Conventions, Symbols, Quantities, Units and Constants for High Resolution Molecular Spectroscopy

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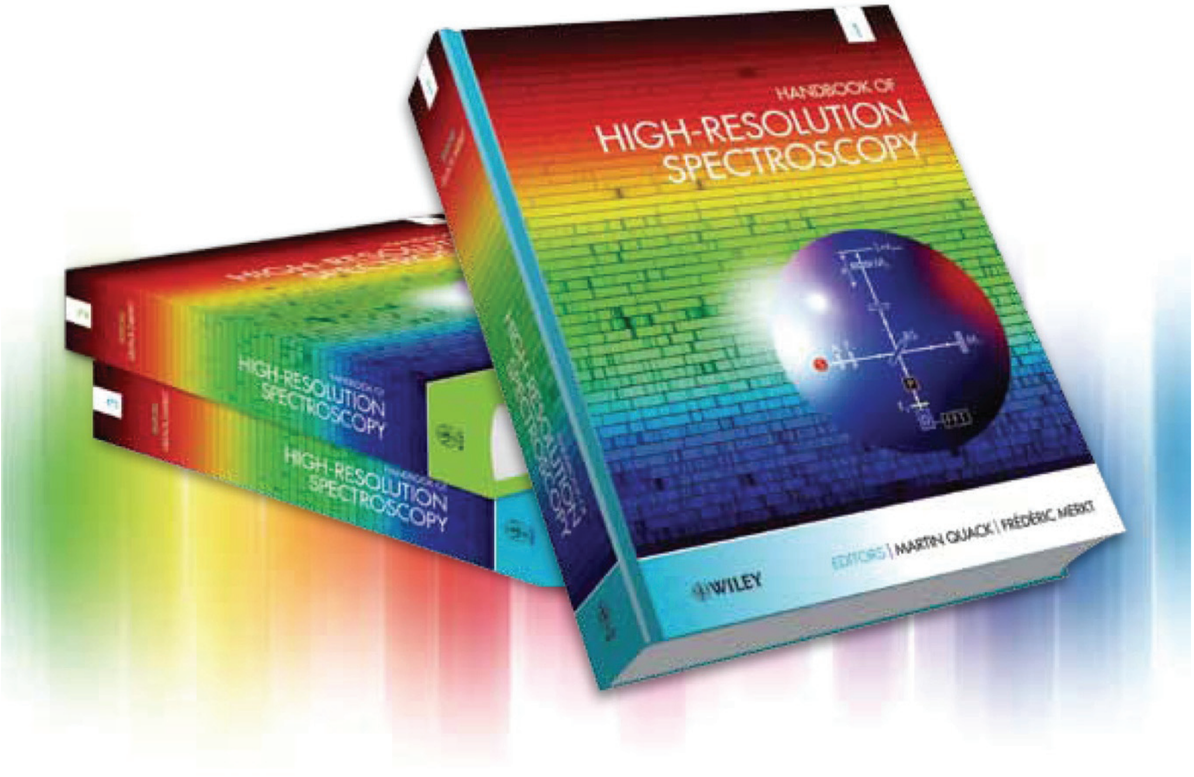

with compliments from Professor Martin Quack, ETH Zürich

Abstract

A summary of conventions, symbols, quantities, units, and constants which are important for high-resolution molecular spectroscopy is provided. In particular, great care is taken to provide definitions which are consistent with the recommendations of the IUPAC “Green Book”, from which large parts of this article are drawn. While the recommendations in general refer to the SI (Système International), the relation to other systems and recommendations, which are frequently used in spectroscopy, for instance atomic units, is also provided. A brief discussion of quantity calculus is provided as well as an up-to-date set of fundamental constants and conversion factors together with a discussion of conventions used in reporting uncertainty of experimentally derived quantities. The article thus should provide an ideal compendium of many quantities of practical importance in high-resolution spectroscopy.

Keywords: conventions; symbols; quantities; units; fundamental constants; high-resolution spectroscopy; quantity calculus; reporting uncertainty in measured quantities; IUPAC

Conventions, Symbols, Quantities, Units and Constants for High-resolution Molecular Spectroscopy

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1 INTRODUCTION

Conventions in spectroscopy, as conventions in science in general, are needed essentially for unambiguous use and exchange of scientific information and data. In essence, one has to define a consistent and correct usage of scientific language, similar to the usage of everyday language. At a first stage, every child learns language intuitively by taking over habits from parents. Similarly, scientists in a given field take over the habits and jargon of that field intuitively and requests for more precise definitions and rules are resisted frequently in both situations with comments of "triviality" on such efforts. However, for an unambiguous exchange of information between different groups of people, different fields of science and technology, a precise definition of language and, in particular, scientific language is primordial. The lack of a common, unambiguous scientific language can lead to enormous losses. A prominent example is the Mars Climate Orbiter story, which we may quote from the preface to Cohen *et al.* (2008):

> A spectacular example of the consequences of confusion of units is provided by the loss of the United States NASA satellite, the "Mars Climate Orbiter" (MCO). The Mishap Investigation Board (Phase I Report, November 10, 1999)[a] found that the root cause for the loss of the MCO was "the failure to use metric units in the coding of the ground (based) software file". The impulse was reported in Imperial units of pounds (force)-seconds (lbf-s) rather than in the metric units of Newton (force)-seconds (N-s). This caused an error of a factor of 4.45 and threw the satellite off course.[b]

One can estimate that in the modern economic world, which is characterized by science and technology in most areas of everyday life, enormous economic losses still occur through inconsistencies in conventions and units. Indeed, such losses are expected to be quite gigantic on a worldwide scale compared to the example given above. Thus, there are great international efforts in providing conventions on symbols, quantities, and units in science and technology. The most prominent effort along those lines is clearly the development of the international system of units, the SI.

Turning specifically to the field of molecular spectroscopy, many of the habits and current language of this subfield of science can be found well represented in the famous set of books by Herzberg (1946, 1950, 1966). However, modern spectroscopy has many interactions with other branches of chemistry, physics, and engineering sciences.

A consistent summary of conventions in these areas closely related to spectroscopy can be found in the volume "Quantities, Units and Symbols in Physical Chemistry" (third edition, 2nd printing, Cohen *et al.* 2008) edited on behalf of IUPAC (third printing 2011).

In this article, we have drawn from this book those parts that are most relevant to spectroscopy and have supplemented them with a few examples referring specifically to spectroscopy. To avoid errors in transcription, many of the tables are taken over literally by permission in line with the general policy of IUPAC, favoring the widest possible dissemination of their publications.

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After a brief introduction, we discuss the basics of quantity calculus and presentation of data as well as some general rules for presentation of scientific texts in Section 2. In Section 3, we present tables of quantities used in spectroscopy and most closely related fields such as electromagnetism, quantum mechanics, quantum chemistry, statistical thermodynamics, and kinetics related to spectroscopy. This section is largely drawn from Section 2 of Cohen *et al.* (2008). It includes a discussion of quantities of units on absorption intensities, a field where one can find many inconsistencies in the literature. In Section 4, we discuss SI units and atomic units as useful for spectroscopy. Section 5 deals with mathematical symbols and includes a table of the Greek alphabet. Section 6 provides an up-to-date summary of some fundamental physical constants and particle properties. Section 7 provides a brief introduction into the reporting of uncertainty in measurements. We conclude with a brief table of acronyms used in spectroscopy and related fields and a little practical table of conversion factors for quantities related to energy.

While it is at present still impossible to have a completely consistent usage of symbols and terminology throughout all of spectroscopy and, indeed just throughout this Handbook, there are nevertheless a few general rules to be remembered for all scientific texts and the individual articles of this Handbook.

Authors are generally free in defining their usage:

(i) Clear and unambiguous definitions for all conventions, symbols, and units within each publication must be explicit, given without exceptions, unless the internationally recognized SI conventions are respected.
(ii) To the greatest possible extent, we recommend the use of the conventions provided as a brief summary here and found more completely in Cohen *et al.* (2008).
(iii) Deprecated usage must be avoided completely. Also, internal laboratory jargon, while acceptable within a local environment, must be avoided. Units and terminology, which can lead to misinterpretation and ambiguities must be avoided, even if frequently used within certain restricted communities of science.

In respecting these rules and conventions, one will find that not only the exchange of scientific information is facilitated but also every day scientific work and thinking is helped by taking the habit of a clear, well-defined and long-term consistent scientific language.

One more word may be useful concerning the use of the SI system. Sometimes, the use of other systems may be preferable, for instance, atomic units in theoretical, spectroscopic, and quantum chemical work. One can argue that the SI system can be intellectually clumsy by comparison and may have disadvantages in some respect. However, for the exchange of information, the use of the SI system has clear advantages and is often to be preferred.

Some key references to this article are, thus, the IUPAC Green Book (Cohen *et al.* 2008) from which much of this article is cited, the International Organization for Standardization Handbook (ISO 1993), the Guide to Expression of Uncertainty in Measurement (GUM 1995), the International Vocabulary of Metrology (VIM 2008), and the SI Brochure from the Bureau International des Poids et Mesures (BIPM) (BIPM 2006), to which we refer for further details.

We are indebted to the International Union of Pure and Applied Chemistry (IUPAC) for allowing us to reproduce within their general policy the relevant sections of the IUPAC Green Book, with modifications as required by the context of this Handbook.

2 QUANTITIES, QUANTITY CALCULUS AND PRESENTATION OF SPECTROSCOPIC DATA

2.1 Introductory Discussion with Examples

The value of a *physical quantity* Q can be expressed as the product of a *numerical value* $\{Q\}$ and a *unit* $[Q]$

$$Q = \{Q\}\,[Q] \tag{1}$$

Neither the name of the physical quantity nor the symbol used to denote it implies a particular choice of unit.

Physical quantities, numerical values, and units may all be manipulated by the ordinary rules of algebra. Thus, we may write, for example, for the wavelength λ of one of the yellow sodium lines

$$\lambda = 5.896 \times 10^{-7}\,\mathrm{m} = 589.6\ \mathrm{nm} \tag{2}$$

where m is the symbol for the unit of length called the metre (or meter, see Sections 2.2 and 4.1), nm is the symbol for the nanometre, and the units metre and nanometre are related as

$$1\,\mathrm{nm} = 10^{-9}\,\mathrm{m} \quad \text{or} \quad \mathrm{nm} = 10^{-9}\ \mathrm{m} \tag{3}$$

The equivalence of the two expressions for λ in equation (2) follows at once when we treat the units by the rules of algebra and recognize the identity of 1 nm and $10^{-9}\,\mathrm{m}$

in equation (3). The wavelength may equally well be expressed in the form

$$\lambda/\mathrm{m} = 5.896 \times 10^{-7} \quad \text{or} \quad \lambda/\mathrm{nm} = 589.6 \qquad (4)$$

It can be useful to work with variables that are defined by dividing the quantity by a particular unit. For instance, in tabulating the numerical values of physical quantities or labeling the axes of graphs, it is particularly convenient to use the quotient of a physical quantity and a unit in such a form that the values to be tabulated are numerical values, as in equation (4). We provide three introductory examples to demonstrate the use of this presentation of quantities in spectroscopy.

Examples

Presentation of tables of spectroscopic parameters

A typical application of quantity calculus arises in the presentation of spectroscopic parameters. For instance, a rotational constant B_v of the vibrational level $v = 0$ may be given as

$$B_0/(hc) = \widetilde{B}_0 = 0.236\,\mathrm{cm}^{-1} \qquad (5)$$

This can be represented in a table in the form $\widetilde{B}_0/\mathrm{cm}^{-1} = 0.236$. The centrifugal distortion constant $\widetilde{D}$ as another quantity in the same table may have a very different order of magnitude

$$D_0/(hc) = \widetilde{D}_0 = 0.225 \times 10^{-6}\,\mathrm{cm}^{-1} \qquad (6)$$

which can be written in the table as $\widetilde{D}_0/10^{-6}\,\mathrm{cm}^{-1} = 0.225$, thus avoiding repeated use of $10^{-6}\,\mathrm{cm}^{-1}$ if several results with this order of magnitude appear, although one might, of course, as well use $\widetilde{D}_0/\mathrm{cm}^{-1} = 0.225 \times 10^{-6}$. Finally, one may have in the same table parameters of different dimension, which could be written in the table similarly and consistently as equations with only numbers appearing in the main body of the table. This simple and consistent use of quantity calculus in tables is, thus, preferred over captions showing "spectroscopic parameters are given in cm^{-1}", "$\widetilde{D} \times 10^6$ is given in cm^{-1}", or even "$\widetilde{D}$ ($10^{-6}\,\mathrm{cm}^{-1}$)"; especially the latter can easily lead to ambiguities or even erroneous representations.

Presentation of spectra

A more detailed discussion on the presentation of spectra is given in Section 3.7.4. Figure 1 presents a small part of the far infrared spectrum of the CO molecule. The ordinate (vertical or y-axis) represents the decadic absorbance $A_{10} = \log_{10}(I_0/I)$ of the sample of CO, where I_0 is the incident and I the transmitted radiation intensity at the frequency considered correcting for effects from windows etc. A_{10} is by its definition a quantity of dimension 1 (without dimension or unit), as given on the vertical axis. The abscissa (horizontal or x-axis) can either represent the frequency ν with dimension T^{-1} and possible unit Hz or the wavenumber $\tilde{\nu}$ with dimension L^{-1} and common unit cm^{-1}. Dividing the corresponding quantities by their respective unit results in a number to be represented on the horizontal axes (ν/THz on the upper and $\tilde{\nu}$/cm^{-1} on the lower axis); see Section 4.4 for the prefixes and Section 3.7.4 for further details.

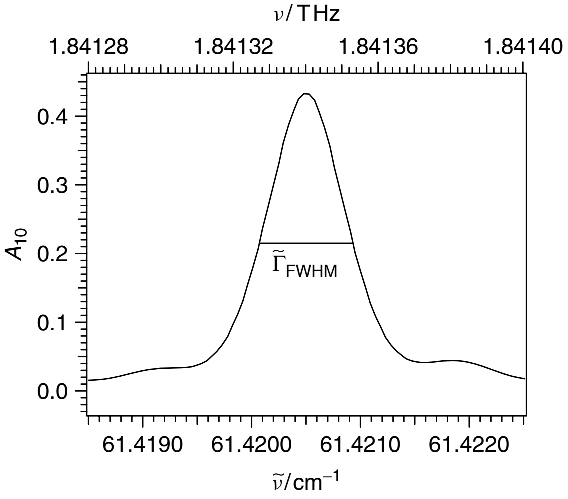

Figure 1 The figure shows a CO absorption line (adapted from Figure 2 in Albert and Quack (2007), by permission) in the far-infrared spectral region measured with the Bruker IFS HR Zürich prototype (ZP) 2001 spectrometer at the highest resolution. The decadic absorbance A_{10} is shown as a function of wavenumber $\tilde{\nu}$ (bottom abscissa) and frequency ν (top abscissa); see Figure 3, Section 3.7.4.

Analysis of absorbance data for different lines in a spectrum in view of the determination of the sample rotational temperature

The relative maximum absorbance A of a single rovibrational line in a diatomic molecule such as CO is approximately given by

$$A = \ln(I_0/I) = C\,\tilde{\nu}\,(J'' + J' + 1)\exp(-E/k_\mathrm{B}T_\mathrm{rot}) \qquad (7)$$

where C is a constant (with unit cm), $\tilde{\nu}$ is the transition wavenumber (unit cm^{-1}), k_B is Boltzmann's constant, T_rot the rotational temperature to be determined, and the ground vibrational state rotational energy E is given by

$$E/(hc) = \widetilde{E} = \left[\widetilde{B}_0 J''(J''+1) - \widetilde{D}_0 (J'')^2 (J''+1)^2 + \widetilde{H}_0 (J'')^3 (J''+1)^3\right] \quad (8)$$

where $\widetilde{B}_0$, $\widetilde{D}_0$, and $\widetilde{H}_0$ are the conventional rotational parameters (unit cm^{-1}). J'' is the rotational quantum number in the lower state and J' in the upper state of the transition. The linearized form of equation (7) can be used as follows:

$$\ln\left[\frac{A}{(\tilde{\nu}(J''+J'+1)\ \mathrm{cm})}\right] = a + b\,\widetilde{E} \quad \text{with} \quad T_{\mathrm{rot}} = -\frac{hc}{k_{\mathrm{B}} b} \quad (9)$$

where the slope b of the graph is related to the rotational temperature. By multiplying the quantity $\tilde{\nu}\ (J''+J'+1)$ with dimension L^{-1} (unit cm^{-1}) by the inverse of its unit (i.e., cm), one obtains again a quantity of dimension 1, resulting also in a number for the argument of the logarithm. Figure 2 shows the results again with the ordinate and the abscissa drawn as quantities with dimension 1 (pure numbers). For instance, the abscissa can be read as $E/(hc\ \mathrm{cm}^{-1}) = \widetilde{E}/\mathrm{cm}^{-1} = 10.1$ or $E/(hc) = \widetilde{E} = 10.1\ \mathrm{cm}^{-1}$ at the appropriate point, similar to the following table given with Figure 2.

$\widetilde{E}/\mathrm{cm}^{-1}$	$\ln[A/(\tilde{\nu}(J''+J'+1)\ \mathrm{cm})]$
0.0	3.727
4.0	2.758
4.0	2.788
11.6	0.955
11.6	0.909

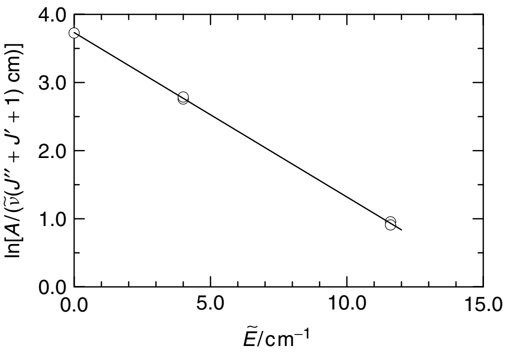

Figure 2 The Boltzmann diagram for the CO absorption measured in a molecular beam within a distance of 11.0 mm from the nozzle (adapted from Figure 4 in Amrein *et al.* (1988), by permission) gives a slope which corresponds to a rotational temperature of $T_{\mathrm{rot}} \approx 6.0$ K.

Equations between numerical values depend on the choice of units, whereas equations between quantities have the advantage of being independent of this choice. Therefore, the use of equations between quantities should generally be preferred.

The method described here for handling physical quantities and their units is known as *quantity calculus* (Guggenheim 1942, de Boer 1994/95, Mills 1997). It is recommended for use throughout science and technology. The use of quantity calculus does not imply any particular choice of units; indeed one of the advantages of quantity calculus is that it makes changes between units particularly easy to follow.

2.2 Base Quantities and Derived Quantities

By convention, physical quantities are organized in a dimensional system built upon seven *base quantities*, each of which is regarded as having its own dimension. These base quantities in the International System of Quantities (ISQ) on which the International System of units (SI) is based, and the principal symbols used to denote them and their dimensions are as follows:

	SI base unit		Symbol for	
Base quantity	Name	Symbol	Quantity	Dimension
length	metre	m	l	L
mass	kilogram	kg	m	M
time	second	s	t	T
electric current	ampere	A	I	I
thermodynamic temperature	kelvin	K	T	Θ
amount of substance	mole	mol	n	N
luminous intensity	candela	cd	I_{v}	J

All other quantities are called *derived quantities* and are regarded as having dimensions derived algebraically from the seven base quantities by multiplication and division.

Example

The dimension of energy is equal to the dimension of $m \cdot l^2 \cdot t^{-2}$. This can be written with the symbol dim for dimension $\dim(E) = \dim(m \cdot l^2 \cdot t^{-2}) = \mathsf{M}\,\mathsf{L}^2\,\mathsf{T}^{-2}$

The quantity *amount of substance* is of special importance to chemists. Amount of substance, n, is proportional to the number of specified elementary entities of the substance considered. The proportionality factor is the same for all substances; its reciprocal is the *Avogadro constant* (Chapter 6). The SI unit of amount of substance is the mole, defined in Section 4.1. The physical quantity "amount of substance" should no longer be called "number of moles", just as the physical quantity mass should not be called "number of kilograms". The name "amount of substance", sometimes also called "chemical amount", may often be usefully abbreviated to the single word "amount", particularly in phrases such as "amount concentration",[c] and "amount of N_2". A possible name for international usage has been suggested: "enplethy" from Greek, similar to enthalpy and entropy (Quack 1998a).

The number and choice of base quantities is pure convention. Other quantities could be considered to be more fundamental, such as electric charge Q instead of electric current I:

$$Q = \int_{t_1}^{t_2} I \, \mathrm{d}t \tag{10}$$

However, in the ISQ, electric current is chosen as base quantity and ampere is the SI base unit. In atomic and molecular physics, the so-called *atomic units* are useful (Section 4.7).

2.3 Symbols for Physical Quantities and Units

A clear distinction should be drawn between the names and symbols for physical quantities, and the names and symbols for units. Names and symbols for many quantities are given in Chapter 3; the symbols given there are *recommendations*. If other symbols are used, they should be clearly defined. Names and symbols for units are given in Chapter 4; the symbols for units listed there are quoted from the Bureau International des Poids et Mesures (BIPM) and are *mandatory*.

2.3.1 General Rules for Symbols for Quantities

The symbol for a physical quantity should be a single letter[d] of the Latin or Greek alphabet (Section 2.5). Capital or lower case letters may both be used. The letter should be printed in italic (sloping) type. When necessary the symbol may be modified by subscripts and superscripts of specified meaning. Subscripts and superscripts that are themselves symbols for physical quantities or for numbers should be printed in italic type; other subscripts and superscripts should be printed in roman (upright) type.

Examples

	C_p	for heat capacity at constant pressure
	p_i	for partial pressure of the ith substance
but	p_B	for partial pressure of substance B
	μ_r	for relative permeability
	A	for absorbance
	A_{10}	for decadic absorbance

When such symbols appear as factors in a product, they should be separated from other symbols by a space, multiplication sign, or parentheses.

The meaning of symbols for physical quantities may be further qualified by the use of one or more subscripts or by information contained in parentheses.

Examples

$$\Delta_\mathrm{f} S^\ominus(\mathrm{HgCl_2, cr, 25\,^\circ C}) = -154.3\ \mathrm{J\ K^{-1}\ mol^{-1}}$$
$$\mu_i = (\partial G/\partial n_i)_{T,p,\ldots,n_j,\ldots;\ j\neq i} \text{ or } \mu_i = (\partial G/\partial n_i)_{T,p,n_{j\neq i}}$$

Vectors and matrices shall be printed in bold-face italic type, e.g., $\boldsymbol{A}, \boldsymbol{a}$. Tensors shall be printed in bold-face italic sans serif type, e.g., $\boldsymbol{\mathsf{S}}$, $\boldsymbol{\mathsf{T}}$. Vectors may alternatively be characterized by an arrow, $\vec{A}$, $\vec{a}$ and second-rank tensors by a double arrow, $\overset{\rightrightarrows}{S}$, $\overset{\rightrightarrows}{T}$.

2.3.2 General Rules for Symbols for Units

Symbols for units should be printed in roman (upright) type. They should remain unaltered in the plural and should not be followed by a full stop except at the end of a sentence.

Examples

$r = 10\,\mathrm{cm}$, not cm. or cms.

Symbols for units shall be printed in lower case letters, unless they are derived from a personal name when they shall begin with a capital letter. An exception is the symbol for the litre, which may be either L or l, i.e., either capital or lower case.[e]

Examples

m (metre), s (second), but J (joule), Hz (hertz)

Decimal multiples and submultiples of units may be indicated by the use of prefixes as defined in Section 4.4.

Examples

nm (nanometre), MHz (megahertz), kV (kilovolt)

A space separates the numerical value $\{Q\}$ of a quantity Q from the unit $[Q]$. This is also applicable for special non-SI units accepted for use with the SI, e.g., degree (symbol $^\circ$), minute (symbol $'$), and second (symbol $''$) (Section 4.5).

Example

One minute is composed of 60 s, $1' = 60''$

Similarly, a space shall be left between the numerical value and the unit for symbols for fractions, e.g., percent (symbol %) and permille (symbol ‰) (Section 4.8.1).

Example

The mass fraction is $w = 2.25 \times 10^{-2} = 22.5$ mg/g $= 2.25$ %

2.4 Products and Quotients of Physical Quantities and Units

Products of physical quantities may be written in any of the ways

$$a\,b \quad \text{or} \quad ab \quad \text{or} \quad a \cdot b \quad \text{or} \quad a \times b$$

and similarly quotients may be written

$$a/b \quad \text{or} \quad \frac{a}{b} \quad \text{or by writing the product of } a \text{ and } b^{-1} \text{ as } ab^{-1}$$

Examples

$$U = RI, \quad R = U/I = UI^{-1}$$

Not more than one solidus (/) shall be used in the same expression unless parentheses are used to eliminate ambiguity.

Example

$$(a/b)/c \text{ or } a/(b/c) \text{ (in general different)}, \quad \text{not} \quad a/b/c$$

In evaluating combinations of many factors, multiplication written without a multiplication sign takes precedence over division in the sense that a/bc is interpreted as $a/(bc)$ and not as $(a/b)c$; however, it is necessary to use parentheses to eliminate ambiguity under all circumstances, thus avoiding expressions of the kind such as a/bcd. Furthermore, $a/b + c$ is interpreted as $(a/b) + c$ and not as $a/(b + c)$. Again, the use of parentheses is recommended (required for $a/(b + c)$).

Products and quotients of units may be written in a similar way, except that the cross (×) is not used as a multiplication sign between units. When a product of units is written without any multiplication sign, a space shall be left between the unit symbols.

Example

$1\,\mathrm{N} = 1\,\mathrm{m\,kg\,s^{-2}} = 1\,\mathrm{m{\cdot}kg{\cdot}s^{-2}} = 1\ \mathrm{m\,kg/s^2}$, not $1\,\mathrm{mkgs^{-2}}$

2.5 The Use of Italic and Roman Fonts for Symbols in Scientific Publications

Scientific manuscripts should follow the accepted conventions concerning the use of italic and roman fonts for symbols. An italic font is generally used for emphasis in running text, but it has a quite specific meaning when used for symbols in scientific text and equations. The following summary is intended to help in the correct use of italic fonts in preparing manuscript material.

1. The general rules concerning the use of italic (sloping) font or roman (upright) font are presented in Sections 2.3 and 5.1 in relation to mathematical symbols and operators. These rules are also presented in the International Standards ISO 31 (successively being replaced by ISO 1993) and in the SI Brochure (BIPM 2006).
2. The overall rule is that symbols representing physical quantities or variables are italic, but symbols representing units, mathematical constants, or labels are roman. Sometimes there may seem to be doubt as to whether a symbol represents a quantity or has some other meaning (such as label): a good rule is that quantities, or variables, may have a range of numerical values, but labels cannot. Vectors, tensors and matrices are denoted using a bold-face (heavy) font, but they shall be italic since they are quantities.

   Examples

   The Planck constant $h = 6.626\,068\,96(33) \times 10^{-34}$ J s.
   The electric field strength $\boldsymbol{E}$ has components E_x, E_y, and E_z.
   The mass of my pen is $m = 24$ g $= 0.024$ kg.

3. The above rule applies equally to all letter symbols from both the Greek and the Latin alphabet, although some authors resist putting Greek letters into italic.

   Example

   When the symbol μ is used to denote a physical quantity (such as permeability or reduced mass), it should be italic, but when it is used as a prefix in a unit such as microgram (μg) or when it is used as the symbol for the muon (μ) (see Note 5), it should be roman.

4. Numbers and labels are roman (upright).

Examples

The ground and first excited electronic state of the $\mathrm{CH_2}$ molecule are denoted . . . $(2\mathrm{a}_1)^2(1\mathrm{b}_2)^2(3\mathrm{a}_1)^1(1\mathrm{b}_1)^1$, $\tilde{\mathrm{X}}\ ^3\mathrm{B}_1$, and . . .$(2\mathrm{a}_1)^2(1\mathrm{b}_2)^2(3\mathrm{a}_1)^2$, $\tilde{\mathrm{a}}\ ^1\mathrm{A}_1$, respectively. The π-electron configuration and symmetry of the benzene molecule in its ground state are denoted . . .$(\mathrm{a}_{2\mathrm{u}})^2(\mathrm{e}_{1\mathrm{g}})^4$, $\tilde{\mathrm{X}}\ ^1\mathrm{A}_{1\mathrm{g}}$. All these symbols are labels and are roman.

5. Symbols for elements in the periodic system should be roman. Similarly, the symbols used to represent elementary particles are always roman. (See, however, Note 9 for the use of italic font in chemical-compound names.)

Examples

H, He, Li, Be, B, C, N, O, F, Ne, . . . for atoms; e for the electron, p for the proton, n for the neutron, μ for the muon, α for the alpha-particle, etc.

6. Symbols for physical quantities are single, or exceptionally two letters of the Latin or Greek alphabet, but they are frequently supplemented with subscripts, superscripts, or information in parentheses to specify further the quantity. Further symbols used in this way are either italic or roman depending on what they represent.

Example

H denotes enthalpy, but H_m denotes molar enthalpy (m is a mnemonic label for molar and is therefore roman). C_p and C_V denote the heat capacity at constant pressure p and volume V, respectively (note the roman m but italic p and V). The chemical potential of argon might be denoted μ_Ar or $\mu(\mathrm{Ar})$, but the chemical potential of the ith component in a mixture would be denoted μ_i, where i is italic because it is a variable subscript.

7. Symbols for mathematical operators are always roman. This applies to the symbol Δ for a difference, δ for an infinitesimal variation, d for an infinitesimal difference (in calculus), and to capital Σ and Π for summation and product signs, respectively. The symbols π (3.141 592. . .), e (2.718 281. . ., base of natural logarithms), i (square root of minus one), etc., are always roman, as are the symbols for specified functions such as log (lg for $\log_{10}$, ln for $\log_\mathrm{e}$, or lb for $\log_2$), exp, sin, cos, tan, erf, ***div***, ***grad***, ***rot***, etc. The particular operators ***grad*** and ***rot*** and the corresponding symbols $\boldsymbol{\nabla}$ for ***grad***, $\boldsymbol{\nabla}\times$ for ***rot***, and $\boldsymbol{\nabla}\cdot$ for ***div*** are printed in bold-face to indicate the vector or tensor character following ISO (1993). Some of these letters, e.g., e for elementary charge, are also sometimes used to represent physical quantities; then, they should be italic, to distinguish them from the corresponding mathematical symbol.

Example

$\Delta H = H(\text{final}) - H(\text{initial})$; $(\mathrm{d}p/\mathrm{d}t)$ used for the rate of change of pressure; δx used to denote an infinitesimal variation of x. However, for a damped linear oscillator, the amplitude F as a function of time t might be expressed by the equation $F = F_0 \exp(-\delta t)\sin(\omega t)$, where δ is the decay coefficient (SI unit: $\mathrm{Np\ s^{-1}}$) and ω is the angular frequency (SI unit: $\mathrm{rad\ s^{-1}}$). Note the use of roman δ for the operator in an infinitesimal variation of x, δx, but italic δ for the decay coefficient in the product δt. Note that the products δt and ωt are both dimensionless, but are described as having the unit neper ($\mathrm{Np} = 1$) and radian ($\mathrm{rad} = 1$), respectively.

8. The fundamental physical constants are always regarded as quantities subject to measurement (even though they are not considered to be variables) and they should accordingly always be italic. Sometimes fundamental physical constants are used as though they were units, but they are still given italic symbols; for example, the hartree, E_h (Section 4.7.1). However, the electronvolt (eV), the dalton (Da), or the unified atomic mass unit (u), and the astronomical unit (ua) have been recognized as units by the Comité International des Poids et Mesures (CIPM) of the BIPM and they are accordingly given roman symbols.

Example

c_0 for the speed of light in vacuum, m_e for the electron mass, h for the Planck constant, N_A or L for the Avogadro constant, e for the elementary charge, a_0 for the Bohr radius, etc. The electronvolt $1\,\mathrm{eV} = e \cdot 1\,\mathrm{V} = 1.602\,176\,487(40) \times 10^{-19}\,\mathrm{J}$.

9. Greek letters are used in systematic organic, inorganic, macromolecular, and biochemical nomenclature. These should be roman (upright), since they are not symbols for physical quantities. They designate the position of substitution in side chains, ligating-atom attachment and bridging mode in coordination compounds, end groups in structure-based names for macromolecules, and stereochemistry in carbohydrates and natural products. Letter symbols for elements are italic when they are locants in chemical-compound names, indicating attachments to heteroatoms, e.g., *O*-, *N*-, *S*-, and *P*-. The italic symbol *H* denotes indicated or added hydrogen (Rigaudy and Klesney 1979).

   Examples

   α-ethylcyclopentaneacetic acid
   α-D-glucopyranose
   5α-androstan-3β-ol
   N-methylbenzamide
   3*H*-pyrrole
   naphthalen-2(1*H*)-one

10. Symbols for symmetry operators are printed in italic. Subscripts and superscripts are printed in roman (upright) except for variables that are replaced by numbers for a specific operator. The power k of an operator should always be specified even when it is 1, e.g., $C_n{}^1$ instead of C_n. Symbols for symmetry groups are printed italic with roman (upright) subscripts. Symbols for irreducible representations of point groups (called *symmetry species* in spectroscopy) are printed in roman (upright); subscripts are also printed in roman except when they are variables to be replaced by numbers. $\mathit{\Gamma}$ used as symbol for an irreducible representation is printed italic when it is a variable to be replaced by other symbols in specific cases.

    Examples

    E is the identity operator.
    $C_n{}^k$ is the n-fold rotation operator for k successive rotations through an angle $2\pi/n$ about an n-fold rotation axis where $n = 2, 3, \ldots;\ k = 1, 2, \ldots, n-1$.
    σ_d is the reflection operator for reflection in a plane bisecting two C_2-axes that are perpendicular to the principal C_n-axis.
    D_2d is the group of operators of the group D_2 plus $2\sigma_\mathrm{d}$ operators.
    $\mathrm{A_1}$, $\mathrm{A_2}$, E, $\mathrm{F_1}$, and $\mathrm{F_2}$ are the irreducible representations of T_d, the molecular symmetry group of methane, $\mathrm{CH_4}$.
    $\Sigma_\mathrm{g}{}^+$, $\Sigma_\mathrm{g}{}^-$, $\Sigma_\mathrm{u}{}^+$, and $\Sigma_\mathrm{g}{}^-$ are the irreducible representations of $D_{\infty\mathrm{h}}$, the molecular symmetry group of carbon dioxide, $\mathrm{CO_2}$.

3 TABLES OF QUANTITIES USED IN HIGH-RESOLUTION SPECTROSCOPY

The following tables contain the internationally recommended names and symbols for the physical quantities most likely to be used in spectroscopy. Further quantities and symbols may be found in recommendations by Cohen *et al.* (2008) from which the present tables are largely reproduced and references cited therein.

Although authors are free to choose any symbols they wish for the quantities they discuss, provided that they define their notation and conform to the general rules indicated in Chapter 2, it is clearly an aid to scientific communication if we all generally follow a standard notation. The symbols below have been chosen to conform with current usage and to minimize conflict as far as possible. Small variations from the recommended symbols may often be desirable in particular situations, perhaps by adding or modifying subscripts or superscripts, or by the alternative use of upper or lower case. Within a limited subject area, it may also be possible to simplify notation, for example, by omitting qualifying subscripts or superscripts, without introducing ambiguity. The notation adopted should in any case always be defined. Major deviations from the recommended symbols should be particularly carefully defined.

The tables are arranged by subject. The five columns in each table give the name of the quantity, the recommended symbol(s), a brief definition, the symbol for the coherent SI unit (without multiple or submultiple prefixes; see Section 4.4), and note references. When two or more symbols are recommended, commas are used to separate symbols that are equally acceptable, and symbols of second choice are put in parentheses. A semicolon is used to separate symbols of slightly different quantities. The definitions are given primarily for identification purposes and are not necessarily complete; they should be regarded as useful relations rather than formal definitions. For some of the quantities listed in this article, the definitions given in various IUPAC documents are collected in McNaught and Wilkinson (1997). Useful definitions of physical quantities in physical organic chemistry can be found in Müller (1994) and those in polymer chemistry in Jenkins *et al.* (1996). For dimensionless quantities, a 1 is entered in the SI unit column (Section 4.8). Further information is added in notes, and in text inserts between the tables, as appropriate. Other symbols used are defined within the same table (not necessarily in the order of appearance) and in the notes.

3.1 Electricity and Magnetism

The names and symbols recommended here are in agreement with those recommended by IUPAP (Cohen and Giacomo 1987) and ISO (ISO 1993).

Name	Symbol	Definition	SI unit	Notes
electric current	I, i		A	1
electric current density	$\boldsymbol{j}, \boldsymbol{J}$	$I = \int \boldsymbol{j} \cdot \boldsymbol{e}_\mathrm{n}\, \mathrm{d}A$	A m^{-2}	2
electric charge, quantity of electricity	Q	$Q = \int I\, \mathrm{d}t$	C	1
charge density	ρ	$\rho = Q/V$	C m^{-3}	
surface density of charge	σ	$\sigma = Q/A$	C m^{-2}	
electric potential	V, ϕ	$V = \mathrm{d}W/\mathrm{d}Q$	V, J C^{-1}	
electric potential difference, electric tension	U, ΔV, $\Delta\phi$	$U = V_2 - V_1$	V	
electromotive force	E	$E = \oint (\boldsymbol{F}/Q)\cdot\mathrm{d}\boldsymbol{r}$	V	3
electric field strength	$\boldsymbol{E}$	$\boldsymbol{E} = \boldsymbol{F}/Q = -\nabla V$	V m^{-1}	
electric flux	Ψ	$\Psi = \int \boldsymbol{D} \cdot \boldsymbol{e}_\mathrm{n}\, \mathrm{d}A$	C	2
electric displacement	$\boldsymbol{D}$	$\nabla \cdot \boldsymbol{D} = \rho$	C m^{-2}	
capacitance	C	$C = Q/U$	F, C V^{-1}	
permittivity	ε	$\boldsymbol{D} = \varepsilon \boldsymbol{E}$	F m^{-1}	4
electric constant, permittivity of vacuum	ε_0	$\varepsilon_0 = {\mu_0}^{-1}{c_0}^{-1}$	F m^{-1}	5
relative permittivity	ε_r	$\varepsilon_\mathrm{r} = \varepsilon/\varepsilon_0$	1	6
dielectric polarization, electric polarization (electric dipole moment per volume)	$\boldsymbol{P}$	$\boldsymbol{P} = \boldsymbol{D} - \varepsilon_0 \boldsymbol{E}$	C m^{-2}	
electric susceptibility	χ_e	$\chi_\mathrm{e} = \varepsilon_\mathrm{r} - 1$	1	
1st hyper-susceptibility	${\chi_\mathrm{e}}^{(2)}$	${\chi_\mathrm{e}}^{(2)} = {\varepsilon_0}^{-1}\, (\partial^2 P/\, \partial E^2)$	C m J^{-1}, m V^{-1}	7
2nd hyper-susceptibility	${\chi_\mathrm{e}}^{(3)}$	${\chi_\mathrm{e}}^{(3)} = {\varepsilon_0}^{-1}(\partial^3 P/\partial E^3)$	C^2 m^2 J^{-2}, m^2 V^{-2}	7

(1) The electric current I is a base quantity in ISQ.

(2) $\boldsymbol{e}_\mathrm{n}\mathrm{d}A$ is a vector element of area.

(3) The name electromotive force is no longer recommended, since an electric potential difference is not a force.

(4) ε can be a second-rank tensor.

(5) c_0 is the speed of light in vacuum.

(6) This quantity was formerly called *dielectric constant*.

(7) The hyper-susceptibilities are the coefficients of the non-linear terms in the expansion of the magnitude P of the dielectric polarization $\boldsymbol{P}$ in powers of the electric field strength $\boldsymbol{E}$, quite related to the expansion of the dipole moment vector described in Section 3.3, Note 17. In isotropic media, the expansion of the component i of the dielectric polarization is given by

$$P_i = \varepsilon_0[{\chi_\mathrm{e}}^{(1)} E_i + (1/2){\chi_\mathrm{e}}^{(2)} E_i^2 + (1/6){\chi_\mathrm{e}}^{(3)} E_i^3 + \cdots]$$

where E_i is the ith component of the electric field strength, and ${\chi_\mathrm{e}}^{(1)}$ is the usual electric susceptibility χ_e, equal to $\varepsilon_\mathrm{r} - 1$ in the absence of higher terms. In anisotropic media, ${\boldsymbol{\chi}_\mathrm{e}}^{(1)}$, ${\boldsymbol{\chi}_\mathrm{e}}^{(2)}$, and ${\boldsymbol{\chi}_\mathrm{e}}^{(3)}$ are tensors of rank 2, 3, and 4, respectively. For an isotropic medium (such as a liquid) or for a crystal with a centrosymmetric unit cell, ${\chi_\mathrm{e}}^{(2)}$ is zero by symmetry. These quantities are macroscopic properties and characterize a dielectric medium in the same way that the microscopic quantities polarizability (α) and hyper-polarizabilities (β, γ) characterize a molecule. For a homogeneous, saturated, isotropic dielectric medium of molar volume V_m, one has $\alpha_\mathrm{m} = \varepsilon_0 \chi_\mathrm{e} V_\mathrm{m}$, where $\alpha_\mathrm{m} = N_\mathrm{A}\alpha$ is the molar polarizability (Section 3.3, Note 17, and Section 3.10).

Name	Symbol	Definition	SI unit	Notes
electric dipole moment	$\boldsymbol{p}, \boldsymbol{\mu}$	$\boldsymbol{p} = \sum_i Q_i \boldsymbol{r}_i$	C m	8
magnetic flux density, magnetic induction	$\boldsymbol{B}$	$\boldsymbol{F} = Q\boldsymbol{v}\times\boldsymbol{B}$	T	9
magnetic flux	Φ	$\Phi = \int \boldsymbol{B}\cdot\boldsymbol{e}_\mathrm{n}\,\mathrm{d}A$	Wb	2
magnetic field strength, magnetizing field strength	$\boldsymbol{H}$	$\nabla\times\boldsymbol{H} = \boldsymbol{j}$	A m^{-1}	
permeability	μ	$\boldsymbol{B} = \mu\boldsymbol{H}$	N A^{-2}, H m^{-1}	10
magnetic constant, permeability of vacuum	μ_0	$\mu_0 = 4\pi\times10^{-7}\ \mathrm{H\ m^{-1}}$	H m^{-1}	
relative permeability	μ_r	$\mu_\mathrm{r} = \mu/\mu_0$	1	
magnetization (magnetic dipole moment per volume)	$\boldsymbol{M}$	$\boldsymbol{M} = \boldsymbol{B}/\mu_0 - \boldsymbol{H}$	A m^{-1}	
magnetic susceptibility	$\chi, \kappa, (\chi_\mathrm{m})$	$\chi = \mu_\mathrm{r} - 1$	1	11
molar magnetic susceptibility	χ_m	$\chi_\mathrm{m} = V_\mathrm{m}\chi$	$\mathrm{m}^3\ \mathrm{mol}^{-1}$	
magnetic dipole moment	$\boldsymbol{m}, \boldsymbol{\mu}$	$E = -\boldsymbol{m}\cdot\boldsymbol{B}$	A m^2, J T^{-1}	
electric resistance	R	$R = U/I$	Ω	12
conductance	G	$G = 1/R$	S	12
loss angle	δ	$\delta = \varphi_U - \varphi_I$	rad	13
reactance	X	$X = (U/I)\sin\delta$	Ω	
impedance, (complex impedance)	Z	$Z = R + \mathrm{i}X$	Ω	
admittance, (complex admittance)	Y	$Y = 1/Z$	S	
susceptance	B	$Y = G + \mathrm{i}B$	S	
resistivity	ρ	$\boldsymbol{E} = \rho\boldsymbol{j}$	Ω m	14
conductivity	κ, γ, σ	$\boldsymbol{j} = \boldsymbol{\kappa}\boldsymbol{E}$	S m^{-1}	14, 15
self-inductance	L	$E = -L(\mathrm{d}I/\mathrm{d}t)$	H, V s A^{-1}	
mutual inductance	M, L_{12}	$E_1 = -L_{12}(\mathrm{d}I_2/\mathrm{d}t)$	H, V s A^{-1}	
magnetic vector potential	$\boldsymbol{A}$	$\boldsymbol{B} = \boldsymbol{\nabla}\times\boldsymbol{A}$	Wb m^{-1}	
Poynting vector	$\boldsymbol{S}$	$\boldsymbol{S} = \boldsymbol{E}\times\boldsymbol{H}$	W m^{-2}	16

(8) When a dipole is composed of two point charges Q and $-Q$ separated by a distance r, the direction of the dipole vector is taken to be from the negative to the positive charge. The opposite convention is sometimes used, but is to be discouraged. The dipole moment of an ion depends on the choice of the origin.

(9) This quantity should not be called *magnetic field*.

(10) μ is a second-rank tensor in anisotropic materials.

(11) The symbol χ_m is sometimes used for magnetic susceptibility, but it should be reserved for molar magnetic susceptibility.

(12) In a material with reactance $R = (U/I)$ cos δ and $G = R/(R^2 + X^2)$.

(13) φ_I and φ_U are the phases of current and potential difference.

(14) This quantity is a tensor in anisotropic materials.

(15) ISO gives only γ and σ, but not κ.

(16) This quantity is also called the *Poynting–Umov vector*.

3.2 Quantum Mechanics and Quantum Chemistry

The names and symbols for quantities used in quantum mechanics and recommended here are in agreement with those recommended by IUPAP (Cohen and Giacomo 1987). The names and symbols for quantities used mainly in the field of quantum chemistry have been chosen on the basis of the current practice in the field. Guidelines for the presentation of methodological choices in publications of computational results have been presented (Boggs 1998). A list of acronyms used in theoretical chemistry has been published by IUPAC (Brown *et al.* 1996); see also Chapter 8.

Name	Symbol	Definition	SI unit	Notes
momentum operator	$\widehat{\boldsymbol{p}}$	$\widehat{\boldsymbol{p}} = -\mathrm{i}\hbar\,\boldsymbol{\nabla}$	J s m^{-1}	1
kinetic energy operator	$\widehat{T}$	$\widehat{T} = -(\hbar^2/2m)\boldsymbol{\nabla}^2$	J	1
Hamiltonian operator, Hamiltonian	$\widehat{H}$	$\widehat{H} = \widehat{T} + \widehat{V}$	J	1
wavefunction, state function	Ψ, ψ, ϕ	$\widehat{H}\psi = E\psi$	(m$^{-3/2}$)	2, 3
hydrogen-like wavefunction	$\psi_{nlm}(r, \theta, \phi)$	$\psi_{nlm} = R_{nl}(r) Y_{lm}(\theta, \phi)$	(m$^{-3/2}$)	3
spherical harmonic function	$Y_{lm}(\theta, \phi)$	$Y_{lm} = N_{l\vert m\vert} P_l^{\vert m\vert}(\cos\theta) e^{\mathrm{i}m\phi}$	1	4
probability density	P	$P = \psi^* \, \psi$	(m^{-3})	3, 5
charge density of electrons	ρ	$\rho = -eP$	(C m^{-3})	3, 5, 6
probability current density, probability flux	$\boldsymbol{S}$	$\boldsymbol{S} = -(\mathrm{i}\hbar/2m)\times$ $(\psi^* \, \boldsymbol{\nabla}\psi - \psi \boldsymbol{\nabla}\psi^*)$	(m^{-2} s^{-1})	3
electric current density of electrons	$\boldsymbol{j}$	$\boldsymbol{j} = -e\boldsymbol{S}$	(A m^{-2})	3, 6
integration element	$\mathrm{d}\tau$	$\mathrm{d}\tau = \mathrm{d}x \; \mathrm{d}y \; \mathrm{d}z$	(varies)	
matrix element of operator $\widehat{A}$	$A_{ij}, \left\langle i \middle\vert \widehat{A} \middle\vert j \right\rangle$	$A_{ij} = \int \psi_i^* \, \widehat{A} \psi_j \mathrm{d}\tau$	(varies)	7
expectation value of operator $\widehat{A}$	$\langle \widehat{A} \rangle, \overline{A}$	$\langle \widehat{A} \rangle = \int \psi^* \, \widehat{A} \psi \mathrm{d}\tau$	(varies)	7
hermitian conjugate of operator $\widehat{A}$	$\widehat{A}^\dagger$	$\left(A^\dagger\right)_{ij} = \left(A_{ji}\right)^*$	(varies)	7
commutator of $\widehat{A}$ and $\widehat{B}$	$[\widehat{A}, \widehat{B}]$, $[\widehat{A}, \widehat{B}]_-$	$[\widehat{A}, \widehat{B}] = \widehat{A}\widehat{B} - \widehat{B}\widehat{A}$	(varies)	8
anticommutator of $\widehat{A}$ and $\widehat{B}$	$[\widehat{A}, \widehat{B}]_+$	$[\widehat{A}, \widehat{B}]_+ = \widehat{A}\widehat{B} + \widehat{B}\widehat{A}$	(varies)	8
angular momentum operators	see Section 3.5			
spin wavefunction	$\alpha; \beta$		1	9

(1) The circumflex (or "hat"), $\widehat{\ }$, serves to distinguish an operator from an algebraic quantity. This definition applies to a coordinate representation, where $\boldsymbol{\nabla}$ denotes the nabla operator (Section 5.2).

(2) Capital and lower case ψ are commonly used for the time-dependent function $\Psi(x, t)$ and the amplitude function $\psi(x)$, respectively. Thus, for a stationary state, $\Psi(x, t) = \psi(x)\exp(-\mathrm{i}Et/\hbar)$.

(3) For the normalized wavefunction of a single particle in three-dimensional space, the appropriate SI unit is given in parentheses. Results in quantum chemistry, however, are commonly expressed in terms of atomic units (Section 4.7.1; Whiffen 1978). If distances, energies, angular momenta, charges, and masses are all expressed as dimensionless ratios $r/a_{0,} E/E_\mathrm{h}$, etc., then all quantities are dimensionless.

(4) $P_l^{|m|}$ denotes the associated Legendre function (degree l, order $|m|$, normalization factor $N_{l|m|}$).

(5) ψ^* is the complex conjugate of ψ. For an anti-symmetrized n electron wavefunction $\Psi\ (r_1, \cdots, r_n, s_1, \cdots, s_n)$, the total probability density of electrons irrespective of spin is $\sum_{s_1} \cdots \sum_{s_n} \int_2 \cdots \int_n \Psi^* \Psi \ \mathrm{d}\tau_2 \cdots \mathrm{d}\tau_n$, where the integration extends over the space coordinates of all electrons but one and the sum extends over all spins.

(6) $-e$ is the charge of an electron.

(7) The unit is the same as for the physical quantity A that the operator represents.

(8) The unit is the same as for the product of the physical quantities A and B.

(9) The spin wavefunctions of a single electron, α and β, are defined by the matrix elements of the z-component of the spin angular momentum, $\widehat{s}_z$, by the relations $\langle \alpha \,|\widehat{s}_z|\, \alpha \rangle = +(1/2)$, $\langle \beta \,|\widehat{s}_z|\, \beta \rangle = -(1/2)$, $\langle \beta \,|\widehat{s}_z|\, \alpha \rangle = \langle \alpha \,|\widehat{s}_z|\, \beta \rangle = 0$ in units of $\hbar$. The total electron–spin wavefunctions of an atom with many electrons are denoted by Greek letters α, β, γ, etc., according to the value of $\sum m_s$, starting from the greatest down to the least.

Name	Symbol	Definition	SI unit	Notes
	Hückel molecular orbital theory (HMO)			
atomic-orbital basis function	χ_r		$\mathrm{m}^{-3/2}$	3
molecular orbital	ϕ_i	$\phi_i = \sum_r \chi_r c_{ri}$	$\mathrm{m}^{-3/2}$	3, 10
Coulomb integral	H_{rr}, α_r	$H_{rr} = \int \chi_r^* \widehat{H} \chi_r \mathrm{d}\tau$	J	3, 10, 11
resonance integral	H_{rs}, β_{rs}	$H_{rs} = \int \chi_r^* \widehat{H} \chi_s \mathrm{d}\tau$	J	3, 10, 12
energy parameter	x	$-x = (\alpha - E)/\beta$	1	13
overlap integral	S_{rs}, S	$S_{rs} = \int \chi_r^* \chi_s \mathrm{d}\tau$	1	10
charge order	q_r	$q_r = \sum_{i=1}^{n} b_i c_{ri}^2$	1	14, 15
bond order	p_{rs}	$p_{rs} = \sum_{i=1}^{n} b_i c_{ri} c_{si}$	1	15, 16

(10) $\widehat{H}$ is an effective Hamiltonian for a single electron, i and j label the molecular orbitals, and r and s label the atomic orbitals. In Hückel MO theory, H_{rs} is taken to be non-zero only for bonded pairs of atoms r and s, and all S_{rs} are assumed to be zero for $r \neq s$.

(11) Note that the name "coulomb integral" has a different meaning in HMO theory (where it refers to the energy of the orbital χ_r in the field of the nuclei) from Hartree–Fock theory discussed below (where it refers to a two-electron repulsion integral).

(12) This expression describes a bonding interaction between atomic orbitals r and s. For an anti-bonding interaction, the corresponding resonance integral is given by the negative value of the resonance integral for the bonding interaction.

(13) In the simplest application of Hückel theory to the π electrons of planar conjugated hydrocarbons, α is taken to be the same for all carbon atoms, and β to be the same for all bonded pairs of carbon atoms; it is then customary to write the Hückel secular determinant in terms of the dimensionless parameter x.

(14) $-eq_r$ is the electronic charge on atom r. q_r specifies the contribution of all n π electrons to the total charge at centre r, with $\sum q_r = n$.

(15) b_i gives the number of electrons which occupy a given orbital energy level ε_i; for non-degenerate orbitals, b_i can take the values 0, 1, or 2.

(16) p_{rs} is the bond order between atoms r and s.

3.2.1 *Ab initio Hartree–Fock Self-consistent Field Theory (ab initio SCF)*

Results in quantum chemistry are typically expressed in atomic units (Section 4.7.1). In the remaining tables of this section, all lengths, energies, masses, charges and angular momenta are expressed as dimensionless ratios to the corresponding atomic units, a_0, E_h, m_e, e, and $\hbar$, respectively. Thus all quantities become dimensionless, and the SI unit column is therefore omitted.

Name	Symbol	Definition	Notes
molecular orbital	$\phi_i(\mu)$		17
molecular spin orbital	$\phi_i(\mu)\alpha(\mu)$; $\phi_i(\mu)\beta(\mu)$		17
total wavefunction	Ψ	$\Psi = (n!)^{-1/2} \lVert \phi_i(\mu) \rVert$	17, 18
core Hamiltonian of a single electron	$\widehat{H}_\mu{}^{\mathrm{core}}$	$\widehat{H}_\mu = -(1/2)\nabla_\mu^2 - \sum_A Z_A/r_{\mu A}$	17, 19

(17) The indices i and j label the molecular orbitals, and either μ or the numerals 1 and 2 label the electron coordinates.

(18) The double vertical bars denote an anti-symmetrized product of the occupied molecular spin orbitals $\phi_i\alpha$ and $\phi_i\beta$ (sometimes denoted ϕ_i and $\overline{\phi}_i$); for a closed-shell system, Ψ would be a normalized Slater determinant. $(n!)^{-1/2}$ is the normalization factor and n the number of electrons.

(19) Z_A is the proton number (charge number) of nucleus A, and $r_{\mu\mathrm{A}}$ is the distance of electron μ from nucleus A. H_{ii} is the energy of an electron in orbital ϕ_i in the field of the core.

Name	Symbol	Definition	Notes
one-electron integrals expectation value of the core Hamiltonian	H_{ii}	$H_{ii} = \int \phi_i^*(1)\widehat{H}_1{}^{\text{core}}\phi_i(1)\mathrm{d}\tau_1$	17, 19
two-electron repulsion integrals			
Coulomb integral	J_{ij}	$J_{ij} = \iint \phi_i^*(1)\phi_j^*(2)\frac{1}{r_{12}}\phi_i(1)\phi_j(2)\mathrm{d}\tau_1\mathrm{d}\tau_2$	17, 20
exchange integral	K_{ij}	$K_{ij} = \iint \phi_i^*(1)\phi_j^*(2)\frac{1}{r_{12}}\phi_j(1)\phi_i(2)\mathrm{d}\tau_1\mathrm{d}\tau_2$	17, 20
one-electron orbital energy	ε_i	$\varepsilon_i = H_{ii} + \sum_j \left(2J_{ij} - K_{ij}\right)$	17, 21
total electronic energy	E	$E = 2\sum_i H_{ii} + \sum_i\sum_j \left(2J_{ij} - K_{ij}\right)$ $= \sum_i(\varepsilon_i + H_{ii})$	17, 21, 22
Coulomb operator	$\widehat{J}_i$	$\widehat{J}_i\phi_j(2) = \left\langle \phi_i(1) \left\| \frac{1}{r_{12}} \right\| \phi_i(1)\right\rangle \phi_j(2)$	17
exchange operator	$\widehat{K}_i$	$\widehat{K}_i\phi_j(2) = \left\langle \phi_i(1) \left\| \frac{1}{r_{12}} \right\| \phi_j(1)\right\rangle \phi_i(2)$	17
Fock operator	$\widehat{F}$	$\widehat{F} = \widehat{H}^{\text{core}} + \sum_i \left(2\widehat{J}_i - \widehat{K}_i\right)$	17, 21, 23

(20) The inter-electron repulsion integral is written in various shorthand notations: In $J_{ij} = \langle ij|ij\rangle$, the first and third indices refer to the index of electron 1 and the second and fourth indices to electron 2. In $J_{ij} = (i^*i|j^*j)$, the first two indices refer to electron 1 and the second two indices to electron 2. Usually the functions are real and the stars are omitted. The exchange integral is written in various shorthand notations with the same index convention as described: $K_{ij} = \langle ij|ji\rangle$ or $K_{ij} = (i^*j|j^*i)$.

(21) These relations apply to closed-shell systems only, and the sums extend over the occupied molecular orbitals.

(22) The sum over j includes the term with $j = i$, for which $J_{ii} = K_{ii}$, so that this term in the sum simplifies to give $2J_{ii} - K_{ii} = J_{ii}$.

3.2.2 Hartree–Fock–Roothaan SCF Theory, Using Molecular Orbitals Expanded as Linear Combinations of Atomic-Orbital Basis Functions (LCAO–MO theory)

Name	Symbol	Definition	Notes
atomic-orbital basis function	χ_r		24
molecular orbital	ϕ_i	$\phi_i = \sum_r \chi_r c_{ri}$	
overlap matrix element	S_{rs}	$S_{rs} = \int \chi_r^*\ \chi_s \mathrm{d}\tau, \quad \sum_{r,s} c_{ri}^*\, S_{rs} c_{sj} = \delta_{ij}$	
density matrix element	P_{rs}	$P_{rs} = 2\sum_i^{\text{occ}} c_{ri}^*\, c_{si}$	25
integrals over the basis functions			
one-electron integrals	H_{rs}	$H_{rs} = \int \chi_r^*\ (1)\hat{H}_1{}^{\text{core}}\chi_s(1)\mathrm{d}\tau_1$	
two-electron integrals	$(rs\|tu)$	$(rs\|tu) = \iint \chi_r^*\ (1)\chi_s(1)\frac{1}{r_{12}}\chi_t^*(2)\chi_u(2)\mathrm{d}\tau_1\mathrm{d}\tau_2$	26, 27
total electronic energy	E	$E = \sum_r\sum_s P_{rs}H_{rs}$ $+(1/2)\sum_r\sum_s\sum_t\sum_u P_{rs}P_{tu}\left[(rs\|tu) - (1/2)\,(ru\|ts)\right]$	25, 27
matrix element of the Fock operator	F_{rs}	$F_{rs} = H_{rs} + \sum_t\sum_u P_{tu}\left[(rs\|tu) - (1/2)\,(ru\|ts)\right]$	25, 28

(23) The Hartree–Fock equations read $(\widehat{F} - \varepsilon_j)\phi_j = 0$. Note that the definition of the Fock operator involves all of its eigenfunctions ϕ_i through the Coulomb and exchange operators, $\widehat{J}_i$ and $\widehat{K}_i$.

(24) The indices r and s label the basis functions. In numerical computations, the basis functions are either taken as Slater-type orbitals (STO) or as Gaussian-type orbitals (GTO). An STO basis function in spherical polar coordinates has the general form $\chi\,(r, \theta, \phi) = Nr^{n-1}\exp\left(-\zeta_{nl} r\right) Y_{lm}\,(\theta, \phi)$, where ζ_{nl} is a shielding parameter representing the effective charge in the state with quantum numbers n and l. GTO functions are typically expressed in Cartesian space coordinates, in the form $\chi\,(x, y, z) = Nx^a y^b z^c \exp\left(-\alpha r^2\right)$. Commonly, a linear combination of such functions with varying exponents α is used in such a way as to model an STO. N denotes a normalization factor.

(25) For closed-shell species with two electrons per occupied orbital. The sum extends over all occupied molecular orbitals. P_{rs} is also called the *bond order* between atoms r and s.

(26) The contracted notation for two-electron integrals over the basis functions, $(rs|tu)$, is based on the same convention outlined in Note 20.

(27) Here, the two-electron integral is expressed in terms of integrals over the spatial atomic-orbital basis functions. The matrix elements H_{ii}, J_{ij}, and K_{ij} may be similarly expressed in terms of integrals over the spatial atomic-orbital basis functions according to the following equations:

$$H_{ii} = \sum_r \sum_s c^*_{ri}\, c_{si}\, H_{rs}$$

$$J_{ij} = (i^*i|j^*j) = \sum_r \sum_s \sum_t \sum_u c^*_{ri}\, c_{si} c^*_{tj}\, c_{uj}\, (r^*s|t^*u)$$

$$K_{ij} = (i^*j|j^*i) = \sum_r \sum_s \sum_t \sum_u c^*_{ri}\, c_{si} c^*_{tj}\, c_{uj}\, (r^*u|t^*s)$$

(28) The Hartree–Fock–Roothaan SCF equations, expressed in terms of the matrix elements of the Fock operator F_{rs} and the overlap matrix elements S_{rs}, take the form:

$$\sum_s (F_{rs} - \varepsilon_i S_{rs})\, c_{si} = 0$$

3.3 Atoms and Molecules

The names and symbols recommended here follow Cohen *et al.* (2008) are in agreement with those recommended by IUPAP and ISO (1993). Additional quantities and symbols used in atomic, nuclear, and plasma physics can be found in Cohen and Giacomo (1987).

Name	Symbol	Definition	SI unit	Notes
nucleon number, mass number	A		1	
proton number, atomic number	Z		1	
neutron number	N	$N = A - Z$	1	
electron mass	m_e		kg	1, 2
mass of atom, atomic mass	m_a, m		kg	
atomic mass constant	m_u	$m_\mathrm{u} = m_\mathrm{a}(^{12}\mathrm{C})/12$	kg	1, 3
mass excess	Δ	$\Delta = m_\mathrm{a} - Am_\mathrm{u}$	kg	
elementary charge	e	proton charge	C	2
Planck constant	h		J s	
Planck constant divided by 2π	$\hbar$	$\hbar = h/2\pi$	J s	2
Bohr radius	a_0	$a_0 = 4\pi\varepsilon_0\hbar^2/m_\mathrm{e}e^2$	m	2
Hartree energy	E_h	$E_\mathrm{h} = \hbar^2/m_\mathrm{e}{a_0}^2$	J	2
Rydberg constant	R_∞	$R_\infty = E_\mathrm{h}/2hc$	m^{-1}	
fine-structure constant	α	$\alpha = e^2/4\pi\varepsilon_0\hbar c$	1	
ionization energy	E_i, I		J	4
electron affinity	E_ea, A		J	4
electronegativity	χ	$\chi = (1/2)\,(E_\mathrm{i} + E_\mathrm{ea})$	J	5
dissociation energy	E_d, D		J	
from the ground state	D_0		J	6
from the potential minimum	D_e		J	6
principal quantum number (hydrogen-like atom)	n	$E = hcZ^2R_\infty/n^2$	1	7

Name	Symbol	Definition	SI unit	Notes
angular momentum quantum numbers	see Section 3.5			
magnetic dipole moment of a molecule	$\boldsymbol{m}, \boldsymbol{\mu}$	$E_\mathrm{p} = -\boldsymbol{m} \cdot \boldsymbol{B}$	$\mathrm{J\ T^{-1}}$	8
magnetizability of a molecule	ξ	$\boldsymbol{m} = \xi \boldsymbol{B}$	$\mathrm{J\ T^{-2}}$	
Bohr magneton	μ_B	$\mu_\mathrm{B} = e\hbar/2m_\mathrm{e}$	$\mathrm{J\ T^{-1}}$	
nuclear magneton	μ_N	$\mu_\mathrm{N} = e\hbar/2m_\mathrm{p} = \left(m_\mathrm{e}/m_\mathrm{p}\right) \mu_\mathrm{B}$	$\mathrm{J\ T^{-1}}$	
gyromagnetic ratio, (magnetogyric ratio)	γ	$\gamma_\mathrm{e} = g_\mathrm{e}\mu_\mathrm{B}/\hbar$	$\mathrm{s^{-1}\ T^{-1}}$	9, 10
g-factor	g, g_e	$g_\mathrm{e} = \gamma_\mathrm{e}(2m_\mathrm{e}/e)$	1	9, 10
nuclear g-factor	g_N	$g_\mathrm{N} = \gamma_\mathrm{N}(2m_\mathrm{p}/e)$	1	9, 10
Larmor angular frequency	$\boldsymbol{\omega}_\mathrm{L}$	$\boldsymbol{\omega}_\mathrm{L} = -\gamma \boldsymbol{B}$	$\mathrm{s^{-1}}$	11
Larmor frequency	ν_L	$\nu_\mathrm{L} = \omega_\mathrm{L}/2\pi$	Hz	
relaxation time,				
longitudinal	T_1		s	12
transverse	T_2		s	12
electric dipole moment of a molecule	$\boldsymbol{p}, \boldsymbol{\mu}$	$E_\mathrm{p} = -\boldsymbol{p} \cdot \boldsymbol{E}$	C m	13

(1) Analogous symbols are used for other particles with subscripts: p for proton, n for neutron, a for atom, N for nucleus, etc.

(2) This quantity is also used as an atomic unit (Section 4.7.1).

(3) m_u is equal to the unified atomic mass unit, with symbol u, i.e., $m_\mathrm{u} = 1$ u (Section 4.5). The name dalton, with symbol Da, is used as an alternative name for the unified atomic mass unit (Mohr *et al.* 2008).

(4) The ionization energy is frequently called the *ionization potential* (I_p). The electron affinity is the energy needed to detach an electron.

(5) The concept of electronegativity was introduced by L. Pauling as the power of an atom in a molecule to attract electrons to itself. There are several ways of defining this quantity (Mullay 1987). The one given in the table has a clear physical meaning of energy and is due to R. S. Mulliken. The most frequently used scale, due to Pauling, is based on bond dissociation energies E_d in eV and it is relative in the sense that the values are dimensionless and that only electronegativity differences are defined. For atoms A and B

$$\chi_\mathrm{r,A} - \chi_\mathrm{r,B} = \sqrt{\frac{E_\mathrm{d}\,(\mathrm{AB})}{\mathrm{eV}} - \frac{1}{2}\frac{[E_\mathrm{d}\,(\mathrm{AA}) + E_\mathrm{d}\,(\mathrm{BB})]}{\mathrm{eV}}}$$

where χ_r denotes the Pauling relative electronegativity. The scale is chosen so as to make the relative electronegativity of hydrogen $\chi_\mathrm{r,H} = 2.1$. There is a difficulty in choosing the sign of the square root, which determines the sign of $\chi_\mathrm{r,A} - \chi_\mathrm{r,B}$. Pauling made this choice intuitively.

(6) The symbols D_0 and D_e are used for dissociation energies of diatomic and polyatomic molecules.

(7) For an electron in the central Coulomb field of an infinitely heavy nucleus of atomic number Z.

(8) Magnetic moments of specific particles may be denoted by subscripts, e.g., μ_e, μ_p, μ_n for an electron, a proton, and a neutron. Tabulated values usually refer to the maximum expectation value of the z-component.

(9) The gyromagnetic ratio for a nucleus is $\gamma_\mathrm{N} = g_\mathrm{N}\mu_\mathrm{N}/\hbar$.

(10) The convention used here follows (iii) Brown *et al.* (2000) with a negative g_e (see Chapter 6 and Mohr *et al.* 2008). Further different sign conventions for the electronic g-factor are discussed in Brown *et al.* (2000). Historically, g_e was defined positive ($g_\mathrm{e} > 0$), e is the (positive) elementary charge, therefore $\gamma_\mathrm{e} < 0$ and a minus sign would have to be introduced in the equation for γ_e given here. For nuclei, γ_N and g_N have the same sign.

(11) This is a vector quantity with magnitude ω_L and is sometimes called *Larmor circular frequency.*

(12) These quantities are used in the context of saturation effects in spectroscopy, particularly spin–resonance spectroscopy (Section 3.4).

(13) See Section 3.4, Note 9.

Name	Symbol	Definition	SI unit	Notes
quadrupole moment of a molecule	$\boldsymbol{Q}; \boldsymbol{\Theta}$	$E_\mathrm{p} = (1/2)\boldsymbol{Q} : \boldsymbol{V}'' = (1/3)\boldsymbol{\Theta} : \boldsymbol{V}''$	$\mathrm{C\ m^2}$	14
quadrupole moment of a nucleus	eQ	$eQ = 2\,\langle \Theta_{zz} \rangle$	$\mathrm{C\ m^2}$	15
electric field gradient tensor	$\boldsymbol{q}$	$q_{\alpha\beta} = -\partial^2 V/\partial\alpha\partial\beta$	$\mathrm{V\ m^{-2}}$	
quadrupole interaction energy tensor	$\boldsymbol{\chi}$	$\chi_{\alpha\beta} = eQq_{\alpha\beta}$	J	16
electric polarizability of a molecule	$\boldsymbol{\alpha}$	$\alpha_{ab} = \partial p_a/\partial E_b$	$\mathrm{C^2\ m^2\ J^{-1}}$	17
1st hyper-polarizability	$\boldsymbol{\beta}$	$\beta_{abc} = \partial^2 p_a/\partial E_b \partial E_c$	$\mathrm{C^3\ m^3\ J^{-2}}$	17
2nd hyper-polarizability	$\boldsymbol{\gamma}$	$\gamma_{abcd} = \partial^3 p_a/\partial E_b \partial E_c \partial E_d$	$\mathrm{C^4\ m^4\ J^{-3}}$	17
activity (of a radio-active substance)	A	$A = -\mathrm{d}N_\mathrm{B}/\mathrm{d}t$	Bq	18
decay (rate) constant, disintegration (rate) constant	λ, k	$A = \lambda N_\mathrm{B}$	$\mathrm{s^{-1}}$	18
half-life	$t_{1/2}, T_{1/2}$	$N_\mathrm{B}(t_{1/2}) = N_\mathrm{B}(0)/2$	s	18, 19
mean life, lifetime	τ	$\tau = 1/\lambda$	s	19
level width	Γ	$\Gamma = \hbar/\tau$	J	
disintegration energy	Q		J	
cross section	σ		$\mathrm{m^2}$	
electroweak charge of a nucleus	Q_W	$Q_\mathrm{W} \approx Z(1 - 4\sin^2\theta_\mathrm{W}) - N$	1	20

(14) The quadrupole moment of a molecule may be represented either by the tensor $\boldsymbol{Q}$, defined by an integral over the charge density ρ:

$$Q_{\alpha\beta} = \int r_\alpha r_\beta \rho \ \mathrm{d}V$$

in which α and β denote x, y, or z or by the tensor $\boldsymbol{\Theta}$ of trace zero defined by

$$\Theta_{\alpha\beta} = (1/2) \int \left(3r_\alpha r_\beta - \delta_{\alpha\beta}\ r^2\right) \rho \ \mathrm{d}V = (1/2)\left[3Q_{\alpha\beta} - \delta_{\alpha\beta}\left(Q_{xx} + Q_{yy} + Q_{zz}\right)\right]$$

$\boldsymbol{V}''$ is the second derivative of the electronic potential:

$$V''_{\alpha\beta} = -q_{\alpha\beta} = \partial^2 V/\partial\alpha\partial\beta$$

The contribution to the potential energy is then given by

$$E_\mathrm{p} = (1/2)\boldsymbol{Q} : \boldsymbol{V}'' = (1/2) \sum_\alpha \sum_\beta Q_{\alpha\beta} V_{\alpha\beta}''$$

(15) Nuclear quadrupole moments are conventionally defined in a different way from molecular quadrupole moments. Q has the dimension of an area and e is the elementary charge. eQ is taken to be twice the maximum expectation value of the zz tensor element (see Note 14).

(16) The nuclear quadrupole interaction energy tensor $\boldsymbol{\chi}$ is usually quoted in MHz, corresponding to the value of eQq/h, although the h is usually omitted.

(17) The polarizability $\boldsymbol{\alpha}$ and the hyper-polarizabilities $\boldsymbol{\beta}, \boldsymbol{\gamma}, \ldots$ are the coefficients in the expansion of the dipole moment $\boldsymbol{p}$ in powers of the electric field strength $\boldsymbol{E}$ (see Section 3.1, Note 7). The expansion of the component a is given by

$$p_a = p_a^{(0)} + \sum_b \alpha_{ab} E_b + (1/2) \sum_{bc} \beta_{abc} E_b E_c + (1/6) \sum_{bcd} \gamma_{abcd} E_b E_c E_d + \cdots$$

α_{ab}, β_{abc}, and γ_{abcd} are elements of the tensors $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, and $\boldsymbol{\gamma}$ of rank 2, 3, and 4, respectively. The components of these tensors are distinguished by the subscript indices $abc\ldots$, as indicated in the definitions, the first index a always denoting the component of p, and the subsequent indices the components of the electric field. The polarizability and the hyper-polarizabilities exhibit symmetry properties. Thus, $\boldsymbol{\alpha}$ is commonly a symmetric tensor, and all components of $\boldsymbol{\beta}$ are 0 for a molecule with a centre of symmetry, etc. Values of the polarizability are commonly quoted as the value $\alpha/4\pi\varepsilon_0$, which is a volume. The value is commonly expressed in the unit Å^3 (Å should not be used, see Section 3.4, Note 11) or in the unit ${a_0}^3$ (atomic units, see Section 4.7.1). Similar comments apply to the hyper-polarizabilities with $\beta/(4\pi\varepsilon_0)^2$ in units of ${a_0}^5 e^{-1}$, and $\gamma/(4\pi\varepsilon_0)^3$ in units of ${a_0}^7 e^{-2}$, etc.

(18) N_B is the number of decaying entities B ($1\ \mathrm{Bq} = 1\ \mathrm{s^{-1}}$, see Section 4.2).

(19) Half lives and mean lives are commonly given in years (unit a). $t_{1/2} = \tau \ln 2$ for exponential decays.

(20) The electroweak charge of a nucleus is approximately given by the neutron number N and the proton number Z with the weak mixing angle θ_W (Chapter 6). It is important in the calculations of atomic and molecular properties including the weak nuclear interaction (Quack and Stohner 2003).

3.4 Spectroscopy

This section essentially follows Cohen *et al.* (2008). It is based on the recommendations of the ICSU Joint Commission for Spectroscopy (Jenkins 1953, Mulliken 1955, Mulliken 1956) and current practice in the field, which is well represented in the books by Herzberg (Herzberg 1946, Herzberg 1950, Herzberg 1966). The IUPAC Commission on Molecular Structure and Spectroscopy has also published recommendations, which have been taken into account (Becker 1978, Becker *et al.* 1981, Physical Chemistry Division, Commission on Molecular Structure and Spectroscopy 1972, Physical Chemistry Division, Commission on Molecular Structure and Spectroscopy 1976a, Physical Chemistry Division, Commission on Molecular Structure and Spectroscopy 1976b, Physical Chemistry Division, Commission on Molecular Structure and Spectroscopy 1976c, Beynon 1978, Schutte *et al.* 1997a, Schutte *et al.* 1997b, Bunker *et al.* 1997, Harris *et al.* 1997, Markley *et al.* 1998).

Name	Symbol	Definition	SI unit	Notes
total term	T	$T = E_{\mathrm{tot}}/hc$	$\mathrm{m^{-1}}$	1, 2
transition wavenumber	$\widetilde{\nu}$	$\widetilde{\nu} = T' - T''$	$\mathrm{m^{-1}}$	1
transition frequency	ν	$\nu = \left(E' - E''\right)/h$	Hz	
electronic term	T_{e}	$T_{\mathrm{e}} = E_{\mathrm{e}}/hc$	$\mathrm{m^{-1}}$	1, 2
vibrational term	G	$G = E_{\mathrm{vib}}/hc$	$\mathrm{m^{-1}}$	1, 2
rotational term	F	$F = E_{\mathrm{rot}}/hc$	$\mathrm{m^{-1}}$	1, 2
spin–orbit coupling constant	A	$T_{\mathrm{so}} = A\langle\widehat{\boldsymbol{L}}\cdot\widehat{\boldsymbol{S}}\rangle$	$\mathrm{m^{-1}}$	1, 3
principal moments of inertia	$I_A; I_B; I_C$	$I_A \leq I_B \leq I_C$	kg $\mathrm{m^2}$	
rotational constants,				
in wavenumber	$\widetilde{A}; \widetilde{B}; \widetilde{C}$	$\widetilde{A} = h/8\pi^2 c I_A$	$\mathrm{m^{-1}}$	1, 2
in frequency	$A; B; C$	$A = h/8\pi^2 I_A$	Hz	
inertial defect	$\varDelta$	$\varDelta = I_C - I_A - I_B$	kg $\mathrm{m^2}$	
asymmetry parameter	κ	$\kappa = \dfrac{2B - A - C}{A - C}$	1	4
centrifugal distortion constants,				
S reduction	$D_J; D_{JK}; D_K; d_1; d_2$		$\mathrm{m^{-1}}$	2, 5
A reduction	$\varDelta_J; \varDelta_{JK}; \varDelta_K; \delta_J; \delta_K$		$\mathrm{m^{-1}}$	2, 5
harmonic vibration wavenumber	$\omega_{\mathrm{e}}; \omega_r$		$\mathrm{m^{-1}}$	2, 6
vibrational anharmonicity constant	$\omega_{\mathrm{e}}x_{\mathrm{e}}; x_{rs}; g_{tt'}$		$\mathrm{m^{-1}}$	2, 6

(1) In spectroscopy the unit $\mathrm{cm^{-1}}$ is almost always used for the quantity wavenumber, and *term values* and *wavenumbers* always refer to the reciprocal wavelength of the equivalent radiation in vacuum. The symbol c in the definition E/hc refers to the speed of light in vacuum. Because "wavenumber" is not a number ISO suggests the use of repetency in parallel with wavenumber (ISO 1993). The use of the word "wavenumber" instead of the unit $\mathrm{cm^{-1}}$ must be avoided.

(2) Term values and spectroscopic constants are sometimes defined as wavenumber (e.g., $T = E/hc$), and sometimes as frequency (e.g., $T = E/h$). When the symbol is otherwise the same, it is convenient to distinguish wavenumber quantities with a tilde (e.g., $\widetilde{\nu}$, $\widetilde{T}$, $\widetilde{A}$, $\widetilde{B}$, $\widetilde{C}$ for quantities defined as wavenumber), although this is not a universal practice.

(3) $\widehat{\boldsymbol{L}}$ and $\widehat{\boldsymbol{S}}$ are electron orbital and electron–spin operators, respectively.

(4) The Wang asymmetry parameters are also used: for a near prolate top, $b_{\mathrm{p}} = (C - B)/(2A - B - C)$ and for a near oblate top $b_{\mathrm{o}} = (A - B)/(2C - A - B)$.

(5) S and A stand for the symmetric and asymmetric reductions of the rotational Hamiltonian respectively; see Watson (1977) for more details on the various possible representations of the centrifugal distortion constants.

(6) For a diatomic molecule, $G(v) = \omega_{\mathrm{e}}\left(v + \frac{1}{2}\right) - \omega_{\mathrm{e}}x_{\mathrm{e}}\left(v + \frac{1}{2}\right)^2 + \cdots$. For a polyatomic molecule, the $3N - 6$ vibrational modes ($3N - 5$ if linear) are labeled by the indices $r, s, t, \cdots$, or $i, j, k, \cdots$. The index r is usually assigned to be increasing with descending wavenumber, symmetry species by symmetry species starting with the totally symmetric species. The index t is kept for degenerate modes. The vibrational term formula is

$$G(v) = \sum_r \omega_r\,(v_r + d_r/2) + \sum_{r\leq s} x_{rs}\,(v_r + d_r/2)\,(v_s + d_s/2) + \sum_{t\leq t'} g_{tt'} l_t l_{t'} + \cdots$$

Another common term formula is defined with respect to the vibrational ground state

$$T(v) = \sum_i v_i \widetilde{\nu}_i{}' + \sum_{r\leq s} x_{rs}{}' v_r v_s + \sum_{t\leq t'} g_{tt'}{}' l_t l_{t'} + \cdots$$

these being commonly used as the diagonal elements of effective vibrational Hamiltonians.

Name	Symbol	Definition	SI unit	Notes
vibrational quantum numbers	$v_r;\ l_t$		1	6
vibrational fundamental wavenumber	$\widetilde{\nu}_r,\ \widetilde{\nu}_r^0,\ \nu_r$	$\widetilde{\nu}_r = T(v_r = 1) - T(v_r = 0)$	m^{-1}	2, 6
Coriolis ζ-constant	$\zeta_{rs}{}^{\alpha}$		1	7
angular momentum quantum numbers	see Section 3.5			
degeneracy, statistical weight	g, d, β		1	8
electric dipole moment of a molecule	$\boldsymbol{p}, \boldsymbol{\mu}$	$E_\mathrm{p} = -\boldsymbol{p}\cdot\boldsymbol{E}$	C m	9
transition dipole moment of a molecule	$\boldsymbol{M}, \boldsymbol{R}$	$\boldsymbol{M} = \int \psi^{*\prime}\boldsymbol{p}\ \psi''\ \mathrm{d}\tau$	C m	9, 10
interatomic distances,				11, 12
equilibrium	r_e		m	
zero-point average	r_z		m	
ground state	r_0		m	
substitution structure	r_s		m	
vibrational coordinates,				11
internal	R_i, r_i, θ_j, etc.		(varies)	
symmetry	S_j		(varies)	
normal				
mass adjusted	Q_r		$\mathrm{kg}^{1/2}$ m	
dimensionless	q_r		1	
vibrational force constants				
diatomic	$f, (k)$	$f = \partial^2 V/\partial r^2$	$\mathrm{J\ m}^{-2}$, $\mathrm{N\ m}^{-1}$	11, 13
polyatomic				
internal coordinates	f_{ij}	$f_{ij} = \partial^2 V/\partial r_i \partial r_j$	(varies)	
symmetry coordinates	F_{ij}	$F_{ij} = \partial^2 V/\partial S_i \partial S_j$	(varies)	
dimensionless normal coordinates	$\phi_{rst\cdots}, k_{rst\cdots}, C_{rst\cdots}$		m^{-1}	2, 14

(7) Frequently the Coriolis coupling constants $\xi_\alpha{}^{v'v}$ with units of cm^{-1} are used as effective Hamiltonian constants ($\alpha = x, y, z$). For two fundamental vibrations with harmonic wavenumbers ω_r and ω_s, these are connected with $\zeta_{rs}{}^{\alpha}$ by the equation ($v_r = 1$ and $v_s = 1$)

$$\xi_\alpha{}^{v'v} = \widetilde{B}_\alpha\ \zeta_{rs}{}^{\alpha}\left[\sqrt{\omega_s/\omega_r} + \sqrt{\omega_r/\omega_s}\right]$$

where $\widetilde{B}_\alpha$ is the α rotational constant. A similar equation applies with B_α if $\xi_\alpha{}^{v'v}$ is defined as a quantity with frequency units.

(8) d is usually used for vibrational degeneracy and β for nuclear spin degeneracy.

(9) E_p is the potential energy of a dipole with electric dipole moment $\boldsymbol{p}$ in an electric field of strength $\boldsymbol{E}$. Molecular dipole moments are commonly expressed in the non-SI unit debye, where 1 D $\approx$ 3.335 64×10^{-30} C m. The SI unit C m is inconvenient for expressing molecular dipole moments, which results in the continued use of the deprecated debye (D). A convenient alternative is to use the atomic unit, ea_0. Another way of expressing dipole moments is to quote the electric dipole lengths, $l_p = p/e$, analogous to the way the nuclear quadrupole areas are quoted (see Section 3.3, Notes 14 and 15). This gives the distance between two elementary charges of the equivalent dipole and conveys a clear picture in relation to molecular dimensions (see also Section 3.1, Note 8).

Examples	Dipole moment			Dipole length
	SI		a.u.	
	p/(C m)	p/D	$p/(ea_0)$	l_p/(pm)
HCl	3.60×10^{-30}	1.08	0.425	22.5
$\mathrm{H_2O}$	6.23×10^{-30}	1.87	0.736	38.9
NaCl	3.00×10^{-29}	9.00	3.54	187

(10) For quantities describing line and band intensities, see Section 3.8.

(11) Interatomic (internuclear) distances and vibrational displacements are commonly expressed in the non-SI unit ångström, where 1 Å = 10^{-10} m = 0.1 nm = 100 pm. Å should not be used.

(12) The various slightly different ways of representing interatomic distances, distinguished by subscripts, involve different vibrational averaging contributions; they are discussed in Graner *et al.* (2000), where the geometrical structures of many free molecules are listed. Only the equilibrium distance r_e is isotopically invariant, to a good approximation. The effective distance parameter r_0 is estimated from the rotational constants for the ground vibrational state and has a more complicated physical significance for polyatomic molecules.

Name	Symbol	Definition	SI unit	Notes
		Electron–spin resonance (ESR), Electron paramagnetic resonance (EPR)		
gyromagnetic ratio	γ	$\gamma = \mu/\hbar\sqrt{S(S+1)}$	$\mathrm{s^{-1}\,T^{-1}}$	15
g-factor	g	$h\nu = \lvert g\rvert\mu_{\mathrm{B}}B$	1	16
hyperfine coupling constant				
in liquids	a, A	$\widehat{H}_{\mathrm{hfs}}/h = a\widehat{\boldsymbol{S}}\cdot\widehat{\boldsymbol{I}}$	Hz	17
in solids	$\boldsymbol{T}$	$\widehat{H}_{\mathrm{hfs}}/h = \widehat{\boldsymbol{S}}\cdot\boldsymbol{T}\cdot\widehat{\boldsymbol{I}}$	Hz	17
		Nuclear magnetic resonance (NMR)		
static magnetic flux density of a NMR spectrometer	$\boldsymbol{B}_0$		T	18
radiofrequency magnetic flux densities	$\boldsymbol{B}_1, \boldsymbol{B}_2$		T	18
spin–rotation interaction tensor	$\boldsymbol{C}$		Hz	19
spin-rotation coupling constant of nucleus A	C_{A}		Hz	19
dipolar interaction tensor	$\boldsymbol{D}$		Hz	19
dipolar coupling constant between nuclei A, B	D_{AB}	$D_{\mathrm{AB}} = \dfrac{\mu_0\hbar}{8\pi^2}\dfrac{\gamma_{\mathrm{A}}\gamma_{\mathrm{B}}}{{r_{\mathrm{AB}}}^3}$	Hz	19
frequency variables of a two-dimensional spectrum	$F_1, F_2;\ f_1, f_2$		Hz	
nuclear spin operator for nucleus A	$\widehat{\boldsymbol{I}}_{\mathrm{A}}, \widehat{\boldsymbol{S}}_{\mathrm{A}}$		1	20
quantum number associated with $\widehat{\boldsymbol{I}}_{\mathrm{A}}$	I_{A}		1	
indirect spin coupling tensor	$\boldsymbol{J}$		Hz	
nuclear spin–spin coupling through n bonds	${}^{n}J$		Hz	21
reduced nuclear spin–spin coupling constant	K_{AB}	$K_{\mathrm{AB}} = \dfrac{J_{\mathrm{AB}}}{h}\dfrac{2\pi}{\gamma_{\mathrm{A}}}\dfrac{2\pi}{\gamma_{\mathrm{B}}}$	$\mathrm{T^2\,J^{-1}}$, $\mathrm{N\,A^{-2}\,m^{-3}}$	20
eigenvalue of $\widehat{\boldsymbol{I}}_{\mathrm{A}z}$	m_{A}		1	22
equilibrium macroscopic magnetization per volume	$\boldsymbol{M}_0$		$\mathrm{J\,T^{-1}\,m^{-3}}$	23

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(13) Force constants are commonly expressed in mdyn Å^{-1} = aJ Å^{-2} for stretching coordinates, mdyn Å = aJ for bending coordinates, and mdyn = aJ Å^{-1} for stretch–bend interactions. Å should not be used (see Note 11). See Morino and Shimanouchi (1978) for further details on definitions and notation for force constants.

(14) The force constants in dimensionless normal coordinates are usually defined in wavenumber units by the equation $V/hc = \sum \phi_{rst\cdots}q_r q_s q_t \ldots$, where the summation over the normal coordinate indices $r, s, t, \cdots$ is unrestricted.

(15) The magnitude of γ is obtained from the magnitudes of the magnetic dipole moment μ and the angular momentum (in ESR: electron spin $\boldsymbol{S}$ for a Σ-state, $L = 0$; in NMR: nuclear spin $\boldsymbol{I}$).

(16) This gives an effective g-factor for a single spin ($S = 1/2$) in an external static field (concerning various sign conventions, see Section 3.3, Note 10).

(17) $\hat{H}_{\mathrm{hfs}}$ is the hyperfine coupling Hamiltonian. $\widehat{\boldsymbol{S}}$ is the electron–spin operator with quantum number S (Section 3.5). The coupling constants a are usually quoted in MHz, but they are sometimes quoted in magnetic induction units (G or T) obtained by dividing by the conversion factor $\lvert g\rvert\mu_{\mathrm{B}}/h$, which has the SI unit Hz T^{-1}; $\lvert g\rvert_{\mathrm{e}}\mu_{\mathrm{B}}/h \approx 28.025$ GHz T^{-1} $\left(= 2.8025 \text{ MHz G}^{-1}\right)$, where g_{e} is the g-factor for a free electron. If in liquids the hyperfine coupling is isotropic, the coupling constant is a scalar a. In solids the coupling is anisotropic, and the coupling constant is a 3×3 tensor $\boldsymbol{T}$. Similar comments apply to the g-factor and to the analogous NMR parameters. A convention for the g-factor has been proposed, in which the sign of g is positive when the dipole moment is parallel to its angular momentum and negative when it is antiparallel. Such a choice would require the g-factors for the electron orbital and spin angular momenta to be negative (Brown *et al.* 2000) (see Section 3.3, Note 10).

(18) The observing ($\boldsymbol{B}_1$) and irradiating ($\boldsymbol{B}_2$) radiofrequency flux densities are associated with frequencies ν_1, ν_2 and with nutation angular frequencies Ω_1, Ω_2 (around $\boldsymbol{B}_1$, $\boldsymbol{B}_2$, respectively). They are defined through $\Omega_1 = -\gamma\boldsymbol{B}_1$ and $\Omega_2 = -\gamma\boldsymbol{B}_2$ (see Section 3.1, Notes 8 and 9).

(19) The units of interaction strengths are Hz. In the context of relaxation, the interaction strengths should be converted to angular frequency units (rad s^{-1}, but commonly denoted s^{-1}, see Note 25).

(20) $\widehat{\boldsymbol{I}}_{\mathrm{A}}$, $\widehat{\boldsymbol{S}}_{\mathrm{A}}$ have components $\widehat{I}_{\mathrm{A}x}$, $\widehat{I}_{\mathrm{A}y}$, $\widehat{I}_{\mathrm{A}z}$, and $\widehat{S}_{\mathrm{A}x}$, $\widehat{S}_{\mathrm{A}y}$, $\widehat{S}_{\mathrm{A}z}$, respectively. Another way of defining angular momentum operators is with unit J s (Section 3.5).

Name	Symbol	Definition	SI unit	Notes
nuclear quadrupole moment	eQ		$\mathrm{C\ m^2}$	24
electric field gradient	$\boldsymbol{q}$	$q_{\alpha\beta} = -\partial^2 V/\partial\alpha\partial\beta$	$\mathrm{V\ m^{-2}}$	25
nuclear quadrupole coupling constant	χ	$\chi = eq_{zz}Q/h$	Hz	19
time dimensions for two-dimensional NMR	t_1, t_2		s	
spin–lattice relaxation time (longitudinal) for nucleus A	${T_1}^{\mathrm{A}}$		s	26, 27
spin–spin relaxation time (transverse) for nucleus A	${T_2}^{\mathrm{A}}$		s	26
spin wavefunctions	$\alpha; \beta$			28
gyromagnetic ratio	γ	$\gamma = \mu/\hbar\sqrt{I(I+1)}$	$\mathrm{s^{-1}\ T^{-1}}$	15, 29
chemical shift for nucleus A	δ_{A}	$\delta_{\mathrm{A}} = (\nu_{\mathrm{A}} - \nu_{\mathrm{ref}})/\nu_{\mathrm{ref}}$	1	30
nuclear Overhauser enhancement	η		1	31
nuclear magneton	μ_{N}	$\mu_{\mathrm{N}} = (m_{\mathrm{e}}/m_{\mathrm{p}})\mu_{\mathrm{B}}$	$\mathrm{J\ T^{-1}}$	32
resonance frequency	ν		Hz	18
of a reference molecule	ν_{ref}			
of the observed rf field	ν_1			
of the irradiating rf field	ν_2			
standardized resonance frequency	Ξ_{A}		Hz	33
shielding tensor	$\boldsymbol{\sigma}$		1	34
shielding constant	σ_{A}	$B_{\mathrm{A}} = (1 - \sigma_{\mathrm{A}})B_0$	1	34
correlation time	τ_{c}		s	26

(21) Parentheses may be used to indicate the species of the nuclei coupled, e.g., $J(^{13}\mathrm{C}, {}^1\mathrm{H})$ or, additionally, the coupling path, e.g., $J(\mathrm{POCF})$. Where no ambiguity arises, the elements involved can be, alternatively, given as subscripts, e.g., J_{CH}. The nucleus of higher mass should be given first. The same applies to the reduced coupling constant.

(22) M rather than m is frequently recommended, but most NMR practitioners use m so as to avoid confusion with magnetization.

(23) This is for a spin system in the presence of a magnetic flux density $\boldsymbol{B}_0$.

(24) See Section 3.3, Notes 14 and 15.

(25) The symbol $\boldsymbol{q}$ is recommended by IUPAC for the field gradient tensor, with the units of $\mathrm{V\ m^{-2}}$ (Section 3.3). With $\boldsymbol{q}$ defined in this way, the quadrupole coupling constant is $\chi = eq_{zz}Q/h$. It is common in NMR to denote the field gradient tensor as $e\boldsymbol{q}$ and the quadrupole coupling constant as $\chi = e^2 q_{zz}Q/h$. $\boldsymbol{q}$ has principal components q_{XX}, q_{YY}, and q_{ZZ}.

(26) The relaxation times and the correlation times are normally given in the units of s. Strictly speaking, this refers to s $\mathrm{rad^{-1}}$.

(27) The spin–lattice relaxation time of nucleus A in the frame of reference rotating with $\boldsymbol{B}_1$ is denoted ${T_{1\rho}}^{\mathrm{A}}$.

(28) See Section 3.2, Note 9.

(29) μ is the magnitude of the nuclear magnetic moment.

(30) Chemical shift (of the resonance) for the nucleus of element A (positive when the sample resonates to high frequency of the reference); for conventions, see Harris *et al.* (2001). Further information regarding solvent, references, or nucleus of interest may be given by superscripts, subscripts, or in parentheses.

(31) The nuclear Overhauser effect, $1 + \eta$, is defined as the ratio of the signal intensity for the I nuclear spin, obtained under conditions of saturation of the S nuclear spin, and the equilibrium signal intensity for the I nuclear spin.

(32) m_{e} and m_{p} are the electron and proton mass, respectively. μ_{B} is the Bohr magneton (see Section 3.3, Notes 1 and 2, and Chapter 6).

(33) Resonance frequency for the nucleus of element A in a magnetic field such that the protons in tetramethylsilane (TMS) resonate exactly at 100 MHz.

(34) The symbols σ_{A} (and related terms of the shielding tensor and its components) refer to shielding on an absolute scale (for theoretical work). For shielding relative to a reference, symbols such as $\sigma_{\mathrm{A}} - \sigma_{\mathrm{ref}}$ should be used. B_{A} is the corresponding effective magnetic flux density (see Section 3.1, Note 9).

3.5 Symbols for Angular Momentum Operators and Quantum Numbers

In the following table, all of the operator symbols denote the dimensionless ratio *angular momentum* divided by $\hbar$. Although this is a universal practice for the quantum numbers, some authors use the operator symbols to denote *angular momentum*, in which case the operators would have SI units: J s. The column heading "*Z-axis*" denotes the space-fixed component, and the heading "*z-axis*" denotes the molecule-fixed component along the symmetry axis (linear or symmetric top molecules), or the axis of quantization.

Angular momentum[1]	Operator symbol	Quantum number symbol Total	 Z-axis	 z-axis	Notes
electron orbital	$\widehat{\boldsymbol{L}}$	L	M_L	Λ	2
one electron only	$\widehat{\boldsymbol{l}}$	l	m_l	λ	2
electron spin	$\widehat{\boldsymbol{S}}$	S	M_S	Σ	
one electron only	$\widehat{\boldsymbol{s}}$	s	m_s	σ	
electron orbital plus spin	$\widehat{\boldsymbol{L}}+\widehat{\boldsymbol{S}}$			$\Omega = \Lambda + \Sigma$	2
nuclear orbital (rotational)	$\widehat{\boldsymbol{R}}$	R		K_R, k_R	
nuclear spin	$\widehat{\boldsymbol{I}}$	I	M_I		
internal vibrational					
spherical top	$\widehat{\boldsymbol{l}}$	$l\,(l\zeta)$		K_l	3
other	$\widehat{\boldsymbol{j}}, \widehat{\boldsymbol{\pi}}$			$l\,(l\zeta)$	2, 3
sum of $R + L\,(+j)$	$\widehat{\boldsymbol{N}}$	N		K, k	2
sum of $N + S$	$\widehat{\boldsymbol{J}}$	J	M_J	K, k	2, 4
sum of $J + I$	$\widehat{\boldsymbol{F}}$	F	M_F		

(1) In all cases, the vector operator and its components are related to the quantum numbers by eigenvalue equation analogous to

$$\widehat{\boldsymbol{J}}^2\psi = J\,(J+1)\,\psi, \quad \widehat{J}_Z\psi = M_J\psi, \quad \text{and} \quad \widehat{J}_z\ \psi = K\psi$$

where the component quantum numbers M_J and K take integral or half-odd values in the range $-J \le M_J \le +J, -J \le K \le +J$. (If the operator symbols are taken to represent *angular momentum*, rather than *angular momentum* divided by $\hbar$, the eigenvalue equations should read $\widehat{\boldsymbol{J}}^2\psi = J\,(J+1)\,\hbar^2\psi$, $\widehat{J}_Z\psi = M_J\hbar\psi$, and $\widehat{J}_z\psi = K\hbar\psi$.) l is frequently called the *azimuthal quantum number* and m_l the *magnetic quantum number*.

(2) Some authors, notably Herzberg (1950, 1946, 1966), treat the component quantum numbers Λ, Ω, l, and K as taking positive or zero values only, so that each non-zero value of the quantum number labels two wavefunctions with opposite signs for the appropriate angular momentum component. When this is done, lower case k is commonly regarded as a signed quantum number, related to K by $K = |k|$. However, in theoretical discussions, all component quantum numbers are usually treated as signed, taking both positive and negative values.

(3) There is no uniform convention for denoting the internal vibrational angular momentum; j, π, p, and G have all been used. For symmetric top and linear molecules, the component of j in the symmetry axis is always denoted by the quantum number l, where l takes values in the range $-v \le l \le +v$ in steps of 2. The corresponding component of angular momentum is actually $l\zeta\hbar$, rather than $l\hbar$, where ζ is the Coriolis ζ-constant (see Section 3.4, Note 7).

(4) Asymmetric top rotational states are labeled by the value of J (or N if $S \neq 0$), with subscripts K_a, K_c, where the latter correlate with the $K = |k|$ quantum number about the a and c axes in the prolate and oblate symmetric top limits, respectively.

Example $J_{K_a,K_c} = 5_{2,3}$ for a particular rotational level.

3.6 Symbols for Symmetry Operators and Labels for Symmetry Species

Although it is desirable to distinguish between symmetry elements (e.g., a rotation axis) and symmetry operators (also called symmetry operations) by typographical conventions, no established convention exists so far. The conventions used here coincide with those of Schutte *et al.* (1997a, b) and Bunker *et al.* (1997). Symbols for symmetry elements and for irreducible representations of point groups (in spectroscopy frequently called *symmetry species*) are printed in roman (upright) fonts, whereas those for symmetry operators are printed in italics. Sometimes, the notations of Wilson *et al.* (1980) and Herzberg (1946, 1950, 1966) differ; in any case, it is recommended that authors clearly identify the conventions they follow. This section follows spectroscopic usage of group theoretical symbols as represented in Wilson *et al.* (1980) and Herzberg (1946, 1950, 1966).

3.6.1 *Symmetry Operators in Molecule-fixed Coordinates (Schönflies symbols)*

Detailed rules on symmetry operators in molecule-fixed coordinates can be found in Herzberg (1950, 1946, 1966) and Mulliken (1955, 1956):

identity	E; I
rotation by $2\pi/n$ about an n-fold axis	C_n
reflection across a plane	$\sigma, \sigma_{\rm v}, \sigma_{\rm d}, \sigma_{\rm h}$
inversion through a centre of symmetry	i
rotation-reflection about an n-fold axis	$S_n\ (= C_n\sigma_{\rm h})$

If C_n is the primary axis of symmetry, wavefunctions that are unchanged or change sign under the operator C_n are given species labels A and B, respectively; otherwise, wavefunctions that are multiplied by $\exp(\pm 2\pi i s/n)$ are given the species label E_s. Wavefunctions that are unchanged or change sign under i are labeled g (gerade) and u (ungerade), respectively. Wavefunctions that are unchanged and change sign under $\sigma_{\rm h}$ have species labels with a prime $'$ and a double prime $''$, respectively. For more detailed rules, see also Section 2.5, Note 10.

3.6.2 *Point Groups and Irreducible Representations*

Point groups are composed of symmetry operators, which are listed in the preceding subsections. To distinguish symmetry operators from symmetry group symbols, the latter are often written in different fonts, e.g., bold-faced italics (Bunker and Jensen 1998) or script (Wilson *et al.* 1980). Here, we do not use a special font as it is clear from the context whether symmetry operators or symmetry group symbols are referred to. The following table lists some selected symmetry point groups labeled by their group symbol together with their irreducible representations (also called species).

Group symbol	Irreducible representation
C_1	A
$C_{\rm i}$	$\mathrm{A_g}$, $\mathrm{A_u}$
$D_2\ (= V)$	A, B_i $(i = 1, 2, 3)$
$C_{3\rm v}$	A_i $(i = 1, 2)$, E
$D_{2\rm h}\ (= V_{\rm h})$	$\mathrm{A_g}$, $\mathrm{B}_{i\rm g}$ $(i = 1, 2, 3)$, $\mathrm{A_u}$, $\mathrm{B}_{i\rm u}$ $(i = 1, 2, 3)$
S_4	A, B, E
$C_{\rm s} (= C_{1\rm h})$	A', A''
C_2	A, B
$C_{2\rm v}$	A_i, B_i $(i = 1, 2)$
$C_{2\rm h}$	A_i, B_i $(i = \mathrm{u}, \mathrm{g})$
$D_{6\rm h}$	$\mathrm{A}_{i\rm g}$, $\mathrm{B}_{i\rm g}$, $\mathrm{E}_{i\rm g}$ $(i = 1, 2)$, $\mathrm{A}_{i\rm u}$, $\mathrm{B}_{i\rm u}$, $\mathrm{E}_{i\rm u}$ $(i = 1, 2)$
$T_{\rm d}$	A_i, E, F_i $(i = 1, 2)$

As an example, we reproduce the character tables of the point groups $C_{2\rm v}$ and $T_{\rm d}$ in the axes convention as given by Wilson *et al.* (1980) and many other tables of point groups:

$C_{2\rm v}$	E	C_2	$\sigma_{\rm v}(xz)$	$\sigma_{\rm v}(yz)$	
$\mathrm{A_1}$	1	1	1	1	T_z
$\mathrm{A_2}$	1	1	−1	−1	R_z
$\mathrm{B_1}$	1	−1	1	−1	T_x; R_y
$\mathrm{B_2}$	1	−1	−1	1	T_y; R_x

$T_{\rm d}$	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_{\rm d}$	
$\mathrm{A_1}$	1	1	1	1	1	
$\mathrm{A_2}$	1	1	1	−1	−1	
E	2	−1	2	0	0	
$\mathrm{F_1}$	3	0	−1	1	−1	R_x, R_y, R_z
$\mathrm{F_2}$	3	0	−1	−1	1	T_x, T_y, T_z

The symbols have historical origin from the early days of quantum mechanics. Generally, the symbols A and B are used for non-degenerate species, the symbol E for doubly degenerate species, and the symbol F for triply degenerate species (sometimes also denoted T). Finally, for the rare higher degeneracy one continues following the order of the alphabet (G for four-fold degenerate species, H for five-fold degenerate species etc.). The last column relates the translational (T) and rotational (R) motion to the corresponding irreducible representations.

The point group $C_{2\rm v}$ is an example for the ambiguity of the use of symmetry species symbols $\mathrm{B_1}$ and $\mathrm{B_2}$, depending on the axis convention used. By exchanging the role of the symmetry planes $\sigma_\mathrm{v}(xz)$ and $\sigma_\mathrm{v}(yz)$ through a change of the axis convention, one exchanges the role of B_1 and B_2. Therefore, it is strongly recommended that in all such cases one gives an explicit definition of the axis convention used in the given context, although some general conventions have been proposed in the literature.

3.6.3 Permutation–inversion Groups and Symmetry Operators in Space-fixed Coordinates

Symmetry operators for permutation–inversion goups can be found in Longuet-Higgins (1963), Bunker *et al.* (1997) and Bunker and Jensen (1998):

identity	E; I
permutation	P, p
space-fixed inversion	E^*, (P)
permutation–inversion	$P^*\ (= PE^*)$, p^*

The permutation operation P permutes the labels of identical nuclei. Here, one uses the usual cyclic notation from the group theory of permutations (Hamermesh 1962).

Example

In the NH_3 molecule, if the hydrogen nuclei are labeled 1, 2 and 3, then $P = (123)$ would symbolize the permutation where 1 is replaced by 2, 2 by 3, and 3 by 1.

The inversion operation E^* reverses the sign of all Cartesian particle coordinates in the coordinate system with space-fixed origin or with origin at the molecule-fixed centre of mass, if translation has been separated. It is also called the *parity operator* and then frequently denoted by P, although this cannot be done in parallel with P for permutation, which then should be denoted by lower case p. In field-free space and in the absence of parity violation (Quack and Stohner 2003, 2005), true eigenfunctions of the Hamiltonian are either of positive parity + (unchanged) or of negative parity $-$ (change sign) under E^*. The label may be used to distinguish the two nearly degenerate components formed by Λ-doubling (in a degenerate electronic state) and l-doubling (in a degenerate vibrational state) in linear molecules, or by K-doubling (asymmetry-doubling) in slightly asymmetric tops. For linear molecules, Λ- or l-doubled components may also be distinguished by the labels e or f (Brown *et al.* 1975); for singlet states, these correspond respectively to parity $+$ or $-$ for J even and vice versa for J odd (but see Brown *et al.* (1975)). For linear molecules in degenerate electronic states the Λ-doubled levels may alternatively be labeled $\Pi(\mathrm{A}')$ or $\Pi(\mathrm{A}'')$(or $\Delta(\mathrm{A}')$, $\Delta(\mathrm{A}'')$, etc.) (Alexander *et al.* 1988). Here, the labels A' and A'' describe the symmetry of the electronic wavefunction at high J with respect to reflection in the plane of rotation (but see Alexander *et al.* (1988) for further details). The A' and A'' labels are particularly useful for the correlation of states of molecules involved in reactions or photodissociation.

In relation to permutation–inversion symmetry species, the superscript $+$ or $-$ may be used to designate parity, whereas a letter is used to designate symmetry with respect to the permutation group. One can also use the systematic notation from the theory of the symmetric group (permutation group) S_n (Hamermesh 1962), the permutation–inversion group being denoted by $S_n{}^*$ in this case, if one considers the full permutation group. The species is then given by the partition $P(S_n)$ (Longuet-Higgins 1963, Mills and Quack 2002, Quack 1977). The examples give the species for $S_4{}^*$, where the partition is conventionally given in square brackets [ ]. Conventions with respect to these symbols still vary (Schutte *et al.* 1997a, 1997b, Bunker *et al.* 1997, Hamermesh 1962, Longuet-Higgins 1963, Mills and Quack 2002, Quack 1977, Schnell 2011, Quack 2011).

Examples

A_1^+ totally symmetric species with respect to permutation, positive parity, $[4]^+$.

A_1^- totally symmetric species with respect to permutation, negative parity, $[4]^-$.

E^+ doubly degenerate species with respect to permutation, positive parity, $[2^2]^+$.

E^- doubly degenerate species with respect to permutation, negative parity, $[2^2]^-$.

F_1^+ triply degenerate species with respect to permutation, positive parity, $[2,1^2]^+$.

F_1^- triply degenerate species with respect to permutation, negative parity, $[2,1^2]^-$.

3.7 Other Symbols and Conventions in Optical Spectroscopy

3.7.1 Term Symbols for Atomic States

The electronic states of atoms are labeled by the value of the quantum number L for the state. The value of L is indicated by an upright capital letter: S, P, D, F, G, H, I, K, . . ., are used for $L = 0, 1, 2, 3, 4, 5, 6, 7, \ldots$, respectively. The corresponding lower case letters are used for the orbital angular momentum of a single electron. For a many-electron atom, the electron–spin multiplicity $(2S + 1)$ may be indicated as a left-hand superscript to the letter, and the value of the total angular momentum J as a right-hand subscript. If either L or S is 0, only one value of J is possible, and the subscript is then usually suppressed. Finally, the electron configuration of an atom is indicated by giving the occupation of each one-electron orbital as in the examples below.

Examples

B: $(1\mathrm{s})^2\,(2\mathrm{s})^2\,(2\mathrm{p})^1,\ {}^2\mathrm{P}^{\circ}_{1/2}$
C: $(1\mathrm{s})^2\,(2\mathrm{s})^2\,(2\mathrm{p})^2,\ {}^3\mathrm{P}_0$
N: $(1\mathrm{s})^2\,(2\mathrm{s})^2\,(2\mathrm{p})^3,\ {}^4\mathrm{S}^{\circ}$

A right superscript $^{\mathrm{o}}$ may be used to indicate odd parity (negative parity $-$). Omission of the superscript $^{\mathrm{e}}$ is then to be interpreted as even parity (positive parity $+$). To avoid ambiguities, it can be useful to always designate parity by $+$ or $-$ as a right superscript (i.e., ${}^4\mathrm{S}^{-}_{3/2}$ for N and ${}^3\mathrm{P}^{+}_{0}$ for C).

3.7.2 *Term Symbols for Molecular States*

The electronic states of molecules are labeled by the symmetry species label of the wavefunction in the molecular point group. These should be Latin or Greek upright capital letters. As for atoms, the spin multiplicity $(2S+1)$ may be indicated by a left superscript. For linear molecules, the value of $\Omega\ (=\Lambda+\Sigma)$ may be added as a right subscript (analogous to J for atoms). If the value of Ω is not specified, the term symbol is taken to refer to all component states, and a right subscript r and i may be added to indicate that the components are regular (energy increases with Ω) or inverted (energy decreases with Ω), respectively.

The electronic states of molecules are also given empirical single letter labels as follows. The ground electronic state is labeled X, excited states of the same multiplicity are labeled A, B, C, . . ., in ascending order of energy, and excited states of different multiplicity are labeled with lower case letters a, b, c, ... In polyatomic molecules (but not diatomic molecules), it is customary to add a tilde (e.g., $\widetilde{\mathrm{X}}$) to these empirical labels to prevent possible confusion with the symmetry species label.

Finally, the one-electron orbitals are labeled by the corresponding lower case letters, and the electron configuration is indicated in a manner analogous to that for atoms.

Examples

The ground state of CH is $(1\sigma)^2\,(2\sigma)^2\,(3\sigma)^2\,(1\pi)^1$, $\mathrm{X}\ {}^2\Pi_{\mathrm{r}}$, in which the ${}^2\Pi_{1/2}$ component lies below the ${}^2\Pi_{3/2}$ component, as indicated by the subscript r for regular.

The ground state of OH is $(1\sigma)^2\,(2\sigma)^2\,(3\sigma)^2\,(1\pi)^3$, X ${}^2\Pi_{\mathrm{i}}$, in which the ${}^2\Pi_{3/2}$ component lies below the ${}^2\Pi_{1/2}$ component, as indicated by the subscript i for inverted.

The two lowest electronic states of $\mathrm{CH_2}$ are
$\cdots(2\mathrm{a}_1)^2\,(1\mathrm{b}_2)^2\,(3\mathrm{a}_1)^2$, $\tilde{\mathrm{a}}\ {}^1\mathrm{A}_1$,
$\cdots(2\mathrm{a}_1)^2\,(1\mathrm{b}_2)^2\,(3\mathrm{a}_1)^1\,(1\mathrm{b}_1)^1$, $\widetilde{\mathrm{X}}\ {}^3\mathrm{B}_1$.

The ground state of $\mathrm{C_6H_6}$ (benzene) is $\cdots(\mathrm{a}_{2\mathrm{u}})^2\,(\mathrm{e}_{1\mathrm{g}})^4$, $\widetilde{\mathrm{X}}\,{}^1\mathrm{A}_{1\mathrm{g}}$.

The vibrational states of molecules are usually indicated by giving the vibrational quantum numbers for each normal mode.

Examples

For a bent triatomic molecule
$(0,0,0)$ denotes the ground state,
$(1,0,0)$ denotes the ν_1 state, i.e., $v_1=1$, and
$(1,2,0)$ denotes the $\nu_1+2\nu_2$ state, i.e., $v_1=1$, $v_2=2$, etc.

3.7.3 *Notation for Spectroscopic Transitions*

The upper and lower levels of a spectroscopic transition are indicated by a prime $'$ and a double prime $''$, respectively.

Example

$$h\nu = E' - E''$$

Transitions are generally indicated by giving the excited-state label, followed by the ground-state label, separated by a dash or an arrow to indicate the direction of the transition (emission to the right, absorption to the left).

Examples

B$-$A	indicates a transition between a higher energy state B and a lower energy state A;
B$\rightarrow$A	indicates emission from B to A;
B$\leftarrow$A	indicates absorption from A to B;
A$\rightarrow$B	indicates more generally a transition from the initial state A to final state B in kinetics;
$(0,2,1)\leftarrow(0,0,1)$	labels the $2\nu_2+\nu_3-\nu_3$ hot band in a bent triatomic molecule.

A more compact notation (Brand *et al.* 1983) may be used to label vibronic (or vibrational) transitions in polyatomic molecules with many normal modes, in which each vibration index r is given a superscript v_r' and a subscript v_r'' indicating the upper electronic and the lower electronic state values of the vibrational quantum number. When $v_r'=v_r''=0$, the corresponding index is suppressed.

Examples

1_0^1	denotes the transition (1,0,0)$-$(0,0,0);
$2_0^2\ 3_1^1$	denotes the transition (0,2,1)$-$(0,0,1).

When spoken and when staggering is necessary in print, the superscript should precede the subscript.

Examples

$1^1{}_0$ denotes the transition (1,0,0)−(0,0,0);
$2^2{}_0\ 3^1{}_1$ denotes the transition (0,2,1)−(0,0,1).

To denote transitions within the same electronic state, one may use matrix notation or an arrow.

Example

2_{20} or $2_{2\leftarrow 0}$ denotes a vibrational transition within the electronic ground state from $v_2 = 0$ to $v_2 = 2$.

For rotational transitions, the value of $\Delta J = J' - J''$ is indicated by a letter labeling the branches of a rotational band: $\Delta J = -2, -1, 0, 1$, and 2 are labeled as the O-branch, P-branch, Q-branch, R-branch, and S-branch, respectively. The changes in other quantum numbers (such as K for a symmetric top, or K_a and K_c for an asymmetric top) may be indicated by adding lower case letters as a left superscript according to the same rule.

Example

${}^{\mathrm{p}}\mathrm{Q}$ labels a "p-type Q-branch" in a symmetric top molecule, i.e., $\Delta K = -1$, $\Delta J = 0$.

The value of K in the lower level is indicated as a right subscript, e.g., ${}^{\mathrm{p}}\mathrm{Q}_{K''}$ or ${}^{\mathrm{p}}\mathrm{Q}_2(5)$ indicating the transition from $K'' = 2$ to $K' = 1$, the value of J'' being added in parentheses.

3.7.4 Graphical Presentation of Spectra

The presentation of spectra is among the routine tasks in spectroscopy. It turns out that a number of ambiguities can arise which should be avoided. While a short description on the representation of spectra was included in the section on spectroscopy of the first and second edition of the IUPAC Green Book (Mills *et al.* 1988, 1993), this was removed from the third edition (Cohen *et al.* 2008). Here, we provide some discussion that should be helpful in choosing an appropriate presentation under most circumstances. Generally, some measure of absorption, reflection, emission, or scattering properties of a sample is taken for presentation as ordinate (y-axis), while some quantity related to the frequency of radiation is chosen for presentation as abscissa (x-axis). In absorption spectroscopy, the ordinate shows frequently either transmittance or transmission factor, $T = I/I_0$, or absorptance or absorbance factor, $\alpha = 1 - T$, as quantities of dimension 1 (between 0 and 1 or 0 % and 100 %). I_0 and I are incident and transmitted intensities, corrected for window effects and reflection. Alternatively, absorbance $A_{\mathrm{e}} = \ln(I_0/I)$ and decadic absorbance $A_{10} = \log_{10}(I_0/I) = \mathrm{lg}(I_0/I)$ are given. One can report directly the molecular property absorption cross section, ideally $\sigma = (C\,l)^{-1}\ \ln(I_0/I)$, where C is the number concentration or number density of molecules (e.g., with unit cm^{-3} or m^{-3}) and l is the length of the absorption path (e.g., with unit cm or m). Ambiguities can arise in the choice of A_{e} or A_{10} (both are frequently represented by the symbol A) or in the choice of molecular or molar absorption cross section or extinction coefficient (decadic ϵ_{10} or ϵ or Napierian κ, sometimes represented also as ϵ). Many of these quantities can be represented either as a function of frequency ν, wavenumber $\widetilde{\nu}$, transition energy $E = h\nu$, or wavelength $\lambda = \nu/c_0$, all of these being quite frequently used. There has been some tradition to invert the common axis direction (that is values on the x-axis decreasing to the right). We take the opportunity and advocate to present spectra graphically with increasing values on the abscissa to the right, no matter whether the x-axis is plotted in wavenumber (in cm^{-1}), wavelength (in nm), frequency (in Hz), etc., as the axes display quantities of dimension 1 which are obtained by dividing the physical quantity by the proper unit (see Example in Section 2.1 and Figure 3). However, this seems to be against some recommendations of IUPAC (Sheppard *et al.* 1976a, b, Becker 1978, 1981, Lamola and Wrighton 1984), but it is in agreement with standard mathematical presentations of abscissa (x-axis) and ordinate (y-axis).

As an example, Figure 3 represents a CO absorption line (adapted from Figure 2 in Albert and Quack 2007) in the far-infrared spectral region measured with the Bruker IFS HR Zürich prototype (ZP) 2001 spectrometer at the highest resolution. The decadic absorbance A_{10} is shown as a function of wavenumber $\widetilde{\nu}$ (bottom abscissa) and frequency ν (top abscissa). The full width at half maximum (FWHM)

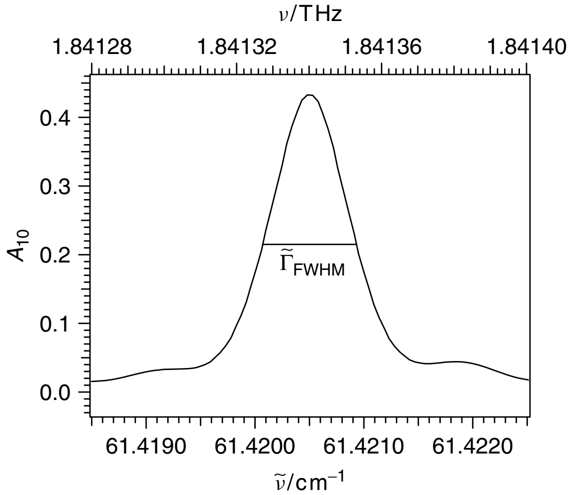

Figure 3 CO absorption line (adapted from Figure 2 in Albert and Quack (2007), by permission.). The decadic absorbance A_{10} is shown as a function of wavenumber $\widetilde{\nu}$ (bottom abscissa) and frequency ν (top abscissa).

($p_{\mathrm{CO}} = 2$ mbar, path length $l = 20$ cm, room temperature) is $\widetilde{\Gamma}_{\mathrm{FWHM}} = 0.000\,83\ \mathrm{cm}^{-1}$, which corresponds to about 24.88 MHz. One should note that $\widetilde{\Gamma}_{\mathrm{FWHM}}$ has not been determined by a thorough statistical analysis but simply by measuring the width of the line at half-height.

A note may be useful on the very common use of the quantity wavenumber with the unit cm^{-1}. The corresponding coherent SI unit would be m^{-1}, but cm^{-1} is acceptable with the SI system as well, with an accepted prefix c (centi, see Section 4.4). As a consequence, however, no further prefixes of cm^{-1} are allowed (i.e., kcm^{-1} is not acceptable for $1000\,\mathrm{cm}^{-1}$). Replacing cm^{-1} by K (Kayser), a one-letter unit, would have allowed further prefixing (kilokayser kK or millikayser mK). However, the use of this unit (found in some older literature) is now deprecated. It has also been suggested to introduce an SI unit Bg (Berg) with 1 Bg = 1 m^{-1} (Quack and Kutzelnigg 1995), which would be fully consistent with the SI and only used in connection with the wavenumber $\widetilde{\nu}$ as customary in spectroscopy. This would facilitate its distinction from the quantity $k = 2\pi/\lambda$ formerly called 'angular wavenumber' or 'circular wavenumber' often in short 'wavenumber' in physics (now magnitude of "angular wave vector or propagation vector", see Section 2.8 in Cohen *et al.* 2008). It appears quite often that different physical quantities have the same dimension or SI unit, for example, 1 Hz = 1 s^{-1}, where Hz is used only in connection with the frequency $\nu = 1/\tau$ and not with the angular frequency $\omega = 2\pi\nu$. The choice of Bg would, thus, resolve a frequently occurring ambiguity (similar to Hz). However, introducing new names for units in the SI is a slow process and Bg has not found acceptance so far. It might furthermore be noted that by definition of the metre in the SI (Section 4.1) the wavenumber $\widetilde{\nu}$ of radiation in vacuo and the frequency ν are connected by a defined constant c_0, the speed of light in vacuo $\nu = c_0\,\widetilde{\nu}$ where it is always understood that wavenumbers $\widetilde{\nu}$ in presentations of spectra refer to wavenumber in vacuo (i.e., corrected for the index of refraction if they are measured in a medium other than vacuum, such as air). As long as the current definition of the metre with a defined speed of light in vacuo, $c_0 = 299\,792\,458\ \mathrm{m\,s^{-1}}$ is maintained, the presentation of spectra in terms of either $\widetilde{\nu}$ or ν is, thus, exactly equivalent to within a defined constant and generally one could recommend the use of frequency ν (with unit Hz, MHz, THz, etc.). Figure 3 gives an example from the literature. It remains true, however, that in the infrared and visible spectral ranges, the use of the quantity wavenumber, $\widetilde{\nu}$, with the unit cm^{-1} is widespread; in fact, it seems to be the most frequently used unit in all of the optical domain of the spectrum (far-infrared to ultraviolet).

3.8 Electromagnetic Radiation

We refer to the corresponding tables in Cohen *et al.* (2008) which take spectroscopic usage into account as well as the practice in the field of laser physics. Terms used in photochemistry (Verhoeven 1996) have been considered as well, but definitions still vary. Terms used in high-energy ionizing electromagnetic radiation, radiation chemistry, radiochemistry, and nuclear chemistry are not included or discussed here.

Name	Symbol	Definition	SI unit	Notes
wavelength	λ		m	
speed of light				
in vacuum	c_0	$c_0 = 299\ 792\ 458\ \mathrm{m\ s^{-1}}$	$\mathrm{m\ s^{-1}}$	1
in a medium	c	$c = c_0/n$	$\mathrm{m\ s^{-1}}$	1
wavenumber in vacuum	$\widetilde{\nu}$	$\widetilde{\nu} = \nu/c_0 = 1/\lambda$	$\mathrm{m^{-1}}$	2
wavenumber (in a medium)	σ	$\sigma = 1/\lambda$	$\mathrm{m^{-1}}$	
frequency	ν	$\nu = c/\lambda$	Hz	
angular frequency, pulsatance	ω	$\omega = 2\pi\nu$	$\mathrm{s^{-1}}$, $\mathrm{rad\ s^{-1}}$	
refractive index	n	$n = c_0/c$	1	
Planck constant	h		J s	
Planck constant divided by 2π	$\hbar$	$\hbar = h/2\pi$	J s	
radiant energy	Q, W		J	3
radiant energy density	ρ, w	$\rho = \mathrm{d}Q/\mathrm{d}V$	$\mathrm{J\ m^{-3}}$	3
spectral radiant energy density				3
in terms of frequency	ρ_ν, w_ν	$\rho_\nu = \mathrm{d}\rho/\mathrm{d}\nu$	$\mathrm{J\ m^{-3}\ Hz^{-1}}$	
in terms of wavenumber	$\rho_{\widetilde{\nu}}, w_{\widetilde{\nu}}$	$\rho_{\widetilde{\nu}} = \mathrm{d}\rho/\mathrm{d}\widetilde{\nu}$	$\mathrm{J\ m^{-2}}$	
in terms of wavelength	ρ_λ, w_λ	$\rho_\lambda = \mathrm{d}\rho/\mathrm{d}\lambda$	$\mathrm{J\ m^{-4}}$	

Name	Symbol	Definition	SI unit	Notes
radiant power (radiant energy per time)	P, Φ	$P = \mathrm{d}Q/\mathrm{d}t$	W	3
radiant intensity	I_e	$I_\mathrm{e} = \mathrm{d}P/\mathrm{d}\Omega$	W sr^{-1}	3, 4
radiant exitance	M	$M = \mathrm{d}P/\mathrm{d}A_\mathrm{source}$	W m^{-2}	3, 4
radiance	L	$I_\mathrm{e} = \int L \cos\Theta \, \mathrm{d}A_\mathrm{source}$	W sr^{-1} m^{-2}	3, 4
intensity, irradiance	I, E	$I = \mathrm{d}P/\mathrm{d}A$	W m^{-2}	3, 5
spectral intensity, spectral irradiance	$I_{\tilde{\nu}}, E_{\tilde{\nu}}$	$I_{\tilde{\nu}} = \mathrm{d}I/\mathrm{d}\tilde{\nu}$	W m^{-1}	6
fluence	$F, (H)$	$F = \int I \mathrm{d}t = \int (\mathrm{d}P/\mathrm{d}A)\mathrm{d}t$	J m^{-2}	7
Einstein coefficient,				
spontaneous emission	A_{ij}	$\mathrm{d}N_j/\mathrm{d}t = -\sum_i A_{ij} N_j$	s^{-1}	8, 9
stimulated or induced				
emission	B_{ij}	$\mathrm{d}N_j/\mathrm{d}t = -\sum_i \rho_{\tilde{\nu}}(\tilde{\nu}_{ij}) B_{ij} N_j$	s kg^{-1}	
absorption	B_{ji}	$\mathrm{d}N_i/\mathrm{d}t = -\sum_j \rho_{\tilde{\nu}}(\tilde{\nu}_{ij}) B_{ji} N_i$	s kg^{-1}	

(1) When there is no risk of ambiguity, the subscript denoting vacuum is often omitted. n denotes the refraction index of the medium.

(2) The unit cm^{-1} is widely used for the quantity wavenumber in vacuum.

(3) The symbols for the quantities such as *radiant energy* and *intensity* are also used for the corresponding quantities concerning visible radiation, i.e., luminous quantities and photon quantities. Subscripts e for energetic, v for visible, and p for photon may be added whenever confusion between these quantities might otherwise occur. The units used for luminous quantities are derived from the base unit candela (cd) (Section 4.1).

Examples

radiant intensity	I_e, $I_\mathrm{e} = \mathrm{d}P/\mathrm{d}\Omega$	SI unit: W sr^{-1}
luminous intensity	I_v	SI unit: cd
photon intensity	I_p	SI unit: s^{-1} sr^{-1}

The radiant intensity I_e should be distinguished from the plain intensity or irradiance I (see Note 5). Additional subscripts to distinguish absorbed (abs), transmitted (tr), and reflected (refl) quantities may be added, if necessary.

(4) The radiant intensity is the radiant power per solid angle in the direction of the point from which the source is being observed. The radiant exitance is the total emitted radiant power per area A_source of the radiation source, for all wavelengths. The radiance is the radiant intensity per area of radiation source; Θ is the angle between the normal to the area element and the direction of observation as seen from the source.

(5) The intensity or irradiance is the radiation power per area that is received at a surface. Intensity, symbol I, is usually used in discussions involving collimated beams of light, as in applications of the Beer–Lambert law for spectrometric analysis. Intensity of electromagnetic radiation can also be defined as the modulus of the Poynting vector (Section 3.1). In photochemistry, the term *intensity* is sometimes used as an alias for radiant intensity and must not be understood as an irradiance, for which the symbol E is preferred (Verhoeven 1996).

(6) Spectral quantities may be defined with respect to frequency ν, wavelength λ, or wavenumber $\tilde{\nu}$; see the entry for spectral radiant energy density in this table.

(7) Fluence is used in photochemistry to specify the energy per area delivered in a given time interval (for instance by a laser pulse); fluence is the time integral of the fluence rate. Sometimes distinction must be made between irradiance and fluence rate (Verhoeven 1996); fluence rate reduces to irradiance for a light beam incident from a single direction perpendicularly to the surface. The time integral of irradiance is called *radiant exposure*.

(8) The indices i and j refer to individual states; $E_j > E_i$, $E_j - E_i = hc\tilde{\nu}_{ij}$, and $B_{ji} = B_{ij}$ in the defining equations. The coefficients B are defined here using energy density $\rho_{\tilde{\nu}}$ in terms of wavenumber; they may alternatively be defined using energy density in terms of frequency ρ_ν, in which case B has SI units m kg^{-1}, and $B_\nu = c_0 B_{\tilde{\nu}}$ where B_ν is defined using frequency and $B_{\tilde{\nu}}$ using wavenumber. The defining equations refer to the *partial* contributions to the rate of change.

(9) The relation between the Einstein coefficients A and $B_{\tilde{\nu}}$ is $A = 8\pi h c_0 \tilde{\nu}^3 B_{\tilde{\nu}}$. The Einstein stimulated absorption or emission coefficient B may also be related to the transition moment between the states i and j; for an electric dipole transition, the relation is

$$B_{\tilde{\nu},ij} = \frac{8\pi^3}{3h^2 c_0 \, (4\pi\varepsilon_0)} \sum_\rho |\langle i|\mu_\rho|j\rangle|^2$$

in which the sum over ρ runs over the three space-fixed Cartesian axes, and μ_ρ is a space-fixed component of the dipole moment operator. Again, these equations are based on a wavenumber definition of the Einstein coefficient B (i.e., $B_{\tilde{\nu}}$ rather than B_ν).

Name	Symbol	Definition	SI unit	Notes
emissivity, emittance	ε	$\varepsilon = M/M_{\mathrm{bb}}$	1	10
Stefan–Boltzmann constant	σ	$M_{\mathrm{bb}} = \sigma T^4$	W $\mathrm{m^{-2}\ K^{-4}}$	10
étendue (throughput, light gathering power)	E, (e)	$E = A\Omega = P/L$	$\mathrm{m^2}$ sr	11
resolution	$\delta\tilde{\nu}$		$\mathrm{m^{-1}}$	2, 12, 13
resolving power	R	$R = \tilde{\nu}/\delta\tilde{\nu}$	1	13
free spectral range	$\Delta\tilde{\nu}$	$\Delta\tilde{\nu} = 1/2l$	$\mathrm{m^{-1}}$	2, 14
finesse	f	$f = \Delta\tilde{\nu}/\delta\tilde{\nu}$	1	14
quality factor	Q	$Q = 2\pi\nu\dfrac{W}{-\mathrm{d}W/\mathrm{d}t}$	1	14, 15
1st radiation constant	c_1	$c_1 = 2\pi hc_0^2$	W $\mathrm{m^2}$	
2nd radiation constant	c_2	$c_2 = hc_0/k_{\mathrm{B}}$	K m	16
transmittance, transmission factor	τ, T	$\tau = P_{\mathrm{tr}}/P_0$	1	17, 18
absorptance, absorption factor	α	$\alpha = P_{\mathrm{abs}}/P_0$	1	17, 18
reflectance, reflection factor	ρ, R	$\rho = P_{\mathrm{refl}}/P_0$	1	17, 18
(decadic) absorbance	$A_{10},\ A$	$A_{10} = -\lg(1-\alpha_{\mathrm{i}})$	1	17–20
napierian absorbance	$A_{\mathrm{e}}, B, (A)$	$A_{\mathrm{e}} = -\ln(1-\alpha_{\mathrm{i}})$	1	17–20
absorption coefficient,				
(linear) decadic	a, K	$a = A_{10}/l$	$\mathrm{m^{-1}}$	18, 21
(linear) napierian	α	$\alpha = A_{\mathrm{e}}/l$	$\mathrm{m^{-1}}$	18, 21

(10) The emittance of a sample is the ratio of the radiant exitance, M, emitted by the sample to the radiant exitance, M_{bb}, emitted by a black body at the same temperature. See Chapter 6 for the value of the Stefan–Boltzmann constant.

(11) Étendue is a characteristic of an optical instrument. It is a measure of the light gathering power, i.e., the power transmitted per radiance of the source. A is the area of the source or image stop; Ω is the solid angle accepted from each point of the source by the aperture stop.

(12) The precise definition of resolution depends on the lineshape, but usually resolution is taken as the full line width at half maximum (FWHM) intensity on a wavenumber, $\delta\tilde{\nu}$, or frequency, $\delta\nu$, scale. Frequently the use of resolving power, of dimension 1, is preferable.

(13) This quantity characterizes the performance of a spectrometer or the degree to which a spectral line (or a laser beam) is monochromatic. It may also be defined using frequency ν or wavelength λ.

(14) These quantities characterize a Fabry–Perot cavity, or a laser cavity. l is the cavity spacing and $2l$ is the round-trip path length. The free spectral range is the wavenumber interval between successive longitudinal cavity modes.

(15) W is the energy stored in the cavity and $-\mathrm{d}W/\mathrm{d}t$ is the rate of decay of stored energy. Q is also related to the linewidth of a single cavity mode: $Q = \nu/\delta\nu = \tilde{\nu}/\delta\tilde{\nu}$. Thus, high Q cavities give narrow linewidths.

(16) k_{B} is the Boltzmann constant (see Chapter 6).

(17) If scattering and luminescence can be neglected, $\tau + \alpha + \rho = 1$. In optical spectroscopy, internal properties (denoted by subscript i) are defined to exclude surface effects and effects of the cuvette such as reflection losses, so that $\tau_{\mathrm{i}} + \alpha_{\mathrm{i}} = 1$, if scattering and luminescence can be neglected. This leads to the customary form of the Beer–Lambert law, $P_{\mathrm{tr}}/P_0 = I_{\mathrm{tr}}/I_0 = \tau_{\mathrm{i}} = 1 - \alpha_{\mathrm{i}} = \exp(-\kappa cl)$. Hence, $A_{\mathrm{e}} = -\ln(\tau_{\mathrm{i}})$, $A_{10} = -\lg(\tau_{\mathrm{i}})$.

(18) In spectroscopy, all of these quantities are commonly taken to be defined in terms of the spectral intensity, $I_{\tilde{\nu}}(\tilde{\nu})$; hence, they are all regarded as functions of wavenumber $\tilde{\nu}$ (or frequency ν) across the spectrum. Thus, for example, the absorption coefficient $\alpha(\tilde{\nu})$ as a function of wavenumber $\tilde{\nu}$ defines the absorption spectrum of the sample; similarly, $T(\tilde{\nu})$ defines the transmittance spectrum. Spectroscopists use $I(\tilde{\nu})$ instead of $I_{\tilde{\nu}}(\tilde{\nu})$.

(19) The definitions given here relate the absorbance A_{10} or A_{e} to the *internal* absorptance α_{i} (see Note 17). However, the subscript i on the absorptance α is often omitted. Experimental data must include corrections for reflections, scattering, and luminescence, if the absorbance is to have an absolute meaning. In practice, the absorbance is measured as the logarithm of the ratio of the light transmitted through a reference cell (with solvent only) to that transmitted through a sample cell.

(20) In Sheppard *et al.* (1985), the symbol A is used for decadic absorbance and B for napierian absorbance.

(21) l is the absorbing path length and c is the amount (of substance) concentration.

Name	Symbol	Definition	SI unit	Notes
molar (decadic)	ε	$\varepsilon = a/c = A_{10}/cl$	$\mathrm{m^2\ mol^{-1}}$	18, 21, 22
molar napierian	κ	$\kappa = \alpha/c = A_\mathrm{e}/cl$	$\mathrm{m^2\ mol^{-1}}$	18, 21, 22
net absorption cross section	σ_net	$\sigma_\mathrm{net} = \kappa/N_\mathrm{A}$	$\mathrm{m^2}$	23
absorption coefficient				
integrated over $\tilde{\nu}$	$A, \overline{A}$	$A = \int \kappa(\tilde{\nu})\ \mathrm{d}\tilde{\nu}$	$\mathrm{m\ mol^{-1}}$	23, 24
	S	$S = A/N_\mathrm{A}$	m	23, 24
	$\overline{S}$	$\overline{S} = (1/pl)\int \ln(I_0/I)\ \mathrm{d}\tilde{\nu}$	$\mathrm{Pa^{-1}\ m^{-2}}$	23–25
integrated over $\ln\tilde{\nu}$	Γ	$\Gamma = \int \kappa(\tilde{\nu})\tilde{\nu}^{-1}\ \mathrm{d}\tilde{\nu}$	$\mathrm{m^2\ mol^{-1}}$	23, 24
integrated net absorption cross section	G_net	$G_\mathrm{net} = \int \sigma_\mathrm{net}(\tilde{\nu})\tilde{\nu}^{-1}\ \mathrm{d}\tilde{\nu}$	$\mathrm{m^2}$	23, 24
absorption index, imaginary refractive index	k	$k = \alpha/4\pi\tilde{\nu}$	1	26
complex refractive index	$\hat{n}$	$\hat{n} = n + \mathrm{i}k$	1	
molar refraction, molar refractivity	R	$R = \left(\dfrac{n^2-1}{n^2+2}\right)V_\mathrm{m}$	$\mathrm{m^3\ mol^{-1}}$	
angle of optical rotation	α		1, rad	27
specific optical rotatory power	$[\alpha]_\lambda{}^\theta$	$[\alpha]_\lambda{}^\theta = \alpha/\gamma l$	$\mathrm{rad\ m^2\ kg^{-1}}$	27
molar optical rotatory power	α_m	$\alpha_\mathrm{m} = \alpha/cl$	$\mathrm{rad\ m^2\ mol^{-1}}$	27

(22) The molar decadic absorption coefficient ε is sometimes called the *extinction coefficient* in the published literature. Unfortunately, numerical values of the "extinction coefficient" are often quoted without specifying units; the absence of units usually means that the units are $\mathrm{mol^{-1}\ dm^3\ cm^{-1}}$ (see also Lamola and Wrighton 1984). The word *extinction* should properly be reserved for the sum of the effects of absorption, scattering, and luminescence.

(23) Note that these quantities give the net absorption coefficient κ, the net absorption cross section σ_net, and the net values of A, S, $\overline{S}$, Γ, and G_net, in the sense that they are the sums of effects due to absorption and induced emission (see the discussion in Section 3.9).

(24) The definite integral defining these quantities may be specified by the limits of integration in parentheses, e.g., $G(\tilde{\nu}_1, \tilde{\nu}_2)$. In general, the integration is understood to be taken over an absorption line or an absorption band. A, $\overline{S}$, and Γ are measures of the strength of the band in terms of amount concentration; $G_\mathrm{net} = \Gamma/N_\mathrm{A}$ and $S = A/N_\mathrm{A}$ are corresponding molecular quantities. For a single spectral line, the relation of these quantities to the Einstein transition probabilities is discussed in Section 3.9. The symbol $\overline{A}$ may be used for the integrated absorption coefficient A when there is a possibility of confusion with the Einstein spontaneous emission coefficient A_{ij}. The integrated absorption coefficient of an electronic transition is often expressed in terms of the oscillator strength or "f-value", which is dimensionless, or in terms of the Einstein transition probability A_{ij} between the states involved, with SI unit $\mathrm{s^{-1}}$. Whereas A_{ij} has a simple and universally accepted meaning (see Note 9, Section 3.8), there are differing uses of f. A common practical conversion is given by the following equation:

$$f_{ij} = [(4\pi\varepsilon_0)\, m_\mathrm{e} c_0/8\pi^2 e^2]\lambda^2 A_{ij} \qquad \text{or} \qquad f_{ij} \approx \left(1.4992 \times 10^{-14}\right)(A_{ij}/\mathrm{s^{-1}})\,(\lambda/\mathrm{nm})^2$$

where λ is the transition wavelength, and i and j refer to individual states. For strongly allowed electronic transitions, f is of order unity.

(25) The quantity $\overline{S}$ is only used for gases; it is defined in a manner similar to A, except that the partial pressure p of the gas replaces the concentration c. At low pressures $p_i \approx c_i RT$, so that $\overline{S}$ and A are related by the equation $\overline{S} \approx A/RT$. Thus, if $\overline{S}$ is used to report line or band intensities and the temperature should be specified. I_0 is the incident, I the transmitted intensity; thus, $\ln(I_0/I) = -\ln(I/I_0) = -\ln(1 - P_\mathrm{abs}/P_0) = A_\mathrm{e}$ (see also Section 3.8, Notes 17 and 19).

(26) α in the definition is the napierian absorption coefficient.

(27) The sign convention for the angle of optical rotation is as follows: α is positive if the plane of polarization is rotated clockwise as viewed looking toward the light source. If the rotation is anticlockwise, then α is negative. The optical rotation due to a solute in solution may be specified by a statement of the type

$$\alpha(589.3\ \mathrm{nm},\ 20\ {}^\circ\mathrm{C},\ \text{sucrose},\ 10\ \mathrm{g\ dm^{-3}}\ \text{in}\ \mathrm{H_2O},\ 10\,\mathrm{cm}\ \text{path}) = +0.6647^\circ$$

The same information may be conveyed by quoting either the specific optical rotatory power $\alpha/\gamma l$ or the molar optical rotatory power α/cl, where γ is the mass concentration, c is the amount (of substance) concentration, and l is the path length. Most tabulations give the specific optical rotatory power, denoted $[\alpha]_\lambda{}^\theta$. The wavelength of light used λ (frequently the sodium D line) and the Celsius temperature θ are conventionally written as a subscript and superscript to the specific rotatory power $[\alpha]$. For pure liquids and solids, $[\alpha]_\lambda{}^\theta$ is similarly defined as $[\alpha]_\lambda{}^\theta = \alpha/\rho l$, where ρ is the mass density.

Specific optical rotatory powers are customarily called *specific rotations* and are unfortunately usually quoted without units. The absence of units may usually be taken to mean that the units are $^\circ\ \mathrm{cm^3\ g^{-1}\ dm^{-1}}$ for pure liquids and solutions, or $^\circ\ \mathrm{cm^3\ g^{-1}\ mm^{-1}}$ for solids, where $^\circ$ is used as a symbol for degrees of plane angle.

3.9 Quantities and Symbols Concerned with the Measurement of Absorption Intensity

"Absorption intensity" is in itself not well defined as there are many different definitions for quantities related to the strength of absorption. In most experiments designed to measure the intensity of spectral absorption, the measurement gives the net absorption due to the effects of absorption from the lower energy level m to the upper energy level n, minus induced emission from n to m. The populations depend on the temperature and so does the measured net absorption. This comment applies to all the quantities defined in the table to measure absorption intensity, although for transitions where $hc_0\tilde{\nu} \gg kT$ the temperature dependence is small and for $\tilde{\nu} > 1000\,\mathrm{cm}^{-1}$ at ordinary temperatures induced emission can generally be neglected.

In a more fundamental approach, one defines the cross section $\sigma_{ji}(\tilde{\nu})$ for an induced radiative transition from the state i to the state j (in either absorption or emission). For an ideal absorption experiment with only the lower state i populated, the integrated absorption cross section for the transition $j \leftarrow i$ is given by

$$G_{ji} = \int \sigma_{ji}(\tilde{\nu})\tilde{\nu}^{-1}\mathrm{d}\tilde{\nu} = \int \sigma_{ji}(\nu)\,\nu^{-1}\mathrm{d}\nu$$

If the upper and lower energy levels are degenerate, the observed line strength is given by summing over transitions between all states i in the lower energy level m and all states j in the upper energy level n, multiplying each term by the fractional population p_i in the appropriate initial state. Neglecting induced emission, this gives

$$G_{\mathrm{net}}(n \leftarrow m) = \sum_{i,j} p_i G_{ji}$$

If induced emission is significant, then the net integrated cross section becomes

$$\begin{aligned} G_{\mathrm{net}}(n \leftarrow m) &= \sum_{i,j} \left(p_i - p_j\right) G_{ji} \\ &= \left(\frac{p_m}{d_m} - \frac{p_n}{d_n}\right) \sum_{i,j} G_{ji} \end{aligned}$$

Here, p_i and p_j denote the fractional populations of states i and j ($p_i = \exp\{-E_i/kT\}/q$ in thermal equilibrium, where q is the partition function); p_m and p_n denote the corresponding fractional populations of the energy levels; and d_m and d_n represent the degeneracies ($p_i = p_m/d_m$, etc.). The absorption intensity G_{ji} and the Einstein coefficients A_{ij} and B_{ji} are fundamental measures of the line strength between the individual states i and j; they are related to each other by the general equations

$$G_{ji} = hB_{\tilde{\nu},ji} = \left(\frac{h}{c_0}\right) B_{\nu,ji} = \frac{A_{ij}}{(8\pi c_0 \tilde{\nu}^3)}$$

Finally, for an electric dipole transition these quantities are related to the square of the transition moment by the equation

$$G_{ji} = hB_{\tilde{\nu},ji} = \frac{A_{ij}}{(8\pi c_0 \tilde{\nu}^3)} = \frac{8\pi^3}{3hc_0(4\pi\varepsilon_0)} \left|M_{ji}\right|^2$$

where the transition moment M_{ji} is given by

$$\left|M_{ji}\right|^2 = \sum_{\rho} \left|\langle i \left|\mu_\rho\right| j\rangle\right|^2$$

Here, the sum is over the three space-fixed Cartesian axes and μ_ρ is a space-fixed component of the electric dipole moment. Substituting numerical values for the constants the relation between G_{ji} and M_{ji} may be expressed in a practical representation as

$$\left(\frac{G_{ji}}{\mathrm{pm}^2}\right) \approx 41.6238 \left|\frac{M_{ji}}{\mathrm{D}}\right|^2$$

where 1 D $\approx 3.335\ 641 \times 10^{-30}$ C m (D is the symbol of the debye) (Quack 1990).

Net integrated absorption band intensities are usually characterized by one of the quantities A, S, $\overline{S}$, Γ, or G_{net}. The SI unit and commonly used units of those quantities are as in the following table. Numerical transformation coefficients in commonly used units, from A, S, $\overline{S}$,, and Γ to G_{net}, are also given in the following page table.

The relation between these quantities is given by the (approximate) equations:

$$G_{\mathrm{net}} = \Gamma/N_{\mathrm{A}} \approx A/(\tilde{\nu}_0 N_{\mathrm{A}}) \approx S/\tilde{\nu}_0 \approx \overline{S}\,(kT/\tilde{\nu}_0)$$

However, only the first equality is exact. The relation to A, $\overline{S}$, and S involves dividing by the band centre wavenumber $\tilde{\nu}_0$ for a band, to correct for the fact that A, $\overline{S}$, and S are obtained by integrating over wavenumber rather than integrating over the logarithm of wavenumber used for G_{net} and Γ. This correction is only approximate for a band (although negligible error is involved for single-line intensities in gases). The relation to $\overline{S}$ involves the assumption that the gas is ideal (which is approximately true at low pressures), and also involves the temperature. Thus, the quantities Γ and G_{net} are most simply related to more fundamental quantities such as the Einstein transition probabilities and the transition moment and are the preferred quantities for reporting integrated line or band intensities.

Quantity	SI unit	Common unit	Transformation coefficient
$A, \overline{A}$	$\mathrm{m\ mol^{-1}}$	$\mathrm{km\ mol^{-1}}$	$\left(G/\mathrm{pm}^2\right) = 16.605\ 40 \dfrac{A/(\mathrm{km\ mol^{-1}})}{\widetilde{\nu}_0/\mathrm{cm^{-1}}}$
$\overline{S}$	$\mathrm{Pa^{-1}\ m^{-2}}$	$\mathrm{atm^{-1}\ cm^{-2}}$	$\left(G/\mathrm{pm}^2\right) = 1.362\ 603 \times 10^{-2}\ \dfrac{\left(\overline{S}/\mathrm{atm^{-1}\ cm^{-2}}\right)(T/\mathrm{K})}{\left(\widetilde{\nu}_0/\mathrm{cm^{-1}}\right)}$
S	m	cm	$\left(G/\mathrm{pm}^2\right) = 10^{20}\ \dfrac{(S/\mathrm{cm})}{\widetilde{\nu}_0/\mathrm{cm^{-1}}}$
Γ	$\mathrm{m^2\ mol^{-1}}$	$\mathrm{cm^2\ mol^{-1}}$	$\left(G/\mathrm{pm}^2\right) = 1.660\ 540 \times 10^{-4}\left(\Gamma/\mathrm{cm^2\ mol^{-1}}\right)$
G	$\mathrm{m^2}$	$\mathrm{pm^2}$	

The situation is further complicated by some authors using the symbol S for any of the above quantities, particularly for any of the quantities here denoted A, S, and $\overline{S}$. It is, therefore, particularly important to define quantities and symbols used in reporting integrated intensities.

For transitions between individual states, any of the more fundamental quantities G_{ji}, $B_{\widetilde{\nu},ji}$, A_{ij}, or $\left|M_{ji}\right|$ may be used; the relations are as given above and are exact. The integrated absorption coefficient A should not be confused with the Einstein coefficient A_{ij} (nor with absorbance, for which the symbol A is also used). Where such confusion might arise, we recommend writing $\overline{A}$ for the band intensity expressed as an integrated absorption coefficient over wavenumber.

Quantities concerned with spectral absorption intensity and relations among these quantities are discussed in Quack (1990), Maki and Wells (1991), Pugh and Rao (1978), Smith *et al.* (1985), and a list of published measurements of line intensities and band intensities for gas phase infrared spectra may be found in Maki and Wells (1991), Pugh and Rao (1978), Smith *et al.* (1985). For relations between spectroscopic absorption intensities and kinetic radiative transition rates, see also Quack (1998b, 1995).

3.10 Conventions for Absorption Intensities in Condensed Phases

Provided transmission measurements are accurately corrected for reflection and other losses, the absorbance, absorption coefficient, and integrated absorption coefficient, A, that are described above may be used for condensed phases. The corrections typically used are adequate for weak and medium bands in neat liquids and solids and for bands of solutes in dilute solution. To make the corrections accurately for strong bands in neat liquids and solids, it is necessary to determine the real and imaginary refractive indices n and k, of the sample throughout the measured spectral range. Then, the resulting n and k themselves provide a complete description of the absorption intensity in the condensed phase. For liquids, this procedure requires knowledge of n and k of the cell windows. Reflection spectra are also processed to yield n and k. For nonisotropic solids, all intensity properties must be defined with respect to specific crystal axes. If the n and k spectra are known, spectra of any optical property or measured quantity of the sample may be obtained from them. Physicists prefer to use the complex relative permittivity (Section 3.1), $\widehat{\varepsilon}_\mathrm{r} = \varepsilon_\mathrm{r}{}' + \mathrm{i}\,\varepsilon_\mathrm{r}{}'' = \mathrm{Re}\,\widehat{\varepsilon}_\mathrm{r} + \mathrm{i}\,\mathrm{Im}\,\widehat{\varepsilon}_\mathrm{r}$ instead of the complex refractive index $\widehat{n}$. $\varepsilon_\mathrm{r}{}' = \mathrm{Re}\,\widehat{\varepsilon}_\mathrm{r}$ denotes the real part and $\varepsilon_\mathrm{r}{}'' = \mathrm{Im}\,\widehat{\varepsilon}_\mathrm{r}$ the imaginary part of $\widehat{\varepsilon}_\mathrm{r}$, respectively. They are related through $\widehat{\varepsilon}_\mathrm{r} = \widehat{n}^2$, so that $\varepsilon_\mathrm{r}{}' = n^2 - k^2$ and $\varepsilon_\mathrm{r}{}'' = 2nk$.

The refractive indices and relative permittivities are properties of the bulk phase. To obtain information about the molecules in the liquid free from dielectric effects of the bulk, the local field that acts on the molecules, $\boldsymbol{E}_\mathrm{loc}$, must be determined as a function of the applied field $\boldsymbol{E}$. A simple relation is the Lorentz local field, $\boldsymbol{E}_\mathrm{loc} = \boldsymbol{E} + \boldsymbol{P}/3\varepsilon_0$, where $\boldsymbol{P}$ is the dielectric polarization. This local field is based on the assumption that long-range interactions are isotropic, so it is realistic only for liquids and isotropic solids.

The use of this local field gives the Lorentz–Lorenz formula (this relation is usually called the Clausius–Mossotti formula when applied to static fields) generalized to treat absorbing materials at any wavenumber:

$$\frac{\widehat{\varepsilon}_\mathrm{r}(\widetilde{\nu}) - 1}{\widehat{\varepsilon}_\mathrm{r}(\widetilde{\nu}) + 2} = \frac{1}{3\varepsilon_0 V_\mathrm{m}}\widehat{\alpha}_\mathrm{m}(\widetilde{\nu})$$

Here, V_m is the molar volume and $\widehat{\alpha}_\mathrm{m}$ is the complex molar polarizability (see Section 3.1, Note 7). The imaginary part $\alpha_\mathrm{m}{}''$ of the complex molar polarizability describes the absorption by molecules in the liquid, corrected for the long-range isotropic dielectric effects but influenced by the anisotropic environment formed by the first few nearest neighbor molecules. The real part $\alpha_\mathrm{m}{}'$ is the molar polarizability (Sections 3.1 and 3.3) in the limit of infinite frequency.

The integrated absorption coefficient of a molecular absorption band in the condensed phase is described by Bertie *et al.* (1993), Bertie and Dale Keefe (1994)[f]

$$C_j = \frac{1}{4\pi\varepsilon_0}\int_{\text{band } j} \widetilde{\nu}\alpha_{\text{m}}''(\widetilde{\nu})\text{d}\widetilde{\nu}$$

Theoretical analysis usually assumes that the measured band includes the transition $j \leftarrow i$ with band centre wavenumber $\widetilde{\nu}_0$ and all of its hot-band transitions. Then,

$$C_j = \frac{N_{\text{A}}\pi}{3hc_0(4\pi\varepsilon_0)}\widetilde{\nu}_0 f(T)|M_{ji}|^2$$

where $f(T)|M_{ji}|^2$ is the population-weighted sum over all contributing transitions of the wavenumber times the square of the electric dipole moment of the transition (f is, in general, a temperature-dependent function, which includes effects from the inhomogeneous band structure). The traditional relation between the gas and liquid phase values of the absorption coefficient of a given band j is the Polo–Wilson equation (Polo and Wilson 1955):

$$A_{\text{liq}} = \frac{(\overline{n}^2+2)^2}{9\overline{n}}A_{\text{gas}}$$

where $\overline{n}$ is the estimated average value of n through the absorption band. This relation is valid under the following conditions:

1. bands are sufficiently weak, i.e., $2nk \ll n^2 - k^2$;
2. the double harmonic approximation yields a satisfactory theoretical approximation of the band structure; in this case, the function f is nearly temperature independent and the gas and liquid phase values of f are equal;
3. $\widetilde{\nu}_0|M_{ji}|^2$ are identical in the gas and liquid phases.

A more recent and more general relation that requires only the second and the third of these conditions is $A_{\text{gas}} = 8\pi^2 C_j$. It follows that for bands that meet all three of the conditions

$$A_{\text{liq}} = 8\pi^2 C_j\frac{(\overline{n}^2+2)^2}{9\overline{n}}$$

This relation shows that, while the refractive index n is automatically incorporated in the integrated absorption coefficient C_j for a liquid, the traditional absorption coefficient A needs to be further corrected for permittivity or refraction.

4 SI UNITS AND ATOMIC UNITS USED IN SPECTROSCOPY

The International System of Units (SI) was adopted by the 11th General Conference of Weights and Measures (CGPM) in 1960 (BIPM 2006). It is a coherent system of units built from seven *SI base units*, one for each of the seven dimensionally independent base quantities (Section 2.2); they are as follows: metre, kilogram, second, ampere, kelvin, mole, and candela for the base quantities length, mass, time, electric current, thermodynamic temperature, amount of substance, and luminous intensity, respectively. The definitions of the SI base units are given in Section 4.1. The *SI-derived units* are expressed as products of powers of the base units, analogous to the corresponding relations between physical quantities. If no numerical factors other than 1 are used in the defining equations for derived units, then the derived units defined in this way are called *coherent derived units*. The SI base units (including the kilogram) and the derived units without any multiple or submultiple prefixes form a coherent set of units and are called the *coherent SI units*.

In the International System of Units, there is only one coherent SI unit for each physical quantity. This is either the appropriate SI base unit itself (Section 4.1) or the appropriate SI-derived unit (Sections 4.2 and 4.3). However, any of the approved decimal prefixes, called *SI prefixes*, may be used to construct decimal multiples or submultiples of SI units (Section 4.4). The SI units and the decimal multiples and submultiples constructed with the SI prefixes are called the *complete set of SI units*, simply the *SI units*, or the *units of the SI.*

It is recommended that only units of the SI be used in science and technology (with SI prefixes where appropriate). Where there are special reasons for making an exception to this rule, it is recommended always to define the units in terms of SI units.

4.1 Definitions of the SI Base Units

The following definitions of the seven SI base units are adopted by the General Conference on Weights and Measures (CGPM) (BIPM 2006).

metre (symbol: m)

The metre is the length of path traveled by light in vacuum during a time interval of 1/299 792 458 of a second.
(17th CGPM, 1983)

kilogram (symbol: kg)

The kilogram is the unit of mass; it is equal to the mass of the international prototype of the kilogram.
(3rd CGPM, 1901)[g]

second (symbol: s)

The second is the duration of 9 192 631 770 periods of the radiation corresponding to the transition between the two hyperfine levels of the ground state of the caesium

133 atom.
(13th CGPM, 1967)
This definition refers to a caesium atom at rest at a temperature of 0 K.
(CIPM, 1997)

In this definition, it is understood that the Cs atom at a temperature of $T = 0$ K is unperturbed by black-body radiation. The frequency of primary frequency standards should, therefore, be corrected for the frequency shift due to the ambient radiation, as stated by the Consultative Committee for Time and Frequency (CCTF, 1999).

ampere (symbol: A)

The ampere is that constant current which, if maintained in two straight parallel conductors of infinite length, of negligible circular cross-section, and placed 1 metre apart in vacuum, would produce between these conductors a force equal to 2×10^{-7} newton per metre of length.
(9th CGPM, 1948)

kelvin (symbol: K)

The kelvin, unit of thermodynamic temperature, is the fraction 1/273.16 of the thermodynamic temperature of the triple point of water.
(13th CGPM, 1967)
This definition refers to water having the isotopic composition defined exactly by the following amount-of-substance ratios: 0.000 155 76 mole of ^{2}H per mole of ^{1}H, 0.000 379 9 mole of ^{17}O per mole of ^{16}O, and 0.002 005 2 mole of ^{18}O per mole of ^{16}O.
(CIPM, 2005)

mole (symbol: mol)

1. The mole is the amount of substance of a system that contains as many elementary entities as there are atoms in 0.012 kilogram of carbon 12; its symbol is "mol".

2. When the mole is used, the elementary entities must be specified and may be atoms, molecules, ions, electrons, other particles, or specified groups of such particles.
(14th CGPM, 1971)
In this definition, it is understood that unbound atoms of carbon 12, at rest and in their ground state, are referred to.
(CIPM, 1980)

Examples of the use of the mole

1 mol of $^1H_2$ contains about 6.022×10^{23} $^1H_2$ molecules, or 12.044×10^{23} ^{1}H atoms.

1 mol of HgCl has a mass of 236.04 g.

1 mol of Hg_2^{2+} has a mass of 401.18 g and a charge of 192.97 kC.

1 mol of $Fe_{0.91}S$ has a mass of 82.88 g.

1 mol of e^- has a mass of 548.58 μg and a charge of −96.49 kC.

1 mol of photons whose frequency is 5×10^{14} Hz has an energy of about 199.5 kJ.

Specification of the entity does not imply that the entities are identical: one may have 1 mol of an isotope mixture or gas mixture.

candela (symbol: cd)

The candela is the luminous intensity, in a given direction, of a source that emits monochromatic radiation of frequency 540×10^{12} hertz and that has a radiant intensity in that direction of 1/683 watt per steradian.
(16th CGPM, 1979)

4.2 SI-derived Units with Special Names and Symbols

	SI-derived unit			
Derived quantity	Name	Symbol	Expressed in terms of other SI units	Notes
plane angle	radian	rad	$m\ m^{-1} = 1$	1
solid angle	steradian	sr	$m^2\ m^{-2} = 1$	1
frequency	hertz	Hz	s^{-1}	2
force	newton	N	$m\ kg\ s^{-2}$	
pressure, stress	pascal	Pa	$N\ m^{-2} = m^{-1}\ kg\ s^{-2}$	
energy, work, heat	joule	J	$N\ m = m^2\ kg\ s^{-2}$	
power, radiant flux	watt	W	$J\ s^{-1} = m^2\ kg\ s^{-3}$	
electric charge	coulomb	C	A s	

(1) Radian and steradian are derived units. Since they are then of dimension 1, this leaves open the possibility of including them or omitting them in expressions of SI-derived units. In practice, this means that rad and sr may be used when appropriate and may be omitted if clarity is not lost.
(2) For angular frequency and for angular velocity, the unit rad s^{-1}, or simply s^{-1}, should be used, and this may *not* be replaced with Hz. The unit Hz shall be used *only* for frequency in the sense of cycles per second.

	SI-derived unit			
Derived quantity	Name	Symbol	Expressed in terms of other SI units	Notes
electric potential, electric tension	volt	V	$\mathrm{J\ C^{-1} = m^2\ kg\ s^{-3}\ A^{-1}}$	
electric resistance	ohm	Ω	$\mathrm{V\ A^{-1} = m^2\ kg\ s^{-3}\ A^{-2}}$	
electric conductance	siemens	S	$\Omega^{-1} = \mathrm{m^{-2}\ kg^{-1} s^3\ A^2}$	
electric capacitance	farad	F	$\mathrm{C\ V^{-1} = m^{-2}\ kg^{-1}\ s^4 A^2}$	
magnetic flux	weber	Wb	$\mathrm{V\ s = m^2\ kg\ s^{-2}\ A^{-1}}$	
magnetic flux density	tesla	T	$\mathrm{Wb\ m^{-2} = kg\ s^{-2}\ A^{-1}}$	
inductance	henry	H	$\mathrm{V\ A^{-1}\ s = m^2\ kg\ s^{-2}\ A^{-2}}$	
Celsius temperature	degree Celsius	°C	K	3
luminous flux	lumen	lm	cd sr = cd	
illuminance	lux	lx	$\mathrm{lm\ m^{-2} = cd\ m^{-2}}$	
activity, (radioactivity) referred to a radio-nuclide	becquerel	Bq	$\mathrm{s^{-1}}$	4
absorbed dose, kerma	gray	Gy	$\mathrm{J\ kg^{-1} = m^2\ s^{-2}}$	4
dose equivalent (dose equivalent index)	sievert	Sv	$\mathrm{J\ kg^{-1} = m^2\ s^{-2}}$	4
catalytic activity	katal	kat	$\mathrm{mol\ s^{-1}}$	4, 5

(3) The Celsius temperature t is defined by the following equation: $t/^\circ\mathrm{C} = T/\mathrm{K} - 273.15$
The SI unit of Celsius temperature is the degree Celsius, °C, which is equal to the kelvin, K. °C shall be treated as a single symbol, with no space between the ° sign and the C. The symbol °K, and the symbol °, shall no longer be used for the unit of thermodynamic temperature.

(4) Becquerel is the basic unit to be used in nuclear and radiochemistry; becquerel, gray, and sievert are admitted for reasons of safeguarding human health (BIPM 2006).

(5) When the amount of a catalyst cannot be expressed as a number of elementary entities, an amount of substance, or a mass, a "catalytic activity" can still be defined as a property of the catalyst measured by a catalyzed rate of conversion under specified optimized conditions. The katal, $1\ \mathrm{kat} = 1\ \mathrm{mol\ s^{-1}}$, should replace the "(enzyme) unit", $1\ \mathrm{U} = \mu\mathrm{mol\ min^{-1}} \approx 16.67\ \mathrm{nkat}$ (Dybkaer 2001).

4.3 SI-derived Units for Other Quantities

This table gives examples of other SI-derived units; the list is merely illustrative.

	SI-derived unit		
Derived quantity	Symbol	Expressed in terms of SI base units	Notes
efficiency	$\mathrm{W\ W^{-1}}$	= 1	
area	$\mathrm{m^2}$		
volume	$\mathrm{m^3}$		
speed, velocity	$\mathrm{m\ s^{-1}}$		
angular velocity	$\mathrm{rad\ s^{-1}}$	$= \mathrm{s^{-1}}$	
acceleration	$\mathrm{m\ s^{-2}}$		
moment of force	N m	$= \mathrm{m^2\ kg\ s^{-2}}$	
repetency, wavenumber	$\mathrm{m^{-1}}$		1
density, mass density	$\mathrm{kg\ m^{-3}}$		
specific volume	$\mathrm{m^3\ kg^{-1}}$		
amount concentration	$\mathrm{mol\ m^{-3}}$		2

Derived quantity	SI-derived unit			Notes
	Symbol	Expressed in terms of SI base units		
molar volume	$\mathrm{m^3\ mol^{-1}}$			
heat capacity, entropy	$\mathrm{J\ K^{-1}}$	=	$\mathrm{m^2\ kg\ s^{-2}\ K^{-1}}$	
molar heat capacity, molar entropy	$\mathrm{J\ K^{-1}\ mol^{-1}}$	=	$\mathrm{m^2\ kg\ s^{-2}\ K^{-1}\ mol^{-1}}$	
specific heat capacity, specific entropy	$\mathrm{J\ K^{-1}\ kg^{-1}}$	=	$\mathrm{m^2\ s^{-2}\ K^{-1}}$	
molar energy	$\mathrm{J\ mol^{-1}}$	=	$\mathrm{m^2\ kg\ s^{-2}\ mol^{-1}}$	
specific energy	$\mathrm{J\ kg^{-1}}$	=	$\mathrm{m^2\ s^{-2}}$	
energy density	$\mathrm{J\ m^{-3}}$	=	$\mathrm{m^{-1}\ kg\ s^{-2}}$	
surface tension	$\mathrm{N\ m^{-1}}$	=	$\mathrm{kg\ s^{-2}}$	
heat flux density, irradiance	$\mathrm{W\ m^{-2}}$	=	$\mathrm{kg\ s^{-3}}$	
thermal conductivity	$\mathrm{W\ m^{-1}\ K^{-1}}$	=	$\mathrm{m\ kg\ s^{-3}\ K^{-1}}$	
kinematic viscosity, diffusion coefficient	$\mathrm{m^2\ s^{-1}}$			
dynamic viscosity, shear viscosity	$\mathrm{Pa\ s}$	=	$\mathrm{m^{-1}\ kg\ s^{-1}}$	
electric charge density	$\mathrm{C\ m^{-3}}$	=	$\mathrm{m^{-3}\ s\ A}$	
electric current density	$\mathrm{A\ m^{-2}}$			
conductivity	$\mathrm{S\ m^{-1}}$	=	$\mathrm{m^{-3}\ kg^{-1}\ s^3\ A^2}$	
molar conductivity	$\mathrm{S\ m^2\ mol^{-1}}$	=	$\mathrm{kg^{-1}\ s^3\ A^2\ mol^{-1}}$	
permittivity	$\mathrm{F\ m^{-1}}$	=	$\mathrm{m^{-3}\ kg^{-1}\ s^4\ A^2}$	
permeability	$\mathrm{H\ m^{-1}}$	=	$\mathrm{m\ kg\ s^{-2}\ A^{-2}}$	
electric field strength	$\mathrm{V\ m^{-1}}$	=	$\mathrm{m\ kg\ s^{-3}\ A^{-1}}$	
magnetic field strength	$\mathrm{A\ m^{-1}}$			
exposure (X and γ rays)	$\mathrm{C\ kg^{-1}}$	=	$\mathrm{kg^{-1}\ s\ A}$	
absorbed dose rate	$\mathrm{Gy\ s^{-1}}$	=	$\mathrm{m^2\ s^{-3}}$	

(1) The word “wavenumber” denotes the quantity “reciprocal wavelength”. Its widespread use to denote the unit $\mathrm{cm^{-1}}$ should be discouraged.

(2) The words “amount concentration” are an abbreviation for “amount-of-substance concentration”. When there is not likely to be any ambiguity, this quantity may simply be called “concentration”.

4.4 SI Prefixes and Prefixes for Binary Multiples

The following prefixes (BIPM 2006) are used to denote decimal multiples and submultiples of SI units.

Submultiple	Prefix	
	Name	Symbol
10^{-1}	deci	d
10^{-2}	centi	c
10^{-3}	milli	m
10^{-6}	micro	µ
10^{-9}	nano	n
10^{-12}	pico	p
10^{-15}	femto	f
10^{-18}	atto	a
10^{-21}	zepto	z
10^{-24}	yocto	y

Multiple	Prefix	
	Name	Symbol
10^{1}	deca	da
10^{2}	hecto	h
10^{3}	kilo	k
10^{6}	mega	M
10^{9}	giga	G
10^{12}	tera	T
10^{15}	peta	P
10^{18}	exa	E
10^{21}	zetta	Z
10^{24}	yotta	Y

Prefix symbols shall be printed in roman (upright) type with no space between the prefix and the unit symbol.

Example

kilometre, km

When a prefix is used with a unit symbol, the combination is taken as a new symbol that can be raised to any power without the use of parentheses.

Example

$1\ \mathrm{cm}^3 = (10^{-2}\ \mathrm{m})^3 = 10^{-6}\ \mathrm{m}^3$
$1\ \mu\mathrm{s}^{-1} = (10^{-6}\ \mathrm{s})^{-1} = 10^6\ \mathrm{s}^{-1}$
$1\ \mathrm{V/cm} = 1\ \mathrm{V}/(10^{-2}\ \mathrm{m}) = 10^2\ \mathrm{V/m}$
$1\ \mathrm{mmol/dm}^3 = 10^{-3}\ \mathrm{mol}/(10^{-3}\ \mathrm{m}^3) = 1\ \mathrm{mol\ m}^{-3}$

A prefix shall never be used on its own, and prefixes are not to be combined into compound prefixes.

Example

pm, not μμm

The names and symbols of decimal multiples and submultiples of the SI base unit of mass, the kilogram, symbol kg, which already contains a prefix, are constructed by adding the appropriate prefix to the name gram and symbol g.

Example

mg, not μkg; Mg, not kkg

The International Electrotechnical Commission (IEC) has standardized the following prefixes for binary multiples, mainly used in information technology, to be distinguished from the SI prefixes for decimal multiples (IEC 2005).

Multiple	Prefix		
	Name	Symbol	Origin
$(2^{10})^1 = (1024)^1$	kibi	Ki	kilobinary
$(2^{10})^2 = (1024)^2$	mebi	Mi	megabinary
$(2^{10})^3 = (1024)^3$	gibi	Gi	gigabinary
$(2^{10})^4 = (1024)^4$	tebi	Ti	terabinary
$(2^{10})^5 = (1024)^5$	pebi	Pi	petabinary
$(2^{10})^6 = (1024)^6$	exbi	Ei	exabinary
$(2^{10})^7 = (1024)^7$	zebi	Zi	zettabinary
$(2^{10})^8 = (1024)^8$	yobi	Yi	yottabinary

4.5 Non-SI Units Accepted for Use with the SI

The following units are not part of the SI, but it is recognized by the CGPM (BIPM 2006) that they will continue to be used in appropriate contexts. SI prefixes may be attached to some of these units, such as millilitre, mL; megaelectronvolt, MeV; and kilotonne, kt.

Physical quantity	Unit accepted for use with the SI			Notes
	Name	Symbol	Value in SI units	
time	minute	min	= 60 s	
time	hour	h	= 3600 s	
time	day	d	= 86 400 s	
plane angle	degree	°, deg	= (π/180) rad	
plane angle	minute	′	= (π/10 800) rad	
plane angle	second	″	= (π/648 000) rad	
volume	litre	l, L	$= 1\ \mathrm{dm}^3 = 10^{-3}\ \mathrm{m}^3$	1
mass	tonne	t	$= 1\ \mathrm{Mg} = 10^3\ \mathrm{kg}$	
level of a field quantity, level of a power quantity	neper	Np	$= \ln \mathrm{e} = (1/2) \ln \mathrm{e}^2 = 1$	2
level of a field quantity, level of a power quantity	bel	B		2
energy	electronvolt	eV ($= e \cdot 1$ V)	$= 1.602\ 176\ 487(40)\times10^{-19}$ J	3

(1) The alternative symbol L is the only exception of the general rule that symbols for units shall be printed in lower case letters unless they are derived from a personal name. In order to avoid the risk of confusion between the letter l and the number 1, the use of L is accepted. However, only the lower case l is used by ISO and IEC.

(2) For logarithmic ratio quantities and their units, see Mills and Morfey (2005).

(3) The values of these units in terms of the corresponding SI units are not exact, since they depend on the values of the physical constants e (for electronvolt) and $m_a(^{12}\mathrm{C})$ or N_A (for the unified atomic mass unit), which are determined by experiment (Section 6).

Physical quantity	Unit accepted for use with the SI			Notes
	Name	Symbol	Value in SI units	
mass	dalton, unified atomic mass unit	Da, u	$= 1.660\ 538\ 782(83)\times 10^{-27}$ kg	3, 4
length	nautical mile	M	$= 1852$ m	5
	astronomical unit	ua	$= 1.495\ 978\ 706\ 91(6)\times 10^{11}$ m	6

(4) The dalton, with symbol Da, and the unified atomic mass unit, with symbol u, are alternative names for the same unit, 1 Da = 1 u $= m_a(^{12}\mathrm{C})/12$. The dalton may be combined with SI prefixes to express the masses of large or small entities.

(5) There is no agreed symbol for the nautical mile. The SI Brochure uses the symbol M.

(6) The astronomical unit is a unit of length approximately equal to the mean Earth–Sun distance. Its value is such that, when used to describe the motion of bodies in the Solar System, the heliocentric gravitational constant is $(0.017\ 202\ 098\ 95)^2$ ua^3 d^{-2} (see also BIPM 2006).

4.6 Coherent Units and Checking Dimensions

If equations between numerical values have the same form as equations between physical quantities, then the system of units defined in terms of base units avoids numerical factors between units and is said to be a *coherent system*. For example, the kinetic energy T of a particle of mass m moving with a speed v is defined by the following equation:

$$T = \left(\frac{1}{2}\right) mv^2$$

but the SI unit of kinetic energy is the joule, defined by the following equation:

$$\mathrm{J} = \mathrm{kg}\ (\mathrm{m/s})^2 = \mathrm{kg\ m^2\ s^{-2}}$$

where it is to be noted that the factor (1/2) is omitted. In fact, the joule, symbol J, is simply a special name and symbol for the product of units kg m^2 s^{-2}.

The International System (SI) is a coherent system of units. The advantage of a coherent system of units is that if the value of each quantity is substituted for the quantity symbol in any quantity equation, then the units may be canceled, leaving an equation between numerical values that is exactly similar (including all numerical factors) to the original equation between the quantities. Checking that the units cancel in this way is sometimes described as checking the dimensions of the equation. The use of a coherent system of units is not essential. In particular, the use of multiple or submultiple prefixes destroys the coherence of the SI, but is nonetheless often convenient.

4.7 Fundamental Physical Constants Used as Units

Sometimes fundamental physical constants, or other well-defined physical quantities, are used as though they were units in certain specialized fields of science. For example, in astronomy it may be more convenient to express the mass of a star in terms of the mass of the sun, and to express the period of the planets in their orbits in terms of the period of the Earth's orbit, rather than to use SI units. In atomic and molecular physics, it is similarly more convenient to express masses in terms of the electron mass, m_e, or in terms of the unified atomic mass unit, 1 u = 1 Da $= m_u = m(^{12}\mathrm{C}/12)$, and to express charges in terms of the elementary charge e, rather than to use SI units. One reason for using such physical quantities as though they were units is that the nature of the experimental measurements or calculations in the specialized field may be such that results are naturally obtained in such terms and can only be converted to SI units at a later stage. When physical quantities are used as units in this way, their relation to the SI must be determined by experiment, which is subject to uncertainty, and the conversion factor may change as new and more precise experiments are developed. Another reason for using such units is that uncertainty in the conversion factor to the SI may be greater than the uncertainty in the ratio of the measurements expressed in terms of the physical constant as a unit. Both reasons make it preferable to present experimental results without converting to SI units.

Three such physical quantities that have been recognized as units by the CIPM are the electronvolt (eV), the dalton (Da) or the unified atomic mass unit (u), and the astronomical unit (ua), listed below (BIPM 2006). The electronvolt is the product of a fundamental constant (the elementary charge, e) and the SI unit of potential difference (the volt, V). The dalton is related to the mass of the carbon-12 nuclide and is thus a fundamental constant. The astronomical unit is a more arbitrarily defined constant that is convenient to astronomers. However, there are many other physical quantities or fundamental constants that are sometimes used in this way as though they were units, so that it is hardly possible to list them all.

Physical quantity	Name of unit	Symbol for unit	Value in SI units	Notes
energy	electronvolt	eV	$1\,\mathrm{eV} = 1.602\ 176\ 487(40) \times 10^{-19}\ \mathrm{J}$	1
mass	dalton, unified atomic mass unit	Da, u	$1\,\mathrm{Da} = 1.660\ 538\ 782(83) \times 10^{-27}\ \mathrm{kg}$	2
length	astronomical unit	ua	$1\,\mathrm{ua} = 1.495\ 978\ 706\ 91(6) \times 10^{11}\ \mathrm{m}$	3

(1) The electronvolt is the kinetic energy acquired by an electron in passing through a potential barrier of 1 V in vacuum.

(2) The dalton and the unified atomic mass unit are alternative names for the same unit. The dalton may be combined with the SI prefixes to express the masses of large molecules (in kDa, MDa) or to express uncertainties with highly accurate determinations of atomic and molecular masses (i.e., nDa, pDa, etc.).

(3) The value of the astronomical unit in SI units is defined such that, when used to describe the motion of bodies in the solar system, the heliocentric gravitational constant is $(0.017\ 202\ 098\ 95)^2\ \mathrm{ua}^3\ \mathrm{d}^{-2}$. The value must be obtained from experiment and is, therefore, not known exactly (see also BIPM 2006).

4.7.1 Atomic Units

One particular group of physical constants that are used as though they were units deserves special mention. These are the so-called atomic units (Whiffen 1978) and arise in calculations of electronic wavefunctions for atoms and molecules, i.e., in quantum chemistry. The first five atomic units in the table on the following page have special names and symbols. Only four of these are independent; all others may be derived by multiplication and division in the usual way, and the table includes a number of examples. The relation between the five named atomic units may be expressed by any one of the equations:

$$E_\mathrm{h} = \frac{\hbar^2}{m_\mathrm{e}{a_0}^2} = \frac{e^2}{4\pi\varepsilon_0 a_0} = \frac{m_\mathrm{e}e^4}{(4\pi\varepsilon_0)^2\hbar^2}$$

The relation of atomic units to the corresponding SI units involves the values of the fundamental physical constants and is, therefore, not exact. The numerical values in the following page table are from the CODATA compilation (Mohr *et al.* 2008) and based on the fundamental constants given here in Chapter 6. The numerical results of calculations in theoretical chemistry are frequently quoted in atomic units, or as numerical values in the form *physical quantity* divided by *atomic unit*, so that the reader may make the conversion using the current best estimates of the physical constants.

4.7.2 The Equations of Quantum Chemistry Expressed in Terms of Reduced Quantities using Atomic Units

It is customary to write the equations of quantum chemistry in terms of reduced quantities. Thus, energies are expressed as reduced energies E^*, distances as reduced distances r^*, masses as reduced masses m^*, charges as reduced charges Q^*, and angular momenta as reduced angular momenta J^*, where the reduced quantities are given by the following equations:

$$E^* = E/E_\mathrm{h}, \quad r^* = r/a_0, \quad m^* = m/m_\mathrm{e}, \quad Q^* = Q/e, \quad \text{and} \quad J^* = J/\hbar \tag{1}$$

The reduced quantity in each case is the dimensionless ratio of the actual quantity to the corresponding atomic unit. The advantage of expressing all the equations in terms of reduced quantities is that the equations are simplified since all the physical constants disappear from the equations (although this simplification is achieved at the expense of losing the advantage of dimensional checking, since all reduced quantities are dimensionless). For example, the Schrödinger equation for the hydrogen atom, expressed in the usual physical quantities, has the following form:

$$-\frac{\hbar^2}{2m_\mathrm{e}}{\nabla_r}^2\ \psi(r,\theta,\phi) + V(r)\psi(r,\theta,\phi) = E\psi(r,\theta,\phi) \tag{2}$$

Here r, θ, and ϕ are the coordinates of the electron, and the operator ∇_r involves derivatives $\partial/\partial r$, $\partial/\partial\theta$, and $\partial/\partial\phi$. However in terms of reduced quantities, the corresponding equation has the form

$$-\left(\frac{1}{2}\right)\nabla_{r^*}^2\ \psi(r^*,\theta,\phi) + V^*(r^*)\psi(r^*,\theta,\phi) = E^*\psi(r^*,\theta,\phi) \tag{3}$$

where ∇_{r^*} involves derivatives $\partial/\partial r^*, \partial/\partial\theta$, and $\partial/\partial\phi$. This may be shown by substituting the reduced (starred) quantities for the actual (unstarred) quantities in equation (2), which leads to equation (3).

Physical quantity	Name of unit	Symbol for unit	Value in SI units	Notes
mass	electron mass	m_e	$= 9.109\ 382\ 15(45) \times 10^{-31}$ kg	
charge	elementary charge	e	$= 1.602\ 176\ 487(40) \times 10^{-19}$ C	
action, (angular momentum)	Planck constant divided by 2π	$\hbar$	$= 1.054\ 571\ 628(53) \times 10^{-34}$ J s	1
length	Bohr radius	a_0	$= 5.291\ 772\ 085\ 9(36) \times 10^{-11}$ m	1
energy	Hartree energy	E_h	$= 4.359\ 743\ 94(22) \times 10^{-18}$ J	1
time		$\hbar/E_h$	$= 2.418\ 884\ 326\ 505(16) \times 10^{-17}$ s	
speed		$a_0E_h/\hbar$	$= 2.187\ 691\ 254\ 1(15) \times 10^{6}$ m s^{-1}	2
force		E_h/a_0	$= 8.238\ 722\ 06(41) \times 10^{-8}$ N	
linear momentum		$\hbar/a_0$	$= 1.992\ 851\ 565(99) \times 10^{-24}$ N s	
electric current		$eE_h/\hbar$	$= 6.623\ 617\ 63(17) \times 10^{-3}$ A	
electric field		E_h/ea_0	$= 5.142\ 206\ 32(13) \times 10^{11}$ V m^{-1}	
electric dipole moment		ea_0	$= 8.478\ 352\ 81(21) \times 10^{-30}$ C m	
electric quadrupole moment		$ea_0{}^2$	$= 4.486\ 551\ 07(11) \times 10^{-40}$ C m^2	
electric polarizability		$e^2a_0{}^2/E_h$	$= 1.648\ 777\ 253\ 6(34) \times 10^{-41}$ C^2 m^2 J^{-1}	
1st hyper-polarizability		$e^3a_0{}^3/E_h^2$	$= 3.206\ 361\ 533(81) \times 10^{-53}$ C^3 m^3 J^{-2}	
2nd hyper-polarizability		$e^4a_0{}^4/E_h^3$	$= 6.235\ 380\ 95(31) \times 10^{-65}$ C^4 m^4 J^{-3}	
magnetic flux density		$\hbar/ea_0{}^2$	$= 2.350\ 517\ 382(59) \times 10^{5}$ T	
magnetic dipole moment		$e\hbar/m_e$	$= 1.854\ 801\ 830(46) \times 10^{-23}$ J T^{-1}	3
magnetizability		$e^2a_0{}^2/m_e$	$= 7.891\ 036\ 433(27) \times 10^{-29}$ J T^{-2}	

(1) $\hbar = h/2\pi$; $a_0 = 4\pi\varepsilon_0\hbar^2/m_e e^2$; $E_h = \hbar^2/m_e a_0^2$.

(2) The numerical value of the speed of light, when expressed in atomic units, is equal to the reciprocal of the fine-structure constant α; $c/(\text{au of speed}) = c\hbar/a_0E_h = \alpha^{-1} = 137.035\ 999\ 679(94)$.

(3) The atomic unit of magnetic dipole moment is twice the Bohr magneton, μ_B.

In the field of quantum chemistry, it is customary to write all equations in terms of reduced (starred) quantities, so that all quantities become dimensionless, and all fundamental constants such as $e, m_e, \hbar, E_h$, and a_0 disappear from the equations. As observed above, this simplification is achieved at the expense of losing the possibility of dimensional checking. To compare the results of a numerical calculation with experiment, it is of course necessary to transform the calculated values of the reduced quantities back to the values of the actual quantities using equation (1).

Unfortunately, it is also customary not to use the star that has been used here, but instead to use exactly the same symbol for the dimensionless reduced quantities and the actual quantities. This makes it impossible to write equations such as equation (1). (It is analogous to the situation that would arise if we were to use exactly the same symbol for h and $\hbar$, where $\hbar = h/2\pi$, thus making it impossible to write the relation between h and $\hbar$.) This may perhaps be excused on the grounds that it becomes tedious to include a star on the symbol for every physical quantity when writing the equations in quantum chemistry, but it is important that readers unfamiliar with the field should realize what has been done. It is also important to realize how the values of quantities "expressed in atomic units", i.e., the values of reduced quantities, may be converted back to the values of the original quantities in SI units.

It is also customary to make statements such as "in atomic units $e, m_e, \hbar, E_h$, and a_0 are all equal to 1", which is not a correct statement. The correct statement would be that in atomic units the elementary charge is equal to $1e$, the mass of an electron is equal to $1m_e$, etc. The difference between equations, such as equation (3) that contains no fundamental constants and equation (2) that contains fundamental constants, concerns the quantities rather than the units. In equation (3) all the quantities are dimensionless reduced quantities, defined by equation (1), whereas in equation (2) the quantities are the usual (dimensioned) physical quantities with which we are familiar in other circumstances.

Finally, many authors make no use of the symbols for the atomic units listed in the tables above, but instead use the symbol "a.u." or "au" for all atomic units. This custom should not be followed. It leads to confusion, just as it would if we were to write "SI" as a symbol for every SI unit or "CGS" as a symbol for every CGS unit.

Example

For the hydrogen molecule the equilibrium bond length r_e and the dissociation energy D_e are given by

$$r_\mathrm{e} = 2.1\ a_0 \quad \text{not} \quad r_\mathrm{e} = 2.1\ \text{a.u.}$$

$$D_\mathrm{e} = 0.16\ E_\mathrm{h} \quad \text{not} \quad D_\mathrm{e} = 0.16\ \text{a.u.}$$

4.8 Quantities of Dimension One

Values of physical quantities of dimension one, frequently called *dimensionless quantities*, are often expressed in terms of mathematically exactly defined values denoted by special symbols or abbreviations, such as % (percent). These symbols are then treated as units and are used as such in calculations.

4.8.1 Fractions (Relative Values, Yields, and Efficiencies)

Fractions such as relative uncertainty, amount-of-substance fraction x (also called *amount fraction*), mass fraction w, and volume fraction φ are sometimes expressed in terms of the symbols in the table below.

Name	Symbol	Value	Example
percent	%	10^{-2}	The isotopic abundance of carbon-13 expressed as an amount-of-substance fraction is $x = 1.1\,\%$.
permille	‰	10^{-3}	The mass fraction of water in a sample is $w = 2.3\,‰$.

These multiples of the unit one are not part of the SI and ISO recommends that these symbols should never be used. They are also frequently used as units of "concentration" without a clear indication of the type of fraction implied, e.g., amount-of-substance fraction, mass fraction, or volume fraction. To avoid ambiguity, they should be used only in a context where the meaning of the quantity is carefully defined. Even then, the use of an appropriate SI unit ratio may be preferred.

Example

The mass fraction $w = 1.5 \times 10^{-6} = 1.5\ \mathrm{mg\ kg^{-1}}$.
The amount-of-substance fraction $x = 3.7 \times 10^{-2} = 3.7\,\%$ or $x = 37\ \mathrm{mmol\ mol^{-1}}$.
Atomic absorption spectroscopy shows the aqueous solution to contain a mass concentration of nickel $\rho(\mathrm{Ni}) = 2.6\ \mathrm{mg\ dm^{-3}}$, which is approximately equivalent to a mass fraction $w(\mathrm{Ni}) = 2.6 \times 10^{-6}$.

Note the importance of using the recommended name and symbol for the quantity in each of the above examples. Statements such as "the concentration of nickel was 2.6×10^{-6}" are ambiguous and should be avoided.

The last example illustrates the approximate equivalence of $\rho/(\mathrm{mg\ dm^{-3}})$ and $w/10^{-6}$ in aqueous solution, which follows from the fact that the mass density of a dilute aqueous solution is always approximately $1.0\,\mathrm{g\,cm^{-3}}$. Dilute solutions are often measured or calibrated to a known mass concentration in mg dm^{-3}, and this unit is then to be preferred to using ppm (or other corresponding abbreviations, which are language dependent) to specify a mass fraction.

4.8.2 Deprecated Usage

Adding extra labels to % and similar symbols, such as % (V/V) (meaning % by volume), should be avoided. Qualifying labels may be added to symbols for physical quantities, but never to units.

Example

A mass fraction $w = 0.5\,\%$, but *not* $0.5\,\%\ (m/m)$.

The symbol % should not be used in combination with other units. In table headings and in labeling the axes of graphs, the use of % in the denominator is to be avoided. Although one would write $x(^{13}\mathrm{C}) = 1.1\,\%$, the notation $100\,x$ is to be preferred to $x/\%$ in tables and graphs.

The further symbols listed in the table below are also found in the literature, but their use is not recommended. Note that the names and symbols for 10^{-9} and 10^{-12} in this table are here based on the American system of names. In other parts of the world, a billion often stands for 10^{12} and a trillion for 10^{18}. Note also that the symbol ppt is sometimes used for part per thousand, and sometimes for part per trillion. In 1948 the word billion had been proposed for 10^{12} and trillion for 10^{18} (Jerrard and McNeill 1980). Although ppm, ppb, ppt, and alike are widely used in various applications of analytical and environmental chemistry, it is suggested to abandon completely their use because of the ambiguities involved. These units are unnecessary and can be easily replaced by SI-compatible expressions such as pmol/mol (picomole per mole), which are unambiguous. The last column contains suggested replacements (similar replacements can be formulated as mg/g, µg/g, pg/g, etc., depending on the precise context). The advantage of these representations of the units (strictly speaking of dimension one) is to remind one of the definition of the quantity used in the equation (e.g., mass fraction), although that definition could be stated explicitly as well. While the mass fraction 5.65 ‰ in the example on the element Ti in the table below is replaced meaningfully by 5.65 mg/g, a replacement of the form 5.65 mA/A would not make much sense in connection

Name	Symbol	Value	Examples with a suggested replacement	
part per hundred	pph[(b)], %	10^{-2}	The degree of dissociation is 1.5 %.	
part per thousand, permille[(a)]	ppt[(b)], ‰	10^{-3}	A preindustrial value of the CO_2 amount-of-substance content of the Earth's atmosphere was about 0.275 ‰ (0.275 ppt). The element Ti has a mass fraction 5.65‰ (5.65×10^3 ppm) in the Earth's crust.	mmol mol^{-1} mg g^{-1}
part per million	ppm[(b)]	10^{-6}	The volume fraction of helium is 20 ppm. The proton chemical shift of chloroform is $\delta_{\mathrm{H}}(\mathrm{CHCl_3}) = 7.27$ ppm.	µL L^{-1} µHz Hz^{-1}
part per hundred million	pphm[(b)]	10^{-8}	The mass fraction of impurity in the metal was less than 5 pphm.	
part per billion	ppb[(b)]	10^{-9}	The air quality standard for ozone is a volume fraction of $\varphi = 120$ ppb.	nL L^{-1}
part per trillion	ppt[(b)]	10^{-12}	The natural background volume fraction of NO in air was found to be $\varphi = 140$ ppt.	pL L^{-1}
part per quadrillion	ppq[(b)]	10^{-15}		

[(a)] The permille is also spelled per mill, permill, per mil, permil, per mille, or promille.
[(b)] Deprecated, see text.

with a mass fraction, although formally correct within the framework of quantity calculus.

4.8.3 Units for Logarithmic Quantities: neper, bel, and decibel

In some fields, especially in acoustics and telecommunications, special names are given to the number 1 when expressing physical quantities defined in terms of the logarithm of a ratio (Mills and Morfey 2005). For a damped linear oscillation, the amplitude of a quantity as a function of time is given by

$$F(t) = A\ \mathrm{e}^{-\delta t} \cos \omega t = A\ \mathrm{Re}[\mathrm{e}^{(-\delta + \mathrm{i}\omega)t}]$$

From this relation it is clear that the coherent SI unit for the decay coefficient δ and the angular frequency ω is the second to the power of minus one, s^{-1}. However, the special names neper (Np) and radian (rad) (Sections 4.2 and 4.5) are used for the units of the dimensionless products δt and ωt, respectively. Thus the quantities δ and ω may be expressed in the units Np/s and rad/s, respectively. Used in this way, the neper (Np) and the radian (rad) may both be thought of as special names for the number 1.

In the fields of acoustics and signal transmission, signal power levels and signal amplitude levels (or field level) are usually expressed as the decadic or the napierian logarithm of the ratio of the power P to a reference power P_0, or of the field F to a reference field F_0. Since power is often proportional to the square of the field or amplitude (when the field acts on equal impedances in linear systems), it is convenient to define the power level and the field level to be equal in such a case. This is done by defining the field level and the power level according to the relations

$$L_F = \ln(F/F_0) \quad \text{and} \quad L_P = (1/2)\ln(P/P_0)$$

so that if $(P/P_0) = (F/F_0)^2$, then $L_P = L_F$. The above equations may be written in the form

$$L_F = \ln(F/F_0)\ \mathrm{Np} \quad \text{and} \quad L_P = (1/2)\ln(P/P_0)\ \mathrm{Np}$$

The bel (B) and its more frequently used submultiple the decibel (dB) are used when the field and power levels are calculated using decadic logarithms according to the relations

$$L_P = \lg(P/P_0)\ \mathrm{B} = 10\ \lg(P/P_0)\ \mathrm{dB} \qquad \text{and}$$
$$L_F = 2\ \lg(F/F_0)\ \mathrm{B} = 20\ \lg(F/F_0)\ \mathrm{dB}$$

The relation between the bel and the neper follows from comparing these equations with the preceding equations. We obtain

$$L_F = \ln\left(\frac{F}{F_0}\right)\mathrm{Np} = 2\lg\left(\frac{F}{F_0}\right)\mathrm{B} = \ln(10)\ \lg\left(\frac{F}{F_0}\right)\mathrm{Np}$$

giving

$$\mathrm{B} = 10\ \mathrm{dB}\ = (1/2)\ \ln(10)\ \mathrm{Np}\ \approx 1.151\,293\ \mathrm{Np}$$

Name	Quantity	Numerical value multiplied by unit	Notes
field level	$L_F = \ln(F/F_0)$	$= \ln(F/F_0)$ Np $= 2\ \lg(F/F_0)$ B $= 20\ \lg(F/F_0)$ dB	1–3
power level	$L_P = (1/2)\ln(P/P_0)$	$= (1/2)\ln(P/P_0)$ Np $= \lg(P/P_0)$ B $= 10\ \lg(P/P_0)$ dB	4–6

(1) F_0 is a reference field quantity, which should be specified.

(2) In the context of acoustics, the field level is called the *sound pressure level* and given the symbol L_p, and the reference pressure $p_0 = 20\ \mu$Pa.

(3) For example, when $L_F = 1$ Np, $F/F_0 = \mathrm{e} \approx 2.718\ 281\ 8$.

(4) P_0 is a reference power, which should be specified. The factor 1/2 is included in the definition to make $L_P \mathrel{\hat{=}} L_F$.

(5) In the context of acoustics, the power level is called the *sound power level* and given the symbol L_W, and the reference power $P_0 = 1$ pW.

(6) When $L_P = 1$ B $= 10$ dB, $P/P_0 = 10$; when $L_P = 2$ B $= 20$ dB, $P/P_0 = 100$; etc.

In practice, the bel is hardly ever used. Only the decibel is used, to represent the decadic logarithm, particularly in the context of acoustics and in labeling the controls of power amplifiers. Thus, the statement $L_P = n$ dB implies that $10\,\lg(P/P_0) = n$.

The general use of special units for logarithmic quantities is discussed in Mills and Morfey (2005). The quantities power level and field level, and the units bel, decibel, and neper are given in the above table and notes that follow.

4.9 Other Systems of Quantities and Units

Today, only three countries, namely, Liberia, Union of Myanmar (Burma), and the United States, have not yet adopted the SI unit system. Before the metric convention established in 1875, a very large number of different systems of measurement were in use, e.g., Arabic, Chinese, Egyptian, Greek, Hebrew, Indian, Prussian, Roman, and the so-called Old Dutch, French, German, Italian, Japanese, Portuguese, Russian, Spanish, and the Old Swedish System, of which detailed conversion tables between the above mentioned systems and the metric system are listed in Cardarelli (1999). More 'modern' systems such as atomic units, cgs units (esu, emu), Gauss units, international electrical units, Imperial units, US customary units, and the FPS (foot, pound, and second) system are still partly in use and the corresponding conversions to the metric SI system are also collected in Cardarelli (1999).

In the twentieth century, special units have been introduced in physics mainly to simplify expressions when developing a theory. A few of such systems are shown in the following table, where the numerical value, $\{Q\}$, of certain fundamental constants, Q (velocity of light, c; elementary charge, e; Planck constant divided by 2π, $\hbar$; gravitational constant, G; electron or proton mass, $m_\mathrm{e}, m_\mathrm{p}$; electric constant, ϵ_0), have been set to 1 (Flowers and Petley 2008):

Unit system name	$\{c\}$	$\{e\}$	$\{\hbar\}$	$\{G\}$	$\{m_\mathrm{e}\}$	$\{m_\mathrm{p}\}$	$\{4\pi\epsilon_0\}$
Stoney units	1	1		1			1
Planck units	1		1	1			1
Schrödinger units		1	1	1			1
atomic units, Hartree units		1	1		1		1
electronic system of units, Dirac units	1	1			1		1
natural units, quantum relativistic units	1		1		1		1
quantum electrodynamic system of units	1	1	1			1	

While a few other systems of quantities and units find occasional use in spectroscopy, we generally recommend the use of the SI or perhaps of atomic units, but some authors may find some other systems of units particularly useful in a special context. In such cases, it becomes primordial to give explicit and complete definitions within the publication under consideration, not just by reference to some source of common usage, in order to avoid ambiguities.

In view of the very many different systems of units mentioned above, the international efforts to unify scientific language in an international system of units is strongly encouraged and supported.

5 RECOMMENDED MATHEMATICAL SYMBOLS

A detailed list of symbols can be found in Chapter 4 of the IUPAC Green book (Cohen *et al.* 2008) and in the ISO Handbook (ISO 1993).

5.1 Printing of Numbers and Mathematical Symbols

1. Numbers in general shall be printed in roman (upright) type. The decimal sign between digits in a number should be a point (e.g., 2.3) or a comma (e.g., 2,3). When the decimal sign is placed before the first significant digit of a number, a zero shall always precede the decimal sign. To facilitate the reading of long numbers, the digits may be separated into groups of three about the decimal sign, using only a thin space (but never a point or a comma, nor any other symbol). However, when there are only four digits before or after the decimal marker, we recommend that no space is required and no space should be used.

   Examples

   2573.421 736 or 2573,421 736 or
   $0.257\,342\,173\,6 \times 10^4$ or $0{,}257\,342\,173\,6 \times 10^4$
   32 573.4215 or 32 573,4215

2. Numerical values of physical quantities that have been determined experimentally are usually subject to some uncertainty. The experimental uncertainty should always be specified. The magnitude of the uncertainty may be represented as follows:

   Examples

   $l = [5.3478 - 0.0064, 5.3478 + 0.0064]\,\mathrm{cm}$
   $l = 5.3478(32)\,\mathrm{cm}$

   In the first example, the range of uncertainty is indicated directly as $[a - b, a + b]$. It is recommended that this notation should be used only with the meaning that the interval $[a - b, a + b]$ contains the true value with a high degree of certainty, such that $b \geq 2\sigma$, where σ denotes the standard uncertainty or standard deviation (see Chapter 7).

   In the second example, $a(c)$, the range of uncertainty c indicated in parentheses is assumed to apply to the least significant digits of a. It is recommended that this notation be reserved for the meaning that b represents 1σ in the final digits of a.

3. Letter symbols for mathematical constants (e.g., e, π, $\mathrm{i} = \sqrt{-1}$) shall be printed in roman (upright) type, but letter symbols for numbers other than constants (e.g., quantum numbers) should be printed in italic (sloping) type, similar to physical quantities.
4. Symbols for specific mathematical functions and operators (e.g., lb, ln, lg, exp, sin, cos, d, δ, Δ, ∇, . . .) shall be printed in roman type, but symbols for a general function (e.g., $f(x)$, $F(x, y)$, . . .) shall be printed in italic type.
5. The operator p (as in $\mathrm{p}a_{\mathrm{H}^+}$, $\mathrm{p}K = -\lg K$, etc.) shall be printed in roman type.
6. Symbols for symmetry species in group theory (e.g., S, P, D, . . ., s, p, d, . . ., Σ, Π, Δ, . . ., $\mathrm{A}_{1\mathrm{g}}$, B_2'', . . .) shall be printed in roman (upright) type when they represent the state symbol for an atom or a molecule, although they are often printed in italic type when they represent the symmetry species of a point group.
7. Vectors and matrices shall be printed in bold italic type.

   Examples

   force $\boldsymbol{F}$, electric field $\boldsymbol{E}$, position vector $\boldsymbol{r}$

   Ordinary italic type is used to denote the magnitude of the corresponding vector.

   Example

   $r = |\boldsymbol{r}|$

   Tensor quantities may be printed in bold-face italic sans serif type.

   Examples

   $\boldsymbol{\mathsf{S}}, \boldsymbol{\mathsf{T}}$

   Vectors may alternatively be characterized by an arrow, $\vec{A}$, $\vec{a}$ and second-rank tensors by a double arrow, $\overset{\rightrightarrows}{S}$, $\overset{\rightrightarrows}{T}$.

5.2 Symbols, Operators, and Functions

Description	Symbol	Notes
signs and symbols		
equal to	$=$	
not equal to	$\neq$	
identically equal to	$\equiv$	
equal by definition to	$\overset{\mathrm{def}}{=}$, $:=$	
approximately equal to	$\approx$	
asymptotically equal to	$\simeq$	
corresponds to	$\widehat{=}$	
proportional to	$\sim$, $\propto$	
tends to, approaches	$\rightarrow$	
infinity	∞	
less than	$<$	
greater than	$>$	
less than or equal to	$\leq$	
greater than or equal to	$\geq$	
much less than	$\ll$	
much greater than	$\gg$	
operations		
plus	$+$	
minus	$-$	
plus or minus	$\pm$	
minus or plus	$\mp$	
a multiplied by b	$a\ b$, ab, $a \cdot b$, $a \times b$	1
a divided by b	a/b, ab^{-1}, $\dfrac{a}{b}$	2
magnitude of a	$\lvert a \rvert$	
a to the power n	a^n	
square root of a, and of $a^2 + b^2$	$\sqrt{a}$, $a^{1/2}$, and $\sqrt{a^2+b^2}$, $\left(a^2+b^2\right)^{1/2}$	
nth root of a	$a^{1/n}$, $\sqrt[n]{a}$	
mean value of a	$\langle a \rangle$, $\overline{a}$	
sign of a (equal to $a/\lvert a \rvert$ if $a \neq 0$, 0 if $a = 0$)	$\operatorname{sgn} a$	
n factorial	$n!$	
binominal coefficient, $n!/p!(n-p)!$	C_p^n, $\binom{n}{p}$	
sum of a_i	$\sum a_i$, $\sum_i a_i$, $\sum\limits_{i=1}^{n} a_i$	
product of a_i	$\prod a_i$, $\prod_i a_i$, $\prod\limits_{i=1}^{n} a_i$	
functions		
sine of x	$\sin x$	
cosine of x	$\cos x$	
tangent of x	$\tan x$	
cotangent of x	$\cot x$	
arc sine of x	$\arcsin x$	3

---

(1) When multiplication is indicated by a dot, the dot shall be half high: $a \cdot b$.

(2) $a : b$ is as well used for "divided by". However, this symbol is mainly used to express ratios such as length scales in maps.

(3) These are the inverse of the parent function, i.e., $\arcsin x$ is the operator inverse of $\sin x$.

Description	Symbol	Notes
arc cosine of x	$\arccos x$	3
arc tangent of x	$\arctan x$	3
arc cotangent of x	$\operatorname{arccot} x$	3
hyperbolic sine of x	$\sinh x$	
hyperbolic cosine of x	$\cosh x$	
hyperbolic tangent of x	$\tanh x$	
hyperbolic cotangent of x	$\coth x$	
area hyperbolic sine of x	$\operatorname{arsinh} x$	3
area hyperbolic cosine of x	$\operatorname{arcosh} x$	3
area hyperbolic tangent of x	$\operatorname{artanh} x$	3
area hyperbolic cotangent of x	$\operatorname{arcoth} x$	3
base of natural logarithms	e	
exponential of x	$\exp x$, e^x	
logarithm to the base a of x	$\log_a x$	4
natural logarithm of x	$\ln x$, $\log_\mathrm{e} x$	4
logarithm to the base 10 of x	$\lg x$, $\log_{10} x$	4
logarithm to the base 2 of x	$\operatorname{lb} x$, $\log_2 x$	4
greatest integer $\leq x$	$\operatorname{ent} x$	
integer part of x	$\operatorname{int} x$	
integer division	$\operatorname{int}(n/m)$	
remainder after integer division	$n/m - \operatorname{int}(n/m)$	
change in x	$\Delta x = x(\text{final}) - x(\text{initial})$	
infinitesimal variation of f	δf	
limit of $f(x)$ as x tends to a	$\lim\limits_{x \to a} f(x)$	
1st derivative of f	$\mathrm{d}f/\mathrm{d}x$, f', $(\mathrm{d}/\mathrm{d}x)f$	
2nd derivative of f	$\mathrm{d}^2 f/\mathrm{d}x^2$, f''	
nth derivative of f	$\mathrm{d}^n f/\mathrm{d}x^n$, $f^{(n)}$	
partial derivative of f	$\partial f/\partial x$, $\partial_x f$, $\mathrm{D}_x f$	
total differential of f	$\mathrm{d}f$	
inexact differential of f	đf	5
1st derivative of x with respect to time	$\dot{x}$, $\mathrm{d}x/\mathrm{d}t$	
2nd derivative of x with respect to time	$\ddot{x}$, $\mathrm{d}^2x/\mathrm{d}t^2$	
integral of $f(x)$	$\int f(x)\,\mathrm{d}x$, $\int \mathrm{d}x f(x)$	
Kronecker delta	$\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$	
Levi-Civita symbol	$\varepsilon_{ijk} = \begin{cases} 1 & \text{if } ijk \text{ is a cyclic permutation of 123} \\ & \varepsilon_{123} = \varepsilon_{231} = \varepsilon_{312} = 1 \\ -1 & \text{if } ijk \text{ is an anticyclic permutation of 123} \\ & \varepsilon_{132} = \varepsilon_{321} = \varepsilon_{213} = -1 \\ 0 & \text{otherwise} \end{cases}$	
Dirac delta function (distribution)	$\delta(x)$, $\int f(x)\delta(x)\,\mathrm{d}x = f(0)$	
unit step function, Heaviside function	$\varepsilon(x)$, $\mathrm{H}(x)$, $\mathrm{h}(x)$, $\varepsilon(x) = 1$ for $x > 0$, $\varepsilon(x) = 0$ for $x < 0$.	

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(4) For positive x.

(5) Notation used in thermodynamics.

Description	Symbol	Notes
gamma function	$\Gamma(x) = \int_0^\infty t^{x-1} \mathrm{e}^{-t} \mathrm{d}t$ $\Gamma(n+1) = (n)!$ for positive integers n	
zeta function (Riemann)	$\zeta(z) = \sum\limits_{n=1}^{\infty} 1/n^z$, z complex with Re $z > 1$	
convolution of functions f and g	$f * g = \int_{-\infty}^{+\infty} f(x - x') g(x')\, \mathrm{d}x'$	
complex numbers		
square root of -1, $\sqrt{-1}$	i	
real part of $z = a + \mathrm{i}\, b$	Re $z = a$	
imaginary part of $z = a + \mathrm{i}\, b$	Im $z = b$	
modulus of $z = a + \mathrm{i}\, b$, absolute value of $z = a + \mathrm{i}\, b$	$\lvert z \rvert = \left(a^2 + b^2\right)^{1/2}$	
argument of $z = a + \mathrm{i}\, b$	arg z; tan(arg z) $= b/a$	
complex conjugate of $z = a + \mathrm{i}\, b$	$z^* = a - \mathrm{i}\, b$	
polar form of z (Gaussian plane)	$z = \lvert z \rvert\ \exp(+\mathrm{i}\alpha) = \lvert z \rvert\ (\cos\alpha + \mathrm{i}\ \sin\alpha)$	
polar form of z^*	$z^* = \lvert z \rvert\ \exp(-\mathrm{i}\alpha) = \lvert z \rvert\ (\cos\alpha - \mathrm{i}\ \sin\alpha)$	
vectors		
vector $\boldsymbol{a}$	$\boldsymbol{a}$, $\vec{a}$	
Cartesian components of $\boldsymbol{a}$	a_x, a_y, a_z	
unit vectors in cartesian coordinate system	$\boldsymbol{e}_x$, $\boldsymbol{e}_y$, $\boldsymbol{e}_z$ or $\boldsymbol{i}, \boldsymbol{j}, \boldsymbol{k}$	
scalar product	$\boldsymbol{a} \cdot \boldsymbol{b}$	
vector or cross product	$\boldsymbol{a} \times \boldsymbol{b}$, $(\boldsymbol{a} \wedge \boldsymbol{b})$	
nabla operator, del operator	$\boldsymbol{\nabla} = \boldsymbol{e}_x \partial/\partial x + \boldsymbol{e}_y \partial/\partial y + \boldsymbol{e}_z \partial/\partial z$	
Laplacian operator	$\boldsymbol{\nabla}^2, \triangle = \partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2$	
gradient of a scalar field V	$\textbf{\textit{grad}}\ V$, $\boldsymbol{\nabla} V$	
divergence of a vector field $\boldsymbol{A}$	$\textbf{\textit{div}}\boldsymbol{A}$, $\boldsymbol{\nabla} \cdot \boldsymbol{A}$	
rotation of a vector field $\boldsymbol{A}$	$\textbf{\textit{rot}}\ \boldsymbol{A}$, $\boldsymbol{\nabla} \times \boldsymbol{A}$, $(\textbf{\textit{curl}}\ \boldsymbol{A})$	
matrices		
matrix of element A_{ij}	$\boldsymbol{A}$	
product of matrices $\boldsymbol{A}$ and $\boldsymbol{B}$	$\boldsymbol{AB}$, where $(\boldsymbol{AB})_{ik} = \sum\limits_j A_{ij} B_{jk}$	
unit matrix	$\boldsymbol{E}$, $\boldsymbol{I}$	
inverse of a square matrix $\boldsymbol{A}$	$\boldsymbol{A}^{-1}$	
transpose of matrix $\boldsymbol{A}$	$\boldsymbol{A}^{\mathsf{T}}$, $\widetilde{\boldsymbol{A}}$	
complex conjugate of matrix $\boldsymbol{A}$	$\boldsymbol{A}^*$	
conjugate transpose (adjoint) of $\boldsymbol{A}$ (hermitian conjugate of $\boldsymbol{A}$)	$\boldsymbol{A}^{\mathsf{H}}$, $\boldsymbol{A}^{\dagger}$, where $\left(\boldsymbol{A}^{\dagger}\right)_{ij} = A_{ji}{}^*$	
trace of a square matrix $\boldsymbol{A}$	$\sum\limits_i A_{ii}$, tr $\boldsymbol{A}$	
determinant of a square matrix $\boldsymbol{A}$	det $\boldsymbol{A}$, $\lvert \boldsymbol{A} \rvert$	
sets and logical operators		
p and q (conjunction sign)	$p \wedge q$	
p or q or both (disjunction sign)	$p \vee q$	
negation of p, not p	$\neg p$	
p implies q	$p \Rightarrow q$	
p is equivalent to q	$p \Leftrightarrow q$	
A is contained in B	$A \subset B$	

Description	Symbol	Notes
union of A and B	$A \cup B$	
intersection of A and B	$A \cap B$	
x belongs to A	$x \in A$	
x does not belong to A	$x \notin A$	
the set A contains x	$A \ni x$	
A but not B	$A \backslash B$	

5.3 Greek Alphabet

This table lists the Greek alphabet with characters displayed in roman and italics fonts, their name together with the pronunciation and a Latin equivalent.

Roman	Italics	Name	Pronounciation and Latin Equivalent	Notes
Α, α	A, α	alpha	A	
Β, β	B, β	beta	B	
Γ, γ	Γ, γ	gamma	G	
Δ, δ	Δ, δ	delta	D	
Ε, ε, ϵ	E, ε, ϵ	epsilon	E	
Ζ, ζ	Z, ζ	zeta	Z	
Η, η	H, η	eta	Ae, Ä, Ee	1
Θ, ϑ, θ	Θ, ϑ, θ	theta	Th	2
Ι, ι	I, ι	iota	I	
Κ, ϰ, κ	K, $\varkappa$, κ	kappa	K	2
Λ, λ	Λ, λ	lambda	L	
Μ, μ	M, μ	mu (my)	M	
Ν, ν	N, ν	nu (ny)	N	
Ξ, ξ	Ξ, ξ	xi	X	
Ο, ο	O, o	omikron	O	
Π, π	Π, π	pi	P	
Ρ, ρ	P, ρ	rho	R	
Σ, σ, ς	Σ, σ, ς	sigma	S	2, 3
Τ, τ	T, τ	tau	T	
Υ, υ	Υ, υ	upsilon, ypsilon	U, Y	
Φ, φ, ϕ	Φ, φ, ϕ	phi	Ph	2
Χ, χ	X, χ	chi	Ch	
Ψ, ψ	Ψ, ψ	psi	Ps	
Ω, ω	Ω, ω	omega	Oo	4

(1) For the Latin equivalent, Ae is to be pronounced as the German Ä. The modern Greek pronounciation of the letter η is like E, long ee as in cheese, or short i as in lips. The Latin equivalent is also often called *long E*.

(2) For the lower case letters theta, kappa, sigma, and phi, there are two variants in each case. For instance, the second variant of the lower case theta is sometimes called *vartheta* in printing.

(3) The second variant for lower case sigma is used in Greek only at the end of the word.

(4) In contrast to omikron (short o), the letter omega is pronounced like a long o.

6 FUNDAMENTAL PHYSICAL CONSTANTS AND PARTICLE PROPERTIES

The data given in this table are from the CODATA recommended values of the fundamental physical constants 2006 (Mohr *et al*. 2008) (online at http://physics. nist.gov/constants) and from the 2008 compilation of the Particle Data Group (Amsler *et al*. 2008) (online at http://pdg.lbl.gov); see notes for details. The standard deviation uncertainty in the least significant digits is given in parentheses.

Quantity	Symbol	Value	Notes
magnetic constant	μ_0	$4\pi\times10^{-7}$ H m^{-1} (defined)	1
speed of light in vacuum	c_0, c	299 792 458 m s^{-1} (defined)	
electric constant	$\varepsilon_0 = 1/\mu_0 c_0^2$	8.854 187 817. . . $\times10^{-12}$ F m^{-1}	1, 2
characteristic impedance of vacuum	$Z_0 = \mu_0 c_0$	376.730 313 461 . . . Ω	2
Planck constant	h	6.626 068 96(33)$\times10^{-34}$ J s	
	$\hbar = h/2\pi$	1.054 571 628(53)$\times10^{-34}$ J s	
	hc_0	1.986 445 501(99)$\times10^{-25}$ J m	
Fermi coupling constant	$G_F/(\hbar c_0)^3$	1.166 37(1)$\times10^{-5}$ GeV^{-2}	3
weak mixing angle θ_W	$\sin^2\theta_W$	0.222 55(56)	4, 5
elementary charge	e	1.602 176 487(40)$\times10^{-19}$ C	
electron mass	m_e	9.109 382 15(45)$\times10^{-31}$ kg	
proton mass	m_p	1.672 621 637(83)$\times10^{-27}$ kg	
neutron mass	m_n	1.674 927 211(84)$\times10^{-27}$ kg	
atomic mass constant	$m_u = 1$ u	1.660 538 782(83)$\times10^{-27}$ kg	6
Avogadro constant	L, N_A	6.022 141 79(30)$\times10^{23}$ mol^{-1}	7
Boltzmann constant	k, k_B	1.380 650 4(24)$\times10^{-23}$ J K^{-1}	
Faraday constant	$F = Le$	9.648 533 99(24)$\times10^{4}$ C mol^{-1}	
molar gas constant	R	8.314 472(15) J K^{-1} mol^{-1}	
zero of the Celsius scale		273.15 K (defined)	
molar volume of ideal gas, $p = 100$ kPa, $t = 0$ °C	V_m	22.710 981(40) dm^3 mol^{-1}	
molar volume of ideal gas, $p = 101.325$ kPa, $t = 0$ °C		22.413 996(39) dm^3 mol^{-1}	
standard atmosphere		101 325 Pa (defined)	
fine-structure constant	$\alpha = \mu_0 e^2 c_0/2h$	7.297 352 537 6(50)$\times10^{-3}$	
	α^{-1}	137.035 999 676(94)	
Bohr radius	$a_0 = 4\pi\varepsilon_0\hbar^2/m_e e^2$	5.291 772 085 9(36)$\times10^{-11}$ m	
Hartree energy	$E_h = \hbar^2/m_e {a_0}^2$	4.359 743 94(22)$\times10^{-18}$ J	
Rydberg constant	$R_\infty = E_h/2hc_0$	1.097 373 156 852 7(73)$\times10^{7}$ m^{-1}	
Bohr magneton	$\mu_B = e\hbar/2m_e$	9.274 009 15(23)$\times10^{-24}$J T^{-1}	
electron magnetic moment	μ_e	-9.284 763 77(23)$\times10^{-24}$ J T^{-1}	
Landé g-factor for free electron	$g_e = 2\mu_e/\mu_B$	-2.002 319 304 362 2(15)	
nuclear magneton	$\mu_N = e\hbar/2m_p$	5.050 783 24(13)$\times10^{-27}$ J T^{-1}	
proton magnetic moment	μ_p	1.410 606 662(37)$\times10^{-26}$ J T^{-1}	
proton gyromagnetic ratio	$\gamma_p = 4\pi\mu_p/h$	2.675 222 099(70)$\times10^{8}$ s^{-1} T^{-1}	
shielded proton magnetic moment (H_2O, sphere, 25 °C)	${\mu_p}'/\mu_B$	1.520 993 128(17)$\times10^{-3}$	
shielded proton gyromagnetic ratio (H_2O, sphere, 25 °C)	${\gamma_p}'/2\pi$	42.576 388 1(12) MHz T^{-1}	

Quantity	Symbol	Value	Notes
Stefan–Boltzmann constant	$\sigma = 2\pi^5 k^4/15h^3{c_0}^2$	$5.670\,400(40)\times10^{-8}$ W m^{-2} K^{-4}	
1st radiation constant	$c_1 = 2\pi h{c_0}^2$	$3.741\,771\,18(19)\times10^{-16}$ W m^2	
2nd radiation constant	$c_2 = hc_0/k$	$1.438\,775\,2(25)\times10^{-2}$ m K	
Newtonian constant of gravitation	G	$6.674\,28(67)\times10^{-11}$ m^3 kg^{-1} s^{-2}	
standard acceleration of gravity	g_n	$9.806\,65$ m s^{-2} (defined)	

(1) H m^{-1} = N A^{-2} = N s^2 C^{-2}; F m^{-1} = C^2 J^{-1} m^{-1}.

(2) ε_0 and Z_0 may be calculated exactly from the defined values of μ_0 and c_0.

(3) The value of the Fermi coupling constant is recommended by the Particle Data Group (Amsler *et al.* 2008).

(4) With the weak mixing angle θ_W, $\sin^2\theta_\mathrm{W}$ is sometimes called *Weinberg parameter*. There are a number of schemes differing in the masses used to determine $\sin^2\theta_\mathrm{W}$ (see Chapter 10 in Amsler *et al.* 2008). The value given here for $\sin^2\theta_\mathrm{W}$ (Mohr *et al.* 2008) is based on the on-shell scheme which uses $\sin^2\theta_\mathrm{W} = 1 - (m_\mathrm{W}/m_\mathrm{Z})^2$, where the quantities m_W and m_Z are the masses of the W$^\pm$- and Z^0-bosons, respectively.

(5) The Particle Data Group (Amsler *et al.* 2008) gives $m_\mathrm{W} = 80.398(25)$ GeV/${c_0}^2$, $m_\mathrm{Z} = 91.1876(21)$ GeV/${c_0}^2$ and recommends $\sin^2\theta_\mathrm{W} = 0.231\,19(14)$, based on the $\overline{\mathrm{MS}}$ scheme. The corresponding value in the on-shell scheme is $\sin^2\theta_\mathrm{W} = 0.223\,08(30)$. The effective parameter also depends on the energy range or momentum transfer considered.

(6) u is the (unified) atomic mass unit (Section 4.7), 1 u = 1 Da.

(7) See Seyfried and Becker (1994) and other papers in the same special issue of *Metrologia* on the precise measurement of the Avogadro constant.

Values of common mathematical constants

Values of some mathematical constants are listed in the table together with a series expansion to calculate the corresponding numerical value.

Mathematical constant	Symbol	Value	Series expansion
ratio of circumference to diameter of a circle	π	3.141 592 653 59···	$\pi = 4\sum_{n=0}^{\infty}\frac{(-1)^n}{2n+1}$
base of natural logarithm	e	2.718 281 828 46···	$\mathrm{e} = \sum_{n=0}^{\infty}\frac{1}{n!}$
natural logarithm of 10	ln 10	2.302 585 092 99···	$\ln 10 = 2\sum_{n=1}^{\infty}\frac{1}{2n-1}\left(\frac{10-1}{10+1}\right)^{2n-1}$

6.1 Properties of Selected Particles

The fonts for symbols of particles, chemical elements, and nuclides are discussed in Section 2.5. The Particle Data Group (Amsler *et al.* 2008) recommends the use of italic symbols for particles and this has been adopted by many physicists. The data given in this table are from the CODATA recommended values of the fundamental physical constants 2006 (Mohr *et al.* 2008) (online at http://physics.nist.gov/constants) and from the 2008 compilation of the (PDG) (Amsler *et al.* 2008) (online at http://pdg.lbl.gov); see notes for details. The standard deviation uncertainty in the least significant digits is given in parentheses.

	Symbol	Spin	Charge number	Mass		
Name		I	z	m/u	mc_0^2/MeV	Notes
photon	γ	1	0	0	0	
neutrino	ν_e	1/2	0	≈ 0	≈ 0	1, 2
electron	e^-	1/2	-1	5.485 799 094 3(23)$\times 10^{-4}$	0.510 998 910(13)	3
muon	$\mu^\pm$	1/2	± 1	0.113 428 925 6(29)	105.658 366 8(38)	2
pion	$\pi^\pm$	0	± 1	0.149 834 76(37)	139.570 18(35)	2
pion	π^0	0	0	0.144 903 35(64)	134.9766(6)	2
proton	p	1/2	1	1.007 276 466 77(10)	938.272 013(23)	
neutron	n	1/2	0	1.008 664 915 97(43)	939.565 346(23)	
deuteron	d	1	1	2.013 553 212 724(78)	1875.612 793(47)	
triton	t	1/2	1	3.015 500 713 4(25)	2808.920 906(70)	4
helion	h	1/2	2	3.014 932 247 3(26)	2808.391 383(70)	4
α-particle	α	0	2	4.001 506 179 127(62)	3727.379 109(93)	
Z-boson	Z^0	1	0		91.1876(21)$\times 10^3$	2, 5
W-boson	$W^\pm$	1	± 1		80.398(25)$\times 10^3$	2, 5

(1) The neutrino and antineutrino have a small mass, $m_{\overline{\nu}_e} < 2\ \mathrm{eV}/c_0^2$ (Amsler *et al.* 2008). In addition to the electron neutrino ν_e, one also finds a tau neutrino, ν_τ, and a myon neutrino, ν_μ (and their antiparticles $\overline{\nu}$).

(2) These data are from the Particle Data Group (Amsler *et al.* 2008).

(3) The electron is sometimes denoted by e or as a β-particle by β^-. Its antiparticle e^+ (positron, also β^+) has the same mass as the electron e^- but opposite charge and opposite magnetic moment.

(4) Triton is the $^3H^+$, and helion the $^3He^{2+}$ particle.

(5) Z^0 and $W^\pm$ are gauge bosons (Amsler *et al.* 2008).

Name	Symbol	Magnetic moment μ/μ_N	Mean life[(a)] τ/s	Notes
photon	γ	0		
neutrino	ν_e	≈ 0		2, 6
electron	e^-	-1.001 159 652 181 11(74)		7, 8
muon	μ^+	8.890 596 98(23)	2.197 019(21)$\times 10^{-6}$	2, 8, 9
pion	$\pi^\pm$	0	2.6033(5)$\times 10^{-8}$	2
pion	π^0	0	8.4(6)$\times 10^{-17}$	2
proton	p	2.792 847 356(23)		8, 10
neutron	n	-1.913 042 73(45)	885.7(8)	8
deuteron	d	0.857 438 230 8(72)		8
triton	t	2.978 962 448(38)		8, 11
helion	h	-2.127 497 718(25)		8, 12
α-particle	α	0		

[(a)] The PDG (Amsler *et al.* 2008) gives the mean life (τ) values.

(6) The Particle Data Group (Amsler *et al.* 2008) gives $\mu/\mu_B < 0.74 \times 10^{-10}$.

(7) The value of the magnetic moment is given in Bohr magnetons μ/μ_B, $\mu_B = e\hbar/2m_e$.

(8) The sign of the magnetic moment is defined with respect to the direction of the spin angular momentum.

(9) μ^- and μ^+ have the same mass but opposite charge and opposite magnetic moment.

(10) The shielded proton magnetic moment, μ_p', is given by $\mu_p'/\mu_N = 2.792\,775\,598(30)$ (H_2O, sphere, 25 °C).

(11) The half-life, $t_{1/2}$, of the triton is about 12.3 a with a corresponding mean life, τ, of 17.7 a.

(12) This is the shielded helion magnetic moment, μ_h', given as μ_h'/μ_N (gas, sphere, 25 °C).

In nuclear physics and chemistry, the masses of particles are often quoted as their energy equivalents (usually in megaelectronvolts). The unified atomic mass unit corresponds to 931.494 028(23) MeV (Mohr *et al.* 2008).

Atom-like pairs of a positive particle and an electron are sometimes sufficiently stable to be treated as individual entities with special names.

Examples

positronium (e^+e^-; Ps)
m(Ps) = 1.097 152 515 21(46) ×10^{-3} u
muonium (μ^+e^-; Mu) m(Mu) = 0.113 977 490 9(29) u

7 REPORTING UNCERTAINTY

It is vital to report an uncertainty estimate along with a measurement. In brief, a report of a quantitative experimental (or theoretical) result should contain a statement about what the expected "best estimate" for the true result is, as well as a statement of the probable range of possible values specifying the uncertainty. The expected dispersion of the measured values arises from a number of sources. The contribution to the uncertainty from all these sources should be estimated as part of an uncertainty budget. The tables show some of the ways in which the contributions to the uncertainty budget can be estimated and combined and the examples below show how a full statement of the resulting combined uncertainty estimate can be presented. The present summary is based on GUM (1995).

7.1 Reporting Uncertainty for a Single Measured Quantity

Uncertainties for a measured quantity X can be reported in several ways by giving the expected best estimate for the quantity together with a second quantity defining an uncertainty that corresponds to some probable range for the true quantity. We use the notation X for measured quantities, x for measurement results, and u_c for uncertainty.

Example 1

$m_s = 100.021\,47$ g with a combined standard uncertainty (i.e., estimated standard uncertainty) of $u_c = 0.35$ mg. Since it can be assumed that the possible estimated values of the standard are approximately normally distributed with approximate standard deviation u_c, the unknown value of the standard is believed to lie in the interval $m_s \pm u_c$ with a level of confidence of approximately 68 %.

Name	Symbol	Definition	Notes
Probability distributions			
probability distribution of x	$f(x)$	The probability density of the quantity having the value x; normal (Gaussian), rectangular, triangular, Student-t, etc.	
expected value of x	$E[x]$	$E[x] = \int x\ f(x)\mathrm{d}x$	
mean	μ	$E[x]$	
variance	σ^2	$E[(x-\mu)^2]$	
standard deviation	σ	$\sigma = +\sqrt{\sigma^2}$	
Statistics			
number of measurements	N		
mean	$\overline{x}$	$\overline{x} = \frac{1}{N}\sum_{i=1}^{N} x_i$	
variance	$s^2(x)$	$s^2(x) = \frac{1}{N-1}\sum_{i=1}^{N}\left(x_i - \overline{x}\right)^2$	1
standard deviation	$s(x)$	$s(x) = +\sqrt{s^2(x)}$	
standard deviation of the mean	$s(\overline{x})$	$s(\overline{x}) = s(x)/\sqrt{N}$	
Uncertainties			
standard uncertainty of x_i	$u(x_i)$	Estimated by Type A or B approaches	2
Type A evaluation		Type A evaluation (of standard uncertainty) is a method of evaluation of a standard uncertainty by the statistical analysis of a series of observations	3

Name	Symbol	Definition	Notes
Type B evaluation		Type B evaluation (of standard uncertainty) is a method of evaluation of a standard uncertainty by means other than the statistical analysis of a series of observations (for instance, it is usually based on scientific judgement using all relevant information that is available)	4
relative standard uncertainty of x	$u_\mathrm{r}(x_i)$	$u_\mathrm{r}(x_i) = u(x_i)/\lvert x_i\rvert \quad (x_i \neq 0)$	
combined standard uncertainty of the measurement result y	$u_\mathrm{c}(y)$	Estimated uncertainty in y from all the component measurement results $y = f(x_1, x_2, \ldots, x_M)$	5
relative combined standard uncertainty of y	$u_{\mathrm{c},r}(y)$	$u_{\mathrm{c},r}(y) = u_\mathrm{c}(y)/\lvert y\rvert \quad (y \neq 0)$	
expanded uncertainty	U	$U = k\, u_\mathrm{c}(y)$	6
coverage factor	k		6

(1) This is an unbiased estimate and takes into account the removal of one degree of freedom because the spread is measured about the mean.

(2) The uncertainty in the result of a measurement generally consists of several components which may be grouped into two categories according to the way in which their numerical value is estimated:

Type A: Those that are evaluated by statistical methods. Type B: Those that are evaluated by other means.

A detailed report on uncertainty should consist of a complete list of the components, specifying for each component the method used to obtain its numerical value. This provides the "uncertainty budget".

(3) Examples of type A evaluations are calculating the standard deviation of the mean of a series of independent observations; using the method of least squares to fit a function to data in order to estimate the parameters of the function and their standard deviations; and carrying out an analysis of variance (ANOVA) in order to identify and quantify random effects in certain kinds of measurements. These components of the uncertainty are characterized by the estimated variances ${s_i}^2$ (or the estimated "standard deviations" s_i) and the number of degrees of freedom ν_i. Where appropriate, the covariances should be given.

(4) This knowledge may include previous measurement data, general knowledge of the behavior and properties of relevant materials and instruments, manufacturer's specifications, and data provided in calibration and other reports. These components of uncertainty should be characterized by quantities ${u_j}^2$, which may be considered approximations to the corresponding variances, the existence of which is assumed. The quantities ${u_j}^2$ may be treated like variances and the quantities u_j like standard deviations.

Examples of Type B evaluations:

(a) If it is reasonable to assume that the quantity, X, can be modeled by a normal probability distribution, then lower and upper limits a_- and a_+ should be estimated such that the best estimated value of the input quantity is $x = (a_- + a_+)/2$ (i.e., the centre of the limits) and there is one chance out of two (i.e., a 50 % probability) that the value of the quantity lies in the interval a_- to a_+, then $u \approx 1.48(a_+ - a_-)/2$.

(b) If however the quantity, X, is better represented by a rectangular distribution then the lower and upper limits a_- and a_+ of the input quantity should be estimated such that the probability that the value lies in the interval a_- and a_+ is, for all practical purposes, 100 %. Provided that there is no contradictory information, treat the quantity as if it is equally probable for its value to lie anywhere within the interval a_- to a_+, that is, model it by a uniform (i.e., rectangular) probability distribution. The best estimate of the value of the quantity is then $x = (a_- + a_+)/2$ with the uncertainty $u = (a_+ - a_-)/2\sqrt{3}$.

(5) The quantity, Y being measured, called the *measurand*, is not measured directly, but is determined from M other quantities $X_1, X_2, \ldots, X_M$ through a function f (sometimes called the measurement equation), $Y = f(X_1, X_2, \ldots, X_M)$. The quantities X_i include corrections (or correction factors), as well as quantities that take into account other sources of variability, such as different observers, instruments, samples, laboratories, etc. An estimate of the measured quantity Y, denoted $y = f(x_1, x_2, \cdots, x_M)$, is obtained from the measurement equation using *input estimates* $x_1, x_2, \ldots, x_M$ for the values of the M *input quantities*. A similar situation exists if other quantities are to be derived from measurements. The propagation of uncertainty is illustrated in the table above.

(6) Some commercial, industrial, and regulatory applications require a measure of uncertainty that defines an interval about a measurement result y within which the value of the measurand Y can be confidently asserted to be. In these cases, the *expanded uncertainty* U is used and is obtained by multiplying the combined standard uncertainty, $u_\mathrm{c}(y)$, by a *coverage factor* k. Thus, $U = k\, u_\mathrm{c}(y)$ and it is confidently believed that Y is greater than or equal to $y - U$ and is less than or equal to $y + U$, which is commonly written as $Y = y \pm U$. The value of the coverage factor k is chosen on the basis of the desired level of confidence to be associated with the interval defined by $U = k\, u_\mathrm{c}$. Typically, k is in the range of two to three. When the normal distribution applies and u_c is a reliable estimate of the standard deviation of y, $U = 2u_\mathrm{c}$ (i.e., $k = 2$) defines an interval having a level of confidence of approximately 95 %, and $U = 3u_\mathrm{c}$ (i.e., $k = 3$) defines an interval having a level of confidence greater than 99 %.

Example 2

$m_\mathrm{s} = (100.021\,47 \pm 0.000\,70)$ g, where the number following the symbol ± is the numerical value of an expanded uncertainty $U = k\,u_\mathrm{c}$, with U determined from a combined standard uncertainty (i.e., estimated standard deviation) $u_\mathrm{c} = 0.35$ mg and a coverage factor of $k = 2$. Since it can be assumed that the possible estimated values of the standard are approximately normally distributed with approximate standard deviation u_c, the unknown value of the standard is believed to lie within the interval defined by U with a level of confidence of 95 % (Section 7.3).

Example 3

$m_\mathrm{s} = 100.021\,47(35)$ g, where the number in parentheses denotes the combined standard uncertainty $u_\mathrm{c} = 0.35$ mg and is assumed to apply to the least significant digits.

7.2 Propagation of Uncertainty for Uncorrelated Measurements

For a discussion of the treatment of correlated uncertainties, see GUM (1995).

Table 1 Spectroscopic parameters for the ground state and the CCl-stretching fundamental ν_4 of CH^{35}ClF$_2$.

$\tilde{\nu}_0$ /cm^{-1}	0.0	809.2725(8)†
$\tilde{A}$ /cm^{-1}	0.341 393 08(7)	0.341 250 65(29)
$\tilde{B}$ /cm^{-1}	0.162 153 86(5)	0.161 332 69(19)
$\tilde{C}$ /cm^{-1}	0.116 996 20(16)	0.116 836 23(12)
$\tilde{D}_J$ /10^{-6} cm^{-1}	0.044 43(11)	0.053 562(30)
$\tilde{D}_{JK}$ /10^{-6} cm^{-1}	0.206 04(53)	0.134 46(16)
$\tilde{D}_K$ /10^{-6} cm^{-1}	0.123 18(45)	0.219 93(26)
$\tilde{d}_1$ /10^{-6} cm^{-1}	−0.014 71(11)	−0.011 482(22)
$\tilde{d}_2$ /10^{-6} cm^{-1}	−0.004 538(82)	−0.004 354 0(77)
$\tilde{H}_J$ /10^{-12} cm^{-1}	0.227(12)	0.227
$\tilde{H}_K$ /10^{-12} cm^{-1}	1.958(45)	1.958
d_rms /cm^{-1}	0.0018	0.0017
N	2452	3994
J_max	90	65

†The value has been corrected by a small average correction of +0.0015 cm^{-1}.
Standard deviations are given in parentheses as uncertainties in the last significant digits (after Luckhaus and Quack (1989)).

Measurement equation	Reported measurement result	Equation for the combined standard uncertainty	Notes
$Y = \sum_{i=1}^{N} a_i X_i$	$y = \sum_{i=1}^{N} a_i x_i$	$u_\mathrm{c}(y) = \left(\sum_{i=1}^{N} a_i^{\,2} u^2(x_i)\right)^{1/2}$	1
$Y = A X_1^{\,a_1} X_2^{\,a_2} \cdots X_N^{\,a_N}$	$y = A x_1^{\,a_1} x_2^{\,a_2} \cdots x_N^{\,a_N}$	$u_\mathrm{c,r}(y) = \left(\sum_{i=1}^{N} a_i^{\,2} u_\mathrm{r}^{\,2}(x_i)\right)^{1/2}$	2

(1) This is sometimes known as *addition in quadrature*. The measurement equation is represented by a sum of quantities X_i multiplied by a constant a_i. The a_i are assumed to be known with certainty.

(2) The measurement equation is represented by a product of quantities X_i raised to powers $a_1, a_2, \ldots, a_N$ and multiplied by a constant A. A and a_i are assumed to be known with certainty.

7.3 Reporting Uncertainties in Terms of Confidence Intervals

One can generally report the uncertainty by defining an interval, within which the quantity is expected to fall with a certain probability. This interval can be specified as $(y - U) \le Y \le (y + U)$.

Example

100.021 40 g $\le m_\mathrm{s} \le$ 100.021 54 g
or $m_\mathrm{s} = 100.021\,47(7)$ g
or $m_\mathrm{s} = (100.021\,47 \pm 0.000\,07)$ g

When specifying such an interval, one should provide the confidence as the estimated probability with which the true quantity is expected to be in the given range (for example, 60, 90, or 95 %). This probability can be estimated using a variety of probability distributions appropriate for the measurement under consideration (Gaussian, Student-t, etc. (GUM 1995, VIM 2008)).

7.4 Reporting Uncertainties in Tables of Spectroscopic Parameters

Presentation of spectroscopic parameters and their uncertainties should conform to the previous sections. The following example gives a table of spectroscopic parameters including the quantities, units, and their uncertainties to be reported. All quantities should be defined in the context of the publication under consideration by appropriate defining equations.

Table 1 summarizes the spectroscopic parameters (band centres, rotational constants, quartic, and some sextic centrifugal distortion constants) as given in the defining equation (1) of Luckhaus and Quack (1989), p. 746. They have been fitted numerically using the Watson S-reduced effective rotational Hamiltonian in the I^{r} representation. It should be noted that the uncertainties of the parameters shown as values in parentheses after the decimal point represent only the standard deviations of the numerical fitting procedure and are not obtained from an analysis of variance (ANOVA) within the GUM as described in this chapter. Parameters held fixed in the least squares procedure are stated without uncertainties.

8 ABBREVIATIONS AND ACRONYMS

Abbreviations and acronyms (words formed from the initial letters of groups of words that are frequently repeated) should be used sparingly. Unless they are well established (e.g., NMR, IR), they should always be defined once in any paper, and they should generally be avoided in titles and abstracts. Some acronyms have been accepted as common words, such as "laser" from the acronym LASER. Abbreviations used to denote physical quantities should if possible be replaced by the recommended symbol for the quantity (e.g., E_{i} rather than IP for ionization energy, see Section 3.3; ρ rather than dens. for mass density). For further recommendations concerning abbreviations, see Lide (1980).

A list of frequently used abbreviations and acronyms is given here to help readers, but not necessarily to encourage their universal usage. In many cases, an acronym can be found written in lower case letters and in capitals. In the list that follows, only the most common usage is given. More extensive lists for different spectroscopic methods have been published by IUPAC (Porter and Turner 1987, Sheppard 1991) and by Wendisch (1990); an extensive list for acronyms used in theoretical chemistry has been published by IUPAC (Brown *et al.* 1996).

A/D	analog-to-digital
AA	atomic absorption
AAS	atomic absorption spectroscopy
ac	alternating current
ACM	adiabatic channel model
ACT	activated complex theory
AD	atom diffraction
ADC	analog-to-digital converter
AES	Auger electron spectroscopy
AFM	atomic force microscopy
AIUPS	angle-integrated ultraviolet photoelectron spectroscopy
AM	amplitude modulated
amu	atomic mass unit
ANOVA	analysis of variance
AO	atomic orbital
APS	appearance potential spectroscopy
ARAES	angle-resolved Auger electron spectroscopy
ARPEFS	angle-resolved photoelectron fine structure
AS	Auger spectroscopy
ATR	attenuated total (internal) reflection
AU	astronomical unit
au	atomic unit
bcc	body-centered cubic
BIPM	Bureau International des Poids et Mesures
BIS	bremsstrahlung isochromat spectroscopy
BM	Bohr magneton (symbol: μ_{B})
bp	boiling point
CARS	coherent anti-Stokes Raman scattering
CAS	complete active space
CAS-SCF	complete active space–self-consistent field
CAT	computer average of transients
CAWIA	Commission on Atomic Weights and Isotopic Abundances (now CIAAW)
CC	coupled cluster
CCD	coupled charge device
CCL	color centre laser
CCSD	coupled-cluster singles and doubles excitation
CCU	Comité Consultatif d'Unités
CD	circular dichroism
CEELS	characteristic electron energy-loss spectroscopy
CELS	characteristic energy-loss spectroscopy
CEPA	coupled electron pair approximation
CGPM	Conférence Générale des Poids et Mesures
cgs, CGS	centimeter–gram–second
CI	chemical ionization
CI	configuration interaction
CIAAW	Commission on Isotopic Abundances and Atomic Weights (formerly CAWIA)
CIDEP	chemically induced dynamic electron polarization
CIDNP	chemically induced dynamic nuclear polarization
CIMS	chemical ionization mass spectroscopy
CIPM	Comité International des Poids et Mesures
CIVR	collision-induced vibrational relaxation
CIVR	classical intramolecular vibrational redistribution
CNDO	complete neglect of differential overlap
CODATA	Committee on Data for Science and Technology
COMAS	Concentration Modulation Absorption Spectroscopy
CRDS	cavity ring-down spectroscopy
CSRS	coherent Stokes–Raman scattering
CT	charge transfer
CVD	chemical vapor deposition
CW	continuous wave
D/A	digital-to-analog

DAC	digital-to-analog converter
D4WM	degenerate 4-wave mixing
DAPS	disappearance potential spectroscopy
dc, DC	direct current
DFG	difference frequency generation
DFT	density functional theory
DHF	Dirac-Hartree-Fock
DQMC	diffusion quantum Monte Carlo
DRIFTS	diffuse reflectance infrared Fourier transform spectroscopy
EAPFS	extended appearance potential fine structure
EC	electron capture
ECD	electron capture detector
ED	electron diffraction
EDA	electron donor−acceptor [complex]
EDX	energy-dispersive X-ray analysis
EELS	electron energy-loss spectroscopy
EH	electron holography
EI	electron impact ionization
EIS	electron impact spectroscopy
EIS	electrochemical impedance spectroscopy
EL	electroluminescence
ELDOR	electron−electron double resonance
ELEED	elastic low-energy electron diffraction
emu	electromagnetic unit
ENDOR	electron−nuclear double resonance
EPR	electron paramagnetic resonance
ESCA	electron spectroscopy for chemical applications (or analysis), see XPS
ESD	electron-stimulated desorption
ESDIAD	electron-stimulated desorption ion angular distribution
ESR	electron spin resonance
esu	electrostatic unit
ETS	electron transmission spectroscopy, electron tunneling spectroscopy
EXAFS	extended X-ray absorption fine structure
EXAPS	electron-excited X-ray appearance potential spectroscopy
EXELFS	extended electron energy-loss fine structure
FAB(MS)	fast atom bombardment (mass spectroscopy)
FD	field desorption
FEESP	field-emitted electron spin-polarization [spectroscopy]
FEM	field emission [electron] microscopy
FES	field emission spectroscopy
FFT	fast Fourier transform
FI	field ionization
FID	flame ionization detector
FID	free induction decay
FIM	field-ion microscopy
FIMS	field-ion mass spectroscopy
FIR	far-infrared
FM	frequency modulated
FPD	flame photometric detector
FSR	free spectral range
FT	Fourier transform
FTD	flame thermionic detector
FTIR	Fourier transform infrared
FWHM	full width at half maximum
GC	gas chromatography
GIXS	grazing-incidence X-ray scattering
GTO	Gaussian-type orbital
GVB	generalized valence bond
HEED	high-energy electron diffraction
HEELS	high-energy electron energy-loss spectroscopy
HEIS	high-energy ion scattering
HF	Hartree−Fock
hfs	hyperfine structure (hyperfine splitting)
HMO	Hückel molecular orbital
HOMO	highest occupied molecular orbital
HREELS	high-resolution electron energy-loss spectroscopy
HTS	Hadamard transform spectroscopy
HWP	half-wave potential
I/O	input−output
IBA	ion beam analysis
IC	integrated circuit
ICISS	impact-collision ion scattering spectroscopy
ICR	ion cyclotron resonance
ICSU	International Council for Science
IEP	isoelectric point
IEPA	independent electron pair approximation
IETS	inelastic electron tunneling spectroscopy
ILEED	inelastic low-energy electron diffraction
INDO	intermediate neglect of differential overlap
INDOR	internuclear double resonance
INS	inelastic neutron scattering
INS	ion neutralization spectroscopy
IP	ionization potential (symbol: E_i)
IPES	inverse photoelectron spectroscopy
IPTS	International Practical Temperature Scale
IR	infrared
IRAS	infrared absorption spectroscopy
IRS	infrared spectroscopy
IS	ionization spectroscopy
ISO	International Organization for Standardization
ISQ	International System of Quantities
ISS	ion scattering spectroscopy
ITS	International Temperature Scale
IUPAC	International Union of Pure and Applied Chemistry
IUPAP	International Union of Pure and Applied Physics
KS	Kohn−Sham
L2TOFMS	laser desorption laser photoionization time-of-flight mass spectroscopy

LASER	light amplification by stimulated emission of radiation
LCAO	linear combination of atomic orbitals
LCMO	linear combination of molecular orbitals
LED	light-emitting diode
LEED	low-energy electron diffraction
LEELS	low-energy electron energy-loss spectroscopy
LEES	low-energy electron scattering
LEF	laser excitation fluorescence
LEIS	low-energy ion scattering
LEPD	low-energy positron diffraction
LET	linear energy transfer
LID	laser-induced desorption
LIDAR	light detection and ranging
LIF	laser-induced fluorescence
LIGS	laser-induced grating spectroscopy
LIMA	laser microprobe mass analysis
LIS	laser isotope separation
LMR	laser magnetic resonance
LUMO	lowest unoccupied molecular orbital
MAR	magic-angle rotation
MAS	magic-angle spinning
MASER	microwave amplification by stimulated emission of radiation
MBE	molecular beam epitaxy
MBGF	many-body Green's function
MBPT	many-body perturbation theory
MC	Monte Carlo
MCA	multichannel analyzer
MCD	magnetic circular dichroism
MCS	multichannel scaler
MCSCF	multiconfiguration self-consistent field
MD	molecular dynamics
MDS	metastable deexcitation spectroscopy
MEED	medium-energy electron diffraction
MEIS	medium-energy ion scattering
MFM	magnetic force microscopy
MINDO	modified intermediate neglect of differential overlap
MIR	mid-infrared
MKS	metre–kilogram–second
MKSA	metre–kilogram–second–ampere
MM	molecular mechanics
MNDO	modified neglect of diatomic overlap
MO	molecular orbital
MOCVD	metal–organic chemical vapor deposition
MOMBE	metal–organic molecular beam epitaxy
MORD	magnetic optical rotatory dispersion
MOS	metal oxide semiconductor
MPI	multiphoton ionization
MPPT	Møller–Plesset perturbation theory
MP2	Møller–Plesset second order
MP-SCF	Møller–Plesset self-consistent field
MRCI	multi-reference configuration interaction
MRD	magnetic rotatory dispersion
MRI	magnetic resonance imaging
MS	mass spectroscopy
MW	microwave
MW	molecular weight (symbol: M_r)
NAA	neutron activation analysis
NDDO	neglect of diatomic differential overlap
Nd:YAG	Nd-doped YAG
NEXAFS	near-edge X-ray absorption fine structure
NIR	near-infrared
NIR	nonionizing radiation
NMA	nuclear microanalysis
NMR	nuclear magnetic resonance
NOE	nuclear Overhauser effect
NQR	nuclear quadrupole resonance
ODMR	optically detected magnetic resonance
OGS	opto-galvanic spectroscopy
ORD	optical rotatory dispersion
PAS	photoacoustic spectroscopy
PD	photoelectron diffraction
PDG	Particle Data Group
PED	photoelectron diffraction
PEH	photoelectron holography
PES	photoelectron spectroscopy
PIES	Penning ionization electron spectroscopy, see PIS
PIPECO	photoion–photoelectron coincidence [spectroscopy]
PIS	Penning ionization (electron) spectroscopy
PMT	photomultiplier tube
ppb	part per billion
pphm	part per hundred million
ppm	part per million
PPP	Pariser–Parr–Pople
PS	see PES
PSD	photon-stimulated desorption
pzc	point of zero charge
QM/MM	quantum mechanical/molecular mechanics methods
QMB	quartz microbalance
QMC	quantum Monte Carlo
QMS	quadrupole mass spectrometer
RADAR	radiowave detection and ranging
RBS	Rutherford (ion) back scattering
RD	rotatory dispersion
REM	reflection electron microscopy
REMPI	resonance enhanced multiphoton ionization
RF	radio frequency
RHEED	reflection high-energy electron diffraction
RHF	restricted Hartree–Fock
RIMS	resonant ionization mass spectroscopy
RKR	Rydberg–Klein–Rees [potential]
rms	root mean square
RRS	resonance Raman spectroscopy

RS	Raman spectroscopy
RSPT	Rayleigh–Schrödinger perturbation theory
S	singlet
SAM	scanning Auger microscopy
SBS	stimulated Brillouin scattering
SBZ	surface Brillouin zone
SCF	self-consistent field
SDCI	singly and doubly excited configuration interaction
SEELFS	surface extended energy-loss fine structure
SEFT	spin-echo Fourier transform
SEM	scanning [reflection] electron microscopy
SEP	stimulated emission pumping
SERS	surface-enhanced Raman spectroscopy
SES	secondary electron spectroscopy
SESCA	scanning electron spectroscopy for chemical applications
SEXAFS	surface extended X-ray absorption fine structure
SFG	sum-frequency generation
SHG	second-harmonic generation
SI	Système International d'Unités
SIMS	secondary ion mass spectroscopy
SMOKE	surface magneto-optic Kerr effect
SOC	spin–orbit coupling
SOR	synchrotron orbital radiation
SPIES	surface Penning ionization electron spectroscopy
SPLEED	spin-polarized low-energy electron diffraction
SPM	scanning probe microscopy
SR	synchrotron radiation
SRS	synchrotron radiation source
SSIMS	static secondary ion mass spectroscopy
STEM	scanning transmission [electron] microscopy
STM	scanning tunneling (electron) microscopy
STO	Slater-type orbital
SVLF	single vibronic level fluorescence
T	triplet
TCF	time correlation function
TDL	tuneable diode laser
TDDFT	time-dependent density functional theory
TDMS	tandem quadrupole mass spectroscopy
TDS	thermal desorption spectroscopy
TED	transmission electron diffraction
TEM	transmission electron microscopy
THEED	transmission high-energy electron diffraction
TOF	time-of-flight [analysis]
TR3	time-resolved resonance Raman scattering
TST	transition state theory
UHF	ultrahigh frequency
UHF	unrestricted Hartree–Fock
UHV	ultrahigh vacuum
UP[E]S	ultraviolet photoelectron spectroscopy
UV	ultraviolet
VB	valence bond
VCD	vibrational circular dichroism
VEELS	vibrational electron energy-loss spectroscopy
VHF	very high frequency
VIS	visible
VLEED	very-low-energy electron diffraction
VLSI	very large scale integration
VPC	vapor-phase chromatography
VSEPR	valence shell electron pair repulsion
VUV	vacuum ultraviolet
WFC	work function change
X	halogen
XAFS	X-ray absorption fine structure
XANES	X-ray absorption near-edge structure [spectroscopy]
XAPS	X-ray appearance potential spectroscopy
XPD	X-ray photoelectron diffraction
XPES	X-ray photoelectron spectroscopy
XPS	X-ray photoelectron spectroscopy
XRD	X-ray diffraction
XSW	X-ray standing wave
YAG	yttrium–aluminium–garnet
ZPE	zero-point energy

END NOTES

[a] The MCO report can be found at ftp://ftp.hq.nasa.gov/pub/pao/reports/1999/MCO_report.pdf.

[b] Impulse (change of momentum) means here the time integral of the force.

[c] The Clinical Chemistry Division of IUPAC recommended that "amount-of-substance concentration" be abbreviated "substance concentration" (Rigg *et al.* 1995).

[d] An exception is made for certain characteristic numbers or "dimensionless quantities" used in the study of transport processes for which the internationally agreed symbols consist of two letters.

Example

pH

[e] However, only the lower case l is used by ISO and the International Electrochemical Commission (IEC).

[f] The SI unit of this quantity is m mol^{-1}. In the Gaussian system, however, the definition of C_j as $C_j = \int_{\mathrm{band}\ j} \tilde{\nu}\alpha_\mathrm{m}''(\tilde{\nu})\mathrm{d}\tilde{\nu}$ is often adopted with unit cm mol^{-1}.

[g] The kilogram is the only base unit which is not defined by a measurement on a system defined by natural microscopic constants or an experimental setup derived from such a system. Rather, it is defined by a human artifact (the international prototype of the kilogram). Therefore, alternative definitions of the kilogram are under current discussion (Kind and Quinn 1999, Mills *et al.* 2005, Mills 2005).

Numerical Energy Conversion Factors

$E = h\nu = hc\tilde{\nu} = kT$; $E_\mathrm{m} = N_\mathrm{A}E$

		wavenumber $\tilde{\nu}$	frequency ν	energy E			molar energy E_m		temperature T
		cm^{-1}	MHz	aJ	eV	E_h	$\mathrm{kJ\ mol}^{-1}$	$\mathrm{kcal\ mol}^{-1}$	K
$\tilde{\nu}$:	$1\,\mathrm{cm}^{-1}$	$\widehat{=}\ 1$	$2.997\,925\times10^{4}$	$1.986\,446\times10^{-5}$	$1.239\,842\times10^{-4}$	$4.556\,335\times10^{-6}$	$11.962\,66\times10^{-3}$	$2.859\,144\times10^{-3}$	$1.438\,775$
ν:	1 MHz	$\widehat{=}\ 3.335\,641\times10^{-5}$	1	$6.626\,069\times10^{-10}$	$4.135\,667\times10^{-9}$	$1.519\,830\times10^{-10}$	$3.990\,313\times10^{-7}$	$9.537\,076\times10^{-8}$	$4.799\,237\times10^{-5}$
E:	1 aJ	$\widehat{=}\ 50\,341.17$	$1.509\,190\times10^{9}$	1	$6.241\,510$	$0.229\,371\,3$	602.2142	143.9326	$7.242\,963\times10^{4}$
	1 eV	$\widehat{=}\ 8065.545$	$2.417\,989\times10^{8}$	$0.160\,217\,6$	1	$3.674\,933\times10^{-2}$	$96.485\,34$	$23.060\,55$	$1.160\,451\times10^{4}$
	$1\ E_\mathrm{h}$	$\widehat{=}\ 219\,474.6$	$6.579\,684\times10^{9}$	$4.359\,744$	$27.211\,38$	1	2625.500	627.5095	$3.157\,747\times10^{5}$
E_m:	$1\ \mathrm{kJ\ mol}^{-1}$	$\widehat{=}\ 83.593\,47$	$2.506\,069\times10^{6}$	$1.660\,539\times10^{-3}$	$1.036\,427\times10^{-2}$	$3.808\,799\times10^{-4}$	1	$0.239\,005\,7$	120.2722
	$1\ \mathrm{kcal\ mol}^{-1}$	$\widehat{=}\ 349.7551$	$1.048\,539\times10^{7}$	$6.947\,694\times10^{-3}$	$4.336\,410\times10^{-2}$	$1.593\,601\times10^{-3}$	4.184	1	503.2189
T:	1 K	$\widehat{=}\ 0.695\,035\,6$	$2.083\,664\times10^{4}$	$1.380\,650\times10^{-5}$	$8.617\,343\times10^{-5}$	$3.166\,815\times10^{-6}$	$8.314\,472\times10^{-3}$	$1.987\,207\times10^{-3}$	1

The symbol $\widehat{=}$ should be read as meaning 'approximately corresponding to' or 'is approximately equivalent to'. The conversion from kJ to kcal is exact by definition of the thermochemical kcal ($1\,\mathrm{kcal} = 4.184\,\mathrm{kJ}$). The values in this table have been obtained from the constants in Chapter 6. The last digit given may not be significant in all cases.

Examples of the use of this table:

$1\ \mathrm{aJ} \ \widehat{=}\ 50\,341.17\,\mathrm{cm}^{-1}$

$1\ \mathrm{eV} \ \widehat{=}\ 96.485\,34\ \mathrm{kJ\ mol}^{-1}$

Examples of the derivation of the conversion factors:

1 aJ to MHz

$$\frac{(1\ \mathrm{aJ})}{h} \ \widehat{=}\ \frac{10^{-18}\ \mathrm{J}}{6.626\,068\,96\times10^{-34}\ \mathrm{J}\ s} \ \widehat{=}\ 1.509\,190\times10^{15}\ \mathrm{s}^{-1} \ \widehat{=}\ 1.509\,190\times10^{9}\ \mathrm{MHz}$$

$1\,\mathrm{cm}^{-1}$ to eV

$$(1\ \mathrm{cm}^{-1})\ hc\left(\frac{e}{e}\right) \ \widehat{=}\ \frac{(1.986\,445\,501\times10^{-25}\ \mathrm{J})\times10^{2}\ e}{1.602\,176\,487\times10^{-19}\ \mathrm{C}} \ \widehat{=}\ 1.239\,842\times10^{-4}\ \mathrm{eV}$$

$1\ E_\mathrm{h}$ to $\mathrm{kJ\ mol}^{-1}$

$$(1\ E_\mathrm{h})\ N_\mathrm{A} \ \widehat{=}\ (4.359\,743\,94\times10^{-18}\ \mathrm{J})\times(6.022\,141\,79\times10^{23}\ \mathrm{mol}^{-1}) \ \widehat{=}\ 2625.500\ \mathrm{kJ\ mol}^{-1}$$

$1\ \mathrm{kcal\ mol}^{-1}$ to cm^{-1}

$$\frac{(1\ \mathrm{kcal\ mol}^{-1})}{hcN_\mathrm{A}} \ \widehat{=}\ \frac{4.184\times(1\ \mathrm{kJ\ mol}^{-1})}{hcN_\mathrm{A}}$$

$$\widehat{=}\ \frac{4.184\times(10^{3}\ \mathrm{J\ mol}^{-1})}{(1.986\,445\,501\times10^{-25}\ \mathrm{J})\times10^{2}\,\mathrm{cm}\times(6.022\,141\,79\times10^{23}\ \mathrm{mol}^{-1})} \ \widehat{=}\ 349.7551\,\mathrm{cm}^{-1}$$

REFERENCES

Albert, S., Albert, K.K., Hollenstein, H., Tanner, C.M., and Quack, M. (2011) Fundamentals of rotation–vibration spectra, in *Handbook of High-resolution Spectroscopy*, Quack, M. and Merkt, F. (eds), John Wiley & Sons, Ltd., Chichester, UK.

Albert, S., Albert, K.K., and Quack, M. (2011) High-resolution Fourier transform infrared spectroscopy, in *Handbook of High-resolution Spectroscopy*, Quack, M. and Merkt, F. (eds), John Wiley & Sons, Ltd., Chichester, UK.

Albert, S. and Quack, M. (2007) Rovibrational spectroscopy of chiral and aromatic compounds. *ChemPhysChem*, **8**, 1271–1281.

Alexander, M.H., Andresen, P., Bacis, R., Bersohn, R., Comes, F.J., Dagdigian, P.J., Dixon, R.N., Field, R.W., Flynn, G.W., Gericke, K.-H. *et al.* (1988) A nomenclature for Λ-doublet levels in rotating linear molecules. *Journal of Chemical Physics*, **89**, 1749–1753.

Amrein, A., Quack, M., and Schmitt, U. (1988) High-resolution interferometric Fourier transform infrared absorption spectroscopy in supersonic free jet expansions: Carbon monoxide, nitric oxide, methane, ethyne, propyne, and trifluoromethane. *Journal of Physical Chemistry*, **92**, 5455–5466.

Amsler, C., Doser, M., Antonelli, M., Asner, D.M., Babu, K.S., Baer, H., Band, H.R., Barnett, R.M., Bergren, E., Beringer, J. *et al.* (2008) Review of particle physics, 2008–2009. Review of particle properties, 2008–2009. *Physics Letters B*, **667**, 1–1340. http://pdg.lbl.gov

Becker, E.D. (1978) Recommendations for the presentation of infrared absorption spectra in data collections — A. Condensed phases. *Pure and Applied Chemistry*, **50**, 231–236.

Becker, E.D., Durig, J.R., Harris, W.C., and Rosasco, G.J. (1981) Presentation of Raman spectra in data collections. *Pure and Applied Chemistry*, **53**, 1879–1885.

Bertie, J.E. and Dale Keefe, C. (1994) Comparison of infrared absorption intensities of benzene in the liquid and gas phases. *Journal of Chemical Physics*, **101**, 4610–4616.

Bertie, J.E., Zhang, S.L., Eysel, H.H., Baluja, S., and Ahmed, M.K. (1993) Infrared intensities of liquids XI: Infrared refractive indices from 8000 to 2 cm^{-1}, absolute integrated intensities, and dipole moment derivatives of methanol at 25 °C. *Applied Spectroscopy*, **47**, 1100–1114.

Beynon, J.H. (1978) Recommendations for symbolism and nomenclature for mass spectroscopy. *Pure and Applied Chemistry*, **50**, 65–73.

BIPM (2006) *Le Système International d'Unités (SI)*, Bureau International des Poids et Mesures, Sèvres, 8th French and English edition.

de Boer, J. (1994/95) On the history of quantity calculus and the international system. *Metrologia*, **31**, 405–429.

Boggs, J.E. (1998) Guidelines for presentation of methodological choices in the publication of computational results. A. *Ab Initio* electronic structure calculations. *Pure and Applied Chemistry*, **70**, 1015–1018.

Brand, J.C.D., Callomon, J.H., Innes, K.K., Jortner, J., Leach, S., Levy, D.H., Merer, A.J., Mills, I.M., Moore, C.B., Parmenter, C.S. *et al.* (1983) The vibrational numbering of bands in the spectra of polyatomic molecules. *Journal of Molecular Spectroscopy*, **99**, 482–483.

Brown, J.M., Buenker, R.J., Carrington, A., di Lauro, C., Dixon, R.N., Field, R.W., Hougen, J.T., Hüttner, W., Kuchitsu, K., Mehring, M. *et al.* (2000) Remarks on the signs of g-factors in atomic and molecular Zeeman spectroscopy. *Molecular Physics*, **98**, 1597–1601.

Brown, J.M., Hougen, J.T., Huber, K.-P., Johns, J.W.C., Kopp, I., Lefebvre-Brion, H., Merer, A.J., Ramsay, D.A., Rostas, J., and Zare, R.N. (1975) The labeling of parity doublet levels in linear molecules. *Journal of Molecular Spectroscopy*, **55**, 500–503.

Brown, R.D., Boggs, J.E., Hilderbrandt, R., Lim, K., Mills, I.M., Nikitin, E., and Palmer, M.H. (1996) Acronyms used in theoretical chemistry. *Pure and Applied Chemistry*, **68**, 387–456.

Bunker, P.R. and Jensen, P. (1998) *Molecular Symmetry and Spectroscopy*, 2nd edition, NRC Research Press, Ottawa.

Bunker, P.R., Schutte, C.J.H., Hougen, J.T., Mills, I.M., Watson, J.K.G., and Winnewisser, B.P. (1997) Notations and conventions in molecular spectroscopy: Part 3. Permutation and permutation-inversion symmetry notation. *Pure and Applied Chemistry*, **69**, 1651–1657.

Cardarelli, F. (1999) *Scientific Unit Conversion*, Springer, London.

Cohen, E.R., Cvitaš, T., Frey, J.G., Holmström, B., Kuchitsu, K., Marquardt, R., Mills, I., Pavese, F., Quack, M., Stohner, J., Strauss, H.L., Takami, M., and Thor, A.J. (2008) *Quantities, Units and Symbols in Physical Chemistry*, 3rd edition, 2nd printing, IUPAC and Royal Society of Chemistry, Cambridge.

Cohen, E.R. and Giacomo, P. (1987) Symbols, units, nomenclature and fundamental constants in physics. Revision. Also published in *Physica (1987)*, **146A**, 1–67. Document IUPAP-25 (IUPAP-SUNAMCO 87-1).

Dybkaer, R. (2001) Unit "katal" for catalytic activity. *Pure and Applied Chemistry*, **73**, 927–931.

Field, R.W., Baraban, J.H., Lipoff, S.H., and Beck, A.R. (2011) Effective hamiltonians for electronic fine structure and polyatomic vibrations, in *Handbook of High-resolution Spectroscopy*, Quack, M. and Merkt, F. (eds), John Wiley & Sons, Ltd., Chichester, UK.

Flaud, J.-M. and Orphal, J. (2011) Spectroscopy of the earth's atmosphere, in *Handbook of High-resolution Spectroscopy*, Quack, M. and Merkt, F. (eds), John Wiley & Sons, Ltd., Chichester, UK.

Flowers, J.L. and Petley, B.W. (2008) Planck, units, and modern metrology. *Annalen der Physik (Berlin)*, **17**, 101–114.

Graner, G., Hirota, E., Iijima, T., Kuchitsu, K., Ramsay, D.A., Vogt, J., and Vogt, N. (2000) Structure data of free polyatomic molecules, in *Landolt-Börnstein, New Series, II/25C*, Kuchitsu, K. (ed), Springer, Berlin, pp. 7–10.

Guggenheim, E.A. (1942) Units and dimensions. *Philosophical Magazine*, **33**, 479–496.

GUM (1995) *Guide to the Expression of Uncertainty in Measurement, BIPM, IEC, IFCC, ISO, IUPAC, IUPAP, OIML*, 1st edition, International Organization for Standardization, Geneva, corrected and reprinted.

Hamermesh, M. (1962) *Group Theory and its Application to Physical Problems*, Addison-Wesley, Reading.

Harris, R.K., Becker, E.D., Cabral de Menezes, S.M., Goodfellow, R., and Granger, P. (1997) Parameters and symbols for use in nuclear magnetic resonance. *Pure and Applied Chemistry*, **69**, 2489–2495.

Harris, R.K., Becker, E.D., Cabral de Menezes, S.M., Goodfellow, R., and Granger, P. (2001) NMR nomenclature. Nuclear spin properties and conventions for chemical shifts. *Pure and Applied Chemistry*, **73**, 1795–1818.

Herzberg, G. (1946) *Molecular Spectra and Molecular Structure Vol. II. Infrared and Raman Spectra of Polyatomic Molecules*, Van Nostrand, Princeton.

Herzberg, G. (1950) *Molecular Spectra and Molecular Structure Vol. I. Spectra of Diatomic Molecules*, Van Nostrand, Princeton.

Herzberg, G. (1966) *Molecular Spectra and Molecular Structure Vol. III. Electronic Spectra and Electronic Structure of Polyatomic Molecules*, Van Nostrand, Princeton.

Hippler, M., Miloglyadov, E., Quack, M., and Seyfang, G. (2011) Mass and isotope-selective infrared spectroscopy, in *Handbook of High-resolution Spectroscopy*, Quack, M. and Merkt, F. (eds), John Wiley & Sons, Ltd., Chichester, UK.

IEC (2005) *International Standard, International Electrochemical Commission*, IEC 60027-2, Geneva.

ISO (1993) *ISO Standards Handbook 2. Quantities and Units*, ISO, Geneva.

Jenkins, F.A. (1953) Report of Subcommittee f (Notation for the Spectra of Diatomic Molecules). *Journal of the Optical Society of America*, **43**, 425–426.

Jenkins, A.D., Kratochvíl, P., Stepto, R.F.T., and Suter, U.W. (1996) Glossary of basic terms in polymer science. *Pure and Applied Chemistry*, **68**, 2287–2311.

Jerrard, H.G. and McNeill, D.B. (1980) *A Dictionary of Scientific Units*, 3rd edition, Chapman Hall, London.

Kind, D. and Quinn, T.J. (1999) Metrology: Quo Vadis? *Physics Today*, **52**, 13–15.

Lamola, A.A. and Wrighton, M.S. (1984) Recommended standards for reporting photochemical data. *Pure and Applied Chemistry*, **56**, 939–944.

Lide, D.R. Jr. (1980) Use of abbreviations in the chemical literature. *Pure and Applied Chemistry*, **52**, 2229–2232.

Longuet-Higgins, H.C. (1963) The symmetry groups of non-rigid molecules. *Molecular Physics*, **6**, 445–460.

Luckhaus, D. and Quack, M. (1989) The far infrared pure rotational spectrum and the Coriolis coupling between ν_3 and ν_8 in $CH^{35}ClF_2$. *Molecular Physics*, **68**, (3), 745–758.

Maki, A.G. and Wells, J.S. (1991) *Wavenumber Calibration Tables from Heterodyne Frequency Measurements*. NIST Special Publication 821, U.S. Department of Commerce.

Markley, J.L., Bax, A., Arata, Y., Hilbers, C.W., Kaptein, R., Sykes, B.D., Wright, P.E., and Wüthrich, K. (1998) Recommendations for the presentation of NMR structures of proteins and nucleic acids. *Pure and Applied Chemistry*, **70**, 117–142.

McNaught, A.D. and Wilkinson, A. (1997) *Compendium of Chemical Terminology – The Gold Book*, 2nd edition, Blackwell, Oxford.

Merkt, F. and Quack, M. (2011) Molecular quantum mechanics and molecular spectra, molecular symmetry, and interaction of matter with radiation, in *Handbook of High-resolution Spectroscopy*, Quack, M. and Merkt, F. (eds), John Wiley & Sons, Ltd., Chichester, UK.

Mills, I.M. (1997) The language of science. *Metrologia*, **34**, 101–109.

Mills, I.M. (2005) On defining base units in terms of fundamental constants. *Molecular Physics*, **103**, 2989–2999.

Mills, I., Cvitaš, T., Homann, K., Kallay, N., and Kuchitsu, K. (1988) *Quantities, Units and Symbols in Physical Chemistry*, 1st edition, Blackwell Science, Oxford.

Mills, I., Cvitaš, T., Homann, K., Kallay, N., and Kuchitsu, K. (1993) *Quantities, Units and Symbols in Physical Chemistry*, 2nd edition, Blackwell Science, Oxford.

Mills, I.M., Mohr, P.J., Quinn, T.J., Taylor, B.N., and Williams, E.R. (2005) Redefinition of the kilogram: A decision whose time has come. *Metrologia*, **42**, 71–80.

Mills, I. and Morfey, C. (2005) On logarithmic ratio quantities and their units. *Metrologia*, **42**, 246–252.

Mills, I.M. and Quack, M. (2002) Introduction to 'The Symmetry Groups of Non-Rigid Molecules' by H. C. Longuet-Higgins. *Molecular Physics*, **100**, 9–10.

Mohr, P.J., Taylor, B.N., and Newell, D.B. (2008) CODATA recommended values of the fundamental physical constants: 2006. *Reviews of Modern Physics*, **80**, 633–730. http://physics.nist.gov/constants

Morino, Y. and Shimanouchi, T. (1978) Definition and symbolism of molecular force constants. *Pure and Applied Chemistry*, **50**, 1707–1713.

Mullay, J. (1987) Estimation of atomic and group electronegativities. *Structure and Bonding (Berlin)*, **66**, 1–25.

Müller, P. (1994) Glossary of terms used in physical organic chemistry. *Pure and Applied Chemistry*, **66**, 1077–1184.

Mulliken, R.S. (1955) Report on notation for the spectra of polyatomic molecules. *Journal of Chemical Physics*, **23**, 1997–2011.

Mulliken, R.S. (1956) Erratum: Report on Notation for the spectra of polyatomic molecules. *Journal of Chemical Physics*, **24**, 1118.

Physical Chemistry Division, Commission on Molecular Structure and Spectroscopy (1972) Recommendations for the presentation of NMR data for publication in chemical journals. *Pure and Applied Chemistry*, **29**, 625–628.

Physical Chemistry Division, Commission on Molecular Structure and Spectroscopy (1976a) Nomenclature and conventions for reporting Mössbauer spectroscopic data. *Pure and Applied Chemistry*, **45**, 211–216.

Physical Chemistry Division, Commission on Molecular Structure and Spectroscopy (1976b) Nomenclature and spectral presentation in electron spectroscopy resulting from excitation by photons. *Pure and Applied Chemistry*, **45**, 221–224.

Physical Chemistry Division, Commission on Molecular Structure and Spectroscopy (1976c) Presentation of NMR data for publication in chemical journals–B. Conventions relating to spectra from nuclei other than protons. *Pure and Applied Chemistry*, **45**, 217–219.

Polo, S.R. and Wilson, M.K. (1955) Infrared intensities in liquid and gas phases. *Journal of Chemistry Physics*, **23**, 2376–2377.

Porter, H.Q. and Turner, D.W. (1987) A descriptive classification of the electron spectroscopies. *Pure and Applied Chemistry*, **59**, 1343–1406.

Pugh, L.A. and Rao, K.N. (1978) Intensities from infrared spectra, in *Molecular Spectroscopy: Modern Research*, Rao, K.N. (ed), Academic Press, New York, Vol. 2.

Quack, M. (1977) Detailed symmetry selection rules for reactive collisions. *Molecular Physics*, **34**, 477–504.

Quack, M. (1990) Spectra and dynamics of coupled vibrations in polyatomic molecules. *Annual Review of Physical Chemistry*, **41**, 839–874.

Quack, M. (1995) Molecular infrared spectra and molecular motion. *Journal of Molecular Structure*, **347**, 245–266.

Quack, M. (1998a) Commission I.1 at the IUPAC general assembly 1995. Summary minutes. *Chemistry International*, **20**, 12.

Quack, M. (1998b) Multiphoton excitation, in *Encyclopedia of Computational Chemistry*, Rague Schleyer, P.V., Allinger, N., Clark, T., Gasteiger, J., Kollman, P.A., Schaefer III, H.F., and Schreiner, P.R. (eds), John Wiley & Sons, Chichester, UK, pp. 1775–1791, Vol. 3.

Quack, M. and Kutzelnigg, W. (1995) Molecular spectroscopy and molecular dynamics: theory and experiment. *Berichte der Bunsen-Gesellschaft für Physikalische Chemie*, **99**(3), 231–245.

Quack, M. and Stohner, J. (2003) Combined multidimensional anharmonic and parity violating effects in CDBrClF. *Journal of Chemical Physics*, **119**, 11228–11240.

Quack, M. and Stohner, J. (2005) Parity violation in chiral molecules. *Chimia*, **59**, 530–538.

Quack, M. (2011) Fundamental symmetries and symmetry violations from high-resolution spectroscopy, in *Handbook of High-resolution Spectroscopy*, Quack, M. and Merkt, F. (eds), John Wiley & Sons, Ltd., Chichester, UK.

Rigaudy, J. and Klesney, S.P. (1979) *IUPAC Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F, and H*, 4th edition, Pergamon Press, Oxford.

Rigg, J.C., Brown, S.S., Dybkaer, R., and Olesen, H. (eds.) (1995) *Compendium of Terminology and Nomenclature of Properties in Clinical Laboratory Sciences*, Blackwell, Oxford.

Schnell, M. (2011) Group theory for high-resolution spectroscopy of nonrigid molecules, in *Handbook of High-resolution Spectroscopy*, Quack, M. and Merkt, F. (eds), John Wiley & Sons, Ltd., Chichester, UK.

Schutte, C.J.H., Bertie, J.E., Bunker, P.R., Hougen, J.T., Mills, I.M., Watson, J.K.G., and Winnewisser, B.P. (1997a) Notations and conventions in molecular spectroscopy: Part 1. General spectroscopic notation. *Pure and Applied Chemistry*, **69**, 1633–1639.

Schutte, C.J.H., Bertie, J.E., Bunker, P.R., Hougen, J.T., Mills, I.M., Watson, J.K.G., and Winnewisser, B.P. (1997b) Notations and conventions in molecular spectroscopy: Part 2. Symmetry notation. *Pure and Applied Chemistry*, **69**, 1641–1649.

Seyfried, P. and Becker, P. (1994) The role of N_A in the SI: An atomic path to the kilogram. *Metrologia*, **31**, 167–172.

Sheppard, N. (1991) English-derived abbreviations for experimental techniques in surface science and chemical spectroscopy. *Pure and Applied Chemistry*, **63**, 887–893.

Sheppard, N., Elyashévich, M.A., Miller, F.A., Becker, E.D., Beynon, J.H., Fluck, E., Hadni, A., Zerbi, G., Herzberg, G., Jeżowska-Trzebiatowska, B. *et al.* (1976a) Nomenclature and spectral presentation in electron spectroscopy resulting from excitation by photons. *Pure and Applied Chemistry*, **45**, 221–224.

Sheppard, N., Elyashévich, M.A., Miller, F.A., Becker, E.D., Beynon, J.H., Fluck, E., Hadni, A., Zerbi, G., Herzberg, G., Jeżowska-Trzebiatowska, B. *et al.* (1976b) Presentation of NMR data for publication in chemical journals—B. Conventions relating to spectra from nuclei other than protons. *Pure and Applied Chemistry*, **45**, 217–219.

Sheppard, N., Willis, H.A., and Rigg, J.C. (1985) Names, symbols, definitions and units of quantities in optical spectroscopy. *Pure and Applied Chemistry*, **57**, 105–120.

Smith, M.A., Rinsland, C.P., Fridovich, B., and Rao, K.N. (1985) Intensities and collision broadening parameters from infrared spectra, in *Molecular Spectroscopy: Modern Research*, Rao, K.N. (ed), Academic Press, New York, Vol. 3.

Tennyson, J. (2011) High accuracy rotation–vibration calculations on small molecules, in *Handbook of High-resolution Spectroscopy*, Quack, M. and Merkt, F. (eds), John Wiley & Sons, Ltd., Chichester, UK.

Verhoeven, J.W. (1996) Glossary of terms used in photochemistry. *Pure and Applied Chemistry*, **68**, 2223–2286.

VIM (2008) *International Vocabulary of Metrology – Basic and General Concepts and Associated Terms*, BIPM/ISO, Paris/Geneva, 3rd edition. http://www.bipm.org.

Watson, J.K.G. (1977) Aspects of quartic and sextic centrifugal effects on rotational energy levels, in *Vibrational Spectra and Structure*, Durig, J.R. (ed), Elsevier, Amsterdam, pp. 1–89, Vol. 6.

Weber, A. (2011) High-resolution Raman spectroscopy of gases, in *Handbook of High-resolution Spectroscopy*, Quack, M. and Merkt, F. (eds), John Wiley & Sons, Ltd., Chichester, UK.

Wendisch, D.A.W. (1990) *Acronyms and Abbreviations in Molecular Spectroscopy*, Springer, Heidelberg.

Whiffen, D.H. (1978) Expression of results in quantum chemistry. *Pure Applied Chemistry*, **50**, 75–79.

Wilson, E.B., Decius, J.C., and Cross, P.C. (1980) *Molecular Vibrations. The Theory of Infrared and Raman Vibrational Spectra*, Dover Publications, New York.

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