1.3.7 General chemistry

Name	*Symbol*	*Definition*	*SI unit*	*Notes*
number of entities (e.g. molecules, atoms, ions, formula units)	N		1	
amount (of substance), chemical amount	n	$n_B = N_B/L$	mol	(1), (2)
Avogadro constant	L, N_A		mol^{-1}	
mass of atom atomic mass	m_a, m		kg	
mass of entity (molecule, formula unit)	m_f, m		kg	(3)
atomic mass constant	m_u	$m_u = m_a(^{12}C)/12$	kg	(4)
molar mass	M	$M_B = m/n_B$	kg mol^{-1}	(2), (5)

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(1) The words 'of substance' may be replaced by the specification of the entity.

Example When the amount of O_2 is equal to 3 moles, $n(O_2) = 3$ mol, then the amount of $\frac{1}{2}O_2$ is equal to 6 moles, $n(\frac{1}{2}O_2) = 6$ mol. Thus $n(\frac{1}{2}O_2) = 2n(O_2)$.

(2) The definition applies to entities B which should always be indicated by a subscript or in parentheses, e.g. n_B of $n(B)$.

(3) A formula unit is not a unit but an entity specified as a group of atoms by the way the chemical formula is written.

(4) m_u is equal to the unified atomic mass unit, with symbol u, i.e. $m_u = 1$ u. In biochemistry this unit is called the dalton, with symbol Da, although the name and symbol have not been approved by CGPM.

(5) The definition applies to pure substance, where m is the total mass and V is the total volume. However, corresponding quantities may also be defined for a mixture as m/n and V/n, where $n = \sum_i n_i$. These quantities are called the mean molar mass and the mean molar volume respectively.

Name	*Symbol*	*Definition*	*SI unit*	*Notes*
relative molecular mass, (relative molar mass, molecular weight)	M_r	$M_r = m_f/m_u$	1	(6)
relative atomic mass, (atomic weight)	A_r	$A_r = m_a/m_u$	1	(6)
molar volume	V_m	$V_{m,B} = V/n_B$	$m^3\ mol^{-1}$	(2), (5)
mass fraction	w	$w_j = m_j/\Sigma m_i$	1	(7)
volume fraction	φ	$\varphi_j = V_j/\Sigma V_i$	1	(7), (8)
mole fraction, amount fraction, number fraction	x, y	$x_B = n_B/\Sigma n_A$	1	(2), (9)
(total) pressure	p, P		Pa	(10)
partial pressure	p_B	$p_B = y_B p$	Pa	(11)

(6) For molecules M_r is the relative molecular mass or molecular weight; for atoms M_r is the relative atomic mass or atomic weight and the symbol A_r may be used. M_r may also be called the relative molar mass, $M_{r,B} = M_B/M^\theta$, where $M^\theta = 1$ g mol^{-1}. The standard atomic weights, recommended by IUPAC, are listed in the Green Book p.94. See also 1.8. Table for atomic weights to five significant figures.

(7) The definition applies to component j.

(8) V_j and V_i are the volumes of appropriate components prior to mixing.

(9) For condensed phases x is used, and for gaseous mixtures y may be used.

(10) Pressures are often expressed in the non-SI unit bar, where 1 bar = 10^5 Pa. The standard pressure p = 1 bar = 10^5 Pa. Low pressures are often expressed in millibars, where 1 mbar =10^{-3} bar = 100 Pa.

(11) The symbol and the definition apply to molecules B, which should be specified. In real (non-ideal) gases there is a difficulty about defining partial pressure. Some workers regard the equation given as an operational definition; the alternative is to regard the partial pressure of B as the pressure exerted by molecules B.

Name	*Symbol*	*Definition*	*SI unit*	*Notes*
mass concentration, (mass density)	γ, ρ	$\gamma_j = m_j/V$	kg m^{-3}	(7),(12),(13)
number concentration, number density of entities	C, n	$C_B = N_B/V$	m^{-3}	(2),(12), (14)
amount concentration, concentration	c	$c_B = n_B/V$	mol m^{-3}	(2), (12), (15)
solubility	s	$s_B = c_B$(saturated soln)	mol m^{-3}	(2)
molality (of a solute)	m, b	$m_B = n_B/m_A$	mol kg^{-1}	(2), (16)
surface concentration	Γ	$\Gamma_B = n_B/A$	mol m^{-2}	(2)

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(12) V is the volume of the mixture.

(13) In polymer science the symbol c is often used for mass concentration.

(14) The term number concentration and symbol C is preferred for mixtures.

(15) The unit mol dm^{-3} is often used for amount concentration. ‘Amount concentration' is an abbreviation for ‘amount-of-substance concentration'. (The Clinical Chemistry Division of IUPAC recommends that amount of substance concentration be abbreviated to ‘substance concentration'.) When there is no risk of confusion the word ‘concentration' may be used alone. The symbol [B] is often used for amount concentration of entities B.

This quantity is also sometimes called molarity. A solution of, for example, 1 mol dm^{-3} is often called a 1 molar solution, denoted 1 M solution. Thus M is often treated as a symbol for mol dm^{-3}.

(16) In the defintion m_B denotes the molality of solute B, and m_A denotes the mass of solvent A; thus the same symbol m is used with two different meaning. This confusion of notation may be avoided by using the symbol b for molality.

A solution of molality 1 mol/kg is occasionally called a 1 molal solution, denoted 1 m solution; however the symbol m should not be treated as a symbol for the unit mol kg^{-1}.

Name	*Symbol*	*Definition*	*SI unit*	*Notes*
stoichiometric number	ν		1	(17)
extent of reaction, advancement	ξ	$n_B = n_{B,0} + \nu_B\xi$	mol	(2), (18)
degree of reaction	α		1	(19)

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(17) The stoichiometric number is defined through the reaction equation. It is negative for reactants and positive for products. The values of the stoichiometric numbers depend on how the reaction equation is written.

Example (½) N_2 + (3/2) H_2 = NH_3: $\nu(N_2) = -½$
$\nu(H_2) = -3/2$
$\nu(NH_3) = +1$

A symbolic way of writing a general chemical equation is

$$0 = \Sigma \nu_j B_j$$

where B_j denotes an entity in the reaction. For multireaction systems it is convenient to write the chemical equations in matrix form

$$\boldsymbol{A}\,\boldsymbol{\nu} = \mathbf{0}$$

where $\boldsymbol{A}$ is the conservation (or formula) matrix with elements A_{ij} representing the number of atoms of the ith element in the jth reaction component (reactant or product) entity and $\boldsymbol{\nu}$ is the stoichiometric number matrix with elements ν_{jk} being the stoichiometric numbers of the jth reaction component entity in the kth reaction. When there are N_s reacting species involved in the system consisting of N_e elements $\boldsymbol{A}$ becomes an $N_e \times N_s$ matrix. Its nullity, $N(\boldsymbol{A}) = N_s$ - rank($\boldsymbol{A}$), gives the number of independent chemical reactions, N_r, and the $N_s \times N_r$ stoichiometric number matrix, $\boldsymbol{\nu}$, can be determined as the null space of $\boldsymbol{A}$. $\mathbf{0}$ is an $N_e \times N_r$ zero matrix.

(18) $n_{B,0}$ is the amount of B when $\xi = 0$. A more general definition is $\Delta\xi = \Delta n_B/\nu_B$. The extent of reaction also depends on how the reaction equation is written, but it is independent of which entity in the reaction equation is used in the defintion.

Example For the reaction is footnote (17), when $\Delta\xi$ = 2 mol, $\Delta n(N_2)$ = -1 mol, $\Delta n(H_2)$ = -3 mol, and $\Delta n(NH_3)$ = +2 mol.

This quantity was originally introduced as *degrè d'avancement* by de Donder.

(19) For a specific reaction terms such as 'degree of dissociation', 'degree of ionization', etc are commonly used.

Other symbols and conventions in chemistry

(i) Symbols for particles and nuclear reactions

neutron	n	helion	h
proton	p	alpha particle	α
deutron	d	electron	e
triton	t	photon	γ
positive muon	μ^+	negative muon	μ^-

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

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

$$\begin{matrix}\text{initial}\\ \text{nuclide}\end{matrix}\left(\begin{matrix}\text{incoming particles}\\ \text{or quanta}\end{matrix},\begin{matrix}\text{outgoing particles}\\ \text{or quanta}\end{matrix}\right)\begin{matrix}\text{final}\\ \text{nuclide}\end{matrix}$$

Examples $^{14}N(\alpha, p)^{17}O$, $^{59}Co(n, \gamma)^{60}Co$,
$^{23}Na(\gamma, 3n)^{20}Na$, $^{31}P(\gamma, pn)^{29}Si$

(ii) Chemical symbols for the elements

The chemical symbols of elements are (in most cases) derived from their Latin names and consist of one or two letters which should always be printed in roman (upright) type. Only for elements of atomic number greater than 103, the systematic symbols consist of three letters.

Examples I, U, Pa, C

The symbols can have different meanings:

(a) They can denote an atom of the element. For example, Cl can denote a chlorine atom having 17 protons and 18 or 20 neutrons (giving a mass number of 35 or 37), the difference being ignored. Its mass is on average 35.4527 u in terrestrial samples.

(b) The symbol may, as a kind of shorthand, denote a sample of the element. For example, Fe can denote a sample of iron, and He a sample of helium gas.

The term *nuclide* implies an atom of specified atomic number (proton number) and mass number (nucleon number). Nuclides having the same atomic number but different mass numbers are called isotopic nuclides or *isotopes*. Nuclides having the same mass number but different atomic numbers are called isobaric nuclides or *isobars*.

A nuclide may be specified by attaching the mass number as a left superscript to the symbol for the element. The atomic number may also be attached as a left subscript, if desired, although this is rarely done. If no left superscript is attached, the symbol is read as inlcuding all isotopes in natural abundance.

Examples ^{14}N, ^{12}C, ^{13}C, ^{1}O, $n(Cl) = n(^{35}Cl) + n(^{37}Cl)$

The ionic charge number is denoted by a right superscript, or by the sign alone when the charge is equal to one.

Examples	Na^{+}	a sodium positive ion (cation)
	$^{79}Br^{-}$	a bromine-79 negative ion (anion, bromide ion)
	Al^{3+} or Al^{+3}	aluminium triply positive ion
	3 S^{2-} or 3 S^{-2}	three sulfur doubly negative ions (sulfide ions)

The right superscript position is also used to convey other information: excited electronic states may be denoted by an asterisk.

Examples H^{*}, Cl^{*}

Oxidation numbers are denoted by positive or negative roman numerals or by zero (see also (iv) below).

Examples Mn^{VII}, O^{-II}, Ni^{0}

The positions and meanings of indices around the symbol of the element are summarized as follows:

left superscript	mass number
left subscript	atomic number
right superscript	charge number, oxidation number, excitation symbol
right subscript	number of atoms per entity (see (iii) below)

(iii) Chemical formulae

Chemical formulae entities composed of more than one atom (molecules, complex ions, groups of atoms, etc.).

Examples N_2, P_4, C_6H_6, $CaSO_4$, $PtCl_4^{2-}$, $Fe_{0.91}S$

They may also be used as a shorthand to denote a sample of the corresponding chemical substance.

Examples	CH_3OH	methanol
	$\rho(H_2SO_4)$	mass density of sulfuric acid

The number of atoms in an entity is indicated by a right subscript (the numeral 1 being omitted). Groups of atoms may also be enclosed in parentheses. Entities may be specified by giving the corresponding formula, often multiplied by a factor. Charge numbers of complex ions, and excitation symbols, are added as right superscripts to the whole formula. The free radical nature of some entities may be stressed by adding a dot to the symbol.

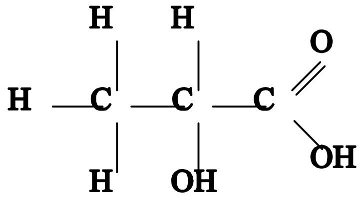
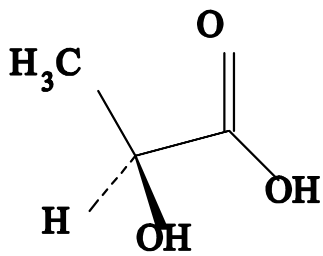
Examples	H_2O	one water molecule, water
	½ O_2	half an oxygen molecule
	$Zn_3(PO_4)_2$	one zinc phosphate formula unit, zinc phosphate
	2 $MgSO_4$	two formula units of magnesium sulfate
	$^1/_5$ $KMnO_4$	one-fifth of a potassium permanganate formula unit
	½ SO^-	half a sulfate ion
	$(CH_3)^\cdot$	methyl free radical
	$CH_3\dot{C}HCH_3$	isopropyl radical
	NO_2*	electronically excited nitrogen dioxide molecule

In the above examples, ½ O_2, $^1/_5$ $KMnO_4$, and ½ SO_4^{2-} are artifical in the sense that such fractions of a molecule cannot exist. However, it may often be convenient to specify entities in this way when calculating amount of substance; see (v) below.

Specific electronic states of entities (atoms, molecules, ions) can be denoted by giving the electronic term symbol (see section 3.5) in parentheses. Vibrational and rotational states can be specified by giving the corresponding quantum numbers.

Examples	$Hg(^3P_1)$	a mercury atom in the triplet -P-one state
	$HF(v = 2, J = 6)$	a hydrogen fluoride molecule in the vibrational state $v = 2$ and the rotational state $J = 6$
	$H_2O^+(^2A_1)$	a water molecule ion in the doublet-A-one state

Chemical formulae may be written in different ways according to the information that they convey, as follows:

Formula	*Information conveyed*	*Example for lactic acid*
empirical	stoichiometric proportion only	CH_2O
molecular	in accord with molecular mass	$C_3H_6O_3$
structural	structural arrangement of atoms	$CH_3CHOHCOOH$
displayed	projection of atoms and bonds	
stereochemical	stereochemical arrangement	

Further conventions for writing chemical formulae are described in Nomenclature of Inorganic Chemistry, Blackwell Sci. Publ., Oxford 1990 and in Nomenclature of Organic Chemistry, Sections A-F, Pergamon Press, Oxford 1979.

(iv) Equations for chemical reactions

Symbols connecting the reactants and products in a chemical reaction equation have the following meanings:

$H_2 + Br_2 = 2\ HBr$	stoichiometric relation
$H_2 + Br_2 \rightarrow 2\ HBr$	net forward reaction
$H_2 + Br_2 \leftrightarrows 2\ HBr$	reaction, both directions
$H_2 + Br_2 \rightleftharpoons 2\ HBr$	equilibrium

A single arrow is also used to designate an elementary reaction, such as $H^{\cdot} + Br_2 \rightarrow HBr + Br^{\cdot}$. It should therefore be made clear if this is the usage intended.

Redox equations are often written so that the absolute value of the stoichiometric number for the electrons transferred (which are normally omitted from the overall equation) is equal to one.

Example $(1/5)\ KMn^{VII}O_4 + (8/5)\ HCl = (1/5)\ Mn^{II}Cl_2 + (½)\ Cl_2 + (1/5)\ KCl + (4/5)\ H_2O$

Similarly a reaction in an electrochemical cell may be written so that the charge number of the cell reaction is equal to one:

Example $(⅓)\ In^0(s) + (½)\ Hg^I{}_2SO_4(s) = (1/6)\ In^{III}{}_2(SO_4)_3(aq) + Hg^0(l)$

(the symbols in parentheses denote the state; see (vi) below).

(v) Amount of substance and the specification of entities

The quantity 'amount of substance' or 'chemical amount' ('Stoffmenge' in German) has been used by chemists for a long time without a proper name. It was simply referred to as the 'number of moles'. This practice should be abandoned, because it is wrong to use 'number of metres' as a synonym for 'length'). The amount of substance is proportional to the number of specified elementary entities of that substance; the proportionality factor is the same for all substances and is the reciprocal of the Avogadro constant. The elementary entities may be chosen as convenient, not necessarily as physically real individual particles. Since the amount of substance and all physical quantities derived from it depend on this choice it is essential to specify the entities to avoid ambiguities.

Examples	n_{Cl}, $n(Cl)$	amount of Cl, amount of chlorine atoms
	$n(Cl_2)$	amount of Cl_2, amount of chlorine molecules
	$n(H_2SO_4)$	amount of (entities) H_2SO_4
	$n(1/5\ KMnO_4)$	amount of (entities) $1/5\ KMnO_4$
	$M(P_4)$	molar mass of (tetraphosphorus) P_4
	c_{HCl}, $c(HCl)$, [HCl]	amount concentration of HCl
	$\Lambda(MgSO_4)$	molar conductivity of (magnesium sulfate entities) $MgSO_4$
	$\Lambda(½\ MgSO_4)$	molar conductivity of (entities) ½ $MgSO_4$
	$n(1/5\ KMnO_4) = 5n(KMnO_4)$	
	$\lambda(½Mg^{2+}) = ½\lambda(Mg^{2+})$	
	$[½H_2SO_4] = 2[H_2SO_4]$	
	(See also examples in section 1.4.1)	

Note that 'amount of sulfur' is an ambiguous statement, because it might imply $n(S)$, $n(S_8)$, or $n(S_2)$, etc. In some cases analogous statements are less ambiguous. Thus for compounds the implied entity is usually the molecule or the common formula entity, and for solid metals it is the atom.

Examples '2 moles of water' implies $n(H_2O)$ = 2 mol; '0.5 moles of sodium chloride' implies n(NaCl) = 0.5 mol; '3 millimoles of iron' implies n(Fe) = 3 mmol, but such statements should be avoided whenever there might be ambiguity.

However, in the equation $pV = nRT$ and in equations involving colligative properties, the entity implied in the definition of n should be an individually translating particle (a whole molecule for a gas), whose nature is unimportant.

(vi) States of aggregation

The following one-, two- or three-letter symbols are used to represent the states of aggregation of chemical species. The letters are appended to the formula symbol in parentheses, and should be printed in roman (upright) type without a full stop (period).

g	gas or vapour	vit	vitreous substance
l	liquid	a, ads	species adsorbed on a substrate
s	solid	mon	monomeric form
cd	condensed phase (i.e. solid or liquid)	pol	polimeric form
		sln	solution
fl	fluid phase (i.e. gas or liquid)	aq	aqueous solution
		aq, ∞	aqueous solution at infinite dilution
cr	crystalline		
lc	liquid crystal	am	amorphous solid

Example	HCl(g)	hydrogen chloride in the gaseous state
	C_V(fl)	heat capacity of a fluid at constant volume
	V_m(lc)	molar volume of a liquid crystal
	U(cr)	internal energy of a crystalline solid
	MnO_2(am)	manganese dioxide as an amophous solid
	MnO_2(cr, I)	manganese dioxide as crystal form I
	NaOH(aq)	aqueous solution of sodium hydroxide
	NaOH(aq, ∞)	...as above, at infinite dilution
	$\Delta_f H^\theta(H_2O, l)$	standard enthalpy of formation of liquid water

The symbols g, l, to denote gas phase, liquid phase, etc., are also sometimes used as a right superscript, and the Greek letter symbols α, β, may be similarly used to denote phase α, phase β, etc., in general notation.

Examples $V_m^{\,l}$, $V_m^{\,s}$ molar volume of the liquid phase, ... of the solid phase
$S_m^{\,\alpha}$, $S_m^{\,\beta}$ molar entropy of phase α, ... of phase β