1 PHYSICAL QUANTITIES AND UNITS

1.1 PHYSICAL QUANTITIES AND QUANTITY CALCULUS

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 (see footnote [1], p. 4).

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 3.2 and 3.3, p. 86 and 87), nm is the symbol for the nanometre, and the units metre and nanometre are related by

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

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} m in Equation (3). The wavelength may equally well be expressed in the form

$$\lambda/\mathrm{m} = 5.896 \times 10^{-7} \tag{4}$$

or

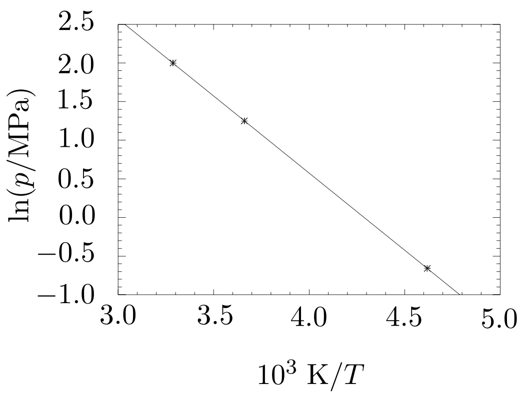
$$\lambda/\mathrm{nm} = 589.6 \tag{5}$$

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 Equations (4) and (5).

Example

$$\ln(p/\mathrm{MPa}) = a + b/T = a + b'(10^3\ \mathrm{K}/T) \tag{6}$$

T/K	10^3 K/T	p/MPa	ln(p/MPa)
216.55	4.6179	0.5180	−0.6578
273.15	3.6610	3.4853	1.2486
304.19	3.2874	7.3815	1.9990



Algebraically equivalent forms may be used in place of 10^3 K/T, such as kK/T or 10^3 $(T/\mathrm{K})^{-1}$. 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* [11–13]. 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. Further examples of the use of quantity calculus are given in Section 7.1, p. 131, which is concerned with the problems of transforming from one set of units to another.

1.2 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:

Base quantity	*Symbol for quantity*	*Symbol for dimension*
length	l	L
mass	m	M
time	t	T
electric current	I	I
thermodynamic temperature	T	Θ
amount of substance	n	N
luminous intensity	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 dimension of energy is equal to dimension of $\mathsf{M\,L^2\,T^{-2}}$
This can be written with the symbol dim for dimension (see footnote [1], below)
$\dim(E) = \dim(m \cdot l^2 \cdot t^{-2}) = \mathsf{M\,L^2\,T^{-2}}$

The quantity *amount of substance* is of special importance to chemists. Amount of substance 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* (see Section 2.10, p. 47, Section 3.3, p. 88, and Chapter 5, p. 111). The SI unit of amount of substance is the mole, defined in Section 3.3, p. 88. 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 such phrases as "amount concentration" (see footnote [2], below), and "amount of N_2". A possible name for international usage has been suggested: "enplethy" [10] (from Greek, similar to enthalpy and entropy).

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.

$$Q = \int_{t_1}^{t_2} I \; \mathrm{d}t \tag{7}$$

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 (see Section 3.9, p. 94).

[1] The symbol $[Q]$ was formerly used for *dimension* of Q, but this symbol is used and preferred for *unit* of Q.
[2] The Clinical Chemistry Division of IUPAC recommended that "amount-of-substance concentration" be abbreviated "substance concentration" [14].

1.3 SYMBOLS FOR PHYSICAL QUANTITIES AND UNITS [5.a]

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 2, p. 11; 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 3, p. 83; the symbols for units listed there are quoted from the Bureau International des Poids et Mesures (BIPM) and are *mandatory*.

1.3.1 General rules for symbols for quantities

The symbol for a physical quantity should be a single letter (see footnote [1], below) of the Latin or Greek alphabet (see Section 1.6, p. 7). 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	C_B	for heat capacity of substance B
		$\mu_\mathrm{B}{}^{\alpha}$	for chemical potential of substance B in phase α
		E_k	for kinetic energy
		μ_r	for relative permeability
		$\Delta_\mathrm{r}H^\ominus$	for standard reaction enthalpy
		V_m	for molar volume
		A_{10}	for decadic absorbance

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 $\Delta_\mathrm{f}S^\ominus(\mathrm{HgCl_2, cr, 25\ °C}) = -154.3\ \mathrm{J\ K^{-1}\ mol^{-1}}$

$\mu_i = (\partial G/\partial n_i)_{T,p,\ldots,n_j,\ldots;\ j\neq i}$ or $\mu_i = (\partial G/\partial n_i)_{T,p,n_{j\neq i}}$

Vectors and matrices may be printed in bold-face italic type, e.g. $\boldsymbol{A}, \boldsymbol{a}$. Tensors may 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, $\vec{\vec{S}}, \vec{\vec{T}}$.

1.3.2 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.

Example $r = 10$ cm, not cm. or cms.

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[1] 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 (see Section 2.15.1, p. 82).

Example Reynolds number, Re; another example is pH (see Sections 2.13 and 2.13.1 (viii), p. 70 and 75).

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

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 (see footnote [2], below).

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 3.6, p. 91.

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

1.4 USE OF THE WORDS "EXTENSIVE", "INTENSIVE", "SPECIFIC", AND "MOLAR"

A quantity that is additive for independent, noninteracting subsystems is called *extensive*; examples are mass m, volume V, Gibbs energy G. A quantity that is independent of the extent of the system is called *intensive*; examples are temperature T, pressure p, chemical potential (partial molar Gibbs energy) μ.

The adjective *specific* before the name of an extensive quantity is used to mean *divided by mass*. When the symbol for the extensive quantity is a capital letter, the symbol used for the specific quantity is often the corresponding lower case letter.

Examples volume, V, and
specific volume, $v = V/m = 1/\rho$ (where ρ is mass density);
heat capacity at constant pressure, C_p, and
specific heat capacity at constant pressure, $c_p = C_p/m$

ISO [5.a] and the Clinical Chemistry Division of IUPAC recommend systematic naming of physical quantities derived by division with mass, volume, area, and length by using the attributes massic or specific, volumic, areic, and lineic, respectively. In addition the Clinical Chemistry Division of IUPAC recommends the use of the attribute entitic for quantities derived by division with the number of entities [14]. Thus, for example, the specific volume could be called massic volume and the surface charge density would be areic charge.

The adjective *molar* before the name of an extensive quantity generally means *divided by amount of substance*. The subscript m on the symbol for the extensive quantity denotes the corresponding molar quantity.

Examples volume, V molar volume, $V_\mathrm{m} = V/n$ (Section 2.10, p. 47)
enthalpy, H molar enthalpy, $H_\mathrm{m} = H/n$

If the name enplethy (see Section 1.2, p. 4) is accepted for "amount of substance" one can use enplethic volume instead of molar volume, for instance. The word "molar" violates the principle that the name of the quantity should not be mixed with the name of the unit (mole in this case). The use of enplethic resolves this problem. It is sometimes convenient to divide all extensive quantities by amount of substance, so that all quantities become intensive; the subscript m may then be omitted if this convention is stated and there is no risk of ambiguity. (See also the symbols recommended for partial molar quantities in Section 2.11, p. 57, and in Section 2.11.1 (iii), p. 60.)

There are a few cases where the adjective *molar* has a different meaning, namely *divided by amount-of-substance concentration*.

Examples absorption coefficient, a
molar absorption coefficient, $\varepsilon = a/c$ (see Section 2.7, note 22, p. 37)
conductivity, κ
molar conductivity, $\Lambda = \kappa/c$ (see Section 2.13, p. 73)

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

1.5 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

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

Examples $F = ma$, $p = nRT/V$

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

Example $(a/b)/c$ or $a/(b/c)$ (in general different), not $a/b/c$

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 a/bcd etc. 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 $1\ \mathrm{mkgs^{-2}}$

1.6 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 Section 1.3.2, p. 5 and in Section 4.1, p. 103 in relation to mathematical symbols and operators. These rules are also presented in the International Standards ISO 31 (successively being replaced by ISO/IEC 80000) [5], ISO 1000 [6], and in the SI Brochure [3].

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 $h = 6.626\ 068\ 96(33)\times10^{-34}$ J s.
   The electric field strength $\boldsymbol{E}$ has components $E_x, E_y,$ and E_z.
   The mass of my pen is $m = 24\ \mathrm{g} = 0.024\ \mathrm{kg}$.

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, $\mathrm{\mu g}$, or when it is used as the symbol for the muon, $\mathrm{\mu}$ (see paragraph 5 below), it should be roman.

4. Numbers, and labels, are roman (upright).

   Examples The ground and first excited electronic state of the CH_2 molecule are denoted $\ldots(2a_1)^2(1b_2)^2(3a_1)^1(1b_1)^1$, $\widetilde{\mathrm{X}}\ {}^3\mathrm{B}_1$, and $\ldots(2a_1)^2(1b_2)^2(3a_1)^2$, $\widetilde{\mathrm{a}}\ {}^1\mathrm{A}_1$, respectively. The π-electron configuration and symmetry of the benzene molecule in its ground state are denoted: $\ldots(\mathrm{a_{2u}})^2(\mathrm{e_{1g}})^4$, $\widetilde{\mathrm{X}}\ {}^1\mathrm{A_{1g}}$. All these symbols are labels and are roman.

5. Symbols for elements in the periodic system shall be roman. Similarly the symbols used to represent elementary particles are always roman. (See, however, paragraph 9 below for 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.

   Examples 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 [5.k]. Some of these letters, e.g. e for elementary charge, are also sometimes used to represent physical quantities; then of course they shall be italic, to distinguish them from the corresponding mathematical symbol.

   Examples $\Delta H = H(\mathrm{final}) - H(\mathrm{initial})$; $(\mathrm{d}p/\mathrm{d}t)$ used for the rate of change of pressure; $\mathrm{\delta}x$ used to denote an infinitesimal variation of x. But 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: Np/s) and ω is the angular frequency (SI unit: rad/s). Note the use of roman δ for the operator in an infinitesimal variation of x, $\mathrm{\delta}x$, 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 (Np = 1) and radian (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. An example is the hartree, E_h (see Section 3.9.1, p. 95). 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.

   Examples 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 $1\ \mathrm{eV} = e{\cdot}1\ \mathrm{V} = 1.602\ 176\ 487(40)\times10^{-19}\ \mathrm{J}$.

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 (see reference [15]).

   Examples α-ethylcyclopentaneacetic acid
   β-methyl-4-propylcyclohexaneethanol
   tetracarbonyl(η^4-2-methylidenepropane-1,3-diyl)chromium
   α-(trichloromethyl)-ω-chloropoly(1,4-phenylenemethylene)
   α-D-glucopyranose
   5α-androstan-3β-ol
   N-methylbenzamide
   O-ethyl hexanethioate
   3*H*-pyrrole
   naphthalen-2(1*H*)-one