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

## MANUAL OF <br> SYMBOLS AND TERMINOLOGY FOR PHYSICOCHEMICAL QUANTITIES AND UNITS

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Second revision prepared for publication by D. H. Whiffen

## 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<br>Chairman<br>Commission on Symbols, Terminology, and Units

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## Preface to 1973 Edition

The text of the 1969 egition 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<br>Chairman<br>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.

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## 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 | $I$ |
| thermodynamic temperature | $T$ |
| amount of substance | $I_{\mathrm{v}}$ |
| luminous intensity |  |

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 election, 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 isrestricted 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: $v=V / m$
heat 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: $V \quad$ molar volume: $V_{\mathrm{m}}=V / n$
Gibbs energy: $G \quad$ molar Gibbs energy: $G_{\mathrm{m}}=G / n$
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 $X_{\mathrm{E}}$, 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:

$$
X_{\mathrm{B}}=\left(\partial X / \partial n_{\mathrm{B}}\right)_{T, p, n_{\mathrm{C}}}, \cdots
$$

For a pure substance B the partial molar quantity $X_{\mathrm{B}}$ and the molar quantity $X_{\mathrm{m}}$ are identical. The partial molar quantity $X_{\mathrm{B}}$ of pure substance B , which is identical with the molar quantity $X_{\mathrm{m}}$ of pure substance B , may be denoted by $X_{\mathrm{B}}^{*}$, where the superscript ${ }^{*}$ denotes 'pure', so as to distinguish it from the partial molar quantity $X_{\mathrm{B}}$ 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:

$$
a b \text { or } a \cdot b \text { or } a . b \text { or } a \times b
$$

[^0]and their quotient in any of the ways:
$$
\frac{a}{b} \text { or } a / b \text { or } a b^{-1}
$$
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 $d_{\mathrm{i}}$ and $d_{\mathrm{e}}$ 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.

| 2.1 | Space, time, 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 | $\lambda$ |
|  | 2.1.07 | wavenumber: $1 / \lambda$ | $\sigma^{(1)}, \tilde{\nu}^{(2)}$ |
|  | 2.1 .08 | plane angle | $\alpha, \beta, \gamma, \theta, \phi$ |
|  | 2.1 .09 | solid angle | $\omega, \Omega$ |
|  | 2.1.10 | area | $A, S, A_{\mathrm{s}}{ }^{(3)}$ |
|  | 2.1.11 | volume | $V$ |
|  | 2.1.12 | time | $t$ |
|  | 2.1.13 | frequency | $\nu, f$ |
|  | 2.1.14 | circular frequency: $2 \pi \nu$ | $\omega$ |

[^1]2.1.15 period: $1 / \nu \quad T$
2.1.16 characteristic time interval, relaxation time, time constant $\tau$
2.1.17 velocity $v, u, w, c$
2.1.18 angular velocity: $\mathrm{d} \phi / \mathrm{d} t \quad \omega$
2.1.19 acceleration $a$
2.1.20 acceleration of free fall $g$

### 2.2 Mechanical and related quantities

2.2.01 mass m
2.2.02 reduced mass $\quad \mu$
2.2.03 specific volume (volume divided by mass) $v$
2.2.04 density (mass divided by volume) $\rho$
2.2.05 relative density (ratio of the density to that $d$
2.2.06 moment of inertia I
2.2.07 momentum $p$
2.2.08 force $F$
2.2.09 weight $G$, (W)
2.2.10 moment of force $\quad M$
2.2.11 angular momentum $L$
2.2.12 work (force times path) $w, W$
2.2.13 energy $E$
2.2.14 potential energy $\quad E_{\mathrm{p}}, V, \Phi$
2.2.15 kinetic energy $\quad E_{\mathrm{k}}, T, K$
2.2.16 Hamiltonian function $H$
2.2.17 Lagrangian function $L$
2.2.18 power (energy divided by time) $P$
2.2.19 pressure $D,(P)$
2.2.20 normal stress $\sigma$
2.2.21 shear stress $\tau$
2.2.22 linear strain (relative elongation): $\Delta l / l_{0} \quad \epsilon, e$
2.2.23 volume strain (bulk strain): $\Delta V / V_{0} \quad \theta$
2.2.24 modulus of elasticity (normal stress divided by linear strain, Young's modulus) $E$
2.2.25 shear modulus (shear stress divided by shear angle)

G
2.2.26 compressibility: $-V^{-1}(\mathrm{~d} V / \mathrm{d} p) \quad \kappa$
2.2.27 compression (bulk) modulus: $-V_{0}(\Delta p / \Delta V) \quad K$
2.2.28 velocity of sound $c$
2.2.29 viscosity $\eta,(\mu)$
2.2.30 fluidity: $1 / \eta \quad \phi$
2.2.31 kinematic viscosity: $\eta / \rho \quad \nu$
2.2.32 friction coefficient (frictional force divided by normal force)
$\mu,(f)$
2.2.33 surface tension
$\gamma, \sigma$
2.2.34 angle of contact
$\theta$
2.2.35 diffusion coefficient $D$
2.2.36 mass transfer coefficient (dimension of length divided by time)
$k_{\mathrm{d}}$

### 2.3 Molecular and related quantities

2.3.01 relative atomic mass of an element (formerly called 'atomic weight')( ${ }^{(1)}$
$A_{\mathrm{r}}$

[^2]Example: $\dot{A_{\mathrm{r}}}(\mathrm{Cl})=35.453$
2.3.02 relative molecular mass of a substance (formerly called 'molecular weight') ${ }^{(1)} \quad M_{r}$
2.3.03 nolar mass (mass divided by amount of substance)
2.3.04 Avogadro constant

M
2.3.05 number of molecules or other entities
$N$
2.3.06 amount of substance ${ }^{(2)}$
$n,(\nu)$
2.3.07 mole fraction of substance $B: n_{B} / \Sigma_{1} n_{i} \quad x_{B}, y_{B}$
2.3.08 mass fraction of substance $B$
2.3.09 volume fraction of substance $B$
$w_{B}$
2.3.10 molality of solute substance $B$ (amount of $B$
2.3.11 amount-of-substance concentration of substance
$\phi_{B}$ $B$ (amount of $B$ divided by the volume of the solution) ${ }^{(4)}$
$c_{B},[B]$
2.3.12 mass concentration of substance $B$ (mass of $B$ divided by the volume of the solution)
$m_{B}$
2.3.11 amount-of-substance concentration of substance
$\begin{array}{ll}\text { 2.3.13 } & \text { surface concentration, surface excess } \\ \text { 2.3.14 } & \text { collision diameter of a molecule }\end{array}$ $\stackrel{\rho_{\mathrm{B}}}{\Gamma}$
$d$, o
2.3.15 mean free path $l, \lambda$
2.3.16 collision number (number of collisions divided by volume and by time)

Z
2.3.17 grand partition function (system) $\Xi$
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 $\sigma, s$
2.3.22 characteristic temperature $\Theta$

### 2.4 Thermodynamic and related quantities

2.4.01 thermodynamic temperature, absolute temperature $\quad T$
2.4.02 Celsius temperature $t, \theta^{(5)}$
2.4.03 (molar) gas constant $\quad R$
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: $U+p V \quad H$
2.4.09 entropy $S$
2.4.10 Helmholtz energy: $U-T S \quad A$
2.4.11 Massieu function: $-A / T \quad J$
2.4.12 Gibbs energy: $H$ - TS $G$
2.4.13 Planck function: $-G / T \quad Y$
2.4.14 compression factor: $p V_{\mathrm{m}} / R T \quad Z$
2.4.15 heat capacity $C$
2.4.16 specific heat capacity (heat capacity divided by mass; the name 'specific heat' is not recommended)
${ }^{(1)}$ The ratio of the average mass per formula unit of a substance to $1 / 12$ of the mass of an atom of nuclide ${ }^{12} \mathrm{C}$.

[^3]| 2.4.17 | ratio $C_{p} / C_{V}$ | $\gamma,(\kappa)$ |
| :---: | :---: | :---: |
| 2.4.18 | Joule-Thomson coefficient | $\mu$ |
| 2.4.19 | thermal conductivity | $\lambda, k$ |
| 2.4 .20 | thermal diffusivity: $\lambda / \rho c_{p}$ | $a$ |
| 2.4.21 | coefficient of heat transfer (density of heat flow rate divided by temperature difference) | $h$ |
| 2.4.22 | cubic expansion coefficient: $V^{-1}(\partial V / \partial T)_{p}$ | $\boldsymbol{a}$ |
| 2.4.23 | isothermal compressibility $-V^{-1}(\partial V / \partial p)_{T}$ | $\kappa$ |
| 2.4.24 | pressure coefficient: $(\partial p / \partial T)_{V}$ | $\beta$ |
| 2.4.25 | chemical potential of substance B | $\mu_{\text {B }}$ |
| 2.4.26 | absolute activity of substance B: $\exp \left(\mu_{\mathrm{B}} / R T\right)$ | $\lambda_{\text {B }}$ |
| 2.4.27 | fugacity | $f, \tilde{p}$ |
| 2.4.28 | osmotic pressure | $\Pi$ |
| 2.4.29 | ionic strength: $\left(I_{m}=\frac{1}{2} \Sigma_{i} m_{1} z_{i}{ }^{2}\right.$ or $\left.I_{c}=\frac{1}{3} \Sigma_{i} c_{i} z_{i}{ }^{2}\right)$ | $I$ |
| 2.4.30 | activity, relative activity of substance $B$ | $a_{\text {B }}$ |
| 2.4.31 | activity coefficient, mole fraction basis | $f_{\text {B }}$ |
| 2.4.32 | activity coefficient, molality basis | $\gamma_{B}$ |
| 2.4.33 | activity coefficient, concentration basis | $y_{B}$ |
| 2.4.34 | osmotic coefficient | $\phi$ |

### 2.5 Chemical reactions

2.5.01 stoichiometric coefficient of substance B (negative for reactants, positive for products)
2.5.02 general equation for a chemical reaction

2.5.03 extent of reaction: $\left(\mathrm{d} \xi=\mathrm{d} n_{\mathrm{B}} / \nu_{\mathrm{B}}\right)$
2.5.04 rate of reaction: $\mathrm{d} \xi / \mathrm{d} t$ (see Section 11)
$\dot{\xi}, J$
2.5.05 rate of increase of concentration of substance B : $\mathrm{d} c_{\mathrm{B}} / \mathrm{d} t$
2.5.06 rate constant
2.5.07 affinity of a reaction: $-\Sigma_{\mathrm{B}} \nu_{\mathrm{B}} \mu_{\mathrm{B}}$
2.5.08 equilibrium constant
$v_{\mathrm{B}}, r_{\mathrm{B}}$
2.5.09 degree of dissociation
$A,(\mathscr{A})$
K
$\alpha$
2.6 Electricity and magnetism
2.6.01 elementary charge (of a proton) e
2.6.02 quantity of electricity $Q$
2.6.03 charge density $\rho$
2.6.04 surface charge density $\sigma$
2.6.05 electric current I
2.6.06 electric current density $j$
2.6.07 electric potential $V, \phi$
2.6.08 electric potential difference: $I R \quad U, \Delta V, \Delta \phi$
2.6.09 electric field strength $\boldsymbol{E}$
2.6.10 electric displacement $\boldsymbol{D}$
2.6.11 capacitance C
2.6.12 permittivity: $(D=\epsilon E) \quad \epsilon$
2.6.13 permittivity of vacuum $\epsilon_{0}$
2.6.14 relative permittivity ${ }^{(1)}: \epsilon / \epsilon_{0} \quad \epsilon \mathrm{r},(\boldsymbol{\epsilon})$
2.6.15 dielectric polarization: $\boldsymbol{D}-\epsilon_{0} \boldsymbol{E} \quad \boldsymbol{P}$
2.6.16 electric susceptibility: $\epsilon_{r}-1 \quad \chi_{e}$
2.6.17 electric dipole moment $p, p_{\mathrm{e}}$
2.6.18 permanent dipole moment of a molecule $\quad \boldsymbol{p}, \mu$
2.6.19 induced dipole moment of a molecule $\quad p, p_{\mathrm{i}}$
2.6.20 electric polarizability of a molecule $\alpha$
2.6.21 magnetic flux $\Phi$
2.6.22 magnetic flux density, magnetic induction $\boldsymbol{B}$
2.6.23 magnetic field strength $\boldsymbol{H}$
2.6.24 permeability: $(\boldsymbol{B}=\boldsymbol{\mu} \boldsymbol{H}) \quad \mu$
2.6.25 permeability of vacuum $\mu_{0}$
${ }^{(1)}$ Also called dielectric constant, and sometimes denoted by $D$, when it is independent of $E$.

| 2.6.26 | relative permeability: $\mu / \mu_{0}$ | $\mu_{\mathrm{r}}$ |
| :---: | :---: | :---: |
| 2.6.27 | magnetization: $\left(\boldsymbol{B} / \mu_{0}\right)-\boldsymbol{H}$ | $\boldsymbol{M}$ |
| 2.6.28 | magnetic susceptibility: $\mu \mathrm{r}-1$ | $\chi,\left(\chi_{m}\right)$ |
| 2.6.29.1 | Bohr magneton | $\mu_{\text {B }}$ |
| 2.6.29.2 | nuclear magneton | $\mu_{\mathrm{N}}$ |
| 2.6.29.3 | $g$-factor | $g$ |
| 2.6.29.4 | gyromagnetic ratio, magnetogyric ratio | $\gamma$ |
| 2.6.30 | electromagnetic moment: $\left(E_{\mathrm{p}}=-m \cdot B\right)$ | $\boldsymbol{m}, \mu$ |
| 2.6.31 | resistance | $R$ |
| 2.6.32 | resistivity (formerly called specific resistance): $(E=\rho j)$ | $\rho$ |
| 2.6.33 | conductivity (formerly called specific conductance): $(j=\kappa \boldsymbol{E})$ | $\kappa$, ( $\sigma$ ) |
| 2.6.34 | self-inductance |  |
| 2.6.35 | mutual inductance | $M, L_{12}$ |
| 2.6.36 | reactance | $X$ |
| 2.6.37 | impedance (complex impedance): $R+\mathrm{i} X$ | $\boldsymbol{Z}$ |
| 2.6.38 | loss angle | $\delta$ |
| 2.6.39 | admittance (complex admittance): $1 / Z$ | $Y$ |
| 2.6.40 | conductance: $(Y=G+\mathrm{i} B)$ | $G$ |
| 2.6.41 | susceptance: $(Y=G+\mathrm{i} B)$ | $B$ |

### 2.7 Electrochemistry

2.7.01 Faraday constant $F$
2.7.02 charge number of an ion $B$ (positive for cations, negative for anions) $\quad z_{B}$
2.7.03 charge number of a cell reaction $n,(z)$
2.7.04 electromotive force $E, E_{\mathrm{MF}}$
2.7.05 electrochemical potential of ionic component B :
$\mu_{\mathrm{B}}+z_{\mathrm{B}} F \phi \quad \tilde{\mu}_{\mathrm{B}}$
2.7.06 electric mobility (velocity divided by electric field strength)
$u, \mu$
2.7.07 electrolytic conductivity (formerly called specific conductance)
$\kappa$, ( $\sigma$
2.7.08 molar conductivity of electrolyte or ion ${ }^{(1)}: \kappa / c \quad \Lambda, \lambda^{(2)}$
2.7.09 transport number (transference number or migration number)
$t$
2.7.10 overpotential $\eta$
2.7.11 exchange current density $j_{0}$
2.7.12 electrochemical transfer coefficient $a$
2.7.13 electrokinetic potential (zeta potential) $\zeta$
2.7.14 thickness of diffusion layer $\delta$
2.7.15 inner electric potential $\phi$
2.7.16 outer electric potential $\psi$
2.7.17 surface electric potential difference: $\phi-\psi \quad \chi$

[^4]$\Lambda$ is used for an electrolyte and $\lambda$ for individual ions.

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

| $l$ | 2.1 .01 | $\tilde{\nu}$ | 2.1 .07 | $\theta$ | 2.1 .08 | $\omega$ | 2.1 .09 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $S$ | 2.1 .10 | $V$ | 2.1 .11 | $t$ | 2.1 .12 | $c_{\mathrm{B}}$ | 2.3 .11 |
| $\rho_{\mathrm{B}}$ | 2.3 .12 | $\Phi$ | 2.8 .04 | $I$ | 2.8 .05 | $E$ | 2.8 .08 |
| $T$ | 2.8 .12 | $A$ | 2.8 .13 .1 | $B$ | 2.8 .13 .2 | $\alpha$ | 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 might otherwise occur.
${ }^{(3)}$ 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 cells; in addition to the physical matching of the sample and reference cells this requires that there be no significant difference between $n_{\text {solvent }}$ and $n_{\text {solution }}$.
${ }^{(8)}$ 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.
2.8.21.1 refractive index (of a non-absorbing
material)
$\begin{array}{ll}\text { 2.8.21.2 } & \text { complex refractive index of an } \\ \text { absorbing material: } n+i k\end{array} \hat{n}$
2.8.22 molar refraction: $\left(n^{2}-1\right) V_{\mathrm{m}} /\left(n^{2}+2\right) \quad R_{\mathrm{m}}$
2.8.23 angle of optical rotation $\quad a$

### 2.9 Transport properties ${ }^{(1)}$

2.9.01 Flux (of a quantity $X$ ) $J_{X}, J$
2.9.02 Reynolds number: $\rho \nu l / \eta \quad \operatorname{Re}$
2.9.03 Euler number: $\Delta p / \rho \nu^{2} \quad E u$
2.9.04 Froude number: $v /(l g)^{\frac{1}{2}} \quad$ Fr
2.9.05 Grashof number: $l^{3} g a \Delta \theta \rho^{2} / \eta^{2} \quad G r$
2.9.06 Weber number: $\rho v^{2} l / \gamma \quad W e$
2.9.07 Mach number: $v / c \quad M a$
2.9.08 Knudsen number: $\lambda / l \quad$ Kn
2.9.09 Strouhal number: lf $/ v \quad \mathrm{Sr}$
2.9.10 Fourier number: $a \Delta t / l^{2} \quad$ Fo
2.9.11 Peclet number: vl/a Pe
2.9.12 Rayleigh number: $l^{3} g \alpha \Delta \theta \rho / \eta a \quad R a$
2.9.13 Nusselt number: $h l / k \quad N u$
2.9.14 Stanton number: $h / \rho v c_{p} \quad$ St
2.9.15 Fourier number for mass transfer: $D t / l^{2} \quad F o^{*}$
2.9.16 Peclet number for mass transfer: $v l / D \quad P e^{*}$
2.9.17 Grashof number for mass transfer: $-l^{3} g(\partial \rho / \partial x)_{T, p} \Delta x \rho / \eta^{2} \quad G r^{*}$
2.9.18 Nusselt number for mass transfer ${ }^{(2)} k_{\mathrm{d}} l / D \quad N u^{*}$
2.9.19 Stanton number for mass transfer: $k_{\mathrm{d}} / v \quad S t^{*}$
2.9.20 Prandtl number: $\eta / \rho a \quad$ Pr
2.9.21 Schmidt number: $\eta / \rho D \quad S c$
2.9.22 Lewis number: $a / D \quad L e$
2.9.23 Magnetic Reynolds number: $v_{\mu \kappa l} \quad R e_{\mathrm{m}}$
2.9.24 Alfvén number: $v(\rho \mu)^{\frac{1}{2}} / B \quad A l$
2.9.25 Hartmann number: $B l(\kappa / \eta)^{\frac{1}{2}} \quad H a$
2.9.26 Cowling number: $B^{2} / \mu \rho v^{2} \quad$ Co

### 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:

$$
\lambda_{\mathrm{NO}_{3}^{-}} \quad \Delta H_{25^{\circ} \mathrm{C}} \quad(p V)_{0}^{p=0}{ }^{\circ} \mathrm{C}
$$

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

[^5]case of concentration. The recommended notation for the formulation of the equilibrium constant $K_{c}$ for the general reaction:
$$
0=\Sigma_{B} \nu_{\mathrm{B}} B
$$
is
$$
K_{c}=\Pi_{\mathrm{B}}\left(c_{\mathrm{B}}\right)^{\nu_{\mathrm{B}}}
$$
but when we turn to a particular example it is better to use a notation such as:
\[

$$
\begin{aligned}
& \mathrm{Br}_{2}+\mathrm{H}_{2} \mathrm{O}=\mathrm{HOBr}+\mathrm{H}^{+}+\mathrm{Br}^{-} \\
& {\left[\frac{[\mathrm{HOBr}]\left[\mathrm{H}^{+}\right]\left[\mathrm{Br}^{-}\right]}{\left[\mathrm{Br}_{2}\right]}=K_{c}\right.} \\
& K_{c}\left(25^{\circ} \mathrm{C}\right)=6 \times 10^{-9} \mathrm{~mol}^{2} \mathrm{dm}^{-6}
\end{aligned}
$$
\]

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:

$$
\begin{aligned}
& \lambda\left(\frac{1}{2} \mathrm{Mg}^{2+}\right)=53 \mathrm{~S} \mathrm{~cm}^{2} \mathrm{~mol}^{-1} \text { at } 25^{\circ} \mathrm{C} \\
& \lambda\left(\mathrm{Cl}^{-}\right)=76 \mathrm{~S} \mathrm{~cm}^{2} \mathrm{~mol}^{-1} \text { at } 25^{\circ} \mathrm{C} \\
& \Lambda\left(\frac{1}{2} \mathrm{MgCl}_{2}\right)=129 \mathrm{~S} \mathrm{~cm}^{2} \mathrm{~mol}^{-1} \text { at } 25^{\circ} \mathrm{C} \\
& \Lambda\left(\mathrm{MgCl}_{2}\right)=258 \mathrm{~S} \mathrm{~cm}^{2} \mathrm{~mol}^{-1} \text { at } 25^{\circ} \mathrm{C}
\end{aligned}
$$

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

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

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

$$
V\left(\mathrm{~K}_{2} \mathrm{SO}_{4}, 0.1 \mathrm{~mol} \mathrm{dm}^{-3} \text { in } \mathrm{H}_{2} \mathrm{O}, 25^{\circ} \mathrm{C}\right)=48 \mathrm{~cm}^{3} \mathrm{~mol}^{-1}
$$

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:

$$
a=n a_{n} / A=N a_{N} / A
$$

where $\alpha_{n}$ is the molar optical rotatory power and $\alpha_{N}$ the molecular optical rotatory power. When on the other hand it is desired to record an experimental measurement, an appropriate notation would be:

$$
\alpha\left(589.3 \mathrm{~nm}, 20^{\circ} \mathrm{C} \text {, sucrose, } 10 \mathrm{~g} \mathrm{dm}^{-3} \text { in } \mathrm{H}_{2} \mathrm{O}, 10 \mathrm{~cm}\right)=+66.470^{\circ}
$$

### 2.11 Recommended superscripts

The following superscripts are recommended:

[^6]
## 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 $m \mu \mathrm{~s}$ for $10^{-9} \mathrm{~s}$

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

### 3.4 Multiplication and division of units

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

$$
\mathrm{Nm} \text { or } \mathrm{N} \cdot \mathrm{~m} \text { or } \mathrm{N} \cdot \mathrm{~m} \text { or } \mathrm{N} \times \mathrm{m}
$$

The representation Nm is not recommended.
A quotient of two units may be represented in any of the ways:

$$
\frac{\mathrm{m}}{\mathrm{~s}} \text { or } \mathrm{m} / \mathrm{s} \text { or } \mathrm{ms}^{-1}
$$

or in any of the other ways of writing the product of $m$ and $\mathrm{s}^{-1}$.
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: $\mathbf{J ~ K}^{-1} \mathrm{~mol}^{-1}$ or $\mathrm{J} /(\mathrm{K} \mathrm{mol})$ but never $\mathrm{J} / \mathrm{K} / \mathrm{mol}$

### 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 $2 \mathrm{p}_{10}$ and $5 \mathrm{~d}_{5}$ 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 9192631770 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 $2 \times 10^{-7}$ 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 $\mathrm{Hg}_{2} \mathrm{Cl}_{2}$ has a mass of 472.08 grams
1 mole of $\mathrm{Hg}_{2}^{2+}$ has a mass of 401.18 grams and a charge of 192.97 kilocoulombs
1 mole of $\frac{1}{2} \mathrm{Ca}^{2+}$ has a mass of 20.04 grams and a charge of 96.49 kilocoulombs
1 mole of $\mathrm{Cu}_{0.5} \mathrm{Zn}_{0.5}$ has a mass of 64.46 grams
1 mole of $\mathrm{Fe}_{0.91} \mathrm{~S}$ has a mass of 82.88 grams
1 mole of $\mathrm{e}^{-}$has a mass of 548.60 micrograms, a charge of -96.49 kilocoulombs, and contains $6.02 \times 10^{23}$ electrons
1 mole of a mixture containing the mole fractions $x\left(\mathrm{~N}_{2}\right)=0.7809, x\left(\mathrm{O}_{2}\right)$ $=0.2905, x(\mathrm{Ar})=0.0093$, and $x\left(\mathrm{CO}_{2}\right)=0.0003$ has a mass of 28.964 grams
1 mole of photons whose frequency is $10^{14} \mathrm{~Hz}$ has energy 39.90 kilojoules (The numerical values in these examples are approximate.)

[^7]
### 3.7 Names and symbols for SI Base Units

physical quantity
length
mass
time
electric current
thermodynamic temperature amount of substance ${ }^{(1)}$
luminous intensity
name of SI Unit metre kilogram second ampe kelvin mole candela
symbol for SI Unit
m
kg
s
A
K
mol
cd

### 3.8 Names and symbols for SI Supplementary Units

physical quantity
plane angle
solid angle
name of SI Unit radian steradian
symbol for SI Unit rad
sr
3.9 Special names and symbols for certain SI Derived Units

|  | name of | symbol for |  |
| :---: | :---: | :---: | :---: |
| physical quantity | SI Unit | SI Unit | definition of SI Unit |
| force | newton | N | $\mathrm{m} \mathrm{kg} \mathrm{s}{ }^{-2}$ |
| pressure, stress | pascal | Pa | $\mathrm{m}^{-1} \mathrm{~kg} \mathrm{~s}^{-2}\left(=\mathrm{N} \mathrm{m}^{-2}\right)$ |
| energy | joule | J | $\mathrm{m}^{2} \mathrm{~kg} \mathrm{~s}^{-2}$ |
| power | watt | W | $\mathrm{m}^{2} \mathrm{~kg} \mathrm{~s}^{-3}\left(=\mathrm{J} \mathrm{s}^{-1}\right)$ |
| electric charge | coulomb | C | s A |
| electric potential difference | volt | V | $\mathrm{m}^{2} \mathrm{~kg} \mathrm{~s}^{-3} \mathrm{~A}^{-1}\left(=\mathrm{JA}^{-1} \mathrm{~s}^{-1}\right)$ |
| electric resistance | ohm | $\Omega$ | $\mathrm{m}^{2} \mathrm{~kg} \mathrm{~s}^{-3} \mathrm{~A}^{-2}\left(=\mathrm{VA}^{-1}\right)$ |
| electric conductance | siemens | S | $\mathrm{m}^{-2} \mathrm{~kg}^{-1} \mathrm{~s}^{3} \mathrm{~A}^{2}\left(=\mathrm{AV}^{-1}=\mathrm{S}^{-1}\right)$ |
| electric capacitance | farad | F | $\mathrm{m}^{-2} \mathrm{~kg}^{-1} \mathrm{~s}^{4} \mathrm{~A}^{2}\left(=A \mathrm{Al}^{-1}\right)$ |
| magnetic flux | weber | Wb | $\mathrm{m}^{2} \mathrm{~kg} \mathrm{~s}^{-2} \mathrm{~A}^{-1}(=\mathrm{V} \mathrm{s})$ |
| inductance | henry | H | $\mathrm{m}^{2} \mathrm{~kg} \mathrm{~s}^{-2} \mathrm{~A}^{-2}\left(=\mathrm{VA}^{-1} \mathrm{~s}\right)$ |
| magnetic flux density | tesla | T | $\mathrm{kg} \mathrm{s}^{-2} \mathrm{~A}^{-1}\left(=\mathrm{V} \mathrm{s} \mathrm{m}^{-2}\right)$ |
| luminous flux | lumen | 1 m | cd sr |
| illuminance | lux | 1 x | $\mathrm{m}^{-2} \mathrm{~cd} \mathrm{sr}$ |
| frequency | hertz | Hz | $\mathrm{s}^{\mathbf{- 1}}$ |
| activity (of radioactive source) | becquerel | Bq | $\mathrm{s}^{-1}$ |
| absorbed dose (of radiation) | gray | Gy | $\mathrm{m}^{2} \mathrm{~s}^{-2}\left(=\mathrm{Jkg}^{-1}\right)$ |

### 3.10 SI Derived Units and Unit-symbols for other quantities

(This list is not exhaustive.)
physical quantity
area
volume
density
velocity
angular velocity
acceleration
kinematic viscosity, diffusion coefficient
dynamic viscosity
molar entropy, molar heat capacity
concentration
electric field strength
magnetic field strength
luminance

SI Unit
square metre
cubic metre
kilogram per cubic metre $\quad \mathrm{kg} \mathrm{m}^{-3}$
metre per second $\quad \mathrm{m} \mathrm{s}^{-1}$
radian per second $\quad \mathrm{rad} \mathrm{s}^{-1}$
metre per second squared $\quad \mathrm{m} \mathrm{s}^{-2}$
square metre per second $\quad \mathrm{m}^{2} \mathrm{~s}^{-1}$
newton-second per square metre
joule per kelvin mole mole per cubic metre volt per metre ampere per metre candela per square metre
symbol for SI Unit
$\mathrm{m}^{2}$
$\mathrm{m}^{3}$
$\mathrm{kg} \mathrm{m}^{-1}$

N s m${ }^{-2}$
$\mathbf{J K K}^{-1} \mathrm{~mol}^{-1}$
$\mathrm{mol} \mathrm{m}^{-3}$
$\mathrm{V} \mathrm{m}^{-1}$
$\mathrm{Am}^{-1}$
$\mathrm{cd} \mathrm{m}^{-2}$

[^8]
### 3.11 SI Prefixes

| fraction | prefix | symbol | multiple | prefix | symbol |
| :--- | :--- | :--- | :--- | :--- | :--- |
| $10^{-1}$ | deci | d | 10 | deca | da |
| $10^{-2}$ | centi | c | $10^{2}$ | hecto | h |
| $10^{-3}$ | milli | m | $10^{3}$ | kilo | k |
| $10^{-6}$ | micro | $\mu$ | $10^{6}$ | mega | M |
| $10^{-9}$ | nano | n | $10^{9}$ | giga | G |
| $10^{-12}$ | pico | p | $10^{12}$ | tera | T |
| $10^{-15}$ | femto | f | $10^{15}$ | peta | P |
| $10^{-18}$ | atto | a | $10^{18}$ | exa | E |

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 $\mu \mathrm{kg} \quad \mu \mathrm{g}$ not nkg Mg not kkg

### 3.12 The degree Celsius

$\begin{array}{ll}\text { physical quantity } & \begin{array}{l}\text { name of unit } \\ \text { degree Celsius }\end{array} \\ \text { Celsius temperature }\end{array}{ }^{\circ} \mathrm{C}$ symbol for unit definition of unit
The Celsius temperature $t$, is defined by $t=T-T_{0}$ where $T_{0}=273.15 \mathrm{~K}$. This leads to $t /{ }^{\circ} \mathrm{C}=T / K-273.15$.

### 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 | $\AA$ | $10^{-10} \mathrm{~m}$ |
| cross section | barn | b | $10^{-28} \mathrm{~m}^{2}$ |
| volume | litre | $1, \mathrm{~L}$ | $10^{-3} \mathrm{~m}^{3}$ |
| mass | tonne | t | $10^{3} \mathrm{~kg}$ |
| pressure | bar | bar | $10^{5} \mathrm{~Pa}$ |

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 $\operatorname{erg}\left(10^{-7} \mathrm{~J}\right)$, the dyne $\left(10^{-5} \mathrm{~N}\right)$, the poise ( 0.1 Pas ), the stokes $\left(10^{-4} \mathrm{~m}^{2} \mathrm{~s}^{-1}\right)$, the gauss (corresponding to $\left.10^{-4} \mathrm{~T}\right)^{(3)}$, the oersted (corresponding to $\left.1000 / 4 \pi \mathrm{Am}^{-1}\right)^{(3)}$, and the maxwell (corresponding to $\left.10^{-8} \mathrm{~Wb}\right)^{(3)}$. The name micron and symbol $\mu$ should not be used for the unit of length, $10^{-6} \mathrm{~m}$, which has the SI name micrometre and symbol $\mu \mathrm{m}$.

### 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.

[^9]| Units in use with the International System |  |  |
| :--- | :---: | :--- |
| name of unit | symbol | definition of unit |
| minutc | min | 60 s |
| hour | h | 3600 s |
| day | d | 86400 s |
| degree | $\circ$ | $(\pi / 180) \mathrm{rad}$ |
| minute | , | $(\pi / 10800) \mathrm{rad}$ |
| second | $\prime$ | $(\pi / 648000) \mathrm{rad}$ |

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 | $3.7 \times 10^{10} \mathrm{~Bq}$ |
| exposure to X or $\gamma$ radiation | röntgen | R | $\stackrel{2.58 \times 10^{-4}}{C \mathrm{~kg}^{-1}}$ |
| ionizing radiation | rad | $\mathrm{rad}^{(1)}$ | $10^{-2} \mathrm{~Gy}$ |

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 generally 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 | 0.45359237 kg |
| force | kilogram-force | kgf | 9.80665 N |
| pressure | standard atmosphere ${ }^{(2)}$ | atm | 101325 Pa |
| pressure | torr | Torr | $\begin{gathered} 101325 \\ 760 \end{gathered} \mathrm{~Pa}$ |
| pressure | conventional millimetre of mercury ${ }^{(3)}$ | mmHg | $\begin{aligned} & 13.5951 \\ & \times 980.665 \\ & \times 10^{-2} \mathrm{~Pa} \end{aligned}$ |
| energy | kilowatt-hour | kW h | $3.6 \times 10^{6} \mathrm{~J}$ |
| energy | thermochemical calorie | $\mathrm{Cal}_{\text {th }}$ | 4.181 J |
|  | British thermal unit degre Rankine | ${ }_{\text {c }}{ }^{\text {Btu }}$ | $\underset{(5 / 9) \mathrm{K}}{1055.055} 85262 \mathrm{~J}$ |
| thermodynamic temperature | degree Rankine | ${ }^{\text {'R }}$ | (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:

| physical quantity <br> energy | name of unit <br> electronvolt | symbol for unit <br> eV | conversion factor <br> mass |
| :--- | :--- | :--- | :--- |
|  | (unified) atomic | u | $\times 10^{-19} \mathbf{j}$ |
|  | mass unit |  |  |

### 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

[^10]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' $=1.00049 \Omega$
1 'mean international volt' $=1.00034 \mathrm{~V}$
1 'US international ohm' $=1.000495 \Omega$
1 'US international volt' $=1.000330 \mathrm{~V}$

### 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. $1 \mathrm{D}=\left(10^{-21} / c\right) \mathrm{A} \mathrm{m}^{2} \approx 3.3356 \times 10^{-30}$ C m.

## 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: 2573,421736 or in English language texts 2573.421736 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: $0,2573 \times 10^{4}$ or in English language texts $0.2573 \times 10^{4}$ 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 $2.573 \times 10^{3}$

### 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 $2,3 \cdot 3,4$
Division of one number by another may be indicated in any of the ways:

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

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 $p_{\mathrm{c}}$ has the value for water:

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

These equations may equally well be written in the forms:

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

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 $\Delta$ ) and mathematical constants (for example e and $\pi$ ) 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 | $\neq$ |
| identically equal to | $\equiv$ |
| corresponds to | $\underline{\underline{=}}$ |
| approximately equal to | * |
| approaches | $\rightarrow$ |
| asymptotically equal to | $\simeq$ |
| proportional to | $\propto \sim$ |
| infinity | $\infty$ |
| less than | $<$ |
| greater than | > |
| less than or equal to | $\leqslant$ |
| greater than or equal to | $\geqslant$ |
| much less than | $\gtrless$ |
| much greater than | $\geqslant$ |
| plus | $+$ |
| minus | - |
| multiplied by |  |
| $a$ divided by $b$ | $\begin{array}{lll} a \\ b \end{array} a / b \quad a b^{-1}$ |
| magnitude of $a$ | $\|a\|$ |
| $a$ raised to the power $n$ | $a^{n}$ |
| square root of $a$ | $a^{1 / 2} a^{\frac{1}{2}} \sqrt{ } a \sqrt{ } a$ |
| $n$ '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 $a$ | $\ln a \quad \log _{e} a$ |
| decadic logarithm of $a$ | $\lg a \log _{10} a \quad \log a$ |
| binary logarithm of $a$ | $\mathrm{lb} a \quad \log _{2} a$ |
| exponential of $a$ | $\exp a \mathrm{e}^{a}$ |

[^11]
## 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: ${ }^{14} \mathrm{~N}_{2},{ }^{35} \mathrm{Cl}^{-}$
Ionic charge: $\mathrm{Cl}^{-}, \mathrm{Ca}^{2+}, \mathrm{PO}_{4}^{3-}$ or $\mathrm{PO}_{4}{ }^{3-}$
Excited electronic state: $\mathrm{He}^{*}$, NO*
Oxidation number: $\mathrm{Pb}_{2}{ }^{\mathrm{II}} \mathrm{Pb}^{\mathrm{IV}} \mathrm{O}_{4}, \mathrm{~K}_{6} \mathrm{M}^{\mathrm{IV}} \mathrm{Mo}_{9} \mathrm{O}_{32}$ (where M denotes a metal)

### 7.3 Particles

| neutron | n | helion |
| :--- | :--- | :--- |
| proton | p | $\alpha-$ particle $\alpha$ |
| deuteron | d | electron |
| e |  |  |
| triton | t | photon |

The electric charge of particles may be indicated by adding the superscript ,+- , or 0 ; e.g., $\mathrm{p}^{+}, \mathrm{n}^{0}, \mathrm{e}^{+}, \mathrm{e}^{-}$. 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:


[^12]
## 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:

$$
\begin{aligned}
& L, l=0: S, s \\
& L, l=4: G, g \\
& =1: \mathrm{P}, \mathrm{p} \quad=5: \mathrm{H}, \mathrm{~h}=9: \mathrm{M}, \mathrm{~m} \\
& L, l=8: \mathrm{L}, 1 \\
& =2: \mathrm{D}, \mathrm{~d} \quad=6: \mathrm{I}, \mathrm{i} \quad=10: \mathrm{N}, \mathrm{n} \\
& =3: \mathrm{F}, \mathrm{f}=7: \mathrm{K}, \mathrm{k}=11: \mathrm{O}, \mathrm{o}
\end{aligned}
$$

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

Examples: ${ }^{2} \mathrm{P}_{3 / 2}$ - state ( $J=3 / 2$, multiplicity 2 )
$\mathrm{p}_{3 / 2}$ - electron ( $j=3 / 2$ )
An atomic electron configuration is indicated symbolically by:

$$
(n l)^{\kappa}\left(n^{\prime} l^{\prime}\right)^{\kappa^{\prime}} \ldots
$$

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

Example: the atomic configuration: $(1 \mathrm{~s})^{2}(2 \mathrm{~s})^{2}(2 \mathrm{p})^{3}$

### 8.3 Molecular spectroscopy

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

$$
\begin{aligned}
\Lambda, \lambda & =0: \Sigma, \sigma \\
& =1: \Pi, \pi \\
& =2: \Delta, \delta
\end{aligned}
$$

and for non-linear molecules:

$$
\mathrm{A}, \mathrm{a} ; \mathrm{B}, \mathrm{~b} ; \mathrm{E}, \mathrm{e} ; \mathrm{etc} .
$$

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 righ ${ }^{+}$-hand superscript indicates the symmetry as regards reflection in any plane through the symmetry axis of the molecules.
Examples: $\Sigma_{\mathbf{d}}, \Pi_{\mathbf{u}},{ }^{2 \Sigma},{ }^{3} \Pi$, etc.
The letter-symbols indicating the vibrational angular momentum states in the case of linear molecules are:

$$
\begin{aligned}
l & =0: \Sigma \\
& =1: \Pi \\
& =2: \Delta
\end{aligned}
$$

[^13]
### 8.4 Spectroscopic transitions

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

## Example: $h \nu=E^{\prime}-E^{\prime \prime}$

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

$$
\begin{array}{cl}
\text { Examples; } ;{ }^{2} \mathrm{P}_{1 / 2}-{ }^{2} \mathrm{~S}_{1 / 2} & \text { for an electronic transition } \\
\left(J^{\prime}, K^{\prime}\right)-\left(J^{\prime \prime}, K^{\prime \prime}\right) & \text { for a rotational transition } \\
v^{\prime}-v^{\prime \prime} & \text { for a vibrational transition }
\end{array}
$$

Absorption transition and emission transition may be indicated by arrows $\leftarrow$ and $\rightarrow$ respectively.
$\begin{array}{ll}\text { Examples: }{ }^{2} \mathrm{P}_{1 / 2} \rightarrow{ }^{2} \mathrm{~S}_{1 / 2} & \text { emission from }{ }^{2} \mathrm{P}_{1 / 2} \text { to }{ }^{2} \mathrm{~S}_{1 / 2} \\ \left(J^{\prime}, K^{\prime}\right) \leftarrow\left(J^{\prime \prime}, K^{\prime \prime}\right) & \text { absorption from }\left(J^{\prime \prime}, K^{\prime \prime}\right) \text { to }\left(J^{\prime}, K^{\prime}\right)\end{array}$
The difference $\Delta$ between two quantum numbers should be that of the upper state minus that of the lower state.
Example: $\Delta J=J^{\prime}-J^{\prime \prime}$
The indications of the branches of the rotation band should be as follows:

$$
\begin{aligned}
\Delta J=J^{\prime}-J^{\prime \prime} & =-2: \text { O-branch } \\
& =-1: \text { P-branch } \\
& =0: \text { Q-branch } \\
& =+1: \text { R-branch } \\
& =+2: \text { S-branch }
\end{aligned}
$$

## 9. CONVENTIONS CONCERNING THE SIGNS OF ELECTRIC POTENTIAL DIFFERENCES, ELECTROMOTIVE 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:

$$
\mathrm{Zn}\left|\mathrm{Zn}^{2+}\right| \mathrm{Cu}^{2+} \mid \mathrm{Cu}
$$

The electric potential difference $\Delta V$ 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:

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

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 $\left[\mathrm{Cu}^{2+}\right] /\left[\mathrm{Zn}^{2+}\right]$ is extremely small), the electric potential difference will be positive.

If, however, the reaction is written as:

$$
\frac{1}{2} \mathrm{Cu}+\frac{1}{2} \mathrm{Zn}^{2+} \rightarrow \frac{1}{2} \mathrm{Cu}^{2+}+\frac{1}{2} \mathbf{Z n}
$$

this implies the diagram:

$$
\mathrm{Cu}\left|\mathrm{Cu}^{2+}\right| \mathbf{Z n}^{2+} \mid \mathbf{Z n}
$$

and the electric potential difference of the cell so specified will be negative (unless the ratio $\left[\mathrm{Cu}^{2+}\right] /\left[\mathrm{Zn}^{2+}\right]$ 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 $E_{\mathrm{MF}}$ 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 $\mathrm{Zn}^{2+} \mid \mathbf{Z n}$ ) the cell in question is:

$$
\mathrm{Pt}\left|\mathrm{H}_{2}\right| \mathrm{H}^{+}\left|\mathrm{Zn}^{2+}\right| \mathrm{Zn}
$$

The reaction taking place at the zinc electrode is:

$$
\mathbf{Z n}^{2+}+2 \mathrm{e}^{-} \rightarrow \mathbf{Z n}
$$

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

$$
\mathrm{Zn}^{2+}+\mathrm{H}_{2} \rightarrow \mathrm{Zn}+2 \mathrm{H}^{+}
$$

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 .

[^14]The symbol $\mathbf{Z n} \mid \mathbf{Z n}^{2+}$ on the other hand implies the cell:

$$
\mathrm{Zn}\left|\mathrm{Zn}^{2+}\right| \mathrm{H}^{+}\left|\mathrm{H}_{2}\right| \mathrm{Pt}
$$

in which the reaction is:

$$
\mathrm{Zn}+2 \mathrm{H}^{+} \rightarrow \mathrm{Zn}^{2+}+\mathrm{H}_{2}
$$

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

## 10. THE QUANTITY $\mathbf{p H}^{(1)}$

### 10.1 Operational definition

In all existing national standards the definition of pH is an operational one. The electromotive force $E_{\mathrm{X}}$ of the cell:
reference electrode | concentrated KCl solution : $^{\text {i solution }} \mathrm{X}\left|\mathrm{H}_{2}\right| \mathrm{Pt}$
is measured and likewise the electromotive force $E_{\mathrm{S}}$ of the cell:
reference electrode | concentrated KCl solution :: solution $\mathrm{S}\left|\mathrm{H}_{2}\right| \mathrm{Pt}$
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 $\mathrm{pH}(\mathrm{X})$, is then related to the pH of the solution S , denoted by $\mathrm{pH}(\mathbf{S})$, by the definition:

$$
\mathrm{pH}(\mathrm{X})=\mathrm{pH}(\mathbf{S})+\frac{\left(E_{\mathrm{S}}-E_{\mathrm{X}}\right) F}{R T \ln 10}
$$

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 $3.5 \mathrm{~mol} \mathrm{~kg}^{-1}$, 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 $\mathrm{pH}(\mathrm{S})$ 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 $E_{\mathrm{X}}$ 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 $\mathbf{S}_{1}$ and $\mathbf{S}_{2}$ such that the $E_{1}$ and $E_{2}$ values are on either side of, and as near as possible to, $E_{\mathbf{X}}$. The pH of solution X is then obtained by assuming linearity between pH and $E$, that is to say:

$$
\frac{\mathrm{pH}(\mathrm{X})-\mathrm{pH}\left(\mathbf{S}_{1}\right)}{\mathrm{pH}\left(\mathbf{S}_{2}\right)-\mathrm{pH}\left(\mathbf{S}_{1}\right)}=\frac{E_{\mathrm{X}}-E_{1}}{E_{2}-E_{1}}
$$

[^15]This procedure is especially recommended when the hydrogen-ion-responsive electrode is a glass electrode.
10.3 Values of $\mathbf{p H}(\mathbf{S})$ for five standard solutions

| $t /{ }^{\circ} \mathrm{C}$ | A | B | C | D | E |
| ---: | :--- | :--- | :--- | :--- | :--- |
| $\mathbf{0}$ |  | 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 |

The compositions of the standard solutions are:
A: KH tartrate (saturated at $25^{\circ} \mathrm{C}$ )
B: KH phthalate, $m=0.05 \mathrm{~mol}^{\mathrm{kg}}{ }^{-1}$
C: $\mathrm{KH}_{2} \mathrm{PO}_{4}, m=0.025 \mathrm{~mol} \mathrm{~kg}^{-1}$; $\mathrm{Na}_{2} \mathrm{HPO}_{4}, m=0.025 \mathrm{~mol} \mathrm{~kg}^{-1}$
D: $\mathrm{KH}_{2} \mathrm{PO}_{4}, m=0.008695 \mathrm{~mol} \mathrm{~kg}^{-1}$; $\mathrm{Na}_{2} \mathrm{HPO}_{4}, m=0.03043 \mathrm{~mol} \mathrm{~kg}^{-1}$
E: $\mathrm{Na}_{2} \mathrm{~B}_{4} \mathrm{O}_{7}, m=0.01 \mathrm{~mol} \mathrm{~kg}^{-1}$
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

$$
0=\Sigma_{\mathbf{B}^{\nu}{ }_{\mathbf{B}} B}
$$

the extent of reaction $\xi$ is defined according to 2.5 .03 by

$$
\mathrm{d} \boldsymbol{\xi}=\nu_{\mathrm{B}}^{-1} \mathrm{~d} n_{\mathrm{B}}
$$

where $n_{\mathrm{B}}$ is the amount, and $\nu_{\mathrm{B}}$ 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

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

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

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

If the specified volume $V$ is independent of time, then

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

If this specified volume $V$ is such that

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

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

$$
V^{-1} \mathrm{~d} \xi / \mathrm{d} t=\nu_{\mathrm{B}}^{-1} \mathrm{~d} c_{\mathrm{B}} / \mathrm{d} t \text { or } \nu_{\mathrm{B}}^{-1} \mathrm{~d}[\mathrm{~B}] / \mathrm{d} t
$$

The quantity

$$
\mathrm{d} n_{\mathrm{B}} / \mathrm{d} t\left(=\nu_{\mathrm{B}} \mathrm{~d} \xi / \mathrm{d} t\right)
$$

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

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

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

$$
v_{\mathrm{B}}=\mathrm{d} c_{\mathrm{B}} / \mathrm{d} t \text { or } \mathrm{d}[\mathrm{~B}] / \mathrm{dt}
$$

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.

### 11.2 Order of reaction

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

$$
v_{\mathrm{B}} \propto[\mathrm{C}]^{c}[\mathrm{D}]^{d} \ldots
$$

then the reaction is described as of order $c$ with respect to C , of order $d$ with respect to $\mathrm{D}, \ldots$, and of overall order $(c+d+\ldots)$.

### 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 |
| :--- | :---: | :--- |
| $\mathrm{Br}_{2}+\mathrm{M} \rightarrow 2 \mathrm{Br}+\mathrm{M}$ | 1 | $k_{1}$ |
| $\mathrm{Br}+\mathrm{H}_{2} \rightarrow \mathrm{HBr}+\mathrm{H}$ | 2 | $k_{2}$ |
| $\mathrm{H}+\mathrm{Br}_{2} \rightarrow \mathrm{HBr}+\mathrm{Br}$ | 3 | $k_{3}$ |
| $\mathrm{H}+\mathrm{HBr} \rightarrow \mathrm{H}_{2}+\mathrm{Br}$ | -2 | $k_{-2}$ |
| $2 \mathrm{Br}+\mathrm{M} \rightarrow \mathrm{Br}_{2}+\mathrm{M}$ | -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) $\times(\text { amount of substance })^{-1}$ and should be denoted by $z$. Thus $z=Z / L c_{\mathrm{A}} c_{\mathrm{B}}$.

## 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 | $\mu_{0}$ | $4 \pi \times 10^{-7} \mathrm{H} \mathrm{m}^{-1}$ exactly |
| Speed of light in vacuum | $c$ | $2.99792458(1) \times 10^{8} \mathrm{~m} \mathrm{~s}^{-1}$ |
| Permittivity of vacuum | $\epsilon_{0}=\left(\mu_{0} c^{2}\right)^{-1}$ | $8.85418782(5) \times 10^{-12} \mathrm{~F} \mathrm{~m}^{-1}$ |
| Fine structure constant | $\underset{a^{-1}}{a=\mu_{0} c e^{2} / 2 h}$ | $\begin{aligned} & 7.2973506(60) \times 10^{-3} \\ & 137.03604(11) \end{aligned}$ |
| Elementary charge | $e$ | $1.6021892(46) \times 10^{-19} \mathrm{C}$ |
| Planck constant | $\stackrel{h}{\hbar}=h / 2 \pi$ | $\begin{aligned} & 6.626176(36) \times 10^{-34} \mathrm{~J} \mathrm{~Hz}^{-1} \\ & 1.0545887(57) \times 10^{-34} \mathrm{~J} \mathrm{~s}^{2} \end{aligned}$ |
| Avogadro constant | $L, N_{\text {A }}$ | $6.022045(31) \times 10^{23} \mathrm{~mol}^{-1}$ |
| Atomic mass unit | $1 \mathrm{u}=10^{-3} \mathrm{~kg} \mathrm{~mol}^{-1} / L$ | $1.6605655(86) \times 10^{-27} \mathrm{~kg}$ |
| Rest mass of electron | $m_{\text {e }}$ | $9.109534(47) \times 10^{-31} \mathrm{~kg}$ |
| Rest mass of proton | $m_{p}$ | $1.6726485(86) \times 10^{-27} \mathrm{~kg}$ |
| Rest mass of neutron | $m_{\mathrm{n}}$ | $1.6749543(86) \times 10^{-27} \mathrm{~kg}$ |
| Faraday constant | $F=L e$ | $9.648456(27) \times 10^{4} \mathrm{C} \mathrm{mol}^{-1}$ |
| Rydberg constant | $R_{\infty}=\mu_{0}{ }^{2} m_{e} e^{4} c^{3} / 8 h^{3}$ | $1.097373177(83) \times 10^{7} \mathrm{~m}^{-1}$ |
| Hartree energy ${ }^{(1)}$ | $E_{\mathrm{h}}=2 h c R_{\infty}$ | $4.359814(24) \times 10^{-18} \mathrm{~J}$ |
| Bohr radius | $a_{0}=a / 4 \pi R_{\infty}$ | $5.2917706(44) \times 10^{-11} \mathrm{~m}$ |
| Bohr magneton | $\mu_{\mathrm{B}}=\boldsymbol{e} \boldsymbol{h} / 2 m_{\mathrm{e}}$ | 9.274078 (36) $\times 10^{-24} \mathrm{~J} \mathrm{~T}^{-1}$ |
| Nuclear magneton | $\mu_{\mathrm{N}}=e \hbar / 2 m_{\mathrm{p}}$ | $5.050824(20) \times 10^{-27} \mathrm{~J} \mathrm{~T}^{-1}$ |
| Electron magnetic moment | $\mu_{\text {e }}$ | $9.284832(36) \times 10^{-24} \mathrm{~J} \mathrm{~T}^{-1}$ |
| Landé $g$-factor for free electron | $g_{\mathrm{e}}=2 \mu_{\mathrm{e}} / \mu_{\mathrm{B}}$ | $2.0023193134(70)$ |
| Proton gyromagnetic ratio | $\gamma_{p}$ | $2.6751987(75) \times 10^{8} \mathrm{~s}^{-1} \mathrm{~T}^{-1}$ |
| Proton resonance frequency $\left(\mathrm{H}_{2} \mathrm{O}\right)$ per unit field ${ }^{(2)}$ | $\gamma_{p}{ }^{\prime} / 2 \pi$ | $4.257602(12) \times 10^{7} \mathrm{~Hz} \mathrm{~T}^{-1}$ |
| Gas constant | $R$ | 8.31441(26) J K ${ }^{-1} \mathrm{~mol}^{-1}$ |
| Zero of the Celsius scale | $\begin{aligned} & T_{0} \\ & R T_{0} \end{aligned}$ | $\begin{aligned} & 273.15 \mathrm{~K} \text { exactly } \\ & 2.271081(71) \times 10^{3} \mathrm{~J} \mathrm{~mol}^{-1} \end{aligned}$ |
| Normal atmosphere | $p_{0}$ | $1.01325 \times 10^{5} \mathrm{~Pa}$ exactly |
| Standard molar volume of ideal gas | $V_{0}=R T_{0} / p_{0}$ | 2.241383 (70) $\times 10^{-2} \mathrm{~m}^{3} \mathrm{~mol}^{-1}$ |
| Boltzmann constant | $k=R / L$ | $1.380662(44) \times 10^{-23} \mathrm{~J} \mathrm{~K}^{-1}$ |
| Gravitational constant | $G$ | $6.6720(27) \times 10^{-11} \mathrm{~m}^{3} \mathrm{~kg}^{-1} \mathrm{~s}^{-2}$ |
| Standard acceleration of free fall | $g_{\text {n }}$ | $9.80665 \mathrm{~m} \mathrm{~s}^{-2}$ exactly |

[^16]
## 13. REFERENCES

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## APPENDIX I

## DEFINITION OF ACTIVITIES AND RELATED QUANTITIES

## A.I. 1 Chemical potential and absolute activity

The chemical potential $\mu_{B}$ of a substance $B$ in a mixture of substances $B$, C, . . ., is defined by

$$
\mu_{\mathrm{B}}=\left(\partial G / \partial n_{\mathrm{B}}\right)_{T, p, n_{\mathrm{c}}} \cdots
$$

where $G$ is the Gibbs energy of the mixture, $T$ is the thermodynamic temperature, $p$ is the pressure, and $n_{\mathrm{B}}, n_{\mathrm{C}}, \ldots$, are the amounts of the substances $\mathrm{B}, \mathrm{C}, \ldots$, in the mixture.
(In molecular theory the symbol $\mu_{\mathrm{B}}$ is sometimes used for the quantity $\mu_{\mathrm{B}} / L$ where $L$ is the Avogadro constant, but this usage is not recommended.)

The absolute activity $\lambda_{\mathrm{B}}$ of the substance B in the mixture is a number defined by

$$
\lambda_{\mathrm{B}}=\exp \left(\mu_{\mathrm{B}} / R T\right) \quad \text { or } \quad \mu_{\mathrm{B}}=R T \ln \lambda_{\mathrm{B}}
$$

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 $f_{\mathrm{B}}{ }^{*}$ of a pure gaseous substance B is a quantity with the same dimensions as pressure, defined in terms of the absolute activity $\lambda_{B}{ }^{*}$ of the pure gaseous substance $B$ by

$$
f_{\mathrm{B}}^{*}=\lambda_{\mathrm{B}} \lim _{p \rightarrow 0}\left(p / \lambda_{\mathrm{B}}{ }^{*}\right)
$$

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

$$
R T \ln f_{\mathrm{B}}^{*}=\mu_{\mathrm{B}}^{*}+\lim _{p \rightarrow 0}\left(R T \ln p-\mu_{\mathrm{B}^{*}}\right)
$$

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

$$
\lim _{p \rightarrow 0}\left(f_{\mathrm{B}}^{*} / p\right)=1
$$

and that

$$
R T \ln \left(f_{\mathrm{B}}{ }^{*} / p\right)=\int_{0}^{p}\left(V_{\mathrm{B}}^{*}-R T / p\right) \mathrm{d} p
$$

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

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

## 2. Mixtures

## A.l. 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 $p_{\mathrm{B}}$ of a substance B in a gascous mixture is a quantity with the same dimensions as pressure defined by

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

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 $f_{\mathrm{B}}$ of the substance B in a gaseous mixture containing mole fractions $y_{\mathrm{B}}, y_{\mathrm{C}}, \ldots$, of the substances $\mathrm{B}, \mathrm{C}, \ldots$, is a quantity with the same dimensions as pressure, defined in terms of the absolute activity $\lambda_{B}$ of the substance $B$ in the gaseous mixture by

$$
f_{\mathrm{B}}=\lambda_{\mathrm{B}} \lim _{p \rightarrow 0}\left(y_{\mathrm{B}} p / \lambda_{\mathrm{B}}\right)
$$

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

$$
R T \ln f_{\mathrm{B}}=\mu_{\mathrm{B}}+\lim _{p \rightarrow 0}\left\{R T \ln \left(y_{\mathrm{B}} p\right)-\mu_{\mathrm{B}}\right\}
$$

It follows from this definition that

$$
\lim _{p \rightarrow 0}\left(f_{\mathrm{B}} / y_{\mathrm{B}} p\right)=1
$$

and that

$$
R T \ln \left(f_{\mathrm{B}} / y_{\mathrm{B}} p\right)=\int_{0}^{p}\left(V_{\mathrm{B}}-R T / p\right) \mathrm{d} p
$$

where $V_{\mathrm{B}}$ is the partial molar volume (see Section 1.4) of the substance B in the gaseous mixture.
A gaseous mixture of $\mathrm{B}, \mathrm{C}, \ldots$, is treated as an ideal gaseous mixture when the approximations $f_{\mathrm{B}}=y_{\mathrm{B}} p, f_{\mathrm{C}}=y_{\mathrm{C}} p, \ldots$, are used. It follows that $p V=\left(n_{\mathrm{B}}+n_{\mathrm{C}}+\ldots\right) R T$ for an ideal gaseous mixture of $\mathrm{B}, \mathrm{C}, \ldots$
The ratio ( $f_{\mathrm{B}} / y_{\mathrm{B}} p$ ) 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 $y_{\mathrm{B}}=1$ 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 $f_{\mathrm{B}}$ of a substance B in a liquid or solid mixture containing mole fractions $x_{\mathrm{B}}, x_{\mathrm{C}}, \ldots$, of the substances $\mathrm{B}, \mathrm{C}, \ldots$, is a number defined in terms of the absolute activity $\lambda_{B}$ of the substance $B$ in the mixture by

$$
f_{\mathrm{B}}=\lambda_{\mathrm{B}} / \lambda_{\mathrm{B}}{ }^{*} x_{\mathrm{B}}
$$

where $\lambda_{\mathrm{B}}{ }^{*}$ is the absolute activity of the pure substance B at the same temperature and pressure, or in terms of the chemical potential $\mu_{\mathrm{B}}$ by

$$
R T \ln \left(x_{\mathrm{B}} f_{\mathrm{B}}\right)=\mu_{\mathrm{B}}-\mu_{\mathrm{B}}^{*}
$$

where $\mu_{\mathrm{B}}{ }^{*}$ is the chemical potential of the pure substance B at the same temperature and pressure.

It follows from this definition that

$$
\lim _{x_{\mathrm{B}} \rightarrow 1} f_{\mathrm{B}}=1 \quad(T, p \text { const. })
$$

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

The relative activity $a_{\mathrm{B}}$ of a substance B in a liquid or solid mixture is a number defined by

$$
a_{\mathrm{B}}=\lambda_{\mathrm{B}} / \lambda_{\mathrm{B}} *
$$

or by

$$
R T \ln a_{\mathrm{B}}=\mu_{\mathrm{B}}-\mu_{\mathrm{B}}^{*}
$$

where the other symbols are as defined in Section A.I.7.
It follows from this definition that

$$
\lim _{x_{\mathrm{B}} \rightarrow 1} a_{\mathrm{B}}=1 \quad \quad(T, p \text { const. })
$$

A mixture of substances $\mathrm{B}, \mathrm{C}, \ldots$, is treated as an ideal mixture when the approximations $a_{\mathrm{B}}=x_{\mathrm{B}}, a_{\mathrm{C}}=x_{\mathrm{C}}, \ldots$, and consequently $f_{\mathrm{B}}=1, f_{\mathrm{C}}=1, \ldots$, 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 $\mathbf{A}$ and the solute substances by B, C, ....

## A.I. 10 Properties of infinitely dilute solutions

The superscript ${ }^{\infty}$ attached to the symbol for a property of a solution denotes the property of an infinitely dilute solution.
For example if $V_{\mathrm{B}}$ denotes the partial molar volume (see Section 1.4) of the solute substance B in a solution containing molalities $m_{\mathrm{B}}, m_{\mathrm{C}}, \ldots$, or mole fractions $x_{\mathrm{B}}, x_{\mathrm{C}}, \ldots$, of solute substances $\mathrm{B}, \mathrm{C}, \ldots$, in a solvent substance A , then

$$
V_{\mathrm{B}}^{\mathrm{X}}=\lim _{\Sigma_{1} m_{1} \rightarrow 0} V_{\mathrm{B}}=\lim _{\Sigma_{1 x_{1} \rightarrow 0}} V_{\mathrm{B}}
$$

$$
\text { ( } T, p \text { const.) }
$$

where $\mathrm{i}=\mathrm{B}, \mathrm{C}, \ldots$.
Similarly if $V_{\mathrm{A}}$ denotes the partial molar volume of the solvent substance A , then

$$
V_{\mathrm{A}}^{\infty}=\lim _{\Sigma_{1} m_{1} \rightarrow 0} V_{\mathrm{A}}=\lim _{\Sigma_{1} \times 1 \rightarrow 0} V_{\mathrm{A}}=V_{\mathrm{A}}^{*}
$$

where $V_{\mathrm{A}}{ }^{*}$ 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 $\gamma_{B}$ of a solute substance $B$ in a solution (especially in a dilute liquid solution) containing molalities $m_{\mathrm{B}}, m_{\mathrm{C}}, \ldots$, of solute substances B, C, . . ., in a solvent substance A, is a number defined in terms of the absolute activity $\lambda_{B}$ of the solute substance $B$ in the solution by

$$
\gamma_{\mathrm{B}}=\left(\lambda_{\mathrm{B}} / m_{\mathrm{B}}\right) /\left(\lambda_{\mathrm{B}} / m_{\mathrm{B}}\right)^{\infty}
$$

$$
\text { ( } T, p \text { const.) }
$$

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

$$
R T \ln \left(m_{\mathrm{B}} \gamma_{\mathrm{B}}\right)=\mu_{\mathrm{B}}-\left(\mu_{\mathrm{B}}-R T \ln m_{\mathrm{B}}\right)^{\infty}
$$

$$
\text { ( } T, p \text { const.) }
$$

It follows from this definition that

$$
\gamma_{\mathrm{B}}{ }^{\infty}=1
$$

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 $m_{\mathrm{B}}$.

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 $\lambda_{\mathrm{B}}$ by

$$
f_{x, \mathrm{~B}}=\left(\lambda_{\mathrm{B}} / x_{\mathrm{B}}\right) /\left(\lambda_{\mathrm{B}} / x_{\mathrm{B}}\right)^{\infty}
$$

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

$$
R T \ln \left(x_{\mathrm{B}} f_{x, \mathrm{~B}}\right)=\mu_{\mathrm{B}}-\left(\mu_{\mathrm{B}}-R T \ln x_{\mathrm{B}}\right)^{\infty} \quad(T, p \text { const. })
$$

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

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

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

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

The relative activity $a_{\mathrm{B}}$ of a solute substance B in a solution (especially in a dilute liquid solution) containing molalities $m_{\mathrm{B}}, m_{\mathrm{C}}, \ldots$, of solute substances $B, C, \ldots$, in a solvent substance $A$, is a number defined in terms of the absolute activity $\lambda_{B}$ by

$$
a_{\mathrm{B}}=\left(\lambda_{\mathrm{B}} / m^{\ominus}\right) /\left(\lambda_{\mathrm{B}} / m_{\mathrm{B}}\right)^{\infty}=m_{\mathrm{B}} \gamma_{\mathrm{B}} / m^{\ominus} \quad(T, p \text { const. })
$$

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

$$
\begin{aligned}
R T \ln a_{\mathrm{B}} & =\mu_{\mathrm{B}}-R T \ln m^{\ominus}-\left(\mu_{\mathrm{B}}-R T \ln m_{\mathrm{B}}\right)^{\infty} \\
& =R T \ln \left(m_{\mathrm{B}} \gamma_{\mathrm{B}} / m^{\ominus}\right)
\end{aligned}
$$

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

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

$$
\left(a_{\mathrm{B}} m^{\ominus} / m_{\mathrm{B}}\right)^{\infty}=1
$$

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

The name relative activity with the symbol $a_{c}, \mathrm{~B}$ may be used for the quantity similarly defined but with concentration $c_{B}$ (see Section 2.3) in place of molality $m_{\mathrm{B}}$, and a standard value $c^{\ominus}$ of concentration (usually chosen to be $1 \mathrm{~mol} \mathrm{dm}^{-3}$ ) 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 $a_{x, \mathrm{~B}}$, is sometimes used. It is defined in terms of the absolute activity $\lambda_{\mathrm{B}}$ by

$$
a_{x, \mathrm{~B}}=\lambda_{\mathrm{B}} /\left(\lambda_{\mathrm{B}} / x_{\mathrm{B}}\right)^{\infty}=x_{\mathrm{B}} f_{x, \mathrm{~B}}
$$

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

$$
\begin{aligned}
R T \ln a_{x, \mathrm{~B}} & =\mu_{\mathrm{B}}-\left(\mu_{\mathrm{B}}-R T \ln x_{\mathrm{B}}\right)^{\infty} \\
& =R T \ln \left(x_{\mathrm{B}} f_{x, \mathrm{~B}}\right)
\end{aligned}
$$

$$
\text { ( } T, p \text { const. })
$$

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

$$
a_{x, \mathrm{~B}}=a_{\mathrm{B}} m^{\ominus} M_{\mathrm{A}}
$$

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

The osmotic coefficient $\phi$ of the solvent substance A in a solution (especially in a dilute liquid solution) containing molalities $m_{\mathrm{B}}, m_{\mathrm{C}}, \ldots$, of solute substances $B, C, \ldots$, is a number defined in terms of the absolute activity $\lambda_{A}$ of the solvent substance $A$ in the solution by

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

where $\lambda_{\mathrm{A}}{ }^{*}$ is the absolute activity of the pure solvent substance A at the same temperature and pressure, and $M_{\mathrm{A}}$ is the molar mass of the solvent substance A , or in terms of the chemical potential $\mu_{\mathrm{A}}{ }^{*}$ by

$$
\phi=\left(\mu_{\mathrm{A}}^{*}-\mu_{\mathrm{A}}\right) / R T M_{\mathrm{A}} \Sigma_{\mathrm{i}} m_{\mathrm{i}}
$$

where $\mu_{A}$ * 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 $\phi_{x}$, is sometimes used. It is defined in terms of the absolute activity $\lambda_{\mathrm{A}}$ by

$$
\phi_{x}=\ln \left(\lambda_{\mathrm{A}} / \lambda_{\mathrm{A}}{ }^{*}\right) / \ln x_{\mathrm{A}}=\ln \left(\lambda_{\mathrm{A}} / \lambda_{\mathrm{A}}{ }^{*}\right) / \ln \left(1-\sum_{\mathrm{i}} x_{\mathrm{i}}\right)
$$

or in terms of the chemical potential $\mu_{\mathrm{A}}$ by

$$
\phi_{x}=\left(\mu_{\mathrm{A}}-\mu_{\mathrm{A}}{ }^{*}\right) / R T \ln x_{\mathrm{A}}=\left(\mu_{\mathrm{A}}-\mu_{\mathrm{A}}^{*}\right) / R T \ln \left(1-\sum_{\mathrm{i}} x_{\mathrm{i}}\right)
$$

where $x_{A}$ is the mole fraction of the solvent substance $A$ in the solution. The rational osmotic coefficient $\phi_{x}$ is related to the (practical) osmotic coefficient $\phi$ by the formula

$$
\phi_{x}=\phi M_{\mathrm{A}} \sum_{\mathrm{i}} m_{\mathrm{i}} / \ln \left(1+M_{\mathrm{A}} \sum_{\mathrm{i}} m_{\mathrm{i}}\right)=-\phi M_{\mathrm{A}} \sum_{\mathrm{i}} m_{\mathrm{i}} / \ln \left(1-\sum_{\mathrm{i}} x_{\mathrm{i}}\right)
$$

## 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 $m_{\mathrm{B}}, m_{\mathrm{C}}, \ldots$, or mole fractions $x_{\mathrm{B}}, x_{\mathrm{C}}, \ldots$, of solute substances $\mathrm{B}, \mathrm{C}, \ldots$, is a number defined in terms of the absolute activity $\lambda_{A}$ of the solvent substance $A$ in the solution by

$$
a_{\mathrm{A}}=\lambda_{\mathrm{A}} / \lambda_{\mathrm{A}}^{*}=\exp \left(-\phi M_{\mathrm{A}} \sum_{\mathrm{i}} m_{\mathrm{i}}\right)=\left(1-\sum_{\mathrm{i}} x_{\mathrm{i}}\right)^{\phi_{x}}
$$

or in terms of the chemical potential $\mu_{\mathrm{A}}$ by

$$
R T \ln a_{\mathrm{A}}=\mu_{\mathrm{A}}-\mu_{\mathrm{A}^{*}}^{*}=-R T \phi M_{\mathrm{A}} \sum_{\mathrm{i}} m_{\mathrm{i}}=\phi_{x} R T \ln \left(1-\sum_{\mathrm{i}} x_{\mathrm{i}}\right)
$$

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.


[^0]:    ${ }^{(1)}$ 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.

[^1]:    ${ }^{(1)}$ In solid-state studies, wavevector $\boldsymbol{k}$ is used ( $|\boldsymbol{k}|=2 \pi / \lambda$ ).
    ${ }^{(2)}$ For electromagnetic radiation referred to a vacuum $\tilde{v}=\nu / c=1 / \lambda_{\text {vac }}$ is preferred.
    ${ }^{(3)}$ The symbol $A_{s}$ may be used when necessary to avoid confusion with the symbol $A$ for Helmholtz energy.

[^2]:    ${ }^{(1)}$ The ratio of the average mass per atom of an element to $1 / 12$ of the mass of an atom of nuclide ${ }^{12} \mathrm{C}$.

[^3]:    Example: $M_{\mathbf{r}}(\mathrm{KCl})=74.555$
    ${ }^{(2)}$ See Section 1.2.
    ${ }^{\text {( }}$ () A solution having a molality equal to $0.1 \mathrm{~mol}^{\mathbf{~ k g}}{ }^{-1}$ 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 $0.1 \mathrm{~mol} \mathrm{dm}^{-3}$ is often called a 0.1 molar 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 $\theta$ for Celsius temperature.
    ${ }^{(6)}$ It is recommended that $q>0$ and $w>0$ both indicate increase of energy of the system under discussion. Thus $\Delta U=q+w$.

[^4]:    ${ }^{(1)}$ 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: $\lambda\left(\mathbf{M g}^{2+}\right)=2 \lambda\left(\frac{1}{2} \mathbf{M g}^{2+}\right)$

[^5]:    ${ }^{(1)}$ See footnote (1) on page 6.
    ${ }^{(2)}$ The name Sherwood number, symbol $S h$ has been widely used.

[^6]:    ${ }^{\circ}$ or * pure substance
    $\infty$ infinite dilution
    id ideal
    ${ }^{\circ}$ or ${ }^{\ominus}$ standard in general
    $\ddagger$ activated complex, transition state

[^7]:    ${ }^{(1)}$ 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 ${ }^{\circ} \mathrm{K}$ and deg be abandoned.

[^8]:    ${ }^{(1)}$ See Section 1.2

[^9]:    ${ }^{(1)}$ The ${ }^{\circ}$ sign and the letter following form one symbol and there should be no space between them. Example: $25^{\circ} \mathrm{C}$ not $25^{\circ} \mathrm{C}$
    ${ }^{(2)}$ By decision of the Twelfth Conférence Générale des Poids et Mesures in October 1964, the old definition of the litre ( $1.000028 \mathrm{dm}^{3}$ ) 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.

[^10]:    ${ }^{(1)}$ 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 101325 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 $13.5951 \mathrm{~g} \mathrm{~cm}^{-3}$ in a place where the acceleration of free fall is exactly $980.665 \mathrm{~cm} \mathrm{~s}^{-2}$. The mmHg differs from the Torr by less than $2 \times 10^{-7}$ Torr.

[^11]:    ${ }^{(1)}$ Taken from Reference 13.1 .11 where a more comprehensive list can be found.

[^12]:    ${ }^{(1)}$ For a more detailed discussion see Reference 13.4.

[^13]:    ${ }^{(1)}$ Taken from Reference 13.2. For further details see Reference 13.10.

[^14]:    (1) The conventions given here are in accordance with the 'Stockholm Convention' of 1953.

[^15]:    ${ }^{(1)}$ The symbol pH is an exception to the general rules given in Section 1.5.

[^16]:    ${ }^{(1)}$ Name and symbol recommended by IUPAC Commission on Symbols, Terminology, and Units.
    (2) The relative temperature dependence of the diamagnetic shielding correction in water is of the order of $1 \times 10^{-8} / \mathrm{K}$, which is negligible in comparison with the present uncertainty in $\gamma_{p}{ }^{\prime} / 2 \pi$. The value given here is based on measurements in the range $20-35^{\circ} \mathrm{C}$.

