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CLINICAL CHEMISTRY

SCIENTIFIC COMMITTEE, ANALYTICAL SECTION
EXPERT PANEL ON pH AND BLOOD GASES†

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

(Recommendations 1983)

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1. INTRODUCTION

1.1. The IUPAC Commission on Quantities and Units in Clinical Chemistry has 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 with the Expert Panel on pH and Blood Gases of the International Federation of Clinical Chemistry.

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.

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.

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.

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:

$$c_B = n_B/V. \quad (1)$$

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. $n_{O,B}$, $c_{O,B}$. 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.):

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

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

$$\lambda_B = \exp(\mu_B / (R \cdot T)). \quad (3)$$

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

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

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:

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

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

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

The general practice in clinical chemistry is to report the substance concentration of the (free) component rather than the chemical activity. Exceptions to 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 below.

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:

$$\text{pH} = -\lg a_{m,H^+} = -\lg(\gamma_{H^+} \cdot m_{H^+} / \tilde{m}_{H^+}^\ominus) = -(\mu_{H^+} - \mu_{H^+}^\ominus) / (R \cdot T \cdot \ln 10). \quad (1)$$

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 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 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.

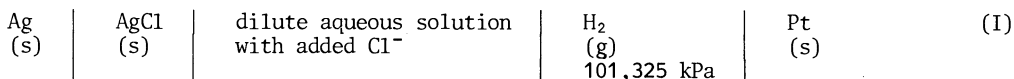
The present convention is based on the assumption that the molal activity coefficient of the chloride ion in dilute aqueous solutions ($I < 0,10 \text{ mol} \cdot \text{kg}^{-1}$) can be estimated by means of the *Debye-Hückel equation*:

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

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

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

$$\text{pH} = -(E_I + E_{II}^\ominus)/(R\cdot T\cdot F^{-1}\cdot \ln 10) + \lg(m_{\text{Cl}^-}/m_{\text{Cl}^-}^\ominus) + \lg\gamma_{\text{Cl}^-} \quad (3)$$

where $\tilde{m}_{\text{Cl}^-}^\ominus = 1 \text{ mol}\cdot\text{kg}^{-1}$. 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).

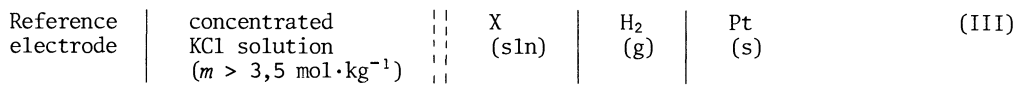
Note:

The standard electrode potential (E^\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:

$$\text{pH}(X) = \text{pH}(S) - (E(X) - E(S))/(R\cdot T\cdot F^{-1}\cdot \ln 10), \quad (4)$$

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 ($\text{mol}\cdot\text{l}^{-1}$) as substance concentration of H^+ is warranted, we recommend reporting the *active* substance concentration (\tilde{c}) of the hydrogen ions, calculated as:

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

where $\tilde{m}_{\text{H}^+}^\ominus = 1 \text{ mol}\cdot\text{kg}^{-1}$ and where $\rho_{\text{H}_2\text{O}}^*$ is the mass density of pure water ($=0,993 \text{ kg}\cdot\text{l}^{-1}$ at 37°C). For example, $\text{pH} = 7,40$ (as measured with a pH-electrode); the active substance concentration of hydrogen ion is then:

$$\tilde{c}_{\text{H}^+} = 10^{-7,40} \cdot (0,993 \text{ kg}\cdot\text{l}^{-1}) \cdot \text{mol}\cdot\text{kg}^{-1} = 39,81 \times 10^{-9} \times 0,993 \text{ mol}\cdot\text{l}^{-1} = 39,53 \text{ nmol}\cdot\text{l}^{-1}.$$

For many practical purposes the mass density of pure water may be taken to be $1,00 \text{ kg}\cdot\text{l}^{-1}$ 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 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:

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

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

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

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

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 (7.16). 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 the value consequently is a pure number. Example: $\text{pH} = 7,40$, *not* $\text{pH} = 7,40 \text{ pH units}$, and *not* $\text{pH} = 7,40 \text{ bel}$.

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

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

$\alpha_{x,B}^{\infty}$ 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 ($\approx 0,018 \text{ kg}\cdot\text{mol}^{-1}$):

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

The unit of osmolality is $\text{mol}\cdot\text{kg}^{-1}$ (not 'osmol'·kg⁻¹).

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

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

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

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:

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

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 vapour pressure ($p_{\text{H}_2\text{O}}$) measured at 37 °C:

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

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_{SOLUTES}), the ratio between the two quantities being the molal osmotic coefficient (ϕ_m), which is generally close to unity for biological fluids:

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

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

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 ($^\infty$) (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 equations 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 (7.12) 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 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	
§	Name	Symbol and definition	Name	Symbol
1.0	number of entities	N		
1.1	length	l	metre	m
1.2	mass	m	kilogram	kg
1.3	time	t	second	s
1.4	electric current	I	ampere	A
1.5	thermodynamic temperature	T	kelvin	K
1.6	amount of substance	n	mole	mol
2.1	energy	$E = m \cdot c^2$	joule	J = $\text{m}^2 \cdot \text{kg} \cdot \text{s}^{-2}$
2.2	entropy	$S = \int T^{-1} \cdot dU$ $dV=0, dQ=0, dn_B=0$	joule per kelvin	$\text{J} \cdot \text{K}^{-1}$ = $\text{m}^2 \cdot \text{kg} \cdot \text{s}^{-2} \cdot \text{K}^{-1}$
2.3	Celsius temperature	$\theta = T - T_0$ $T_0 = 273,15 \text{ K}$	degree Celsius	$^{\circ}\text{C}$
2.4	volume	$V = l^3$	cubic metre, litre	m^3 l = dm^3
2.4.1	(partial) molar volume of component B	$V_B = (\partial V / \partial n_B)_{T,p,n_C,\dots}$	litre per mole	$l \cdot \text{mol}^{-1}$
2.5	pressure	$p = -(\partial U / \partial V)_{S,Q,n_B}$	pascal	Pa = $\text{J} \cdot \text{m}^{-3}$ = $\text{m}^{-1} \cdot \text{kg} \cdot \text{s}^{-2}$
2.6	electric charge; quantity of electricity	$Q = \int I \cdot dt$	coulomb	C = $\text{s} \cdot \text{A}$

6.1	Remarks	References		
		ISO 31 (7.12)	IUPAC Manual (7.21)	CQUCC EPQUCC (7.8)
§				
1.0	1. Base quantity.	8-2.1	2.3.05	
1.1	1. Base quantity and SI base unit.	1-3.1	2.1.01	4.1
1.2	1. Base quantity and SI base unit. 2. In the present text <i>m</i> indicates mass, whereas <i>m</i> is molality (§ 3.3)	3-1.1	2.2.01	4.4
1.3	1. Base quantity and SI base unit.	1-6.1	2.1.12	4.23
1.4	1. Base quantity and SI base unit.	5-1.1	2.6.05	
1.5	1. Base quantity and SI base unit.	4-1.1	2.4.01	4.18
1.6	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 Avogadro constant.	8-3.1	2.3.06	4.6
2.1	1. This definition (the Einstein 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). 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).	4-19.1	2.4.07	
2.2		4-17.1	2.4.06	
2.3	1. $1^\circ\text{C} = 1 \text{ K}$. 2. Alternative symbol: <i>t</i> .	4-2.1	2.4.02	4.19
2.4	1. The definition applies for a cube. 2. In the present context the litre is employed as the unit for volume. 3. The capital L has been adopted by CGPM as an alternative symbol for litre to avoid confusion with the number 1.	1-5.1	2.1.11	4.3
2.4.1	1. The molar volume of a pure substance A is: $V_m = V/n$. 2. For an ideal gas: $V_m = R \cdot T/p$. $V_m \approx (22\,413,83 \pm 0,70) \times 10^{-6} \text{ m}^3 \cdot \text{mol}^{-1}$ for $T = 273,15 \text{ K}$ and $p = 101,325 \text{ kPa}$. 3. The molar gas constant is $R \approx (8,314\,41 \pm 0,000\,26) \cdot \text{J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ 4. $V = \sum(V_B \cdot n_B)$.	8-6.1	1.4	
2.5	1. Pressure is often defined as the force perpendicular to a surface divided by the area of that surface. This may give the erroneous implication that pressure is a vector. 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. Alternative symbol: <i>P</i> .	3-13.1	2.2.19	4.21
2.6	1. The elementary charge is $e \approx (160,218\,92 \pm 0,000\,46) \times 10^{-21} \text{ C}$. 2. The Faraday constant is $F = e \cdot L \approx (96\,484,56 \pm 0,27) \cdot \text{C} \cdot \text{mol}^{-1}$.	5-2.1	2.6.02	

6.1 Quantity		Unit		
§	Name	Symbol and definition	Name	Symbol
2.6.1	charge number of component B	$z_B = Q_B/e$		
2.7	electric potential; electromotive force	$\phi = (\partial U/\partial Q)_{V,S,n_B}$	volt	V =J·C ⁻¹ =m ² ·kg·s ⁻³ ·A ⁻¹
2.8	Gibbs energy	$G = U + p·V - T·S$	joule	J =m ² ·kg·s ⁻²
2.9.1	(absolute) chemical potential of component B	$\mu_B = (\partial U/\partial n_B)_{V,S,Q,n_C,\dots}$	joule per mole	J·mol ⁻¹ =m ² ·kg·s ⁻² ·mol ⁻¹
2.9.2	(absolute) electrochemical potential of component B	$\tilde{\mu}_B = (\partial U/\partial n_B)_{V,S,n_C,\dots}$	joule per mole	J·mol ⁻¹ =m ² ·kg·s ⁻² ·mol ⁻¹
2.9.3	(practical) chemical potential of component B	$\psi_B = \mu_B - \mu_B^e$	joule per mole	J·mol ⁻¹ =m ² ·kg·s ⁻² ·mol ⁻¹
2.10	absolute activity of component B	$\lambda_B = \exp(\mu_B/(R·T))$		
3.0	molar mass	$M = m/n$	kilogram per mole	kg·mol ⁻¹
3.1	mass concentration of component B	$\rho_B = m_B/V$	kilogram per litre	kg·l ⁻¹ =10 ³ ·m ⁻³ ·kg
3.1.1	(mass) density	$\rho = m/V$	kilogram per litre	kg·l ⁻¹ =10 ³ ·m ⁻³ ·kg
3.2	(amount-of-)substance fraction; mole fraction of component B	$x_B = n_B/(n_B+n_C+\dots)$		
3.2.1	saturation fraction of component B	$s_B = n_B/n_B(\text{sat})$		
3.3	molality of solute B	$m_B = n_B/m_A$	mole per kilogram	mol·kg ⁻¹
3.4	(amount-of-)substance concentration of component B	$c_B = n_B/V$	mole per litre	mol·l ⁻¹

6.1	Remarks	References		
		ISO (7.12)	IUPAC Manual (7.21)	CQUCC EPQUCC (7.8)
§				
2.6.1	1. q_B is the charge of one B elementary entity (molecule, ion).	8-41.1	2.7.02	4.4
2.7	1. ϕ is preferred for inner electric potential. Other symbols: V (in the present context V = volume), E (preferred for electromotive force).	5-6.1	2.6.07	
2.8	1. $dG = V \cdot dp - S \cdot dT + \phi \cdot dQ + \sum(\mu_B \cdot dn_B)$.	4-19.4	2.4.12	
2.9.1	1. Only differences in μ_B can be measured (§2.9.3). 2. $\mu_B = (\partial G / \partial n_B)_{p, T, Q, n_B, \dots}$. 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: $\Delta\mu_B = z_B \cdot F \cdot \Delta E$	8-17.1	2.4.25 A.I.1	
2.9.2	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	
2.9.3	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), $\psi_{m, B}$ (§6.2), $\psi_{c, B}$ (§6.3), $\psi_{p, B}$ (§6.4). 3. $\psi_B = R \cdot T \cdot \ln a_B$ (where a_B is relative activity).		Ref. 7.15	
2.10	1. Only the relative λ_B can be measured (§§ 6.1.1, 6.1.2, 6.2, 6.3, 6.4).	8-18.1	2.4.26 A.I.1	
3.0	1. The name 'dalton' is sometimes used as unofficial unit: 1 dalton = 1 g·mol ⁻¹ .			
3.1		8-11.2	2.3.12	4.8
3.1.1	1. The mass density of the solvent A equals the mass concentration of A in pure A: $\rho(A) = \rho_A^*$.	8-11.1		
3.2		8-15.1	2.3.07	4.13
3.2.1	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.			
3.3	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. 3. $m_B = x_B / (x_A \cdot M_A)$.	8-16.1	2.3.10	4.12
3.4	1. $c_B = M_B \cdot \rho_B$. 2. $c_B = m_B \cdot \rho_A$. 3. The symbol [B] is often employed for c_B .	8-13.1	2.3.11	4.11

6.1 Quantity		Unit		
§	Name	Symbol and definition	Name	Symbol
3.5	ionic strength	$I = \frac{1}{2} \cdot \sum (z_B^2 \cdot m_B)$	mole per kilogram	$\text{mol} \cdot \text{kg}^{-1}$
3.6	partial pressure of component B	$p_B = x_B \cdot p$	pascal	Pa $= \text{m}^{-1} \cdot \text{kg} \cdot \text{s}^{-2}$
4.0.1	activity coefficient of solvent A or of component A (in a mixture)	$f_A = (\lambda_A/x_A) / \lim_{x_A \rightarrow 1} (\lambda_A/x_A)$		
4.0.2	rational activity coefficient of solute B	$f_{x,B} = (\lambda_B/x_B) / \lim_{x_A \rightarrow 1} (\lambda_B/x_B)$		
4.1	molal activity coefficient of solute B	$\gamma_B = (\lambda_B/m_B) / \lim_{x_A \rightarrow 1} (\lambda_B/m_B)$		
4.2	(substance)concentrational activity coefficient of solute B	$y_B = (\lambda_B/c_B) / \lim_{x_A \rightarrow 1} (\lambda_B/c_B)$		
4.3	fugacity coefficient of component B (in a gas mixture)	$g_B = (\lambda_B/p_B) / \lim_{p \rightarrow 0} (\lambda_B/p_B)$		

6.1	Remarks	References		
§		ISO 31 (7.12)	IUPAC Manual (7.21)	CQUCC EPQUCC (7.8)
3.5	1. Sometimes ionic strength is calculated from substance concentration (symbol I_O). It is preferable, however, always to define ionic strength on the basis of molality.	8-45.1	2.4.29	
3.6	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.	8-19.1	A.I.5	4.22
4.0.1	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. $\lim_{x_A \rightarrow 1} f_A = f_A^* = 1$ (where * indicates pure substance).	8-22.1	2.3.31 A.I.7 A.I.14	
4.0.2	1. $\lim_{x_A \rightarrow 1} f_{x,B} = f_{x,B}^\infty = 1$ (where ∞ indicates infinite dilution).		A.I.11	
4.1	1. $\lim_{x_A \rightarrow 1} \gamma_B = \gamma_B^\infty = 1$ (where ∞ indicates infinite dilution). 2. $\gamma_B/f_{x,B} = x_A$. 3. For ions in dilute aqueous solutions γ is a function of I and the hydration number h according to the <i>Debye-Hückel</i> theory and the <i>Stokes-Robinson</i> hydration theory (7.4, 7.20): $\ln \gamma_B = -(\ln 10) \cdot z_B^2 \cdot A \cdot I^{1/2} / (1 + \hat{a} \cdot B \cdot I^{1/2}) + h_B \cdot M_{H_2O} \cdot \hat{m} - \ln(1 + M_{H_2O} \cdot \Sigma(m_B \cdot (1 - h_B)))$ 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 osmolality (§8.1). $h_{Cl^-} = 0$ by the <i>Bates-Staples-Robinson</i> convention (7.4). 4. A strong electrolyte B dissociating in solution into cations C and anions D according to $B \rightarrow \nu_C \cdot C + \nu_D \cdot D, \text{ i.e. } \lambda_B = \lambda_C^{\nu_C} \cdot \lambda_D^{\nu_D}$ is described in terms of 'mean ionic' quantities, indicated by subscript \pm , e.g.: $\lambda_{\pm B} = (\lambda_C^{\nu_C} \cdot \lambda_D^{\nu_D})^{1/(\nu_C + \nu_D)} \quad (\S 2.10)$ $m_{\pm B} = (m_C^{\nu_C} \cdot m_D^{\nu_D})^{1/(\nu_C + \nu_D)} \quad (\S 3.3)$ $\gamma_{\pm B} = (\gamma_C^{\nu_C} \cdot \gamma_D^{\nu_D})^{1/(\nu_C + \nu_D)} \quad (\S 4.1)$ $m_{\pm B} = (m_C^{\nu_C} \cdot m_D^{\nu_D})^{1/(\nu_C + \nu_D)} \quad (\S 5.1)$ $a_{\pm m, B} = (a_{m, C}^{\nu_C} \cdot a_{m, D}^{\nu_D})^{1/(\nu_C + \nu_D)} \quad (\S 6.1)$ Analogous definitions and equations apply for $x_{\pm B}$, $f_{x_{\pm B}}$, $a_{x_{\pm B}}$ (§§ 3.2, 4.0.2, 6.0.2) and $e_{\pm B}$, $y_{\pm B}$, $\hat{e}_{\pm B}$, $\alpha_{e_{\pm B}}$ (§§ 3.4, 4.2, 5.2, 6.2).	8-24.1	2.4.32 A.I.11	
4.2	1. $\lim_{x_A \rightarrow 1} y_B = y_B^\infty = 1$ (where ∞ indicates infinite dilution). 2. $\gamma_B/y_B = \rho_A/\rho_A^*$.		2.4.33	
4.3	1. $\lim_{\rho \rightarrow 0} g_B = 1$.		A.I.6	

6.1 Quantity		Unit		
§	Name	Symbol and definition	Name	Symbol
5.1	active molality of solute B	$\tilde{m}_B = \gamma_B \cdot m_B$	mole per kilogram	$\text{mol} \cdot \text{kg}^{-1}$
5.2	active (substance) concentration of solute B	$\tilde{c}_B = \gamma_B \cdot c_B$	mole per litre	$\text{mol} \cdot \text{l}^{-1}$ $= 10^3 \cdot \text{m}^{-3} \cdot \text{mol}$
5.3	fugacity; active partial pressure of component B (in a gas mixture)	$\tilde{p}_B = g_B \cdot p_B$	pascal	Pa $= \text{m}^{-1} \cdot \text{kg} \cdot \text{s}^{-1}$
6.0.1	(relative) activity of solvent A or of a component a (in a mixture)	$a_A = \lambda_A / \lambda_A^\ominus$ $x_A^\ominus = 1$		
6.0.2	(relative) rational activity of solute B	$a_{x,B} = \lambda_B / \lambda_B^\ominus$ $f_{x,B}^\ominus \cdot x_B^\ominus = 1$		
6.1	(relative) molal activity of solute B	$a_{m,B} = \lambda_B / \lambda_B^\ominus$ $\tilde{m}_B^\ominus = 1 \text{ mol} \cdot \text{kg}^{-1}$		
6.1.1	hydrogen ion exponent; pH	$\text{pH} = -\lg a_{m,\text{H}^+}$		
6.2	(relative) (substance-) concentrational activity of solute B	$a_{c,B} = \lambda_B / \lambda_B^\ominus$ $\tilde{c}_B^\ominus = 1 \text{ mol} \cdot \text{l}^{-1}$		
6.3	(relative) baric activity of component B (in gas mixture)	$a_{p,B} = \lambda_B / \lambda_B^\ominus$ $\tilde{p}_B^\ominus = 101,325 \text{ kPa}$		

6.1	Remarks	References		
		ISO 31 (7.12)	IUPAC Manual (7.21)	CQUCC EPQUCC (7.8)
5.1	1. The symbol \tilde{m} was chosen in analogy with the symbol \tilde{p} for fugacity (§5.3). 2. Sometimes this quantity is called the molal activity, but it should be distinguished from <i>relative</i> molal activity (§6.1) which is dimensionless. 3. $\lim_{x_A \rightarrow 1} \tilde{m}_B = m_B$.			
5.2	1. The symbol \tilde{c} was chosen in analogy with the symbol \tilde{p} for fugacity (§5.3). 2. Sometimes this quantity is called the concentrational activity, but it should be distinguished from <i>relative</i> concentrational activity (§6.2) which is dimensionless. 3. $\lim_{x_A \rightarrow 1} \tilde{c}_B = c_B$. 4. $\tilde{c}_B/\tilde{m}_B = \rho_A^*$.			
5.3	1. The symbol \tilde{p} is preferred in this context. An alternative symbol is f . 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 (§3.6) and the fugacity of a component in a solution are identical. See also introductory section 4.1. 3. $\lim_{p \rightarrow 0} \tilde{p}_B = p_B$.	8.20.1	2.4.27 A.I.6	
6.0.1	1. $\alpha_A = \lambda_A/\lambda_A^*$. 2. $\alpha_A = f_A \cdot x_A$.		2.4.30 A.I.8	
6.0.2	1. $\alpha_{x,B} = f_{x,B} \cdot x_B$. 2. $\alpha_{x,B}/\tilde{m}_B = M_A$.		A.I.12	
6.1	1. $\alpha_{m,B} = \tilde{m}_B/\tilde{m}_B^\ominus$. 2. This is the activity generally employed in clinical chemistry for an ion in solution when using ion-selective electrodes. 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 $\alpha_{m,B} = a_{m,C}^{\nu_C} \cdot a_{m,D}^{\nu_D} = \alpha_{m\pm B}^{(\nu_C + \nu_D)}$ (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 ($\tilde{c}_{\pm B}^\ominus = 1 \text{ mol} \cdot \text{l}^{-1}$).	8-23.1	A.I.12	
6.1.1	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 $3,5 \text{ mol} \cdot \text{kg}^{-1}$. Reference solutions with known pH have been described. See also introductory section 3.		10	
6.2	1. $\alpha_{c,B} = \tilde{c}_B/\tilde{c}_B^\ominus$.	8-23.1	A.I.12	
6.3	1. $\alpha_{p,B} = \tilde{p}_B/\tilde{p}_B^\ominus$. 2. Fugacity, \tilde{p}_B , is used more generally than relative baric activity, $\alpha_{p,B}$.			

6.1 Quantity		Unit		
§	Name	Symbol and definition	Name	Symbol
7.0	rational solubility coefficient of solute B	$\alpha_{x,B} = x_B/\tilde{p}_B$	reciprocal pascal	Pa^{-1} $=\text{m}\cdot\text{kg}^{-1}\cdot\text{s}^2$
7.1	molal solubility coefficient of solute B	$\alpha_{m,B} = m_B/\tilde{p}_B$	mole per kilogram pascal	$\text{mol}\cdot\text{kg}^{-1}\cdot\text{Pa}^{-1}$ $=\text{m}\cdot\text{kg}^{-1}\cdot\text{s}^2\cdot\text{mol}$
7.2	(substance-)concentrational solubility coefficient of solute B	$\alpha_{c,B} = c_B/\tilde{p}_B$	mole per litre pascal	$\text{mol}\cdot\text{l}^{-1}\cdot\text{Pa}^{-1}$ $=10^3\cdot\text{m}^{-2}\cdot\text{kg}^{-1}\cdot\text{s}^2\cdot\text{mol}$
8.1	osmolality (of a solution)	$\hat{m} = (-\ln a_A)/M_A$	mole per kilogram	$\text{mol}\cdot\text{kg}^{-1}$
8.2	molal osmotic coefficient (of a solution)	$\phi_m = \hat{m}/\Sigma_B m_B$		
8.3	osmotic concentration (of a solution)	$\hat{c} = (-\ln a_A)/V_A^*$	mole per litre	$\text{mol}\cdot\text{l}^{-1}$ $=10^3\cdot\text{m}^{-3}\cdot\text{mol}$
8.4	concentrational osmotic coefficient (of a solution)	$\phi_c = \hat{c}/\Sigma_B c_B$		
8.5	freezing point depression (of a solution)	$\Delta T_{\text{fus}} = T_{\text{fus}}^\infty - T_{\text{fus}}$	kelvin	K
8.6	molal freezing point depression constant (of a solution)	$K_{\text{fus}} = \Delta T_{\text{fus}}/\hat{m}$	kilogram kelvin per mole	$\text{kg}\cdot\text{K}\cdot\text{mol}^{-1}$
8.7	concentrational freezing point depression constant (of a solution)	$K_{\text{fus},c} = \Delta T_{\text{fus}}/\hat{c}$	litre kelvin per mole	$1\cdot\text{K}\cdot\text{mol}^{-1}$ $=10^{-3}\cdot\text{m}^3\cdot\text{K}\cdot\text{mol}^{-1}$
8.8	osmotic pressure (of a solution)	$\Pi = - \int_{\mu_A^*}^{\mu_A} V_A^{-1} \cdot d\mu_A$	pascal	Pa $=\text{m}^{-1}\cdot\text{kg}\cdot\text{s}^{-2}$
9.1	buffer capacity (for hydrogen ion) (in a solution)	$B = (\partial n_{\text{H}^+}/\partial \lg a_{m,\text{H}^+})$	mole	mol

6.1	Remarks	References
§		ISO 31 IUPAC CQUCC (7.12) Manual EPQUCC (7.21) (7.8)
7.0	<ol style="list-style-type: none"> $\alpha_{x,B} = \alpha_{x,B}^{\infty} / f_{x,B}$, where $\alpha_{x,B}^{\infty}$ refers to infinite dilution. $\alpha_{x,B}^{\infty} = \alpha_{x,B} / \tilde{p}_B$. For the solvent A: $\alpha_{x,A} = \alpha_{x,A}^* / f_A$, where $\alpha_{x,A}^* = 1 / \tilde{p}_A^*$. 	
7.1	<ol style="list-style-type: none"> $\alpha_{m,B} = \alpha_{m,B}^{\infty} / \gamma_B$. $\alpha_{m,B}^{\infty} = \tilde{m}_B / \tilde{p}_B$. 	
7.2	<ol style="list-style-type: none"> $\alpha_{c,B} = \alpha_{c,B}^{\infty} / \gamma_B$. $\alpha_{c,B}^{\infty} = \tilde{c}_B / \tilde{p}_B$. 	
8.1	<ol style="list-style-type: none"> M_A is molar mass of the solvent A. The unit is not 'osmol'·kg⁻¹. $\tilde{p}_A = \tilde{p}_A^* \cdot \exp(-\hat{m} \cdot M_A)$, where \tilde{p}_A^* is vapour pressure (fugacity) of pure solvent. 	
8.2	<ol style="list-style-type: none"> $\Sigma_B m_B$ is the molality of all the solutes. $\Sigma_B m_B = (1 - x_A) / (x_A \cdot M_A)$. $\lim_{x_A \rightarrow 1} \phi_m = \phi_m^{\infty} = 1$. 	8-24.2 A.I.13
8.3	<ol style="list-style-type: none"> V_A^* is molar volume of pure solvent A. The unit is not 'osmol'·l⁻¹. $\hat{c} = \hat{n} \cdot \rho_A^*$. Currently called 'osmolality' because 'molarity' was formerly used for substance concentration. 	
8.4	<ol style="list-style-type: none"> $\Sigma_B c_B$ is the substance concentration of all solutes. $\Sigma_B c_B = c_A \cdot (1 - x_A) / x_A$. $\lim_{x_A \rightarrow 1} \phi_c = \phi_c^{\infty} = 1$. $\phi_c = \phi_m \cdot \rho_A^* / \rho_A$. 	
8.5	<ol style="list-style-type: none"> T_{fus}^{∞} is the freezing point of pure solvent. 	
8.6	<ol style="list-style-type: none"> 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: $K_{fus} = R \cdot T_{fus}^2 / \Delta H_w$. For aqueous solutions: $K_{fus} = 1,855 \text{ kg} \cdot \text{K} \cdot \text{mol}^{-1}$. 	
8.7	<ol style="list-style-type: none"> $K_{fus,c} = K_{fus} / \rho_A^*$. 	
8.8	<ol style="list-style-type: none"> 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. Integration, assuming $V_A = V_A^* = \text{constant}$, gives the <i>van't Hoff</i> equation: $\Pi = -(\mu_A - \mu_A^*) / V_A^* = R \cdot T \cdot \hat{c}$. 	8-26.1
9.1	<ol style="list-style-type: none"> 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 anion (e.g. Cl⁻) or in exchange for a cation (e.g. Na⁺). Other 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. $dn_{H^+} = -dn_{Base}$; $-\lg a_{m,H^+} = \text{pH}$; $B = (\partial n_{Base} / \partial \text{pH})$. 	

(Cont.)

6.1 Quantity		Unit		
§	Name	Symbol and definition	Name	Symbol
9.1 (cont.)				
9.2	buffer value; volumic buffer capacity (for hydrogen ion) (in a solution)	$\beta = B/V$	mole per litre	$\text{mol}\cdot\text{l}^{-1}$ $=10^{-3}\cdot\text{m}^{-3}\cdot\text{mol}$
9.3.1	(partial) molar buffer capacity of solute B	$B_{m,B} = (\partial B/\partial n_B)$		
9.3.2	(partial) specific buffer capacity of solute B	$B_{w,B} = (\partial B/\partial m_B)$	mole per kilogram	$\text{mol}\cdot\text{kg}^{-1}$
10.1	stoichiometric number of component B (in a chemical reaction)	ν_B		
10.2	equilibrium constant (for a chemical reaction)	$K_a = \prod_B (a_B)^{\nu_B}$		
10.3.1	molal equilibrium product (for a chemical reaction)	$K_m = \prod_B (m_B)^{\nu_B}$		$(\text{mol}\cdot\text{kg}^{-1})^{\sum \nu_B}$
10.3.2	concentrational equilibrium product (for a chemical reaction)	$K_c = \prod_B (c_B)^{\nu_B}$		$(\text{mol}\cdot\text{l}^{-1})^{\sum \nu_B}$
10.3.3	baric equilibrium product (for a chemical reaction)	$K_p = \prod_B (p_B)^{\nu_B}$		$(\text{Pa})^{\sum \nu_B}$

6.1	Remarks	References		
§		ISO	IUPAC Manual	CQUCC EPQUCC
		(7.12)	(7.21)	(7.8)
9.1	4. The quantity has been defined for H ⁺ only, although similar (cont.) quantities would apply for other components.			
9.2	1. For <i>V</i> constant: $\beta = (\partial c_{O,H^+} / \partial \lg a_{m,H^+}) = (\partial c_{Base} / \partial pH)$. 2. <i>Donald D. Van Slyke</i> first defined this quantity. The name 'slyke' is sometimes used as an unofficial unit: 1 slyke = 1 mol·l ⁻¹ .			
9.3.1	1. Other independent variables are constant. 2. $B_{m,B} = (\partial \beta / \partial c_{O,B})$. 3. For a H ⁺ binding group at pH = pK _a : $B_{m,B} = 0,576$. 4. $\beta = \Sigma_B (B_{m,B} \cdot c_B)$.			
9.3.2	1. m_B is mass of added B. 2. Other independent variables are constant. 3. $B_{w,B} = (\partial \beta / \partial \rho_B)$. 4. $\beta = \Sigma_B (B_{w,B} \cdot \rho_B)$.			
10.1	1. Base quantity (\approx number of entities, §1.0). 2. $0 = \Sigma_B (\nu_B \cdot B)$ symbolizes a chemical reaction, 3. $\nu_B < 0$ for reactants, $\nu_B > 0$ for products. 4. Equilibrium of a chemical reaction is characterized by: $0 = \Sigma_B (\nu_B \cdot \mu_B)$ or $0 = \Pi_B (\lambda_B)^{\nu_B}$.			
10.2	1. The chemical reaction is $0 = \Sigma_B (\nu_B \cdot B)$. 2. α_B refers to the equilibrium system. 3. The value of K_α depends on the choice of activity scale (choice of standard reference system), e.g. for solutes $a_{x,B}$, $a_{m,B}$, or $a_{c,B}$. 4. $\Delta G_m^\ominus = \Sigma_B (\nu_B \cdot \mu_B^\ominus) = -\Sigma_B (\nu_B \cdot (\mu_B - \mu_B^\ominus)) = -R \cdot T \cdot \ln K_\alpha$ where ΔG_m^\ominus is called the molar standard Gibbs energy of reaction.			
10.3.1	1. Often hybrid equilibrium products are employed for practical purposes, e.g. calculation of $c_{HCO_3^-}$ from pH and p_{CO_2} : Reaction: $CO_2 + H_2O \rightleftharpoons H^+ + HCO_3^-$.			
10.3.2	$K_{hybrid} = 10^{-pH} \cdot c_{HCO_3^-} / p_{CO_2}$, $K_\alpha = a_{m,H^+} \cdot a_{m,HCO_3^-} / (a_{m,CO_2} \cdot a_{H_2O})$. The relationship between the two is:			
10.3.3	$K_{hybrid} = K_\alpha \cdot \alpha_{m,CO_2}^\infty \cdot a_{H_2O} \cdot \rho_{H_2O} / \gamma_{HCO_3^-}$. K_α and α_{m,CO_2}^∞ are temperature dependent constants. a_{H_2O} varies with the total concentration of solutes. ρ_{H_2O} varies primarily with the concentration of macromolecules (e.g. proteins and lipids). $\gamma_{HCO_3^-}$ varies with the 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.

System-Component(s) (specification),	kind of quantity	Symbol	Typical numerical value	Unit	Remarks	Determination
1.1 Ecf - Hydrogen ion (titratable),	substance concentration	$e_{tH^+}(Ecf)$	-1,6	$mmol \cdot l^{-1}$	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, $\theta = 37$ °C, and constant sO_2 (equal to that of arterial blood):
1.2 Ecf - Base (H^+ -binding groups),	substance concentration difference	$\Delta e_{Base}(Ecf)$	+1,6	$mmol \cdot l^{-1}$	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	e_{tCO_2}	25,6	$mmol \cdot l^{-1}$	P = plasma. Total CO_2 comprises: CO_2 (free dissolved), 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 spectrometry.
2.2 P - Carbonate + carbon dioxide,	substance concentration	e_{tCO_2}	25,6	$mmol \cdot l^{-1}$	This name is given in Ref. 7.9. Carbonate here means $CO_3^{2-} + HCO_3^- + H_2CO_3$.	
3.1 aB - Oxygen (total),	substance concentration	e_{tO_2}	9,4	$mmol \cdot l^{-1}$	aB = arterial blood. Total oxygen comprises: O_2 (free dissolved) + Hb O_2 (haemoglobin-bound O_2).	Oxidation of haemoglobin to hemoglobin, extraction of O_2 into a gas phase, and measurement of O_2 in the gas phase, e.g. by gas-mass spectrometry.
3.2 aB - Dioxigen (free + Hb-bound),	substance concentration	e_{tO_2}	9,4	$mmol \cdot l^{-1}$	This name is given in Ref. 7.9. Trivial name: oxygen content.	
4.1 P - Calcium (total),	substance concentration	e_{tCa}	2,5	$mmol \cdot l^{-1}$	Total calcium comprises: Ca^{2+} (free ionized) + Ca (bound).	Gas-mass spectrometry or atomic absorption spectrometry.
4.2 P - Calcium(II) (Ca, total),	substance concentration	e_{tCa}	2,5	$mmol \cdot l^{-1}$	This name is given in Ref. 7.9. II is the oxidation state in <i>Stock</i> 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 to use a fixed value for the concentrational activity coefficient (γ) unless special circumstances warrants 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.

§	System – Component,	kind of quantity	Symbol	Numerical Unit value	Determination	Cf. 6.1 §
1.1.1*	P –	pH	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	$\psi_{m,H^+} = -R \cdot T \cdot (\ln 10) \cdot \text{pH}$.	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	$\tilde{m}_{H^+} = a_{m,H^+} \cdot \tilde{m}_{H^+}^e$, $\tilde{m}_{H^+}^e = 1 \text{ mol} \cdot \text{kg}^{-1}$.	5.1
1.1.5	P –	Hydrogen ion, molality	m_{H^+}	51,7	$m_{H^+} = \tilde{m}_{H^+} / \gamma_{H^+}$.	3.3
1.1.6	P –	Hydrogen ion, concentrational activity	a_{c,H^+}	$39,5 \times 10^{-9}$	$a_{c,H^+} = \tilde{m}_{H^+} \cdot \rho_{H_2O}^* / \tilde{c}_{H^+}^e$, $\tilde{c}_{H^+}^e = 1 \text{ mol} \cdot \text{l}^{-1}$.	6.2
1.1.7	P –	Hydrogen ion, active substance concentration	\tilde{c}_{H^+}	39,5	$\tilde{c}_{H^+} = \tilde{m}_{H^+} \cdot \rho_{H_2O}^*$.	5.2
1.1.8	P –	Hydrogen ion, substance concentration	c_{H^+}	48,2	$c_{H^+} = \tilde{c}_{H^+} / \gamma_{H^+} = m_{H^+} \cdot \rho_{H_2O}$.	3.4
1.2.1	P –	Hydrogen ion, molal activity coefficient	γ_{H^+}	0,77	Estimated from: $\ln \gamma_{H^+} = \ln \gamma_{Na^+} + (h_{H^+} - h_{Na^+}) \cdot M_{H_2O} \cdot \tilde{m}$ 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	γ_{H^+}	0,82	$\gamma_{H^+} = \gamma_{H^+} \cdot \rho_{H_2O}^* / \rho_{H_2O}$.	4.2
1.3.1	P –	Hydrogen ion, buffer value (for H^+)	β	10,4	Determined by titrating plasma with strong acid or base in a closed system, i.e. c_{tCO_2} constant (7.19).	9.2
1.3.2	P –	Hydrogen ion, buffer value (for H^+) (p_{CO_2} constant)	$\beta(p_{\text{CO}_2})$	64,3	Determined by titrating plasma with strong acid or base in an open system with constant p_{CO_2} (7.19).	9.2

6.3 §	System - Component,	kind of quantity	Symbol	Numerical value	Unit	Determination	Cf. 6.1 §
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 _{w,Pr}	0,11	mol·kg ⁻¹	Determined as the slope of β as a function of p _{Pr} .	9.3.2
2.1.1* P -	Carbon dioxide,	partial pressure	p _{CO₂}	5,33	kPa	Measured with a p _{CO₂} electrode.	3.6.5
2.1.2 P -	Carbon dioxide,	active substance concentration	z̄ _{CO₂}	1,32	mmol·l ⁻¹	z̄ _{CO₂} = p _{CO₂} · α _{e,CO₂} [∞] .	5.2
2.1.3 P -	Carbon dioxide,	substance concentration	e _{CO₂}	1,22	mmol·l ⁻¹	e _{CO₂} = p _{CO₂} · α _{e,CO₂} .	3.4
2.2.1 P -	Carbon dioxide,	concentrational solubility coefficient	α _{e,CO₂}	0,225	mmol·l ⁻¹ ·kPa ⁻¹	α _{e,CO₂} = α _{e,CO₂} [∞] /y _{CO₂} . An empirical equation gives slightly higher values (7.1, 7.19): lg{α _{e,CO₂} [∞] } = lg(0,230) - 9,20×10 ⁻³ · {ΔT} + 90×10 ⁻⁶ · {ΔT} ² where {α _{e,CO₂} [∞] } = α _{e,CO₂} [∞] /(mmol·l ⁻¹ ·kPa ⁻¹) and {ΔT} = (T - 310 K)/K.	7.2
2.2.2 P -	Carbon dioxide,	molal activity coefficient	γ _{CO₂}	1,03		Empirical variation with the osmolality (m̂): ln γ _{CO₂} = 5,5 · M _{H₂O} · m̂.	4.1
2.2.3 P -	Carbon dioxide,	concentrational activity coefficient	y _{CO₂}	1,10		y _{CO₂} = γ _{CO₂} · ρ _{H₂O} [*] / ρ _{H₂O} .	4.2
3.1.1* P -	Oxygen,	partial pressure	p _{O₂}	13,0	kPa	Measured with a p _{O₂} electrode.	3.6; 5.3
3.1.2 P -	Oxygen,	substance concentration	e _{O₂}	124	μmol·l ⁻¹	e _{O₂} = p _{O₂} · α _{e,O₂} [∞] .	3.4
3.2.1 P -	Oxygen,	concentrational solubility coefficient	α _{e,O₂}	9,55	μmol·l ⁻¹ ·kPa ⁻¹	α _{e,O₂} [∞] = α _{e,O₂} [∞] /y _{O₂} .	7.2
3.2.2 P -	Oxygen,	molal activity coefficient	γ _{O₂}	1,03		Empirical variation with the osmolality (m̂): ln γ _{O₂} = 5,5 · M _{H₂O} · m̂.	4.1
3.2.3 P -	Oxygen,	concentrational activity coefficient	y _{O₂}	1,10		y _{O₂} = γ _{O₂} · ρ _{H₂O} [*] / ρ _{H₂O} .	4.2

6.3 §	System - Component,	kind of quantity	Symbol	Numerical value	Unit	Determination	Cf. 6.1 §
4.1.1	P - Hydrogen carbonate ion,	active molality	$\tilde{m}_{\text{HCO}_3^-}$	15,9	mmol·kg ⁻¹	$\tilde{m}_{\text{HCO}_3^-} = K_a \cdot p_{\text{CO}_2} \cdot a_{\text{H}_2\text{O}} \cdot 10^{\text{pH}} \cdot a_{\text{CO}_2} \cdot \infty / \rho_{\text{H}_2\text{O}}^*$ K_a is the thermodynamic equilibrium constant (cf. 6.3 §10.3).	5.1
4.1.2*	P - Hydrogen carbonate ion,	substance concentration	$c_{\text{HCO}_3^-}$	20,0	mmol·l ⁻¹	$c_{\text{HCO}_3^-} = \tilde{m}_{\text{HCO}_3^-} \cdot \rho_{\text{H}_2\text{O}} / \gamma_{\text{HCO}_3^-}$ $c_{\text{HCO}_3^-}$ calculated as $c_{\text{CO}_2} - c_{\text{CO}_3^{2-}}$ includes various ion pairs (e.g. NaHCO ₃ , CaHCO ₃ ⁺ , CO ₃ ²⁻ , and carbamate. Empirical equation (37 °C): $c_{\text{HCO}_3^-} = 10^{\text{pH}-6,74} \cdot p_{\text{CO}_2} \text{ mmol} \cdot \text{l}^{-1} \cdot \text{kPa}^{-1}$ (7.14)	3.4
4.2.1	P - Hydrogen carbonate ion,	molal activity coefficient	$\gamma_{\text{HCO}_3^-}$	0,74		$\ln \gamma_{\text{HCO}_3^-} = \ln \gamma_{\text{Na}^+} + (h_{\text{HCO}_3^-} - h_{\text{Na}^+}) \cdot M_{\text{H}_2\text{O}} \cdot \tilde{m}$, where $\gamma_{\text{Na}^+} = 0,75$ (6.3 §5.2.1), $h_{\text{Na}^+} = 3,5$, and $h_{\text{HCO}_3^-} = 0$ (hydration numbers, Ref. 7.4, 7.20).	4.1
4.2.2	P - Hydrogen carbonate ion,	concentrational activity coefficient	$\beta_{\text{HCO}_3^-}$	0,79		$\beta_{\text{HCO}_3^-} = \gamma_{\text{HCO}_3^-} \cdot \rho_{\text{H}_2\text{O}}^* / \rho_{\text{H}_2\text{O}}$	4.2
5.1.1	P - Sodium ion,	active molality	\tilde{m}_{Na^+}	113	mmol·kg ⁻¹	Measured with ion selective electrode.	5.1
5.1.2*	P - Sodium ion,	substance concentration	c_{Na^+}	140	mmol·l ⁻¹	c_{Na^+} measured by flamespectrometry includes some bound Na ⁺ (e.g. NaHCO ₃), possibly about 1% for normal plasma.	3.4
5.2.1	P - Sodium ion,	molal activity coefficient	γ_{Na^+}	0,75		$\gamma_{\text{Na}^+} = \tilde{m}_{\text{Na}^+} / (c_{\text{Na}^+} / \rho_{\text{H}_2\text{O}})$	4.2
6.1.1	P - Potassium ion,	active molality	\tilde{m}_{K^+}	3,2	mmol·kg ⁻¹	Measured with ion selective electrode.	5.1
6.1.2*	P - Potassium ion,	substance concentration	c_{K^+}	4,0	mmol·l ⁻¹	$c_{\text{K}^+} = (\tilde{m}_{\text{K}^+} / \gamma_{\text{K}^+}) \cdot \rho_{\text{H}_2\text{O}}$ c_{K^+} measured by flamespectrometry includes some bound K ⁺ .	3.4
6.2.1	P - Potassium ion,	molal activity coefficient	γ_{K^+}	0,74		$\ln \gamma_{\text{K}^+} = \ln \gamma_{\text{Na}^+} + (h_{\text{K}^+} - h_{\text{Na}^+}) \cdot M_{\text{H}_2\text{O}} \cdot \tilde{m}$, where $h_{\text{K}^+} = 1,9$ and $h_{\text{Na}^+} = 3,5$ (hydration numbers, Ref. 7.4, 7.20).	4.2
7.1.1	P - Calcium ion,	active molality	$\tilde{m}_{\text{Ca}^{2+}}$	0,41	mmol·kg ⁻¹	Measured with ion selective electrode.	5.1
7.1.2*	P - Calcium ion,	substance concentration	$c_{\text{Ca}^{2+}}$	1,23	mmol·l ⁻¹	$c_{\text{Ca}^{2+}} = (\tilde{m}_{\text{Ca}^{2+}} / \gamma_{\text{Ca}^{2+}}) \cdot \rho_{\text{H}_2\text{O}}$	3.4

6.3 §	System - Component,	kind of quantity	Symbol	Numerical value	Unit	Determination	Cf. 6.1 §
7.2.1	P - Calcium ion,	molal activity coefficient	$\gamma_{Ca^{2+}}$	0,31		$\ln \gamma_{Ca^{2+}} = 4 \cdot \ln \gamma_{Na^+} + (\nu_{Ca^{2+}} - 4 \cdot \nu_{Na^+}) \cdot M_{H_2O} \cdot \hat{m} + 3 \cdot \ln(1 + M_{H_2O} \cdot \sum_B \{[1 - \nu_B] \cdot \nu_B\})$ where $\nu_{Ca^{2+}} = 12$ and $\nu_{Na^+} = 3,5$ (hydration numbers, Ref. 7.4, 7.20).	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)	\hat{m}	294	mmol·kg ⁻¹	$\hat{m} = \Delta T_{fus} / K_{fus}$, $K_{fus} = 1,855 \text{ kg} \cdot \text{K} \cdot \text{mol}^{-1}$	
8.1.3	P -	osmotic concentration (0 °C)	\hat{c}	294	mmol·l ⁻¹	$\hat{c} = \Delta T_{fus} / K_{fus, c}$, $K_{fus, c} = K_{fus} / \rho_{H_2O} = 1,855 \text{ l} \cdot \text{K} \cdot \text{mol}^{-1}$	8.1
8.1.4	P - Solutes,	substance concentration	c_{solute}	300	mmol·l ⁻¹	$c_{\text{solute}} = \hat{c} / \phi_c$ $\approx 2 \cdot (c_{Na^+} + c_{K^+}) + c_{\text{Glucose}} + c_{\text{Carbamide}} - c_{\text{Pr}^-}$	8.3
8.1.5	P - Water,	activity (0 °C)	a_{H_2O}	0,9947		$-\ln a_{H_2O} = \Delta T_{fus} \cdot M_{H_2O} / K_{fus}$, or from vapour pressure measurements: $a_{H_2O} = p_{H_2O} / p_{H_2O}^*$	6.0.1 8.1 8.6
8.1.6	P -	osmotic pressure	Π	758	kPa	$\Pi = R \cdot T \cdot \hat{c}$.	8.8
8.1.7	P - Water,	vapour pressure (37 °C)	p_{H_2O}	6,24	kPa	Measured by means of vapour pressure osmometer.	5.3
8.1.8	P - Water,	mass concentration	ρ_{H_2O}	0,933	kg·l ⁻¹	$\rho_{H_2O} = \pi_{H_2O} / V$.	3.1
8.1.9	P - Water,	substance concentration	c_{H_2O}	51,8	mol·l ⁻¹	$c_{H_2O} = \rho_{H_2O} / M_{H_2O}$.	3.4
8.2.1	P -	molal osmotic coefficient	ϕ_m	0,92		Depends on the composition of the plasma.	8.2
8.2.2	P -	concentrational osmotic coefficient	ϕ_c	0,98		Depends on the composition of the plasma.	8.4

6.3 §	System - Component,	kind of quantity	Symbol	Numerical value	Unit	Determination	Cf. 6.1 §
9	P - (water phase)	ionic strength	I	160	$\text{mmol} \cdot \text{kg}^{-1}$	Macro-ions are considered rather immobile and are not included in the calculation of the ionic strength. Albumin in a conc. of $0,6 \text{ mmol} \cdot \text{l}^{-1}$ and with a charge number of about 20 would otherwise contribute $120 \text{ mmol} \cdot \text{kg}^{-1}$ to the ionic strength.	3.5
10.1	Water -	vapour pressure (37 °C)	$p_{\text{H}_2\text{O}}^*$	6,275	kPa		5.3
10.2	Water -	mass density (37 °C)	ρ	0,9930	$\text{kg} \cdot \text{l}^{-1}$	Mass density of water equals mass concentration of water in pure water: $\rho(\text{H}_2\text{O}) = \rho_{\text{H}_2\text{O}}^*$.	3.1
10.3	Water - ($\text{CO}_2 + \text{H}_2\text{O} \rightleftharpoons \text{H}^+ + \text{HCO}_3^-$),	equilibrium constant	K_a	$10^{-6,32}$		$K_a = \alpha_m \cdot \text{H}^+ \cdot \alpha_{\text{HCO}_3^-} / (\alpha_m \cdot \text{CO}_2 \cdot \alpha_{\text{H}_2\text{O}})$. Determined by measuring $K_{\text{hybrid}} = \alpha_m \cdot \text{H}^+ \cdot c_{\text{HCO}_3^-} / c_{\text{CO}_2}$ and extrapolating to infinite dilution. Varies with T (7.18): $-\lg K_a = 6,32 - 2,31 \times 10^{-3} \cdot \{\Delta T\} + 158 \times 10^{-6} \cdot \{\Delta T\}^2$ where $\{\Delta T\} = (T - 310,15 \text{ K})/\text{K}$.	10.2
10.4.1	Water - Carbon dioxide, (infinite dilution)	concentrational solubility coefficient	$\alpha_{\text{C},\text{CO}_2}^\infty$	0,247	$\text{mmol} \cdot \text{l}^{-1} \cdot \text{kPa}^{-1}$	Empirical temperature variation (7.1, 7.11): $\lg\{\alpha_{\text{C},\text{CO}_2}^\infty\} = \lg(0,247) - 9,60 \times 10^{-3} \cdot \{\Delta T\}^2 + 158 \times 10^{-6} \cdot \{\Delta T\}^3$, $\{\alpha_{\text{C},\text{CO}_2}^\infty\} = \alpha_{\text{C},\text{CO}_2}^\infty / (\mu\text{mol} \cdot \text{l}^{-1} \cdot \text{kPa}^{-1})$, $\{\Delta T\} = (T - 310,15 \text{ K})/\text{K}$.	7.2
10.4.2	Water - Oxygen, (infinite dilution)	concentrational solubility coefficient	$\alpha_{\text{C},\text{O}_2}^\infty$	10,50	$\mu\text{mol} \cdot \text{l}^{-1} \cdot \text{kPa}^{-1}$	Empirical temperature variation (7.3): $\lg\{\alpha_{\text{C},\text{O}_2}^\infty\} = \lg(10,50) - 5 \times 10^{-3} \cdot \{\Delta T\}^2 + 9 \times 10^{-5} \cdot \{\Delta T\}^3$, $\{\alpha_{\text{C},\text{O}_2}^\infty\} = \alpha_{\text{C},\text{O}_2}^\infty / (\mu\text{mol} \cdot \text{l}^{-1} \cdot \text{kPa}^{-1})$, $\{\Delta T\} = (T - 310,15 \text{ K})/\text{K}$.	7.2

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, although printed in upright type, 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.

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

Symbol	Name	Cf. 6.1 §
a	relative activity	6.0.1
a_c	concentrational relative activity	6.2
a_m	molal relative activity	6.1
a_p	baric relative activity	6.3
a_x	rational relative activity	6.0.2
B	buffer capacity	9.1
B_m	molar buffer capacity	9.3
B_w	specific buffer capacity	9.4
(b)	(molality)	3.3
c	amount-of-substance concentration	3.4
\tilde{c}	active substance concentration	5.2
\hat{c}	osmotic concentration	8.3
E	energy	2.1
E	electromotive force	2.7
F	Faraday constant	(Remark 2) 2.6
f	activity coefficient	4.0.1
(f)	(fugacity)	5.3
f_x	rational activity coefficient	4.0.2
G	Gibbs energy	2.8
h	hydration number	(Remark 3) 4.1
g	fugacity coefficient	4.3
I	electric current	1.4
I	ionic strength	3.5
K_a	equilibrium constant	10.2
K_c	concentrational equilibrium product	10.3.2
K_{fus}	molal freezing point depression constant	8.6
$K_{fus,c}$	concentrational freezing point depression constant	8.7
K_m	molal equilibrium product	10.3.1
K_p	baric equilibrium product	10.3.3
L	Avogadro constant	(Remark 2) 1.6
l	length	1.1
M	molar mass	3.0
m	mass	1.2
m	molality	3.3
\tilde{m}	active molality	5.1
\hat{m}	osmolality	8.1
N	number of entities	1.0
n	amount of substance	1.6
p	pressure	2.5
p	partial pressure	3.6

6.4 (continued)

Symbol	Name	Cf. 6.1 §
\tilde{p}	fugacity	5.3
Q	electric charge	2.6
R	molar gas constant	2.4.1
S	entropy	2.2
s	saturation fraction	3.2.1
T	thermodynamic temperature	1.5
ΔT_{fus}	freezing point depression	8.5
t	time	1.3
U	internal energy	2.1
V	volume	2.4
(V)	(electric potential)	2.7
V_m	molar volume	(Remark 1) 2.4.1
x	substance fraction	3.2
y	concentrational activity coefficient	4.2
z	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	Celsius temperature	2.3
λ	absolute activity	2.1
μ	absolute chemical potential	2.9.1
$\tilde{\mu}$	electrochemical potential	2.9.2
ν	stoichiometric number	10.1
Π	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_m	molal osmotic coefficient	8.2
ψ	practical chemical potential	2.9.3

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