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Part 9:
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Partie 9: Chimie physique et physique moléculaire

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Contents

Page

Foreword iv
Introduction v
1 Scope 1
2 Normative references 1
3 Terms and definitions 1
Bibliography 15
Index 16

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.

The procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular, the different approval criteria needed for the different types of ISO documents should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see www.iso.org/directives).

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. Details of any patent rights identified during the development of the document will be in the Introduction and/or on the ISO list of patent declarations received (see www.iso.org/patents).

Any trade name used in this document is information given for the convenience of users and does not constitute an endorsement.

For an explanation of the voluntary nature of standards, the meaning of ISO specific terms and expressions related to conformity assessment, as well as information about ISO's adherence to the World Trade Organization (WTO) principles in the Technical Barriers to Trade (TBT), see www.iso.org/iso/foreword.html.

This document was prepared by Technical Committee ISO/TC 12, *Quantities and units*, in collaboration with Technical Committee IEC/TC 25, *Quantities and units*.

This second edition cancels and replaces the first edition (ISO 80000-9:2009), which has been technically revised. It also incorporates the Amendment ISO 80000-9:2009/Amd. 1:2011.

The main changes compared to the previous edition are as follows:

— the table giving the quantities and units has been simplified;

— some definitions and the remarks have been stated physically more precisely.

A list of all parts in the ISO 80000 and IEC 80000 series can be found on the ISO and IEC websites.

Any feedback or questions on this document should be directed to the user's national standards body. A complete listing of these bodies can be found at www.iso.org/members.html.

Introduction

In this document, symbols for substances are shown as subscripts, for example c_B, w_B, p_B for substance 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 $c(H_2SO_4)$.

In the following, the letter s is used to denote the solid state, the letter l the liquid state, and the letter g the gaseous state.

The symbol * used as a superscript means "pure".

The plimsoll sign $\ominus$ is used to denote a standard in general.

EXAMPLE 1 $\mu_B^*(T, p)$ for chemical potential of pure substance B concerning a mixture system including the substance B.

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

In an expression such as

$$\varphi_B = x_B \frac{V_{m,B}}{\sum x_i V_{m,i}}$$

where

φ_B is the volume fraction of a particular substance B in a mixture of substances A, B, C, ...;

x_i is the amount-of-substance fraction of i; and

$V_{m,i}$ is the molar volume of the pure substance i, where all the molar volumes $V_{m,A}$, $V_{m,B}$, $V_{m,C}$, ... 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 $\sum x_i = 1$. Throughout the document sums are running over the respective index.

Additional qualifying information on a quantity symbol may be added as a subscript or superscript (see e.g. item 9-21) or in parentheses after the symbol.

Quantities and units —

Part 9:
Physical chemistry and molecular physics

1 Scope

This document gives names, symbols, definitions and units for quantities of physical chemistry and molecular physics. Where appropriate, conversion factors are also given.

2 Normative references

There are no normative references in this document.

3 Terms and definitions

Names, symbols, definitions and units for quantities used in physical chemistry and molecular physics are given in Table 1.

ISO and IEC maintain terminological databases for use in standardization at the following addresses:

— ISO Online browsing platform: available at https://www.iso.org/obp

— IEC Electropedia: available at http://www.electropedia.org/

Table 1 — Quantities and units used in physical chemistry and molecular physics

Item No.	Quantity			Unit	Remarks
	Name	Symbol	Definition		
9-1	number of entities	$N(\mathrm{X})$, N_X	number of elementary entities of kind X in a system	1	The elementary entities must be specified and can be atoms, molecules, ions, electrons, other particle, or a specified group of such particles. It is important to always give a precise specification of the entity involved; this should preferably be done by the empirical chemical formula of the material involved.
9-2	amount of substance DEPRECATED: number of moles	$n(\mathrm{X})$	quotient of number N of specified elementary entities of kind X (item 9-1) in a sample, and the Avogadro constant N_A (ISO 80000-1): $n(\mathrm{X}) = N(\mathrm{X})/N_\mathrm{A}$	mol	Amount of substance is one of the seven base quantities in the International System of Quantities, ISQ (see ISO 80000-1). Elementary entities, such as molecules, atoms, ions, electrons, holes and other quasi-particles, double bonds can be used. It is necessary to specify precisely the entity involved, e.g. atoms of hydrogen H vs. molecules of hydrogen H_2, preferably by giving the molecular chemical formula of the material involved. In the name “amount of substance”, the words “of substance” could be replaced by words specifying the substance concerned, e.g. “amount of hydrogen chloride, HCl”, or “amount of benzene, C_6H_6”. 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.

Table 1 *(continued)*

Item No.	Quantity			Unit	Remarks
	Name	Symbol	Definition		
9-3	relative atomic mass	$A_r(X)$	quotient of the average mass (ISO 80000-4) of atom X and the unified atomic mass (ISO 80000-10)	1	A similar quantity “relative molecular mass” can be defined for molecules. EXAMPLE $A_r(Cl) \approx 35{,}453$, $A_r(CO_2) \approx 44$. 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.
9-4	molar mass	$M(X)$	for a pure substance X, quotient of mass $m(X)$ (ISO 80000-4) and amount n of substance (item 9-2): $M = m/n$	g/mol kg mol^{-1}	
9-5	molar volume	V_m	for a pure substance, quotient of its volume V (ISO 80000−3) and amount n of substance (item 9-2): $V_m = V/n$	m^3 mol^{-1}	
9-6.1	molar internal energy	U_m	quotient of internal energy U (ISO 80000-5) and amount n of substance (item 9-2): $U_m = U/n$	J/mol kg m^2 s^{-2} mol^{-1}	Molar quantities are normally only used with reference to pure substances.
9-6.2	molar enthalpy	H_m	quotient of enthalpy H (ISO 80000-5) and amount n of substance (item 9-2): $H_m = H/n$	J/mol kg m^2 s^{-2} mol^{-1}	Molar quantities are normally only used with reference to pure substances.

Table 1 *(continued)*

Item No.	Quantity			Unit	Remarks
	Name	Symbol	Definition		
9-6.3	molar Helmholtz energy	F_m	quotient of the Helmholtz energy F (ISO 80000-5) and amount n of substance (item 9-2): $F_m = F/n$	J/mol kg m^2 s^{-2} mol^{-1}	Molar quantities are normally only used with reference to pure substances.
9-6.4	molar Gibbs energy	G_m	quotient of the Gibbs energy G (ISO 80000-5) and amount n of substance (item 9-2): $G_m = G/n$	J/mol kg m^2 s^{-2} mol^{-1}	Molar quantities are normally only used with reference to pure substances.
9-7	molar heat capacity	C_m	quotient of heat capacity C (ISO 80000-5) and amount of substance n (item 9-2): $C_m = C/n$	J/(mol K) kg m^2 s^{-2} K^{-1} mol^{-1}	Conditions (constant pressure or volume etc.) must be specified.
9-8	molar entropy	S_m	quotient of entropy S (ISO 80000-5) and amount n of substance (item 9-2): $S_m = S/n$	J/(mol K) kg m^2 s^{-2} K^{-1} mol^{-1}	Conditions (constant pressure or volume etc.) must be specified.
9-9.1	particle concentration	n, (C)	quotient of number N of particles (item 9-1) and volume V (ISO 80000−3): $n = N/V$	m^{-3}	The term “number density” is also used.
9-9.2	molecular concentration	$C(\mathrm{X})$, C_X	for substance X in a mixture, quotient of number N_X of molecules of substance X and volume V (ISO 80000−3) of the mixture: $C_X = N_X/V$	m^{-3}	
9-10	mass concentration	γ_X, (ρ_X)	for substance X in a mixture, quotient of mass m_X (ISO 80000-4) of substance X and volume V (ISO 80000−3) of the mixture: $\gamma_X = m_X/V$	g/l kg m^{-3}	Decided by the 16th CGPM (1979), both “l” and “L” are allowed for the symbols for the litre.
9-11	mass fraction	w_X	for substance X in a mixture, quotient of mass m_X (ISO 80000-4) of substance X and total mass m of the mixture: $w_X = m_X/m$	1	

Table 1 *(continued)*

Item No.	Quantity			Unit	Remarks
	Name	Symbol	Definition		
9-12.1	amount-of-substance concentration	c_X	for substance X in a mixture, quotient of amount n_X of substance (item 9-2) of X and volume V (ISO 80000−3) of the mixture: $c_X = n_X / V$	mol/l mol m^{-3}	In chemistry, the name “amount-of-substance concentration” is generally abbreviated to the single word “concentration”, it being assumed that the adjective “amount-of-substance” is intended. For this reason, however, the word “mass” should never be omitted from the name “mass concentration” in item 9-10. Decided by the 16th CGPM (1979), both “l” and “L” are allowed for the symbols for the litre.
9-12.2	standard amount-of-substance concentration	$c^{\ominus}(X)$	for substance X, one mole per litre	mol/l mol m^{-3}	Decided by the 16th CGPM (1979), both “l” and “L” are allowed for the symbols for the litre.
9-13	amount-of-substance fraction mole fraction	x_X, y_X	for substance X in a mixture, quotient of amount of substance n_X (item 9-2) of X and total amount n of substance (item 9-2) in the mixture: $x_X = n_X / n$	1	For condensed phases, x_X is used, and for gaseous mixtures y_X may be used. The unsystematic name “mole fraction” is still used. However, the use of this name is deprecated. For this quantity, the entity used to define the amount of substance should always be a single molecule for every species in the mixture.
9-14	volume fraction	φ_X	for substance X, quotient of product of amount of substance fraction x_X (item 9-13) of X and molar volume $V_{m,X}$ (item 9-5) of the pure substance X at the same temperature (ISO 80000-5) and pressure(ISO 80000-4), and sum over all substances i of products of amount-of-substance fractions x_i (item 9-13) of substance i and their molar volumes $V_{m,i}$ (item 9-5): $\varphi_X = \frac{x_X V_{m,X}}{\sum_i x_i V_{m,i}}$	ml/l 1	Generally, the volume fraction is temperature dependent. Decided by the 16th CGPM (1979), both “l” and “L” are allowed for the symbols for the litre.