INTERNATIONAL STANDARD

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Quantities and units —

Part 9:
Physical chemistry and molecular physics

Grandeurs et unités —

Partie 9: Chimie physique et physique moléculaire

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Foreword

ISO (the International Organization for Standardization) is a worldwide federation of national standards bodies (ISO member bodies). The work of preparing International Standards is normally carried out through ISO technical committees. Each member body interested in a subject for which a technical committee has been established 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. ISO collaborates closely with the International Electrotechnical Commission (IEC) on all matters of electrotechnical standardization.

International Standards are drafted in accordance with the rules given in the ISO/IEC Directives, Part 2.

The main task of technical committees is to prepare International Standards. Draft International Standards adopted by the technical committees are circulated to the member bodies for voting. Publication as an International Standard requires approval by at least 75 % of the member bodies casting a vote.

Attention is drawn to the possibility that some of the elements of this document may be the subject of patent rights. ISO shall not be held responsible for identifying any or all such patent rights.

ISO 80000-9 was prepared by Technical Committee ISO/TC 12, *Quantities and units*.

This first edition of ISO 80000-9 cancels and replaces ISO 31-8:1992. It also incorporates the Amendment ISO 31-8:1992/Amd.1:1998. The major technical changes from the previous standard are the following:

— the presentation of *Numerical statements* has been changed;

— the *Normative references* have been changed;

— some new items have been introduced;

— some new chemical elements have been introduced in Annex A;

— Annex C on pH has been revised and given a completely new text.

ISO 80000 consists of the following parts, under the general title *Quantities and units*:

— *Part 1: General*

— *Part 2: Mathematical signs and symbols to be used in the natural sciences and technology*

— *Part 3: Space and time*

— *Part 4: Mechanics*

— *Part 5: Thermodynamics*

— *Part 7: Light*

— *Part 8: Acoustics*

— *Part 9: Physical chemistry and molecular physics*

— *Part 10: Atomic and nuclear physics*

— *Part 11: Characteristic numbers*

— *Part 12: Solid state physics*

IEC 80000 consists of the following parts, under the general title *Quantities and units*:

— *Part 6: Electromagnetism*

— *Part 13: Information science and technology*

— *Part 14: Telebiometrics related to human physiology*

Introduction

0.1 Arrangements of the tables

The tables of quantities and units in this International Standard are arranged so that the quantities are presented on the left-hand pages and the units on the corresponding right-hand pages.

All units between two full lines on the right-hand pages belong to the quantities between the corresponding full lines on the left-hand pages.

Where the numbering of an item has been changed in the revision of a part of ISO 31, the number in the preceding edition is shown in parentheses on the left-hand page under the new number for the quantity; a dash is used to indicate that the item in question did not appear in the preceding edition.

0.2 Tables of quantities

The names in English and in French of the most important quantities within the field of this International Standard are given together with their symbols and, in most cases, their definitions. These names and symbols are recommendations. The definitions are given for identification of the quantities in the International System of Quantities (ISQ), listed on the left-hand pages of the table; they are not intended to be complete.

The scalar, vectorial or tensorial character of quantities is pointed out, especially when this is needed for the definitions.

In most cases only one name and only one symbol for the quantity are given; where two or more names or two or more symbols are given for one quantity and no special distinction is made, they are on an equal footing. When two types of italic letters exist (for example as with ϑ and θ; φ and ϕ; *a* and a; *g* and g) only one of these is given. This does not mean that the other is not equally acceptable. It is recommended that such variants should not be given different meanings. A symbol within parentheses implies that it is a reserve symbol, to be used when, in a particular context, the main symbol is in use with a different meaning.

In this English edition, the quantity names in French are printed in an italic font, and are preceded by *fr*. The gender of the French name is indicated by (m) for masculine and (f) for feminine, immediately after the noun in the French name.

0.3 Tables of units

0.3.1 General

The names of units for the corresponding quantities are given together with the international symbols and the definitions. These unit names are language-dependent, but the symbols are international and the same in all languages. For further information, see the SI Brochure (8th edition 2006) from BIPM and ISO 80000-1[1].

The units are arranged in the following way:

a) The coherent SI units are given first. The SI units have been adopted by the General Conference on Weights and Measures (Conférence Générale des Poids et Mesures, CGPM). The use of coherent SI units

1) To be published.

is recommended; decimal multiples and submultiples formed with the SI prefixes are recommended, even though not explicitly mentioned.

b) Some non-SI units are then given, being those accepted by the International Committee for Weights and Measures (Comité International des Poids et Mesures, CIPM), or by the International Organization of Legal Metrology (Organisation Internationale de Métrologie Légale, OIML), or by ISO and IEC, for use with the SI.

   Such units are separated from the SI units in the item by use of a broken line between the SI units and the other units.

c) Non-SI units currently accepted by the CIPM for use with the SI are given in small print (smaller than the text size) in the “Conversion factors and remarks” column.

d) Non-SI units that are not recommended are given only in annexes in some parts of this International Standard. These annexes are informative, in the first place for the conversion factors, and are not integral parts of the standard. These deprecated units are arranged in two groups:

   1) units in the CGS system with special names;

   2) units based on the foot, pound, second, and some other related units.

e) Other non-SI units are given for information, especially regarding the conversion factors, in informative annexes in some parts of this International Standard.

0.3.2 Remark on units for quantities of dimension one, or dimensionless quantities

The coherent unit for any quantity of dimension one, also called a dimensionless quantity, is the number one, symbol 1. When the value of such a quantity is expressed, the unit symbol 1 is generally not written out explicitly.

EXAMPLE 1 Refractive index $n = 1{,}53 \times 1 = 1{,}53$

Prefixes shall not be used to form multiples or submultiples of this unit. Instead of prefixes, powers of 10 are recommended.

EXAMPLE 2 Reynolds number $Re = 1{,}32 \times 10^3$

Considering that plane angle is generally expressed as the ratio of two lengths and solid angle as the ratio of two areas, in 1995 the CGPM specified that, in the SI, the radian, symbol rad, and steradian, symbol sr, are dimensionless derived units. This implies that the quantities plane angle and solid angle are considered as derived quantities of dimension one. The units radian and steradian are thus equal to one; they may either be omitted, or they may be used in expressions for derived units to facilitate distinction between quantities of different kinds but having the same dimension.

0.4 Numerical statements in this International Standard

The sign $=$ is used to denote “is exactly equal to”, the sign $\approx$ is used to denote “is approximately equal to”, and the sign $:=$ is used to denote “is by definition equal to”.

Numerical values of physical quantities that have been experimentally determined always have an associated measurement uncertainty. This uncertainty should always be specified. In this International Standard, the magnitude of the uncertainty is represented as in the following example.

EXAMPLE $l = 2{,}347\,82(32)$ m

In this example, $l = a(b)$ m, the numerical value of the uncertainty b indicated in parentheses is assumed to apply to the last (and least significant) digits of the numerical value a of the length l. This notation is used when b represents one standard uncertainty (estimated standard deviation) in the last digits of a. The numerical example given above may be interpreted to mean that the best estimate of the numerical value of the length l (when l is expressed in the unit metre) is 2,347 82, and that the unknown value of l is believed to lie between $(2{,}347\,82 - 0{,}000\,32)$ m and $(2{,}347\,82 + 0{,}000\,32)$ m with a probability determined by the standard uncertainty 0,000 32 m and the probability distribution of the values of l.

0.5 Special remarks

In this part of ISO 80000, symbols for substances are shown as subscripts, for example c_B, w_B, p_B.

Generally, it is advisable to put symbols for substances and their states in parentheses on the same line as the main symbol, for example $c(\mathrm{H_2SO_4})$.

The superscript * is used to mean “pure”. The superscript $^\ominus$ is used to mean “standard”.

EXAMPLE 1 V_m ($\mathrm{K_2SO_4}$, 0,1 mol · dm^{-3} in $\mathrm{H_2O}$, 25 °C) for molar volume.

EXAMPLE 2 $C^\ominus_{\mathrm{m},p}$ ($\mathrm{H_2O}$, g, 298,15 K) $=$ 33,58 J · K^{-1} · mol^{-1} for standard molar heat capacity at constant pressure.

In an expression such as $\varphi_\mathrm{B} = x_\mathrm{B} V^*_\mathrm{m,B} / \sum x_i V^*_{\mathrm{m},i}$, where φ_B denotes the volume fraction of a particular substance B in a mixture of substances A, B, C, ..., where x_i denotes the amount-of-substance fraction of i and $V^*_{\mathrm{m},i}$ the molar volume of the pure substance i, and where all the molar volumes $V^*_\mathrm{m,A}$, $V^*_\mathrm{m,B}$, $V^*_\mathrm{m,C}$, ... are taken at the same temperature and pressure, the summation on the right-hand side is that over all the substances A, B, C, ... of which a mixture is composed, so that $\sum x_i = 1$.

The names and symbols of the chemical elements are given in Annex A.

Additional qualifying information on a quantity symbol may be added as a subscript or superscript or in parentheses after the symbol.

Quantities and units —

Part 9:
Physical chemistry and molecular physics

1 Scope

ISO 80000-9 gives names, symbols, and definitions for quantities and units of physical chemistry and molecular physics. Where appropriate, conversion factors are also given.

2 Normative references

The following referenced documents are indispensable for the application of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO 80000-3:2006, *Quantities and units — Part 3: Space and time*

ISO 80000-4:2006, *Quantities and units — Part 4: Mechanics*

ISO 80000-5:2007, *Quantities and units — Part 5: Thermodynamics*

IEC 80000-6:2008, *Quantities and units — Part 6: Electromagnetism*

3 Names, symbols, and definitions

The names, symbols, and definitions for quantities and units of physical chemistry and molecular physics are given on the following pages.

PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS				QUANTITIES
Item No.	**Name**	**Symbol**	**Definition**	**Remarks**
9-1 (*8-3*)	amount of substance *fr quantité* (f) *de matière*	n	amount of substance is one of the seven base quantities in the International System of Quantities, ISQ, on which the SI is based	Amount of substance of a pure sample is that quantity that can often be determined by measuring its mass and dividing by the molar mass of the sample. Amount of substance is defined to be proportional to the number of specified elementary entities in a sample, the proportionality constant being a universal constant which is the same for all samples. The name "number of moles" is often used for "amount of substance", but this is deprecated because the name of a quantity should be distinguished from the name of the unit. In the name "amount of substance", the words "of substance" could, for simplicity, be replaced by words to specify the substance concerned in any particular application, so that one may, for example, talk of "amount of hydrogen chloride, HCl", or "amount of benzene, C_6H_6". It is important to always give a precise specification of the entity involved (as emphasized in the second sentence of the definition of the mole); this should preferably be done by giving the molecular chemical formula of the material involved.

UNITS				PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS
Item No.	**Name**	**International symbol**	**Definition**	**Conversion factors and remarks**
9-1.a	mole	mol	the mole is the amount of substance of a system which contains as many elementary entities as there are atoms in 0,012 kg of carbon 12 [14th CGPM (1971)]	When the mole is used, the elementary entities shall be specified and may be atoms, molecules, ions, electrons, other entities or specified groups of them. The definition applies to unbound atoms of carbon 12, at rest and in their ground state. The mole is also used for entities such as holes and other quasi-particles, double bonds, etc.

(*continued*)

PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS — **QUANTITIES**

Item No.	Name	Symbol	Definition	Remarks
9-2.1 (*8-1.1*)	relative atomic mass *fr masse* (f) *atomique relative*	A_r	ratio of the average mass (ISO 80000-4:2006, item 4-1) per atom of an element to 1/12 of the mass of an atom of the nuclide ^{12}C	EXAMPLE $A_r(Cl) \approx 35{,}453$ The relative atomic or relative molecular mass depends on the nuclidic composition. The International Union of Pure and Applied Chemistry (IUPAC) accepts the use of the special names “atomic weight” and “molecular weight” for the quantities “relative atomic mass” and “relative molecular mass”, respectively. The use of these traditional names is deprecated.
9-2.2 (*8-1.2*)	relative molecular mass *fr masse* (f) *moléculaire relative*	M_r	ratio of the average mass per molecule or specified entity of a substance to 1/12 of the mass of an atom of the nuclide ^{12}C	
9-3 (*8-2*)	number of particles *fr nombre* (m) *de particules*	N_B	N_B equals the number of particles in a system	Different entities may be used as a particle, e.g. number of molecules, number of atoms. A subscript added to the symbol indicates a specific entity, e.g. N_B for the number of molecules of substance B.
9-4 (*8-4*)	Avogadro constant *fr constante* (f) *d'Avogadro*	L, N_A	for a pure sample $L = N/n$ where N is the number of particles (item 9-3) and n is amount of substance (item 9-1)	$L = 6{,}022\ 141\ 79(30) \times 10^{23}\ \text{mol}^{-1}$ $10^{23}\ \text{mol}^{-1}$ [CODATA 2006]
9-5 (*8-5*)	molar mass *fr masse* (f) *molaire*	M	for a pure sample $M = m/n$ where m is mass (ISO 80000-4:2006, item 4-1) and n is amount of substance (item 9-1)	
9-6 (*8-6*)	molar volume *fr volume* (m) *molaire*	V_m	for a pure sample $V_m = V/n$ where V is volume (ISO 80000-3:2006, item 3-4) and n is amount of substance (item 9-1)	The molar volume of an ideal gas at 273,15 K and 101 325 Pa is $V_m = 0{,}022\ 413\ 996\ (39)\ \text{m}^3/\text{mol}$ and, for 273,15 K and 100 000 Pa, the molar volume is $V_m = 0{,}022\ 710\ 981\ (40)\ \text{m}^3/\text{mol}$. [CODATA 2006]

UNITS			PHYSICAL CHEMISTRY AND MOLECULAR PHYSICS	
Item No.	**Name**	**Inter-national symbol**	**Definition**	**Conversion factors and remarks**
9-2.a	one	1		See the Introduction, 0.3.2.
9-3.a	one	1		See the Introduction, 0.3.2.
9-4.a	mole to the power minus one	mol^{-1}		
9-5.a	kilogram per mole	kg/mol		The commonly used unit for molar mass is gram per mole, g/mol, rather than kilogram per mole, kg/mol.
9-6.a	cubic metre per mole	m^3/mol		

(*continued*)