INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

PHYSICAL CHEMISTRY SECTION: COMMISSION ON PHYSICO-CHEMICAL SYMBOLS AND TERMINOLOGY

Manual of Physico-Chemical Symbols and Terminology

Prepared from the publications of the Commission by its President

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CHEMICAL ELEMENTS AND NUCLIDES

Recommendations adopted by the
Symbols, Units and Nomenclature
Commission of the International Union of
Pure and Applied Physics, September, 1958

Apart from minor differences these conventions were adopted by the Physical Chemistry Section of the Commission on Physico-Chemical Symbols and Terminology of the IUPAC in Stockholm, 1953. On behalf of the Commission its Chairman recommends them to be used by chemists.

◆ Comments concerning present conflicts with the practice of American chemists and the rules of *Chemical Abstracts* have been interpolated in the text. It is hoped that the necessity for such comments can be reduced in future years. These comments, in smaller type, are preceded by the symbol ◆.

Symbols for chemical elements should be written in roman type. The symbol is not followed by a period.

Examples: Ca, C, H, He

The attached numerals specify a *nuclide:*

mass number 14

$^{14}_{7}N_2$

atomic number 7   2 atoms/molecule
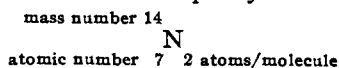
Remark.—It may be of advantage to omit the atomic number when there is no special reason for indicating it.

The right superscript place remains for indicating, if required, a state of ionization or a nuclear excited state.

◆ The practice of American chemists and physicists in general has been to put the mass number at the upper right of the symbol.

CONVENTIONS CONCERNING THE SIGN OF ELECTROMOTIVE FORCES AND ELECTRODE POTENTIALS

At the XVIIth Conference of the International Union of Pure and Applied Chemistry in Stockholm, 1953, the Commission on Physico-Chemical Symbols and Terminology and the Commission on Electrochemistry reached complete agreement on the sign conventions to be recommended with a view to removing the serious confusion that has long existed in this field, especially in the specification of so-called "electrode potentials."

The following statement of the recommendations has been drawn up by the Chairmen of the two Commissions on the basis of a draft prepared by the Commission on Physico-Chemical Symbols and Terminology and of some modifications of the text proposed by the Commission on Electrochemistry.

The Electromotive Force of a Cell.—The cell should be represented by a diagram, *e.g.*

$$Zn\,|\,Zn^{++}\,\|\,Cu^{++}\,|\,Cu$$
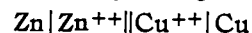
The electromotive force is equal in sign and magnitude to the electrical potential of the metallic conducting lead on the right when that of the similar lead on the left is taken as zero, the cell being open.

When the reaction of the cell is written as

$$\tfrac{1}{2}Zn + \tfrac{1}{2}Cu^{++} \longrightarrow \tfrac{1}{2}Zn^{++} + \tfrac{1}{2}Cu$$
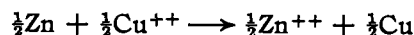
this implies a diagram so drawn that this reaction takes place when positive electricity flows through the cell from left to right. If this is the direction

of the current when the cell is short-circuited, as in the present example, the electromotive force will be positive (unless the ratio Cu^{++}/Zn^{++} is extremely small). If, however, the reaction is written as

$$\tfrac{1}{2}Cu + \tfrac{1}{2}Zn^{++} \longrightarrow \tfrac{1}{2}Cu^{++} + \tfrac{1}{2}Zn$$
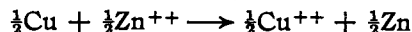
this implies the diagram

$$Cu \,|\, Cu^{++} \| Zn^{++} \,|\, Zn$$

and the electromotive force of the cell so specified will be negative (unless the ratio Cu^{++}/Zn^{++} is extremely small).
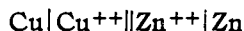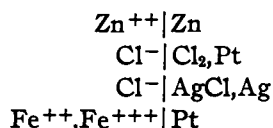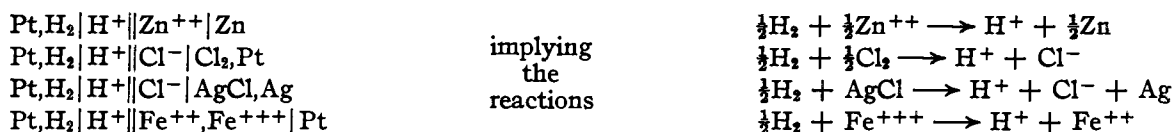
The Electromotive Force of a Half Cell and the So-called "Electrode Potential."—When we speak of the electromotive forces of the half cells
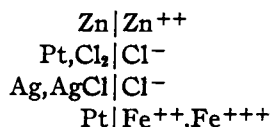
$$Zn^{++} \,|\, Zn$$
$$Cl^- \,|\, Cl_2,Pt$$
$$Cl^- \,|\, AgCl,Ag$$
$$Fe^{++},Fe^{+++} \,|\, Pt$$

we mean the electromotive forces of the cells

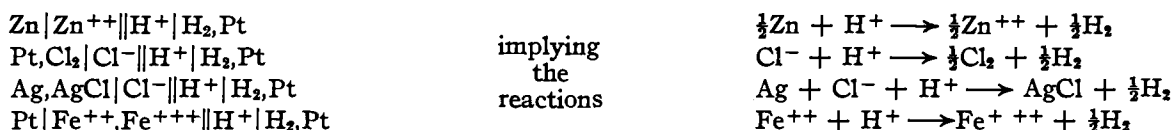|		
$Pt,H_2 \,|\, H^+ \| Zn^{++} \,|\, Zn$		$\tfrac{1}{2}H_2 + \tfrac{1}{2}Zn^{++} \longrightarrow H^+ + \tfrac{1}{2}Zn$
$Pt,H_2 \,|\, H^+ \| Cl^- \,|\, Cl_2,Pt$	implying the reactions	$\tfrac{1}{2}H_2 + \tfrac{1}{2}Cl_2 \longrightarrow H^+ + Cl^-$
$Pt,H_2 \,|\, H^+ \| Cl^- \,|\, AgCl,Ag$		$\tfrac{1}{2}H_2 + AgCl \longrightarrow H^+ + Cl^- + Ag$
$Pt,H_2 \,|\, H^+ \| Fe^{++},Fe^{+++} \,|\, Pt$		$\tfrac{1}{2}H_2 + Fe^{+++} \longrightarrow H^+ + Fe^{++}$

where the electrode on the left is a *standard hydrogen electrode*.

These electromotive forces may also be called *relative electrode potentials* or, in brief, *electrode potentials*.

When, on the other hand, we speak of the electromotive forces of the half cells

$$Zn \,|\, Zn^{++}$$
$$Pt,Cl_2 \,|\, Cl^-$$
$$Ag,AgCl \,|\, Cl^-$$
$$Pt \,|\, Fe^{++},Fe^{+++}$$

we mean the electromotive forces of the cells

$Zn \,|\, Zn^{++} \| H^+ \,|\, H_2,Pt$		$\tfrac{1}{2}Zn + H^+ \longrightarrow \tfrac{1}{2}Zn^{++} + \tfrac{1}{2}H_2$
$Pt,Cl_2 \,|\, Cl^- \| H^+ \,|\, H_2,Pt$	implying the reactions	$Cl^- + H^+ \longrightarrow \tfrac{1}{2}Cl_2 + \tfrac{1}{2}H_2$
$Ag,AgCl \,|\, Cl^- \| H^+ \,|\, H_2,Pt$		$Ag + Cl^- + H^+ \longrightarrow AgCl + \tfrac{1}{2}H_2$
$Pt \,|\, Fe^{++},Fe^{+++} \| H^+ \,|\, H_2,Pt$		$Fe^{++} + H^+ \longrightarrow Fe^{+++} + \tfrac{1}{2}H_2$

where the electrode on the right is a *standard hydrogen electrode*.

These electromotive forces should NOT be called electrode potentials.

THE QUANTITY pH

Paris, 1957

pH has been defined on an experimental basis in a number of papers in the *Journal of Research of the United States National Bureau of Standards* and in the British Standards Institute's Standard 1647 (1950). The Commission notes that these alternative definitions are equivalent for all (or almost all) practical purposes. The Commission recommends that these definitions of pH (printed in roman type) be accepted internationally.

SYMBOLS AND USAGES IN PHYSICAL CHEMISTRY

The recommendations on the following pages are mainly those agreed upon in Amsterdam (1949), with modifications which subsequent discussions in the Commission have made desirable. The Commission refers to the report of 1949 concerning the history and concerning the agreement with recommendations from related bodies, especially the Symbols, Units and Nomenclature Commission of IUPAP.

Referring to section III below, the Commission has found it desirable, however, to quote two paragraphs from the Introduction to the report of 1949.

"It is recognized that recommendations by an international body must involve compromises and will sometimes have to include alternative usages for particular quantities from which the various national organizations can select those most closely in accord with their established practices. The proposals now made are not therefore intended to prescribe rigidly usages that should be universally adopted, but to give guidance in seeking a wider measure of international agreement and warning of instances where existing diversities may cause misunderstandings."

"Even among chemists in different countries, or belonging to different schools, complete agreement has not been attained on the use of symbols for certain quantities and in a few instances it may be necessary, at least temporarily, to agree to disagree and to say so."

I. Numbers and Mathematical Operations

Numbers should be printed in roman figures, with a period or comma only separating whole numbers from the decimals. To facilitate reading of long numbers the figures may be grouped together in threes without using commas or periods to separate the groups.

◆ *Chemical Abstracts* prefers the use of the comma when there are five or more figures, *e.g.*, 53,122. In some countries a comma is used instead of a period for the decimal point, hence the recommendation for the use of spaces in an international system.

Symbols for mathematical operations should be printed in roman type.

II. Abbreviations for Words

◆ General agreement at an international level on abbreviations is difficult to attain. Slight variations seem relatively unimportant in view of other language differences. Periods or no periods after abbreviations is a matter for editorial discretion. A *Chemical Abstracts* approved list of abbreviations is published in each annual Subject Index and in the "Directions for Abstractors and Section Editors of Chemical Abstracts." *Chemical Abstracts* uses periods after abbreviations in order to standardize on unambiguous forms, thus m. (meter), l. (liter), sec. (second), min. (minute), hr. (hour), g. (gram), (ton, dyne, bar) (not abbreviated), j. (joule), w. (watt), cal. (calorie), °C., °F., °K., amp. (ampere), v. (volt), f. (farad). *Chemical Abstracts* prefers italic *M* (for molar concentration) and *N* (for normal concentration).

To be printed in roman type.
Abbreviations for the Names of Units.—Abbreviations for units named after persons begin with a capital letter. Single capital letters used as abbreviations may be printed in smaller type than is used in the body of the text, but practice in this varies and no recommendation is made.

meter	m	degree Celsius*	°C
micron	μ	degree Fahrenheit*	°F
ångström	Å	degree Kelvin*	°K
liter	l	lumen	lm
second	s	lux	lx
minute	min	stilb	sb
hour	h	candela	cd
hertz	Hz	coulomb	C
gram	g	ampère	A
ton	t	volt	V
dyne	dyn	ohm	Ω
newton	N	farad	F
bar	b	henry	H
poise	P	molal (concentration)ᵇ	m
joule	J	molar (concentration)ᵇ	M
watt	W	normal (concentration)ᵇ	N
calorie	cal	formal (concentration)ᵇ	F

Prefixes to abbreviations for the names of units indicating:

Multiples			Sub-multiples		
tera	10^{12}	T	deci	10^{-1}	d
giga	10^{9}	G	centi	10^{-2}	c
mega	10^{6}	M	milli	10^{-3}	m
kilo	10^{3}	k	micro	10^{-6}	μ
			nano	10^{-9}	n
			pico	10^{-12}	p

* The ° sign and the letter following form *one symbol* and there should be no space between them, *e.g.*, 25°C or 25 °C but *not* 25° C. ᵇ Used only when preceded by numerals to indicate the magnitude of a concentration in the specified terms and not as symbols for concentrations in equations.

Abbreviations for Other Words.—These will vary with the language used and no attempt is therefore made to secure uniformity of practice at an international level.

III. Symbols for Physical and Chemical Quantities

Symbols for physical and chemical quantities, in contrast to abbreviations for units, should be printed in italic type whenever these symbols are letters of the Latin alphabet and if practicable when they are letters of the Greek alphabet.

A bold-face italic type may be used to represent certain specified physical constants or conversion factors.

Symbols separated by commas represent equivalent recommendations.

Symbols preceded by three dots are alternatives to be used only when there is some reason for not using a symbol before the three dots.

Space, time, mass and related quantities

1	length	l
2	height	h
3	radius	r
4	diameter	d
5	path, length of arc	s
6	plane angle	$\alpha, \beta, \gamma, \theta, \varphi, \psi$
7	solid angle	ω
8	area	A, S
9	volume	$V \ldots v$
10	specific volume	v
11	wave length	λ
12	wave number	σ, ν
13	time	t
14	period or other characteristic interval	T, τ
15	frequency	ν, f
16	angular frequency $(2\pi\nu)$	ω
17	velocity	$v \ldots u, w$
18	angular velocity	ω
19	acceleration	a
20	acceleration of free fall	g
21	mass	m
22	moment of inertia	I
23	density	ρ
24	relative density	d

Molecular and related quantities

101	molecular mass	m
102	molar mass	M
103	Avogadro's number	N_0, L, N
104	number of molecules	N
105	number of moles	n
106	mole fraction	$x \ldots X, y$
107	molality	m
108	concentration	c
109	molar concentration of substance B	$c_B, [B], c(B)$
110	molecular concentration	C
111	partition function	Q
112	statistical weight	$g \ldots p$
113	symmetry number	σ
114	characteristic temperature	Θ
115	diameter of molecule	$\sigma \ldots D$
116	mean free path	l
117	diffusion coefficient	D
118	osmotic pressure	Π
119	surface concentration	Γ

Mechanical and related quantities

201	force	F
202	force due to gravity (weight)	$G \ldots W$
203	moment of force	M
204	power	P
205	pressure	p, P

206	traction	σ
207	shear stress	τ
208	modulus of elasticity	E
209	shear modulus	G
210	compressibility	κ
211	compression modulus $(1/\kappa)$	K
212	viscosity	η
213	fluidity	φ
214	kinematic viscosity	ν
215	friction coefficient	f
216	surface tension	$\gamma \ldots \sigma$
217	angle of contact	θ

Thermodynamic and related quantities

301	temperature	$\theta \ldots t$
302	temperature, absolute	T
303	gas constant	$R, \boldsymbol{R}$
304	Boltzmann constant	$k, \boldsymbol{k}$
305	heat	q, Q
306	work	w, A

		a	b
307	energy (Gibbs ϵ)	$U \ldots E$	$E \ldots U$

^{a} Recommended by IUPAP (without$\ldots E$), European practice. ^{b} American practice.

308	entropy (Gibbs η)	S	S
309	Helmholtz free energy (Gibbs ψ)	F	A
310	enthalpy (Gibbs χ)	H	H
311	Gibbs function (ζ)	G	$G \ldots F$

◆ American practice is $F \ldots G$, the opposite of the listing shown.

312	heat capacity	C
313	specific heats	c_p, c_v
314	ratio c_p/c_v	γ, κ
315	chemical potential	μ
316	activity, absolute	λ
317	activity (relative)	a
318	activity coefficient	f, γ
319	osmotic coefficient	g, φ
320	thermal conductivity	λ
321	Joule-Thomson coefficient	μ

Chemical reactions

401	stoichiometric number of molecules (negative for reactants, positive for products)	ν
402	standard equation of chemical reaction	$\Sigma \nu_B B = 0$
403	affinity $(-\Sigma \nu_B \mu_B)$ of a reaction	A
404	equilibrium constant	K
405	equilibrium quotient or equilibrium product (of molalities)	Q
406	extent of reaction ($dn_B = \nu_B d\xi$)	ξ
407	degree of reaction (e.g., degree of dissociation)	α
408	rate constant	k
409	collision number (collisions per unit volume and unit time)	Z
410	rate constant corresponding to the rate Z	z
411	rate of reaction	$v \ldots r, s, J$

Light

501	Planck's constant	$h, \boldsymbol{h}$
502	Planck's constant divided by 2π	$\hbar$
503	quantity of light	Q
504	radiant power, flux of light (dQ/dt)	Φ
505	luminous intensity $(d\Phi/d\omega)$	I
506	illumination $(d\Phi/dS)$	E
507	luminance	L, B
508	luminous emittance	H
509	absorption factor (fraction of incident radiant power which is absorbed)	α
510	reflection factor (fraction of incident radiant power which is reflected)	ρ
511	transmission factor (fraction of incident radiant power which is transmitted)	τ
512	transmittance $(T = I/I_0)$	T
513	absorption (extinction) coefficient $(\kappa lc = \ln (1/T))$	κ
514	absorbance (extinction) $(A = \log_{10} (1/T))$	$A \ldots E$
515	absorptivity (specific absorbance) (decadic absorption or extinction coefficient)	a
516	molar absorptivity (molar decadic absorption or extinction coefficient) $(\epsilon lc = A)$	ϵ
517	refraction index	n
518	refractivity	r
519	angle of optical rotation	α

Electricity and magnetism

601	elementary charge	$e, \boldsymbol{e}$
602	quantity of electricity	Q
603	charge density	ρ
604	surface charge density	σ
605	electric current	$I \ldots i$
606	electric current density	J
607	electric potential	V
608	electric field strength	E
609	electric displacement	D
610	electrokinetic potential	ζ
611	capacity	C
612	permittivity (dielectric constant)	ϵ
613	dielectric polarization	P
614	dipole moment	μ
615	electric polarizability of a molecule	α, γ
616	magnetic field strength	H
617	magnetic induction	B
618	magnetic permeability	μ
619	magnetization	M
620	magnetic susceptibility	χ
621	resistance	R
622	resistivity	ρ
623	self inductance	L
624	mutual inductance	M, L_{12}
625	reactance	X
626	impedance	Z
627	admittance	Y

Electrochemistry

701 Faraday's constant (the faraday) $F, \mathbf{F}$
702 charge number of an ion, plus or minus z
703 degree of electrolytic dissociation α
704 ionic strength $I \ldots \mu$
705 electrolytic conductivity (specific conductance) κ
706 equivalent or molar conductance of electrolyte or ion Λ
707 transport number t, T
708 electromotive force E
709 overpotential η

IV. Symbols for Subsidiary Quantities

It is much more difficult to make detailed recommendations on symbols for subsidiary quantities than on symbols for the principal quantities. 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

$$A_{NO_3}\text{- and } H_{25°C}$$
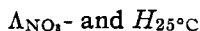
The problem is vastly reduced if it is recognized that two different kinds of notation are required for two different purposes. In the formulation of general fundamental relations the most important requirement is a notation easy to understand and easy to remember. In applications to particular cases, 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 already is accepted to some extent in the case of concentration. The best notation for formulating the laws of homogeneous chemical equilibrium is something such as

$$A + \ldots \rightleftharpoons L + \ldots$$
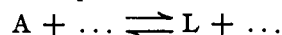
$$\frac{c_L \cdots}{c_A \cdots} = K_c$$

$$\frac{m_L \cdots}{m_A \cdots} = K_m$$

but when we turn to a particular example it is better to use a notation such as

$$Br_2 + H_2O \rightleftharpoons HOBr + H^+ + Br^-$$

$$\frac{[HOBr][H^+][Br^-]}{[Br_2]} = K_c$$

$$K_c(25°C) = 6 \times 10^{-9} \text{ mole}^2 \text{ l}^{-2}$$

Once the principle of dual notation is accepted, its adaptability and usefulness become manifest in all fields of physical chemistry. It will be illustrated here by just a few examples.

The general relation between the equivalent conductance of an electrolyte and the equivalent conductance 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

$$\Lambda(\tfrac{1}{2}Mg^{++}) = 53 \ \Omega^{-1} \text{ cm}^2 \text{ equiv}^{-1} \text{ at } 25°C$$
$$\Lambda(Cl^-) = 76 \ \Omega^{-1} \text{ cm}^2 \text{ equiv}^{-1} \text{ at } 25°C$$
$$\Lambda(\tfrac{1}{2}MgCl_2) = 129 \ \Omega^{-1} \text{ cm}^2 \text{ equiv}^{-1} \text{ at } 25°C$$
$$\Lambda(MgCl_2) = 258 \ \Omega^{-1} \text{ cm}^2 \text{ mole}^{-1} \text{ at } 25°C$$

In both notations the meaning of the symbols is so obvious and so well suited to the purpose that it is hardly necessary even to define them.

Again partial quantities are most simply denoted by the use of a subscript, for example V_1 for partial volume and the general relation between the partial volumes of the two components of a binary system is written most simply

$$n_1 \, dV_1 + n_2 \, dV_2 = 0 \qquad (T, P \text{ const.})$$

and this relation holds whether the partial volumes V_1, V_2 are expressed per mole or per gram or per kilogram according as the quantities n_1, n_2 are measured in moles or grams or kilograms. When it is desired to emphasize the contrast between partial quantities, which are intensive, and the extensive properties from which they are derived, this may be achieved either by use of a bar over the symbol or by use of the corresponding lower case letter. Thus in these notations

$$n_1 \, d\bar{V}_1 + n_2 \, d\bar{V}_2 = 0 \qquad (T, P \text{ const.})$$
$$n_1 \, dv_1 + n_2 \, dv_2 = 0 \qquad (T, P \text{ const.})$$

◆ In journals of the American Chemical Society partial molal quantities are indicated almost exclusively by an italic letter surmounted by a bar, e.g., $\bar{V}$. V_1 and V_2 are not regarded as adequate.

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

$$V(K_2SO_4, \text{ aq., } 0.1 \text{ M, } 25°C) = 48 \text{ ml mole}^{-1}$$
$$= 24 \text{ ml equiv}^{-1}$$
$$= 0.27 \text{ ml g}^{-1}$$

Each kind of notation is appropriate to its purpose.

Incidentally the notation for extensive and partial quantities need not be restricted to purely thermodynamic quantities but is also appropriate to such quantities as refraction. Thus if we define the refraction R (an extensive property) by

$$R = \frac{n^2 - 1}{n^2 + 2} V$$

then it becomes natural to denote the derived partial refractivity by R_i or $\bar{R}_i$ or r_i.

A last example will be given relating to optical rotation. The relations between the angle α of rotation of the plane of polarization and the total number n of moles or N of molecules in the path of a light beam of cross-section A can be clearly expressed in the form

$$\alpha = \frac{n}{A} \alpha_n = \frac{N}{A} \alpha_N$$

where α_n is the molar optical rotatory power and α_N the molecular optical rotatory power (a molecular cross-sectional area). When on the other hand it is desired to record an experimental measurement, an appropriate notation would be

$$\alpha(5900 \text{ Å, } 25°C, \text{ D-sucrose,}$$
$$\text{aq., } 10 \text{ g/l, } 10 \text{ cm}) = \ldots °$$

These superscripts are recommended:

    $\cdot$ = pure substance
    ∞ = infinite dilution
    id = ideal
    $\ominus$ = standard in general
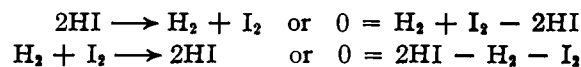   † = pressure independent term

The superscript⁰ is not specifically recommended because it has been used with several meanings.

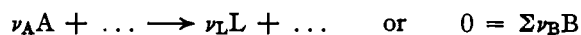## SYMBOLS IN REACTION KINETICS

Paris, 1957

The Commission decided to recommend:

(a) Each reaction should be represented by a formulation which may be written in either of two forms

$$2HI \longrightarrow H_2 + I_2 \quad \text{or} \quad 0 = H_2 + I_2 - 2HI$$
$$H_2 + I_2 \longrightarrow 2HI \quad \text{or} \quad 0 = 2HI - H_2 - I_2$$

and in general

$$\nu_A A + \ldots \longrightarrow \nu_L L + \ldots \quad \text{or} \quad 0 = \Sigma \nu_B B$$

where ν_A, ν_L, ν_B are integral stoichiometric numbers. ν_B is negative for reactants, positive for products.

The rate of reaction is then defined by

$$v = \frac{1}{\nu_B} \frac{d[B]}{dt}$$

where [B] denotes the concentrations of *any* of the substances, either reactant or product.

(b) If *experimentally*

$$v \propto [Q]^q [R]^r$$

then the reaction is described as of order q with respect to Q and of order r with respect to R.

(c) *Elementary* processes should be labeled in such a manner that reverse processes are immediately recognizable, for example, either 2 and -2, or $3 \rightarrow 5$ and $5 \rightarrow 3$.

(d) *Elementary* processes are called unimolecular, bimolecular, trimolecular according to the number of molecules involved.

(e) The collision number defined as the number of collisions per unit time and per unit volume is a rate and should be denoted by Z.

The collision number divided by the product of the two relevant concentrations (or by the square of the relevant concentration) is a second-order rate constant and should be denoted by z.

NOTE BY THE CHAIRMAN, OCTOBER, 1958.—Some of these recommendations, particularly (b), may be subject to later revision.