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PROVISIONAL

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CLINICAL CHEMISTRY DIVISION

COMMISSION ON QUANTITIES AND UNITS IN CLINICAL CHEMISTRY*

in conjunction with

INTERNATIONAL FEDERATION OF CLINICAL CHEMISTRY

EXPERT PANEL ON pH AND BLOOD GASES†

PHYSICOCHEMICAL QUANTITIES AND UNITS IN CLINICAL CHEMISTRY WITH SPECIAL EMPHASIS ON ACTIVITIES AND ACTIVITY COEFFICIENTS

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Comments on these recommendations are welcome and should be sent within 8 months from August 1981 to:

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Comments from the viewpoint of languages other than English are especially encouraged. These may have special significance regarding the publication in various countries of translations of the nomenclature eventually approved by IUPAC.

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Contents

1. Introduction

1.1. In 1976, the Committee on Standards (since 1979 the Scientific Committee) of the International Federation of Clinical Chemistry established the Expert Panel on pH and Blood Gases. Among its terms of reference is the preparation of recommendations on quantities and units for the components H^+, CO_2, and O_2. The present document has been worked out in collaboration with the IUPAC Commission on Quantities and Units in Clinical Chemistry, which has previously published general recommendations on quantities and units in clinical chemistry (7.9).

1.2. The quantities mentioned in the subsequent paragraphs are all defined and described in more detail in the Appendices. The list of quantities and units (6.1) has a similar format as the authoritative documents, ISO-31, from Technical Committee 12 of the International Organization for Standardization (7.8). The purpose of this list is to make the explicit definitions of the various kinds of activities and activity coefficients available to clinical chemists who are using ion-selective electrodes or certain other physico-chemical analytical techniques.

1.3. The number of different kinds of quantities is very large. This is partly due to a considerable redundancy among the different kinds of quantities, e.g. the similarity of the quantities substance fraction, substance concentration, and molality, which lead, for instance, to three different activity scales and three different activity coefficients for solute B in a solution.

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Data reduction is essential in practical clinical work. It is therefore necessary to try to reduce the number of different kinds of quantities that are employed in practical clinical work as much as possible and try to select those quantities that are of significant clinical value.

So a selection has been made among the many alternative ways of indicating the chemical potential of a component in a system (6.4) and those quantities preferred for clinical use have been indicated by an asterisk. Other quantities listed in the Appendices (e.g. activity coefficients, solubility coefficients, osmotic coefficients, etc.) are primarily of interest in the clinical chemical laboratory for purposes of calculation.

2. The extensive and the intensive chemical quantities

2.1. The physico-chemical description of a component in a chemical system is based on two fundamental groups of quantities:

(1) An extensive quantity (or capacity factor): the amount of substance of the component added or removed in the process of formation of the system, positive when added, negative when removed. This quantity is sometimes called the stoichiometric amount of substance of the component in the system, symbol n_0.

(2) An intensive quantity (or intensity factor): the chemical potential of the component in the system, symbol μ.

These chemical quantities are analogous to the spatial quantities, volume and pressure; the thermal quantities, entropy and temperature; the electrical quantities, electric charge and electric potential. The products of the extensive and the intensive quantities all represent energy: chemical energy, spatial energy, thermal energy (heat), and electrical energy, respectively.

2.2. The stoichiometric amount of substance of the component (B) in the system (S) is usually divided by the volume of the system, providing the stoichiometric concentration (c_0) of the component in the system:

$$c_0\mathrm{B(S)} = \frac{n_0\mathrm{B(S)}}{V\mathrm{(S)}} \ .$$

The component added to the system may dissociate or react with other components to form a series of derived components and only a fraction of the original component may actually exist in a free form in the system.

The stoichiometric concentration of the component equals the substance concentration (c) of the component including all the derived forms (or more correctly the change in that quantity as the component is added or removed in the process of formation of the system). This can be formulated as follows:

$$c_0\mathrm{B(S)} = c\mathrm{tB(S)} - c\mathrm{tB(S_0)}$$

where tB indicates total B including free and derived forms, and $\mathrm{S_0}$ indicates the system before adding B. In many cases $c\mathrm{tB(S_0)} = 0$ but this is not the case when B is formed from the other components; for example, in a system consisting of H_2O, H^+, and Cl^-, H^+ is present in the water before any H^+ is added.

In clinical chemistry, the substance concentration is more generally employed than the stoichiometric concentration and several rules have been formulated to indicate the various derived forms of the component, e.g. mixtures of a defined chemical component and its derivatives may be denoted by the plural form of the name of the pure unchanged substance, or to indicate the sum of components specified in individual quantities the specification "total" may be employed (7.5). Examples of such quantity names are given in 6.3.

2.3. The chemical potential of a component in a system is defined as the differential change in internal energy (U) divided by the differential change in the stoichiometric amount of substance of the component, maintaining other independent variables constant, i.e. volume (V), entropy (S), electric charge (Q), and stoichiometric amount of other components (B_2, B_3, etc):

$$\mu\mathrm{B}_1(\mathrm{S}) = \left(\frac{\partial U}{\partial n_0\mathrm{B}_1}\right)_{V,S,\ Q,n_0\mathrm{B}_2,n_0\mathrm{B}_3,\mathrm{etc.}}$$

The chemical potential is generally converted to an exponential function, the absolute chemical activity (λ):

$$\lambda\mathrm{B}(\mathrm{S}) = \exp\frac{\mu\mathrm{B}(\mathrm{S})}{R \cdot T}.$$

Chemical activity can only be measured relative to a standard state, for example relative concentrational activity (a_c):

$$a_c\mathrm{B}(\mathrm{S}) = \frac{\lambda\mathrm{B}(\mathrm{S})}{\lambda\mathrm{B}(\mathrm{S}_c^{\ominus})},$$

where $\mathrm{S}_c^{\ominus}$ is an ideal solution with $c\mathrm{B}(\mathrm{S}_c^{\ominus}) = 1$ mol/l.

The concentrational activity may be divided by the concentrational activity coefficient (y) to provide the substance concentration of the component in the free unbound form:

$$c\mathrm{B}(\mathrm{S}) = \frac{a_c\mathrm{B}(\mathrm{S})}{y\mathrm{B}(\mathrm{S})}\ \mathrm{mol/l}.$$

The general practice in clinical chemistry is to report the substance concentration of the (free) component rather than the chemical activity. Exceptions from this rule are the intensive quantities related to the following components:
(1) hydrogen ions, where the intensive quantity is described in terms of pH;
(2) the blood gases (CO_2 and O_2) which are described in terms of the partial pressure;
(3) water, which is described in terms of the osmolality or the osmotic concentration.
These and related quantities are listed in 6.4 and are discussed in the following.

3. pH and the active substance concentration of hydrogen ions

3.1. The quantity pH is defined as the negative decadic logarithm of the molal activity of hydrogen ions:

$$\mathrm{pH} \overset{\mathrm{def}}{=} -\lg a_m\mathrm{H}^+ = -\lg(\gamma\mathrm{H}^+ \cdot m\mathrm{H}^+/\mathrm{mol}\cdot\mathrm{kg}^{-1}) = -R\cdot T\cdot\ln 10\cdot\mu_m^{\ominus}\mathrm{H}^+ ,$$

where a_m is molal activity, γ is molal activity coefficient, and m is molality. The definition is traditionally based on molality rather than substance concentration (7.1). pH is linearly related to the standard molal chemical potential of hydrogen ion ($\mu_m^{\ominus}\mathrm{H}^+$).

3.2. Chemical potential or activity of *ions* cannot be determined on purely thermodynamical basis. This is due to the fact that the effects of an ion cannot be separated from the effects of the accompanying counter-ion, or in other terms, the electro-chemical potential of the ion cannot be separated into the chemical and the electrical component. Such a separation must necessarily be based on a non-thermodynamic convention.

The present convention is based on the assumption that the molal activity coefficient of the chloride ion in dilute aqueous solutions can be estimated by means of the *Debye-Hückel equation*:

$$-\lg\gamma = \frac{A\cdot z^2\cdot\sqrt{I/\mathrm{mol}\cdot\mathrm{kg}^{-1}}}{1+\mathring{a}\cdot B\cdot\sqrt{I/\mathrm{mol}\cdot\mathrm{kg}^{-1}}} ,$$

where I is ionic strength, z is charge number of the ion, $\mathring{a}$ is ion size parameter, A and B are temperature dependent constants.

According to the *Bates-Guggenheim convention* $\mathring{a}\mathrm{Cl}^-\cdot B$ is taken to be 1.5 at all temperatures (7.1).

3.3. The definitive method for pH measurement in dilute aqueous solutions is based on measuring the electromotive force (E) of a cell without a liquid-liquid junction (without transference):

$\mathrm{Ag(s)}$ | $\mathrm{AgCl(s)}$ | dilute aqueous solution with added Cl^- | $\mathrm{H_2(g,\ 101{,}325\ kPa)}$ | $\mathrm{Pt(s)}$

The calculation function is:

$$\mathrm{pH} = \frac{-E - E^{\ominus}}{R\cdot T\cdot\ln 10}\cdot F + \lg(m\mathrm{Cl}^-/\mathrm{mol}\cdot\mathrm{kg}^{-1}) + \lg\gamma\mathrm{Cl}^- .$$

$E^{\ominus}$ is the standard electrode potential of the Ag/AgCl half cell ($E^{\ominus} = 0{,}21423$ V at 37°C). $m\mathrm{Cl}^-$ is measured and $\gamma\mathrm{Cl}^-$ is calculated from the equation in 3.2. NaCl is added in different amounts and the results are extrapolated linearly to zero molality of added NaCl.

The definitive method is employed for determining the pH in a series of primary aqueous calibration solutions, the so-called NBS-buffers (National Bureau of Standards, U.S.A.) (7.1, 7.3).

Note:

The standard electrode potential ($E^\ominus$) of the Ag/AgCl half cell is defined as the potential of the cell:

$$\begin{array}{l|l|c|l|l} \text{Pt} & H_2(\text{g, } 101{,}325 \text{ kPa}) & \text{aqueous solution of HCl} & \text{AgCl} & \text{Ag} \\ \text{(s)} & ' & a_m\text{HCl} = 1 & \text{(s)} & \text{(s)} \end{array}$$

The cell potential (E) as a function of the molal activity of HCl is given by the Nernst equation:

$$E = E^\ominus - \frac{R \cdot T}{F} \cdot \ln a_m\text{HCl} .$$

We introduce

$$a_m\text{HCl} = (a_{m\pm})^2 = \left(\gamma_\pm \cdot \frac{m\text{HCl}}{\text{mol/kg}}\right)^2 ,$$

where $a_{m\pm}$ is the geometric mean ion activity and $\gamma_\pm$ is the geometric mean ionic activity coefficient and mHCl is the stoichiometric molality of HCl.

According to the Debye-Hückel theory, in dilute aqueous solutions of a one-one electrolyte $-\ln \gamma_\pm = A \cdot \sqrt{m}/\text{mol/kg})$ where A is a constant.

Therefore

$$E + \frac{2 \cdot R \cdot T}{F} \cdot \ln \frac{m\text{HCl}}{\text{mol/kg}} = E^\ominus + \frac{2 \cdot R \cdot T \cdot A}{F} \cdot \sqrt{\frac{m\text{HCl}}{\text{mol/kg}}} .$$

If the quantity on the left is plotted against $\sqrt{m\text{HCl}/(\text{mol/kg})}$, and extrapolated back to $m = 0$, the intercept at $m = 0$ gives the value of $E^\ominus$. In practice an extended form of the Debye-Hückel theory is often used to give a somewhat better extrapolation function.

3.4. The reference method for inorganic aqueous solutions is based on a cell with a liquid-liquid junction:

$$\begin{array}{l|l}\text{Reference electrode} & \text{concentrated} \\ & \text{KCl solution} \\ & (m > 3{,}5 \text{ mol/kg}) \end{array} \begin{array}{c} \vdots\vdots \\ \vdots\vdots \\ \vdots\vdots \end{array} \text{solution X} \mid H_2(\text{g}) \mid \text{Pt(s)}$$

The calculation function is:

$$\text{pH(X)} = \text{pH(S)} - \frac{E(\text{X}) - E(\text{S})}{R \cdot T \cdot \ln 10/F} ,$$

where S is one of the calibration solutions mentioned in 3.3. This equation is generally called the "operational" pH definition (7.14).

The reference method is subject to a small variable bias due to a possible difference between the liquid junction potential for the calibration solution and the unknown solution.

The hydrogen gas electrode is unsuitable for biological fluids where the reference method must be based on the glass electrode. The reference method for pH measurement in blood will be described in more detail in a subsequent document.

3.5. In order to draw analogy to the way in which other quantities are reported in clinical chemistry it has often been suggested to report the substance concentration of hydrogen ion rather than pH. However, in view of the international agreement concerning the pH scale and the reference method for pH measurement (7.14) we recommend to continue to use the quantity pH also in clinical chemistry.

The substance concentration of H^+ is often calculated erroneously as the antilogarithm of the negative pH value, without taking the activity coefficient of the hydrogen ions into account. If a quantity with the same unit (mol/l) as substance concentration of H^+ is warranted, we recommend to report the *active* substance concentration ($\tilde{c}$) of the hydrogen ions, calculated as

$$\tilde{c}H^+ = 10^{-pH} \cdot \rho(H_2O) \cdot mol \cdot kg^{-1} ,$$

where $\rho(H_2O)$ is the mass density of pure water (= 0.993 kg/l at 37°C). For example, pH = 7.40 (as measured with a pH-electrode); the active substance concentration of hydrogen ion is then: $\tilde{c}H^+ = 10^{-7.40} \cdot (0{,}993 \cdot kg \cdot l^{-1}) \cdot mol \cdot kg^{-1} = 39{,}81 \times 10^{-9} \times 0{,}993 \cdot mol \cdot l^{-1} = 39{,}53$ nmol/l. For many practical purposes the mass density of pure water may be taken to be 1,00 kg/l in which case the following approximation applies:

$$\tilde{c}H^+ = 10^{-pH} \cdot mol \cdot l^{-1} .$$

3.6. The pH concept should not be generalized to other ions measured by means of ion-selective electrodes (e.g. Na^+, K^+, Ca^{2+}) or to other components in general.

Ion-selective electrodes should be calibrated in a manner analogous to pH electrodes, i.e. on the basis of molal activity (a_m). However, for clinical chemical purposes the results should be reported as the substance concentration of the (free) ion and calculated by means of the appropriate activity coefficient (y), e.g. for Ca^{2+}:

$$cCa^{2+} = a_m Ca^{2+} \cdot \rho(H_2O) \cdot (yCa^{2+})^{-1} \cdot mol \cdot kg^{-1} .$$

For example, molal activity of calcium ion: $a_m Ca^{2+} = 0{,}36 \times 10^{-3}$ (as measured with a Ca^{2+}-electrode) and concentrational activity coefficient of calcium ion: $yCa^{2+} = 0.3$ (estimated for ionic strength = 0,16 mol/kg) provide a substance concentration of free calcium ion:

$$cCa^{2+} = 0{,}36 \times 10^{-3} \cdot (0{,}993 \cdot kg \cdot l^{-1}) \times 0{,}3^{-1} \cdot mol \cdot kg^{-1} = 1{,}19 \text{ mmol/l} .$$

3.7. It has been suggested to use the unit bel for the pH quantity in order to "flag" that the pH value represents the negative *decadic logarithm* of another quantity (7.13). We recommend to restrict the use of the bel (or decibel) to an amplitude or power level difference (7.8).

The pH quantity is dimensionless and consequently has the unit one (1). Example: pH = 7,40, *not* pH = 7,40 pH units, and *not* pH = 7,40 bel.

3.8. It has been claimed that the mean value of a series of pH values should be calculated as the negative logarithm of the mean value of the corresponding hydrogen ion activities: $\langle pH \rangle = -lg(\Sigma \text{ antilg } pH_i)/N)$.

We recommend to use the arithmetic mean of the pH values: $\langle pH \rangle = (\Sigma\ pH_i)/N$. The arithmetic mean is directly proportional to the mean value of the chemical potentials and it represents the geometric mean of the corresponding chemical activities. The "mean ionic activity" of an electrolyte solution is in fact defined as the geometric mean of the individual ion activities.

4. The partial pressure of gases in solution

4.1. Partial pressure (p) of a component (B) in a gas mixture (G) is defined as the substance fraction (x) of the component times the pressure of the gas mixture:

$$p\text{B(G)} = x\text{B(G)} \cdot p\text{(G)} \ .$$

Partial pressure is a kind of quantity which strictly speaking only applies to a component in a gas mixture. When applied to gases in liquid solution (S) we recommend to interpret the quantity as being equal to the partial pressure in an *ideal* gas mixture in equilibrium with the solution, or alternatively, as being equal to the fugacity ($\tilde{p}$) in a *real* gas mixture in equilibrium with the solution:

$$p\text{B(S)} = p\text{B}(\text{G}_{\text{ideal}}|\text{S}) = \tilde{p}\,\text{B}(\text{G}_{\text{real}}|\text{S}) \ .$$

Fugacity ($\tilde{p}$) of a component in a gas mixture is defined as the fugacity coefficient (g) for the component times the partial pressure:

$$\tilde{p}\,\text{B(G)} = g\text{B(G)} \cdot p\text{B(G)} \ .$$

Therefore the unit of fugacity is the same as the unit of pressure.

4.2. The partial pressure (fugacity) of a solute (B) in a solution is directly proportional to the rational chemical activity (a_x) of the solute. This relationship is called Henry's law:

$$p\text{B(S)} = \frac{1}{\tilde{\alpha}_x\text{B(S)}} \cdot a_x\text{B(S)} \ .$$

$\tilde{\alpha}_x$B(S) is the ideal rational solubility coefficient, the reciprocal of which is called the Henry law constant.

For the solvent (A) the relationship is called Raoult's law, and the proportionality factor is the fugacity of the pure solvent $\tilde{p}\,$A(A)

$$p\text{A(S)} = \tilde{p}\,\text{A(A)} \cdot a\text{A(S)} \ .$$

4.3. The substance concentration of the component in a solution can be derived from the partial pressure by multiplication with the concentrational solubility coefficient (α_c):

$$c\text{B(S)} = \alpha_c\text{B(S)} \cdot p\text{B(S)} \ .$$

For usual clinical chemical purposes we recommend to report the blood gases (CO_2 and O_2) in terms of the partial pressure rather than the substance concentration because of the need for comparison with or evaluation of the composition of the alveolar air.

5. Osmolality and osmotic concentration

5.1. The chemical potential or the activity of water in an aqueous solution is determinative for several 'colligative' properties: water vapour pressure, osmotic pressure, freezing point depression, and boiling point elevation.

5.2. In clinical chemistry the activity (a) of the water is generally expressed in terms of osmolality $\hat{m}$, which is defined as the quotient of negative natural logarithm of the rational activity of water and molar mass (M) of water (18 g/mol):

$$\hat{m}(\mathrm{S}) = \frac{-\ln a\mathrm{H_2O(S)}}{M(\mathrm{H_2O})} .$$

The unit is mol/kg (*not* "osmol"/kg).

In order to obtain the same unit as substance concentration, we recommend to use osmotic concentration ($\hat{c}$), which equals the osmolality times the mass density (ρ) of water:

$$\hat{c}(\mathrm{S}) = \hat{m}(\mathrm{S}) \cdot \rho(\mathrm{H_2O}) .$$

As $\rho(\mathrm{H_2O}) \approx 1$ kg/l the numerical value of osmotic concentration (in mol/l) practically equals that of osmolality (in mol/kg).

5.3. The osmotic concentration (osmolarity) is generally calculated on the basis of measurement of the freezing point depression (ΔT_f) by dividing with the concentrational freezing point depression constant ($K_{\mathrm{f,c}}$), which is 1,855 K/(mol/l) for aqueous solutions:

$$\hat{c}(\mathrm{S}) = \frac{\Delta T_\mathrm{f}(\mathrm{S})}{K_{\mathrm{f,c}}(\mathrm{S})} .$$

It is generally tacitly assumed that the osmotic concentration at the temperature of freezing (of plasma or urine) equals the value at 37°C. In order to obtain the true osmotic concentration at 37°C it is necessary to calculate the value on the basis of vapor pressure ($p\mathrm{H_2O}$) measured at 37°C:

$$\hat{c}(\mathrm{S}) = \frac{-\ln(p\mathrm{H_2O(S)}/p\mathrm{H_2O(H_2O)})}{V_\mathrm{m}(\mathrm{H_2O})}$$

where $p\mathrm{H_2O(H_2O)}$ is the vapour pressure of pure water and $V_\mathrm{m}(\mathrm{H_2O})$ is the molar volume of water (18 ml/mol).

5.4. The reason for using the osmotic concentration in clinical chemistry is that this quantity can be directly compared to the sum of substance concentrations of the solutes (c Solutes), the ratio between the two quantities being the concentrational osmotic coefficient (ϕ_c), which is generally close to unity for biological fluids:

$$\hat{c}(\mathrm{S}) = \phi_c(\mathrm{S}) \cdot c\ \mathrm{Solutes(S)} .$$

In other words, for many practical purposes the osmotic concentration may be adequately estimated on the basis of measurements of the substance concentrations of the principal solutes in a solution.

6. Appendices

6.1. List of quantities and units related to the chemical potential and the chemical activity of solute and solvent in a solution, and the fugacity of a component in a gas mixture

The list contains the following columns:

6.1.1. Quantity

6.1.1.1. Name: the names refer to the kind of quantity. The full designation of a quantity also requires a specification of the system, and often the component, e.g. volume of a given system, mass concentration of a given component in a given system.

A few alternative names are given, e.g. electric charge = quantity of electricity (2.6).

Parentheses indicate a part of the name, which may be omitted if no ambiguity is introduced.

6.1.1.2. Symbol: the symbols refer to "kind of quantity" and should be italicized. An alphabetical index of the symbols is given in 6.4. As far as possible the symbols are consistent with previous recommendations.

The symbol for the quantity requires specification of system, and often of a given component e.g. mass concentration (ρ) of a given component (B) in a given system (S) may be written: $\rho_{\mathrm{B}}(\mathrm{S})$. Although ISO (7.8) and IUPAC (7.11, 7.14) recommend printing the symbol for the component (B) as a subscript, it may in many cases be printed on the line without introducing ambiguity, e.g. $\rho\mathrm{B}(\mathrm{S})$.

For system and component the symbols are always printed in roman type.

A physical system (S) may be a pure component or a mixture of components (B_i, where i is a running index number). $\mathrm{S}^{\ominus}$ is reference system, G is a gas mixture.

Notice that the word *mixture* is used when the components are all treated in the same way. The word *solution* is used when, for convenience, one of the components (A), which is called the solvent (and may itself be a mixture) is treated differently from the other components (B_i) which are called solutes (7.14).

6.1.1.3. Definition: the SI (Système International d'Unités) defines a set of base units corresponding to a set of *base kinds of quantities* which are exclusively defined in terms of a reference method of measurement. All other quantities are considered *derived quantities* which can be defined by means of an algebraic equation containing only base quantities.

An attempt has been made to order the quantities so that all definitions are based on previous quantities in the List. The equations are written in terms of the above mentioned symbols.

All the definitions in the List are consistent with definitions given in the references although sometimes slightly reformulated.

6.1.2. SI unit

6.1.2.1. Name

6.1.2.2. Symbol: the symbol for the SI unit is given and derived units are defined in terms of the SI base units.

6.1.3. Remarks

This column contains various important equations which are not considered to be definitions but which can be derived from previous definitions (with the exception of the equation for dU (∮2.1) and K_f (∮10.6). Cross references to other paragraphs of the List 6.1 are indicated by the symbol ∮.

In the present international document we prefer the decimal comma as recommended for all languages by ISO (7.8) although the decimal point is generally used in English texts.

6.1.4. References

The references given in the different paragraphs of the List indicate where the given quantity has been previously mentioned. The numbers indicate the appropriate paragraph in the reference. The absence of references in several paragraphs indicates that those quantities have not yet been defined or mentioned, neither by ISO (7.8), IUPAC (7.14), or IFCC (7.4).

6.1. List of quantities and units related to the chemical potential and the chemical activity of solute and solvent in a solution, and the fugacity of a component in a gas mixture

For explanation of the columns, see text section 6.1.

6.1	Quantity		
§	Name	Symbol	Definition
1.1	length	l	
1.2	mass	m	
1.3	time	t	
1.4	electric current	I	
1.5	thermodynamic temperature	T	
1.6	amount of substance	n	
2.1	energy	E, U	$E = m \cdot c^2$
2.2	entropy	S	$\mathrm{d}S = \mathrm{d}U/T, \mathrm{d}V = \mathrm{d}nB_i = \mathrm{d}Q = 0$
2.3	Celsius temperature	θ, t	$\theta = T - T_0, T_0 = 273{,}15\ \mathrm{K}$
2.4	volume	V	$V = l^3$
2.4.1.	(partial) molar volume of component B_1 (in system S)	V_m	$V_\mathrm{m}\mathrm{B}_1(\mathrm{S}) = \left(\frac{\partial V(\mathrm{S})}{\partial n\mathrm{B}_1(\mathrm{S})}\right)_{T,p,n\mathrm{B}_2,n\mathrm{B}_3\ldots.}$
2.5	pressure	p, P	$p = -\left(\frac{\partial U}{\partial V}\right)_{S,Q,n\mathrm{B}_i}$
2.6	electric charge; quantity of electricity	Q	$\mathrm{d}Q = I \cdot \mathrm{d}t$
2.7	electric potential; electromotive force	ϕ, V, E	$\phi = \left(\frac{\partial U}{\partial Q}\right)_{V,S,n\mathrm{B}_i}$

Unit		Remarks	References		
Name	Symbol		ISO 31 (7.8)	IUPAC Manual (7.14)	EPQUCC CQUCC (7.4)
metre	m	1. Base quantity and SI base unit	1—3.1	2.1.01	4.1
kilogram	kg	1. Base quantity and SI base unit	3—1.1	2.2.01	4.4
second	s	1. Base quantity and SI base unit	1—6.1	2.1.12	4.23
ampere	A	1. Base quantity and SI base unit	5—1.1	2.6.05	
kelvin	K	1. Base quantity and SI base unit	4—1.1	2.4.01	4.18
mole	mol	1. Base quantity and SI base unit	8—3.1	2.3.06	4.6
joule	$J = m^2 \cdot kg \cdot s^{-2}$	1. E is relativistic energy. U is preferred for internal energy 2. c = speed of light in vacuo (in this paragraph). 3. $dU = -p \cdot dV + T \cdot dS + \phi \cdot dQ + \Sigma_i \mu B_i \cdot dnB_i$	4—19.1	2.4.07	
joule per kelvin	$J/K = m^2 \cdot kg \cdot s^{-2} \cdot K^{-1}$		4—17.1	2.4.06	
degree Celsius	°C		4—2.1	2.4.02	4.19
cubic metre, litre	m^3 $l = dm^3$	1. In the present context the litre is employed as the unit for volume. 2. Conférence Générale de Poids et Mesures has adopted the capital L as an alternative symbol for litre to avoid confusion with the number 1	1—5.1	2.1.11	4.3
litre per mole	l/mol	1. The molar volume of a pure substance A is: $V_m(A) = V(A)/n(A)$. 2. $V(S) = \Sigma_i V_m B_i(S) \cdot nB_i(S)$	8—6.1	1.4	
pascal	$Pa = J \cdot m^{-3} = m^{-1} \cdot kg \cdot s^{-2}$	1. Pressure is often defined as the force perpendicular to a surface divided by the area of that surface. This gives the erroneous implication that pressure is a vector quantity. 2. The non SI unit of pressure mmHg = Torr (= 0,1333 kPa) is still widely employed in the clinical literature especially for blood pressure	3—13.1	2.2.19	4.21
coulomb	$C = s \cdot A$		5—2.1	2.6.02	
volt	$V = J \cdot C^{-1} = m^2 \cdot kg \cdot s^{-3} \cdot A^{-1}$	1. ϕ is preferred for inner electric potential, E is preferred for electromotive force. In the present context V =volume.	5—6.1	2.6.07	

List 6.1 (continued)

6.1	Quantity		
§	Name	Symbol	Definition
2.8	charge number of component B	z	$zB = QB/e$
2.9	Gibbs energy	G	$G = U + p \cdot V - T \cdot S$
2.10	(absolute) chemical potential of component B_1	μ	$\mu B_1 = \left(\frac{\partial U}{\partial nB_1}\right)_{V,S,Q,nB_2,nB_3,---}.$
2.11 ●	(absolute) electrochemical potential of component B_1	$\tilde{\mu}$	$\tilde{\mu} B_1 = \left(\frac{\partial U}{\partial nB_1}\right)_{V,S,nB_2,nB_3,---}.$
2.12	(standard) chemical potential of component B (in system S)	$\mu^{\ominus}$	$\mu^{\ominus}B(S) = \mu B(S) - \mu B(S^{\ominus})$
2.13	absolute activity of component B (in system S)	λ	$\lambda B(S) = \exp \frac{\mu B(S)}{R \cdot T}$
3.1	mass concentration of component B (in system S)	ρ	$\rho B(S) = \frac{mB(S)}{V(S)}$
3.2	(amount-of-)substance fraction; mole fraction of component B_j (in system S)	x	$xB_j(S) = \frac{nB_j(S)}{\Sigma_i nB_i(S)}$
3.2.1	saturation fraction of component B (in system S)	s, S	$sB(S) = nB(S)/nB(S, \text{sat})$
3.3	molality of solute B (in solution S)	m, b	$mB(S) = \frac{nB(S)}{mA(S)}$

Unit		Remarks	References		
Name	Symbol		ISO 31 (7.8)	IUPAC Manual (7.14)	EPQUCC CQUCC (7.4)
one	1	1. QB is the charge of one B elementary entity (molecule, ion). 2. e = elementary charge ≈ (160,21892 ± 0,00046) × 10^{-21} C.	8—41.1	2.7.02	4.4
joule	J = $m^2 \cdot kg \cdot s^{-2}$	1. $dG = V \cdot dp - S \cdot dT + \phi \cdot dQ + \Sigma \mu B_i \cdot dnB_i$	4—19.4	2.4.12	
joule per mole	J/mol $= m^2 \cdot kg \cdot s^{-2} \cdot mol^{-1}$	1. Only differences in μB can be measured (∮2.12). 2. $\mu B_1 = \left(\frac{\partial G}{\partial nB_1}\right)_{p,T,Q,nB_2,nB_3,\cdots}$ (follows from ∮∮ 2.1 and 2.9). 3. Notice: $zB_1 \ddagger 0 \Rightarrow dQ \ddagger 0$. 4. μB is proportional to the electric potential (E) of an ideal electrode for component B: $\Delta\mu B = zB \cdot F \cdot \Delta E$	8—16.1	2.4.25 A.I.1	
joule per mole	J/mol $= m^2 \cdot kg \cdot s^{-2} \cdot mol^{-1}$	1. Notice that Q is not constant. 2. Only differences in $\tilde{\mu}$B can be measured. 3. $\tilde{\mu}B(S) = \mu B(S) + zB \cdot F \cdot \phi(S)$ $F \approx (96\,484{,}56 \pm 0{,}27) \cdot C \cdot mol^{-1}$ 4. See also introductory section 3.2.		2.7.05	
joule per mole	J/mol $= m^2 \cdot kg \cdot s^{-2} \cdot mol^{-1}$	1. $S^{\ominus}$ is a standard reference system, which must be specified. 2. For the solvent A the reference system is the pure solvent, and for a component B in a mixture the reference system is generally the pure B (∮6.1.1). 3. For $\hat{a}$ solute B the reference system may be $S_x^{\ominus}$ (∮6.1.2), $S_m^{\ominus}$ (∮7.2) or $S_c^{\ominus}$ (∮7.3). 4. For a gas mixture the reference system is $G^{\ominus}$ (∮7.4).		Ref. 7.11	
one	1	1. Only the relative λB can be measured (∮∮ 6.1.1, 6.1.2, 7.2, 7.3, 7.4). 2. R = molar gas constant ≈ (8,31441 ± 0,00026) $\cdot J \cdot K^{-1} \cdot mol^{-1}$.	8—17.1	2.4.26 A.I.1	
kilogram per litre	kg/l $= 10^3 \cdot m^{-3} \cdot kg$	1. ρ is also used as symbol for mass density of a system $\rho(S) = \frac{m(S)}{V(S)}$	8—11.2	2.3.12	4.8
one	1		8—14.1	2.3.07	4.13
one	1	1. (S, sat) indicates the system saturated with B. 2. Capital S is used as the symbol of saturation fraction in the physiological literature.			
mole per kilogram	mol/kg	1. A is the solvent. 2. In the present text the m is preferred as the symbol for molality whereas m indicates mass. The symbol b is favoured by ISO/TC 12 as an alternative symbol. In clinical chemistry the symbol b is employed for catalytic activity concentration.	8—15.1	2.3.10	4.12

List 6.1 (continued)

6.1	Quantity		
§	Name	Symbol	Definition
3.4	(amount-of-)substance concentration of component B (in system S)	c	$cB(S) = \frac{nB(S)}{V(S)}$
3.5	partial pressure of component B (in gas mixture G)	p, P	$pB(G) = xB(G) \cdot p(G)$
3.6	ionic strength (of solution S)	I	$I(S) = \frac{1}{2} \cdot \Sigma_i (zB_i(S))^2 \cdot mB_i(S)$
4.1	absolute rational activity coefficient of component B (in system S)	λ_x	$\lambda_x B(S) = \frac{\lambda B(S)}{xB(S)}$
4.2	absolute molal activity coefficient of solute B (in solution S)	λ_m	$\lambda_m B(S) = \frac{\lambda B(S)}{mB(S)}$
4.3	absolute (substance-)concentrational activity coefficient of compoent B (in system S)	λ_c	$\lambda_c B(S) = \frac{\lambda B(S)}{cB(S)}$
4.4	absolute fugacity coefficient of component B (in gas mixture G)	λ_p	$\lambda_p B(G) = \frac{\lambda B(G)}{pB(G)}$
5.1.1	activity coefficient of solvent A (in solution S) or of component A (in a mixture S)	f	$fA(S) = \frac{\lambda_x A(S)}{\lim_{xA(S) \to 1} \lambda_x A(S)}$
5.1.2	rational activity coefficient of solute B (in solution S)	f_x	$f_x B(S) = \frac{\lambda_x B(S)}{\lim_{xA(S) \to 1} \lambda_x B(S)}$

Unit		Remarks	References		
Name	Symbol		ISO 31 (7.8)	IUPAC Manual (7.14)	EPQUCC CQUCC (7.4)
mole per litre	mol/l	1. From §§ 3.1, 3.3, and 3.4 follows: $cB(S) = mB(S) \cdot \rho A(S)$. 2. The symbol [B] is often employed for cB.	8—13.1	2.3.11	4.11
pascal	Pa $= m^{-1} \cdot kg \cdot s^{-2}$	1. Partial pressure applies to a component in a gas mixture; when applied to gases in liquid solution the quantity strictly speaking applies to a hypothetical ideal gas phase in equilibrium with the liquid. The name (gas) tension has been suggested for this kind of quantity, and also the name vapour pressure. See also introductory section 4.1. 2. The capital P is used as the symbol of partial pressure in the physiological literature.	8—18.1	A.I.5	4.22
mole per kilogram	mol/kg	1. Sometimes ionic strength is calculated from substance concentration (symbol I_c). It is preferable, however, always to define ionic strength on the basis of molality.	8—43.1	2.4.29	
one	1	1. This kind of quantity has not been defined in the references but it is useful for the definition of the rational activity coefficient (§5.1). 2. Only the relative $\lambda_x B$ can be measured (§ 5.1).			
kilogram per mole	kg/mol	1. This kind of quantity has not been defined in the references but it is useful for the definition of the molal activity coefficient (§5.2). 2. Only the relative $\lambda_m B$ can be measured (§ 5.2).			
litre per mole	l/mol $= 10^{-3} \cdot m^3 \cdot mol^{-1}$	1. This kind of quantity has not been defined in the references but it is useful for the definition of the concentrational activity coefficient (§ 5.3). 2. Only the relative $\lambda_c B$ can be measured (§ 5.3).			
reciprocal pascal	Pa^{-1} $= m \cdot kg^{-1} \cdot s^2$	1. This kind of quantity has not been defined in the references but it is useful for the definition of the fugacity coefficient (§ 5.4). 2. Only the relative $\lambda_p B$ can be measured (§ 5.4).			
one	1	1. $\lim_{xA(S) \to 1} fA(S) = 1$	8—20.1	2.4.31 A.I.7 A.I.14	
one	1	1. $\lim_{xA(S) \to 1} f_x B(S) = 1.$		A.I.11	

List 6.1 (continued)

6.1	Quantity		
§	Name	Symbol	Definition
5.2	molal activity coefficient of solute B (in solution S)	γ	$\gamma B(S) = \dfrac{\lambda_m B(S)}{\lim\limits_{x A(S) \to 1} \lambda_m B(S)}$
5.3	(substance)concentrational activity coefficient of solute B (in solution S)	y	$y B(S) = \dfrac{\lambda_c B(S)}{\lim\limits_{x A(S) \to 1} \lambda_c B(S)}$
5.4	fugacity coefficient of component B (in gas mixture G)	g	$g B(G) = \dfrac{\lambda_p B(G)}{\lim\limits_{p(G) \to 0} \lambda_p B(G)}$
6.1.1	(relative) activity of solvent A (in solution S) or of a component A (in a mixture S)	a	$a A(S) = f A(S) \cdot x A(S)$
6.1.2	(relative) rational activity of solute B (in solution S)	a_x	$a_x B(S) = f_x B(S) \cdot x B(S)$
6.2	active molality of solute B (in solution S)	$\tilde{m}$, $\tilde{b}$	$\tilde{m} B(S) = \gamma B(S) \cdot m B(S)$
6.3	active (substance) concentration of solute B (in solution S)	$\tilde{c}$	$\tilde{c} B(S) = y B(S) \cdot c B(S)$
6.4	fugacity; active partial pressure of component B (in gas mixture G)	f, $\tilde{p}$	$\tilde{p} B(G) = g B(G) \cdot p B(G)$

Unit	Remarks	Remarks	References		
Name	Symbol		ISO 31 (7.8)	IUPAC Manual (7.14)	EPQUCC CQUCC (7.4)
one	1	1. $\lim\limits_{xA(S)\to 1} \gamma B(S) = 1$. 2. For ions in dilute aqueous solutions ($I <$ 0.1 mol/kg) γB is a function of I according to the Debye-Hückel limiting law: $-\lg \gamma B = \dfrac{A \cdot (zB)^2 \cdot \sqrt{I/\text{mol} \cdot \text{kg}^{-1}}}{1 + B \cdot \mathring{a}B \cdot \sqrt{I/\text{mol} \cdot \text{kg}^{-1}}}$ where A and B are temperature dependent constants. $A = 0{,}5215$ and $B = 3{,}305\ \text{nm}^{-1}$ at 37° C. $\mathring{a}B$ is the ion size parameter for component B. 3. In most biological fluids γB is a more complicated empirical function of the ionic composition of the solution.	8—22.1 8—22.1	2.4.32 2.4.32	A.I.11 A.I.11
one	1	1. $\lim\limits_{xA(S)\to 1} yB(S) = 1$. 2. $yB(S) = \gamma B(S) \cdot \rho(A)/\rho A(S)$ where $\rho(A)$ is the mass density of the pure solvent. (Follows from ∮∮ 3.4, 4.2, 4.3, and 5.3).		2.4.33	
one	1	1. $\lim\limits_{p(G) \to 0} gB(G) = 1$.			A.I.6
one	1	1. $aA(S) = \lambda A(S)/\lambda A(S^{\ominus})$ where $xA(S^{\ominus}) = 1$ (follows from ∮∮ 4.1, 5.11, and 6.1.1). 2. $\lim\limits_{xA(S)\to 1} aA(S) = 1$.		2.4.30	A.I.8
one	1	1. $a_x B(S) = \lambda B(S)/\lambda B(S_x^{\ominus})$, where $f_x B(S_x^{\ominus}) \cdot xB(S_x^{\ominus}) = 1$ (follows from ∮∮ 4.1, 5.1.2, and 6.1.2).			A.I.12
mole per kilogram	mol/kg	1. This quantity has not been defined by ISO or IUPAC although it is analogous to fugacity (∮ 6.4).			
mole per litre	mol/l $= 10^3 \cdot \text{m}^{-3} \cdot$ mol	1. This quantity has not been defined by ISO or IUPAC although it is analogous to fugacity (∮ 6.4). 2. $\tilde{c}B(S) = \tilde{m}B(S) \cdot \rho(A)$ (follows from ∮∮ 3.4, 5.3, 6.2, and 6.3).			
pascal	Pa	1. Symbol $\tilde{p}$ is preferred in this context, where f = activity coefficient (∮ 5.1.1). 2. Fugacity is defined for a component in a gas mixture. When applied to gases in liquid solution the quantity strictly speaking refers to a hypothetical gas phase in equilibrium with the liquid. It follows that the partial pressure (∮ 3.5) and the fugacity of a component in a solution are identical. See also introductory section 4.1.	8—19.1	2.4.27	A.I.6

List 6.1 (continued)

6.1	Quantity		
§	Name	Symbol	Definition
7.2 *	(relative) molal activity of solute B (in solution S)	a_m	$a_m = \frac{\tilde{m}B(S)}{mol/kg}$
7.2.1	hydrogen ion exponent; pH	pH	$pH(S) = -lg\ a_m H^+(S)$
7.3	(relative) (substance-)concentrational activity of solute B (in solution S)	a_c	$a_c B(S) = \frac{\tilde{c}B(S)}{mol/l}$
7.4	(relative) baric activity of component B (in gas mixture G)	a_p	$a_p B(C) = \frac{\tilde{p}B(G)}{101{,}325\ kPa}$
8.1.	ideal rational solubility coefficient; rational activity — fugacity coefficient of component B (in solution S)	$\tilde{\alpha}_x$	$\tilde{\alpha}_x B(S) = \frac{a_x B(S)}{\tilde{p}B(G\|S)}$
8.2	ideal molal solubility coefficient; active molality — fugacity coefficient of component B (in solution S)	$\tilde{\alpha}_m$	$\tilde{\alpha}_m B(S) = \frac{\tilde{m}B(S)}{\tilde{p}B(G\|S)}$

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* 7.1 see § § 6.1.1 and 6.1.2.

Unit		Remarks	References		
Name	Symbol		ISO 31 (7.8)	IUPAC Manual (7.14)	EPQUCC CQUCC (7.4)
one	1	1. $a_m\mathrm{B(S)} = \lambda\mathrm{B(S)}/\lambda\mathrm{B}(\mathrm{S}_m^{\ominus})$, where $\tilde{m}\mathrm{B}(\mathrm{S}_m^{\ominus}) = 1$ mol/kg (follows from ∮∮ 4.2, 5.2, 6.2, and 7.2). 2. This is the activity generally employed in clinical chemistry for an ion in solution when using ion-selective electrodes.	8.21.1	A.I.12	
one	1	1. Sometimes pH is considered the name of the quantity rather than the symbol. 2. pH may be considered a special kind of quantity, or it may be considered a special type of quantity, i.e. the kind of quantity "negative decadic logarithm of molal activity" applied to the hydrogen ions. 3. The reference method for pH measurement is based on the use of a hydrogen-ion-responsive electrode, a reference electrode, and a bridge solution of concentrated KCl of a molality not less than 3,5 mol/kg. Reference solutions with known pH have been described. See also introductory section 3.		10	
one	1	1. $a_c\mathrm{B(S)} = \lambda\mathrm{B(S)}/\lambda\mathrm{B}(\mathrm{S}_c^{\ominus})$, where $\tilde{c}\mathrm{B}(\mathrm{S}_c^{\ominus}) =$ 1 mol/l. (follows from ∮∮ 4.3, 5.3, 6.3, and 7.3). 2. $a_c\mathrm{B(S)} = a_m\mathrm{B(S)} \cdot \rho(\mathrm{A})/(\mathrm{kg/l})$ (follows from ∮∮ 6.3, 7.2, and 7.3).	8—21.1	A.1.12	
one	1	1. $a_p\mathrm{B(G)} = \lambda\mathrm{B(G)}/\lambda\mathrm{B}(\mathrm{G}^{\ominus})$, where $\tilde{p}\mathrm{B}(\mathrm{G}^{\ominus}) = 101, 325$ kPa (follows from ∮∮ 4.4, 5.4, 6.4, and 7.4). 2. The fugacity $\tilde{p}\mathrm{B(G)}$ is used more generally than $a_p\mathrm{B(G)}$.			
reciprocal pascal	Pa^{-1} $= \mathrm{m} \cdot \mathrm{kg}^{-1} \cdot \mathrm{s}^2$	1. G |S means gas phase G in equilibrium with S. 2. $\tilde{\alpha}_x\mathrm{B(S)} = \lim\limits_{x\mathrm{A(S)}\to 1}(x\mathrm{B(S)}/\tilde{p}\mathrm{B(G\|S)})$ (follows from ∮∮ 4.1, 4.4, 5.1, 5.4, 6.1, 6.4). 3. For the solvent A:$\tilde{\alpha}_x\mathrm{A(S)} = 1/\tilde{p}\mathrm{A(A)}$, where $\tilde{p}\mathrm{A(A)}$ is fugacity of pure A. 4. $\tilde{\alpha}$ only depends on the type of component B and the type of solvent A, i.e. $\tilde{\alpha}_x\mathrm{B}(\mathrm{S}_1) = \tilde{\alpha}_x\mathrm{B}(\mathrm{S}_2)$ when the solvent is the same for S_1 and S_2. 5. The coefficient $(\tilde{\alpha}_x)^{-1}$ is called Henry law constant. See also introductory section 4.2.			
mole per kilogram pascal	(mol/kg)/Pa $= \mathrm{m} \cdot \mathrm{kg}^{-2} \cdot \mathrm{s}^2 \cdot \mathrm{mol}$	1. $\tilde{\alpha}_m$ only depends on the type of component and the type of solvent.			

List 6.1 (continued)

6.1	Quantity		
§	**Name**	**Symbol**	**Definition**
8.3	ideal (substance-)concentrational solubility coefficient; active concentration — fugacity coefficient of component B (in solution S)	α_c	$\tilde{\alpha}_c\mathrm{B(S)} = \dfrac{\tilde{c}\mathrm{B(S)}}{\tilde{p}\mathrm{B(G\|S)}}$
9.1	rational solubility coefficient of component B (in solution S in equilibrium with gas phase G)	α_x	$\alpha_x\mathrm{B(S\|G)} = \dfrac{x\mathrm{B(S)}}{p\mathrm{B(G)}}$
9.2	molal solubility coefficient of component B (in solution S in equilibrium with gas phase G)	α_m	$\alpha_m\mathrm{B(S\|G)} = \dfrac{m\mathrm{B(S)}}{p\mathrm{B(G)}}$
9.3	(substance-)concentrational solubility coefficient of component B (in solution S in equilibrium with gas phase G)	α_c	$\alpha_c\mathrm{B(S\|G)} = \dfrac{c\mathrm{B(S)}}{p\mathrm{B(G)}}$
10.1	osmolality (of solution S)	$\hat{m}$	$\hat{m}\mathrm{(S)} = \dfrac{-\ln a\mathrm{A(S)}}{M\mathrm{(A)}}$
10.2	molal osmotic coefficient (of solution S)	ϕ_m	$\phi_m\mathrm{(S)} = \dfrac{\hat{m}\mathrm{(S)}}{\Sigma_i m\mathrm{B}_i\mathrm{(S)}}$
10.3	osmotic concentration (of solution S)	$\hat{c}$	$\hat{c}\mathrm{(S)} = \dfrac{-\ln a\mathrm{A(S)}}{V_\mathrm{m}\mathrm{(A)}}$
10.4	concentrational osmotic coefficient (of solution S)	ϕ_c	$\phi_c\mathrm{(S)} = \dfrac{\hat{c}\mathrm{(S)}}{\Sigma_i c\mathrm{B}_i\mathrm{(S)}}$
10.5	freezing point depression (of solution S)	ΔT_f	$\Delta T_\mathrm{f}\mathrm{(S)} = T_\mathrm{f}\mathrm{(A)} - T_\mathrm{f}\mathrm{(S)}$
10.6	molal freezing point depression constant (for solution S)	K_f	$K_\mathrm{f}\mathrm{(S)} = \dfrac{\Delta T_\mathrm{f}\mathrm{(S)}}{\hat{m}\mathrm{(S)}}$

Unit		Remarks	References		
Name	Symbol		ISO 31 (7.8)	IUPAC Manual (7.14)	EPQUCC CQUCC (7.4)
mole per litre pascal	$(\mathrm{mol/l})/\mathrm{Pa} = 10^3 \cdot \mathrm{m}^{-2} \cdot \mathrm{kg}^{-1} \cdot \mathrm{s}^2 \cdot \mathrm{mol}$	1. $\tilde{\alpha}_c$ only depends on the type of component and the type of solvent.			
reciprocal pascal	$\mathrm{Pa}^{-1} = \mathrm{m} \cdot \mathrm{kg}^{-1} \cdot \mathrm{s}^2$	1. S|G means system in equilibrium with gas phase. 2. $\alpha_x B(S\|G) = \tilde{\alpha}_x B(S) \cdot g B(G)/f_x B(S)$ (follows from §§ 6.1, 6.4, 8.1, and 9.1).			
mole per kilogram pascal	$(\mathrm{mol/kg})/\mathrm{Pa} = \mathrm{m} \cdot \mathrm{kg}^{-2} \cdot \mathrm{s}^2 \cdot \mathrm{mol}$	1. $\alpha_m B(S\|G) = \tilde{\alpha}_m B(S) \cdot g B(G)/\gamma B(S)$ (follows from §§ 6.2, 6.4, 8.2 and 9.2).			
mole per litre pascal	$(\mathrm{mol/l})/\mathrm{Pa} = 10^3 \cdot \mathrm{m}^{-2} \cdot \mathrm{kg}^{-1} \cdot \mathrm{s}^2 \cdot \mathrm{mol}$	1. $\alpha_c B(S\|G) = \tilde{\alpha}_c B(S) \cdot g B(G)/\gamma B(S)$ (follows from §§ 6.3, 6.4, 8.3 and 9.3)			
mole per kilogram	mol/kg	1. $M(A)$ = molar mass of A = $m(A)/n(A)$. 2. The unit is not "osmol"/kg. 3. $pA(S) = pA(A) \cdot \exp(-\tilde{m}(S) \cdot M(A))$, where $pA(A)$ is vapour pressure of pure solvent (follows from §§ 6.1.2, 8.1, and 10.1).			
one	1	1. $\Sigma_i m B_i(S)$ is the molality of all the solutes in S. 2. $\Sigma_i m B_i(S) = \frac{xA(S)^{-1} - 1}{M(A)} \rightarrow \frac{-\ln aA(S)}{M(A)}$ for $xA(S) \rightarrow 1$ (from §§ 3.2, 3.3, 6.1.1, 10.1). 3. $\lim_{xA(S) \rightarrow 1} \phi_m(S) = 1$ 4. $\phi_m(S) = \frac{-xA(S) \cdot \ln(fA(S) \cdot xA(S))}{1 - xA(S)}$		A.I.13	
mole per litre	$\mathrm{mol/l} = 10^3 \cdot \mathrm{m}^{-3} \cdot \mathrm{mol}$	1. $V_m(A) = V(A)/n(A)$ (§2.4.1). 2. The unit is not "osmol"/l. 3. $\tilde{c}(S) = \tilde{m}(S) \cdot \rho(A)$, where $\rho(A)$ is the mass density of the solvent. (follows from §§ 10.1 and 10.3) 4. Currently called "osmolarity" because "molarity" was formerly used for substance concentration.			
one	1	1. $\phi_c(S) = \phi_m(S) \cdot \rho(A)/\rho A(S)$ (follows from §§ 10.2, 10.3, and 10.4).			
kelvin	K	1. $T_f(A)$ is the freezing point of pure solvent.			
kilogram kelvin per mole	$\mathrm{kg} \cdot \mathrm{K} \cdot \mathrm{mol}^{-1}$	1. It can be shown that K_f is related to the specific enthalpy of melting of the solvent $\Delta H_w(A)$: $K_f(S) = R \cdot T_f(A)^2/\Delta H_w(A)$. $K_f(S)$ is therefore only dependent on the type of solvent A. 2. For aqueous solutions: $K_f = 1{,}855\ \mathrm{K/(mol/kg)}$.			

List 6.1 (continued)

6.1	Quantity		
§	**Name**	**Symbol**	**Definition**
10.7	concentrational freezing point depression constant (for solution S)	$K_{f,c}$	$K_{f,c}(S) = \frac{\Delta T_f(S)}{\hat{c}(S)}$
10.8	osmotic pressure (of solution S)	Π	$-\mu^{\ominus}A(S) = \int_0^{\Pi(S)} V_m(A) \cdot dp(A)$
11.1	buffer capacity (for hydrogen ion) (in solution S)	B	$B(S) = \left(\frac{\partial nH^+(S)}{\partial \lg a_m H^+(S)}\right)_{\text{specified conditions}}$ e.g. $T, p, nB_1, \mu B_2, nB_3, \ldots$
11.2	volumic buffer capacity (for hydrogen ion); buffer value (for hydrogen ion) (in solution S)	β	$\beta(S) = \frac{B(S)}{V(S)}$
11.3	(partial) molar buffer capacity of component B (in solution S)	B_m	$B_m B(S) = \left(\frac{\partial B(S)}{\partial nB(S)}\right)_{\text{specified conditions}}$
11.4	(partial) specific buffer capacity of component B (in solution S)	B_w	$B_w B(S) = \left(\frac{\partial B(S)}{\partial mB(S)}\right)_{\text{specified conditions}}$
12.1	stoichiometric number of component B (in a chemical reaction)	ν	$0 = \Sigma_i \nu B_i \cdot B_i$

Unit		Remarks	References		
Name	Symbol		ISO 31 (7.8)	IUPAC Manual (7.14)	EPQUCC CQUCC (7.4)
litre kelvin per mole	$l \cdot K \cdot mol^{-1} = 10^{-3} \cdot m^3 \cdot K \cdot mol^{-1}$	1. $K_{f,c}(S) = K_f/\rho(A)$ (follows from §§ 10.3 and 10.6).			
pascal	$Pa = m^{-1} \cdot kg \cdot s^{-2}$	1. Π is that pressure difference between the solution (S) and the pure solvent (A) which provides the same chemical potential of the solvent in the solution and in the pure solvent. 2. $dV_m(A)/dp(A) = 0 \Rightarrow \Pi(S) = -\mu^{\ominus}A(S)/V_m(A)$, i.e. $\Pi(S) = R \cdot T \cdot \hat{c}(S)$ which is called the van't Hoff equation.	8—24.1		
mole	mol	1. $nH^+(S)$ means amount of substance of added H^+. 2. The independent variables must be specified. The quantity is different when either nB_1 or μB_1 is kept constant. If nothing is specified nB_1 is assumed constant. 3. $dnH^+ = -dn\text{Base}$ and $-\lg a_m H^+ = pH$: $B(S) = \dfrac{\partial n\text{Base}(S)}{\partial pH(S)}$. 4. The quantity has been defined for H^+ only, although similar quantities would apply for other components.			
mole per litre	$mol/l = 10^3 \cdot m^{-3} \cdot mol$	1. For $V(S)$ constant: $\beta(S) = \dfrac{\partial cH^+(S)}{\partial \lg a_m H^+(S)} = \dfrac{\partial c\text{Base}(S)}{\partial\ pH(S)}$. 2. Donald D. Van Slyke first defined this quantity. The name 'slyke' is sometimes used as an unofficial unit: 1 slyke = 1 mol/l.			
one	1	1. $B_m B(S)$ for a H^+ binding group at $pH = pK_A$ is 0,576.			
mole per kilogram	mol/kg				
one	1	1. $0 = \Sigma_i \nu B_i \cdot B_i$ symbolizes a chemical reaction. 2. The stoichiometric numbers for reactants are negative, those for products are positive.	8—26.1	11.1	2.5.01

List 6.1 (continued)

6.1	Quantity		
§	Name	Symbol	Definition
12.2	equilibrium constant (for a chemical reaction)	K_a	$K_a = \prod_i (a\mathrm{B}_i(\mathrm{S}))^{\nu\mathrm{B}i}$
12.3	molal equilibrium product (for a chemical reaction)	K_m	$K_m = \prod_i (m\mathrm{B}_i(\mathrm{S}))^{\nu\mathrm{B}i}$
12.4	concentrational equilibrium product (for a chemical reaction	K_c	$K_c = \prod_i (c\mathrm{B}_i(\mathrm{S}))^{\nu\mathrm{B}i}$
12.5	baric equilibrium product (for a chemical reaction)	K_p	$K_p = \prod_i (p\mathrm{B}_i(\mathrm{S}))^{\nu\mathrm{B}i}$

Unit		Remarks	References		
Name	Symbol		ISO 31 (7.8)	IUPAC Manual (7.14)	EPQUCC CQUCC (7.4)
one	1	1. The reaction is $0 = \Sigma_i \nu\mathrm{B}_i \cdot \mathrm{B}_i$. 2. S is an equilibrium system for the reaction. 3. The value of K_a depends on the choice of activity scale. $a\mathrm{B}_i(\mathrm{S})$ may be rational activity (a_x), molal activity (a_m), or concentrational activity (a_c) for the solutes. 4. K_a is related to the standard free energy of reaction ($\Delta G_{\mathrm{m}}^{\ominus}$) as follows: $K_a = \exp(-\Delta G_{\mathrm{m}}^{\ominus}/R \cdot T)$ where $\Delta G_{\mathrm{m}}^{\ominus} = -\Sigma_i \nu\mathrm{B}_i \cdot \mu^{\ominus}\mathrm{B}_i(\mathrm{S})$ The value of $\Delta G_{\mathrm{m}}^{\ominus}$ depends on the choice of standard states for the reactants and products.			
	$\left(\frac{\mathrm{mol}}{\mathrm{kg}}\right)^{\Sigma\nu\mathrm{B}_i}$ $\left(\frac{\mathrm{mol}}{\mathrm{l}}\right)^{\Sigma\nu\mathrm{B}_i}$ $\mathrm{Pa}^{\Sigma\nu\mathrm{B}_i}$	Often hybrid equilibrium products are employed for practical purposes, e.g. calculation of $c\mathrm{HCO}_3^-$ from pH and $p\mathrm{CO}_2$: Reaction: $\mathrm{CO}_2 + \mathrm{H}_2\mathrm{O} \rightleftharpoons \mathrm{H}^+ + \mathrm{HCO}_3^-$ $K_{\mathrm{hybrid}} = \frac{10^{-\mathrm{pH}} \cdot c\mathrm{HCO}_3^-}{p\mathrm{CO}_2}$ $K_a = \frac{a_m\mathrm{H}^+ \cdot a_m\mathrm{HCO}_3^-}{a_m\mathrm{CO}_2 \cdot a\mathrm{H}_2\mathrm{O}}$ The relationship between the two is: $K_{\mathrm{hybrid}} = K_a \cdot \tilde{\alpha}_m\mathrm{CO}_2 \cdot a\mathrm{H}_2\mathrm{O} \cdot \rho\mathrm{H}_2\mathrm{O}/\gamma\mathrm{HCO}_3^-$ K_a and $\tilde{\alpha}_m$ are temperature dependent constants. $a\mathrm{H}_2\mathrm{O}$ varies with the total concentration of solutes. $\rho\mathrm{H}_2\mathrm{O}$ varies primarily with the concentration of macromolecules (e.g. protein). $\gamma\mathrm{HCO}_3^-$ varies with the ionic composition of the solution (ionic strength).			

6.2. *Flow charts for definitions of activity coefficients and relative activity*

The flow charts illustrate the analogies and the differences between the definitions of the activity of the solvent (6.2.1) and the three different activities of a solute (6.2.2). For comparison the definition of fugacity is also illustrated (6.2.3).

A rounded box is a quantity; a square box is an equation of definition. A dotted arrow indicates an alternative way of defining a quantity.

The quantities in the left column can only be measured relative to a reference quantity: chemical potential μ; absolute activity λ; absolute activity coefficients λ_x, λ_m, λ_c, λ_p.

The quantities in the right column are relative quantities which can be directly measured: activity coefficients f, f_x, γ, y, and fugacity coefficient g; active molality $\tilde{m}$, active substance concentration $\tilde{c}$, fugacity $\tilde{p}$; relative activity a, a_x, a_m, a_c; and standard chemical potential $\mu^{\ominus}$.

6.2.1. *Relative activity of a solvent in a solution or a component in a mixture*

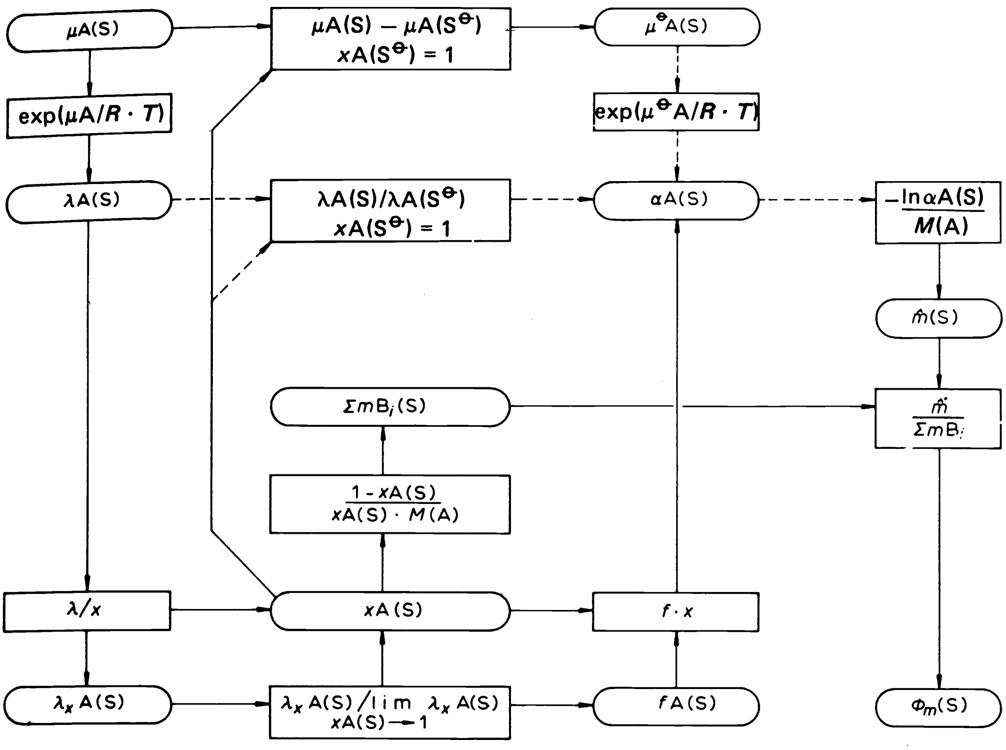
The chart indicates that this quantity may be defined in three different ways:

$aA(S) = fA(S) \cdot xA(S)$, $aA(S) = \lambda A(S)/\lambda A(S^{\ominus})$ for $xA(S^{\ominus}) = 1$,

$aA(S) = \exp(\mu^{\ominus}A(S)/R \cdot T)$.

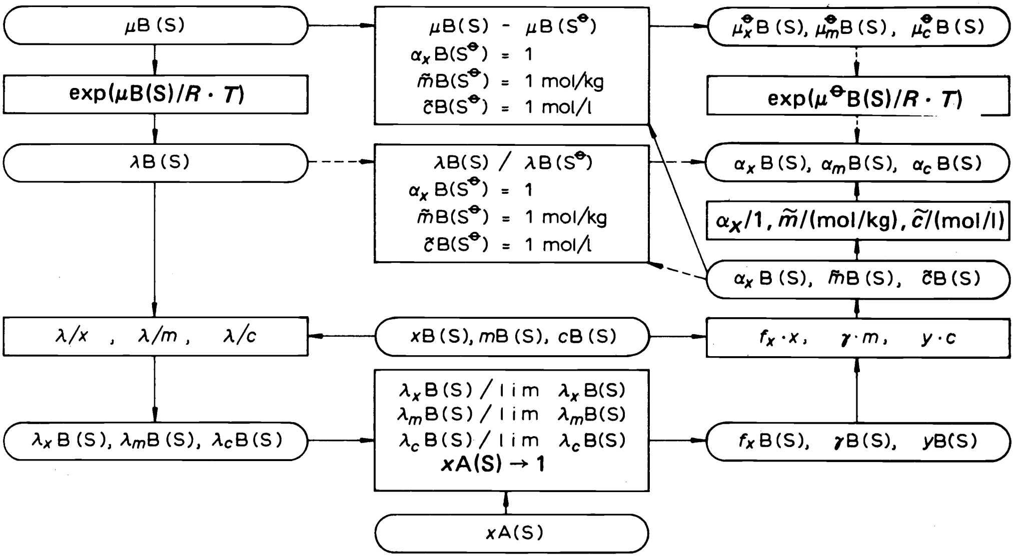
Concerning the words *mixture* and *solution* cf. 6.1.1.2.

This chart also illustrates the definitions of osmolality ($\hat{m}$) and osmotic coefficient (ϕ) of a solution. $\Sigma m B_i(S)$ is the sum of the molalities of all the solutes.



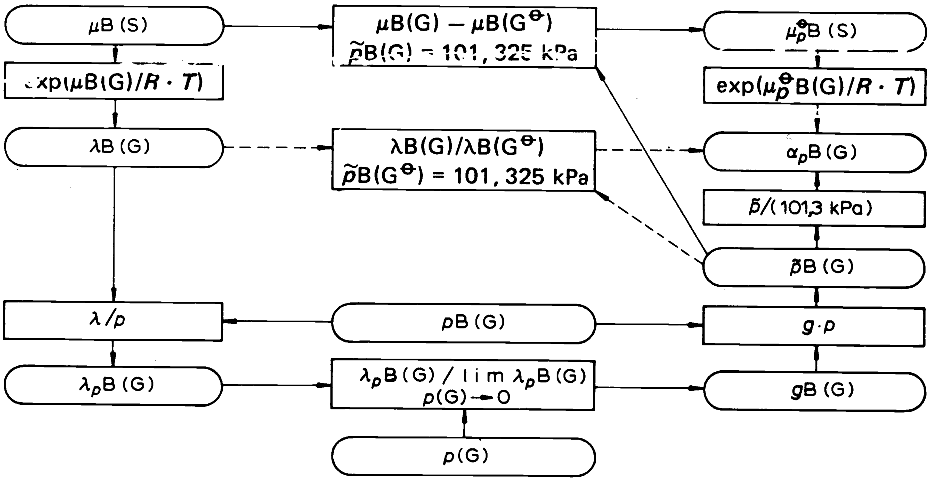
6.2.2. Relative activities of a solute in a solution

The alternative ways of defining rational activity a_x, molal activity a_m, or concentrational activity a_c imply $a_x\mathrm{B(S^{\ominus})} = 1$, or $\tilde{m}\mathrm{B(S^{\ominus})} = 1$ mol/kg, or $\tilde{c}\mathrm{B(S^{\ominus})} = 1$ mol/l, which may not be physically possible if B is slightly soluble. Therefore the definition indicated by full arrows was preferred.



6.2.3. Fugacity of a component in a gas mixture

The relative activity of a component in a gas mixture, $a_p\mathrm{B(G)}$, may be defined in different ways as indicated by the dotted arrows. The simplest definition, from fugacity ($\tilde{p}$), is preferred.



6.3. *List of quantities expressing the stoichiometric concentration of the components H^+, CO_2, O_2, and Ca^{2+}*

Alternative names are shown, indicating that different names for the components may be employed.

6.3 §	System — Component(s) (specification)	Kind of quantity	Typical numerical value	Unit	Remarks	Determination
1.1	Ecf — Hydrogen ion (titratable),	substance concentration	—1.6	mmol/l	Ecf = Extracellular fluid, i.e. blood + interstitial fluid. For purposes of calculation, Ecf in adults may be represented by a model: Ecf = 1aB + 2aP, i.e. arterial blood diluted 3 fold by its own plasma. Titratable means free + bound. Suggested symbol: ctH^+(Ecf)	Titration of the model Ecf with strong acid or base to plasma-pH = 7,40 at $p\mathrm{CO_2}$ = 5,33 kPa, θ = 37°C, and constant $sO_2 = sO_2$(aB). Algorithm for calculating ctH^+(Ecf) from pH and $p\mathrm{CO_2}$ of the arterial blood is given in a subsequent document.
1.2	Ecf — Base (H^+-binding groups),	substance concentration difference	+1.6	mmol/l	This quantity equals the former quantity with opposite sign. Trivial names: Base excess (BE) of the extracellular fluid, or standard base excess (SBE)	
2.1.	P — Carbon dioxide (total),	substance concentration	25.7	mmol/l	P = plasma Total CO_2 implies CO_2 which can be extracted by acidification and vacuum. Comprises $CO_3^{2-} + HCO_3^- + CO_2$ (free dissolved) + Pr-NH-COO$^-$ (carbamino-CO_2). Suggested symbol: $ctCO_2$(P)	Acidification of plasma, extraction of CO_2, into gas phase followed by gas chromatography and mass spectrometry. Algorithm for calculating $ctCO_2$ from plasma pH and $p\mathrm{CO_2}$ is given in a subsequent document.
2.2	P — Carbonate + carbon dioxide,	substance concentration	25.7		This name was suggested by EPQUCC [7.5] Carbonate here means $CO_3^{2-} + HCO_3^- + H_2CO_3$	

3.1	aB — Oxygen (total),	substance concentration	9.4	mmol/l	aB = arterial blood Total oxygen implies O_2 which can be extracted by vacuum. Comprises free dissolved O_2 + hemoglobin-bound O_2	Oxidation of hemoglobin to hemiglobin, extraction of O_2 into a gas phase followed by gas chromatography and mass spectrometry. Algorithm for calculating ctO_2 from blood pO_2, ctHb and pH is given in a subsequent document
3.2	aB — Dioxygen (free + Hb-bound)	substance concentration	9.4	mmol/l	EPQUCC favours the name dioxygen [7.5] Trivial name: oxygen content	
4.1	P — Calcium (total),	substance concentration	2.5	mmol/l	Total calcium comprises Ca^{2+} (free ionized) + Ca (bound)	Gas-mass spectrometry
4.2	P — Calcium(II) (Ca, total),	substance concentration	2.5	mmol/l	This name was suggested by EPQUCC [7.5]. II is the oxidation state in Stock notation.	

6.4. List of quantities related to the chemical activity of the components H^+, CO_2, O_2, HCO_3^-, Ca^{2+}, Na^+, K^+, and H_2O in human blood plasma

Among the many different ways of indicating the chemical activity of a given component (8 possibilities are shown for H^+: §§ 1.1.1 to 1.1.8) the one preferred for practical clinical application is marked by an asterisk..

In the case of measurements in whole blood or serum by means of ion selective electrodes we recommend to use a fixed value for the concentrational activity coefficient unless special circumstances warrant consideration of variations in ionic strength or mass concentration of water.

The typical values given refer to normal arterial plasma at 37° C, and the values are mutually consistent.

6.4 §	Quantity name	Symbol	Typical numerical value	Unit	Determination	Cf. Appendix 6.1
1.1.1 *	P — pH	pH(P)	7,40	1	(measured with a pH electrode)	7.2.1
1.1.2	P — Hydrogen ion, molal chemical potential	$\mu_m^{\ominus}H^+(P)$	—43,9	kJ/mol	$\mu_m^{\ominus}H^+ = -R \cdot T \cdot \ln 10 \cdot pH$	2.12
1.1.3	P — Hydrogen ion, molal activity	$a_m H^+(P)$	39,8	10^{-9}	$a_m H^+ = 10^{-pH}$	7.2
1.1.4	P — Hydrogen ion, active molality	$\tilde{m}H^+(P)$	39,8	nmol/kg	$\tilde{m}H^+ = 10^{-pH} \cdot mol \cdot kg^{-1}$	6.2
1.1.5	P — Hydrogen ion, molality	$mH^+(P)$	48,0	nmol/kg	$mH^+ = 10^{-pH} \cdot (\gamma H^+)^{-1} \cdot mol \cdot kg^{-1}$	3.3
1.1.6	P — Hydrogen ion, concentrational activity	$a_c H^+(P)$	39,5	10^{-9}	$a_c H^+ = 10^{-pH} \cdot \rho(H_2O) \cdot l \cdot kg^{-1}$	7.3
1.1.7	P — Hydrogen ion, active substance concentration	$\tilde{c}H^+(P)$	39,5	nmol/l	$\tilde{c}H^+ = 10^{-pH} \cdot \rho(H_2O) \cdot mol \cdot kg^{-1}$	6.3
1.1.8	P — Hydrogen ion, substance concentration	$cH^+(P)$	44,9	nmol/l	$cH^+ = 10^{-pH} \cdot \rho(H_2O) \cdot (\gamma H^+)^{-1} \cdot mol \cdot kg^{-1}$	3.4

1.2.1	P — Hydrogen ion, molal activity coefficient	$\gamma H^+(P)$	0,83	1	May be estimated from an empirical equation: (7.10) $\lg \gamma H^+(P) = -A \cdot I^{1/2}/(1 + I^{1/2}) + (B - C) \cdot I - D \cdot I^{3/2}$ For 37°C: $A = 0.521$, $B = 0.196$, $C = -0.369$, $D = 0.318$. $I = I(Pw)$ (see 6.4.9)	5.2 5.2
1.2.2	P — Hydrogen ion, concentrational activity coefficient	$y H^+(P)$	0,88	1	$y H^+ = \gamma H^+ \cdot \rho(H_2O) \cdot (\rho H_2O(P))^{-1}$	5.3
1.3.1.	P — buffer value (for H^+)	$\beta(P)$	10,4	mmol/l	Determined by titrating plasma with strong acid or base in a closed system, i.e. $ctCO_2(P)$ constant.	11.2
1.3.2	P — buffer value (for H^+, pCO_2 constant)	β (P, pCO_2 const.)	64,3	mmol/l	Determined by titrating plasma with strong acid or base in an open system with constant $pCO_2(P)$.	11.2
.3.3	P — Albumin, molar buffer capacity (for H^+)	$B_m Alb(P)$	8,0	1	Determined as the slope of $\beta(P)$ as a function of $cAlb(P)$	11.3
.3.4	P — Protein, specific buffer capacity (for H^+)	$B_w Pr(P)$	0,11	mol/kg	Determined as the slope of $\beta(P)$ as a function of $\rho tPr(P)$	11.4
.1.1 *	P — Carbon dioxide, partial pressure	$pCO_2(P)$	5,3	kPa	(Measured with a pCO_2 electrode)	3.5 6.5
.1.2	P — Carbon dioxide, active substance concentration	$\tilde{c}CO_2(P)$	1,33	mmol/l	$\tilde{c}CO_2(P) = pCO_2(P) \cdot \tilde{\alpha}_c CO_2(P)$	6.3
.1.3	P — Carbon dioxide, substance concentration	$cCO_2(P)$	1,22	mmol/l	$cCO_2(P) = pCO_2(P) \cdot \alpha_c CO_2(P)$	3.4
.1.1 *	P — Carbon dioxide, ideal concentrational solubility coefficient	$\tilde{\alpha}_c CO_2(P)$	0,251	$mmol \cdot l^{-1} \cdot kPa^{-1}$ $= 10^{-3}$ mol/J	A temperature dependent constant (7.7): $\lg(\tilde{\alpha}_c CO_2 \cdot mmol^{-1} \cdot l \cdot kPa) = \lg(0.251) - 9.6 \cdot 10^{-3} \cdot \Delta T/K + 90 \cdot 10^{-6} \cdot (\Delta T/K)^2$ $\Delta T = T - 310.15$ K	8.3
.2.2	P — Carbon dioxide, concentrational solubility coefficient	$\alpha_c CO_2(P)$	0,230	$mmol \cdot l^{-1} \cdot kPa^{-1}$ $= 10^{-3}$ mol/J	$\alpha_c CO_2(P) = \tilde{\alpha}_c CO_2(P) \cdot gCO_2(G\|P) \cdot (yCO_2(P))^{-1}$. For all practical purposes $g = 1$. g is the fugacity coefficient in the gas phase in equilibrium with plasma	9.3
.2.3	P — Carbon dioxide, molal activity coefficient	$\gamma CO_2(P)$	1,03	1	Empirical variation with the composition of the plasma (7.10): $\lg \gamma CO_2(P) = 0.085 \cdot I(Pw)/mol \cdot kg^{-1}$, where Pw is the plasma water phase (6.4.9).	5.2

List 6.4 (continued)

6.4 §	Quantity name	Symbol	Typical numerical value	Unit	Determination	Cf. Appendix 6.1
2.2.4	P — Carbon dioxide, concentrational activity coefficient	$y\mathrm{CO_2(P)}$	1,09	1	$y\mathrm{CO_2(P)} = \gamma\mathrm{CO_2(P)} \cdot \rho(\mathrm{H_2O}) \cdot (\rho\mathrm{H_2O(P)})^{-1}$	5.3
3.1.1 *	P — Dioxygen, partial pressure	$p\mathrm{O_2(P)}$	13,0	kPa	(Measured with a $p\mathrm{O_2}$ electrode)	3.5 6.5
3.1.2	P — Dioxygen, substance concentration	$c\mathrm{O_2(P)}$	125	μmol/l	$c\mathrm{O_2(P)} = p\mathrm{O_2(P)} \cdot \alpha_c\mathrm{O_2(P)}$	3.4
3.2.1	P — Dioxygen, ideal concentrational solubility coefficient	$\tilde{\alpha}_c\mathrm{O_2(P)}$	10,50	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1} \cdot \mathrm{kPa}^{-1}$ $= 10^{-6}$ mol/J	Empirical temperature variation (7.2): $\lg(\tilde{\alpha}_c\mathrm{O_2} \cdot \mu\mathrm{mol}^{-1} \cdot \mathrm{l} \cdot \mathrm{kPa}) = \lg(10.50) -$ $5 \cdot 10^{-3} \cdot \Delta T/\mathrm{K} + 9 \cdot 10^{-5} \cdot (\Delta T/\mathrm{K})^2$ $\Delta T = T - 310.15$ K	8.3
3.2.2	P — Dioxygen, concentrational solubility coefficient	$\alpha_c\mathrm{O_2(P)}$	9,63	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1} \cdot \mathrm{kPa}^{-1}$	$\alpha_c\mathrm{O_2(P)} = \tilde{\alpha}_c\mathrm{O_2(P)} \cdot (y\mathrm{O_2(P)})^{-1} \cdot g\mathrm{O_2(G\|P)}$ For all practical purposes $g\mathrm{O_2(G\|P)} = 1$	9.3
3.2.3	P — Dioxygen, molal activity coefficient	$\gamma\mathrm{O_2(P)}$	1,03	1	Empirical variation with the composition of the plasma: $\lg \gamma\mathrm{O_2(P)} = 0.085 \cdot I(\mathrm{Pw})/\mathrm{mol} \cdot \mathrm{kg}^{-1}$, where Pw is the plasma water phase.	5.2
3.2.4	P — Dioxygen, concentrational activity coefficient	$y\mathrm{O_2(P)}$	1,09	1	$y\mathrm{O_2(P)} = \gamma\mathrm{O_2(P)} \cdot \rho(\mathrm{H_2O}) \cdot (\rho\mathrm{H_2O(P)})^{-1}$.	5.3
4.1.1	P — Hydrogen carbonate ion, active molality	$\tilde{m}\mathrm{HCO_3^-(P)}$	16,9	mmol/kg	(Measurable with a combined pH/$p\mathrm{CO_2}$ electrode system). $\tilde{m}\mathrm{HCO_3^-(P)} = K_a \cdot p\mathrm{CO_2(P)} \cdot a\mathrm{H_2O(P)} \cdot 10^{\mathrm{pH}} \cdot$ $\tilde{\alpha}_c\mathrm{CO_2(P)}/\rho(\mathrm{H_2O})$. K_a is the thermodynamic equilibrium constant (cf. § 10.3). At 37°C: $\tilde{m}\mathrm{HCO_3^-(P)} = p\mathrm{CO_2(P)} \cdot 10^{\mathrm{pH}} \cdot 10^{-6.90}$	6.2
4.1.2 *	P — Hydrogen carbonate ion, substance concentration	$c\mathrm{HCO_3^-(P)}$	24,4	mmol/l	$c\mathrm{HCO_3^-(P)} = \tilde{m}\mathrm{HCO_3^-(P)} \cdot (\gamma\mathrm{HCO_3^-(P)})^{-1} \cdot \rho\mathrm{H_2O(P)}$. At 37°C: $c\mathrm{HCO_2(P)} \approx p\mathrm{CO_2(P)} \cdot 10^{\mathrm{pH}} \cdot 10^{-6.74}$	3.4
4.2.1	P — Hydrogen carbonate ion, molal activity coefficient	$\gamma\mathrm{HCO_3^-(P)}$	0,65	1	Empirical variation with ionic strength of plasma water phase (I(Pw)) (7.10): $-\lg \gamma\mathrm{HCO_3^-(P)} = A \cdot I^{1/2}/(1 + I^{1/2}) - C \cdot I - \mathrm{D} \cdot \mathrm{I}^{3/2}$. At 37°C: $A = 0.521$, $C = -0.369$, $D = 0.318$.	5.2

4.2.2	P — Hydrogen carbonate ion, concentrational activity coefficient	$y\text{HCO}_3^-(\text{P})$	0,69	1	$y\text{HCO}_3^-(\text{P}) = \gamma\text{HCO}_3^-(\text{P}) \cdot \rho(\text{H}_2\text{O}) \cdot (\rho\text{H}_2\text{O}(\text{P}))^{-1}$.	5.3
5.1.1	P — Calcium ion, active molality	$\tilde{m}\text{Ca}^{2+}(\text{P})$	0,36	mmol/kg	(Measured with ion selective electrode) .	6.2
5.1.2 *	P — Calcium ion, substance concentration	$c\text{Ca}^{2+}(\text{P})$	1,2	mmol/l	$c\text{Ca}^{2+}(\text{P}) = \tilde{m}\text{Ca}^{2+}(\text{P}) \cdot \rho(\text{H}_2\text{O}) \cdot (y\text{Ca}^{2+})^{-1}$.	3.4
5.2.1	P — Calcium ion, concentrational activity coefficient	$y\text{Ca}^{2+}(\text{P})$	0,30	1	Depends on ionic strength and mass concentration of water.	5.3
6.1.1	P — Sodium ion, active molality	$\tilde{m}\text{Na}^+(\text{P})$	109	mmol/kg	(Measured with ion selective electrode).	6.2
6.1.2 *	P — Sodium ion, substance concentration	$c\text{Na}^+(\text{P})$	143	mmol/l	$c\text{Na}^+(\text{P}) = \tilde{m}\text{Na}^+(\text{P}) \cdot \rho(\text{H}_2\text{O}) \cdot (y\text{Na}^+(\text{P}))^{-1}$.	3.4
6.2.1	P — Sodium ion, concentrational activity coefficient	$y\text{Na}^+(\text{P})$	0,76	1	Depends on ionic strength and mass concentration of water (7.12).	5.3
7.1.1	P — Potassium ion, active molality	$\tilde{m}\text{K}^+(\text{P})$	3,6	mmol/kg	(Measured with ion selective electrode).	6.2
7.1.2 *	P — Potassium ion, substance concentration	$c\text{K}^+(\text{P})$	4,8	mmol/l	$c\text{K}^+(\text{P}) = \tilde{m}\text{K}^+(\text{P}) \cdot \rho(\text{H}_2\text{O}) \cdot (y\text{K}^+(\text{P}))^{-1}$.	3.4
7.2.1	P — Potassium ion, concentrational activity coefficient	$y\text{K}^+(\text{P})$	0,75	1	Depends on ionic strength and mass concentration of water (7.12).	5.3
8.1.1	P — freezing point depression	$\Delta T_\text{f}(\text{P})$	0,545	K	(Measured by means of freezing point osmometer).	10.5
8.1.2	P — osmolality (0° C)	$\hat{m}(\text{P})$	294	mmol/kg	$\hat{m}(\text{P}) = \Delta T_\text{f}(\text{P})/K_\text{f}$. $K_\text{f} = 1.855 \text{ kg} \cdot \text{K} \cdot \text{mol}^{-1}$.	10.1
8.1.3 *	P — osmotic concentration	$\hat{c}(\text{P})$	294	mmol/l	$\hat{c}(\text{P}) = \Delta T_\text{f}(\text{P})/K_{\text{f},c}$. $K_{\text{f},c} = K_\text{f}/\rho(\text{H}_2\text{O}) = 1.855 \text{ litre} \cdot \text{K} \cdot \text{mol}^{-1}$.	10.3
8.1.4	P — Solutes, substance concentration	$c\text{Solutes}(\text{P})$	300	mmol/l	$c\text{Solutes}(\text{P}) = \hat{c}(\text{P})/\phi_c(\text{P}) \approx 2 \cdot (c\text{Na}^+ + c\text{K}^+) + c\text{Glucose} + c\text{Carbamide} - c\text{Pr}^-$.	10.4 3.4
8.1.5	P — Water, activity (0° C)	$a\text{H}_2\text{O}(\text{P})$	0,9946	1	$-\ln a\text{H}_2\text{O}(\text{P}) = \Delta T_\text{f}(\text{P}) \cdot M(\text{H}_2\text{O})/K_\text{f}$, or from vapor pressure measurements: $a\text{H}_2\text{O}(\text{P}) = p\text{H}_2\text{O}(\text{P})/p\text{H}_2\text{O}(\text{H}_2\text{O})$	7.1 10.1 10.6
8.1.6	P — osmotic pressure	$\Pi(\text{P})$	758	kPa	$\Pi = R \cdot T \cdot \hat{c}$	10.8
8.1.7	P — Water, vapor pressure (37° C)	$p\text{H}_2\text{O}(\text{P})$	6.24	kPa	(Measured by means of vapor pressure osmometer)	6.5
8.1.8	P — Water, mass concentration	$\rho\text{H}_2\text{O}(\text{P})$	0,94	kg/l	$\rho\text{H}_2\text{O}(\text{P}) = m\text{H}_2\text{O}(\text{P})/V(\text{P})$	3.1

List 6.4 (continued)

6.4 §	Quantity name	Symbol	Typical numerical value	Unit	Determination	Cf. Appendix 6.1
8.1.9	P — Water, substance concentration	$c\mathrm{H_2O(P)}$	52.2	mol/l	$c\mathrm{H_2O(P)} = \rho\mathrm{H_2O(P)}/M(\mathrm{H_2O})$	3.4
8.2.1	P — molal osmotic coefficient	$\phi_m\mathrm{(P)}$	0,92	1	Depends on the composition of the plasma	10.2
8.2.2	P — concentrational osmotic coefficient	$\phi_c\mathrm{(P)}$	0.98	1	Depends on the composition of the plasma	10.4
9	P (water phase) — ionic strength	$I\mathrm{(Pw)}$	160	mmol/kg	Macro-ions are considered rather immobile and are not included in the calculation of the ionic strength. Albumin in a conc. of 0.6 mmol/l and with a charge number of about 20 would otherwise contribute with 240 mmol/kg to the ionic strength.	3.6
10.1	Water — vapor pressure (37° C)	$p\mathrm{H_2O(H_2O)}$	6,275	kPa		6.5
10.2	Water — mass density (37° C)	$\rho\mathrm{(H_2O)}$	0,9930	kg/l	$\rho\mathrm{H_2O} = m(\mathrm{H_2O})/V(\mathrm{H_2O})$	3.1
10.3	Water — ($\mathrm{CO_2 + H_2O \rightleftharpoons H^+ + HCO_3^-}$), equilibrium constant (37° C)	K_a	$10^{-6.30}$		Determined by measuring $K_{\mathrm{hybrid}} = \dfrac{a_m\mathrm{H^+} \cdot c\mathrm{HCO_3^-}}{a_m\mathrm{CO_2} \cdot a\mathrm{H_2O}}$ and extrapolating to infinite dilution. Varies with T (7.7): $-\lg K_a = 6.30 - 2.6 \cdot 10^{-3} \cdot \Delta T/\mathrm{K} + 0.12 \cdot 10^{-3} \cdot (\Delta T/\mathrm{K})^2$, $\Delta T = T - 310.15\ \mathrm{K}$	12.2

6.5. Alphabetical index of symbols of kinds of quantities.

References are given to the paragraphs of List 6.1 for definitions and remarks

Symbol	name	reference
a	relative activity	6.1.1
a_c	relative activity, concentrational	7.3
a_m	relative activity, molal	7.2
a_p	relative activity, baric	7.4
a_x	relative activity, rational	6.1.2
B	buffer capacity	11.1
B_m	buffer capacity, molar	11.3
B_w	buffer capacity, specific	11.4
b	(molality)	3.3
$\tilde{b}$	(active molality)	6.2
$\hat{b}$	(osmolality)	10.1
c	substance concentration	3.4
$\tilde{c}$	active substance concentration	6.3
$\hat{c}$	osmotic concentration	10.3
E	energy	2.1
E	electromotive force	2.7
F	faraday constant	2.11
f	activity coefficient	5.1.1
f	(fugacity)	6.4
f_x	activity coefficient, rational	5.1.2
G	gibbs energy	2.9
g	fugacity coefficient	5.4
I	electric current	1.4
I	ionic strength	3.6
K_a	equilibrium constant	12.1
K_m	molal equilibrium product	12.2
K_c	concentrational equilibrium product	12.3
K_f	freezing point depression constant, molal	10.6
K_p	baric equilibrium product	12.4
l	length	1.1
M	molar mass	10.1
m	mass	1.2
m	molality	3.3
$\tilde{m}$	active molality	6.2
$\hat{m}$	osmolality	10.1
n	amount of substance	1.6
p	pressure	2.5
p	partial pressure	3.5
$\tilde{p}$	fugacity	6.4
Q	electric charge	2.6
R	molar gas constant	2.13

Symbol	name	reference
S	entropy	2.2
s	saturation fraction	3.2.1
T	thermodynamic temperature	1.5
ΔT_f	freezing point depression	10.5
t	time	1.3
U	energy, internal	2.1
V	volume	2.4
V	(electric potential)	2.7
V_m	molar volume	2.4.1
x	substance fraction	3.2
y	activity coefficient, concentrational	5.3
z	charge number	2.8
α_c	solubility coefficient, concentrational	9.3
$\tilde{\alpha}_c$	solubility coefficient, ideal concentrational	8.3
α_m	solubility coefficient, molal	9.2
$\tilde{\alpha}_m$	solubility coefficient, ideal molal	8.2
α_x	solubility coefficient, rational	9.1
$\tilde{\alpha}_x$	solubility coefficient, ideal rational	8.1
β	buffer value	11.2
γ	activity coefficient, molal	5.2
θ	Celcius temperature	2.3
λ	absolute activity	2.13
λ_c	absolute activity coefficient, concentrational	4.3
λ_m	absolute activity coefficient, molal	4.2
λ_p	absolute activity coefficient, baric	4.4
λ_x	absolute activity coefficient, rational	4.1
μ	chemical potential, absolute	2.10
$\tilde{\mu}$	chemical potential, electrochemical absolute	2.11
$\mu^{\ominus}$	chemical potential, standard	2.12
ν	stoichiometric number	12.1
Π	osmotic pressure	10.8
ρ	mass concentration	3.1
ρ	mass density	3.1
ϕ	electric potential	2.7
ϕ_c	osmotic coefficient, concentrational	10.4
ϕ_m	osmotic coefficient, molal	10.2

7 References

7.1 Bates, R.G. (1973). Determination of pH. Theory and Practice. 3rd ed. pp. 435. John Wiley and Sons, New York.

7.2. Christoforides, C., Laasberg, L.H. and Hedley-White, J. (1969). Effect of temperature on solubility of O_2 in human plasma. J. Appl. Physiol. 26, 56—60.

7.3. Durst, R.A. (1975, revised 1979). Standard reference materials: standardization of pH measurements, pp. 48. NBS Special Publication 260—53, U.S. Government Printing Office. Washington DC, U.S.A.

7.4. Dybkaer, R. (ed.) (1979). Quantities and units in clinical chemistry. Recommendation 1978. International Union of Pure and Applied Chemistry and the International Federation of Clinical Chemistry. Clin. Chim. Acta 96, 157F—183F.

7.5. Dybkaer, R. (ed.) (1979). List of quantities in clinical chemistry. Recommendation 1978. International Union of Pure and Applied Chemistry and the International Federation of Clinical Chemistry. Clin. Chim. Acta, 96, 185F—204F.

7.6. Dybkaer, R. and Jørgensen, K. (1967). Quantities and Units in Clinical Chemistry Including Recommendation 1966 of the Commission on Clinical Chemistry of the IUPAC and of the IFCC. 1st ed., pp. X + 102. Munksgaard, Copenhagen.

7.7. Harned, N.S. and Davis, R. Jr. (1943). The ionization constant of carbonic acid in water and the solubility of carbon dioxide in water and aqueous salt solutions from 0 to 50. J. Am. Chem. Soc. 65, 2030—2037.

7.8. International Standard, ISO 31 Series, Technical Committee ISO/TC 12 (1979). Quantities, units, symbols, conversion factors, and conversion tables, 14 Parts. International Organization for Standardization, Geneva.

7.9. Lowe, D.A. (1975). A Guide to International Recommendations on Names Symbols for Quantities and on Units of Measurement. Progress in Standardization: 2, 1st ed., pp. 314. Bull. WHO, 52, Suppl., World Health Organization, Geneva.

7.10. Maas, A.H.J., Van Heijst, A.N.P. and Visser, B.F. (1971). The determination of the true equilibrium constant ($p\overline{K}_{1g}$) and the practical equilibrium coefficients ($p\overline{K}_{1g}$) for the first ionization of carbonic acid in solutions of sodium bicarbonate, cerebrospinal fluid, plasma, and serum at 25° and 38°. Clin. Chim. Acta, 33, 325—343.

7.11. McGlashan, M.L. (1971). Physicochemical Quantities and Units. The Grammar and Spelling of Physical Chemistry. 2nd ed., pp. X + 117. The Royal Institute of Chemistry, London.

7.12. Neff, G.W., Radke, W.A., Sambucetti, C.J. and Widdowson, G.M. (1970). A computer-assisted electrode system for measuring blood pH, pO_2, pCO_2, sodium and potassium. Clin. Chem. 16, 566—572.

7.13. Page, C.H. (1975). On the dimension group of classical physics. J. Res. Natl. Bur. Stand. 79B, 127—135.

7.14. Whiffen, D.H. (ed.) (1979). Manual of Symbols and Terminology for Physicochemical Quantities and Units. IUPAC, Division of Physical Chemistry, Commission on Symbols, Terminology, and Units. 1978 edition. Pure Appl. Chem. 51, 1—41.