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Scientific Committee, Analytical Section

Expert Panel on pH and Blood Gases³⁾,
Expert Panel on Quantities and Units⁴⁾
and**INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY**

Division of Clinical Chemistry

Commission on Quantities and Units in Clinical Chemistry⁴⁾**Approved Recommendation (1984) on
Physico-Chemical Quantities and Units in Clinical Chemistry
with Special Emphasis on Activities and Activity Coefficients***Prepared for publication⁵⁾ by**O. Siggaard-Andersen**University of Copenhagen Hospital, Herlev, Denmark**R. A. Durst**National Bureau of Standards, Washington DC, U.S.A. and**A. H. J. Maas**University Hospital, Utrecht, The Netherlands*

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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 coefficient for solute B in a solution.

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 to 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 (6.3) 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) are primarily of interest in the clinical chemical laboratory for purposes of calculation.

1. Introduction

1.1. The IUPAC Commission on Quantities and Units in Clinical Chemistry has together with the IFCC Expert Panel on Quantities and Units in Clinical Chemistry previously published general recommendations on quantities and units in clinical chemistry (7.8, 7.9, 7.10). The present document has been prepared in collaboration between the Expert Panel on pH and Blood Gases and the IUPAC Commission. It was published by IUPAC as Recommendations 1983 in Pure & Appl. Chem. 56 (1984) 567 – 594 and has been accepted by the Council of the International Federation of Clinical Chemistry by mail ballot in September 1984. In the present reprinted document some minor corrections and editing changes have been made.

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 (7.12). 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.

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 quantities:

(1) An extensive quantity: 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 .

(2) An intensive quantity: 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 is usually divided by the volume (V) of the system, providing the stoichiometric concentration (c) of the component in the system:

$$c_B = \frac{n_B}{V} \quad (1)$$

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.

It is therefore essential to distinguish between the stoichiometric concentration and the substance concentration of the free form of the component in the system (see 2.3.).

Sometimes stoichiometric quantities are indicated by subscript (0), e. g. $n_{0,B}$, $c_{0,B}$. Concerning the general format for the symbols employed in the present document, see 6.1.1.2. and 6.4.

In clinical chemistry, the term stoichiometric concentration is rarely employed. Instead, the name of the component is modified to indicate inclusion of the various derived forms, 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 (7.9). Examples of such quantity names are given in 6.2.

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 extensive variables constant, i. e. volume (V), entropy (S), electric charge (Q), and stoichiometric amount of other components (C, D, etc):

$$\mu_B = \left(\frac{\partial U}{\partial n_B} \right)_{V, S, Q, n_C, \dots} \quad (2)$$

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

$$\lambda_B = \exp \frac{\mu_B}{R \cdot T} \quad (3)$$

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

$$a_{m,B} = \frac{\lambda_B}{\lambda_B^{\ominus}}, \quad (4)$$

where the standard reference system ($^\ominus$) based on molality is chosen so that $\gamma_B^\ominus \cdot m_B^\ominus = \tilde{m}_B^\ominus = 1 \text{ mol} \cdot \text{kg}^{-1}$. Concerning the different standard reference systems, see List 6.1., §§ 6.0–6.3.

The molal activity may be divided by the molal activity coefficient (γ) to provide the molality of the component in the free unbound form:

$$m_B = \frac{a_{m,B}}{\gamma_B} \cdot \tilde{m}_B^\ominus \quad (5)$$

Substance concentration is obtained by multiplying molality with the mass concentration of water (ϱ_{H_2O}):

$$c_B = m_B \cdot \varrho_{H_2O} \quad (6)$$

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:

$$\begin{aligned} \text{pH} &= - \lg a_{m,H^+} = - \lg \frac{\gamma_{H^+} \cdot m_{H^+}}{\tilde{m}_H^\ominus} \\ &= - \frac{\mu_{H^+} - \mu_H^\ominus}{R \cdot T \cdot \ln 10} \end{aligned} \quad (1)$$

The molal standard reference system is chosen so that $\gamma_{H^+}^\ominus \cdot m_{H^+}^\ominus = \tilde{m}_{H^+}^\ominus = 1 \text{ mol} \cdot \text{kg}^{-1}$. The definition is traditionally based on molality rather than substance concentration (7.2). pH is linearly related to the chemical potential of hydrogen ion (μ_{H^+}).

3.2. Chemical potential or activity of ions cannot be determined on a purely thermodynamic basis. This is due to the fact that the effects of an ion cannot be separated from the effects of the accompanying counterion, 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.

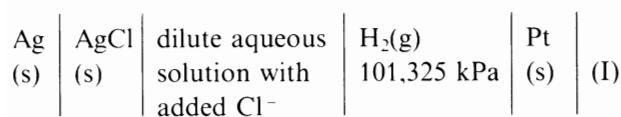
The present convention is based on the assumption that the molal activity coefficient of the chloride ion in dilute aqueous solutions ($I < 0,10 \text{ mol} \cdot \text{kg}^{-1}$) can be estimated by means of the *Debye-Hückel equation*:

$$-\lg \gamma_B = \frac{A \cdot z_B^2 \cdot I^{\frac{1}{2}}}{1 + \bar{a} \cdot B \cdot I^{\frac{1}{2}}}, \quad (2)$$

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

According to the *Bates-Guggenheim convention* $\bar{a} \cdot B$ is taken to be $1,5 (\text{mol} \cdot \text{kg}^{-1})^{-\frac{1}{2}}$ at all temperatures and for all compositions of the solution (7.2).

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



The calculation function is:

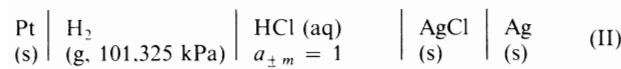
$$\text{pH} = \frac{-E_I - E_{II}^\ominus}{R \cdot T \cdot \ln 10} \cdot F + \lg \frac{m_{\text{Cl}^-}}{\tilde{m}_{\text{Cl}^-}^\ominus} + \lg \gamma_{\text{Cl}^-}, \quad (3)$$

E_{II}^\ominus is the standard electrode potential of the Ag/AgCl half cell ($E_{II}^\ominus = 0,21423 \text{ V}$ at 37°C). m_{Cl^-} is measured and γ_{Cl^-} is calculated from Eqn (2). Cl⁻ is added in different amounts and the results are extrapolated linearly to zero molality of added Cl⁻.

The definitive method is employed for determining the pH in a series of primary aqueous calibration solutions, e. g. the NBS-buffers (National Bureau of Standards, U.S.A.) (7.2, 7.7).

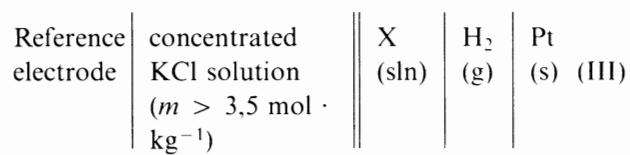
Note:

The standard electrode potential (E_{II}^\ominus) of the Ag/AgCl half cell is defined as the potential of the cell:



where $a_{\pm m} = (a_{m,\text{H}^+} \cdot a_{m,\text{Cl}^-})^{\frac{1}{2}}$ is the mean ionic activity which can be determined without any convention for single ion activities. Hence E^\ominus is independent of such conventions and pH (Eqn. 3) is dependent only on the convention for calculating γ_{Cl^-} (3.2). Values of E^\ominus have been tabulated (7.3).

3.4. The reference method for inorganic aqueous solutions is based on a cell with a liquid-liquid junction (III), measuring the cell potential with the unknown solution, $E(X)$, and the calibration solution, $E(S)$:



The calculation function is:

$$\text{pH}(X) = \text{pH}(S) - \frac{E(X) - E(S)}{R \cdot T \cdot \ln 10} \cdot F, \quad (4)$$

where S is one of the calibration solutions mentioned in 3.3. This equation is generally called the "operational" pH definition (7.21), but it should not be considered a pH definition in the same sense as the definition given in 3.1.

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 standardise the method of reporting quantities in clinical chemistry it has often been suggested that the substance concentration of hydrogen ion should be reported instead of pH. However, in view of the international agreement concerning the pH scale and the reference method for pH measurement (7.21) we recommend the continuing use of the quantity pH also in clinical chemistry.

The "substance concentration" of H⁺ is often calculated 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 reporting the *active* substance concentration (\tilde{c}) of the hydrogen ions, calculated as

$$\tilde{c}_{\text{H}^+} = 10^{-\text{pH}} \cdot \varrho_{\text{H}_2\text{O}}^* \cdot \tilde{m}_{\text{H}^+}^\ominus, \quad (5)$$

where $\tilde{m}_{\text{H}^+}^\ominus = 1 \text{ mol} \cdot \text{kg}^{-1}$ and where $\varrho_{\text{H}_2\text{O}}^*$ 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: $\tilde{c}_{\text{H}^+} = 10^{-7,40} \cdot (0,993 \cdot \text{kg} \cdot \text{l}^{-1}) \cdot \text{mol} \cdot \text{kg}^{-1} = 39,81 \times 10^{-9} \times 0,993 \cdot \text{mol} \cdot \text{l}^{-1} =$

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:

$$\tilde{c}_{\text{H}^+} = 10^{-\text{pH}} \cdot \tilde{c}_{\text{H}^+}^\ominus, \quad (6)$$

where $\tilde{c}_{\text{H}^+}^\ominus = 1 \text{ mol} \cdot \text{l}^{-1}$.

3.6. For clinical purposes 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 may be reported as the 'substance concentration' of the ion, determined as the molal activity multiplied by an appropriate constant depending upon the ion and the type of biological fluid under investigation. For example, for Ca^{2+} in blood plasma:

$$c_{\text{Ca}^{2+}} = a_{m,\text{Ca}^{2+}} \cdot \gamma_{\text{Ca}^{2+}}^{-1} \cdot \varrho_{\text{H}_2\text{O}} \cdot \tilde{m}_{\text{Ca}^{2+}}^\ominus \quad (7)$$

where $\tilde{m}_{\text{Ca}^{2+}}^\ominus = 1 \text{ mol} \cdot \text{kg}^{-1}$. The appropriate constant is

$$k_{\text{Ca}^{2+}} = \gamma_{\text{Ca}^{2+}}^{-1} \cdot \varrho_{\text{H}_2\text{O}} \cdot \tilde{m}_{\text{Ca}^{2+}}^\ominus \quad (8)$$

where $\gamma_{\text{Ca}^{2+}}$ and $\varrho_{\text{H}_2\text{O}}$ should be the mean values for *normal* plasma (see List 6.3, §§ 7.2.1 and 8.1.8).

At present, 'ionized calcium' is reported as the substance concentration of Ca^{2+} in the 'water phase', which equals $m_{\text{Ca}^{2+}} \cdot \varrho_{\text{H}_2\text{O}}^*$.

3.7. It has been suggested that the unit bel should be used for the pH quantity in order to "flag" that the pH value represents the negative *decadic logarithm* of another quantity (7.1.6). We recommend restricting the use of the bel (or decibel) to an amplitude or power level difference (7.12). The pH quantity is dimensionless and consequently is a pure number. Example: $\text{pH} = 7,40$, not $\text{pH} = 7,40$ pH units, and not $\text{pH} = 7,40$ 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:

$$\langle \text{pH} \rangle = -\lg(\{\sum 10^{-\text{pH}_i}\}/N).$$

We recommend the use of the arithmetic mean of the pH values: $\langle \text{pH} \rangle = (\sum_i \text{pH}_i)/N$. 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.

4. The partial pressure of gases in solution

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

$$p_B = x_B \cdot p \quad (1)$$

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 (sln) we recommend interpreting the quantity as being equal to the partial pressure in an *ideal* gas mixture (g^{ideal}) in equilibrium with the solution, or alternatively, as being equal to the fugacity (\tilde{p}) in a *real* gas mixture (g^{real}) in equilibrium with the solution:

$$p_B(\text{sln}) = p_B(g^{\text{ideal}}) = \tilde{p}_B(g^{\text{real}}). \quad (2)$$

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

$$\tilde{p}_B = g_B \cdot p_B. \quad (3)$$

Therefore the unit of fugacity is the same as the unit of pressure. For many gases (CO_2 , O_2 , N_2 etc.) $g_B \approx 1$ when $p < 100 \text{ kPa}$.

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*:

$$p_B = \frac{a_{x,B}}{\alpha_{x,B}^\infty}. \quad (4)$$

$\alpha_{x,B}^\infty$ is the rational solubility coefficient for infinite dilution, i. e. for pure solvent.

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^* :

$$p_A = \tilde{p}_A^* \cdot a_A. \quad (5)$$

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):

$$c_B = \alpha_{c,B} \cdot p_B. \quad (6)$$

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 ($\approx 0.018 \text{ kg} \cdot \text{mol}^{-1}$):

$$\hat{m} = \frac{-\ln a_{\text{H}_2\text{O}}}{M_{\text{H}_2\text{O}}} \quad (1)$$

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

The osmotic concentration (\hat{c}), formerly called the osmolarity, equals the osmolality times the mass density (ϱ) of water:

$$\hat{c} = \hat{m} \cdot \varrho_{\text{H}_2\text{O}}^* \quad (2)$$

As $\varrho_{\text{H}_2\text{O}}^* \approx 1 \text{ kg/l}$ the numerical value of osmotic concentration (in mol/l) practically equals that of osmolality (in mol/kg).

5.3. The osmolality is generally calculated on the basis of measurement of the freezing point depression (ΔT_{fus}) divided by the molal freezing point depression constant (K_{fus}), which is $1,855 \text{ K} \cdot \text{kg} \cdot \text{mol}^{-1}$ for aqueous solutions:

$$\hat{m} = \frac{\Delta T_{\text{fus}}}{K_{\text{fus}}} \quad (3)$$

It is generally tacitly assumed that the osmolality at the temperature of freezing (of plasma or urine) equals the value at 37 °C. In order to obtain the true osmolality at 37 °C it is necessary to calculate the value on the basis of vapor pressure ($p_{\text{H}_2\text{O}}$) measured at 37 °C:

$$\hat{m} = \frac{-\ln(p_{\text{H}_2\text{O}}/p_{\text{H}_2\text{O}}^*)}{M_{\text{H}_2\text{O}}} \quad (4)$$

where $p_{\text{H}_2\text{O}}^*$ is the vapour pressure of pure water.

5.4. The reason for using the osmolality in clinical chemistry is that this quantity can be directly compared to the sum of molalities of the solutes (m_{Solute}), the ratio between the two quantities being the molal osmotic coefficient (ϕ_m):

$$\hat{m} = \phi_m \cdot m_{\text{Solute}} \quad (5)$$

In other words, for many practical purposes the osmolality may be adequately estimated on the basis of measurements of the molalities 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).

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

6.1.1.2. *Symbol and definition:* 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 general format for the symbol of a quantity when the 'kind of quantity' (general symbol Q) and the system (general symbol X) both need specification is either Q^X or $Q(X)$. The format Q^X is employed when X is a standard reference system ($^\ominus$), pure substance (*), or a solution of infinite dilution (^) (7.6, 7.21). The format $Q(X)$ is employed in the present document in other cases. Often specification of the system (X) may be omitted without introducing ambiguity.

Many kinds of quantities need specification of a given component, e. g. partial pressure (p) of a component (B). Generally the component is indicated by a subscript, e. g. p_B , and this format is employed in the present document. However, in clinical chemistry the symbol may often be printed on the line without introducing ambiguity, e. g. $p\text{CO}_2$, $p\text{O}_2$, $c\text{H}^+$, $c\text{HCO}_3^-$.

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, C, D etc.) which are called solutes (7.21).

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 (§§ 1.1 – 1.6). All other quantities are considered *derived quantities* which can be defined by means of an algebraic equation containing only base quantities in addition to the quantity being defined.

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*: only SI units are given in this column. When no unit is given, this indicates that the value of the quantity is a pure number (i. e. quantities of dimension one = 'dimensionless' quantities). Sometimes the number 1 is considered the unit of 'dimensionless' quantities.

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_{fus} (§ 8.6). Cross references to other paragraphs of the List 6.1 are indicated by the symbol §. The values of various constants were obtained from Ref. 7.21.

In the present international document we prefer the decimal comma as recommended for all languages by ISO (7.2) 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 (7.12), IUPAC (7.21), or IFCC (7.8).

6.1. List of quantities and units. For explanation of the columns, see text section 6.1.

6.1. Quantity		Unit	Symbol and definition	Name	Symbol	Remarks	References
§	Name						
1.0	number of entities	N					
1.1	length	<i>l</i>		metre	m	1. Base quantity	8 – 2.1 2.3.05
1.2	mass	<i>m</i>		kilo-gram	kg	1. Base quantity and SI base unit 2. In the present text <i>m</i> indicates mass, whereas <i>m</i> is molarity (§ 3.3).	1 – 3.1 2.1.01 3 – 1.1 2.2.01 4.4
1.3	time	<i>t</i>		second	s	1. Base quantity and SI base unit	1 – 6.1 2.1.12 4.23
1.4	electric current	<i>I</i>		ampere	A	1. Base quantity and SI base unit	5 – 1.1 2.6.05
1.5	thermodynamic temperature	<i>T</i>		K	1. Base quantity and SI base unit	4 – 1.1 2.4.01 4.18	
1.6	amount of substance	<i>n</i>		mole	mol	1. Base quantity and SI base unit 2. $N_B/n_B = L = (602,2045 \pm 0,0031) \times 10^{21} \text{ mol}^{-1}$, where <i>L</i> is the <i>Avogadro</i> - <i>dro</i> constant	8 – 3.1 2.3.06 4.6
2.1	energy	$E = m \cdot c^2$		joule	J = $\text{m}^2 \cdot \text{kg} \cdot \text{s}^{-2}$	1. This definition (the <i>Einstein</i> equation) is the fundamental relationship between the base quantity mass and the derived quantity energy. <i>c</i> is the speed of light in vacuo (in this paragraph only). On the basis of this equation it is possible to derive the following equations for special forms of energy: <i>potential energy</i> $dE_{\text{pot}} = \vec{F} \cdot d\vec{l}$ (where \vec{F} is force), and <i>kinetic energy</i> $dE_{\text{kin}} = \vec{v} \cdot d\vec{p}$ (where \vec{v} is velocity and $\vec{p} = m \cdot \vec{v}$ is momentum).	4 – 19.1 2.4.07
2.2	entropy	$S = \int T^{-1} \cdot dU$ $dV = 0, dQ = 0, dn_B = 0$		joule per kelvin	J/K = $\text{m}^2 \cdot \text{kg} \cdot \text{s}^{-2} \cdot \text{K}^{-1}$	2. <i>U</i> is the preferred symbol for internal energy 3. $dU = -p \cdot dV + T \cdot dS + \phi \cdot dQ$ $+ \sum (\mu_B \cdot dn_{o,b})$ (for derivation see textbooks of physical chemistry)	4 – 17.1 2.4.06

2.3	Celsius temperature	$\theta = T - T_0, T_0 = 273,15 \text{ K}$	${}^\circ\text{C}$ degree Celsius	4 – 2.1	2.4.02	4.19
2.4	volume	$V = \beta$	m^3 cubic metre, litre	1 – 5.1	2.1.11	4.3
2.4.1.	(partial) molar volume of component B	$V_B = \left(\frac{\partial V}{\partial n_B} \right)_{T,p,n_C,\dots}$	litre per mole	8 – 6.1	1.4	
2.5	pressure	$p = - \left(\frac{\partial U}{\partial V} \right)_{S,Q,n_B}$	$\text{Pa} = \text{J} \cdot \text{m}^{-3} = \text{m}^{-1} \cdot \text{kg} \cdot$ s^{-2}	4.21	3 – 13.1	2.2.19
2.6	electric charge; quantity of electricity	$Q = \int I \cdot dt$	coulomb	5 – 2.1	2.6.02	
2.6.1	charge number of component B	$z_B = Q_B/e$		1. Q_B is the charge of one B elementary entity (molecule, ion)	8 – 41.1	2.7.02
2.7	electric potential; electromotive force	$\phi = \left(\frac{\partial U}{\partial Q} \right)_{V,S,n_B}$	volt	5 – 6.1	2.6.07	
2.8	Gibbs energy	$G = U + p \cdot V - T \cdot S$	joule	4 – 19.4	2.4.12	
				$1. \text{d}G = V \cdot dp - S \cdot dT + \phi \cdot dQ + \Sigma (\mu_B \cdot dn_B)$		

6.1. List of quantities and units. (continued)

§	Quantity	Symbol and definition	Name	Unit	Remarks	References
	Name	Symbol	Symbol	Unit		
2.9.1	(absolute) chemical potential of component B	$\mu_B = \left(\frac{\partial U}{\partial n_B} \right)_{V,S,Q,n_C, \dots}$	joule per mole	J/mol = m ² · kg · s ⁻² · mol ⁻¹	1. Only differences in μ_B can be measured (§ 2.9.3) 2. $\mu_B = \left(\frac{\partial G}{\partial n_B} \right)_{P,T,Q,n_A, \dots}$ This equation is often preferred as the definition 3. Notice: $z_B \neq 0 \Rightarrow dQ \neq 0$. Hence μ_B cannot be measured for an ion unless a non-thermodynamic convention is adopted (see Section 3.2) 4. μ_B is proportional to the electric potential (E) of an ideal electrode for component B: $\Delta\mu_B = z_B \cdot F \cdot \Delta E$	ISO 31 (7.12) IUPAC Manual (7.21) EPQUCC CQUCC (7.8)
2.9.2	(absolute) electrochemical potential of component B	$\tilde{\mu} = \left(\frac{\partial U}{\partial n_B} \right)_{V,S,n_C, \dots}$	joule per mole	J/mol = m ² · kg · s ⁻² · mol ⁻¹	1. Notice that Q is not constant. 2. Only differences in $\tilde{\mu}_B$ can be measured. 3. $\tilde{\mu}_B = \mu_B + z_B \cdot F \cdot \phi$ 4. See also introductory section 3.2.	2.7.05 Ref.7.15
2.9.3	(practical) chemical potential of component B	$\psi_B = \mu_B - \mu_B^\ominus$	joule per mole	J/mol = m ² · kg · s ⁻² · mol ⁻¹	1. The symbol ψ is tentative. 2. The standard reference system (\ominus) may be indicated by subscript (compare relative activity): ψ_A (§ 6.1.1), $\psi_{x,B}$ (§ 6.1.2), ψ_{mb} (§ 6.2), ψ_{cb} (§ 6.3), ψ_{pb} (§ 6.4). 3. $\psi_B = R \cdot T \cdot \ln a_B$ (where a_B is relative activity).	Ref.7.15
2.10	absolute activity of component B	$\lambda_B = \exp \frac{\mu_B}{R \cdot T}$	kilogram per mole	kg/l = 10 ³ · m ⁻³ · kg	1. Only the relative λ_B can be measured (§§ 6.1.1, 6.1.2, 6.2, 6.3, 6.4). 1. The name 'dalton' is sometimes used as unofficial unit: 1 dalton = 1 g · mol ⁻¹	8 – 18.1 A.I.1 2.4.26
3.0	molar mass	$M = m/n$				8 – 11.2 2.3.12 4.8
3.1	mass concentration of component B	$\varrho_B = \frac{m_B}{V}$				

3.1.1	(mass) density	$\varrho = m/V$	kilogram per litre	$\text{kg/l} = 10^3 \cdot \text{m}^{-3} \cdot \text{kg}$	1. The mass density of the solvent A equals the mass concentration of A in pure A: $\varrho(A) = \varrho(A)^*$	8–11.1
3.2	(amount-of-)substance fraction; mole fraction of component B	$x_B = \frac{n_B}{n_B + n_C + \dots}$			1. (sat) indicates the system saturated with B at constant T, p, n_C, \dots 2. Capital S is used as the symbol of saturation fraction in the physiological literature.	4.13
3.2.1	saturation fraction of component B	$s_B = n_B/n_B(\text{sat})$			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.	4.12
3.3	molality of solute B	$m_B = \frac{n_B}{M_A}$	mole per kilogram	mol/kg	3. $m_B = x_B/(x_A \cdot M_A)$ 1. $c_B = M_B \cdot \varrho_B$ 2. $c_B = m_B \cdot \varrho_A$ 3. The symbol [B] is often employed for c_B .	8–16.1
3.4	(amount-of-)substance concentration of component B	$c_B = \frac{n_B}{V}$	mole per litre	mol/l	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.	2.3.11
3.5	ionic strength	$I = \frac{1}{2} \cdot \sum(z_B^2 \cdot m_B)$	mole per kilogram	mol/kg	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.	2.4.29
3.6	partial pressure of component B	$p_B = x_B \cdot p$	pascal	$\text{Pa} = \text{m}^{-1} \cdot \text{kg} \cdot \text{s}^{-2}$	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.	4.22

6.1. List of quantities and units. (continued)

§	Quantity	Symbol and definition	Name	Symbol	Unit	Remarks	References
4.0.1	activity coefficient of solvent A or of component A (in a mixture)	$f_A = \frac{\lambda_A/x_A}{\lim_{x_A \rightarrow 1} (\lambda_A/x_A)}$				ISO 31 (7.12)	IUPAC Manual CQUCC (7.8)
4.02	rational activity coefficient of solute B	$f_{x,B} = \frac{\lambda_B/x_B}{\lim_{x_A \rightarrow 1} (\lambda_B/x_B)}$				8 – 22.1 A.I.7 A.I.14	EPQUCC
4.1	molal activity coefficient of solution B	$\gamma_B = \frac{\lambda_B/m_B}{\lim_{x_A \rightarrow 1} (\lambda_B/m_B)}$				4.3	

1. λ_A/x_A may be interpreted as an 'absolute' activity coefficient while f_A is a relative activity coefficient. A similar remark applies in §§ 4.0.2, 4.1, 4.2 and 4.3

2. $f_A = (\lambda_A/\lambda_A^*)/x_A^*$

3. $\lim_{x_A \rightarrow 1} f_A = f_A^*$ (where * indicates pure substance)

1. $\lim_{x_A \rightarrow 1} f_{x,B}^o = 1$ (where o indicates infinite dilution)

1. $\lim_{x_A \rightarrow 1} \gamma_B = \gamma_B^o = 1$ (where o indicates infinite dilution)

2. $\gamma_B/f_{x,B} = x_A$

3. For ions in dilute aqueous solutions γ_B is a function of I and the hydration number h according to the Debye-Hückel theory and the Stokes-Robinson hydration theory (7.4, 7.20):

$$\gamma_B = -\ln 10 \cdot \frac{A \cdot z_B^2 \cdot I^{1/2}}{1 + B \cdot \hat{a} \cdot I^{1/2}} + h_B \cdot M_{H_2O} \cdot \hat{m} - \ln(1 + M_{H_2O}) \cdot \sum (m_B \cdot (1 - h_B)),$$

where A and B are temperature dependent constants: $A = 0.5215 \text{ (mol} \cdot \text{kg}^{-1})^{-1/2}$ and $B = 3.305 \text{ nm}^{-1} \cdot (\text{mol} \cdot \text{kg}^{-1})^{-1/2}$, \hat{a} is the ion size parameter (a length), \hat{m} is the osmolarity (§ 8.1). $h_{Cl^-} = 0$ by the Bates-Staples-Robinson convention (7.4).

4. A strong electrolyte B dissociating in solution into cations C and anions D according to

$$B \rightarrow v_C \cdot C + v_D \cdot D, \text{ i. e.}$$

$$\lambda_B = \lambda_C^o \cdot \lambda_D^o, \text{ is described in terms of 'mean ionic' quantities, indicated by subscript } \pm, \text{ e.g.:}$$

4.2	(substance) concentrational activity coefficient of solute B	$y_B = \frac{\lambda_B/c_B}{\lim_{x_A \rightarrow 1} (\lambda_B/c_B)}$		1. $\lim_{x_A \rightarrow 1} y_B^\infty = 1$ (where $^\infty$ indicates infinite dilution)	2.4.33
4.3	fugacity coefficient of component B (in a gas mixture)	$g_B = \lim_{p \rightarrow 0} \frac{\lambda_B/p_B}{(\lambda_B/p_B)}$		2. $\gamma_B/y_B = \varrho_A/\varrho_A^*$	A.I.6
5.1	active molality of solute B	$\tilde{m}_B = \gamma_B \cdot m_B$	mole per kilogram	1. $\lim_{x_A \rightarrow 1} \tilde{m}_B = m_B$.	
5.2	active (substance) concentration of solute B	$\tilde{c}_B = y_B \cdot c_B$	mole per litre	2. $\tilde{c}_B = \tilde{m}_B / M_B$	
5.3	fugacity; active partial pressure of component B (in a gas mixture)	$\tilde{p}_B = g_B \cdot p_B$	pascal	3. $\tilde{p}_B = \tilde{m}_B \cdot R_B T$	
6.0.1	(relative) activity of solvent A or of a component A (in a mixture)	$a_A = \lambda_A/\lambda_A^\ominus$ $x_A^\ominus = 1$		4. $\tilde{a}_A = \tilde{m}_A \cdot R_A T$	2.4.30 A.I.8

6.1. List of quantities and units. (continued)

§	Quantity	Unit	Name	Symbol	Remarks	References
	Name	Symbol and definition				
6.02	(relative) rational activity of solute B	$a_{x,B} = \lambda_B / \lambda_B^\ominus$ $f_{x,B}^\ominus \cdot x_B^\ominus = 1$			1. $a_{x,B} = f_{x,B} \cdot x_B$ 2. $a_{x,B}/\tilde{m}_B = M_A$	A.1.12
6.1	(relative) molal activity of solute B	$a_{m,B} = \lambda_B / \lambda_B^\ominus$ $\tilde{m}_B^\ominus = 1 \text{ mol} \cdot \text{kg}^{-1}$			1. $a_{m,B} = \tilde{m}_B / \tilde{m}_B^\ominus$ 2. This is the activity generally employed in clinical chemistry for an ion in solution when using ion-selective electrodes.	8.23.1 A.1.12
6.1.1	hydrogen ion exponent; pH	$\text{pH} = -\lg a_{m,H^+}$			3. For a strong electrolyte B, the standard reference system is defined by $\tilde{m}_{\pm B}^\ominus = 1 \text{ mol} \cdot \text{kg}^{-1}$ (see § 4.1 remark 4). It follows that $a_{m,B} = a_{m,C} \cdot a_{m,C}^\text{vp} = a_{m,\pm B}^{(vc+vp)}$ (from §§ 6.1, 5.1, 4.1). Analogous remarks apply in § 6.0.2 ($f_{x,\pm B}^\ominus \cdot x_{\pm B}^\ominus = 1$) and § 6.2 ($\tilde{c}_{\pm B}^\ominus = 1 \text{ mol} \cdot \text{l}^{-1}$).	10
6.2	(relative) (substance-) concentrational activity of solute B	$a_{c,B} = \lambda_B / \lambda_B^\ominus$ $\tilde{c}_B^\ominus = 1 \text{ mol} \cdot \text{l}^{-1}$			1. Sometimes pH is considered the name of the quantity rather than the symbol. 2. 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.	8-23.1 A.1.12
6.3	(relative) baric activity of component B (in a gas mixture)	$a_{p,B} = \lambda_B / \lambda_B^\ominus$ $\tilde{p}_B^\ominus = 101,325 \text{ kPa}$			1. $a_{p,B} = \tilde{p}_B / \tilde{p}_B^\ominus$ 2. Fugacity $\tilde{\rho}_B$ is used more generally than relative baric activity, $a_{p,B}$	1. $a_{x,B} = \alpha_{x,B}^\text{co} / f_{x,B}$, where $\alpha_{x,B}^\text{co}$ refers to infinite dilution. 2. $\alpha_{x,B} = \alpha_{x,B} / \tilde{p}_B$.
7.0	rational solubility coefficient of solute B			reciprocal pascal	$\text{Pa}^{-1} = \text{m} \cdot \text{kg}^{-1} \cdot \text{s}^2$	1. For the solvent A: $\alpha_{x,A} = \alpha_{x,A}^* / f_A$, where $\alpha_{x,A}^* = 1 / \tilde{p}_A^*$

7.1	molal solubility coefficient of solute B	$\alpha_{m,B} = m_B/\bar{p}_B$	mole per kilogram pascal	(mol/kg)/Pa = m · kg ⁻² · s ² · mol pascal	1. $\alpha_{m,B} = \alpha_m^{\infty}/\gamma_B$ 2. $\alpha_{m,B}^{\infty} = \bar{m}_B/\bar{p}_B$
7.2	(substance-) concentrational solubility coefficient of solute B	$\alpha_{c,B} = c_B/\bar{p}_B$	mole per litre pascal	(mol/l)/Pa = 10 ³ · m ⁻² · kg ⁻¹ · s ⁻² · mol pascal	1. $\alpha_{c,B} = \alpha_c^{\infty}/\gamma_B$ 2. $\alpha_{c,B}^{\infty} = \bar{c}_B/\bar{p}_B$
8.1	osmolality (of a solution)	$\hat{m} = -\frac{\ln a_A}{M_A}$	mole per kilogram	mole/mol	1. M_A is molar mass of the solvent A 2. The unit is not "osmol"/kg 3. $\bar{p}_A = \bar{p}_A^* \cdot \exp(-\hat{m} \cdot M_A)$, where \bar{p}_A^* is vapour pressure (fugacity) of pure solvent
8.2	molal osmotic coefficient (of a solution)	$\phi = \frac{\hat{m}}{\Sigma_B m_B}$	mole per litre	mol/l = 10 ³ · m ⁻³ · mol per litre	1. $\Sigma_B m_B$ is the molality of all the solutes 2. The unit is not "osmol"/l. 3. $\hat{c} = \hat{m} \cdot \varrho_A^*$ 4. Currently called "osmolarity" because "molarity" was formerly used for substance concentration.
8.3	osmotic concentration (of a solution)	$\hat{c} = \frac{-\ln a_A}{V_A^*}$	mole per litre	mol/l = 10 ³ · m ⁻³ · mol per litre	1. V_A^* is molar volume of pure solvent A 2. The unit is not "osmol"/l. 3. $\hat{c} = \hat{m} \cdot \varrho_A^*$ 4. Currently called "osmolarity" because "molarity" was formerly used for substance concentration.
8.4	concentrational osmotic coefficient (of a solution)	$\phi_c = \frac{\hat{c}}{\Sigma_B c_B}$	kelvin	K	1. $\Sigma_B c_B$ is the substance concentration of all solutes 2. $\Sigma_B c_B = c_A \frac{1 - x_A}{x_A}$ 3. $\lim_{x_A \rightarrow 1} \phi_c = \phi_c^{\infty} = 1$ 4. $\phi_c = \phi_m \cdot \varrho_A^* \varrho_A$
8.5	freezing point depression (of a solution)	$\Delta T_{fus} = T_{fus}^{\infty} - T_{fus}$	kelvin	kg · K · mol ⁻¹	1. T_{fus}^{∞} is the freezing point of pure solvent.
8.6	molal freezing point depression constant (of a solution)	$K_{fus} = \frac{\Delta T_{fus}}{\hat{m}}$	kelvin	kg · K · mol ⁻¹	1. It can be shown that K_{fus} is related to the specific enthalpy of melting, ΔH_w , and the freezing point, T_{fus} , of the solvent: $K_{fus} = R \cdot T_{fus}^2 / \Delta H_w$ 2. For aqueous solutions: $K_{fus} = 1.855 \text{ K/(mol/kg).}$
8.7	concentrational freezing point depression constant (of a solution)	$K_{fus,c} = \frac{\Delta T_{fus}}{\hat{c}}$	litre kelvin	1 · K · mol ⁻¹ K · mol ⁻¹	1. $K_{fus,c} = K_{fus} / \varrho_A^*$

6.1. List of quantities and units. (continued)

6.1.	Quantity	Unit		Remarks	References
§	Name	Symbol and definition	Name	Symbol	ISO 31 (7.12) IUPAC (7.21) Manual (7.8) CQUCC (7.8)
8.8	osmotic pressure (of a solution) $\Pi = - \int_{\mu_A^*}^{\mu_A} V_A^{-1} \cdot d\mu_A$	pascal	$P_A = m^{-1} \cdot kg \cdot s^{-2}$	1. Π is that pressure difference between the solution and the pure solvent (A) which provides the same chemical potential of the solvent in the solution and in the pure solvent. 2. Integration, assuming $V_A = V_A^*$ constant, gives the <i>van't Hoff</i> equation: $\Pi = - \frac{\mu_A - \mu_A^*}{V_A^*} = R \cdot T \cdot \bar{c}$	8–26.1
9.1	buffer capacity (for hydrogen ion) (in a solution) $B = \frac{\partial n_{H^+}}{\partial \lg a_{m,H^+}}$	mole	mol	1. n_{H^+} is amount of substance of added H^+ (stoichiometric amount of H^+). In order to maintain electroneutrality, H^+ must be added together with an indifferent ion (e. g. Cl^-) or in exchange for a cation (e. g. Na^+) 2. The independent variables are constant, usually T, p, n_B, \dots . Occasionally μ_B rather than n_B is considered the independent variable, e. g. p_{CO_2} rather than n_{CO_2} . This must be clearly specified, because the value of B will be different when either n_B or μ_B is constant 3. $d n_{H^+} = - dn_{Base} - \lg a_{m,H^+} = pH:$ $B = \frac{\partial n_{Base}}{\partial pH}.$ 4. The quantity has been defined for H^+ only, although similar quantities would apply for other components.	
9.2	buffer value; volumic buffer capacity (for hydrogen ion) (in a solution) $\beta = \frac{B}{V}$	mol/l = $10^3 \cdot m^{-3} \cdot mol$ per litre		1. For V constant: $\beta = \frac{\partial c_{o,H^+}}{\partial \lg a_{m,H^+}} = \frac{\partial c_{Base}}{\partial pH}.$ 2. Donald D. Wan Slyke first defined this quantity. The name 'slyke' is sometimes used as an unofficial unit: 1 slyke = 1 mol/l. 3. Other independent variables are constant	
9.3.1	(partial) molar buffer capacity of solute B	$B_{m,B} = \frac{\partial B}{\partial n_B}$		2. $B_{m,B} = \frac{\partial \beta}{\partial c_{o,B}}$ 3. For a H^+ binding group at pH = $pK_w \cdot B_{m,B} = 0,576$. 4. $\beta = \sum_B (B_{m,B} \cdot c_B)$	

9.3.2	(partial) specific buffer capacity of solute B	$B_{w,B} = \frac{\partial B}{\partial m_B}$	mole per kilogram	mol/kg	1. m_B is mass of added B 2. Other independent variables are con- stant
10.1	stoichiometric number of com- ponent B (in a chemical reac- tion)	v_B			3. $B_{w,B} = \frac{\partial \beta}{\partial Q_B}$ 4. $\beta = \Sigma_B (B_{w,B} \cdot Q_B)$
10.2	equilibrium constant (for a chemical reaction)	$K_a = \Pi_B (a_B)^{v_B}$			1. Base quantity (\approx number of entities, § 1.0) 2. $0 = \Sigma_B (v_B \cdot B)$ symbolizes a chemical reaction. 3. $v_B < 0$ for reactants, $v_B > 0$ for products 4. Equilibrium of a chemical reaction is characterized by: $0 = \Sigma_B (v_B \cdot \mu_B)$ or $0 = \Pi_B (\lambda_B)^{v_B}$
10.3.1	molal equilibrium product (for a chemical reaction)	$K_m = \Pi_B (m_B)^{v_B}$			1. The chemical reaction is $0 = \Sigma_B (v_B \cdot$ B) 2. a_B refers to the equilibrium system 3. The value of K_a depends on the choice of activity scale (choice of standard reference system), e. g. for solutes $a_{x,B}$, $a_{m,B}$ or $a_{e,B}$.
10.3.2	concentrational equilibrium product (for a chemical reac- tion)	$K_c = \Pi_B (c_B)^{v_B}$			4. $\Delta G_m^\ominus = \Sigma_B (v_B \cdot \mu_B^\ominus) =$ $- \Sigma_B (v_B \cdot (u_B - \mu_B^\ominus)) =$ $- R \cdot T \cdot \ln K_a$ where ΔG_m^\ominus is called the molar stan- dard Gibbs energy of reaction.
10.3.3	baric equilibrium product (for a chemical reaction)	$K_p = \Pi_B (p_B)^{v_B}$			Often hybrid equilibrium products are employed for practical purposes, e. g. calculation of $c_{\text{HCO}_3^-}$ from pH and p_{CO_2} : Reaction: $\text{CO}_2 + \text{H}_2\text{O} \rightleftharpoons \text{H}^+ + \text{HCO}_3^-$
					$K_{\text{hybrid}} = \frac{10^{-\text{pH}} \cdot c_{\text{HCO}_3^-}}{p_{\text{CO}_2}}$ $K_a = a_{m,\text{H}^+} \cdot a_{m,\text{HCO}_3^-}$ The relationship between the two is: $P_{\text{a}^{\Sigma_B}} = K_a \cdot \alpha_{m,\text{CO}_2} \cdot a_{\text{H}_2\text{O}} \cdot Q_{\text{H}_2\text{O}} / \gamma_{\text{HCO}_3^-}$ K_a and α_{m,CO_2} are temperature dependent constants. $a_{\text{H}_2\text{O}}$ varies with the total concentration of solutes. $Q_{\text{H}_2\text{O}}$ varies primarily with the concentra- tion of macro-molecules (e. g. proteins and lipids). $\gamma_{\text{HCO}_3^-}$ varies with ionic composition of the solution (ionic strength).

6.2 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.

6.2 §	System – Component(s) (specification)	Kind of quantity	Symbol	Typical numerical value	Unit	Remarks	Determination
1.1	Ecf – Hydrogen ion (titratable),	substance concen- tration	$c_{H^+}(Ecf)$	-1,6	mmol/l	Ecf = Extracellular fluid \approx blood + interstitial fluid. For purposes of calculation, Ecf in adults may be represented by a model: Ecf = 1 aB + 2 aP, i.e. arterial blood diluted 3 fold by its own plasma. Titratable means free + bound.	Titration of the model Ecf with strong acid or base to plasma $-pH = 7,40$ at $pCO_2 = 5,33$ kPa, $\theta = 37^\circ C$, and constant sO_2 (equal to that of arterial blood).
1.2	Ecf – Base (H^+ -bind- ing groups),	substance concen- tration difference	$\Delta c_{Base}(Ecf)$	+1,6	mmol/l	This quantity equals the former quantity with op- posite sign. Trivial names: Base excess (BE) of the extracellular fluid, or standard base excess (SBE).	Acidification of plasma, extraction of CO_2 into gas phase, and measurement of CO_2 in the gas phase, e.g. by gas-mass spectro- metry.
2.1	P – Carbon dioxide (total),	substance concen- tration	c_{CO_2}	25,6	mmol/l	$P = \text{plasma}$ Total CO_2 comprises: CO_2 (free dissolved), and HCO_3^- and CO_3^{2-} (and ion-pairs including these), $Pr-NH-COO^-$ (carbamino- CO_2).	Acidification of plasma, extraction of CO_2 into gas phase, and measurement of CO_2 in the gas phase, e.g. by gas-mass spectro- metry.
2.2	P – Carbonate + car- bon dioxide, aB – Oxygen (total),	substance concen- tration	$c_{CO_3^{2-}}$	25,6	mmol/l	This name is given in Ref. 7.9. Carbonate here means $CO_3^{2-} + HCO_3^- + H_2CO_3$	Oxidation of haemoglobin to haemiglobin, extraction of O_2 into a gas phase, and meas- urement of O_2 in the gas phase, e.g. by gas- mass spectrometry.
3.1	aB – Oxygen (total),	substance concen- tration	c_{O_2}	9,4	mmol/l	aB = arterial blood Total oxygen comprises: O_2 (free dissolved) + HbO_2 (haemoglobin-bound O_2).	Oxidation of haemoglobin to haemiglobin, extraction of O_2 into a gas phase, and meas- urement of O_2 in the gas phase, e.g. by gas- mass spectrometry.
3.2	aB – Dioxygen (free + Hb-bound)	substance concen- tration	c_{O_2}	9,4	mmol/l	This name is given in Ref. 7.9. Trivial name: oxygen content	
4.1	P – Calcium (total),	substance concen- tration	c_{Ca}	2,5	mmol/l	Total calcium comprises: Ca^{2+} (free ionized) + Ca (bound)	Gas-mass spectrometry or atomic absorp- tion spectrometry
4.2	P – Calcium(II) (Ca, total),	substance concen- tration	c_{Ca}	2,5	mmol/l	This name is given in Ref. 7.9. II is the oxidation state in Stock notation.	

6.3. 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 using a fixed value for the concentrational activity coefficient (γ) unless special circumstances warrant consideration of variations in ionic strength or mass concentration of water.

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

6.3	System-Component	Kind of quantity	Symbol	Numerical value	Unit	Determination	Cf. 6.1 §
1.1.1*	P –	pH		7,40		(measured with a pH electrode)	6.1.1
1.1.2	P – Hydrogen ion,	molal chemical potential	ψ_{m,H^+}	-43,9	kJ/mol	$\psi_{m,H^+} = - R \cdot T \cdot (\ln 10) \cdot \text{pH}$	2.9.3
1.1.3	P – Hydrogen ion,	molal activity	a_{m,H^+}	$39,8 \times 10^{-9}$		$a_{m,H^+} = 10^{-\text{pH}}$	6.1
1.1.4	P – Hydrogen ion,	active molality	\tilde{m}_{H^+}	39,8	nmol/kg	$\tilde{m}_{H^+} = a_{m,H^+} \cdot \tilde{m}_{H^+}^\ominus = 1 \text{ mol/kg}$	5.1
1.1.5	P – Hydrogen ion,	molality	m_{H^+}	51,7	nmol/kg	$m_{H^+} = \tilde{m}_{H^+} / \gamma_{H^+}$	3.3
1.1.6	P – Hydrogen ion,	concentrational activity	a_{c,H^+}	$39,5 \times 10^{-9}$		$a_{c,H^+} = \tilde{m}_{H^+} \cdot \varrho_{H_2O}^* / c_{H^+}$, $\tilde{c}_{H^+}^\ominus = 1 \text{ mol/l}$	6.2
1.1.7	P – Hydrogen ion,	active substance concentration	\tilde{c}_{H^+}	39,5	nmol/l	$\tilde{c}_{H^+} = \tilde{m}_{H^+} \cdot \varrho_{H_2O}^*$	5.2
1.1.8	P – Hydrogen ion,	substance concentration	c_{H^+}	48,2	nmol/l	$c_{H^+} = c_{H^+} / \gamma_{H^+} = m_{H^+} \cdot \varrho_{H_2O}$	3.4
1.2.1	P – Hydrogen ion,	molal activity coefficient	γ_{H^+}	0,77		Estimated from: $\ln \gamma_{H^+} = \ln \gamma_{Na^+} + (h_{H^+} - h_{Na^+}) \cdot M_{H_2O} \cdot \dot{m}_{Na^+}$ where $\gamma_{Na^+} = 0,75$ (6.3 § 5.2.1), $h_{H^+} = 8$, and $h_{Na^+} = 3,5$ (hydration numbers, Ref. 7.4, 7.20)	4.1
1.2.2	P – Hydrogen ion,	concentrational activity coefficient	y_{H^+}	0,82		$y_{H^+} = \gamma_{H^+} \cdot \varrho_{H_2O}^* / \varrho_{H_2O}$	4.2
1.3.1.	P –	buffer value (for H^+)	β	10,4	mmol/l	Determined by titrating plasma with strong acid or base in a closed system, i. e. c_{CO_2} constant (7.19)	9.2
1.3.2	P –	buffer value, (for H^+) (p_{CO_2} constant)	$\beta (p_{CO_2})$	64,3	mmol/l	Determined by titrating plasma with strong acid or base in an open system with constant p_{CO_2} (7.19)	9.2
1.3.3	P – Albumin,	molar buffer capacity (for H^+)	$B_{m,Alb}$	8,0		Determined as the slope of β as a function of c_{Alb}	9.3.1
1.3.4	P – Protein,	specific buffer capacity (for H^+)	$B_{s,Pr}$	0,11	mol/kg	Determined as the slope of β as a function of Q_{Pr}	9.3.2
2.1.1*	P – Carbon dioxide,	partial pressure	p_{CO_2}	5,33	kPa	Measured with a p_{CO_2} electrode	3.6; 5.3
2.1.2	P – Carbon dioxide,	active substance concentration	\tilde{c}_{CO_2}	1,32	mmol/l	$\tilde{c}_{CO_2} = p_{CO_2} \cdot \alpha_{c,CO_2}^\infty$	5.2
2.1.3	P – Carbon dioxide,	substance concentration	c_{CO_2}	1,22	mmol/l	$\tilde{c}_{CO_2} = p_{CO_2} \cdot \alpha_{c,CO_2}$	3.4
2.2.1	P – Carbon dioxide,	concentrational solubility coefficient	α_{c,CO_2}	0,230	mmol · 1 ⁻¹ · kPa ⁻¹	$\alpha_{c,CO_2} = \alpha_{c,CO_2}^\infty / y_{CO_2}$, Empirical temperature variation (7.1, 7.2) 7.19;	7.2
						$\lg \{\alpha_{c,CO_2}\} = \lg (0,230) - 9,20 \times 10^{-3} \cdot \{\Delta T\} + 90 \times 10^{-6} \cdot \{\Delta T\}^2$ where $\{\alpha_{c,CO_2}\} = \alpha_{c,CO_2}^\infty / (mmol \cdot l^{-1} \cdot kPa^{-1})$ and $\{\Delta T\} = (T - 310 \text{ K})$	

6.3. 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 (continued)

6.3 §	System-Component	Kind of quantity	Symbol	Numerical value	Unit	Determination	Cf. 6.1 §
2.2.2	P – Carbon dioxide,	molal activity coefficient	γ_{CO_2}	1,009		Empirical variation with the osmolarity (\hat{m}): $\ln \gamma_{CO_2} = 5,5 \cdot M_{H_2O} \cdot \hat{m} - 0,020$	4.1
2.2.3	P – Carbon dioxide,	concentrational activity coefficient	y_{CO_2}	1,074		$\gamma_{CO_2} = \gamma_{CO_2} \cdot Q_{H_2O}^* / Q_{H_2O}$	4.2
3.1.1*	P – Oxygen,	partial pressure	p_{O_2}	13,0	kPa	Measured with a p_{O_2} electrode	3.6; 5.3
3.1.2	P – Oxygen,	substance concentration	c_{O_2}	124	$\mu\text{mol/l}$	$c_{O_2} = p_{O_2} \cdot \alpha_{c,O_2}$	3.4
3.2.1	P – Oxygen,	concentrational solubility coefficient	α_{c,O_2}	9,55	$\mu\text{mol} \cdot l^{-1} \cdot k\text{Pa}^{-1}$	$\alpha_{c,O_2} = \sigma_{c,O_2}^{\infty} / y_{O_2}$	7.2
3.2.2	P – Oxygen,	molal activity coefficient	γ_{O_2}	1,03		Empirical variation with the osmolarity (\hat{m}): $\ln \gamma_{O_2} = 5,5 \cdot M_{H_2O} \cdot \hat{m}$	4.1
3.2.3	P – Oxygen,	concentrational activity coefficient	y_{O_2}	1,10		$y_{O_2} = \gamma_{O_2} \cdot Q_{H_2O}^* / Q_{H_2O}$	4.2
4.1.1	P – Hydrogen carbonate ion,	active molality	$\tilde{m}_{HCO_3^-}$	15,9	mmol/kg	$\tilde{m}_{HCO_3^-} = K_a \cdot p_{CO_2} \cdot a_{H_2O} \cdot 10^{pH} \cdot \alpha_{c,CO_2}^{\infty} / Q_{H_2O}^*$ K_a is the thermodynamic equilibrium constant (cf. 6.3 § 10.3).	5.1
4.1.2*	P – Hydrogen carbonate ion,	substance concentration	$c_{HCO_3^-}$	20,0	mmol/l	$c_{HCO_3^-} = \tilde{m}_{HCO_3^-} \cdot \varrho_{H_2O} / \gamma_{HCO_3^-}$ $c_{HCO_3^-}$, calculated as $c_{CO_2} - c_{CO_2}$ includes various ion pairs (e.g. NaHCO_3 , CaHCO_3^+ , CO_3^{2-} , and carbamate). Empirical equation (37°C): $c_{HCO_3^-} = 10^{pH} \cdot 6,74 \cdot p_{CO_2} \text{ mmol} \cdot l^{-1} \cdot k\text{Pa}^{-1}$. (7.1.14)	3.4
4.2.1	P – Hydrogen carbonate ion,	molal activity coefficient	$\gamma_{HCO_3^-}$	0,74		$\ln \gamma_{HCO_3^-} = \ln \gamma_{Na^+} + (h_{HCO_3^-} - h_{Na^+}) \cdot M_{H_2O} \cdot \hat{m}$, where $4,1$ $\gamma_{Na^+} = 0,75$ ($6,3$ § 5.2.1), $h_{Na^+} = 3,5$, and $h_{HCO_3^-} = 0$ (hydration numbers, Ref. 7.4, 7.20).	
4.2.2	P – Hydrogen carbonate ion,	concentrational activity coefficient	$y_{HCO_3^-}$	0,79		$y_{HCO_3^-} = \gamma_{HCO_3^-} \cdot p_{H_2O}^* / \varrho_{H_2O}$	4.2
5.1.1	P – Sodium ion,	active molality	\tilde{m}_{Na^+}	11,3	mmol/kg	Measured with ion selective electrode.	5.1
5.1.2*	P – Sodium ion,	substance concentration	c_{Na^+}	140	mmol/l	c_{Na^+} measured by flame spectrometry includes some bound Na^+ (e.g. NaHCO_3), possibly 1% for normal plasma	3.4
5.2.1	P – Sodium ion,	molal activity coefficient	γ_{Na^+}	0,75		$\gamma_{Na^+} = \tilde{m}_{Na^+} / (c_{Na^+} / \varrho_{H_2O})$.	4.2
6.1.1	P – Potassium ion,	active molality	\tilde{m}_{K^+}	3,2	mmol/kg	Measured with ion selective electrode.	5.1
6.1.2*	P – Potassium ion,	substance concentration	c_{K^+}	4,0	mmol/l	$c_{K^+} = (\tilde{m}_{K^+} / \gamma_{K^+}) \cdot \varrho_{H_2O}$ c_{K^+} measured by flame spectrometry includes some bound K^+ .	3.4
6.2.1	P – Potassium ion,	molal activity coefficient	γ_{K^+}	0,74		$\ln \gamma_{K^+} = \ln \gamma_{Na^+} + (h_{K^+} - h_{Na^+}) \cdot M_{H_2O} \cdot \hat{m}$, where $h_{K^+} = 1,9$ and $h_{Na^+} = 3,5$ (hydration numbers, Ref. 7.4, 7.20).	4.2
7.1.1	P – Calcium ion,	active molality	$\tilde{m}_{Ca^{2+}}$	0,38	mmol/kg	Measured with ion selective electrode.	5.1
7.1.2*	P – Calcium ion,	substance concentration	$c_{Ca^{2+}}$	1,15	mmol/l	$c_{Ca^{2+}} = (\tilde{m}_{Ca^{2+}} / \gamma_{Ca^{2+}}) \cdot \varrho_{H_2O}$	3.4
7.2.1	P – Calcium ion,	molal activity coefficient	$\gamma_{Ca^{2+}}$	0,31		$\ln \gamma_{Ca^{2+}} = 4 \cdot \ln \gamma_{Na^+} + (h_{Ca^{2+}} - 4 \cdot h_{Na^+}) / M_{H_2O} \cdot \hat{m} + 3 \cdot \ln (1 + M_{H_2O} \cdot \Sigma \{ [1 - h_B] \cdot m_B \})$	4.2

8.1.1	P –	freezing point depression	ΔT_{fus}	0,545	K	Measured by means of freezing point osmometer.	8.5
8.1.2*	P –	osmolality (0 °C)	\dot{m}	294	mmol/kg	$\dot{m} = \Delta T_{\text{fus}}/K_{\text{fus}}$	8.1
8.1.3	P –	osmotic concentration (0 °C)	\hat{c}	294	mmol/l	$\hat{c} = \Delta T_{\text{fus}}/K_{\text{fus},c}$	8.3
8.1.4	P – Solute,	substance concentration	c_{Solute}	300	mmol/l	$c_{\text{Solute}} = \hat{c}/\phi_c \approx 2 \cdot (c_{\text{Na}^+} + c_K^+) + c_{\text{Glucose}} + c_{\text{Carbamide}}$	10.4.3.4
8.1.5	P – Water,	activity (0 °C)	$a_{\text{H}_2\text{O}}$	0,9947		$- c_{\text{Pr}^-}$	
8.1.6	P –	osmotic pressure	P	758	kPa	$-\ln a_{\text{H}_2\text{O}} = \Delta T_{\text{fus}} \cdot M_{\text{H}_2\text{O}}/K_{\text{fus}}$, or from vapor pressure measurements:	6.01
8.1.7	P – Water,	vapor pressure (37 °C)	$p_{\text{H}_2\text{O}}$	6,24	kPa	$a_{\text{H}_2\text{O}} = p_{\text{H}_2\text{O}}/p_{\text{H}_2\text{O}}^*$.	8.1
8.1.8	P – Water,	mass concentration	$\varrho_{\text{H}_2\text{O}}$	0,933	kg/l	$P = R \cdot T \cdot \hat{c}$	8.8
8.1.9	P – Water,	substance concentration	$c_{\text{H}_2\text{O}}$	51,8	mol/l	Measured by means of vapor pressure osmometer	5.3
8.2.1	P –	molal osmotic coefficient	ϕ_m	0,92		$\varrho_{\text{H}_2\text{O}} = m_{\text{H}_2\text{O}}/V$.	3.1
8.2.2	P –	concentrational osmotic coefficient	ϕ_c	0,98		$c_{\text{H}_2\text{O}} = \varrho_{\text{H}_2\text{O}}/M_{\text{H}_2\text{O}}$	3.4
9	P – (water phase)	ionic strength	I	160	mmol/kg	Depends on the composition of the plasma.	8.4
10.1	Water –	vapor pressure (37 °C)	$p_{\text{H}_2\text{O}}^*$	6,275	kPa	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 120 mmol/kg to the ionic strength.	3.5
10.2	Water –	mass density (37 °C)	ϱ	0,9930	kg/l	Mass density of water equals mass concentration of water in pure water: $\varrho(\text{H}_2\text{O}) = \varrho_{\text{H}_2\text{O}}^*$.	3.1
10.3	Water –	equilibrium constant (37 °C)	K_a	$10^{-6,32}$		$K_a = a_{\text{m,H}^+} \cdot a_{\text{HCO}_3^-} / (a_{\text{m,CO}_2} \cdot a_{\text{H}_2\text{O}})$.	10.2
	$(\text{CO}_2 + \text{H}_2\text{O} \rightleftharpoons \text{H}^+ + \text{HCO}_3^-)$,					Determined by measuring $K_{\text{hybrid}} = \frac{a_{\text{m,H}^+} \cdot a_{\text{HCO}_3^-}}{c_{\text{CO}_2}}$ and extrapolating to infinite dilution. Varies with T (7.18):	
10.4.1	Water – Carbon dioxide, (infinite dilution)	concentrational solubility coefficient	$\alpha_{\text{c,CO}_2}^\infty$	0,247	mmol · l ⁻¹ · kPa ⁻¹	$-\lg K_a = 6,32 - 2,31 \cdot 10^{-3} \cdot \{\Delta T\} + 158 \cdot 10^{-6} \cdot (\Delta T)^2$, where $\{\Delta T\} = (T - 310,15 \text{ K})/\text{K}$.	7.2
10.4.2	Water – Oxygen, (infinite dilution)	concentrational solubility coefficient	$\alpha_{\text{c,CO}_2}^\infty$	10,50	μmol · l ⁻¹ · kPa ⁻¹	Empirical temperature variation (7.3): $\lg \{\alpha_{\text{c,CO}_2}^\infty\} = \lg (10,50) - 5 \times 10^{-3} \cdot \{\Delta T\} + 9 \times 10^{-5}$.	7.2
						$\{\alpha_{\text{c,CO}_2}^\infty\} = \alpha_{\text{c,CO}_2}^\infty / (\mu\text{mol} \cdot \text{l}^{-1} \cdot \text{kPa}^{-1})$, $\{\Delta T\} = (T - 310,15 \text{ K})/\text{K}$.	

6.4. Alphabetical index of symbols of kinds of quantities.

Symbols of physical or chemical quantities should be single letters of the Latin or Greek alphabet printed in sloping type (7.21). Unfortunately Greek letters of sloping type are unavailable for common typewriters. In the present document, Greek letters are printed in upright type and generally represent physical quantities, with the following exceptions (which should always be printed in upright type): Δ = difference, μ = prefix micro (not to be confused with μ = chemical potential), Π = product (not to be confused with Π = osmotic pressure), Σ = sum.

Sym-	Name	cf. 6.1
bol		§
<i>a</i>	relative activity	6.01
<i>a_c</i>	concentrational relative activity	6.2
<i>a_m</i>	molal relative activity	6.1
<i>a_p</i>	baric relative activity	6.3
<i>a_x</i>	rational relative activity	6.02
<i>B</i>	buffer capacity	9.1
<i>B_m</i>	molar buffer capacity	9.3
<i>B_w</i>	specific buffer capacity	9.4
(<i>b</i>)	(molality)	3.3
<i>c</i>	substance concentration	3.4
<i>c̄</i>	active substance concentration	5.2
<i>c̄̄</i>	osmotic concentration	8.3
<i>E</i>	energy	2.1
<i>E</i>	electromotive force	2.7
<i>F</i>	Faraday constant	(Remark 2)
<i>f</i>	activity coefficient	4.0.1
(<i>f</i>)	(fugacity)	5.3
<i>f_x</i>	rational activity coefficient	4.0.2
<i>G</i>	Gibbs energy	2.8
<i>g</i>	fugacity coefficient	4.3
<i>h</i>	hydration number	(Remark 3)
<i>I</i>	electric current	1.4
<i>I</i>	ionic strength	3.5
<i>K_a</i>	equilibrium constant	10.2
<i>K_c</i>	concentrational equilibrium product	10.3.2
<i>K_{fus}</i>	molal freezing point depression constant	8.6
<i>K_{fus,c}</i>	concentrational freezing point depression constant	8.7

<i>K_m</i>	molal equilibrium product	10.3.1
<i>K_p</i>	baric equilibrium product	10.3.3
<i>L</i>	Avogadro constant	(Remark 2)
<i>l</i>	length	1.1
<i>M</i>	molar mass	3.0
<i>m</i>	mass	1.2
<i>m̄</i>	molality	3.3
<i>m̄̄</i>	active molality	5.1
<i>m̄̄̄</i>	osmolality	8.1
<i>N</i>	number of entities	1.0
<i>n</i>	amount of substance	1.6
<i>p</i>	pressure	2.5
<i>p</i>	partial pressure	3.6
<i>p̄</i>	fugacity	5.3
<i>Q</i>	electric charge	2.6
<i>R</i>	molar gas constant	2.4.1
<i>S</i>	entropy	2.2
<i>s</i>	saturation fraction	3.2.1
<i>T</i>	thermodynamic temperature	1.5
ΔT_{fus}	freezing point depression	8.5
<i>t</i>	time	1.3
<i>U</i>	energy, internal	2.1
<i>V</i>	volume	2.4
(<i>V</i>)	(electric potential)	2.7
<i>V_m</i>	molar volume	(Remark 1)
<i>x</i>	substance fraction	3.2
<i>y</i>	concentrational activity coefficient	4.2
<i>z</i>	charge number	2.6.1
α_c	concentrational solubility coefficient	7.2
α_m	molal solubility coefficient	7.1
α_x	rational solubility coefficient	7.0
β	buffer value	9.2
γ	molal activity coefficient	4.1
θ	Celcius temperature	2.3
λ	absolute activity	2.1
μ	absolute chemical potential	2.9.1
$\tilde{\mu}$	electrochemical potential	2.9.2
<i>v</i>	stoichiometric number	10.1
	osmotic pressure	8.8
ϱ	mass concentration	3.1
ϱ	mass density	3.1
ϕ	electric potential	2.7
ϕ_c	concentrational osmotic coefficient	8.4
ϕ	molal osmotic coefficient	8.2
ψ	practical chemical potential	2.9.3

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