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Quantities and units of physical chemistry and molecular physics

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FOREWORD

ISO (the International Organization for Standardization) is a worldwide federation of national standards institutes (ISO Member Bodies). The work of developing International Standards is carried out through ISO Technical Committees. Every Member Body interested in a subject for which a Technical Committee has been set up has the right to be represented on that Committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work.

Draft International Standards adopted by the Technical Committees are circulated to the Member Bodies for approval before their acceptance as International Standards by the ISO Council.

International Standard ISO 31/VIII (originally Draft No. 1777) was drawn up by Technical Committee ISO/TC 12, *Quantities, units, symbols, conversion factors and conversion tables*.

It was approved in August 1969 by the Member Bodies of the following countries :

Australia	Greece	South Africa, Rep. of
Austria	Hungary	Spain
Belgium	India	Sweden
Canada	Israel	Switzerland
Czechoslovakia	Japan	Thailand
Denmark	Netherlands	United Kingdom
Egypt, Arab Rep. of	New Zealand	U.S.A.
France	Norway	U.S.S.R.
Germany	Poland	

No Member Body expressed disapproval of the document.

Quantities and units of physical chemistry and molecular physics

INTRODUCTION

General remarks

This document, containing a table of *quantities and units of physical chemistry and molecular physics*, is the eighth part of a more comprehensive publication dealing with quantities and units in various fields of science and technology. The parts of this publication are :

Part 0 : *General introduction — General principles concerning quantities, units and symbols.*¹⁾

Part I (2nd edition) : *Basic quantities and units of the SI and quantities and units of space and time.*²⁾

Part II : *Quantities and units of periodic and related phenomena.*

Part III : *Quantities and units of mechanics.*

Part IV : *Quantities and units of heat.*

Part V : *Quantities and units of electricity and magnetism.*

Part VI : *Quantities and units of light and related electromagnetic radiations.*

Part VII : *Quantities and units of acoustics.*

Part VIII : *Quantities and units of physical chemistry and molecular physics.*

Part IX : *Quantities and units of atomic and nuclear physics.*

Part X : *Quantities and units of nuclear reactions and ionizing radiations.*

Part XI : *Mathematical signs and symbols for use in the physical sciences and technology.*

General information regarding the arrangement of the tables and the symbols and abbreviations used is to be found in the introduction to Part I, where the full definitions of base units are given as an appendix.

The statements in the definition column for quantities are given merely for identification; they are not intended to be complete definitions.

Special remarks

In this document the amount of substance is treated as an independent base quantity. The base unit of this quantity is the mole, defined under item 8-3.a.

Following a decision of the 13th Conférence Générale des Poids et Mesures, the name kelvin and symbol K have been used for the unit of thermodynamic temperature.

For simplicity this document includes only a selection of units, preferably from the International System of Units. Other units can be derived from units given in Parts III, IV and V. Some conversion factors are added for information.

Decimal multiples and submultiples of units are in general not explicitly mentioned in the tables; this does not mean, however, that they are not recommended. General recommendations for decimal multiples and submultiples of units are given in Part 0.

The names and symbols of the chemical elements are given in Appendix I on page 12.

1) At present at the stage of draft (No. 2180).

2) The title of the first edition of this document was : "Fundamental quantities and units of the MKSA system and quantities and units of space and time".

8. Physical chemistry and molecular physics

Item No.	Quantity	Symbol	Definition 1)	Remarks 2)
8-1.1	relative atomic mass of an element	A_r	The ratio of the average mass per atom of the natural isotopic composition of an element to 1/12 of the mass of an atom of nuclide ^{12}C .	These quantities are dimensionless. Example: $A_r(\text{Cl}) = 35.453$ Formerly called atomic weight.
8-1.2	relative molecular mass of a substance	M_r	The ratio of the average mass per molecule of the natural isotopic composition of a substance to 1/12 of the mass of an atom of nuclide ^{12}C .	Formerly called molecular weight. The concept of relative atomic or molecular mass is also applicable to other specified isotopic compositions, but the natural isotopic composition is assumed unless the composition is specified.
8-2.1	number of molecules or particles	N	Number of molecules or particles in a system.	This quantity is dimensionless.
8-3.1	amount of substance	$n, (\nu)$		This quantity is treated in this document as a basic quantity. ν may be used as an alternative to n when n is used for number density of particles, see 8-10.1
8-4.1	Avogadro constant	L, N_A	Number of molecules divided by the amount of substance.	$N_A = N/n$ $N_A = (6.022\,52 \pm 0.000\,28) \times 10^{23} \text{ mol}^{-1}$
8-5.1	molar mass	M	Mass divided by amount of substance.	$M = m/n$, where m is the mass of the substance.
8-6.1	molar volume	V_m	Volume divided by amount of substance.	The subscript m is often omitted, or can be replaced by the chemical formula of the substance. $V_m = V/n$ The molar volume of an ideal gas under standard conditions (0 °C and 1 atm) is $V_0 = (22.4136 \pm 0.0030) \times 10^{-3} \text{ m}^3/\text{mol}$ For a gas, the "Amagat volume" is defined by $V_A = V_m/V_m^\circ$, where V_m° is the molar volume of this gas at 0 °C and 1 atm.
8-7.1	molar internal energy	$U_m, (E_m)$	Internal energy divided by amount of substance.	The subscript m is often omitted, or can be replaced by the chemical formula of the substance. $U_m = U/n$ See ISO/R 31/Part IV, item 4-15.1 Similar definitions apply to other molar thermodynamic functions.

1) The statements in this column are given merely for identification and they are not intended to be complete definitions.

2) The numerical values in this column are derived from J.W.M. DuMond and E.R. Cohen, Recommended Values of the Physical Constants — 1963 U.I.P.A. Commission on Nuclidic Masses, Doc. MN 632 — Sept. 4. 1963, see also Doc. U.I.P. 11 (1965) of the U.I.P.A.

8. Physical chemistry and molecular physics

Units
8-3.a...8-7.a

Item No.	Name of unit and in certain cases abbreviation for this name	International symbol for unit	Definition	Conversion factors	Remarks
8-3.a	mole	mol	1 mol is the amount of substance of a system which contains as many elementary entities as there are atoms in 0.012 kg (exactly) of ^{12}C . 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.		The numerical value of the quantity 8-3.1 expressed in moles is also called number of moles.
8-3.b	kilomole	kmol			
8-4.a	reciprocal mole	mol^{-1}			The numerical value of the quantity 8-4.1 expressed in mol^{-1} is called Avogadro number.
8-5.a	kilogram per mole	kg/mol			$M = 10^{-3} M_r \text{ kg/mol}$ $= M_r \text{ kg/kmol}$ $= M_r \text{ g/mol},$ where M_r is the relative molecular mass of a substance of definite chemical composition.
8-5.b	gram per mole	g/mol			
8-6.a	cubic metre per mole	m^3/mol			In 1964 the Conférence Générale des Poids et Mesures redefined the litre as $1 \text{ l} = 1 \text{ dm}^3$.
8-6.b	litre per mole	l/mol		$1 \text{ l/mol} = 10^{-3} \text{ m}^3/\text{mol}$ (exactly)	
8-7.a	joule per mole	J/mol			For other units of energy, e.g. the calories, see ISO/R31/Part III $1 \text{ cal}_{\text{IT}} = 4.1868 \text{ J}$ (exactly) $1 \text{ cal}_{\text{th}} = 4.1840 \text{ J}$ (exactly) $1 \text{ cal}_{15} = 4.1855 \text{ J}$

8. Physical chemistry and molecular physics (continued)

Quantities

8-8.1...8-19.1

Item No.	Quantity	Symbol	Definition 1)	Remarks 2)
8-8.1	molar heat capacity	C_m	Heat capacity divided by amount of substance.	The subscript m is often omitted, or can be replaced by the chemical formula of the substance. $C_m = C/n$ See ISO/R 31/Part IV, item 4-10.1
8-9.1	molar entropy	S_m	Entropy divided by amount of substance.	The subscript m is often omitted, or can be replaced by the chemical formula of the substance. $S_m = S/n$ See ISO/R 31/Part IV, item 4-13.1
8-10.1	number density of molecules (or particles)	n	The number of molecules or particles divided by volume.	$n = N/V$ The number density of an ideal gas under standard conditions (0 °C and 1 atm) is $n_0 = N_A/V_0 = (2.6870 \pm 0.0003) \times 10^{25} \text{ m}^{-3}$, this constant is called Loschmidt constant. See 8-4.1 and 8-6.1
8-10.2	molecular concentration of component B	C_B	The number of molecules of component B divided by volume of mixture.	
8-11.1	density	ρ	Mass divided by volume.	The dimensionless quantity $\rho_A = 1/V_A$ is called "Amagat density", see 8-6.1
8-11.2	mass concentration of component B	ρ_B	Mass of component B divided by volume of the mixture.	
8-12.1	mass fraction of component B	w_B	Ratio of the mass of component B to the mass of the mixture.	This quantity is dimensionless.
8-13.1	concentration of component B, amount of substance concentration of component B	c_B	Amount of substance of component B divided by volume of the mixture.	Formerly also called molarity of component B In chemistry also indicated as [B]
8-14.1	mole fraction of component B	x_B	Ratio of the amount of substance of component B to the amount of substance of the mixture.	These quantities are dimensionless.
8-14.2	mole ratio of solute component B	r_B	Ratio of the amount of substance of solute component B to the amount of substance of the solvent.	For a one-solute solution $r = x / (1-x)$
8-15.1	molality of solute component B	m_B	The amount of substance of solute component B in a solution divided by the mass of the solvent.	
8-16.1	chemical potential of component B	μ_B	For a mixture with components B, C, ..., $\mu_B = (\partial G / \partial n_B)_{T, p, n_C, \dots}$, where n_B is the amount of substance of component B and G is the Gibbs function.	For a pure substance $\mu = G/n = G_m$ where G_m is the molar Gibbs function. The symbol μ is also used for the quantity G_m/N_A , where N_A is the Avogadro constant.
8-17.1	absolute activity of component B	λ_B	$\lambda_B = \exp [\mu_B/RT]$	This quantity is dimensionless. For R and T , see 8-33.1
8-18.1	partial pressure of component B (in a gaseous mixture)	p_B	For a gaseous mixture, $p_B = x_B \cdot p$ where p is the pressure.	
8-19.1	fugacity of component B (in a gaseous mixture)	f_B, p_B^*	For a gaseous mixture, f_B is proportional to the absolute activity λ_B , the proportionality factor, which is a function of temperature only, being determined by the condition that at constant temperature and composition f_B/p_B tends to 1 for an infinitely dilute gas.	$f_B = \lambda_B \cdot \lim_{p \rightarrow 0} (x_B p / \lambda_B)$ For a pure gas $p^* = \lambda \cdot \lim_{p \rightarrow 0} (p / \lambda)$ where λ is the absolute activity. (For the symbol, see also 8-20.1)

1) See footnote 1 on page 2.

2) See footnote 2 on page 2.

8. Physical chemistry and molecular physics (continued)

Units
8-8.a....8-19.a

Item No.	Name of unit and in certain cases abbreviation for this name	International symbol for unit	Definition	Conversion factors	Remarks
8-8.a	joule per mole kelvin	J/(mol · K)			
8-9.a	joule per mole kelvin	J/(mol · K)			
8-10.a	reciprocal cubic metre	m ⁻³			
8-11.a	kilogram per cubic metre	kg/m ³			
8-13.a	mole per cubic metre	mol/m ³			
8-13.b	mole per litre	mol/l		1 mol/l = 10 ³ mol/m ³ (exactly)	A solution with the concentration <i>y</i> mol/l is called a <i>y</i> molar solution.
8-15.a	mole per kilo-gram	mol/kg			
8-16.a	joule per mole	J/mol			
8-18.a	pascal	Pa	1 Pa = 1 N/m ²		For other units of pressure, see ISO/R 31/Part III, in particular 1 atm = 101 325 Pa (exactly)
8-19.a	pascal	Pa			See 8-18.a

8. Physical chemistry and molecular physics (continued)

Quantities

8-20.1...8-30.1

Item No.	Quantity	Symbol	Definition 1)	Remarks 2)
8-20.1	activity coefficient of component B (in a liquid or a solid mixture)	f_B	For a liquid mixture $f_B = \lambda_B / (\lambda_B^\circ x_B)$, where λ_B° is the absolute activity of the pure substance B at the same temperature and pressure.	This quantity is dimensionless.
8-21.1	activity of solute component B, relative activity of solute component B (especially in a dilute liquid solution)	$a_B, a_{m,B}$	For a solution, a_B is proportional to the absolute activity λ_B , the proportionality factor, which is a function of temperature and pressure only, being determined by the condition that at constant temperature and pressure a_B divided by the molality ratio m_B/m° tends to 1 for infinite dilution; m° is a reference molality, usually 1 mol/kg	This quantity is dimensionless. $a_B = \lambda_B \cdot \lim_{m_B \rightarrow 0} \frac{m_B/m^\circ}{\lambda_B}$ The quantity $a_{c,B}$ similarly defined in terms of the concentration ratio c_B/c° is also called: activity or relative activity of solute component B; c° is a reference molarity, usually 1 mol/l $a_{c,B} = \lambda_B \cdot \lim_{c_B \rightarrow 0} \frac{c_B/c^\circ}{\lambda_B}$ The subscript c in $a_{c,B}$ is often omitted.
8-22.1	activity coefficient of solute component B (especially in a dilute liquid solution)	γ_B	For a solution, $\gamma_B = \frac{a_B}{m_B/m^\circ}$	This quantity is dimensionless. The name activity coefficient of solute component B is also used for the quantity γ_B , defined as $\gamma_B = \frac{a_{c,B}}{c_B/c^\circ}$ See item 8-21.1
8-23.1	osmotic coefficient of a solution	g, φ	The ratio of the difference between the chemical potential of the pure solvent and that of the solvent in solution to the corresponding difference for an ideal dilute solution.	This quantity is dimensionless.
8-24.1	osmotic pressure	Π	The excess pressure required to maintain osmotic equilibrium between a solution and the pure solvent separated by a membrane, permeable only to the solvent.	
8-25.1	stoichiometric number of component B	ν_B	The integers or simple fractions occurring in the standard expression for a chemical reaction: $0 = \sum \nu_B B$, where the symbol B indicates the molecules or atoms involved in the reaction.	This quantity is dimensionless. In the present formulation the stoichiometric numbers for reactants are negative and those for products are positive.
8-26.1	affinity	A	$A = -\sum \nu_B \mu_B$	
8-27.1	equilibrium constant	K_p	For gaseous reactions, K_p is the equilibrium value of the product $\Pi_B (p_B^*)^{\nu_B}$	K_p is a function of temperature. Instead of fugacities (or partial pressures), concentrations, mole fractions or molalities are also used to define equilibrium constants. These constants are denoted by K_c , K_x and K_m .
8-28.1	mass of molecule	m		$m = M_r \cdot m_u$ where m_u is the (unified) atomic mass constant, see ISO/R 31/Part IX.
8-29.1	electric dipole moment of molecule	p, μ	The electric dipole moment is a vector quantity, the vector product of which with the electric field strength is equal to the torque.	The subscripts e and m may be used to distinguish between electric and magnetic moment.
8-30.1	electric polarizability of a molecule	α	Induced electric dipole moment divided by electric field strength.	γ is also used.

1) See footnote 1 on page 2.

2) See footnote 2 on page 2.

8. Physical chemistry and molecular physics (continued)

Units
8-24.a...8-30.a

Item No.	Name of unit and in certain cases abbreviation for this name	International symbol for unit	Definition	Conversion factors	Remarks
8-24.a	pascal	Pa			
8-26.a	joule per mole	J/mol			
8-27.a	pascal raised to the power $\Sigma \nu_R$	$\text{Pa}^{\Sigma \nu_R}$			
8-28.a	kilogram	kg			For (unified) atomic mass unit, $1 \text{ u} = m(^{12}\text{C})/12$ see ISO/R 31/Part IX
8-29.a	coulomb metre	$\text{C} \cdot \text{m}$			The electrostatic CGS unit of electric dipole moment of a molecule corresponds to $3.335\,63 \times 10^{-12} \text{ C} \cdot \text{m}$
8-30.a	coulomb metre squared per volt	$\text{C} \cdot \text{m}^2/\text{V}$			The electrostatic CGS unit of polarizability of a molecule equal to 1 cm^3 , corresponds to $1.112\,65 \times 10^{-16} \text{ C} \cdot \text{m}^2/\text{V}$

Item No.	Quantity	Symbol	Definition 1)	Remarks 2)
8-31.1	partition function	Q, Z	The sum of the quantities $\exp(-E_i/kT)$ over all quantum states i , where E_i is the energy of state i .	This quantity is dimensionless. For k see 8-34.1 Z is used for the total partition function.
8-32.1	statistical weight	g	Multiplicity of quantum state.	This quantity is dimensionless.
8-33.1	molar gas constant	R	The universal constant of proportionality in the ideal gas law: $pV_m = RT$	$R = (8.3143 \pm 0.0012) \text{ J/(mol} \cdot \text{K)}$
8-34.1	Boltzmann constant	k	$k = R/N_A$	$k = (1.38054 \pm 0.00018) \times 10^{-23} \text{ J/K}$ β is used for $1/kT$, where T is the thermodynamic temperature.
8-35.1	mean free path	l, λ	For a molecule, the average distance between two successive collisions.	
8-36.1	diffusion coefficient	D	$n_B \langle \mathbf{v}_B \rangle = -D \text{grad } n_B$, where n_B is the local number density of component B in the mixture and $\langle \mathbf{v}_B \rangle$ is the local average velocity of the component.	
8-37.1	thermal diffusion ratio	k_T	In the stationary state of a binary mixture in which thermal diffusion occurs: $\text{grad } x_B = -(k_T/T) \text{grad } T$, where x_B is the local mole fraction of the heavier component B and T is the local temperature.	These quantities are dimensionless.
8-37.2	thermal diffusion factor	α_T	$\alpha_T = k_T/x_A x_B$, where x_A and x_B are the local mole fractions of the two components.	
8-38.1	thermal diffusion coefficient	D_T	$D_T = k_T \cdot D$	
8-39.1	atomic number	Z	The number of electrons in a neutral atom.	This quantity is dimensionless.
8-40.1	elementary charge	e	The electric charge of a proton.	The magnitude of the electric charge of an electron is equal to e . $e = (1.60210 \pm 0.00007) \times 10^{-19} \text{ C}$
8-41.1	charge number of ion	z	The ratio of the charge of the ion to the elementary charge.	This quantity is dimensionless. This quantity is negative for a negative ion.
8-42.1	Faraday constant	F	$F = N_A e$	$F = (9.64870 \pm 0.00016) \times 10^4 \text{ C/mol}$
8-43.1	ionic strength	I	The ionic strength of a solution is defined as $I = \frac{1}{2} \sum z_i^2 m_i$, where the summation is carried out over all ions with molalities m_i .	
8-44.1	degree of dissociation	α	The ratio of the number of dissociated molecules to the total number of molecules.	This quantity is dimensionless.

1) See footnote 1 on page 2.

2) See footnote 2 on page 2.

8. Physical chemistry and molecular physics (continued)

Units
8-33.a...8-43.a

Item No.	Name of unit and in certain cases abbreviation for this name	International symbol for unit	Definition	Conversion factors	Remarks
8-33.a	joule per mole kelvin	J/(mol·K)			
8-34.a	joule per kelvin	J/K			
8-35.a	metre	m			
8-36.a	square metre per second	m ² /s			
8-38.a	square metre per second	m ² /s			
8-40.a	coulomb	C			
8-42.a	coulomb per mole	C/mol			
8-43.a	mole per kilo-gram	mol/kg			

8. Physical chemistry and molecular physics (end)

Quantities

8-45.1...8-47.1

Item No.	Quantity	Symbol	Definition 1)	Remarks 2)
8-45.1	electrolytic conductivity	$\gamma, \kappa, K, \sigma$	The electrolytic current density divided by the electric field strength.	This quantity was formerly called specific conductance.
8-46.1	molar conductivity	Λ_m	Conductivity divided by concentration	
8-47.1	transport number	t	The ratio of the current carried by a specified kind of ions to the total current.	This quantity is dimensionless.
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1) See footnote 1 on page 2.

2) See footnote 2 on page 2.