INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY DIVISION OF PHYSICAL CHEMISTRY COMMISSION ON SYMBOLS, TERMINOLOGY, AND UNITS

MANUAL OF SYMBOLS AND TERMINOLOGY FOR PHYSICOCHEMICAL QUANTITIES AND UNITS

Adopted by the IUPAC Council at Cortina d'Ampezzo, Italy, on 7 July 1969

> Prepared for publication by M. L. MCGLASHAN

> > 1973 Edition

Adopted by the IUPAC Council at Munich, Federal Republic of Germany, on 31 August 1973

> Revision prepared for publication by M. A. PAUL

Second revision prepared for publication by D. H. WHIFFEN

PERGAMON PRESS

PREFACE

The Commission on Symbols, Terminology, and Units is a part of the Division of Physical Chemistry of the International Union of Pure and Applied Chemistry. Its general responsibilities are to secure clarity and precision, and wider agreement in the use of symbols, by chemists in different countries, among physicists, chemists, and engineers, and by editors of scientific journals. In pursuing these aims, liaison is maintained with other international organizations and in particular with the Commission on Symbols, Units and Nomenclature of the International Union of Pure and Applied Physics (SUN Commission) and Technical Committee 12 of the International Organization for Standardization (ISO/TC 12). References to the publications of these organizations are given in 13.1 and 13.2 of this Manual. These publications may be referred to for more extended coverage of symbols for quantities, and related information, not commonly used by chemists. The recommendations presented here are generally in agreement with those of the SUN Commission and ISO/TC 12.

The present publication supersedes the Commission's publication of 1959 (Reference 13.3) in English and French and its translations into other languages.

M. L. MCGLASHAN Chairman

Commission on Symbols, Terminology, and Units

Department of Chemistry University of Exeter Exeter August 1969

Preface to 1973 Edition

The text of the 1969 edition of this Manual has been revised to take account of recent decisions by the Comité International des Poids et Mesures concerning use of the International System of Units, summarized in the document, 'Le Système International d'Unités (SI)', published by the Bureau International des Poids et Mesures in a second edition in 1973 (translations of this document into English have been prepared jointly and published separately by the National Physical Laboratory, UK, and the National Bureau of Standards, USA). Section 2.8 of the Manual has been revised in collaboration with IUPAC's Commission on Molecular Structure and Spectroscopy. Attention is called also to separate publication by IUPAC of an Appendix entitled, 'Definitions, Terminology, and Symbols in Colloid and Surface Chemistry—I', prepared by the Commission on Colloid and Surface Chemistry. References to the publications cited are included in Section 13.

M. A. PAUL Chairman Commission on Symbols, Terminology, and Units National Academy of Sciences Washington, DC October 1973

Preface to 1979 Edition

The 1979 edition is not greatly changed from the earlier editions, but many minor corrections have been incorporated as a consequence of decisions by relevant bodies both within IUPAC and on the broader international scientific stage.

Appendix I, 'Definition of Activities and Related Quantities' is printed with this text. Appendix II, 'Definitions, Terminology and Symbols in Colloid and Surface Chemistry' in two parts, is published in *Pure and Applied Chemistry* Part I (1972), 31, 577 and Part II, 'Heterogeneous Catalysis' (1976), 46, 71. Appendix III, 'Electrochemical Nomenclature' published in *Pure and Applied Chemistry* (1974), 37, 503.

> D. H. WHIFFEN Former Chairman Commission on Symbols, Terminology, and Units

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CONTENTS

Pre	face						1
1.		cal quantities and symbols for physical quantiti	es	•	•	•	5
	1.1		00	•	•	•	5
	1.2		•	•	•	•	5
	1.3			•	•	•	5
	1.4	Use of the words 'specific' and 'molar' in the		nocofr	hvoio	01	3
	1.4	and white a		nes or f	JIIYSIC	ai	~
	1.5	Printing of symbols for physical quantities	·	•	•	•	5
	1.6	Printing of subscripts and superscripts .		•	•	•	6
	1.7	Products and quotients of physical quantities		•	•	•	6
	1.7	Froducts and quotients of physical quantities	5.	•	·	•	6
2.	Dagor	nmended names and symbols for quantities	:	ahamiat			
4.	physic		ш	chenus	ry an	iu.	8
	2.1	Space, time, and related quantities	·	•	•	•	8
	2.2	Mechanical and related quantities .	•	•	•	•	° 9
	2.3	Molecular and related quantities	•	•	•	•	9
	2.4	Thermodynamic and related quantities .	·	•	•	•	
	2.5		·	•	•	•	10
	2.6	Chemical reactions	•	•	•	•	11
	2.0			•	•	•	11
	2.7	Electrochemistry	•	•	•	•	12
	2.8 2.9	Transport properties	•	•	•	•	13
			•	•	•	•	14
	2.10 2.11	Symbols for particular cases of physical quan			•	•	14
	2.11	Recommended superscripts	•	•	•	•	15
•	.						
3.		and symbols for units	•	•	•	•	16
	3.1	Printing of symbols for units	•	•	•	•	16
	3.2	Printing of prefixes	•	•	•	•	16
	3.3	Combination of prefixes and symbols .	•	•	•	•	16
	3.4	Multiplication and division of units .	•	•	•	•	16
	3.5	The International System of Units .	•	•	•	•	16
	3.6	Definitions of the SI Base Units		•			17
	3.7	Names and symbols for SI Base Units .	•			•	18
	3.8	Names and symbols for SI Supplementary U	nits	•		•	18
	3.9	Special names and symbols for certain SI De					18
	3.10	SI Derived Units and Unit-symbols for other	r qua	Intities	•	•	18
	3.11	SI Prefixes		•		•	19
	3.12	The degree Celsius				•	19
	3.13	Decimal fractions and multiples of SI Units ha	aving	g special	l name	es	19
	3.14	Some other units now exactly defined in term	ıs of	the SI	Units		19
•	3.15	Units defined in terms of the best available e					.,
		of certain physical constants					20
	3.16	'International' electrical units					20
	3.17	Electrical and magnetic units belonging to	unit	-system	s othe	er	20
		than the International System of Units .					21
				-			-1
4.	Num	bers					22
	4.1	Printing of numbers		•			22
	4.2	Multiplication and division of numbers .				•	22
F	D				-	-	
5.		ical quantities, units, and numerical values .	•	•	•	•	23
6.	Reco	mmended mathematical symbols					24

4

7.	Symt	ols for chen	nical ele	ments	. nuc	lides.	and n	article	s				25
	7.1	Definition					-	•					25
	7.2	Elements a											25
	7.3	Particles											25
	7.4	Abbreviate	ed notat	tion fo	or nu	clear	reaction		•			•	25
8.	Symt	ols for spec	troscopy	<i>.</i>									26
	8.1	General ru											26
	8.2	Atomic sp	ectrosco										26
	8.3	Molecular											26
	8.4	Spectrosco	pic trar	sition	IS					•			27
-	_	•	•										
9.		entions con						-				s,	• •
		omotive for							•		•	•	28
	9.1	The electri					-		cell	•	•	•	28
	9.2	Electrode	potentia	u.		•	•	•	•	•	•	•	28
10.	The c	quantity pH											30
	10.1												30
	10.2	Standards											30
	10.3	Values of						ons		•	•	•	31
11.		ition of rate											32
11.	11.1	Rate of rea							•	•	•	•	32
		Order of r				•		:	•	•	•	•	33
	11.2	Labelling of		-					•	•	•	•	33
	11.5			-	-			•	•	•	•	•	33
	11.4	Consion	umber	•		•	•	•	•	•	•	•	33
12.	Value	es of some fu	ındamer	ital co	onstar	nts	•	•	•	•	•	•	34
13.	Refer	ences .					•	•	•	•	•	•	36
App	endix]	I. Definitio	n of act	ivities	and	relate	d qua	ntities		•			37
		ure substan				•				•		•	37
	2. N	Mixtures						•			•		38
	3. S	Solutions		-						. '			39

1. PHYSICAL QUANTITIES AND SYMBOLS FOR PHYSICAL QUANTITIES

1.1 Physical quantities

A physical quantity is the product of a numerical value (a pure number) and a unit.

1.2 Base physical quantities

Physical quantities are generally organized in a dimensional system built upon seven base quantities. These base quantities, each of which has its own dimension, and the symbols used to denote them, are as follows:

base physical quantity	symbol for quantity
length	l
mass	m
time	t
electric current	Ι
thermodynamic temperature	T
amount of substance	п
luminous intensity	$I_{ m v}$

Luminous intensity is seldom if ever needed in physical chemistry.

One of these independent base quantities is of special importance to chemists but until recently had no generally accepted name, although units such as the mole have been used for it. The name 'amount of substance' is now reserved for this quantity.

The definition of amount of substance, as of all other physical quantities (see Section 5), has nothing to do with any choice of *unit*, and in particular has nothing to do with the particular unit of amount of substance called the mole (see Section 3.6). It is now as inconsistent to call n the 'number of moles' as it is to call m the 'number of kilograms' or l the 'number of metres', since n, m, and l are symbols for quantities not for numbers.

The amount of a substance is proportional to the number of *specified* elementary entities of that substance. The proportionality factor is the same for all substances; its reciprocal is the Avogadro constant. The specified elementary entity may be an atom, a molecule, an ion, a radical, an electron, etc., or any *specified* group of such particles.

1.3 Derived physical quantities

All other physical quantities are regarded as being derived from, and as having dimensions derived from, the seven independent base physical quantities by definitions involving only multiplication, division, differentiation, and/or integration. Examples of derived physical quantities are given, often with brief definitions, in Section 2.

1.4 Use of the words 'specific' and 'molar' in the names of physical quantities

The word 'specific' before the name of an extensive physical quantity is

restricted to the meaning 'divided by mass'. For example specific volume is the volume divided by the mass. When the extensive quantity is represented by a capital letter, the corresponding specific quantity may be represented by the corresponding lower case letter.

Examples; volume: V

specific volume: v = V/mheat capacity at constant pressure: C_p specific heat capacity at constant pressure: $c_p = C_p/m$

The word 'molar' before the name of an extensive quantity is restricted to the meaning 'divided by amount of substance'. For example molar volume is the volume divided by the amount of substance. The subscript m attached to the symbol for the extensive quantity denotes the corresponding molar quantity.

Examples; volume: V molar volume: $V_m = V/n$ Gibbs energy: G molar Gibbs energy: $G_m = G/n$

The subscript m may be omitted when there is no risk of ambiguity. Lower case letters may be used to denote molar quantities when there is no risk of misinterpretation.

The symbol X_B , where X denotes an extensive quantity and B is the chemical symbol for a substance, denotes the partial molar quantity of the substance B defined by the relation:

$$X_{\rm B} = (\partial X / \partial n_{\rm B})_{T, p, n_{\rm C}}, \ldots$$

For a pure substance B the partial molar quantity X_B and the molar quantity X_m are identical. The partial molar quantity X_B of pure substance B, which is identical with the molar quantity X_m of pure substance B, may be denoted by X_B^* , where the superscript * denotes 'pure', so as to distinguish it from the partial molar quantity X_B of substance B in a mixture.

1.5 Printing of symbols for physical quantities

The symbols for physical quantities should be single letters⁽¹⁾ of the Latin or Greek alphabets which, when necessary, may be modified by subscripts and superscripts of specified meaning. The symbols for physical quantities should always be printed in italic (sloping) type.

The symbols for vector quantities should be printed in **bold-faced** italic type.

1.6 Printing of subscripts and superscripts

Subscripts or superscripts which are themselves symbols for physical quantities or numbers should be printed in italic (sloping) type and all others in roman (upright) type.

Examples: C_p for heat capacity at constant pressure, but C_B for heat capacity of substance B

1.7 Products and quotients of physical quantities

A product of two quantities a and b may be represented in any of the ways:

ab or $a \cdot b$ or $a \cdot b$ or $a \times b$

⁽¹⁾ An exception to this rule has been made for certain numbers used in the study of transport processes (see Section 2.9), for which the internationally agreed symbols consist of two letters. When such a symbol appears as a factor in a product, it is recommended that it be separated from the other symbols by a space, by a multiplication sign, or by parentheses. *Example:* Reynolds number: Re.

and their quotient in any of the ways:

 $\frac{a}{b}$ or a/b or ab^{-1}

or in any of the other ways of writing the product of a and b^{-1} .

These rules may be extended to more complex groupings but more than one solidus (/) should never be used in the same expression unless parentheses are used to eliminate ambiguity.

Example; (a/b)/c or a/(b/c) but never a/b/c

2. RECOMMENDED NAMES AND SYMBOLS FOR QUANTITIES IN CHEMISTRY AND PHYSICS

The following list contains the recommended symbols for the most important quantities likely to be used by chemists. Whenever possible the symbol used for a physical quantity should be that recommended. In a few cases where conflicts were foreseen alternative recommendations have been made. Bold-faced italic (sloping) as well as ordinary italic (sloping) type can also sometimes be used to resolve conflicts. Further flexibility can be obtained by the use of capital letters as variants for lower-case letters, and *vice versa*, when no ambiguity is thereby introduced.

For example, d and D may be used instead of d_i and d_e for internal and external diameter in a context in which no quantity appears, such as diffusion coefficient, for which the recommended symbol is D. Again, the recommended symbol for power is P and for pressure is p or P, but P and p may be used for two powers or for two pressures; if power and pressure appear together, however, P should be used only for power and p only for pressure, and necessary distinctions between different powers or between different pressures should be made by the use of subscripts or other modifying signs.

When the above recommendations are insufficient to resolve a conflict or where a need arises for other reasons, an author is of course free to choose an *ad hoc* symbol. Any *ad hoc* symbol should be particularly carefully defined.

In the following list, where two or more symbols are indicated for a given quantity and are separated only by commas (without parentheses), they are on an equal footing; symbols within parentheses are reserve symbols.

Any description given after the name of a physical quantity is merely for identification and is not intended to be a complete definition.

Vector notation (bold-faced italic or sloping type) is used where appropriate in Section 2.6; it may be used when convenient also for appropriate quantities in other Sections.

Space, i	mic, and related quantities	
2.1.01	length	l
2.1.02	height	h
2.1.03	radius	r
2.1.04	diameter	d
2.1.05	path, length of arc	S
2.1.06	wavelength	λ
2.1.07	wavenumber: $1/\lambda$	$\sigma^{(1)}, \tilde{\nu}^{(2)}$
2.1.08	plane angle	α, β΄, γ, θ, φ
2.1.09	solid angle	ω, Ω
2.1.10	area	$A, S, A_{\rm s}^{(3)}$
2.1.11	volume	V
2.1.12	time	t
2.1.13	frequency	ν, f
2.1.14	circular frequency: $2\pi\nu$	ω

2.1 Space, time, and related quantities

⁽¹⁾ In solid-state studies, wavevector **k** is used $(|\mathbf{k}| = 2\pi/\lambda)$.

⁽²⁾ For electromagnetic radiation referred to a vacuum $\tilde{\nu} = \nu/c = 1/\lambda_{\rm vac}$ is preferred.

(3) The symbol A_s may be used when necessary to avoid confusion with the symbol A for Helmholtz energy.

9

2.1.15	period: $1/\nu$	T
2.1.16	characteristic time interval, relaxation time,	
	time constant	au
2.1.17	velocity	v, u, w, c
2.1.18	angular velocity: $d\phi/dt$	ω
2.1.19	acceleration	а
2.1.20	acceleration of free fall	g

2.2 Mechanical and related quantities

2.2.01	mass	m
2.2.02	reduced mass	μ
2.2.03	specific volume (volume divided by mass)	v
2.2.04	density (mass divided by volume)	ρ
2.2.05	relative density (ratio of the density to that	
	of a reference substance)	d
2.2.06	moment of inertia	Ι
2.2.07	momentum	р
2.2.08	force	F
2.2.09	weight	G,(W)
2.2.10	moment of force	M
2.2.11	angular momentum	L
2.2.12	work (force times path)	w, W
2.2.13	energy	É
2.2.14	potential energy	$E_{\rm p}, V, \Phi$
2.2.15	kinetic energy	$E_{\mathbf{k}}, T, K$
2.2.16	Hamiltonian function	H,
2.2.17	Lagrangian function	Ĺ
2.2.18	power (energy divided by time)	P
2.2.19	pressure	D, (P)
2.2.20	normal stress	σ
2.2.20	shear stress	τ
2.2.22	linear strain (relative elongation): $\Delta l/l_0$	ε, e
2.2.23	volume strain (bulk strain): $\Delta V/V_0$	θ
2.2.23	modulus of elasticity (normal stress divided by	0
2.2.27	linear strain, Young's modulus)	Ε
2.2.25	shear modulus (shear stress divided by shear	-
2.2.23	angle)	G
2.2.26	compressibility: $-V^{-1}(dV/dp)$	ĸ
2.2.20	compression (bulk) modulus: $-V_0(\Delta p/\Delta V)$	ĸ
2.2.27	velocity of sound	к с
2.2.28	viscosity	τ η, (μ)
2.2.30	fluidity: $1/\eta$	ϕ
2.2.31	kinematic viscosity: η/ρ	ν
2.2.32	friction coefficient (frictional force divided by	
	normal force)	μ, (f)
2.2.33	surface tension	γ, σ
2.2.34	angle of contact	θ
2.2.35	diffusion coefficient	D
2.2.36	mass transfer coefficient (dimension of lengt	
	divided by time)	k_{d}

2.3 Molecular and related quantities

2.3.01 relative atomic mass of an element (formerly called 'atomic weight')⁽¹⁾

Ar

.

 $^{^{(1)}}$ The ratio of the average mass per atom of an element to 1/12 of the mass of an atom of nuclide $^{12}\mathrm{C}.$

2.3.02	relative molecular mass of a substance	
	(formerly called 'molecular weight') ⁽¹⁾	$M_{\rm r}$
2.3.03	molar mass (mass divided by amount of	
	substance)	M
2.3.04	Avogadro constant	$L, N_{\mathbf{A}}$
2.3.05	number of molecules or other entities	Ν
2.3.06	amount of substance ⁽²⁾	n, (v)
2.3.07	mole fraction of substance B : $n_{\rm B}/\Sigma_{\rm i}n_{\rm i}$	$x_{\rm B}, y_{\rm B}$
2.3.08	mass fraction of substance B	w _B
2.3.09	volume fraction of substance B	$\phi_{\rm B}$
2.3.10	molality of solute substance B (amount of B	
	divided by mass of solvent) ⁽³⁾	$m_{\rm B}$
2.3.11	amount-of-substance concentration of substance	9
	B (amount of B divided by the volume of the	
	solution) ⁽⁴⁾	с _в , [В]
2.3.12	mass concentration of substance B (mass of B	
	divided by the volume of the solution)	$\Gamma^{\rho_{\mathbf{B}}}$
2.3.13	surface concentration, surface excess	-
2.3.14	collision diameter of a molecule	d, o
2.3.15	mean free path	<i>l</i> , λ
2.3.16	collision number (number of collisions divided	
	by volume and by time)	Ζ
2.3.17	grand partition function (system)	Ξ
2.3.18	partition function (system)	Q, Z
2.3.19	partition function (particle)	q, z
2.3.20	statistical weight	g
2.3.21	symmetry number	σ, s
2.3.22	characteristic temperature	Θ

2.4 Thermodynamic and related quantities

2.4.01	thermodynamic temperature, absolute	
	temperature	Т
2.4.02	Celsius temperature	$t, \theta^{(5)}$
2.4.03	(molar) gas constant	R
2.4.04	Boltzmann constant	k
2.4.05	heat	$q, Q^{(0)}$
2.4.06	work	w, W ⁽⁶⁾
2.4.07	internal energy	U, (E)
2.4.08	enthalpy: $U + pV$	H
2.4.09	entropy	S
2.4.10	Helmholtz energy: $U - TS$	A
2.4.11	Massieu function: $-A/T$	J
2.4.12	Gibbs energy: $H - TS$	G
2.4.13	Planck function: $-G/T$	Y
2.4.14	compression factor: pV_m/RT	Z
2.4.15	heat capacity	С
2.4.16	specific heat capacity (heat capacity divided by	
	mass; the name 'specific heat' is not	
	recommended)	С

 $^{(1)}$ The ratio of the average mass per formula unit of a substance to 1/12 of the mass of an atom of nuclide $^{12}C.$

Example: $M_r(KCl) = 74.555$

⁽²⁾ See Section 1.2.

⁽³⁾ A solution having a molality equal to 0.1 mol kg⁻¹ is sometimes called a 0.1 molal solution or a 0.1 m solution.

⁽⁴⁾ This quantity may be simply called 'concentration' when there is no risk of ambiguity. A solution with an amount-of-substance concentration of 0.1 mol dm^{-3} is often called a 0.1 mol ar solution or a 0.1 M solution.

(5) Where symbols are needed to represent both time and Celsius temperature, t is the preferred symbol for time and θ for Celsius temperature. (6) It is recommended that q > 0 and w > 0 both indicate *increase* of energy of the system under discussion. Thus $\Delta U = q + w$.

2.4.17	ratio C_p/C_V	γ, (κ)	
2.4.18	Joule-Thomson coefficient	μ	
2.4.19	thermal conductivity	μ λ, k	
2.4.20	thermal diffusivity: $\lambda/\rho c_p$	а	
2.4.21	coefficient of heat transfer (density of heat flow		
	rate divided by temperature difference)	h	
2.4.22	cubic expansion coefficient: $V^{-1}(\partial V/\partial T)_p$	a	
2.4.23	isothermal compressibility: $-V^{-1}(\partial V/\partial p)_T$	κ	
2.4.24	pressure coefficient: $(\partial p/\partial T)_V$	β	
2.4.25	chemical potential of substance B	$\dot{\mu}_{\rm B}$	
2.4.26	absolute activity of substance B: $exp(\mu_B/RT)$	$\lambda_{\rm B}$	
2.4.27	fugacity	f, p	
2.4.28	osmotic pressure	Π	
2.4.29	ionic strength: $(I_m = \frac{1}{2}\sum_i m_i z_i^2)$ or $I_c = \frac{1}{2}\sum_i c_i z_i^2)$	1	
2.4.30	activity, relative activity of substance B	$a_{\rm B}$	
2.4.31	activity coefficient, mole fraction basis	$f_{\rm B}$	
2.4.32	activity coefficient, molality basis	ŶΒ	
2.4.33	activity coefficient, concentration basis	y _B	
2.4.34	osmotic coefficient	ϕ	
		•	

2.5 Chemical reactions

2.5.01	stoichiometric coefficient of substance B	
	(negative for reactants, positive for products)	$\nu_{\rm B}$
2.5.02	general equation for a chemical reaction	$0 = \Sigma_{\mathrm{B}} \mathbf{v}_{\mathrm{B}} \mathbf{B}$
2.5.03	extent of reaction: $(d\xi = dn_B/\nu_B)$	ξ ξ, J
2.5.04	rate of reaction: $d\xi/dt$ (see Section 11)	ξ, J
2.5.05	rate of increase of concentration of	
	substance B : dc_B/dt	$v_{\rm B}, r_{\rm B}$
2.5.06	rate constant	k
2.5.07	affinity of a reaction: $-\Sigma_{\rm B}\nu_{\rm B}\mu_{\rm B}$	A, (A)
2.5.08	equilibrium constant	K
2.5.09	degree of dissociation	a
Electric	sity and magnetism	
2.6.01	elementary charge (of a proton)	е

2.6

2.6.01	elementary charge (of a proton)	е
2.6.02	quantity of electricity	Q
2.6.03	charge density	ρ
2.6.04	surface charge density	σ
2.6.05	electric current	Ι
2.6.06	electric current density	j
2.6.07	electric potential	ν, φ
2.6.08	electric potential difference: IR	$U, \Delta V, \Delta \phi$
2.6.09	electric field strength	Ē
2.6.10	electric displacement	D
2.6.11	capacitance	С
2.6.12	permittivity: $(D = \epsilon E)$	ε
2.6.13	permittivity of vacuum	€0
2.6.14	relative permittivity ⁽¹⁾ : ϵ/ϵ_0	$\epsilon_{\rm r}, (\epsilon)$
2.6.15	dielectric polarization: $D - \epsilon_0 E$	P
2.6.16	electric susceptibility: $\epsilon_r - 1$	χ _e
2.6.17	electric dipole moment	p, p_e
2.6.18	permanent dipole moment of a molecule	p , μ
2.6.19	induced dipole moment of a molecule	p, p_i
2.6.20	electric polarizability of a molecule	a
2.6.21	magnetic flux	${ { \Phi} }$
2.6.22	magnetic flux density, magnetic induction	B
2.6.23	magnetic field strength	H
2.6.24	permeability: $(B = \mu H)$	μ
2.6.25	permeability of vacuum	μο

⁽¹⁾ Also called dielectric constant, and sometimes denoted by D, when it is independent of E.

۰.

2.6.26 2.6.27 2.6.28 2.6.29.1 2.6.29.2	relative permeability: μ/μ_0 magnetization: $(B/\mu_0) - H$ magnetic susceptibility: $\mu r - 1$ Bohr magneton nuclear magneton	$ \begin{array}{l} \mu_{\rm r} \\ \boldsymbol{M} \\ \boldsymbol{\chi}, (\boldsymbol{\chi}_{\rm m}) \\ \boldsymbol{\mu}_{\rm B} \\ \boldsymbol{\mu}_{\rm H} \end{array} $
2.6.29.3	g-factor	μ_{N}
2.6.29.4	gyromagnetic ratio, magnetogyric ratio	γ
2.6.30	electromagnetic moment: $(E_p = -m \cdot B)$	m , μ
2.6.31	resistance	R
2.6.32	resistivity (formerly called specific resistance):	
	$(E = \rho \mathbf{j})$	ρ
2.6.33	conductivity (formerly called specific	
	conductance): $(j = \kappa E)$	к, (σ)
2.6.34	self-inductance	L
2.6.35	mutual inductance	M, L_{12}
2.6.36	reactance	Х
2.6.37	impedance (complex impedance): $R + iX$	Ζ
2.6.38	loss angle	δ
2.6.39	admittance (complex admittance): $1/Z$	Y
2.6.40	conductance: $(Y = G + iB)$	G
2.6.41	susceptance: $(Y = G + iB)$	B

2.7 Electrochemistry

2.7.01	Faraday constant	F
2.7.02	charge number of an ion B (positive for cations	,
	negative for anions)	$z_{\rm B}$
2.7.03	charge number of a cell reaction	n, (z)
2.7.04	electromotive force	E, E_{MF}
2.7.05	electrochemical potential of ionic component B	:
	$\mu_{ m B}+z_{ m B}Foldsymbol{\phi}$	$\tilde{\mu}_{\mathbf{B}}$
2.7.06	electric mobility (velocity divided by electric	
	field strength)	u , μ
2.7.07	electrolytic conductivity (formerly called	
	specific conductance)	κ, (σ)
2.7.08	molar conductivity of electrolyte or $ion^{(1)}$: κ/c	$\Lambda, \lambda^{(2)}$
2.7.09	transport number (transference number or	
	migration number)	t
2.7.10	overpotential	η
2.7.11	exchange current density	j _o
2.7.12	electrochemical transfer coefficient	a
2.7.13	electrokinetic potential (zeta potential)	ζ
2.7.14	thickness of diffusion layer	δ
2.7.15	inner electric potential	φ
2.7.16	outer electric potential	ψ
2.7.17	surface electric potential difference: $\phi - \psi$	x

⁽¹⁾ The word molar, contrary to the general rule given in Section 1.4, here means 'divided by amount-of-substance concentration'. ⁽²⁾ The formula unit whose concentration is c must be specified. Example: $\lambda(Mg^{2+}) = 2\lambda(\frac{1}{2}Mg^{2+})$

 $[\]Lambda$ is used for an electrolyte and λ for individual ions.

2.8 Light and related electromagnetic radiation ⁽¹⁾

Light a	inu related creetromagnetic radiation V	
2.8.01	Planck constant	h
2.8.02	Planck constant divided by 2π	ħ
2.8.03	radiant energy	$Q^{(2)}$
2.8.04	radiant flux, radiant power	$\widetilde{\Phi}^{(2)}, P$
2.8.05	radiant intensity: $d\Phi/d\omega$	I ⁽²⁾
2.8.06	radiance: $(dI/dS)/\cos\theta$	$L^{(2)}$
2.8.07	radiant excitance: $d\Phi/dS$	$M^{(2)}$
2.8.08	irradiance: $d\Phi/dS$	$E^{(2)}$
2.8.09	absorptance, absorption-factor ⁽³⁾	
	(ratio of absorbed to incident	
	radiant or luminous flux)	a ⁽³⁾
2.8.10	reflectance, reflection factor ⁽³⁾	
	(ratio of reflected to incident	
	radiant or luminous flux)	$\rho^{(3)}, R$
2.8.11	transmittance, transmission factor ⁽³⁾	•
	(ratio of transmitted to incident	
	radiant or luminous flux)	$ au^{(3)}$
2.8.12	internal transmittance ⁽³⁾	
	(transmittance of the medium itself,	
	disregarding boundary or container	
	influence)	$ au_{\mathbf{i}^{(3)}}, T$
2.8.13.1	internal transmission density ⁽³⁾ ,	
	(decadic) absorbance ⁽⁴⁾ : $\log_{10}(1/T)$	$D_{i^{(3)}}, A$
2.8.13.2	Napierian absorbance: $\ln(1/T)$	В
2.8.14.1	(linear) (decadic) absorption	
	$\operatorname{coefficient}^{(3,4)}: A/l$	$a^{(3)}, K$
2.8.14.2	Napierian absorption coefficient: B/l	a
2.8.15	absorption index: $B/4\pi\tilde{\nu}l = a/4\pi\tilde{\nu}$	k
2.8.16.1	specific (decadic) absorption	
	coefficient ⁽⁵⁾ : $A/\rho_{\rm B}l$	a ^(7,8)
2.8.16.2	specific Napierian absorption	
	$\operatorname{coefficient}^{(5)}: B/\rho_{\mathrm{B}}/$	$\mu^{(7,8)}$
2.8.17.1	molar (decadic) absorption	
	$coefficient^{(4,6)}$: $A/c_{\rm B}l$	$\epsilon^{(7,8)}$
2.8.17.2	molar Napierian absorption	
	coefficient ⁽⁶⁾ : $B/c_{\rm B}l$	$\kappa^{(7,8)}$
2.8.18	quantum yield	Φ
2.8.19	exposure: $\int E dt$	H
2.8.20	velocity of light in vacuo	с

⁽¹⁾ References to the symbols used in defining the quantities in 2.8 are as follows:

1	2.1.01	ĩ	2.1.07	θ	2.1.08	ω	2.1.09
S	2.1.10	V	2.1.11	t	2.1.12	СВ	2.3.11
ρΒ	2.3.12	Φ	2.8.04	Ι	2.8.05	E	2.8.08
	2.8.12	A	2.8.13.1	. B	2.8.13.2	a	2.8.14.2
k	2.8.15	n	2.8.21.1				

⁽²⁾ The same symbol is often used also for the corresponding luminous quantity. Subscripts e for energetic and v for visible may be added whenever confusion between these quantities

⁽³⁾ These names and symbols are in agreement with those adopted jointly by the International Commission of Illumination (CIE) and the International Electrotechnical Commission (IEC).

⁽⁴⁾ The terms extinction (for 2.8.13.1) and extinction coefficient (for 2.8.14.1) are unsuitable because extinction is reserved for diffusion of radiation rather than absorption. Molar absorptivity (for 2.8.17.1) should be avoided because the meaning, absorptance per unit length, has been accepted internationally for the term absorptivity. ⁽⁵⁾ The word specific, contrary to the general rule given in Section 1.4, here means

'divided by mass concentration'.

⁽⁶⁾ The word molar, contrary to the general rule given in Section 1.4, here means 'divided by amount-of-substance concentration'.

⁽⁷⁾ For measurements on solutions, 1/T is ordinarily replaced by T_0/T where T_0 is the internal transmittance of the solvent medium and T is the internal transmittance of the solution. If a double-beam spectrometer is used in solution spectrometry, T_0/T is given directly, provided the boundary and container influences have been equalized between the two collections of the solution. two cells; in addition to the physical matching of the sample and reference cells this requires that there be no significant difference between nsolvent and nsolution.

⁽⁸⁾ For measurements on solutions, it is tacitly assumed that the solution obeys the Beer-Lambert law unless the solute concentration is specified. The temperature should be specified.

refractive index (of a non-absorbing	
material)	n
complex refractive index of an	
absorbing material: $n + ik$	ĥ
molar refraction: $(n^2 - 1)V_m/(n^2 + 2)$	$R_{\rm m}$
angle of optical rotation	a
	complex refractive index of an absorbing material: $n + ik$ molar refraction: $(n^2 - 1)V_m/(n^2 + 2)$

2.9 Transport properties⁽¹⁾

Transpo	at properties	
2.9.01	Flux (of a quantity X)	J_X, J
2.9.02	Reynolds number: $\rho v l / \eta$	Re
2.9.03	Euler number: $\Delta p/\rho v^2$	Eu
2.9.04	Froude number: $v/(lg)^{\frac{1}{2}}$	Fr
2.9.05	Grashof number: $l^3ga\Delta\theta \rho^2/\eta^2$	Gr
2.9.06	Weber number: $\rho v^2 l/\gamma$	We
2.9.07	Mach number: v/c	Ma
2.9.08	Knudsen number: λ/l	Kn
2.9.09	Strouhal number: lf/v	Sr
2.9.10	Fourier number: $a\Delta t/l^2$	Fo
2.9.11	Peclet number: vl/a	Pe
2.9.12	Rayleigh number: $l^3g_a\Delta\theta\rho/\eta a$	Ra
2.9.13	Nusselt number: hl/k	Nu
2.9.14	Stanton number: $h/\rho vc_p$	St
2.9.15	Fourier number for mass transfer: Dt/l^2	Fo*
2.9.16	Peclet number for mass transfer: vl/D	Pe*
2.9.17	Grashof number for mass transfer:	
	$-l^{3}g(\partial \rho/\partial x)_{T,p}\Delta x \rho/\eta^{2}$	Gr*
2.9.18	Nusselt number for mass transfer ⁽²⁾ $k_d l/D$	Nu*
2.9.19	Stanton number for mass transfer: k_d/v	St*
2.9.20	Prandtl number: $\eta/\rho a$	Pr
2.9.21	Schmidt number: $\eta/\rho D$	Sc
2.9.22	Lewis number: a/D	Le
2.9.23	Magnetic Reynolds number: $v_{\mu\kappa}l$	<i>Re</i> m
2.9.24	Alfvén number: $v(\rho\mu)^{\frac{1}{2}}/B$	Al
2.9.25	Hartmann number: $Bl(\kappa/\eta)^{\frac{1}{2}}$	На
2.9.26	Cowling number: $B^2/\mu\rho v^2$	Со

2.10 Symbols for particular cases of physical quantities

It is much more difficult to make detailed recommendations on symbols for physical quantities in particular cases than in general cases. The reason is the incompatibility between the need for specifying numerous details and the need for keeping the printing reasonably simple. Among the most awkward things to print are superscripts to subscripts and subscripts to subscripts. Examples of symbols to be avoided are:

> $(pV)_{0}^{p=0}$ $\Delta H_{25^{\circ}C}$ λ_{NO_1}

The problem is vastly reduced if it is recognized that two different kinds of notation are required for two different purposes. In the formation of general fundamental relations the most important requirement is a notation that is easy to understand and easy to remember. In applications to particular cases, in quoting numerical values, and in tabulation, the most important requirement is complete elimination of any possible ambiguity even at the cost of an elaborate notation.

The advantage of a dual notation is already to some extent accepted in the

⁽¹⁾ See footnote (1) on page 6.
⁽²⁾ The name Sherwood number, symbol Sh has been widely used.

case of concentration. The recommended notation for the formulation of the equilibrium constant K_c for the general reaction:

is

$$K_{c} = \Pi_{\mathbf{B}} (c_{\mathbf{B}})^{\mathbf{v}_{\mathbf{B}}}$$

 $0 = \sum_{B} \nu_{B} B$

but when we turn to a particular example it is better to use a notation such as:

$$Br_{2} + H_{2}O = HOBr + H^{+} + Br^{-}$$

$$\frac{[HOBr] [H^{+}] [Br^{-}]}{[Br_{2}]} = K_{c}$$

$$K_{c}(25 \text{ °C}) = 6 \times 10^{-9} \text{ mol}^{2} \text{ dm}^{-6}$$

Once the principle of dual notation is accepted, its adaptability and usefulness become manifest in all fields of physical chemistry. It will here be illustrated by just a few examples.

The general relation between the molar conductivity of an electrolyte and the molar conductivities of the two ions is written most simply and most clearly as:

$$\Lambda = \lambda^+ + \lambda^-$$

but when it comes to giving values in particular cases a much more appropriate notation is:

$$\lambda(\frac{1}{2}Mg^{2+}) = 53 \text{ S cm}^{2} \text{ mol}^{-1} \text{ at } 25^{\circ}\text{C}$$

$$\lambda(\text{Cl}^{-}) = 76 \text{ S cm}^{2} \text{ mol}^{-1} \text{ at } 25^{\circ}\text{C}$$

$$\Lambda(\frac{1}{2}Mg\text{Cl}_{2}) = 129 \text{ S cm}^{2} \text{ mol}^{-1} \text{ at } 25^{\circ}\text{C}$$

$$\Lambda(\text{MgCl}_{2}) = 258 \text{ S cm}^{2} \text{ mol}^{-1} \text{ at } 25^{\circ}\text{C}$$

The general relation between the partial molar volumes of the two components A and B of a binary mixture is written most simply:

$$n_{\rm A} \mathrm{d} V_{\rm A} + n_{\rm B} \mathrm{d} V_{\rm B} = 0$$
 (*T*, *p* const.)

But when it comes to specifying values, a completely different notation is called for, such as:

$$V(K_2SO_4, 0.1 \text{ mol dm}^{-3} \text{ in } H_2O, 25 \text{ }^\circ\text{C}) = 48 \text{ cm}^3 \text{ mol}^{-1}$$

Each kind of notation is appropriate to its purpose.

A last example will be given relating to optical rotation. The relations between the angle a of rotation of the plane of polarization and the amount n, or the number N of molecules, of the optically active substance in the path of a light beam of cross-section A can be clearly expressed in the form:

$$a = na_n/A = Na_N/A$$

where α_n is the molar optical rotatory power and α_N the molecular optical rotatory power. When on the other hand it is desired to record an experimental measurement, an appropriate notation would be:

 α (589.3 nm, 20 °C, sucrose, 10 g dm⁻³ in H₂O, 10 cm) = +66.470°

2.11 Recommended superscripts

The following superscripts are recommended:

° or * pure substance

- ∞ infinite dilution
- ^{id} ideal
- ° or ^o standard in general
 - [‡] activated complex, transition state

3. UNITS AND SYMBOLS FOR UNITS

3.1 Printing of symbols for units

The symbol for a unit should be printed in roman (upright) type, should remain unaltered in the plural, and should not be followed by a full stop except when it occurs at the end of a sentence in text.

Example; 5 cm but not 5 cms and not 5 cm. and not 5 cms.

The symbol for a unit derived from a proper name should begin with a capital roman (upright) letter.

Examples: J for joule and Hz for hertz

Any other symbol for a unit should be printed in lower case roman (upright) type.

3.2 Printing of prefixes

Symbols for prefixes for units should be printed in roman (upright) type with no space between the prefix and the unit. Compound prefixes should be avoided. (See Section 3.11)

Example: ns but not mus for 10^{-9} s

3.3 Combination of prefixes and symbols

A combination of prefix and symbol for a unit is regarded as a single symbol which may be raised to a power without the use of brackets.

Examples: cm^2 means $(cm)^2$ and μs^{-1} means $(\mu s)^{-1}$

3.4 Multiplication and division of units

A product of two units may be represented in any of the ways:

Nm or N·m or N.m or N \times m

The representation Nm is not recommended.

A quotient of two units may be represented in any of the ways:

$$\frac{m}{s}$$
 or m/s or m s⁻¹

or in any of the other ways of writing the product of m and s^{-1} .

These rules may be extended to more complex groupings but more than one solidus (/) should never be used in the same expression unless parentheses are used to eliminate ambiguity.

Example: $J K^{-1} mol^{-1}$ or J/(K mol) but never J/K/mol

3.5 The International System of Units

The name International System of Units has been adopted by the Conférence Générale des Poids et Mesures for the system of units based on a selected set of dimensionally independent *SI Base Units*. The SI Base Units are the metre, kilogram, second, ampere, kelvin, candela, and mole. In the International System of Units there is one and only one *SI Unit* for each physical quantity. This is either the appropriate SI Base Unit itself (see Section 3.7) or the appropriate *SI Derived Unit* formed by multiplication and/or division of two or more SI Base Units (see Section 3.10). A few such SI Derived Units have been given special names and symbols (see Section 3.9). There are also two *SI Supplementary Units* for which it is not decided whether they are SI Base Units or SI Derived Units (see Section 3.8).

Any of the approved decimal prefixes, called *SI Prefixes*, may be used to construct decimal multiples or submultiples of SI Units (see Section 3.11).

It is recommended that only units composed of SI Units and SI Prefixes be used in science and technology.

3.6 Definitions of the SI Base Units

metre: The metre is the length equal to 1650763.73 wavelengths in vacuum of the radiation corresponding to the transition between the levels $2p_{10}$ and $5d_5$ of the krypton-86 atom.

kilogram: The kilogram is the unit of mass; it is equal to the mass of the international prototype of the kilogram.

second: The second is the duration of 9192 631770 periods of the radiation corresponding to the transition between the two hyperfine levels of the ground state of the caesium-133 atom.

ampere: The ampere is that constant current which, if maintained in two straight parallel conductors of infinite length, of negligible 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.

kelvin: The kelvin, unit of thermodynamic temperature, is the fraction 1/273.16 of the thermodynamic temperature of the triple point of water⁽¹⁾. *candela:* The candela is the luminous intensity, in the perpendicular direction, of a surface of 1/600000 square metre of a black body at the temperature of freezing platinum under a pressure of 101325 newtons per square metre.

mole: The mole is the amount of substance of a system which contains as many elementary entities as there are atoms in 0.012 kilogram of carbon-12. 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.

Some examples of the use of the mole:

- 1 mole of HgCl has a mass of 236.04 grams
- 1 mole of Hg₂Cl₂ has a mass of 472.08 grams
- 1 mole of Hg_2^{2+} has a mass of 401.18 grams and a charge of 192.97 kilocoulombs
- 1 mole of $\frac{1}{2}Ca^{2+}$ has a mass of 20.04 grams and a charge of 96.49 kilo-coulombs
- 1 mole of $Cu_{0.5}Zn_{0.5}$ has a mass of 64.46 grams
- 1 mole of $Fe_{0.91}S$ has a mass of 82.88 grams
- 1 mole of e⁻ has a mass of 548.60 micrograms, a charge of -96.49 kilocoulombs, and contains 6.02×10^{23} electrons
- 1 mole of a mixture containing the mole fractions $x(N_2) = 0.7809$, $x(O_2) = 0.2905$, x(Ar) = 0.0093, and $x(CO_2) = 0.0003$ has a mass of 28.964 grams
- 1 mole of photons whose frequency is 10¹⁴ Hz has energy 39.90 kilojoules (The numerical values in these examples are approximate.)

17

⁽¹⁾ In October 1967 the thirteenth Conférence Générale des Poids et Mesures recommended that the kelvin, symbol K, be used for thermodynamic temperature and for thermodynamic temperature interval, and that the unit-symbols °K and deg be abandoned.

3.7 Names and symbols for SI Base Units

physical quantity	name of SI Unit	symbol for SI Unit
length	metre	m
mass	kilogram	kg
time	second	S
electric current	ampere	Α
thermodynamic temperature	kelvin	K
amount of substance ⁽¹⁾	mole	mol
luminous intensity	candela	cd

3.8 Names and symbols for SI Supplementary Units

physical quantity	name of SI Unit	symbol for SI Unit
plane angle	radian	rad
solid angle	steradian	sr

3.9 Special names and symbols for certain SI Derived Units

1			
		symbol for	
physical quantity	SI Unit	SI Unit	definition of SI Unit
force	newton	N	m kg s ⁻²
pressure, stress	pascal	Pa	$m^{-1} \text{ kg s}^{-2} (= N m^{-2})$
energy	joule	J	$m^2 kg s^{-2}$
power	watt	W	$m^2 kg s^{-3} (=J s^{-1})$
electric charge	coulomb	С	s A
electric potential			
difference	volt	v	$m^2 kg s^{-3} A^{-1} (= J A^{-1} s^{-1})$
electric resistance	ohm	Ω	$m^2 kg s^{-3} A^{-2} (= V A^{-1})$
electric conductance	siemens	S	$m^{-2} kg^{-1} s^3 A^2 (= A V^{-1} = \Omega^{-1})$
electric capacitance	farad	F	$m^{-2} kg^{-1} s^4 A^2 (=A s V^{-1})$
magnetic flux	weber	Wb	$m^2 kg s^{-2} A^{-1} (= V s)$
inductance	henry	н	$m^2 kg s^{-2} A^{-2} = V A^{-1} s$
magnetic flux density	•	Т	$kg s^{-2} A^{-1} (= V s m^{-2})$
luminous flux	lumen	lm	cd sr
illuminance	lux	lx	m ^{−2} cd sr
frequency	hertz	Hz	s ⁻¹
activity (of radioactive	e		
source)	becquerel	Bq	s ⁻¹
absorbed dose (of			
radiation)	gray	Gy	$m^2 s^{-2} (= J kg^{-1})$

3.10 SI Derived Units and Unit-symbols for other quantities

(This list is not exhaustive.)

<i>physical quantity</i> area volume density velocity angular velocity	SI Unit square metre cubic metre kilogram per cubic metre metre per second radian per second	symbol for SI Unit m ² m ³ kg m ⁻³ m s ⁻¹ rad s ⁻¹
acceleration	metre per second squared	m s ⁻²
kinematic viscosity, diffusion coefficient dynamic viscosity	square metre per second newton-second per square metre	$m^2 s^{-1}$ N s m ⁻²
molar entropy, molar heat capacity concentration electric field strength magnetic field strength luminance	joule per kelvin mole mole per cubic metre volt per metre ampere per metre candela per square metre	J K ⁻¹ mol ⁻¹ mol m ⁻³ V m ⁻¹ A m ⁻¹ cd m ⁻²

3.11 SI Prefixes

fraction	prefix	symbol	multiple	prefix	symbol
10-1	deci	d	10	deca	da
10^{-2}	centi	с	102	hecto	h
10-3	milli	m	10 ³	kilo [.]	k
10-6	micro	μ	106	mega	Μ
10 ⁻⁹	nano	n	109	giga	G
10-12	pico	р	10 ¹²	tera	Т
10 ⁻¹⁵	femto	f	10 ¹⁵	peta	Р
10-18	atto	a	1018	exa	Е

The names and symbols of decimal multiples and sub-multiples of the unit of mass, which already contains a prefix, are constructed by adding the appropriate prefix to the word gram and symbol g:

Examples: mg not μ kg μ g not nkg Mg not kkg

3.12 The degree Celsius

physical quantity	name of unit	symbol for unit	definition of unit
Celsius temperature	degree Celsius	°C (1)	$^{\circ}C = K$

The Celsius temperature t, is defined by $t = T - T_0$ where $T_0 = 273.15$ K. This leads to $t/^{\circ}C = T/K - 273.15$.

3.13 Decimal fractions and multiples of SI Units having special names

The following units do not belong to the International System of Units, but in view of existing practice the Comité International des Poids et Mesures has considered (1969) that it was preferable to keep them for the time being (along with several other specified units not particularly relevant to chemistry) for use with those of the International System.

physical quantity	name of unit	symbol for unit	definition of unit
length	ångström	Å	10 ⁻¹⁰ m
cross section	barn	b	10 ⁻²⁸ m ²
volume	litre ⁽²⁾	l, L	10 ⁻³ m ³
mass	tonne	t	10 ³ kg
pressure	bar	bar	10 ⁵ Pa

Other units with special names based on the c.g.s. system and the electromagnetic c.g.s. system⁽³⁾ are preferably not to be used; among these are the erg (10⁻⁷ J), the dyne (10⁻⁵ N), the poise (0.1 Pa s), the stokes $(10^{-4} \text{ m}^2 \text{ s}^{-1})$, the gauss (corresponding to 10^{-4} T)⁽³⁾, the oersted (corresponding to $1000/4\pi$ A m⁻¹)⁽³⁾, and the maxwell (corresponding to 10^{-8} Wb)⁽³⁾. The name micron and symbol μ should not be used for the unit of length, 10^{-6} m, which has the SI name micrometre and symbol μm .

3.14 Some other units now exactly defined in terms of the SI units

The CIPM (1969) recognized that users of the SI will wish to employ with it certain units not part of it but which are important and are widely used. These units are given in the following table. The combination of units of this table with SI units to form compound units should, however, be authorized only in limited cases.

⁽¹⁾ The ° sign and the letter following form one symbol and there should be no space between them. Example: 25 °C not 25° C.

⁽²⁾ By decision of the Twelfth Conférence Générale des Poids et Mesures in October 1964, the old definition of the litre (1.000 028 dm³) was rescinded. The word litre is now regarded as a special name for the cubic decimetre. Neither the word litre nor its symbol should be used to express results of high precision. The alternative symbol L was recommended by CIPM to CGPM in 1978.

⁽³⁾ The electromagnetic c.g.s. system is a three-dimensional system of units in which the unit of electric current and units for other electric and magnetic quantities are considered to be derived from the centimetre, gram, and second as base units. The electric and magnetic units of this system cannot strictly speaking be compared to the corresponding units of the SI, which has four dimensions when only units derived from the metre, kilogram, second, and ampere are considered.

Units in use with the International System

Units in use with the International System				
symbol	definition of unit			
min	60 s			
h	3 600 s			
d	86 400 s			
G	$(\pi/180)$ rad			
,	$(\pi/10\ 800)\ rad$			
"	$(\pi/648 \ 000)$ rad			
	s <u>vmbol</u> min h d			

In view of existing practice, as in the case of those units listed in Section 3.13, the CIPM (1969) has considered it preferable to retain the following units for the time being, for use with those of the SI. The definitions given in the fourth column of this table are exact.

Units to be used with the International System for a limited time				
physical quantity	name of unit	symbol for unit	definition of unit	
radioactivity	curie	Ci	$3.7 \times 10^{10} \text{ Bg}$	
exposure to X or γ radiation	röntgen	R	2.58×10^{-4} C kg ⁻¹	
ionizing radiation absorbed	rad	rad ⁽¹⁾	10 ⁻² Ğy	

The use of the following units is to be progressively discouraged and eventually abandoned. In the meantime it is recommended that any author who uses these units will define them in terms of SI units once in each publication in which he uses them. The definitions given here are exact. This list is not exhaustive.

	Other units generall	y deprecated	
physical quantity	name of unit	symbol for unit	definition of unit
length	inch	in	$2.54 \times 10^{-2} \mathrm{m}$
mass	pound (avoirdupois)	lb	0.453 592 37 kg
force	kilogram-force	kgf	9.806 65 N
pressure	standard atmosphere ⁽²⁾	atm	101 325 Pa
pressure	torr	Torr	101 325 760 Pa
pressure	conventional millimetre of mercury ⁽³⁾	mmHg	13.5951 × 980.665 × 10 ⁻² Pa
energy	kilowatt-hour	kW h	$3.6 \times 10^6 \text{ J}$
cnergy	thermochemical calorie	calth	4.184 J
energy	British thermal unit	Btu	1055.055 852 62 J
thermodynamic temperature	degree Rankine	R	(5/9) K

3.15 Units defined in terms of the best available experimental values of certain physical constants

It is necessary to recognize outside the International System some units, useful in specialized fields, the values of which expressed in SI units can be obtained only by experiment and are therefore not known exactly. Among such units recognized by the CIPM (1969) that are relevant to chemistry are the following:

<i>physical quantity</i>	<i>name of unit</i>	symbol for unit	conversion factor $1 \text{ eV} \approx 1.6021892$
energy	electronvolt	eV	
mass	(unified) atomic mass unit	u	× 10^{-19} J 1 u ≈ 1.6605655 × 10^{-27} kg

3.16 'International' electrical units

These units are obsolete having been replaced by the 'absolute' (SI) units in 1948. The conversion factors which should be used with electrical measurements quoted in 'international' units depend on where and when the

⁽¹⁾ Where there is a risk of confusion with the symbol for radian, rd may be used as the symbol for the unit, rad.

⁽²⁾ The phrase 'standard atmosphere' remains admissable for the reference pressure 101 325 Pa.

⁽³⁾ The conventional millimetre of mercury, symbol mmHg (not mm Hg), is the pressure exerted by a column exactly 1 mm high of a fluid of density exactly 13.5951 g cm⁻³ in a place where the acceleration of free fall is exactly 980.665 cm s⁻². The mmHg differs from the Torr by less than 2×10^{-7} Torr.

instruments used to make the measurements were calibrated. The following two sets of conversion factors refer respectively to the 'mean international' units estimated by the ninth Conférence Générale des Poids et Mesures in 1948, and to the 'US international' units estimated by the National Bureau of Standards (USA) as applying to published measurements made with instruments calibrated by them prior to 1948.

1 'mean international ohm' = 1.00049Ω 1 'mean international volt' = 1.00034 V 1 'US international ohm' = 1.000495Ω

1 'US international volt' = 1.000330 V

3.17 Electrical and magnetic units belonging to unit-systems other than the **International System of Units**

Definitions of units used in the obsolescent 'electrostatic CGS' and 'electromagnetic CGS' unit-systems can be found in References 13.1.05 and 13.2.

Another 'electrostatic CGS' unit used in chemistry for electric dipole moment is the debye, symbol D. $1D = (10^{-21}/c) \text{ A m}^2 \approx 3.3356 \times 10^{-30}$ Cm.

4. NUMBERS

4.1 Printing of numbers

Numbers should be printed in upright type. The decimal sign between digits in a number should be a comma (,) or (especially in English-language texts) a point (.). To facilitate the reading of long numbers the digits may be grouped in threes but no comma or point should ever be used except for the decimal sign.

Example: 2 573,421 736 or in English language texts 2 573.421 736 but never 2,573.421,736

When the decimal sign is placed before the first digit of a number a zero should always be placed before the decimal sign.

Example: 0.2573×10^4 or in English language texts 0.2573×10^4 but not $.2573 \times 10^4$ and not $.2573 \times 10^4$

It is often convenient to print numbers with just one digit before the decimal sign.

Example: $2,573 \times 10^3$ or in English language texts 2.573×10^3

4.2 Multiplication and division of numbers

The multiplication sign between numbers should be a cross (\times) or (but never when a point is used as the decimal sign) a centred dot (\cdot) . *Example:* 2.3 \times 3.4 or 2,3.3,4

Division of one number by another may be indicated in any of the ways: 136

 $\frac{130}{273}$ or 136/273 or $136 \times (273)^{-1}$

These rules may be extended to more complex groupings, but more than one solidus (/) should never be used in the same expression unless parentheses are used to eliminate ambiguity.

Example: (136/273)/2.303 or $136/(273 \times 2.303)$ but never 136/273/2.303

5. PHYSICAL QUANTITIES, UNITS, AND NUMERICAL VALUES

As stated in Section 1.1 the value of a *physical quantity* is equal to the product of a *numerical value* and a *unit*:

physical quantity = numerical value \times unit.

Neither any physical quantity, nor the symbol used to denote it, should imply a particular choice of unit.

Operations on equations involving physical quantities, units, and numerical values, should follow the ordinary rules of algebra.

Thus the physical quantity called the critical pressure and denoted by p_c has the value for water:

 $p_{\rm c} = 221.2$ bar or better $p_{\rm c} = 22.12$ MPa.

These equations may equally well be written in the forms:

 $p_{\rm c}/{\rm bar} = 221.2$ or better $p_{\rm c}/{\rm MPa} = 22.12$,

which are especially useful for the headings in tables and as labels on the axes of graphs.

6. RECOMMENDED MATHEMATICAL SYMBOLS⁽¹⁾

Mathematical operators (for example d and Δ) and mathematical constants (for example e and π) should always be printed in roman (upright) type. Letter symbols for numbers other than mathematical constants should be printed in italic type.

equal to	-
not equal to	 +
identically equal to	
corresponds to	~
	<u> </u>
approximately equal to	\approx
approaches	
asymptotically equal to	~
proportional to	$\sim \sim$
infinity	8
less than	$\vee \land \lor \land \lor \land \lor \land \lor \land \lor \land \lor$
greater than	>
less than or equal to	\leq
greater than or equal to	≥
much less than	\ll
much greater than	\gg
plus	
minus	
multiplied by	× •
	a
a divided by b	$b^{u}a/b ab^{-1}$
	D
magnitude of a	a
a raised to the power n	a^n
square root of a	$\begin{array}{ccc} a^{1/2} & a^{\frac{1}{2}} & \sqrt{a} & \sqrt{a} \\ a^{1/n} & a^{\frac{1}{n}} & \sqrt[n]{a} & \sqrt[n]{a} \end{array}$
n'th root of a	$a^{1/n} a^{\frac{1}{n}} \sqrt[n]{a} \sqrt[n]{a}$
mean value of a	$\langle a \rangle \bar{a}$
natural logarithm of <i>a</i>	$\ln a \log_{e}a$
decadic logarithm of a	$\log a \log_{10} a \log a$
binary logarithm of a	$lb a log_2 a$
exponential of a	$exp a e^{a}$
• • • • • •	

24

⁽¹⁾ Taken from Reference 13.1.11 where a more comprehensive list can be found.

7. SYMBOLS FOR CHEMICAL ELEMENTS, NUCLIDES, AND PARTICLES

7.1 Definitions

A nuclide is a species of atoms of which each atom has identical atomic number (proton number) and identical mass number (nucleon number). Different nuclides having the same value of the atomic number are named isotopes or isotopic nuclides. Different nuclides having the same mass number are named isobars or isobaric nuclides.

7.2 Elements and nuclides

Symbols for chemical elements should be written in roman (upright) type. The symbol is not followed by a full stop except when it occurs at the end of a sentence in text.

Examples: Ca C H He

The nuclide may be specified by attaching numbers. The mass number should be placed in the left superscript position; the atomic number, if desired, may be placed as a left subscript. The number of atoms per molecule is indicated as a right subscript. lonic charge, or state of excitation, or oxidation number⁽¹⁾ may be indicated in the right superscript space.

Examples: Mass number: 14N2, 35Cl-

Ionic charge: Cl⁻, Ca²⁺, PO₄³⁻ or PO₄³⁻
 Excited electronic state: He*, NO*
 Oxidation number: Pb^{II}₂Pb^{IV}O₄, K₆M^{IV}Mo₉O₃₂ (where M denotes a metal)

7.3 Particles

neutron	n	helion	h
proton	р	∝-particle	α
deuteron	d	electron	e
triton	t	photon	γ

The electric charge of particles may be indicated by adding the superscript +, -, or 0; e.g., p⁺, n⁰, e⁺, e⁻. If the symbols p and e are used without charge, they refer to the positive proton and negative electron respectively.

7.4 Abbreviated notation for nuclear reactions

The meaning of the symbolic expression indicating a nuclear reaction should be the following:

			b) outgoing particle(s)	final
	nuclide	or quanta	, or quanta	nuclide
Examples:	$^{14}N(a,p)$	Ì7 O	⁵⁹ Co(n,γ) ⁶⁰ Co	/
•	²³ Na(γ,3	n) ²⁰ Na	³¹ P(y,pn) ²⁹ Si	

⁽¹⁾ For a more detailed discussion see Reference 13.4.

8. SYMBOLS FOR SPECTROSCOPY⁽¹⁾

8.1 General rules

A letter-symbol indicating the quantum state of *a system* should be printed in capital upright type. A letter-symbol indicating the quantum state of *a* single particle should be printed in lower case upright type.

8.2 Atomic spectroscopy

The letter-symbols indicating quantum states are:

L, l = 0: S, s	<i>L</i> , <i>l</i> = 4: G, g	L, l = 8: L, 1
= 1: P, p	= 5: H, h	= 9: M, m
= 2: D,d	= 6: I, i	= 10: N, n
= 3: F, f	= 7: K, k	= 11: O, o

A right-hand subscript indicates the total angular momentum quantum number J or j. A left-hand superscript indicates the spin multiplicity 2S + 1.

Examples: ${}^{2}P_{3/2}$ - state (J = 3/2, multiplicity 2) $p_{3/2}$ - electron (j = 3/2)

An atomic electron configuration is indicated symbolically by:

 $(nl)^{\kappa}(n'l')^{\kappa'}\ldots$

Instead of l = 0, 1, 2, 3, ... one uses the quantum state symbols s, p, d, f, ...

Example: the atomic configuration: (1s)²(2s)²(2p)³

8.3 Molecular spectroscopy

The letter-symbols indicating molecular electronic quantum states are, in the case of *linear molecules*:

$$\begin{array}{l} \Lambda, \ \lambda = 0; \ \Sigma, \ \sigma \\ = 1; \ \Pi, \ \pi \\ = 2; \ \Delta, \ \delta \end{array}$$

and for non-linear molecules:

Remarks: A left-hand superscript indicates the spin multiplicity. For molecules having a symmetry centre the parity symbol g or u, indicating respectively symmetric or antisymmetric behaviour on inversion, is attached as a right-hand subscript. A + or - sign attached as a right-hand superscript indicates the symmetry as regards reflection in any plane through the symmetry axis of the molecules.

Examples: Σ_{g}^{+} , Π_{u} , ${}^{2}\Sigma$, ${}^{3}\Pi$, etc.

The letter-symbols indicating the vibrational angular momentum states in the case of *linear molecules* are:

 $l = 0: \Sigma$ = 1: Π = 2: Δ

⁽¹⁾ Taken from Reference 13.2. For further details see Reference 13.10.

8.4 Spectroscopic transitions

The upper level and the lower level are indicated by ' and " respectively.

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

A spectroscopic transition should be indicated by writing the upper state first and the lower state second, connected by a dash in between.

<i>Examples</i> ; ${}^{2}P_{1/2} - {}^{2}S_{1/2}$	for an electronic transition
(J',K') - (J'',K'')	for a rotational transition
v' - v''	for a vibrational transition

Absorption transition and emission transition may be indicated by arrows \leftarrow and \rightarrow respectively.

Examples:
$${}^{2}P_{1/2} \rightarrow {}^{2}S_{1/2}$$
emission from ${}^{2}P_{1/2}$ to ${}^{2}S_{1/2}$ $(J',K') \leftarrow (J'',K'')$ absorption from (J'',K'') to (J',K')

The difference Δ between two quantum numbers should be that of the upper state minus that of the lower state.

Example: $\Delta J = J' - J''$

The indications of the branches of the rotation band should be as follows:

$$\Delta J = J' - J'' = -2: \text{ O-branch}$$

= -1: P-branch
= 0: Q-branch
= +1: R-branch
= +2: S-branch

9. CONVENTIONS CONCERNING THE SIGNS OF ELECTRIC POTENTIAL DIFFERENCES, ELECTRO-MOTIVE FORCES, AND ELECTRODE POTENTIALS⁽¹⁾

9.1 The electric potential difference for a galvanic cell

The cell should be represented by a diagram, for example:

$$Zn | Zn^{2+} | Cu^{2+} | Cu$$

The electric potential difference ΔV is equal in sign and magnitude to the electric potential of a metallic conducting lead on the right minus that of an identical lead on the left.

When the reaction of the cell is written as:

$$\frac{1}{2}Zn + \frac{1}{2}Cu^{2+} \rightarrow \frac{1}{2}Zn^{2+} + \frac{1}{2}Cu$$

this implies a diagram so drawn that this reaction takes place when positive electricity flows through the cell from left to right. If this is the direction of the current when the cell is short-circuited, as it will be in the present example (unless the ratio $[Cu^{2+}]/[Zn^{2+}]$ is extremely small), the electric potential difference will be positive.

If, however, the reaction is written as:

$$\frac{1}{2}Cu + \frac{1}{2}Zn^{2+} \rightarrow \frac{1}{2}Cu^{2+} + \frac{1}{2}Zn$$

this implies the diagram:

$$Cu | Cu^{2+} | Zn^{2+} | Zn$$

and the electric potential difference of the cell so specified will be negative (unless the ratio $[Cu^{2+}]/[Zn^{2+}]$ is extremely small).

The limiting value of the electric potential difference for zero current through the cell is called the electromotive force and denoted by $E_{\rm MF}$ or E.

9.2 Electrode potential

The so-called electrode potential of an electrode (half-cell) is defined as the electromotive force of a cell in which the electrode on the left is a *standard* hydrogen electrode and that on the right is the electrode in question. For example, for the zinc electrode (written as $Zn^{2+} | Zn$) the cell in question is:

$$Pt | H_2 | H^+ | Zn^{2+} | Zn$$

The reaction taking place at the zinc electrode is:

$$Zn^{2+} + 2e^- \rightarrow Zn$$

The latter is to be regarded as an abbreviation for the reaction in the mentioned cell:

$$Zn^{2+} + H_2 \rightarrow Zn + 2H^+$$

In the standard state the electromotive force of this cell has a negative sign and a value of -0.763 V. The standard electrode potential of the zinc electrode is therefore -0.763 V.

⁽¹⁾ The conventions given here are in accordance with the 'Stockholm Convention' of 1953.

The symbol $Zn \mid Zn^{2+}$ on the other hand implies the cell:

 $Zn \mid Zn^{2+} \mid H^+ \mid H_2 \mid Pt$

in which the reaction is:

$$Zn + 2H^+ \rightarrow Zn^{2+} + H_2$$

The electromotive force of this cell should not be called an electrode potential.

10. THE QUANTITY pH⁽¹⁾

10.1 Operational definition

In all existing national standards the definition of pH is an operational one. The electromotive force E_X of the cell:

reference electrode | concentrated KCl solution \therefore solution X | H₂ | Pt is measured and likewise the electromotive force E_8 of the cell:

reference electrode | concentrated KCl solution : solution S | H₂ | Pt

both cells being at the same temperature throughout and the reference electrodes and bridge solutions being identical in the two cells. The pH of the solution X, denoted by pH(X), is then related to the pH of the solution S, denoted by pH(S), by the definition:

$$pH(X) = pH(S) + \frac{(E_S - E_X)F}{RT \ln 10}$$

where R denotes the gas constant, T the thermodynamic temperature, and F the Faraday constant. Thus defined the quantity pH is a number.

To a good approximation, the hydrogen electrodes in both cells may be replaced by other hydrogen-ion-responsive electrodes, e.g. glass or quinhydrone. The two bridge solutions may be any molality not less than 3.5 mol kg^{-1} , provided they are the same (see Reference 13.5).

10.2 Standards

The difference between the pH of two solutions having been defined as above, the definition of pH can be completed by assigning a value of pH at each temperature to one or more chosen solutions designated as standards. A series of pH(S) values for five suitable standard reference solutions is given in Section 10.3.

If the definition of pH given above is adhered to strictly, then the pH of a solution may be slightly dependent on which standard solution is used. These unavoidable deviations are caused not only by imperfections in the response of the hydrogen-ion electrodes but also by variations in the liquid junctions resulting from the different ionic compositions and mobilities of the several standards and from differences in the geometry of the liquidliquid boundary. In fact such variations in measured pH are usually too small to be of practical significance. Moreover, the acceptance of several standards allows the use of the following alternative definition of pH.

The electromotive force E_X is measured, and likewise the electromotive forces E_1 and E_2 of two similar cells with the solution X replaced by the standard solutions S_1 and S_2 such that the E_1 and E_2 values are on either side of, and as near as possible to, E_X . The pH of solution X is then obtained by assuming linearity between pH and E, that is to say:

$$\frac{\mathrm{pH}(\mathrm{X}) - \mathrm{pH}(\mathrm{S}_1)}{\mathrm{pH}(\mathrm{S}_2) - \mathrm{pH}(\mathrm{S}_1)} = \frac{E_{\mathrm{X}} - E_1}{E_2 - E_1}$$

⁽¹⁾ The symbol pH is an exception to the general rules given in Section 1.5.

This procedure is especially recommended when the hydrogen-ion-responsive electrode is a glass electrode.

t/°C	Α	В	С	D	E
0		4.003	6.984	7.534	9.464
5		3.999	6.951	7.500	9.395
10		3.998	6.923	7.472	9.332
15		3.999	6.900	7.448	9.276
20		4.002	6.881	7.429	9.225
25	3.557	4.008	6.865	7.413	9.180
30	3.552	4.015	6.853	7.400	9.139
35	3.549	4.024	6.844	7.389	9.102
38	3.548	4.030	6.840	7.384	9.081
40	3.547	4.035	6.838	7.380	9.068
45	3.547	4.047	6.834	7.373	9.038
50	3.549	4.060	6.833	7.367	9.011
55	3.554	4.075	6.834		8.985
60	3.560	4.091	6.836		8.962
70	3.580	4.126	6.845		8.921
80	3.609	4.164	6.859		8.885
90	3.650	4.205	6.877		8.850
95	3.674	4.227	6.886		8.833

10.3 Values of pH(S) for five standard solu

The compositions of the standard solutions are:

A: KH tartrate (saturated at 25 °C)

B: KH phthalate, $m = 0.05 \text{ mol kg}^{-1}$ C: KH₂PO₄, $m = 0.025 \text{ mol kg}^{-1}$;

$$Ma_2HPO_4, m = 0.025 \text{ mol kg}^{-1};$$

Na₂HPO₄, $m = 0.025 \text{ mol kg}^{-1};$

D: KH_2PO_4 , m = 0.008 695 mol kg⁻¹;

Na₂HPO₄, m = 0.030 43 mol kg⁻¹

E: Na₂B₄O₇,
$$m = 0.01 \text{ mol kg}^{-1}$$

where m denotes molality and the solvent is water.

11. DEFINITION OF RATE OF REACTION AND RELATED QUANTITIES

11.1 Rate of reaction

For the reaction

 $0 = \sum_{\mathbf{B}} \nu_{\mathbf{B}} \mathbf{B}$

the extent of reaction ξ is defined according to 2.5.03 by

$$\mathrm{d}\boldsymbol{\xi} = \nu_{\mathrm{B}}^{-1} \mathrm{d}\boldsymbol{n}_{\mathrm{B}}$$

where $n_{\rm B}$ is the amount, and $\nu_{\rm B}$ is the stoichiometric number, of the substance B.

It is recommended that the *rate of reaction* be defined as the rate of increase of the extent of reaction, namely

$$\xi = \mathrm{d}\xi/\mathrm{d}t = \nu_{\mathrm{p}}^{-1}\mathrm{d}n_{\mathrm{B}}/\mathrm{d}t$$

This definition is independent of the choice of B and is valid regardless of the conditions under which a reaction is carried out, e.g. it is valid for a reaction in which the volume varies with time, or for a reaction involving two or more phases, or for a reaction carried out in a flow reactor.

If both sides of this equation are divided by any specified volume V, not necessarily independent of time, and not necessarily that of a single phase in which the reaction is taking place, then

$$V^{-1}\mathrm{d}\boldsymbol{\xi}/\mathrm{d}t = V^{-1}\nu_{\mathrm{B}}^{-1}\mathrm{d}\boldsymbol{n}_{\mathrm{B}}/\mathrm{d}t$$

If the specified volume V is independent of time, then

$$V^{-1}\mathrm{d}\xi/\mathrm{d}t = \nu_{\mathrm{B}}^{-1}\mathrm{d}(n_{\mathrm{B}}/V)/\mathrm{d}t$$

If this specified volume V is such that

 $n_{\rm B}/V = c_{\rm B}$ or [B]

where $c_{\rm B}$ or [B] is the amount-of-substance concentration of B, then

$$V^{-1}d\xi/dt = v_{\rm p}^{-1}dc_{\rm B}/dt \text{ or } v_{\rm p}^{-1}d[{\rm B}]/dt$$

The quantity

$$dn_{\rm B}/dt (= \nu_{\rm B} d\xi/dt)$$

may be called the rate of formation of B, and the quantity

$$V^{-1}\nu_{\rm p}^{-1}{\rm d}n_{\rm B}/{\rm d}t \ (=V^{-1}{\rm d}\xi/{\rm d}t)$$

may be called the rate of reaction divided by volume, and the quantity

 $v_{\rm B} = {\rm d}c_{\rm B}/{\rm d}t$ or d[B]/dt

which has often been called the rate of reaction, may be called the rate of increase of the concentration of B, but none of these three quantities should be called the rate of reaction.

Manual of symbols and terminology for physicochemical quantities and units 33

11.2 Order of reaction

If it is found *experimentally* that the rate of increase of the concentration of B is given by

 $v_{\rm B} \propto [{\rm C}]^{c}[{\rm D}]^{d} \dots$

then the reaction is described as of order c with respect to C, of order d with respect to D, ..., and of overall order (c + d + ...).

11.3 Labelling of elementary processes

Elementary processes should be labelled in such a manner that reverse processes are immediately recognizable.

Example:

elementary process	label	rate constant
$Br_2 + M \rightarrow 2Br + M$	1	k_1
$Br + H_2 \rightarrow HBr + H$	2	k_2
$H + Br_2 \rightarrow HBr + Br$	3	k_3
$H + HBr \rightarrow H_2 + Br$	-2	k_{-2}
$2\mathbf{Br} + \mathbf{M} \rightarrow \mathbf{Br}_2 + \mathbf{M}$	-1	k_{-1}

11.4 Collision number

The collision number defined as the number of collisions per unit time and per unit volume and having dimensions $(time)^{-1} \times (volume)^{-1}$ should be denoted by Z.

The collision number divided by the product of two relevant concentrations (or by the square of the relevant concentration) and by the Avogadro constant is a second-order rate constant having dimensions $(time)^{-1} \times (volume)$ \times (amount of substance)⁻¹ and should be denoted by z. Thus $z = Z/Lc_Ac_B$.

12. VALUES OF SOME FUNDAMENTAL CONSTANTS

At its General Assembly in Stockholm on September 11, 1973, the Committee on Data for Science and Technology (CODATA) of the International Council of Scientific Unions recommended a revised set of consistent values of the fundamental constants for international use. For details and especially for the correlation of errors the reader is referred to the CODATA report (Reference 13.11) and to the full description of the procedures by which these values were obtained (Reference 13.12). For convenience, selected constants most useful for chemists are listed here, including several defined constants and derived constants not mentioned in the CODATA report. In each case, the digit(s) in parentheses following a numerical value represent the standard deviation of that value in the decimal place(s) indicated for its final digit(s).

Quantity	Symbol and equivalences	Value
Permeability of vacuum	μο	$4\pi \times 10^{-7}$ H m ⁻¹ exactly
Speed of light in vacuum	с	$2.99792458(1) \times 10^8 \text{ m s}^{-1}$
Permittivity of vacuum	$\epsilon_0 = (\mu_0 c^2)^{-1}$	$8.85418782(5) \times 10^{-12} \mathrm{Fm}^{-1}$
Fine structure constant	$a = \mu_0 c e^2/2h$ a^{-1}	$7.2973506(60) \times 10^{-3}$ 137.03604(11)
Elementary charge	е	1.6021892(46) × 10 ⁻¹⁹ C
Planck constant	$\overset{h}{\hbar}=h/2\pi$	$6.626176(36) imes 10^{-34} \text{ J Hz}^{-1}$ 1.0545887(57) $ imes 10^{-34} \text{ J s}$
Avogadro constant	$L, N_{\rm A}$	$6.022045(31) \times 10^{23} \mathrm{mol}^{-1}$
Atomic mass unit	$1 \text{ u} = 10^{-3} \text{ kg mol}^{-1}/L$	$1.6605655(86) \times 10^{-27} \text{ kg}$
Rest mass of electron	me	9.109534(47) $ imes$ 10 ⁻³¹ kg
Rest mass of proton	mp	$1.6726485(86) \times 10^{-27} \mathrm{kg}$
Rest mass of neutron	m _n	$1.6749543(86) imes 10^{-27} \mathrm{kg}$
Faraday constant	F = Le	9.648456(27) × 10 ⁴ C mol ⁻¹
Rydberg constant	$R_{\infty}=\mu_0^2m_{ m e}e^4c^3/8h^3$	$1.097373177(83) \times 10^{7} \mathrm{m^{-1}}$
Hartree energy ⁽¹⁾	$E_{\rm h}=2hcR_{\infty}$	$4.359814(24) \times 10^{-18} \text{ J}$
Bohr radius	$a_0 = a/4\pi R_{\infty}$	5.2917706(44) × 10 ⁻¹¹ m
Bohr magneton	$\mu_{ m B}=e\hbar/2m_{ m e}$	9.274078(36) $ imes$ 10 ⁻²⁴ J T ⁻¹
Nuclear magneton	$\mu_{ m N} = e\hbar/2m_{ m p}$	5.050824(20) $ imes$ 10 ⁻²⁷ J T ⁻¹
Electron magnetic moment	μe	9.284832(36) $ imes$ 10 ⁻²⁴ J T ⁻¹
Landé g-factor for free electron	$g_{ m e}=2\mu_{ m e}/\mu_{ m B}$	2.0023193134(70)
Proton gyromagnetic ratio	γρ	$2.6751987(75) \times 10^8 s^{-1} T^{-1}$
Proton resonance frequency (H ₂ O) per unit field ⁽²⁾	$\gamma_{p}'/2\pi$	4.257602(12) \times 10 ⁷ Hz T ⁻¹
Gas constant	R	8.31441(26) J K ⁻¹ mol ⁻¹
Zero of the Celsius scale	To RTo	273.15 K exactly 2.271081(71) \times 10 ³ J mol ⁻¹
Normal atmosphere	Po	1.01325×10^5 Pa exactly
Standard molar volume of ideal gas	$V_0 = RT_0/P_0$	$2.241383(70) \times 10^{-2} \mathrm{m^3 mol^{-1}}$
Boltzmann constant	k = R/L	1.380662(44) $ imes$ 10 ⁻²³ J K ⁻¹
Gravitational constant	G	6.6720(27) \times 10 $^{-11}m^3kg^{-1}s^{-2}$
Standard acceleration of free fall	gn	9.80665 m s ^{-2} exactly

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⁽¹⁾ Name and symbol recommended by IUPAC Commission on Symbols, Terminology,

⁽a) Name and symbol recommended by FOLAC commission on symbols, remained by, (a) The relative temperature dependence of the diamagnetic shielding correction in water is of the order of $1 \times 10^{-8}/\text{K}$, which is negligible in comparison with the present uncertainty in $\gamma_p'/2\pi$. The value given here is based on measurements in the range 20–35 °C.

13. REFERENCES

13.1	The ISO 31 International Standard Series will, when complete, form a com- prehensive publication dealing with quantities and units in various fields of science and technology. The following parts have so far been published and can be purchased in any country belonging to ISO from the 'Member Body', usually the national standardizing organization of the country.
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APPENDIX I

DEFINITION OF ACTIVITIES AND RELATED QUANTITIES

A.I.1 Chemical potential and absolute activity

The chemical potential μ_B of a substance B in a mixture of substances B, C, . . ., is defined by

$$\mu_{\rm B} = (\partial G/\partial n_{\rm B})_{T,p,n_{\rm C}} \dots$$

where G is the Gibbs energy of the mixture, T is the thermodynamic temperature, p is the pressure, and $n_{\rm B}$, $n_{\rm C}$, ..., are the amounts of the substances B, C, ..., in the mixture.

(In molecular theory the symbol μ_B is sometimes used for the quantity μ_B/L where L is the Avogadro constant, but this usage is not recommended.)

The absolute activity λ_B of the substance B in the mixture is a number defined by

$$\lambda_{\rm B} = \exp(\mu_{\rm B}/RT)$$
 or $\mu_{\rm B} = RT \ln \lambda_{\rm B}$

where R is the gas constant.

The definitions given below often take simpler, though perhaps less familiar, forms when they are expressed in terms of absolute activity rather than in terms of chemical potential. Each of the definitions given below is expressed in both of these ways.

1. Pure substances

A.I.2 Properties of pure substances

The superscript * attached to the symbol for a property of a substance denotes the property of the *pure* substance. It is sometimes convenient to treat a mixture of constant composition as a pure substance.

A.I.3 Fugacity of a pure gaseous substance

The fugacity f_B^* of a pure gaseous substance B is a quantity with the same dimensions as pressure, defined in terms of the absolute activity λ_B^* of the pure gaseous substance B by

$$f_{\rm B}^* = \lambda_{\rm B}^* \lim_{p \to 0} (p/\lambda_{\rm B}^*)$$
(*T* const.)

or in terms of the chemical potential $\mu_{\rm B}$ by

$$RT \ln f_{\rm B}^* = \mu_{\rm B}^* + \lim_{p \to 0} (RT \ln p - \mu_{\rm B}^*)$$
 (T const.)

where p is the pressure of the gas and T is its thermodynamic temperature. It follows from this definition that

$$\lim_{p \to 0} (f_B^*/p) = 1 \qquad (T \text{ const.})$$

and that

$$RT \ln(f_{\mathbf{B}}^*/p) = \int_{0}^{p} (V_{\mathbf{B}}^* - RT/p) \,\mathrm{d}p$$
 (*T* const.)

where $V_{\rm B}^*$ is the molar volume of the pure gaseous substance B.

A pure gaseous substance B is treated as an *ideal gas* when the approximation $f_{B}^{*} = p$ is used. The ratio (f_{B}^{*}/p) may be called the fugacity coefficient.

The name activity coefficient has sometimes been used for this ratio but is not recommended.

2. Mixtures

A.I.4 Definition of a mixture

The word *mixture* is used to describe a gaseous or liquid or solid phase containing more than one substance, when the substances are all treated in the same way (contrast the use of the word *solution* in Section A.I.9).

A.I.5 Partial pressure

The partial pressure $p_{\rm B}$ of a substance B in a gaseous mixture is a quantity with the same dimensions as pressure defined by

 $p_{\rm B} = y_{\rm B} p$

where y_B is the mole fraction of the substance B in the gaseous mixture and p is the pressure.

A.I.6 Fugacity of a substance in a gaseous mixture

The fugacity f_B of the substance B in a gaseous mixture containing mole fractions y_B , y_C , ..., of the substances B, C, ..., is a quantity with the same dimensions as pressure, defined in terms of the absolute activity λ_B of the substance B in the gaseous mixture by

$$f_{\rm B} = \lambda_{\rm B} \lim_{n \to \infty} (y_{\rm B} p / \lambda_{\rm B})$$
 (*T* const.)

or in terms of the chemical potential $\mu_{\rm B}$ by

$$RT \ln f_{\rm B} = \mu_{\rm B} + \lim_{p \to 0} \{RT \ln(y_{\rm B}p) - \mu_{\rm B}\}$$
(T const.)

It follows from this definition that

$$\lim_{n \to \infty} (f_{\rm B}/y_{\rm B}p) = 1 \qquad (T \text{ const.})$$

and that

$$RT \ln(f_{\rm B}/y_{\rm B}p) = \int_{0}^{p} (V_{\rm B} - RT/p) \,\mathrm{d}p \qquad (T \,\mathrm{const.})$$

where V_B is the partial molar volume (see Section 1.4) of the substance B in the gaseous mixture.

A gaseous mixture of B, C, ..., is treated as an *ideal gaseous mixture* when the approximations $f_B = y_B p$, $f_C = y_C p$, ..., are used. It follows that $pV = (n_B + n_C + ...)RT$ for an ideal gaseous mixture of B, C, ...

The ratio (f_B/y_Bp) may be called the fugacity coefficient of the substance B. The name activity coefficient has sometimes been used for this ratio but is not recommended.

When $y_B = 1$ the definitions given in this Section for the fugacity of a substance in a gaseous mixture reduce to those given in Section A.I.3 for the fugacity of a pure gaseous substance.

A.I.7 Activity coefficient of a substance in a liquid or solid mixture

The activity coefficient f_B of a substance B in a liquid or solid mixture containing mole fractions x_B , x_C ,..., of the substances B, C,..., is a number defined in terms of the absolute activity λ_B of the substance B in the mixture by

$$f_{\rm B} = \lambda_{\rm B} / \lambda_{\rm B} * x_{\rm B}$$

where λ_{B}^{*} is the absolute activity of the pure substance B at the same temperature and pressure, or in terms of the chemical potential μ_{B} by

$$RT\ln(x_{\rm B}f_{\rm B})=\mu_{\rm B}-\mu_{\rm B}^*$$

where μ_B^* is the chemical potential of the pure substance B at the same temperature and pressure.

It follows from this definition that

$$\lim_{x_{\rm B}\to 1} f_{\rm B} = 1 \qquad (T, p \text{ const.})$$

A.I.8 Relative activity of a substance in a liquid or solid mixture

The relative activity a_B of a substance B in a liquid or solid mixture is a number defined by

$$a_{\rm B} = \lambda_{\rm B}/\lambda_{\rm B}^*$$

or by

$$RT \ln a_{\rm B} = \mu_{\rm B} - \mu_{\rm B}^*$$

where the other symbols are as defined in Section A.I.7.

It follows from this definition that

$$\lim_{x_{\rm B}\to 1} a_{\rm B} = 1 \qquad (T, p \text{ const.})$$

A mixture of substances B, C, ..., is treated as an *ideal mixture* when the approximations $a_{\rm B} = x_{\rm B}$, $a_{\rm C} = x_{\rm C}$, ..., and consequently $f_{\rm B} = 1, f_{\rm C} = 1, \ldots$, are used.

3. Solutions

A.I.9 Definition of solution

The word *solution* is used to describe a liquid or solid phase containing more than one substance, when for convenience one of the substances, which is called the *solvent* and may itself be a mixture, is treated differently from the other substances, which are called *solutes*. When, as is often but not necessarily the case, the sum of the mole fractions of the solutes is small compared with unity, the solution is called a *dilute solution*. In the following definitions the solvent substance is denoted by A and the solute substances by B, C,

A.I.10 Properties of infinitely dilute solutions

The superscript ∞ attached to the symbol for a property of a solution denotes the property of an *infinitely dilute solution*.

For example if V_B denotes the partial molar volume (see Section 1.4) of the solute substance B in a solution containing molalities m_B, m_C, \ldots , or mole fractions x_B, x_C, \ldots , of solute substances B, C, ..., in a solvent substance A, then

$$V_{\rm B}^{\rm c} = \lim_{\Sigma_1 m_1 \to 0} V_{\rm B} = \lim_{\Sigma_1 x_1 \to 0} V_{\rm B} \qquad (T, p \text{ const.})$$

where $i = B, C, \ldots$

Similarly if V_A denotes the partial molar volume of the *solvent* substance A, then

$$V_{\mathbf{A}}^{\infty} = \lim_{\Sigma_{1} \neq \mathbf{n} \to \mathbf{0}} V_{\mathbf{A}} = \lim_{\Sigma_{1} \neq \mathbf{n} \to \mathbf{0}} V_{\mathbf{A}} = V_{\mathbf{A}}^{*} \qquad (T, p \text{ const.})$$

where V_A^* is the molar volume of the pure solvent substance A.

A.I.11 Activity coefficient of a solute substance in a solution

The activity coefficient γ_B of a *solute* substance B in a solution (especially in a dilute liquid solution) containing molalities m_B, m_C, \ldots , of solute substances B, C, ..., in a solvent substance A, is a number defined in terms of the absolute activity λ_B of the solute substance B in the solution by

$$\gamma_{\rm B} = (\lambda_{\rm B}/m_{\rm B})/(\lambda_{\rm B}/m_{\rm B})^{\infty} \qquad (T, p \text{ const.})$$

or in terms of the chemical potential $\mu_{\rm B}$ by

$$RT \ln(m_{\rm B}\gamma_{\rm B}) = \mu_{\rm B} - (\mu_{\rm B} - RT \ln m_{\rm B})^{\infty} \qquad (T, p \text{ const.})$$

It follows from this definition that

$$\gamma_{\rm B}^{\infty} = 1$$
 (*T*, *p* const.)

The name activity coefficient with the symbol y_B may be used for the quantity similarly defined but with amount-of-substance concentration c_B (see Section 2.3) in place of molality m_B .

Another activity coefficient, called the *rational activity coefficient* of a solute substance B and denoted by $f_{x,B}$ is sometimes used. It is defined in terms of the absolute activity λ_B by

$$f_{x,B} = (\lambda_B/x_B)/(\lambda_B/x_B)^{\infty}$$
 (*T*, *p* const.)

or in terms of the chemical potential $\mu_{\rm B}$ by

$$RT \ln(x_{\rm B} f_{x,\rm B}) = \mu_{\rm B} - (\mu_{\rm B} - RT \ln x_{\rm B})^{\infty} \qquad (T, p \text{ const.})$$

where x_B is the mole fraction of the solute substance B in the solution. The rational activity coefficient $f_{x,B}$ is related to the (practical) activity coefficient γ_B by the formula

$$f_{x,\mathrm{B}} = \gamma_{\mathrm{B}}(1 + M_{\mathrm{A}}\sum_{\mathrm{i}}m_{\mathrm{i}}) = \gamma_{\mathrm{B}}/(1 - \sum_{\mathrm{i}}x_{\mathrm{i}})$$

A solution of solute substances B, C, ..., in a solvent substance A is treated as an *ideal dilute solution* when the activity coefficients are approximated to unity, for example $\gamma_B = 1, \gamma_C = 1, \ldots$

A.I.12 Relative activity of a solute substance in a solution

The relative activity a_B of a *solute* substance B in a solution (especially in a dilute liquid solution) containing molalities m_B, m_C, \ldots , of solute substances B, C, ..., in a solvent substance A, is a number defined in terms of the absolute activity λ_B by

$$a_{\rm B} = (\lambda_{\rm B}/m^{\Theta})/(\lambda_{\rm B}/m_{\rm B})^{\infty} = m_{\rm B}\gamma_{\rm B}/m^{\Theta} \qquad (T, p \text{ const.})$$

or in terms of the chemical potential $\mu_{\rm B}$ by

$$RT \ln a_{\rm B} = \mu_{\rm B} - RT \ln m^{\ominus} - (\mu_{\rm B} - RT \ln m_{\rm B})^{\infty}$$
$$= RT \ln(m_{\rm BYB}/m^{\ominus})$$

where m^{\ominus} is a standard value of molality (usually chosen to be 1 mol kg⁻¹) and where the other symbols are as defined in Section A.I.11.

It follows from this definition of $a_{\rm B}$ (compare Section A.I.8) that

$$(a_{\rm B}m^{\Theta}/m_{\rm B})^{\infty} = 1 \qquad (T, p \text{ const.})$$

The name activity is often used instead of the name relative activity for this quantity.

The name relative activity with the symbol $a_{c,B}$ may be used for the quantity similarly defined but with concentration c_B (see Section 2.3) in place of molality m_B , and a standard value c^{\ominus} of concentration (usually chosen to be 1 mol dm⁻³) in place of the standard value m^{\ominus} of molality.

Another relative activity, called the *rational relative activity* of the solute substance B and denoted by $a_{x,B}$, is sometimes used. It is defined in terms of the absolute activity λ_B by

$$a_{x,B} = \lambda_{B} / (\lambda_{B} / x_{B})^{\infty} = x_{B} f_{x,B} \qquad (T, p \text{ const.})$$

or in terms of the chemical potential $\mu_{\rm B}$ by

$$RT \ln a_{x,B} = \mu_{B} - (\mu_{B} - RT \ln x_{B})^{\infty}$$

= $RT \ln(x_{B} f_{x,B})$ (T, p const.)

where x_B is the mole fraction of the substance B in the solution. The rational relative activity $a_{x,B}$ is related to the (practical) relative activity a_B by the formula

$$a_{x,B} = a_B m^{\Theta} M_A$$

A.I.13 Osmotic coefficient of the solvent substance in a solution

The osmotic coefficient ϕ of the *solvent* substance A in a solution (especially in a dilute liquid solution) containing molalities m_B, m_C, \ldots , of solute substances B, C, ..., is a number defined in terms of the absolute activity λ_A of the solvent substance A in the solution by

$$\phi = (M_{\rm A} \sum_{\rm i} m_{\rm i})^{-1} \ln(\lambda_{\rm A}^* / \lambda_{\rm A})$$

where λ_A^* is the absolute activity of the pure solvent substance A at the same temperature and pressure, and M_A is the molar mass of the solvent substance A, or in terms of the chemical potential μ_A^* by

$$\phi = (\mu_{\rm A}^* - \mu_{\rm A})/RTM_{\rm A}\sum_{\rm i}m_{\rm i}$$

where μ_A^* is the chemical potential of the pure solvent substance A at the same temperature and pressure.

For an *ideal dilute solution* as defined in Section A.I.11 or A.I.12 it can be shown that $\phi = 1$.

Another osmotic coefficient, called the *rational osmotic coefficient* of the solvent substance A and denoted by ϕ_x , is sometimes used. It is defined in terms of the absolute activity λ_A by

$$\phi_x = \ln(\lambda_A/\lambda_A^*)/\ln x_A = \ln(\lambda_A/\lambda_A^*)/\ln(1 - \sum_i x_i)$$

or in terms of the chemical potential μ_A by

$$\phi_x = (\mu_{\rm A} - \mu_{\rm A}^*)/RT \ln x_{\rm A} = (\mu_{\rm A} - \mu_{\rm A}^*)/RT \ln(1 - \sum_i x_i)$$

where x_A is the mole fraction of the solvent substance A in the solution. The rational osmotic coefficient ϕ_x is related to the (practical) osmotic coefficient ϕ by the formula

$$\phi_x = \phi M_{\rm A} \sum_{\rm i} m_{\rm i} / \ln(1 + M_{\rm A} \sum_{\rm i} m_{\rm i}) = -\phi M_{\rm A} \sum_{\rm i} m_{\rm i} / \ln(1 - \sum_{\rm i} x_{\rm i})$$

A.I.14 Relative activity of the solvent substance in a solution

The relative activity a_A of the *solvent* substance A in a solution (especially in a dilute liquid solution) containing molalities m_B, m_C, \ldots , or mole fractions x_B, x_C, \ldots , of solute substances B, C, ..., is a number defined in terms of the absolute activity λ_A of the solvent substance A in the solution by

$$a_{\rm A} = \lambda_{\rm A}/\lambda_{\rm A}^* = \exp(-\phi M_{\rm A} \sum_{\rm i} m_{\rm i}) = (1 - \sum_{\rm i} x_{\rm i})^{\phi_x}$$

or in terms of the chemical potential μ_A by

1

$$RT \ln a_{\mathbf{A}} = \mu_{\mathbf{A}} - \mu_{\mathbf{A}}^* = -RT\phi M_{\mathbf{A}} \sum_{i} m_{i} = \phi_{x}RT \ln(1 - \sum_{i} x_{i})$$

where the other quantites are as defined in Section A.I.13. Note: The definition in this Section of the relative activity of the *solvent* in a *solution*, is identical with the definition in Section A.I.8 of the relative activity of any substance in a *mixture*. See also Section A.I.12.