_o$	The vacuum wavenumber of the radiation used to excite Raman spectra.
Excitation wavelength	λ_o	The wavelength of the radiation used to excite Raman spectra. It is usually given as the wavelength in air, so the vacuum wavenumber is usually related to it by $\tilde{\nu}_o = 1/(\lambda_o n_a)$, where n_a is the refractive index of air.

Quantity	Symbol	Meaning
Exciton splitting		Splitting of vibrational bands in crystals due to dynamic intermolecular forces. Essentially the same as Davydov splitting.
Experimental absorbance		A term sometimes used instead of "absorbance" (see above) to describe $-\log_{10}$ of the transmittance spectrum of a cell full of liquid, to emphasize that radiation is lost from the beam by reflection, and possibly vignetting, and not solely by absorption.
External reflection spectroscopy		Spectroscopy in which radiation is reflected from a sample of higher refractive index than that of the incident medium.
Extinction coefficient	ε	A term that has been widely used for the molar absorptivity, unfortunately often with values given in ill-defined units. Use of this term has been discouraged since the 1960s, when international agreement with non-chemical societies reserved the word "extinction" for diffusion of radiation, i.e. the sum of the effects of absorption, scattering and luminescence.
Extraordinary wave Extraordinary ray		In uniaxial crystals the optic axis coincides with the symmetry axis. The refractive index of the crystal is the same in all directions perpendicular to the optic axis but is different along the optic axis. Consequently, electromagnetic rays or waves that do not travel along the optic axis experience different refractive indices in different directions perpendicular to their direction of propagation. Two waves result, one has its electric vector perpendicular to the optic axis and forms the ordinary wave (see below). The other has its electric vector oblique to the optic axis, and does not obey the normal laws of refraction. The latter wave is called the extraordinary wave or extraordinary ray.
F matrix	*F*	The square symmetric matrix that contains the potential energy information, in the form of the force constants, F_{ij}, in normal coordinate analysis. See also "Force constant" and "Vibrational potential energy".
Factor Group		The mathematical group formed by the cosets of the invariant sub-group of pure translations in the space group. The factor group is isomorphic with (so uses the same character table as) the point group of the crystal class. In vibrational spectroscopy, the term factor group analysis nearly always means unit cell group analysis, because it is usually the individual elements of the unit cell group that are used not the coset elements of the factor group.
Factor group splitting		The same as "unit cell group splitting" (see below).
Far-infrared Far-IR		The spectral region in which vacuum wavenumbers range from $\sim 400 \, \text{cm}^{-1}$ to $\sim 10 \, \text{cm}^{-1}$.
Fermi resonance		Traditionally, the anharmonic interaction between a fundamental state and one or more overtone or combination state. Usually identified by the presence of more than one band of comparable intensity when only one fundamental is expected. Also seen as an Evans hole (see above). Fermi resonance is often regarded today as any cubic anharmonic resonance, i.e. any interaction caused by the cubic terms in the vibrational potential energy.

Quantity	Symbol	Meaning
Finesse		The finesse of an instrument is the free spectral range divided by the resolution.
Fingerprint bands		Infrared and Raman bands that are characteristic of a given molecule rather than a particular functional group.
Fingerprint region		The spectral region that contains fingerprint bands (see above) as well as bands with characteristic group frequencies; often thought of as the region of the mid-infrared or Raman spectrum between $1500 \, \text{cm}^{-1}$ and $200 \, \text{cm}^{-1}$.
Flicker noise		Any noise in excess of the quantum or shot noise that is proportional to the magnitude of the photon signal. It is usually caused by variations in the experimental variables that control the radiance of the source (source flicker noise) or by fluctuations in the sample (analyte flicker noise). Sometimes called multiplicative noise.
Folding		In vibrational spectroscopy folding occurs when the analog signal is undersampled (see 'Undersampling'). When a spectrum is sampled correctly only up to $\tilde{v}_M$, radiation of wavenumber $\tilde{v} > \tilde{v}_M$ appears to have a wavenumber between 0 and $\tilde{v}_M$, as follows: For $\tilde{v}$ between $\tilde{v}_M$ and $2\tilde{v}_M$, $\tilde{v}_{app} = \tilde{v}_M - (\tilde{v} - \tilde{v}_M) = 2\tilde{v}_M - \tilde{v}$; for $\tilde{v}$ between $2\tilde{v}_M$ and $3\tilde{v}_M$, $\tilde{v}_{app} = \tilde{v} - 2\tilde{v}_M$; for $\tilde{v}$ between $3\tilde{v}_M$ and $4\tilde{v}_M$, $\tilde{v}_{app} = 4\tilde{v}_M - \tilde{v}$; for $\tilde{v}$ between $4\tilde{v}_M$ and $5\tilde{v}_M$, $\tilde{v}_{app} = \tilde{v} - 4\tilde{v}_M$, etc. This process can be simulated by *folding* a spectrum that shows the correct wavenumbers back onto itself at $\tilde{v}_M$ and its multiples. Folding is sometimes called aliasing.
Force constant	F_{ii}, F_{ij}	The second derivative of the potential energy with respect to one or two displacement coordinates. $$F_{ii} = \frac{\partial^2 V}{\partial R_i^2}; \quad F_{ij} = \frac{\partial^2 V}{\partial R_i \partial R_j}.$$ SI unit: $\text{J m}^{-2} = \text{N m}^{-1}$, $\text{J m}^{-1} \, \text{rad}^{-1}$, or J rad^{-2}, depending on whether the R_i and R_j are changes in bond lengths or angles. Common unit: $\text{mdyn} \, \text{Å}^{-1} = \text{aJ} \, \text{Å}^{-2} = 100 \, \text{N m}^{-1}$, $\text{mdyn} = \text{aJ} \, \text{Å}^{-1} \, \text{rad}^{-1} = 10^{-8} \, \text{J m}^{-1} \, \text{rad}^{-1}$, or $\text{mdyn} \, \text{Å} = \text{aJ} \, \text{rad}^{-2}$. The unit rad is frequently omitted.
Fourier transform infrared spectroscopy	FT-IR	Infrared spectroscopy practiced by the use of a Fourier transform spectrometer (see below). Often abbreviated to FTIR but FT-IR is preferred to avoid confusion with frustrated total internal reflection.
Fourier transform Raman spectroscopy		Raman spectroscopy in which a Fourier transform spectrometer (see below) is used to separate the scattered radiation into its component wavenumbers. This technique usually uses near-infrared excitation.
Fourier transform spectrometer		A spectrometer in which radiation is separated into its component wavenumbers by Fourier transformation of the interferogram produced by an interferometer.

Quantity	Symbol	Meaning
Free spectral range	$\Delta\tilde{v}$	For a Fabry–Perot or laser cavity the free spectral range is the wavenumber interval between successive longitudinal cavity modes; $\Delta\tilde{v} = 1/2nl$, where l is the cavity spacing and n is the refractive index of the material in the cavity. SI unit: m^{-1}.
Frequency	v, f	The number of cycles of periodic motion in unit time. In spectroscopy the periodic motion is of the electric and magnetic vectors of electromagnetic radiation. SI unit: Hz, where $1\,Hz = 1\,s^{-1}$. Frequency is related to the energy change, ΔE, induced when electromagnetic radiation is absorbed through $\Delta E = hv$ per photon.
Fresnel equations Fresnel's equations		Equations that give, for s- and p-polarized radiation, the coefficients of transmission, t_s, t_p, and reflection, r_s, r_p, of the electric field at the boundary between two materials in terms of the optical constants of the materials and the angles of incidence and refraction. The transmittance and reflectance are then given by the sum of the squares of the coefficients appropriate to the polarization of the incident beam.
Fresnel reflection		Reflection of radiation from a surface that is smooth and large with respect to the wavelength of the radiation. A reflected beam, of intensity governed by the Fresnel equations, is produced at an angle of reflection equal to the angle of incidence. Sometimes called "specular reflection" for non-scattering samples.
Frustrated multiple internal reflection	FMIR	A term sometimes used for multiple attenuated total reflection.
Frustrated total internal reflection	FTIR	A name sometimes used for attenuated total reflection.
Full width at half height Full width at half maximum	FWHH FWHM	The full width of a band at half of the peak height. For infrared absorption spectra, the FWHH must be measured from a spectrum that is plotted linear in absorbance, not transmittance. For Raman spectra, the FWHH can be measured directly from the spectrum of scattered light intensity, unless the instrument response function varies significantly across the band.
Fundamental band Fundamental transition		A fundamental band results from a fundamental transition – a transition between the ground state and a state in which one vibration is singly excited; i.e. a transition between the ground state and the state: $v_i = 1$, $v_{j \neq i} = 0$.
G matrix	*G*	The square symmetric matrix that contains the kinetic energy information in normal coordinate analysis. See also "Vibrational kinetic energy".
Gaussian band		A band with the shape $H_G \exp[-2.7726(\tilde{v} - \tilde{v}_o)^2/W^2]$, where H_G is the peak height, W is the full width at half height, $\tilde{v}_o$ is the peak wavenumber and 2.7726 is 4ln(2).
Glide Plane		A symmetry element in solids which consists of reflection in a plane followed by translation by one half of the length of the primitive unit cell length parallel to the plane.
Grating spectrometer		A spectrometer in which radiation is separated spatially into its component wavenumbers by a diffraction grating.

Quantity	Symbol	Meaning
Grazing incidence		When the angle of incidence of a radiation beam onto a surface is very high, ideally over 80° but frequently over 70° in practice.
Ground state		The state of lowest intramolecular energy. In vibrational spectroscopy, "ground state" usually means "ground vibrational state", the lowest vibrational state of the molecule, i.e. the state in the lowest electronic state in which all vibrational quantum numbers, υ_i, equal zero.
Group frequency		A vibrational frequency (usually wavenumber) that is characteristic of a particular chemical functional group.
Hadamard transform spectrometer		A Hadamard transform spectrometer is a multiplexing spectrometer that uses the optical components of a dispersive spectrometer with a Hadamard encoding mask. Hadamard encoding is based on the studies of determinants made by the French mathematician J. Hadamard.
Half width at half height	HWHH	One half of the full width at half height (see above).
Harmonic constant	ω_e	The coefficient of $(v + \frac{1}{2})$ in the vibrational term value, determined
Harmonic wavenumber	ω_k	by the harmonic terms in the vibrational potential energy. SI unit: m^{-1}; Common unit: $cm^{-1} = 100\,m^{-1}$.
Harmonicity		See "Mechanical harmonicity" and "Electrical harmonicity".
Harmonics		A term widely used in music and physics for $2f, 3f, 4f$, etc., the overtones of frequency f.
High-pass filter		Either: An optical filter that excludes the radiation of wavenumber lower than a certain cut-on value and passes radiation of wavenumber above this value. Or: An electrical filter that blocks signal with a modulation frequency lower than a certain cut-on value and passes signals of frequency above this value.
High-resolution electron energy loss spectroscopy	HREELS	Electron energy loss spectroscopy in which the energy resolution is between 1 and 5 meV, i.e. between 8 and 40 cm^{-1}. Used to detect vibrational motion.
Hilbert transforms		The Hilbert transforms are used, inter alia, to interrelate the real part, f', and imaginary part, f'', of many function. For example, the real refractive index, n, and imaginary refractive index, k, or the real and imaginary spectra computed from an interferogram by the complex Fourier transform may be related through $$f'(\nu_a) - f'_\infty = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{f''(\tilde{\nu})}{\tilde{\nu} - \tilde{\nu}_a}\,d\tilde{\nu}$$ $$f''(\nu_a) = \frac{-1}{\pi} P \int_{-\infty}^{\infty} \frac{f''(\tilde{\nu}) - f'_\infty}{\tilde{\nu} - \tilde{\nu}_a}\,d\tilde{\nu}$$ where P means the principal part of the integral is taken at the singularity.
Homogeneous broadening		Line broadening by mechanisms that affect every molecule of the same species in the sample in the same way. Such mechanisms do not require an ensemble of spectroscopically non-equivalent

Quantity	Symbol	Meaning
		molecules of the same species. Such mechanisms are the natural linewidth, which is usually negligible in vibrational spectroscopy, and intra- or intermolecular interactions, including anharmonic vibrational interactions, that reduce the lifetime of the upper state.
Hot band Hot transition		A hot band arises from a hot transition – a transition between an excited state and a state in which all vibrational quantum numbers are the same or greater. A hot transition has the same changes in vibrational quantum numbers as a fundamental, overtone or sum transition but it originates in an excited vibrational state not the ground state.
Hyper-polarizabilities	β, γ	The coefficients of the higher than linear terms in the relation between the electric dipole moment μ of a molecule and the electric field E which acts on the molecule $$\mu = \mu_o + \alpha E + \tfrac{1}{2}\beta E^2 + \tfrac{1}{6}\gamma E^3 + \cdots$$ where β is the first hyperpolarizability, a $3 \times 3 \times 3$ tensor, with SI unit: $C^3\,m^3\,J^{-2}$. γ is the second hyperpolarizability, a $3 \times 3 \times 3 \times 3$ tensor, with SI unit: $C^4\,m^4\,J^{-3}$.
Hyper Raman spectroscopy		Raman spectroscopy in which the scattering occurs through the hyper-polarizabilities.
Hyperspectral imaging		Use of a spectrometer to obtain information about the spatial composition of a sample by imaging the surface of the sample onto an array detector; the spectrum of each spatially resolved point of the sample is measured.
Imaginary dielectric constant	ε''	The same as the dielectric loss (see above).
Imaginary refractive index	k	The imaginary part of the refractive index. It describes absorption. SI unit: none, a dimensionless quantity. See also "Absorption index".
Imaging		See "Hyperspectral imaging".
Improper rotation axis	S_n	In spectroscopy, a rotation–reflection axis, which is a symmetry element such that rotation by $2\pi/n$ about the axis followed by reflection through a plane perpendicular to the axis transforms an object into itself. N.B. In crystallography, a rotation-inversion axis, which is a symmetry element such that rotation by $2\pi/n$ about the axis followed by inversion through the center of symmetry transforms an object into itself.
Inelastic electron tunneling spectroscopy		In inelastic electron tunneling spectroscopy the current, I, due to tunneling through a thin non-conducting sample is measured as a function of the applied voltage, V. For vibrational spectroscopy V lies between $\sim 1\,\text{mV}$ ($\cong 8\,\text{cm}^{-1}$) and $1\,\text{V}$ ($\cong 8100\,\text{cm}^{-1}$). In practice the ordinate is usually d^2I/dV^2 or $d^2I/dV^2 \div (dI/dV)$, instead of I.

Quantity	Symbol	Meaning
Inelastic neutron scattering spectroscopy		In inelastic neutron scattering spectroscopy neutrons pass through the sample and are scattered by interaction with the molecular vibrations, i.e. gain or lose energy by interaction with the vibrations. The incident and final energies of the neutrons are measured and their difference gives the wavenumber of the vibration via $\Delta E = h c_o \tilde{v}$, where h is Planck's constant and c_o is the velocity of light in vacuum. For crystalline solids the change in momentum of the neutrons is also measured and provides information about the wave vector of the vibrations. Selection rules restrict infrared and Raman spectra to the very small number of crystal vibrations that have approximately zero-wave-vector. A particular value of inelastic neutron scattering is that it gives information about all of the vibrations in a crystal.
Infrared intensity		A term usually used to refer qualitatively to the amount of infrared radiation absorbed at a particular wavenumber by the system under study. The term "absolute infrared intensity" or "integrated infrared intensity" is usually used when quantitative reference is intended. "Relative infrared intensity" is used when the ratios of intensities at different wavenumbers are known quantitatively but none are known absolutely. See also "Integrated intensity".
Infrared reflection–absorption spectroscopy	IRRAS	See "Reflection–absorption at grazing incidence".
Infrared spectrum		A graph of a measure of the radiant power resulting from the direct interaction of infrared radiation with a sample plotted against the wavelength, frequency or wavenumber of the radiation as abscissa.
Inhomogeneous broadening		Line broadening by mechanisms that require an ensemble of spectroscopically non-equivalent molecules of the same species. Such molecules exist, for example, when molecules occupy non-equivalent sites in a condensed phase, and when gaseous molecules have different velocities and, thus, shift the observed wavenumber differently through the Doppler effect (see above).
Instrument line shape	ILS	The shape of an infinitely sharp line measured by the instrument. For dispersive spectrometers, the ILS varies with the slit width and, for very high resolution, the number of lines on the grating; for Fourier transform spectrometers the ILS varies with the maximum optical path difference, apodization function and beam divergence.
Integrated intensity		In integrated spectroscopy, the area under an absorption band where the absorption quantity is, unlike transmittance or percent transmission, linearly proportional to the amount of absorber in unit area. The absorption quantity is usually a Beer–Lambert absorption coefficient, but recently $\tilde{v}\alpha''_m$, the wavenumber times the imaginary local molar polarizability, has been used for neat liquids to correct for dielectric effects. See also "Infrared intensity". SI unit: $\mathrm{km\,mol^{-1}}$.

Quantity	Symbol	Meaning
Integration range		In vibrational spectroscopy this usually refers to the wavenumber range over which the integrated intensity of a band is found by numerical integration of the area under the band. For Gaussian bands integration over 1 FWHH to each side of the band center yields 98% of the area under the band. For Lorentzian bands integration over 3.1 or 15.9 FWHH to each side yields 90% or 98% of the band area.
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: $W\,m^{-2}$.
Interaction force constant	F_{ij}	The second derivative of the potential energy with respect to two displacement coordinates; e.g. the F_{ij} in the vibrational potential energy (see below) in terms of internal coordinates. See also "Force constant".
Interference fringes		A sinusoidal intensity variation due to interference of radiation that undergoes multiple reflection between two flat and parallel surfaces. They are frequently observed in transmission spectra of cells with flat windows and in polymer films.
Interference record Interference function		The record of the signal from the detector of a Michelson or other two-beam interferometer as the path difference between the two beams is varied. It contains a part that is constant and a part that varies with the path difference.
Interferogram		The part of the signal from the detector of a Michelson or other two-beam interferometer that varies with path difference. See also "Interference record".
Interferometer		An instrument in which two or more radiation beams interfere with each other after passing through different optical paths. In vibrational spectroscopy, a two-beam interferometer of the Michelson or related design is usually used, and the output is an interferogram or interference record. See also "Interferogram" and "Interference record".
Internal absorbance	A_i	A rarely used term that is useful in quantitative absolute intensity studies to emphasize that the necessary corrections of the transmittance for reflection and other cell effects have been made. Instrument manufacturers usually use the raw, uncorrected transmittance when calculating the absorbance. Formally, $A_i = -\log_{10}(1 - \alpha_i)$, whence $A_i = -\log_{10}(T_i)$ for a sample that does not scatter or luminesce. Here α_i is the internal absorptance (see below) and T_i is the internal transmittance (see below). SI unit: none, a dimensionless quantity.
Internal absorptance	α_i	The absorptance fully corrected for surface effects and effects of the cell such as reflection and vignetting losses. If scattering and luminescence in the sample are negligible $$\alpha_i + T_i = 1.$$ SI unit: none, a dimensionless quantity.

Quantity	Symbol	Meaning
Internal coordinate	$\boldsymbol{R}$, R_j	R_j represents an interatomic valence displacement within a molecule that causes no translational or rotational displacement of the molecule. The collection of R_j form the vector $\boldsymbol{R}$. R_j is a general symbol for all displacements, and r_i, θ_j or τ_κ are frequently used to describe a change in length of bond i, a change in angle j, or a change in dihedral angle k, respectively. SI unit: m for length, rad for angle. Common unit: $\text{Å} = 10^{-10}$ m, or nm, for length, rad for angle.
Internal reflection		Reflection of radiation from a material of lower refractive index than that of the incident medium.
Internal reflection element		A material of high refractive index that carries the radiation to the sample in internal reflection and attenuated total reflection measurements. The sample is mounted in optical contact with the element.
Internal reflection spectroscopy	IRS	A name sometimes used for attenuated total reflection spectroscopy.
Internal transmission		A term used instead of transmission (see below) to emphasize that the radiation does not undergo reflection or scattering. See also "Internal Transmission Spectroscopy".
Internal transmission spectroscopy		The measurement of a spectrum produced by the transmission through a very thin layer of relatively low index of refraction located in between two high index materials, such as silicon, at an incidence angle larger than the critical angle between the substrate and the film. The enhancement of the component perpendicular to the interface arises from the large intensity of the evanescent field within the layer.
Internal transmittance	T_i, τ_i	The transmittance fully corrected for surface effects and effects of the cell such as reflection and vignetting losses. If scattering and luminescence in the sample are unimportant, then $\alpha_i + T_i = 1$, where α_i is the internal absorptance (see above). SI unit: none, a dimensionless quantity.
Invariant of the polarizability		See "Polarizability invariant".
Inverse Raman scattering		When a sample is simultaneously illuminated by coincident beams from a continuum source and a giant-pulse laser at $\tilde{\nu}_o$, energy is absorbed from the continuum at $\tilde{\nu}_o + \tilde{\nu}_s$, where $\tilde{\nu}_s$ is the wavenumber of a Raman-active vibration in the sample which is excited by this process, and this energy is emitted at $\tilde{\nu}_o$.
Irradiance	I	The radiant power received on unit area. See also "Intensity". SI unit: W m^{-2}
IRTRAN™		IRTRAN 1™ to IRTRAN 6™ are hot-pressed forms of MgF_2, ZnS, CaF_2, ZnSe, MgO and CdTe, respectively. IRTRAN™ is a registered trade mark of Eastman Kodak Co.
Isotropic		Having properties that are the same in all directions.
Isotropic Raman scattering		Raman scattering by the isotropic part of the derived polarizability tensor (see above). See also "Polarizability invariant".

Quantity	Symbol	Meaning
Jacquinot stop, J-stop		An aperture in the optics of a Fourier transform spectrometer, typically between the source and the interferometer, designed to be the limiting aperture when no other optical element such as the detector serves this purpose.
Johnson noise		Noise generated by the thermal motion of electrons.
Kinetic coupling		Coupling of vibrational displacements through terms in the vibrational kinetic energy (see below). Two displacement coordinates must share a common atom if they are to couple kinetically.
Kramers–Kronig transforms		Transforms based on the physical principle of causality that interconvert the real and imaginary parts of complex optical quantities when they are known over a sufficiently wide (strictly infinite) wavenumber range. They are frequently used to interconvert the real part, f', and imaginary part, f'', of the refractive index, $\hat{n} = n + \mathrm{i}k$, dielectric constant, $\hat{\varepsilon} = \varepsilon' + \mathrm{i}\varepsilon''$, or logarithm of the complex reflection coefficient $r\mathrm{e}^{\mathrm{i}\phi}$ through $$f'\left(\tilde{\nu}_{\mathrm{a}}\right) - f'_{\infty} = \frac{2}{\pi}P\int_{\mathrm{o}}^{\infty}\frac{\tilde{\nu}f''\left(\tilde{\nu}\right)}{\tilde{\nu}^2 - \tilde{\nu}_{\mathrm{a}}^2}\,\mathrm{d}\tilde{\nu}$$ $$f''\left(\tilde{\nu}_{\mathrm{a}}\right) = \frac{-2\tilde{\nu}_{\mathrm{a}}}{\pi}P\int_{\mathrm{o}}^{\infty}\frac{f'\left(\tilde{\nu}\right) - f'_{\infty}}{\tilde{\nu}^2 - \tilde{\nu}_{\mathrm{a}}^2}\,\mathrm{d}\tilde{\nu}$$ where P means that the principal part of the integral is taken at the singularity. All functions used to model vibrational spectra obey the Kramers–Kronig transforms as long as the real parts are even functions of wavenumber and the imaginary parts are odd functions of wavenumber so that the Kramers–Kronig transforms are equivalent to the Hilbert transforms (see above).
KRS-5		Thallium bromide iodide, an infrared window material; A eutectic (42% TlBr, 58% TlI) mixture of thallium bromide and thallium iodide, that transmits well down to $200\,\mathrm{cm}^{-1}$. It is practically insoluble in water but its refractive index is rather high ($\sim$2.35), it is rather plastic and deforms with time, and it is poisonous.
Kubelka–Munk function		The Kubelka–Munk function, $f(R_{\infty})$, 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, $f(R_{\infty})$ 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. See also "Remission function".
Kubelka–Munk reflection		See "Volume reflection".
Lateral resolution		See "Spatial resolution".

Quantity	Symbol	Meaning
Lattice vibration		In an atomic crystal, an interatomic vibration, and all vibrations are lattice vibrations. In a molecular crystal, an intermolecular vibration, so a crystal containing M molecules in the primitive unit cell has $6M$ or $5M$ branches of lattice vibrations for non-linear or linear molecules, respectively. Three branches of lattice vibrations are the three acoustic branches. See also "Crystal vibrations", "Acoustic vibration" and "Optic vibration", "Translational lattice vibration" and "Rotational lattice vibration".
Libration		A lattice vibration based on rotational motion of the molecules on sites that prevent overall rotation. More descriptively called "rotational vibration" (see below).
Lifetime broadening		Homogeneous broadening due to the limited lifetime of the states involved in the transition. The lifetime may be limited by the natural lifetime, by collisions as in pressure broadening, or by anharmonic vibrational interactions as in phonon–phonon collisions in solids.
Light		Electromagnetic radiation that is visible to the human eye. In general spectroscopic usage "light" is usually synonymous with "radiation" when the specific wavelength is not important.
Line width		The width of a spectral line. In vibrational spectroscopy this is usually measured as the full width at half height (see above) and abbreviated to FWHH. The half width at half height (see above), HWHH, is also used, although rarely in vibrational spectroscopy.
Linear absorption coefficient	α	Usual name for the linear napierian absorption coefficient (see below). See also "Optical absorption depth".
Linear decadic absorption coefficient	a, K	The decadic absorbance (see above) divided by the path-length, $a = A_{10}/l$. SI unit: m^{-1}. Common unit: $cm^{-1} = 100\, m^{-1}$.
Linear dichroism		The phenomenon of different optical absorption properties in different directions in the sample and, consequently, of different optical behavior under different linear polarizations of the radiation.
Linear napierian absorption coefficient	α	The napierian absorbance (see below) divided by the path-length, $\alpha = A_{e}/l$. SI unit: m^{-1}. Common unit: $cm^{-1} = 100\, m^{-1}$.
Linear remission coefficient	b	The negative napierian logarithm (see below) of the fraction of light remitted by a non-absorbing scattering sample, divided by the path length l. $$b = -\frac{\ln(I_R/I_o)}{l}$$ SI unit: m^{-1}.
Liquid crystal tunable filter	LCTF	An optical device, based on polarization interference caused by transmission through a series of birefringent liquid crystals of different thicknesses, that allows a narrow wavelength region to be selected and tuned over a broad spectral range.

Quantity	Symbol	Meaning
Local mode		An abbreviation of "local mode of vibration", i.e. a vibration localized in one type of bond. For highly excited CH stretching vibrations anharmonic interactions mix the normal vibrations to the point that each observed vibration behaves as a local mode.
Local molar polarizability	$\hat{\alpha}_m$	Usually simply called the molar polarizability. It is defined under the assumption of the Lorentz local field (see below) by the Lorentz–Lorenz formula: $$\hat{\alpha}_m(\tilde{v}) = \frac{3V_m}{4\pi}\frac{\hat{\varepsilon}(\tilde{v})-1}{\hat{\varepsilon}(\tilde{v})+2} = \frac{3V_m}{4\pi}\frac{\hat{n}^2(\tilde{v})-1}{\hat{n}^2(\tilde{v})+2}$$ where V_m is the molar volume and $\hat{\varepsilon}$ and $\hat{n}$ are the complex dielectric constant and refractive index, respectively. To allow description of absorption, $\hat{\alpha}(\tilde{v})$ is complex:
Local molar polarizability (continued)		$\hat{\alpha}_m(\tilde{v}) = \alpha'_m(\tilde{v}) + i\alpha''_m(\tilde{v})$. The imaginary molar polarizability spectrum shows absorption bands free from long range dielectric effects which distort the shapes of very strong absorption bands. SI unit: $J^{-1}\,C^2\,m^2\,mol^{-1}$. (In the rationalized MKS system on which SI units are based, the term $3V_m/(4\pi)$ in the above equations is replaced by $3V_m\varepsilon_o$, where ε_o is the permittivity of vacuum.) Common unit: $cm^3\,mol^{-1}$, as an abbreviation of $4\pi\varepsilon_o\,cm^3\,mol^{-1}$; $1\,cm^3\,mol^{-1} = 1.11265 \times 10^{-16}\,J^{-1}\,C^2\,m^2\,mol^{-1}$. See also "Polarizability volume".
Local molar polarizability volume		The term recommended to avoid confusion about the local molar polarizability when it is expressed in $cm^3\,mol^{-1}$, because under the SI system the polarizability is $4\pi\varepsilon_o$ times this quantity. See also "Local molar polarizability".
Local susceptibility	$\widehat{C}$	The (complex) local susceptibility, $\widehat{C} = C' + iC''$ was defined by Bryce Crawford, Jr under the Gaussian system of units as the proportionality factor between the polarization induced in a material and the Lorentz local field (see below) that acts on its molecules; thus $\boldsymbol{P} = \widehat{C}\boldsymbol{E}_{loc}$ and $\widehat{C}^{-1} = \hat{\chi}^{-1} + 4\pi/3$, where $\hat{\chi}$ is the macroscopic susceptibility (defined by $\boldsymbol{P} = \hat{\chi}\boldsymbol{E}$, where $\boldsymbol{E}$ is the applied macroscopic field). $\widehat{C}$ equals the local molar polarizability volume (see above) divided by the molar volume and is useful for comparison of different materials. SI units: none, a dimensionless quantity. Common unit: none, a dimensionless quantity, but numerically 4π times smaller than when expressed in the dimensionless SI units.
Lock-in Amplifier	LIA	An amplifier that amplifies only those signals that have, within a specified bandwidth, the same frequency as, and a specified phase relationship with, the selected reference signal.
Longitudinal vibration		A crystal vibration in which the atomic displacements are parallel to the wavevector, i.e. to the propagation direction of the wave. Longitudinal vibrations may be longitudinal optic vibrations or

Quantity	Symbol	Meaning
		longitudinal acoustic vibrations. Strictly longitudinal vibrations only occur for propagation along a direction of sufficiently high symmetry. See also "Acoustic vibration", "Crystal vibrations", "Optic vibration", and "Transverse vibration".
Lorentzian band		A band with the shape $H_L W^2/[W^2 + 4(\tilde{v} - \tilde{v}_o)^2]$, where H_L is the peak height, W is the full width at half height, and $\tilde{v}_o$ is the peak wavenumber.
Lorentz local field		The relation $\boldsymbol{E}_{\text{loc}} = \boldsymbol{E} + \boldsymbol{P}/(3\varepsilon_o)$, between the applied macroscopic field, $\boldsymbol{E}$, the local field acting on a molecule, $\boldsymbol{E}_{\text{loc}}$, the polarization, $\boldsymbol{P}$, of the material and the permittivity of vacuum, ε_o. The relation is exact for molecules in isotropic materials. In the esu and Gaussian systems of electricity and magnetism the relation is $\boldsymbol{E}_{\text{loc}} = \boldsymbol{E} + 4\pi\boldsymbol{P}/3$.
Low pass filter		Either: An optical filter that excludes the radiation of wavenumber higher than a certain cut-on value and passes radiation of wavenumber below this value. Or: An electrical filter that blocks signal with a modulation frequency above a certain cut-on value and passes signals of frequency below this value.
Magic angle		The magic angle is 54.74°, the angle at which the Legendre polynomial $P_2(\cos\theta) = \frac{1}{2}(3\cos^2\theta - 1)$ equals zero. This angle is important in the estimation of the molecular orientation in polymer fibers by vibrational spectroscopy. In particular, if for a particular vibrational band the dichroic ratio measured parallel and perpendicular to the fiber axis is unity for many degrees of orientation of the fiber, then the oscillating dipole must lie very close to 54.74° to the axis of the polymer chain. The name arises from solid state nuclear magnetic resonance, in which rapidly spinning a sample about an axis at 54.74 degrees to the magnetic field "magically" converts into sharp lines the very broad bands that are due to coupling of the magnetic dipoles in the solid.
Mapping		Use of microspectroscopy to obtain information about the spatial composition of a sample by measuring its spectrum in different parts by moving the sample or, in Raman spectroscopy, by moving the exciting laser beam to different parts of the sample.
Mass concentration	ρ, γ, c	The mass of the component divided by the volume of the mixture, e.g. for solute j, $\rho_j = m_j/V$. SI unit: kg m^{-3}. Common unit: $\text{g dm}^{-3} = \text{g L}^{-1} = \text{kg m}^{-3}$; $\text{mg L}^{-1} = 10^{-3} \text{ kg m}^{-3}$. N.B. In analytical and polymer science c is often used for mass concentration as well as for amount concentration.
Mass fraction	w	The mass of the component divided by the total mass of the sample, e.g. for component j, $w_j = m_j/\Sigma m_i$. SI unit: none, a dimensionless quantity. Common unit: ppm, ppmg, ppb, or ppt. See "Parts per zillion".

Quantity	Symbol	Meaning
Matrix isolation		A technique in which the molecules of interest are co-deposited with a large excess of an inert diluent onto a cold plate sufficiently slowly that no rearrangement of the molecules occurs on condensation. The technique is used to study isolated molecules at low temperature in the absence of free molecular rotation.
Mechanical anharmonicity		The influence of the cubic and higher order terms in the vibrational potential energy (see below).
Mechanical harmonicity		The influence of the quadratic terms in the vibrational potential energy (see below).
Mertz phase correction		Also known as multiplicative phase correction. The phase angles at each wavenumber required to correct the asymmetric interferogram are computed from the complex Fourier transform of a short, double-sided interferogram that is extracted from the recorded interferogram as $\theta_{\tilde{v}\%} = \arctan[im(\tilde{v}\%)/re(\tilde{v}\%)]$ where $im(\tilde{v})$ and $re(\tilde{v})$ are the imaginary and real transforms of the short interferogram. The entire interferogram, which is essentially one-sided with just a few points on the short side, is then Fourier transformed to give $RE(\tilde{v})$ and $IM(\tilde{v})$ after being multiplied by a ramp function which weights the points on both sides of the center burst correctly and being multiplied by the apodization function. The intensity is then calculated as $$B(\tilde{v}\%) = RE(\tilde{v}\%)\cos(\theta_{\tilde{v}\%}) + IM(\tilde{v}\%)\sin(\theta_{\tilde{v}\%}).$$
Mid-infrared mid-IR		The spectral region in which vacuum wavenumbers range from $\sim 4000\,\text{cm}^{-1}$ to $\sim 400\,\text{cm}^{-1}$.
Mie scattering		Light scattering by particles with diameters that are greater than or similar to the wavelength of radiation but are too small to yield specular or diffuse reflection.
Mode		In vibrational spectroscopy "mode" usually means "mode of vibration". This is the same as "normal vibration" or, as is usually said, simply "vibration".
Modulation frequency f		The frequency at which the intensity of an optical beam, the polarization of a beam, or some property of the sample is changed. SI unit: Hz; common unit, Hz.
Molar absorptivity Molar (decadic) absorption coefficient	ε	Decadic absorbance divided by the path-length, l, and mole concentration, c, of the absorbing material. $\varepsilon = A_{10}/cl$. The molar absorptivity is a Beer–Lambert absorption coefficient. SI unit: $\text{m}^2\,\text{mol}^{-1}$. Common unit: $\text{L}\,\text{mol}^{-1}\,\text{cm}^{-1} = 0.1\,\text{m}^2\,\text{mol}^{-1}$; $\text{cm}^2\,\text{mol}^{-1} = 10^{-4}\,\text{m}^2\,\text{mol}^{-1}$.
Molar concentration		The number of moles of the component in unit volume of mixture. Also called "mole concentration" and "amount concentration" (see above).

Quantity	Symbol	Meaning
		SI unit: $mol\,m^{-3}$.
		Common unit: $mol\,L^{-1} = mol\,dm^{-3} = 1000\,mol\,m^{-3}$.
Molar ellipticity	$[\Theta]_\lambda^T$	The ellipticity divided by the amount concentration of the optically active absorbing material and by the path length, all at temperature T and wavelength λ.
		SI unit: $rad\,m^2\,mol^{-1}$.
Molar napierian absorption coefficient	κ	Napierian absorbance divided by the path-length, l, and mole concentration, c, of absorbing material. $\kappa = A_e/cl$. The molar napierian absorption coefficient is a Beer–Lambert absorption coefficient.
		SI unit: $m^2\,mol^{-1}$.
		Common unit: $L\,mol^{-1}\,cm^{-1} = 0.1\,m^2\,mol^{-1}$;
		$cm^2\,mol^{-1} = 10^{-4}\,m^2\,mol^{-1}$.
Molar polarizability	$\hat{\alpha}_m$	The polarizability per mole of absorber. Usually means the same as the "local molar polarizability" (see above).
Mole concentration	c	Same as "molar concentration" (see above).
Mole fraction	x	The number of moles of the component divided by the total number of moles in the mixture, e.g. for component j, $x_j = n_j/\Sigma n_I$.
		SI unit: none, a dimensionless quantity. Commonly given as a fraction, a percentage, or ppm, ppb, or ppt. See "Parts per zillion".
Moment of inertia	I_a, I_b, I_c	The standard measure of the inertial resistance to rotational motion about a principal axis of inertia. $$I = \sum_\alpha m_\alpha x_\alpha^2,$$ where m_α is the mass of atom α and x_α is its distance from the principal axis of rotation. I_a, I_b, I_c are respectively the smallest, middle and largest moments of inertia of a non-linear polyatomic molecule.
Multichannel advantage		The increase in measurement efficiency obtained by measuring the intensity at many different wavenumbers simultaneously with many detectors, as with a CCD or other array detector.
Multiple attenuated total reflection		The process in which attenuated total reflection occurs sequentially several times with the same sample. It has also been called multiple internal reflection, MIR, and frustrated multiple internal reflection, FMIR.
Multiple internal reflection	MIR	A term sometimes used for multiple attenuated total reflection.
Multiplex advantage		The increase in measurement efficiency obtained by measuring the intensity at many different wavenumbers simultaneously with a single detector, as is done, for example, in Fourier transform spectroscopy.
Multiplicative noise		See "Flicker noise".
Napierian		Relating to the base e, e.g. e^x or $\ln x = \log_e x$.

Quantity	Symbol	Meaning
Napierian absorbance	A_e, B	$A_e = -\ln(1 - \alpha_i)$, whence $A_e = -\ln(T_i)$ for a sample that does not scatter or luminesce. Here the internal absorptance, α_i (see above) or internal transmittance, T_i (see above) are the absorptance or transmittance corrected for reflection and other non-absorption effects, and must be used if the napierian absorbance is to have absolute numerical significance. SI unit: none, a dimensionless quantity. Care must be taken to avoid confusion with the decadic absorbance $A_{10} = -\log_{10}(1 - \alpha_i)$.
Napierian logarithm	ln	The logarithm to the base e.
Natural lifetime		The lifetime of an excited state of a molecule that is isolated from radiation fields and other molecules or entities. The lifetime is limited by the probability of spontaneous emission to a lower state. If the state n can only emit spontaneously to a single lower state m, the natural lifetime of state n equals the reciprocal of A_{mn}, the Einstein transition probability of spontaneous emission.
Natural line width		The natural linewidth of a molecular line arises from the probability of spontaneous emission, which would limit the lifetime of the upper state n if the molecule were isolated from radiation fields and other molecules or entities. The natural linewidth (measured as the FWHH (see "Linewidth" above)) equals $1/(2\pi c_o \Delta t)$, where Δt is the natural lifetime of the upper state. If the upper state n can only emit spontaneously to a single lower state m the natural linewidth is $1.86 \times 10^{-38} \tilde{\nu}_{mn}^3 \langle m|\mu|n \rangle^2$, when the transition wavenumber $\tilde{\nu}_{mn}$ is in cm^{-1} and the dipole moment μ is in Debye ($1\,D = 3.33564 \times 10^{-30}\,C\,m$). In the infrared, typical natural linewidths are $\sim 10^{-7}\,cm^{-1}$.
Near-infrared Near-IR		The spectral region in which vacuum wavenumbers range from $\sim 12\,500\,cm^{-1}$ to $\sim 4000\,cm^{-1}$ and wavelengths range from $\sim 800\,nm$ to $\sim 2500\,nm$. The region is often divided into the silicon region between $12\,500\,cm^{-1}$ and $9000\,cm^{-1}$ ($800\,nm$ and $1100\,nm$) and the lead sulfide region between $9000\,cm^{-1}$ and $4000\,cm^{-1}$ ($1100\,nm$ and $2500\,nm$), where the names reflect the common detector for the region.
Neper		A special name sometimes given to the number 1. Its usual use in vibrational spectroscopy is as the unit of a napierian logarithm. Thus the unit of the linear napierian absorption coefficient is sometimes given as neper m^{-1} instead of m^{-1}.
Noise		A measure of the random excursions of a signal. Noise can be defined as peak-to-peak noise, which is the difference between the largest and smallest values of these fluctuations in a given region, or as root-mean-square noise, which is the standard deviation of the noise in that region. For digital data with ~ 100 independent data points, the peak-to-peak noise is about five times greater than the root-mean-square noise.

Quantity	Symbol	Meaning
Noise equivalent power	ϕ_N NEP	The incident radiation power that yields a signal-to-noise ratio of 1 within a bandwidth of 1 Hz at the wavelength or wavenumber of interest. SI unit: $W\,Hz^{-1/2}$.
Non-dispersive infrared methods		A term for methods, such as correlation spectroscopy, mainly used to obtain adequate spectral throughput for process measurement and monitoring, in which the effect of the sample on the radiation from the source is measured as a whole without exploring the wavenumber dependence.
Nonsymmorphic space group		A space group that contains screw axes (see below) and glide planes (see above).
Normal coordinate	Q_k	The formal mathematical description of a normal vibration. When the potential energy, V, is harmonic and the kinetic energy, T, is calculated in the limit of infinitesimally small displacements, the normal coordinates are defined as independent entities such that $$V = \frac{1}{2} \sum_{k=1}^{3N-6} \lambda_k Q_k^2 \text{ and } T = \frac{1}{2} \sum_{k=1}^{3N-6} \dot{Q}_k^2$$ where λ_k is the kth eigenvalue and $\dot{Q}$ is $\partial Q/\partial t$. Normal coordinate Q_k is related to the internal displacement coordinates, R_i, through the elements, $L_{ik} = \partial R_i/\partial Q_k$ of the kth column of the eigenvector matrix $\boldsymbol{L}$. The normal coordinates are not independent when the potential energy is anharmonic or the displacements are not infinitesimal. See also "Normal coordinate analysis" and "Vibrational eigenvector". SI unit: $kg^{1/2}\,m$. Common unit: $u^{1/2}\,\text{Å} = 4.07497 \times 10^{-24}\,kg^{1/2}\,m$.
Normal coordinate analysis		The calculation of the normal modes of vibration of a molecule or crystal under the assumptions that the potential energy is harmonic and the displacements from equilibrium are infinitesimal. If internal coordinates are used the calculation is usually through the $\boldsymbol{G}$ and $\boldsymbol{F}$ matrices (see above) and the equation $\boldsymbol{GFL} = \boldsymbol{L}\lambda$. See also "Normal coordinate" and "Vibrational eigenvector".
Normal dispersion		In non-absorbing regions far from regions of strong absorption, the real refractive index of a material decreases slowly as the wavenumber decreases. This behavior is termed normal dispersion (of the refractive index).
Normal incidence		When the angle of incidence of a radiation beam onto a surface is $0°$, i.e. the incident radiation beam is normal to the surface.
Normalized Tunneling Intensity	NTI	The quantity $d^2I/dV^2 \div (dI/dV)$ which is plotted against the bias voltage V to report inelastic electron tunneling spectroscopy data. Also called constant resolution tunneling intensity.

Quantity	Symbol	Meaning
Normal mode		An abbreviation of "normal mode of vibration" which means "normal vibration".
Normal vibration		One of the 3N-6 (3N-5 for a linear molecule) independent vibrational motions that would add to give the total vibrational motion in a molecule if the displacements from equilibrium were infinitesimal and the interatomic potential were strictly quadratic in the displacements. This never occurs, so normal vibrations are an idealized concept that has proved extremely useful.
Norton–Beer-apodization function		A set of apodization functions explored by R.H. Norton and R. Beer in 1976 of the form $$A(\delta) = \sum_{i=0}^{n} C_i \left[1 - \left(\frac{\delta}{\Delta} \right)^2 \right]^i$$ where δ is the optical retardation and Δ is the maximum optical retardation in the interferogram. They defined three functions for general use: a weak function with $C_0 = 0.348093$, $C_1 = -0.087577$, $C_2 = 0.703484$, and other $C_i = 0$; a medium function with $C_0 = 0.152442$, $C_1 = -0.136176$, $C_2 = 0.983734$, and other $C_i = 0$; a strong function with $C_0 = 0.045335$, $C_1 = 0.0$, $C_2 = 0.554883$, $C_3 = 0.399782$, and other $C_i = 0$.
Null-balance		See "Optical null".
Number concentration Number density	C	The number of molecules (or atoms, ions, formula units, etc.) of interest divided by the volume of the mixture, e.g. for component j, $C_j = N_j/V$. SI unit: m^{-3}.
Numerical aperture	NA	For a typical optical system, the NA is the sine of the half-angle of the beam at an aperture. For a fiber, the NA is equal to $n_o \sin \theta_\alpha$, where n_o is the refractive index of the exterior medium and θ_α is the maximum input half angle that can support propagation.
Nyquist criterion		A result of information theory that a sine wave can be completely reconstructed if its ordinate is known at two or more points in a cycle.
Nyquist wavenumber		The highest wavenumber that is correctly sampled with the digitization interval used. See "Folding" and "Nyquist criterion".
O-branch		See "Rotational branches".
Off-diagonal force constant	F_{ij}	The same as "interaction force constant" (see above).
Optical absorption depth	μ_β	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 (see above). SI unit: m. Common unit: μm.
Optical constants		A collective name for the real and imaginary refractive indices, n and k.
Optical density		An old term meaning absorbance (see above). The use of optical density is now discouraged.
Optically active materials		Optically active materials show different behavior to right and left circularly polarized radiation. They are chiral molecules and materials.

Quantity	Symbol	Meaning
Optical null		In an optical null double beam spectrometer the ratio of the radiant power in the two beams at each wavenumber is determined opto-mechanically by inserting a linear optical attenuator into the reference beam until the two signals measured by the detector are equal, then measuring the displacement of the optical attenuator.
Optical path difference	OPD	The same as "Optical retardation" (see below).
Optical retardation		The optical path difference between the two arms of a Michelson or other two-beam interferometer. The term is derived from phase retardation which refers to the change in the phase of the electromagnetic radiation in the interferometer. Also commonly called "retardation". SI unit: m. Common unit: cm.
Optical rotatory dispersion	ORD	The wavelength dependence of the angle of rotation of the plane of linearly-polarized radiation when transmitted through optically active materials. See also "Optically active materials".
Optical throughput		An alternative name for "étendue" (see above).
Optic vibration Optic branch		If there are A atoms in the primitive unit cell, $(3A\text{-}3)$ branches of dispersion curves tend to finite frequency as the wavevector tends to zero, i.e. as the wavelength tends to infinity. These are the optic branches and the vibrations in them are the optic vibrations. See also "Crystal vibrations", "Longitudinal vibration", "Transverse vibration" and "Acoustic vibration".
Orbital mediated tunneling spectroscopy	OMTS	A technique based on electron tunneling in which bands are observed in dI/dV spectra that are associated with resonance-like interactions between the tunneling electron and oxidized or reduced states of the molecular system studied. Usually used for analyzing data obtained from metal−insulator−analyte−metal tunnel diodes or from the metal−analyte−tip structure in STM (scanning tunneling microscopy).
Ordinary wave Ordinary ray		In a uniaxial crystal electromagnetic waves that have their electric vector perpendicular to the optic axis obey the normal laws of refraction and are called ordinary waves or ordinary rays. See also "Extraordinary wave".
Overtone band Overtone transition		An overtone band results from an overtone transition, which is a transition between the ground state and a state in which a single vibration is multiply excited, e.g. a transition from the ground state to the state in which $v_i \geq 2$, $v_{j \neq i} = 0$.
pATR spectrum		A term used and recommended for the spectrum of $-\log_{10}$ of the attenuated total reflectance (see above) to avoid the confusing, but common and incorrect, practice of calling it the absorbance spectrum.
P-branch		See "Rotational branches".
p-polarization		The polarization when electromagnetic radiation is incident upon a surface with its electric vector in the plane of incidence and, therefore, inclined to the reflecting surface unless the incidence is normal. Also called transverse magnetic, TM, polarization.

Quantity	Symbol	Meaning
Parfocal		A parfocal optical system has no chromatic aberration. Thus in a parfocal infrared microscope the focal points of the infrared and visible beams coincide.
Parts per zillion	ppz ppzg ppzv	Where zillion (z) is usually thousand (t or th), million (m), billion (b) or trillion (t or tr). Commonly used to express a mole, gram, or volume fraction. ppzg or ppzv are often used to mean parts per zillion by mass, i.e. a mass fraction, or parts per zillion by volume, i.e. a volume fraction (for gases essentially a mole fraction), respectively. Use of these terms to express a concentration (mass/volume) is confusing and should be defined if it is unavoidable. Also, billion and trillion have different meanings in Europe (10^{12} and 10^{18}) and North America (10^9 and 10^{12}) and should be defined.
Path-length Path length Pathlength	l, s	The length of the optical path through the sample. In a transmission cell, this is usually taken as the distance between the windows. SI unit: m. Common unit: μm, mm.
Penetration depth	d_p	See "Depth of penetration". SI unit: m. Common unit: μm.
Percent transmission	$\%T$	Transmittance × 100%.
Permittivity of vacuum	ε_o	In the rationalized mks system on which the SI units of electricity and magnetism are based, the permittivity of vacuum is defined by the equation $\varepsilon_o\mu_o = 1/c^2$, where $c = 2.99792458 \times 10^8\,\text{m s}^{-1}$ is the speed of light in vacuum and $\mu_o = 4\pi \times 10^{-7}\,\text{H m}^{-1}$ is the magnetic permeability of vacuum, where H = henry. Thus, $\varepsilon_o = 8.854187816 \times 10^{-12}\,\text{F m}^{-1}$, where F = farad.
Phase correction		The correction of an interferogram for asymmetry about zero path difference.
Phase modulation		The process of modulating the phase, or path, difference between the two beams of a step-scan interferometer by rapidly cycling (dithering) the position of the mirror that reflects one of the beams over a small range about a constant average. Here "small" means "comparable with the step size".
Phonon		The quantum of energy in a crystal vibration.
Photoacoustic saturation		A condition in photoacoustic spectroscopy (see below) in which all bands with greater than a certain absorption intensity appear to have the same intensity. It arises when the sample is optically opaque and thermally thin, i.e. when the thermal diffusion depth, L (see below) is greater than the optical absorption depth, μ_β (see above) and less than the sample thickness. The condition may be relieved by increasing the modulation frequency sufficiently that L becomes less than μ_β, i.e. that the sample becomes thermally thick.
Photoacoustic spectroscopy	PAS	A form of spectroscopy in which the absorption of radiation by the sample is detected by the emission of sound generated by a thermal pressure wave in the sample.
Photomultiplier multiplication noise		Noise caused by random fluctuations in the gain within a photomultiplier tube due to the random nature of the secondary emission of electrons at the dynodes.
Photothermal spectroscopy		A form of spectroscopy in which the absorption of radiation by a sample is detected as a result of the heat caused by the absorption.

Quantity	Symbol	Meaning
Planck's constant	h	The fundamental constant $h = 6.6260755 \times 10^{-34}$ J s which relates the frequency of the radiation ν to the energy of a photon, and hence to the energy change ΔE caused by the absorption of the photon, via $\Delta E = h\nu$.
Point Group		The mathematical group formed by the symmetry operations, including the identity, that pass through a point and transform a molecule into itself, i.e. leave a molecule unchanged. More generally, one of the 32 mathematical groups formed by the identity, the inversion center, symmetry planes, and proper and improper rotation axes that pass through a single point.
Polarizability	α	The coefficient of the first order term in the relation between the electric dipole moment $\boldsymbol{\mu}$ of a molecule and the electric field $\boldsymbol{E}$ which acts on the molecule, $\boldsymbol{\mu} = \boldsymbol{\mu}_o + \boldsymbol{\alpha}E + \frac{1}{2}\boldsymbol{\beta}E^2 + \frac{1}{6}\boldsymbol{\gamma}E^3 + \cdots$. The polarizability is a scalar for isotropic entities and a 3×3 tensor for others. SI unit: $J^{-1} C^2 m^2$. Common unit: cm^3, as an abbreviation of $4\pi\varepsilon_o \, cm^3$; $cm^3 = 1.11265 \times 10^{-16} \, J^{-1} C^2 m^2$.
Polarizability derivative tensor		See "Derived polarizability tensor".
Polarizability invariant	$\bar{\alpha}_o, \gamma_o^2$	The rows and columns of the 3×3 polarizability tensor correspond to x, y and z Cartesian directions. The two quantities $\bar{\alpha}_o = \frac{1}{3}(\alpha_{xx} + \alpha_{yy} + \alpha_{zz})$ and $\gamma_o^2 = \frac{1}{2}[(\alpha_{xx} - \alpha_{yy})^2 + (\alpha_{yy} - \alpha_{zz})^2 + (\alpha_{zz} - \alpha_{xx})^2 + 6(\alpha_{xy}^2 + \alpha_{yz}^2 + \alpha_{zx}^2)]$ are invariant to reorientation of the axes of the tensor. $\bar{\alpha}_0$ is the isotropic invariant of the polarizability and γ_0^2 is the anisotropic invariant of the polarizability.
Polarizability volume	α	A term sometimes used for the polarizability when it is expressed in volume units. This results when polarizability is defined in equations under the esu or Gaussian system. To obtain the SI unit $J^{-1} C^2 m^2$, the polarizability volume must be multiplied by $4\pi\varepsilon_o$ before converting the volume unit to m^3. ε_o is the permittivity of vacuum (see above). See also "Polarizability" and "Local molar polarizability".
Polarized Raman band		In normal Raman spectroscopy a polarized band has depolarization ratio $\rho \leq 0.75$ for linear polarized incident radiation.
Potential coupling		Coupling of vibrational displacements through terms in the vibrational potential energy (see below). The second-order (quadratic) terms cause harmonic potential coupling while the cubic and higher terms cause anharmonic potential coupling.
Potential energy		See "Vibrational potential energy".
Pressure broadening		Broadening of spectral lines of gases due to molecular collisions and other intermolecular interactions that reduce the lifetime of quantum states. At pressures sufficiently low that the linewidth is far smaller than the line wavenumber, the linewidth increases linearly with pressure, the broadening is homogeneous and the lineshape is Lorentzian.

Quantity	Symbol	Meaning
Primitive translation		One of the three translation vectors that carries one lattice point into another in a crystal. Crystallographers sometimes prefer to use the larger and more symmetrically oriented translation vectors of centered cells (which contain more than one lattice point) instead of the primitive translation vectors.
Primitive unit cell		The parallelepiped between lattice points of a crystal defined by the three primitive translation vectors. For body-centered and face-centered structures the primitive cell is two or four times smaller than the centered cell that is used by crystallographers, and the primitive unit cell can be chosen in more than one way. For all other structures the primitive unit cell is simply called the unit cell.
Proper rotation axis	C_n	A symmetry element such that rotation by $2\pi/n$ about the axis transforms an object into itself.
Q-branch		See "Rotational branches".
Quantization noise		Noise due to the finite resolution of any readout device; also known as digitization noise.
Quantum noise		The fundamental noise due to the random emission of photons from a source.
R-branch		See "Rotational branches".
Radial frequency		The same as "angular frequency".
Radiance	L	A normalized measure of the brightness of a source. It is the radiant power emitted by unit area of the source into unit solid angle of the radiation beam. SI unit: $W\,sr^{-1}\,m^{-2}$.
Radiant energy density	ρ, w	The radiant energy in unit volume. SI unit: $J\,m^{-3}$.
Radiant flux (emitted) Radiant excitance	M	The radiant power emitted by unit area of the source. SI unit: $W\,m^{-2}$
Radiant flux received irradiance	I, E	The radiant power incident on unit area. See also "Intensity". SI unit: $W\,m^{-2}$.
Radiant power	Φ, P	Radiant energy in unit time. SI unit: W.
Radiation		See "Electromagnetic radiation".
Radiative lifetime		The same as "natural lifetime" (see above).
Raman excitation wavelength		See "Excitation wavelength".
Raman excitation wavenumber		See "Excitation wavenumber".
Raman optical activity	ROA	The phenomenon that vibrations in chiral molecules and materials Raman-scatter right circularly polarized incident radiation to a different extent than left circularly polarized incident radiation. In practice, the circular polarization of the exciting beam, or of the scattered beam, or of both beams simultaneously, may be selected. Raman optical activity is usually specified as "right minus left" circular polarization, in unfortunate contrast to the "left minus right" specification that is universal in vibrational circular polarization and other forms of optical activity.

Quantity	Symbol	Meaning
Raman spectrum		A graph of the radiant energy, or number of photons, scattered by the sample through the indirect interaction between the molecular vibrations in the sample and monochromatic radiation of frequency much higher than that of the vibrations. The abscissa is usually the difference in wavenumber between the incident and scattered radiation.
(Normal) Raman scattering		Raman scattering that occurs through the polarizability, not the hyper-polarizabilities, and is excited by radiation that is not in resonance with electronic transitions in the sample. The scattering, in fact, occurs through the derived polarizability tensors, i.e. through changes in the polarizability during the vibrations.
Raman wavenumber shift	$\Delta\tilde{\nu}$	The wavenumber of the exciting line minus the wavenumber of the scattered radiation. SI unit: m^{-1}. Common unit: $cm^{-1} = 100\,m^{-1}$. $\Delta\tilde{\nu}$ is positive for Stokes scattering and negative for anti-Stokes scattering.
Rapid-scan FT-IR		Fourier transform infrared spectroscopy in which the path difference is continually changed at a rate $\geq 0.05\,cm\,s^{-1}$. See also "Continuous scan interferometers".
Ratio recording		In a ratio-recording double beam spectrometer the ratio of the radiant power in the two beams at each wavenumber is determined by electronically taking the ratio of the two signals from the detector.
Rayleigh criterion		The Rayleigh criterion of resolution was proposed to define the resolution obtainable from a diffraction limited grating spectrometer. It is based on the properties of the sinc-squared, i.e. $[(\sin(x)/x)^2]$, instrument line shape that is given by such a spectrometer and also by a Fourier transform spectrometer that uses triangular apodization. The criterion states that two lines of equal intensity and width are just resolved when the peak of one line is at the wavenumber of the zero-crossing of the second line closest to its peak. Under these conditions the measured spectrum shows a dip between the two peaks that is 20% of the peak height. For spectra measured with a different instrument line shape, the separation of two lines required to give a dip of 20% between them has sometimes been incorrectly called the Rayleigh resolution.
Rayleigh scattering		Light scattering in which the incident and scattered radiation has the same frequency. Also called elastic scattering.
Real dielectric constant Real relative permittivity	ε'	The real part of the dielectric constant, simply called the dielectric constant for non-absorbing materials. Related to the real, n, and imaginary, k, refractive indices through $\varepsilon' = n^2 - k^2$. SI unit: none, a dimensionless quantity.
Real refractive index	n	The real part of the complex refractive index $\hat{n}$. When no absorption occurs, n is the ratio of the velocity of radiation in vacuum to that in the medium and is usually called simply the refractive index. SI unit: none, a dimensionless quantity.

Quantity	Symbol	Meaning
Reflectance	ρ	In spectroscopy, the ratio of the "spectral intensity" (see below) at wavenumber $\tilde{\nu}$ reflected by the sample to that incident on the sample. For non-scattering and non-luminescent samples the sum of absorptance (α), transmittance (T) and reflectance (ρ) equals one. SI unit: none, a dimensionless quantity.
Reflectance spectrum		A term sometimes used instead of "reflection spectrum". The word "reflectance" is reserved for the fraction of the incident radiation that is reflected by a sample. Thus, the term "reflectance spectrum" should only be used when the intensity axis shows the reflectance. In other cases "reflection spectrum" (see below) is the term to use.
Reflection		The process by which radiation is reflected by a sample. For non-scattering samples the term means "Fresnel reflection" (see above) or "specular reflection" (see below); for scattering samples the term includes "regular reflection" (see below) and "volume reflection" (see below) or "diffuse reflection" (see above).
Reflection–absorption		A sampling method in which the radiation enters and travels through an absorbing medium, is reflected by a smooth surface that originally was, and still is usually, metallic, and again travels through the absorbing medium before exiting. The primary process is the absorption of radiation by the absorbing medium if the path-length in that medium is of the order of the wavelength of the light or greater, but absorption by species at the surface can be detected if the path-length in the absorbing medium is much less than the wavelength of the radiation. In recent years the former case has been called transflection (see below), and reflection–absorption at grazing incidence (see below) has been used in the latter case for the observation of surface species.
Reflection–absorption at grazing incidence		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 travelling 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. This technique is also known as reflection–absorption infrared spectroscopy (RAIRS) or infrared reflection–absorption spectroscopy (IRRAS).
Reflection–absorption infrared spectroscopy	RAIRS	See 'Reflection–absorption at grazing incidence'.
Reflection spectrum		A general term for the spectrum of radiation reflected by a sample. The spectrum may be called a reflectance spectrum if the ordinate quantity is the reflectance, but not otherwise.
Refractive index		See "Real refractive index" and "Imaginary refractive index".
Regular reflection		A term sometimes used for front-surface reflection from scattering samples instead of "specular reflection" (see below) to distinguish it from "diffuse reflection".

Quantity	Symbol	Meaning
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 (see above).
Remission fraction	R	The fraction of the incident radiation that undergoes remission. The sum of the remission fraction (R), the transmission fraction (T) (see below) and the absorption fraction (A) (see above) equals one.
Remission function		A name sometimes used for the Kubelka–Munk function.
Remittance		Another term for remission fraction.
Resolution		A term that usually means spectral resolution and is used in two different ways. First, (spectral) resolution of an instrument can be defined as the full width at half height of an infinitely sharp isolated line measured by the instrument. An equivalent definition is the minimum separation of two infinitely sharp lines of equal intensity that allows the presence of two lines to be seen in the measured spectrum. Resolution depends strongly on the instrument line shape function of the spectrometer and on the natural line width. Second, the nominal (spectral) resolution that a user uses to obtain a spectrum. The actual resolution achieved is related to this, to the width of the bands studied and to the alignment of the instrument. SI unit: m^{-1}. Common unit: $cm^{-1} = 100\,m^{-1}$. See also "Rayleigh criterion", "Spectral resolution".
Resolving power	R	The wavelength (or wavenumber or frequency) divided by the resolution at that wavelength (or wavenumber or frequency); $R = \lambda/d\lambda = \tilde{\nu}/d\tilde{\nu} = \nu/d\nu$. SI unit: none, a dimensionless quantity.
Resonance Raman scattering		Raman scattering that occurs through the polarizability, not the hyper-polarizabilities and is excited by radiation that is in resonance with electronic or vibronic transitions in the sample.
Reststrahlen		An adjective used to describe bands, regions, reflection, etc., associated with the extremely intense absorption by the lattice vibrations of ionic crystals. Infrared radiation with the wavenumbers of the absorption by the lattice vibrations is reflected from an ionic crystal very efficiently, while radiation with all other wavenumbers is largely transmitted. This separation is so effective that reflection from such a crystal was used as an optical filter to isolate these "remaining rays", or "reststrahlen" as they are called in German.
Retardation		See "Optical retardation".
Rotational branch, O, P, Q, R, S.		In rotation–vibration spectra of gases, branches of lines that derive from the same change in rotation quantum number, J. $\Delta J = J_{upper} - J_{lower} = -2, -1, 0, +1$ and $+2$ for the O, P, Q, R and S branches, respectively. The most commonly observed branches for simple molecules are the P, Q and R branches in infrared spectroscopy and the O, Q and S branches in Raman spectroscopy.

Quantity	Symbol	Meaning
Rotational lattice vibration		If the molecules in a crystal are located on centers of symmetry, the displacements due to molecular rotation are separated by symmetry from those due to molecular translation. The same separation occurs if the frequencies of the two types of vibration differ markedly, as they do for water. Hence, with M molecules per primitive unit cell, $3M$ (non-linear) or $2M$ (linear) branches of the lattice vibrations are termed rotational vibrations. These branches are all optic branches.
Rotational vibration		Same as "Rotational lattice vibration" (see above).
Rotational–Vibrational		Adjective usually used to characterize a transition. A rotational–vibrational transition is a transition in which both the rotational state and the vibrational state of a molecule change.
Rotation–vibration spectra		Spectra which show the absorption or emission of radiation during transitions between rotational–vibrational states of a molecule.
Ro-vibrational		See "Rotational–Vibrational".
Salt optics		Windows and lenses made from salts such as LiF, NaCl, KBr, CsBr,
Salt windows		CsI, TlBrI (KRS-5), CaF_2 and AgCl.
S-branch		See "Rotational branches".
s-polarization		The polarization when electromagnetic radiation is incident upon a surface with its electric vector perpendicular to the plane of incidence and, therefore, parallel to the reflecting surface. Also called transverse electric, TE, polarization.
Sampling depth		The same as "penetration depth".
Scattering coefficient		A term with two definitions:

Scattering coefficient — definitions (continued):

1. The negative napierian logarithm of the ratio of the intensity transmitted by a scattering, non-absorbing sample to the incident intensity, divided by the path length, l.

$$s = -\frac{\ln(I_\mathrm{T}/I_\mathrm{o})}{l}$$

2. The negative napierian logarithm of the ratio of the intensity of radiation scattered by a non-absorbing sample to the incident intensity, divided by the path length, l.

$$s = -\frac{\ln(I_\mathrm{s}/I_\mathrm{o})}{l}$$

SI unit: m^{-1}.

Quantity	Symbol	Meaning
Scattering geometry		The relation between the propagation directions, k_i, k_s, and the polarization directions, p_i, p_s, of the incident and scattered radiation, usually expressed in terms of laboratory-fixed or crystal-fixed Cartesian axes. A common notation, due to Porto, is $k_\mathrm{i}(p_\mathrm{i}\,p_\mathrm{s})k_\mathrm{s}$.
Schottky noise		Noise that is observed whenever a current passes through or is generated at an interface.
Screw axis		Symmetry element in solids consisting of a C_n rotation axis followed by translation by one nth of the length of the primitive unit cell parallel to the axis.

Quantity	Symbol	Meaning
Shot noise		Noise in the current or readout voltage that is due to both quantum noise and photomultiplier multiplication noise.
Signal-to-noise ratio		The ratio of the size of the signal to the size of the noise, usually calculated as the average signal divided by the root-mean-square noise.
Single-beam spectrometer		An instrument that measures the radiant power from the source that reaches the detector at each wavenumber and does not reference it to another spectrum in real time. Most Fourier transform spectrometers are single-beam spectrometers.
Single-beam spectrum		The output of a single-beam spectrometer as a function of wavenumber or wavelength. A single-beam spectrum is often called an intensity spectrum (the measured radiant power is the intensity (see above) times the area of the detector) and does not have a flat baseline.
Site splitting		The appearance of more than one band in the spectrum of the crystal when only one is seen in that of the gas, when this splitting is attributed either to the molecule lying on a crystal site of lower symmetry than that of the gaseous molecule or to molecules occupying more than one type of crystal site. Site splitting arises from the static intermolecular forces in the crystal.
Slit width		In a dispersive spectrometer, the physical slit width is the distance between the blades of the entrance or exit slits in the monochromator. The spectral slit width is the range of wavenumbers that the physical slit widths allow to be passed by the monochromator and is often determined as the full width at half height measured by the instrument for a line that is known to be extremely sharp.
Snell's law of refraction		$n_i \sin \theta_i = n_f \sin \theta_f$, where n_i and n_f are the (real) refractive indices of the incident and final media, θ_i is the angle of incidence and θ_f is the angle of refraction.
Space group		A mathematical group formed by the complete set of symmetry operations that transform an infinite crystal into itself. These operations include the identity, inversions, reflections, proper and improper rotations, screw axes, glide planes, and primitive translations and their multiples and combinations, and do not pass through a single point. The 230 space groups completely describe the ways in which identical objects may be arranged in an infinite lattice.
Spatial resolution		The smallest physical distance between measured positions on the sample in either single-point, mapping, or imaging spectroscopy.
Spectral intensity	$I_{\tilde{v}}(\tilde{v})$	The intensity in unit wavenumber interval at wavenumber $\tilde{v}$. Spectral intensity and spectral irradiance are formally the same quantity, but the term intensity is usually used for collimated beams of radiation. SI unit: $W\,m^{-1}$. Common unit: $W\,m^{-2}/cm^{-1}$.
Spectral irradiance	$I_{\tilde{v}}(\tilde{v})$	The radiant power in unit wavenumber interval at wavenumber $\tilde{v}$ received on unit area. Formally the derivative of the irradiance with respect to wavenumber at wavenumber $\tilde{v}$. SI unit: $W\,m^{-1}$. Common unit: $W\,m^{-2}/cm^{-1}$.

Quantity	Symbol	Meaning
Spectral radiance Spectral brightness	$L_{\tilde{\nu}}(\tilde{\nu})$	The radiance in unit wavenumber interval at wavenumber $\tilde{\nu}$. SI unit: $W\,sr^{-1}\,m^{-1}$ or photons $s^{-1}\,sr^{-1}\,m^{-1}$.
Spectral radiant energy density	$\rho_{\tilde{\nu}}(\tilde{\nu})$	The radiant energy density in unit wavenumber interval at wavenumber $\tilde{\nu}$. SI unit: $J\,m^{-2}$.
Spectral resolution		The smallest difference between wavenumbers (or wavelengths or frequencies) at which one can distinguish different spectral properties. There are several specific definitions about how the distinction is made. See "Rayleigh criterion", "Resolution".
Spectral slit width		See "Slit width".
Spectral subtraction		The subtraction of one spectrum from another spectrum, usually in order to improve the visibility of minor components of a mixture. Successful use of the technique requires spectra, like absorbance and Raman spectra, in which the intensity is linear in concentration, an extremely precise wavenumber scale and a very high signal-to-noise ratio.
Spectrometer		An instrument that separates radiation into its component wavenumbers and transforms the radiant power at each wavenumber into an electrical signal.
Spectrum		A graph of a quantity derived from the radiant power at each wavenumber as ordinate plotted against the wavenumber, wavelength or frequency of the radiation as abscissa. In mid-infrared and Raman spectroscopy wavenumber is universally used while it is frequently replaced by wavelength in near-infrared spectroscopy.
Specular reflection		A term with more than one meaning. Traditionally it meant reflection from a shiny surface, and is used for non-scattering samples to mean the same as Fresnel reflection. In discussion of scattering samples it refers to radiation that is reflected from the front surface of the sample at an angle of reflection equal to the angle of incidence; however, some authors include radiation that has penetrated into the particles before emerging at that angle and thus carries the absorption signature of the sample.
Spherical top		A molecule whose three principal moments of inertia are all the same. An isotropic molecule.
Stark effect		The effect of an electric field on molecular energy levels and, hence, spectra. The spectral changes may be manifested as single lines splitting into multiplets, frequency shifts, inactive vibrations becoming active, or changed intensities of active vibrations.
Step-scan interferometers		Interferometers typically used for FT-IR spectroscopy in which the optical path difference is changed by a certain amount, held constant, or modulated if phase modulation (see above) is desired, while the signal at the current path difference is recorded, then the process is repeated. Also known as "step-and-integrate" and "stepping mode" interferometers.
Stokes scattering		Light scattering in which the molecules gain energy and the scattered radiation has lower wavenumber than the exciting radiation.

Quantity	Symbol	Meaning
Stray light		Radiation that does not follow the usual path through a spectrometer and consequently appears in a spectrum at a wavenumber different from its true wavenumber. The term is also used to refer to radiation that passes around the sample instead of through in infrared spectroscopy, and consequently is not modified by the sample and seriously affects absolute and relative intensities.
Sum band Sum transition		A sum band results from a sum transition. A sum transition is a combination transition (see above) between the ground state and a state in which more than one vibration is excited; i.e. a transition from the ground state in which more than one quantum number increases.
Sum-frequency spectroscopy		Nonlinear optical technique in which pulsed lasers at frequencies ω_1 and ω_2 are overlapped at a surface and light emitted at the sum of the two frequencies, $\omega_1 + \omega_2$, is detected. One laser is normally in the mid-infrared and the other in the visible or near-infrared.
Sum tone		Synonymous with sum band or transition (see above).
Surface-enhanced infrared absorption	SEIRA	The phenomenon by which the intensity of absorption bands of molecules within a few nanometers of the surface of metal particles is increased by interactions with surface plasmons (the collective resonance of electrons near the surface of metal islands). The metals that give the largest enhancement are silver and gold, but this phenomenon has been reported to occur with at least eight other metals.
Surface-enhanced Raman spectroscopy	SERS	The phenomenon by which the intensity of vibrational bands in the Raman spectra of molecules within a few nanometers of the surface of microscopically rough metals, metal colloids and metal nanoparticles is increased by several orders of magnitude. The metals that give the largest enhancement are silver, gold and copper, but this phenomenon has been reported to occur more weakly with a few other metals.
Symmetric		A term used in at least three senses in vibrational spectroscopy. In general usage, a symmetric molecule is a molecule with high symmetry. In more specific usage, a property is symmetric with respect to a symmetry element if it remains unchanged by the action of the corresponding symmetry operation. And spectral bands are often said to be symmetric.
Symmetry coordinate	$\boldsymbol{S}, S_i$	Each S_i is a linear combination of general coordinates, usually internal coordinates, constructed to take advantage of the molecular symmetry. The S_i are elements of the vector $\boldsymbol{S}$. They have the same units as the general coordinates from which they were constructed.
Symmetric top		A molecule that has two equal principal moments of inertia with the third one different.
Symmorphic space group		A space group that does not contain screw-axes and glide planes.
Tangential baseline		For many practical purposes the area under a band is frequently measured above a tangential baseline, namely a baseline drawn tangentially to the spectral curve on each side of a band.

Quantity	Symbol	Meaning
Thermal diffusion depth, Thermal wave decay length	L, μ_s	In photoacoustic spectroscopy, equals $\sqrt{(D/\pi f)}$, where D is the thermal diffusivity and f is the modulation frequency of the radiation. 63% of the PAS signal originates within the thermal diffusion depth. SI unit: m. Common unit: μm.
Thermal diffusivity	D, a	The thermal conductivity divided by the product of the specific heat and the density. SI unit: $m^2 s^{-1}$.
Thermal wave decay coefficient	a_s	The reciprocal of the thermal diffusion depth (see above). SI unit: m^{-1}.
Throughput		An alternative name for "étendue" (see above). Also sometimes used for the product of the étendue and the transmittance of the optics of a spectrometer.
Total internal reflection		Internal reflection from a non-absorbing material at angles of incidence at or above the critical angle.
Total transmission		The combination of "direct transmission" (see above) and "diffuse transmission" (see above). Thus total transmission describes the collection of processes by which radiation incident on one side of a scattering sample leaves the opposite side of sample. Usually called simply transmission.
Total transmission fraction	T	The fraction of the spectral intensity incident upon a scattering sample that leaves the opposite side of the sample. The sum of the total transmission fraction (T), the remission fraction (R) (see above), and the absorption fraction (A) (see above) equals one.
Total transmittance		Another term for "transmission fraction" (see below) and "total transmission fraction" (see above).
Transflectance		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" (see below), and this usage is strongly discouraged.
Transflection		A term that has become common in recent years for reflection absorption at "near-normal incidence" when the thickness of the absorbing medium is large enough to yield an interpretable spectrum. The substrate is usually a mirror for mid-infrared measurements and a ceramic disk for near-infrared measurements. The angle of incidence is typically between 0° and 45°. Transflection is widely used in IR microscopy and is particularly convenient for measuring transmission-like spectra in a near-infrared instrument configured for diffuse reflection measurements by mounting the sample on a non-absorbing diffusely reflecting substrate.
Transition		A change of energy states which, in spectroscopy, is caused by interaction with radiation and is the cause of a spectral line at wavenumber $\tilde{\nu} = (E^{upper} - E^{lower})/hc_o$, where the Es are the energies of the states involved, h is Planck's constant and c_o is the velocity of light in vacuum.

Quantity	Symbol	Meaning
Transition dipole moment Transition moment	M_{ij}, R_{ij}	For electric dipole transitions, $M_{ij} = \int \psi_i^* \mu \psi_j \, d\tau$, where μ is the electric dipole moment and the ψ are the wave functions of the states involved. ψ_i^* is the complex conjugate of ψ_i. SI unit: C m. Common unit: Debye, $D = 3.33564 \times 10^{-30}$ C m. For magnetic dipole transitions, μ is replaced by the magnetic dipole moment.
Transition probability		The probability that a transition will occur in unit time. For dipole transitions it is proportional to the square of the transition dipole moment. For absorption and induced emission transitions it is also proportional to the spectral radiant energy density (see above) at the transition wavenumber. See also "Einstein transition probability". SI unit: s^{-1}.
Translational lattice vibration		If the molecules in a crystal are located on centers of symmetry, the displacements due to molecular translation are separated by symmetry from those due to molecular rotation. The same separation occurs if the frequencies of the two types of vibration differ markedly, as they do for water. Hence, with M molecules per primitive unit cell, $3M$ branches of the lattice vibrations are termed translational vibrations. Three of these branches are the three acoustic branches.
Transmission		The process in which radiation passes through a sample, entering it on one side and leaving it on the other. For non-scattering, non-luminescent samples the transmitted ray obeys Snell's law of refraction (see above), and the term internal transmission (see above) is used for transmission within the sample, i.e. when surface reflection effects are not included. For scattering, non-luminescent samples, transmission consists of two processes, direct transmission (see above), and diffuse transmission (see above) and is sometimes called total transmission.
Transmission fraction	T	The term usually used instead of "total transmission fraction" (see above) for scattering samples.
Transmission spectrum		A general term for the spectrum of transmitted radiation. The ordinate quantity is usually the percentage of the incident radiation that is transmitted, usually called the percent transmission, with range 0 to 100%. If the ordinate quantity is the fraction transmitted, i.e. the transmittance (see below), the ordinate range is 0 to 1 and the spectrum may be called a transmittance spectrum.
Transmittance	T, τ	In spectroscopy, the ratio of the spectral intensity (see above) at wavenumber $\tilde{\nu}$ transmitted by the sample to that incident on the sample. For non-scattering, non-luminescent samples the sum of absorptance (α), transmittance (T), and reflectance (ρ) equals one. For scattering, non-luminescent samples the term transmission fraction (see above) is usually used instead of transmittance. SI unit: none, a dimensionless quantity.

Quantity	Symbol	Meaning
Transverse vibration		A crystal vibration in which the atomic displacements are perpendicular to the wavevector, i.e. to the propagation direction of the wave. Transverse vibrations may be transverse optic vibrations or transverse acoustic vibrations. Strictly transverse vibrations only occur for propagation along a direction of sufficiently high symmetry. See also "Acoustic vibration", "Crystal vibrations", "Optic vibration" and "Longitudinal vibration".
Undersampling		Sampling less frequently than is required by the Nyquist criterion (see above). It occurs when an analog signal is digitized with less than two data points per wavelength of the shortest wavelength (highest wavenumber) radiation that reaches the detector.
Unified atomic mass unit	u	One twelfth of the mass of an atom of Carbon-12. Sometimes called the Dalton, Da.
Unit cell group		The mathematical group formed by the elements of the space group modulo primitive translations. "Modulo primitive translations" means that equivalent positions in different primitive unit cells are regarded as identical. The unit cell group is isomorphic with (so uses the same character table as) the point group of the crystal class. The symmetry elements in the unit cell group are the essential symmetry elements in the primitive unit cell, modulo primitive translations.
Unit cell group splitting		The combined effect of site splitting and Davydov splitting in the spectra of crystals.
Vacuum wavenumber Vacuum wavelength		See "Wavenumber in vacuum" or "Wavelength in vacuum".
Vibrational circular dichroism	VCD	Specifically, circular dichroism, $k^{\mathrm{L}} - k^{\mathrm{R}}$, for vibrational transitions. See "Circular dichroism". In general, the phenomenon that vibrations in chiral molecules and materials absorb left circularly polarized radiation to a different extent than right circularly polarized radiation.
Vibrational eigenvector	$\boldsymbol{L}$, L_{ik}	Part of the solution of the matrix equation of normal coordinate analysis, $\boldsymbol{GFL} = \boldsymbol{L}\lambda$. Each element L_{ik} of $\boldsymbol{L}$ gives the change in internal coordinate R_i during unit change in the normal coordinate Q_k, as shown in matrix form by $\boldsymbol{R} = \boldsymbol{LQ}$, i.e. $L_{ik} = \partial R_i / \partial Q_k$. Eigenvectors are sometimes expressed in terms of symmetry coordinates or Cartesian coordinates. SI unit: $\mathrm{kg}^{-1/2}$. Common unit: $\mathrm{u}^{-1/2} = 2.45400 \times 10^{13}\,\mathrm{kg}^{-1/2}$.
Vibrational electron energy loss spectroscopy	VEELS	See "High-resolution electron energy loss spectroscopy".
Vibrational kinetic energy	T	The kinetic energy of the molecule as a function of the displacements of the atoms from equilibrium positions. For

Quantity	Symbol	Meaning
		Cartesian displacement coordinates, x, y, z

$$T = \sum_{\alpha} \frac{1}{2} m_{\alpha} \left(\dot{x}_{\alpha}^2 + \dot{y}_{\alpha}^2 + \dot{z}_{\alpha}^2 \right)$$

where the sum is over all atoms and $\dot{x}_{\alpha}$, etc., are the displacement velocities.

For internal coordinates, R_i

$$T = \frac{1}{2} \mathbf{P}^t \mathbf{G} \mathbf{P} = \frac{1}{2} \dot{\mathbf{R}}^t \mathbf{G}^{-1} \dot{\mathbf{R}} = \frac{1}{2} \sum_{ij} G_{ij}^{-1} \dot{R}_i \dot{R}_j$$

where $\dot{\mathbf{R}}^t$ and $\dot{\mathbf{R}}$ are the row and column vector, respectively, of the $\partial R_i / \partial t$, $\mathbf{P}^t$ and $\mathbf{P}$ are the row and column vector, respectively, of the momenta conjugate to the R_i, $\mathbf{G}^{-1}$ is the inverse of the $\mathbf{G}$ matrix and G_{ij}^{-1} is the ijth element of $\mathbf{G}^{-1}$. The elements of the $\mathbf{G}$ matrix are defined by

$$G_{ij} = \sum_{\alpha} \frac{1}{m_{\alpha}} B_{i\alpha} B_{j\alpha}$$

where $B_{i\alpha}$ and $B_{j\alpha}$ relate the ith and jth internal coordinate to the αth Cartesian displacement coordinate through the equation $\mathbf{R} = \mathbf{B}\mathbf{X}$ in which $\mathbf{X}$ is the column vector of the Cartesian displacement coordinates.

SI unit: J.

Quantity	Symbol	Meaning
Vibrational mode		One of the 3N-6 (3N-5 for a linear molecule) normal vibrations of a molecule.
Vibrational potential energy	V	The potential energy of the molecule as a function of the displacements of the atoms from equilibrium positions. The harmonic terms are quadratic in the displacements and the anharmonic terms are of cubic, quartic and higher orders in the displacements.

In terms of normal coordinates

$$2V = \sum_{k} \lambda_k Q_k^2 + \sum_{ijk} k_{ijk} Q_i Q_j Q_k + \text{higher terms}$$

In terms of internal coordinates, R_i,

$$2V = \sum_{i} F_{ii} R_i^2 + \sum_{i,j \neq i} F_{ij} R_i R_j + \sum_{i,j,k} F_{ijk} R_i R_j R_k + \text{higher terms.}$$

SI unit: J.

Quantity	Symbol	Meaning
Vibrational term value	G	The vibrational energy, E, expressed in wavenumber units. $G = E/(hc_o)$, where h is Planck's constant and c_o is the velocity of light in vacuum. G is usually written with zero-energy at the minimum of the potential energy curve as:

Quantity	Symbol	Meaning
		For a diatomic molecule $$G = \omega_e(\upsilon + \tfrac{1}{2}) - \omega_e x_e(\upsilon + \tfrac{1}{2})^2 + \omega_e y_e(\upsilon + \tfrac{1}{2})^3$$ $$+ \text{ higher terms}$$ and for a polyatomic molecule $$G = \sum_k \omega_k \left(\upsilon_k + \frac{d_k}{2}\right) + \sum_{i \leq j} X_{ij}\left(\upsilon_i + \frac{d_i}{2}\right)\left(\upsilon_j + \frac{d_j}{2}\right)$$ $$+ \text{ higher terms}$$ where υ, υ_k, etc. $= 0, 1, 2, 3, \ldots$, and the d_ls are the degeneracies of the vibrations. SI unit: m^{-1} Common unit: $cm^{-1} = 100\,m^{-1}$.
Vibronic transition		A transition that changes both the electronic state and the vibrational state of the molecule.
Voigt function		The convolution of Gaussian and Lorentzian (Cauchy) functions.
Volume fraction	ϕ	The volume of component divided by the total volume of the components, all measured prior to mixing, e.g. for component j, $\phi_j = V_j / \sum_i V_i$. For gases, the volume fraction essentially equals the mole fraction. SI unit: none, a dimensionless quantity. Common unit: ppm, ppmv, ppb, or ppt. See "Parts per zillion".
Volume reflection		The process of light penetrating into a powdered sample and re-emerging from the surface of incidence; sometimes called Kubelka–Munk reflection and diffuse reflection.
Wavelength	λ	Distance traveled by the electromagnetic wave in one cycle in a non-absorbing medium of real refractive index n. $$\lambda = \frac{\lambda_o}{n}.$$ N.B. In spectroscopy the unqualified term "wavelength" frequently means the wavelength in vacuum, and λ frequently means λ_o. SI unit: m. Common unit: nm or μm.
Wavelength in vacuum	λ_o	Distance traveled by an electromagnetic wave in one cycle in vacuum. SI unit: m. Common unit: nm or μm.
Wavenumber	σ	The reciprocal of the wavelength of the radiation in a material of refractive index n. $\sigma = n\tilde{\upsilon}$. SI unit: m^{-1}. Common unit: $cm^{-1} = 100\,m^{-1}$. N.B. In spectroscopy the unqualified term "wavenumber" almost always means the wavenumber in vacuum.

Quantity	Symbol	Meaning
Wavenumber in vacuum	$\tilde{v}$	The reciprocal of the vacuum wavelength of the radiation, $1/\lambda_{\mathrm{o}}$. $\tilde{v}$ is related to the energy change, ΔE, induced when the radiation is absorbed by $\Delta E = hc_{\mathrm{o}}\tilde{v}$. v has often been used instead of $\tilde{v}$. It should only be used when no confusion with frequency is possible. SI unit: m^{-1}. Common unit: $\mathrm{cm}^{-1} = 100\,\mathrm{m}^{-1}$.
Wavenumber shift	$\Delta\tilde{v}$	See "Raman wavenumber shift".
Wavevector Wave vector	$\boldsymbol{k}$	The vector with direction along the propogation direction of a wave and with magnitude equal to $2\pi/\lambda$, where λ is the wavelength. See also "Crystal vibrations" above.
White noise		Noise that has approximately the same amplitude at all frequencies.
Zero filling		The addition of zeros to an interferogram to decrease the wavenumber spacing between points in the Fourier transformed spectrum.
Zero path difference		In a Michelson or other two-beam interferometer, the position of the moving mirror at which the optical paths are equal in the two beams.
Zero-wave-vector selection rule		One selection rule for the absorption of radiation by crystal vibrations is that the wave vector of the radiation in the crystal must equal the wave vector of the vibration, i.e. the vibration wave and the radiation wave must travel in the same direction and have the same wavelength in the crystal. The wave vector of the radiation is very small compared to wave vectors of crystal vibrations, so a first approximation to the selection rule is that the wave vector of the vibration must be zero, i.e. that vibrational displacements must be the same in all primitive unit cells. In a crystal with A atoms in a unit cell and n moles of unit cells there are $3A \times 6.02 \times 10^{23} \times n$ vibrations, three of which are the zero-frequency, zero-wave-vector acoustic vibrations that are the three translations of the crystal. See "Acoustic branch". If the crystal is disordered, all $3A \times 6.02 \times 10^{23} \times n$ vibrations are active. If the crystal is ordered, the zero-wave-vector selection rule allows only the $3A$ zero-wave-vector vibrations to be active. Further, three of these $3A$ vibrations are the three zero-frequency translations of the crystal and others may be forbidden by the unit cell group symmetry.