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Glossary of Terms Related to Solubility

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INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

ANALYTICAL CHEMISTRY DIVISION*

SUBCOMMITTEE ON SOLUBILITY AND EQUILIBRIUM DATA**

GLOSSARY OF TERMS RELATED TO SOLUBILITY

(IUPAC RECOMMENDATIONS 200-)

Prepared for publication by

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Glossary of Terms Related to Solubility

(IUPAC Recommendations 200-)

Abstract:

This glossary defines 151 terms used to describe solubility and related phenomena. The definitions are consistent with one another and with recommendations of the International Union of Pure and Applied Chemistry for terminology and nomenclature.

1. INTRODUCTION

Disciplines concerned with solubility and related phenomena extend well beyond the traditional branches of chemistry to a wide range of bio-medical, environmental, and industrial fields including, for example, mineralogy, pharmacology, oceanography, and petroleum engineering. The diversity in the technical backgrounds and training of individuals concerned with solubility heightens the potential for confusion and miscommunication of both concepts and data related to solubility. This glossary seeks to reduce such confusion and miscommunication by presenting a set of solubility related terms that are consistent with one another and with IUPAC recommendations for chemical terminology [1] and quantities, units, and symbols [2] at the time of its preparation (2006).

This glossary defines 151 terms which were selected by the authors as the central set related to solubility. Within each definition terms defined elsewhere in the glossary are indicated by *italics* at their first use. Inevitably some users will seek terms that are not defined here or will wish to consult definitions of terms used in these definitions. In both cases the authors recommend the IUPAC *Compendium of Chemical Terminology* (Gold Book), particularly the online version [1]. The authors also recommend the IUPAC publication *Quantities, Units and Symbols in Physical Chemistry* (Green Book) [2] as an authoritative and consistent guide to the presentation of chemical data.

Definitions of particular terms have, in many cases, been expanded or modified compared to the corresponding definitions given in the Gold Book [1], which means that such definitions have been modified compared to the original IUPAC recommendations used to prepare entries in the Gold Book. The object has been to make the definitions as clear and as useful as possible within the general format of the glossary, but without changing significantly the meaning of the Gold Book entries. Where synonymous terms are in common usage the recommended term ("main term") is followed on the second line of the glossary entry by the synonym or synonyms which are then followed by the definition and notes, if any. The synonyms are also listed separately in their proper alphabetical position, with the annotation "See (main term)".

2. GLOSSARY OF TERMS

1. absorption coefficient, β^* (in gas solubility)

Volume V^{g} of an *amount* n_{B}^{-1} of a dissolved gas at a given *standard temperature*, usually $T^{e} = 273.15$ K, and total *standard pressure* p^{e} divided by the volume of the pure dissolving liquid of volume V^{I} that contains an amount n_{A} of *solvent* at the same temperature T and pressure p.

Note 1: There is only one absorption coefficient, as compared to the *Bunsen, Ostwald* and *Kuenen coefficients*, because the volume of gas in the definition contains both solute and solvent. The mathematical definition is:

absorption coefficient, pure solvent reference

 $\beta_{\rm B}^* = V^{\rm g}(T, p_{\rm A} + p_{\rm B} = p^{\rm e}, n_{\rm B}^{\rm l}) / V^{\rm l}(T, p^{\rm e}, n_{\rm A})$ where $p_{\rm A}, p_{\rm B}$ are the partial pressures of solvent and gas.

Note 2: For an ideal gas, the absorption coefficient and Bunsen coefficient are related by:

$$\beta/\alpha = \beta^*/\alpha^* = p_{\rm B}/p^{\rm e} = (1 - p_{\rm A}/p^{\rm e})$$

since V^{g} is inversely proportional to pressure.

Note 3: The relations between the *molality* $m_{\rm B}(p^{\rm e})$ or *amount fraction* $x_{\rm B}(p^{\rm e})$ of dissolved gas and the absorption coefficients are:

$$\frac{1}{x_{\rm B}} = 1 + \frac{1}{m_{\rm B}(p^{\rm e})M_{\rm A}} = 1 + \frac{RT^{\rm e}Z_{\rm B}^{\rm e}(1 + p_{\rm A}/p^{\rm e})}{p^{\rm e}V_{\rm m,A}\beta_{\rm B}^{*}}$$

where $V_{\rm A}$, $V_{\rm m,A}$ are the respective partial molar volume and molar volume of the solvent and $Z_{\rm B}$ is the compression factor of the gas.

Note 4: The absorption coefficient and the related quantities for expression of gas solubility; Bunsen coefficient, Kuenen coefficient, and Ostwald coefficient appear frequently in the older literature of gas solubility determination. However, the modern practice, recommended here, is to express gas solubility as *molality*, *amount fraction* or *amount ratio*.

2. activity coefficient, *f*, γ_m , γ_c

Dimensionless correction factor that multiplies the quantity used to express the composition of the substance (usually *amount fraction*, *molality* or *amount concentration*) to produce the (relative) activity of the substance.

(a) Referenced to *Raoult's law*, and for a substance B in a liquid or solid *mixture* containing amount fractions $x_B, x_C, ...$ of the substances B, C,...: a dimensionless quantity f_B defined in terms of the chemical potential μ_B of B in the mixture by:

$$RT \ln (x_{\rm B} f_{\rm B}) = RT \ln a_{\rm B} = \mu_{\rm B} (T, p, x) - \mu^{*}_{\rm B} (T, p)$$

where x denotes the set of amount fractions x_B, x_C, \dots and μ^*_B is the standard chemical potential, defined as the value for pure B. The activity coefficient has the value 1 for pure substance B. (b) Referenced to *Henry's law*, and for a *solute* B in a *solution* (especially a dilute liquid solution) containing molalities $m_{\rm B}, m_{\rm C}, \dots$ because $m_{\rm B}$ denotes the molality of solute B and $m_{\rm A}$ denotes the mass of solvent A) of *solutes* B, C,... in a *solvent* A: a dimensionless quantity $\gamma_{m,B}$ defined in terms of the chemical potential $\mu_{\rm B}$ of B in the solution by:

$$RT\ln(\gamma_{m,B}m_{B}/m^{e}) = RT\ln a_{B} = \mu_{B} - \mu_{m,B}^{e}$$
$$\mu_{m,B}^{e} = \lim_{m_{D} \to 0} [\mu_{B} - RT\ln(m_{B}/m^{e})]$$

where $m^{\theta} = 1 \mod \text{kg}^{-1}$ is the standard molality and μ^{θ}_{B} is the standard chemical potential, defined as the value at infinite dilution of all solutes. The activity coefficient has the value 1 at infinite dilution of all solutes.

(c) Referenced to Henry's law, and for a solute B in a solution (especially a dilute liquid solution) containing amount concentrations $c_{\rm B}$, $c_{\rm C}$, ... of solutes B, C,... in a solvent A: a dimensionless quantity $\gamma_{c,B}$ defined in terms of the chemical potential μ_B of B in the solution by:

$$RT\ln(\gamma_{c,B}c_{B}/c^{e}) = RT\ln a_{B} = \mu_{B} - \mu_{c,B}$$
$$\mu_{c,B} = \lim_{c_{B} \to 0} [\mu_{B} - RT\ln(c_{B}/c^{e}_{B})]$$

where $c^{\Theta} = 1 \text{ mol dm}^{-3}$ is the standard amount concentration and $\mu^{\Theta}_{c,B}$ is the standard chemical potential, defined as the value at infinite dilution of all solutes. The activity coefficient has the value 1 at infinite dilution of all solutes.

See also activity coefficient at infinite dilution Modified from [1, 2].

3. activity coefficient at infinite dilution, f°

For a substance B, *activity coefficient* $f_{\rm B}$ extrapolated to *infinite dilution*:

$$\ln f_{\rm B}^{\infty} = \lim_{x_{\rm B} \to 0} \left(\frac{\mu_{\rm B} - \mu_{\rm B}^*}{RT} - \ln x_{\rm B} \right)$$

Note 1: Useful for dilute *mixtures* as an alternative to the standard chemical potential on a *molality* basis, and as such a fundamental thermodynamic property.

Note 2: The relation between the activity coefficient at infinite dilution and the standard chemical potentials is, for a solute B in a solvent A:

$$\ln f_{\rm B}^{\infty} = \frac{\mu_{\rm m,B}^{\rm e} - \mu_{\rm B}^{*}}{RT} - \ln(M_{\rm A}m_{\rm B}^{\rm e})$$

where M_A is the molar mass of the *solvent*. See also activity coefficient

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4. amount, n

amount of substance

Base quantity in the system of quantities upon which SI is based. It is the number of elementary entities divided by the Avogadro constant.

Note 1: Since amount is proportional to the number of entities, the proportionality constant being the reciprocal Avogadro constant and the same for all substances, it has to be treated almost identically with the number of entities. Thus the counted elementary entities must always be specified.

Note 2: The words 'of substance' may be replaced by the specification of the entity, for example: amount of chlorine atoms, n(Cl), amount of chlorine molecules, $n(Cl_2)$. No specification of the entity might lead to ambiguities [amount of sulfur could stand for n(S), $n(S_s)$, etc.], but in many cases the implied entity is assumed to be known: for molecular compounds it is usually the molecule [e.g. amount of benzene usually means $n(C_6H_6)$], for ionic compounds the simplest formula unit [e.g. amount of sodium chloride usually means n(NaCl)] and for metals the atom [e.g. amount of silver usually stands for n(Ag)].

Note 3: In some derived quantities the words 'of substance' are also omitted, e.g. amount concentration, amount fraction. Thus in many cases the name of the base quantity is shortened to amount and to avoid possible confusion with the general meaning of the word the attribute chemical is added. The chemical amount is hence the alternative name for amount of substance. In the field of clinical chemistry the words 'of substance' should not be omitted and abbreviations such as substance concentration (for amount of substance concentration) and substance fraction are in use. The quantity had no name prior to 1969 and was simply referred to as the number of moles. [1]

5. amount concentration, c

amount-of-substance concentration, substance concentration (in clinical chemistry), molarity (in older literature).

Amount of a constituent divided by the volume of a mixture.

Note 1: For constituent B it is often denoted [B].

Note 2: The common unit is mole per cubic decimeter (mol dm^{-3}) or mole per liter (mol L^{-1}) sometimes denoted by (small capital) M. Modified from [1].

6. amount fraction, x

mole fraction Amount of substance of a constituent divided by the total amount of all constituents in a mixture. Modified from [1].

7. amount ratio, r

mole ratio

Amount of one constituent divided by the amount of a second constituent in the same system. For constituents 1 and 2,

 $r_{12} = n_1 / n_2$

[3]

8. analytical method

Class of experimental procedures for *solubility* determination in which a *saturated solution* is prepared and then analyzed to determine composition.

See also synthetic method.

9. binary system

System containing two components.

See also ternary system, higher-order system.

10. binodal curve

See coexistence curve.

11. Bunsen coefficient, α

Volume V^{g} of an *amount* n_{B}^{1} of a gas dissolved at a given standard temperature T^{e} (usually 273.15 K) and given standard (partial) pressure p_{B}^{e} (usually 1 atm or 1 bar = 0.1 MPa) divided by the volume of the solvent V⁴ containing an amount n_A of solvent at temperature T and the given total pressure p° .

Note 1: There are two Bunsen coefficients, depending on whether the liquid is the equilibrium solution or the pure liquid, with mathematical definitions:

```
Bunsen coefficient, solution reference \alpha_{\rm B} = V^{\rm g}(T^{\rm e}, p^{\rm e}, n_{\rm B}^{\rm l}) / V^{\rm f}(T, p^{\rm e}, n_{\rm A}, n_{\rm B}^{\rm l})
Bunsen coefficient, pure solvent reference \alpha_{\rm B}^{*} = V^{\rm g}(T^{\rm e}, p^{\rm e}, n_{\rm B}^{\rm l}) / V^{\rm f}(T, p^{\rm e}, n_{\rm A}, n_{\rm B}^{\rm l})
```

where $n_{\rm B}^{-1}$ is the amount of dissolved gas in the liquid solution.

Note 2: The relations between the *molality* $m_{\rm B}(p^{\rm e})$ or mole fraction $x_{\rm B}(p^{\rm e})$ of dissolved gas and the Bunsen coefficients are:

$$\frac{1}{x_{\rm B}^{\rm o}} = 1 + \frac{1}{m_{\rm B}(p^{\rm o})M_{\rm A}} = 1 + \frac{RT^{\rm o}Z_{\rm B}^{\rm o}(T^{\rm o})}{p^{\rm o}V_{\rm A}\alpha_{\rm B}}$$

$$\frac{1}{x_{\rm B}^{\rm o}} = 1 + \frac{1}{m_{\rm B}(p^{\rm o})M_{\rm A}} = 1 + \frac{RT^{\rm b}Z_{\rm B}^{\rm o}(T^{\rm b})}{p^{\rm o}V_{\rm m,A}\alpha_{\rm B}^{*}}$$

where $V_{\rm A}$, $V_{\rm m,A}$ are the respective partial molar volume and molar volume of the solvent and $Z_{\rm B}$ is the compression factor of the gas.

Note 3: The Bunsen coefficient and the related quantities for expression of gas solubility; absorption coefficient, Kuenen coefficient, and Ostwald coefficient appear frequently in the older literature of gas solubility determination. However, the modern practice, recommended here, is to express gas solubility as molality, amount fraction or amount ratio.

12. catatectic reaction See metatectic reaction

13. chlorinity, Cl

Mass of chlorine (in all forms, usually chloride) divided by mass of saline solution.

Note 1: Used in describing composition of saline solutions, e.g., seawater, brackish waters and brines.

Note 2. Usual unit for this mass fraction is permil.

See also *salinity*. [4]

14. Clarke-Glew equation

Semi-empirical equation describing the temperature dependence of the standard Gibbs energy of solution:

$$\Delta_{\rm sln}G^{\rm e}(T, p^{\rm e}) / RT = A_{\rm o} + A_1(T_{\rm r} / T) + A_2 \ln(T / T_{\rm r}) + A_3(T / T_{\rm r}) + A_4(T / T_{\rm r})^2 + \dots$$

A .ties and . where the A_i are constants that can be related to thermodynamic quantities and T_r is a reference temperature.

See also Clarke-Glew-Weiss equation [5, 6]

15. Clarke-Glew-Weiss equation

Clarke-Glew equation with $T_r = 100$ K. [5, 7]

16. cloud point

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Critical solution point, particularly when used as an end point of a turbidometric titration to determine solubility.

See also synthetic method

17. coexistence curve

- binodal curve
- conodal curve

Boundary of stable phase separation (limits of solubility) in a liquid or solid system of two or more components.

Note: In a *binary system*, a plot of experimental variables such as temperature or pressure, or of theoretical variables such as Gibbs energy, against amount fraction displays the coexistence curve. In ternary or higher-order systems, coexistence curves are displayed on a plot of composition at constant temperature or pressure, usually on a *ternary diagram*.

See also spinodal curve, conjugate phases. From [8]

18. common ion effect

Decrease in solubility of a salt when a second *non-saturating* salt with one ion in common with the salt is added to its saturated solution.

Note: Restricted in practice to salts with sufficiently low *solubility* and at sufficiently *low ionic* strengths that the activity coefficient of the salt is close to unity. At higher ionic strengths, or for salts with high solubility, the activity coefficient usually decreases with addition of nonsaturating salt, resulting in a higher solubility.

19. component

thermodynamic component

independent component

Constituent of a mixture the amount or concentration of which can be varied independently. The number of components in a given system is the minimum number of independent species necessary to define the composition of all *phases* of that system. Relations among the constituents, such as charge balance or chemical *equilibria*, must be taken into account in determining the number of components. The term component is also often used in the more general sense defined here under constituent. Modified from [1].

20. compression factor, Z

compressibility factor

Product of pressure and molar volume divided by the gas constant and thermodynamic

temperature. For an ideal gas it is equal to 1. [1]

21. conjugate phases

Two phases of variable composition in mutual thermodynamic equilibrium.

See also *coexistence curve*. From [8]

22. conodal

connodal See *tie line* From [8]

23. conodal (connodal) curve

See coexistence curve.

24. constituent

Chemical species present in a system.

See also component

Modified from [1].

25. critical index β

Index in the basic equation describing a coexistence curve:

$$\beta = \lim_{T \to T_{c}} \left(\frac{\partial \ln(x'' - x')}{\partial \ln[T - T_{c}]} \right)$$

3

where x'', x' are the compositions of one *component* in the respective concentrated and dilute phases and T_c is the *critical solution temperature*. From [8]

26. critical point

Temperature and pressure at which intensive properties of liquid and vapor (density, heat capacity, etc.) become equal.

Note: The highest temperature (*critical temperature*) and pressure (*critical pressure*) at which both a gaseous and a liquid phase of a given compound can exist.

27. critical pressure, p_c

In binary, ternary and higher-order liquid-liquid systems, the point on a phase diagram of pressure against composition (at constant temperature) at which the liquid and vapor composition become equal.

28. critical solution point

cloud point

consolute point

plait point (ternary and higher-order systems)

In a binary system, point with coordinates critical solution temperature (CST) or critical solution pressure (CSP) and critical composition on a temperature-composition or pressure-composition phase diagram at which the distinction between coexistent phases disappears.

In *ternary* and *higher-order systems*, composition below or above which, on a ternary or higher composition phase diagram at constant temperature and pressure, the distinction between coexistent phases disappears.

Note 1: Disappearance of the distinction between phases corresponds to disappearance of a miscibility gap; see mutual solubility.

Note 2: In solid-solid, solid-liquid and liquid-liquid systems both upper and lower critical solution temperatures (UCST, LCST) or upper and lower critical solution pressures (UCSP, LCSP) can occur. In some systems, both can be observed. Modified from [1].

29. critical temperature, $T_{\rm c}$

In binary, ternary and higher-order liquid-liquid or solid-solid systems, point on a phase *diagram* of temperature against composition (at constant pressure) at which the liquid and vapor composition become equal.

Note: The highest temperature at which vapor-liquid equilibrium can exist. Modified from [1].

30. crystallization

Formation of a crystalline solid *phase* from either (a) a solid, liquid or gaseous *mixture* or solution, or (b) a pure liquid or gas.

Note: Crystallization usually occurs under laboratory conditions by altering the temperature or pressure of a *system*, or by evaporation of a *solvent*. [1]

31. data

Experimental results, often numerical

Note 1: The term is plural; its singular form is datum.

Note 2: Data directly obtained from experimental apparatus may be referred to as raw data. Raw data may be subjected to numerical operations (unit conversions, etc) to give transformed data, which maintain a point-for-point correspondence with the raw data. However, the use of the term data to refer to the results of numerical modeling operations or other elaborate calculations is controversial and discouraged. The latter are better referred to as "results" and, when presented graphically, represented by smooth lines.

32. dissolution

Process of mixing of two or more phases with the formation of one new homogeneous phase (i.e., the *solution*)

Modified from [1].

33. dystectic reaction

congruent melting < indifferent melting [9]

Isobaric, reversible melting or *dissolution* with either complete or partial dissociation on heating of a solid compound, A_aB_b, formed by *components* A and B:

$$A_{a}B_{b}(s) \Rightarrow A_{a}B_{b}(l) \Rightarrow aA(l) + bB(l)$$

where the forward arrow indicates the direction of heating.

Note 1: The dystectic temperature is a maximum (dT/dx = 0) of the melting temperature composition curve. The dystectic point is the isobarically invariant maximum at the dystectic composition and dystectic temperature, where the compositions of the liquid and solid *phases* are equal. The composition of a non-stoichiometric compound is also equal to that of the *melt* at the dystectic temperature and composition.

[9]

Note 2: Derived from Greek, meaning "difficult (or highest) melting".

Examples: systems Mg-Sn [10], H₂SO₄ – H₂O

Note 3: Occasionally a similar reaction takes place in the subsolidus region. Quite appropriately it is called dystectoid reaction.

34. dystonic reaction

congruent dissolution

Reversible *dissolution* in an isothermal, isobaric *system* of three or more *components* characterized by congruent dissolution of and *saturation* with a stoichiometric compound consisting of two or more of these components. The equilibrium process is, for example:

$$AB \cdot pH_2O \Rightarrow A(aq, sat) + B(aq, sat) + pH_2O(l)$$

Note 1: The chemical potential of *solvent* and consequently its *partial pressure* reaches a maximum value at the dystonic composition or point, which is isothermally and isobarically invariant.

Note 2: Dystonic points have been detected in aqueous media only.

Note 3: Derived from Greek, meaning "difficult (or highest) tension (or vapor pressure)".

Examples: systems Na₂SO₄-ZnSO₄-H₂O, Na₂SO₄-CdSO₄-H₂O, Na₂SO₄-CuSO₄-H₂O

35. equilibrium

State of a *system* in which the macroscopic properties of the system become uniform, independent of time. If the temperature is uniform throughout the system, a state of thermal equilibrium has been reached; if the pressure is uniform, a state of mechanical equilibrium has been reached; and if the chemical potential of each component is uniform, a state of chemical equilibrium has been reached. If all these quantities become uniform, the system is said to be in a state of complete thermodynamic equilibrium.

Note 1: Complete thermodynamic equilibrium can also be expressed in many ways, depending on which variables are of interest. For solubility purposes, the important variables are *T*, *p* and the chemical potentials μ_i of the *C* components. For these variables, the condition for stable equilibrium is that a variation in the total Gibbs energy at equilibrium caused by variations in any of the variables is zero, $\delta G(T, p, \mu_i) = 0$; i.e., the Gibbs energy is a minimum. If the variation is negative, an irreversible change of the system can occur.

Note 2: Solubility equilibrium is an example of a state of complete thermodynamic equilibrium. For example, a saturated solution of a solid in a liquid at a fixed temperature and pressure is in a state of complete thermodynamic equilibrium. If the system is subjected to a small increase in temperature, a small amount of solid will dissolve to restore the equilibrium (if the solubility increases with temperature), while if there is a small decrease in temperature, a small amount of solid will precipitate. This is the basis for determining accurate values of solubility by approaching the equilibrium solubility from both *supersaturation* and *undersaturation* directions.

36. eutectic reaction

Isothermal reversible reaction of a liquid *phase* l which is transformed into two (or more) different solid phases α and β during the cooling of a *system*. In a binary system:

 $1 \Rightarrow \alpha + \beta$

where l is a liquid phase, α , β are solid phases and the forward arrow indicates the direction of cooling. The *equilibrium* reaction occurs along the eutectic line at the eutectic temperature. At the eutectic composition, the composition of the liquid and solid phases are equal, and intermediate to the compositions of the solid phases of the system.

Note 1: The solid phases may be pure phases, solid mixtures, or binary compounds.

Note 2: The eutectic line and composition (hence point) are isobaric invariants of the system, and represent the composition and the minimum melting temperature along the two intersecting melting curves.

Note 3: Derived from Greek, meaning "easy (or lowest) melting".

Example: system Ag-Cu [10] and many salt-water systems

37. eutectoid reaction

Isothermal reversible reaction of a solid mixture *phase* γ which is transformed into two (or more) different solid (pure, binary compound or mixture) phases α and β during the cooling of a *system*. In a *binary system*:

 $\gamma \Rightarrow \alpha + \beta$

where the forward arrow indicates the direction of cooling. The *equilibrium* reaction occurs along the eutectoid line at the eutectoid temperature. At the eutectoid composition, the compositions of the high temperature solid phase and the mechanical mixture of the low temperature solid phases are equal, and intermediate to the compositions of the pure solid phases α and β . This composition and the eutectoid temperature, which are isobaric univariants of the system, define the eutectoid point.

Note: Derived from Greek and Latin, meaning "resembling a eutectic".

Example: system Fe-C [10]

38. eutonic reaction

isothermally invariant reaction

(isothermally invariant) reaction of double saturation

Reversible isoplethic dissolution in a system of three or more components characterized by the composition of a *solution* that is simultaneously saturated with respect to all (at least two or more) dissolved *solutes*. The two simultaneous equilibrium processes are, for example:

$$A \cdot pH_2O \Rightarrow A(aq, sat) + pH_2O(l)$$

 $B \cdot qH_2O \Rightarrow B(aq, sat) + qH_2O(l)$

Note 1: The eutonic point is invariant in a *ternary system* at a given temperature and pressure.-

Note 2: The chemical potential of solvent decreases along the two solubility curves that intersect at the eutonic point, and thus reaches a minimum value at that point. Thus, colligative properties

(that depend on solvent activity) reach a minimum value at the eutonic point. For example, if the solutes are non-volatile and the solvent is volatile, the vapor pressure reaches a minimum value.

Note 3: Eutonic points have been detected in aqueous media only.

Note 4: The term is derived from Greek meaning "easy (or lowest) tension (or vapor pressure)".

Examples: systems Na₂SO₄-ZnSO₄-H₂O, Na₂SO₄-CdSO₄-H₂O, Na₂SO₄-CuSO₄-H₂O

See also peritonic reaction

39. fitting equation smoothing equation

Theoretically-based or empirical equation for interpolation of *data* over a range of temperature, pressure, composition, or other variable.

Note: The use of a fitting equation for extrapolation of data beyond the equation's known range of validity is a potential source of extreme error.

40. fugacity

Of a substance B, $f_{\rm B}$ or $\tilde{p}_{\rm B}$, in a gaseous *mixture* is defined by $f_{\rm B} = \lambda_{\rm B} \lim_{n \to \infty} (p_{\rm B} / \lambda_{\rm B})_T$, where $p_{\rm B}$

is the *partial pressure* of B and λ_B its absolute activity.

SI unit: Pa. [1], [2]

41. fugacity coefficient, φ

fugacity divided by the partial pressure of a gaseous constituent.

Modified from [1]

42. Gibbs-Duhem equation

Equation relating the intensive variables T, p and the C chemical potentials μ_i in a phase:

$$SdT - Vdp + \sum_{i=1}^{C} n_i d\mu_i = 0$$

where C is the total number of components i in a phase.

Note 1: Note that the variables in this equation are the intensive quantities T, p and μ_i .

Note 2: The Gibbs-Duhem equation may be written in terms of intensive quantities:

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$$\sum_{i=1}^{C} x_i \left(\mathrm{d}\mu_i + S_i \mathrm{d}T - V_i \mathrm{d}p \right) = 0$$

where S_i , V_i , x_i are the respective partial molar entropy, partial molar volume and amount fraction of component *i*.

Note 3: There is a Gibbs-Duhem equation for each phase in a *system* exhibiting multi-phase equilibria. Application of the conditions for an *equilibrium* state leads to the *phase rule* as one example of the application of this equation. When equilibrium conditions are applied, T, p and μ are equal in all phases of an equilibrated system, while S_i , V_i and x_i are not. [9]

43. Gibbs energy of transfer

Change in Gibbs energy at a given temperature and pressure for transfer of a substance between two different phases.

44. Gibbs-Konovalov equations

Van der Waals' equations

Pair of equations for a binary *mixture* of *components* A and B that relate the variables T, p, in one *phase* of variable composition, α , to the variables T, p, in a coexisting *equilibrium* phase of variable composition, β : (n) +

$$-\frac{(1-x_{\rm B}^{\beta})\Delta_{\alpha}^{\beta}H_{\rm A}+x_{\rm B}^{\beta}\Delta_{\alpha}^{\beta}H_{\rm B}}{T}dT + [(1-x_{\rm B}^{\beta})\Delta_{\alpha}^{\beta}V_{\rm A}+x_{\rm B}^{\beta}\Delta_{\alpha}^{\beta}V_{\rm B}]dp + (x_{\rm B}^{\alpha}-x_{\rm B}^{\beta})\left(\frac{\partial^{2}G_{\rm m}^{\alpha}}{\partial x_{\rm B}^{\alpha}^{2}}\right)_{T, p}dx_{\rm B}^{\alpha} = 0$$

$$-\frac{(1-x_{\rm B}^{\alpha})\Delta_{\alpha}^{\beta}H_{\rm A}+x_{\rm B}^{\alpha}\Delta_{\alpha}^{\beta}H_{\rm B}}{T}dT + [(1-x_{\rm B}^{\alpha})\Delta_{\alpha}^{\beta}V_{\rm A}+x_{\rm B}^{\alpha}\Delta_{\alpha}^{\beta}V_{\rm B}]dp + (x_{\rm B}^{\alpha}-x_{\rm B}^{\beta})\left(\frac{\partial^2 G_{\rm m}^{\beta}}{\partial x_{\rm B}^{\beta^2}}\right)_{T, p}dx_{\rm B}^{\beta} = 0$$

where $\Delta_{\alpha}^{\beta} H_{A} = H_{A}^{\beta} - H_{A}^{\alpha}$, $\Delta_{\alpha}^{\beta} V_{A} = V_{A}^{\beta} - V_{A}^{\alpha}$ are the enthalpy and volume of transfer of component A from phase α to phase β , and similarly for component B.

Note 1: $\left(\frac{\partial^2 G_{\rm m}}{\partial x_{\rm R}^2}\right)_{T, p} > 0$ (condition for diffusional stability). This quantity may also be expressed

in terms of the derivatives of the chemical potentials, using

$$\left(\frac{\partial^2 G_{\rm m}}{\partial x_{\rm B}^2}\right)_{T, p} = -\frac{1}{x_{\rm B}} \left(\frac{\partial \mu_{\rm A}}{\partial x_{\rm B}}\right)_{T, p} = \frac{1}{x_{\rm A}} \left(\frac{\partial \mu_{\rm B}}{\partial x_{\rm B}}\right)_{T, p}$$

Note 2: These equations show that an extremum occurs for each phase equation when the compositions of the two phases are equal, and that the slope of the T -composition or p composition curve is zero for each phase equation at the extremum. Í S

Note 3: Sometimes these equations are called van der Waals' equations.

Note 4: Sometimes the spelling Konovalow is found.

[9]

45. Henry's law

Partial pressure (fugacity) of a *solute* (B) in a *solution* is directly proportional to the relative *activity*, $a_{\rm B}$, of the *solute*:

 $p_{\rm B} = a_{\rm B}/a^{\infty}_{\rm B}$

where a_{B}^{∞} is the activity at *infinite dilution*, i.e., for pure *solvent*.

Note 1: For the solvent (A) the relationship is called Raoult's law, and the proportionally factor is the fugacity of the pure solvent, $p_A = p_A^* a_A$.

Note 2. Henry's law is a limiting law, but can sometimes be used for converting solubility *data* from the experimental pressure to standard partial pressure, provided the amount(mole) fraction of the gas in the liquid is small and that the difference in pressures is small.

See also Henry's law constant. Modified from [1].

46. Henry's law constant, $k_{\rm H}$

Henry coefficient, Henry's law coefficient, Henry constant For a gas B,

 $k_{\rm H} = \lim_{x_{\rm B} \to 0} (f_{\rm B} / x_{\rm B}) = (\partial f_{\rm B} / \partial x_{\rm B})_{x_{\rm B} \to 0}$

where $f_{\rm B}$ is the fugacity of B.

Note 1: At low pressures, $f_{\rm B}$ becomes equal to the partial pressure $p_{\rm B}$.

Note 2: Henry's law constant in terms of amount fractions has units Pa, but is sometimes expressed in terms of molalities or *amount concentrations*, with corresponding units Pa kg mol⁻¹, Pa m³ mol⁻¹, respectively.

the forms a. Note 3: Henry's law constant is sometimes given as the reciprocal of the forms defined above, so its exact definition must always be given.

See also *Henry's law*. From [2, 5].

47. higher-order system multicomponent system

System containing more than three *components*.

48. incongruent reaction

See *peritectic reaction*

49. independent component

See component

50. infinite dilution

Limiting composition or other variable in a *solution* obtained by extrapolating to a value of zero for the variable describing the composition of the solution.

51. infinite miscibility

Property of a system of forming a single phase at all relative proportions of its components.

See also *mutual solubility*

52. initial complex method

See wet residue method

53. ionic amount (mole) fraction, x_{+} , x_{-}

species amount fraction, species mole fraction

(a) For an ionized salt B in *solution*:

$$x_{+B} = \frac{\nu_{+B} x_{B}}{1 + \sum_{i=1}^{s} (\nu_{i} - 1) x_{i}}, x_{-B} = \frac{\nu_{-B} x_{+B}}{\nu_{+B}}$$

where the summation is over all *s* solute components *i* and $v_i = v_{+i} + v_{-i}$ is the sum of the stoichiometric numbers of the ions formed from salt *i*.

(b) For a single solvent A:

$$x'_{\rm A} = \frac{x_{\rm A}}{1 + \sum_{i=1}^{s} (v_i - 1)x}$$

Note 1: These are generalizations of terms defined in [11], and are used in formulating fitting equations for *solubility* of salts, in defining *activity coefficients* on the *amount fraction* scale, and in discussing salt effects on solubilities of gases.

Note 2: Note that:

$$\sum_{i=1}^{s} (x_{+i} + x_{-i}) + x'_{A} = 1$$

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54. ionic strength

Measure of effective molality or amount concentration of ionic species in solution:

(a) on molality basis: $I_{\rm m} = \frac{1}{2} \sum z_i^2 m_i$ (b) on amount concentration basis: $I_{\rm c} = \frac{1}{2} \sum z_i^2 c_i$

where z_i is the charge number of species *i*, and the summation is over all ionic species. From [2].

55. Ising model

Theory of *coexistence curves* or other discontinuities in the properties of *phases* (such as orderdisorder or magnetic transitions) in *binary systems*, based on a one-, two- or three-dimensional statistical mechanical nearest-neighbor lattice theory.

Note: The theory predicts phase separation in a wide variety of systems, including binary liquid or solid systems that possess *critical solution points*.

[12]

56. isobar

Line joining points of equal pressure on a phase diagram.

57. isopleth

Line joining points of equal composition on a phase diagram.

58. isotherm

Line joining points of equal temperature on a phase diagram.

59. isothermal method

See: synthetic method

60. Jänecke coordinates

solute amount (mass) fraction.

Coordinates used mainly in representation of multicomponent *phase diagrams* that distinguish *solutes* and a single *solvent*. The *amount* or *mass fractions* of the *s* solutes are chosen as the primary composition variables and the amount or mass fraction of solvent as a secondary variable, so that the solute amount (mass) fractions may be represented, for example in ternary and quaternary *systems*, as linear (ternary) or planar triangular or square planar (quaternary)

diagrams, with the solvent amount or mass fraction along an axis perpendicular to the chosen diagram of solute variables. Quantitatively:

$$x_{\mathrm{s,B}} = x_{\mathrm{B}} / \sum_{i=1}^{s} x_i$$

where the summation is over the *s* solute substances. Note that $\sum_{s,B}^{s} x_{s,B} = 1$

Note 1: The amount fraction of solvent component A is replaced by a special case of the solvent

amount fraction $x_{v,A} = x_A / \sum_{i=1}^{p} x_i$, which becomes infinite for pure solvent.

Note 2: This quantity can be scaled to a finite value by adding an arbitrary constant to the denominator.

See also Solvent amount (mass) fraction.

[5, 13]

61. Kuenen coefficient, S

Volume V^{g} of an *amount* n_{B}^{1} of a dissolved gas at a given standard temperature T^{e} (usually 273.15 K) and given standard pressure p^{θ} (usually 1 atm) divided by the mass m^{1} of the dissolving liquid containing an amount n_A of solvent at temperature T and the given pressure p° .

Note 1: There are two Kuenen coefficients, depending on whether the liquid is the *equilibrium solution* or the pure liquid, with mathematical definitions:

Kuenen coefficient, solution reference $S_{\rm B} = V^{\rm g}(T^{\rm e}, p^{\rm e}, n_{\rm B}^{\rm l}) / m^{\rm l}(T, p^{\rm e}, n_{\rm A}, n_{\rm B}^{\rm l})$ Kuenen coefficient, pure solvent reference $S_{\rm B}^{*} = V^{\rm g}(T^{\rm e}, p^{\rm e}, n_{\rm B}^{\rm l}) / m^{\rm l}(T, p^{\rm e}, n_{\rm A})$

Note 2: The relations between the *molality* $m_{\rm B}(p^{\theta})$ or *amount fraction* $x_{\rm B}(p^{\theta})$ of dissolved gas and the Kuenen coefficients are:

$$\frac{1}{x_{\rm B}^{\rm e}} = 1 + \frac{1}{m_{\rm B}(p^{\rm e})M_{\rm A}} = 1 + \frac{RT^{\rm e}Z_{\rm B}^{\rm e}(T^{\rm e})}{p^{\rm e}M_{\rm A}S_{\rm B}}$$
$$\frac{1}{x_{\rm B}^{\rm e}} = 1 + \frac{1}{m_{\rm B}(p^{\rm e})M_{\rm A}} = 1 + \frac{RT^{\rm e}Z_{\rm B}^{\rm e}(T^{\rm e})}{p^{\rm e}M_{\rm A}S_{\rm B}}$$

where $M_{\rm A}$ is the molar mass the solvent and $Z_{\rm B}$ is the compression factor of the gas.

Note 3: The Kuenen coefficient and the related quantities for expression of gas solubility; absorption coefficient, Bunsen coefficient, and Ostwald coefficient appear frequently in the older literature of gas solubility determination. However, the modern practice, recommended here, is to express gas solubility as *molality*, *amount fraction* or *amount ratio*.

62. lower critical solution temperature

See critical solution point

63. mass concentration, γ , ρ

mass density Mass of a *constituent* divided by the volume of a *mixture*. From [2].

64. mass density

Mass of a pure substance, *mixture* or *solution* divided by its volume. From [2].

65. mass fraction, w

Mass of a particular *constituent* divided by the sum of the masses of all *system* constituents.

$$w_B = m_B / \sum_i m_i$$

Note: Solubility may be expressed in terms of mass fraction as mg(1) / kg solution. However, it is recommended that the term "parts per million, ppm" be avoided since "parts" may be measured on either a mass or volume basis. If it is used, the physical quantity to which it refers must be specified.

From [2].

66. mass percent For a *system constituent* 100 times the *mass fraction* of that constituent.

67. mass ratio

Mass of one *constituent* divided by the mass of a second constituent in the same system.

68. mass solubility, C_w

Obsolete term for *molality* of a dissolved gas.

69. melt

Liquid state of *system* that is a solid at room temperature.

70. metastable state

State of a *system* in which a perturbation of any one of its defining variables may cause a change to a more stable state.

Note 1: A system in a metastable state is in a state of metastable *equilibrium*, and so can be described consistently by thermodynamic methods.

Note 2: Although a driving force for the transition of a metastable state to a stable state exists $(\Delta_{tr}G < 0 \text{ at constant } T \text{ and } p)$ the transition is retarded during the time of observation.

Modified from [1].

71. metatectic reaction

catatectic reaction [14]

Isothermal reversible reaction of a solid *mixture phase* β which is transformed into a different solid phase a plus a liquid phase I during cooling of a system. For a binary system:

 $\beta \Rightarrow \alpha + 1$

where the forward arrow indicates the direction of cooling. The *equilibrium* transformation occurs along the metatectic line characterized by the metatectic temperature. The metatectic composition and temperature, isobaric invariants of the system, define the metatectic point, which lies between the compositions of liquid l and solid phase α .

Note 1: Derived from Greek, meaning "behind, or second-order, after melting".

Example: system Fe-Zr [10]

Note 2: Occasionally a similar reaction takes place in the subsolidus region. Quite appropriately it is called metatectoid reaction.

72. miscibility

Ability of two liquids to undergo spontaneous mixing to form a homogeneous *mixture*.

73. miscibility gap

See *mutual solubility*.

74. mixture

.bstance, whe. Gaseous, liquid or solid *phase* containing more than one substance, when all the substances are treated in the same way.

See also solution. [2, 15]

75. molality, m, b

Amount of a solute divided by the mass of the solvent. Modified from [1]

76. mole fraction, x See amount fraction

IUPAC

77. mole percent

For a system constituent 100 times the amount fraction of that constituent.

78. mole ratio, r

See amount ratio

79. monotectic reaction

Isothermal reversible reaction of a solid and a liquid *phase* to form a new solid phase during cooling of a system. In a binary system:

 $l_1 \rightleftharpoons \alpha + l_2$

where the forward arrow indicates the direction of cooling. The *equilibrium* transformation occurs along the monotectic line, characterized by the monotectic temperature. The monotectic composition and temperature, isobaric invariants of the system, define the monotectic point, which lies between the compositions of liquid l_2 and solid phase α .

Note: Derived from Greek, meaning "single melting".

Examples: systems Pb-Zn [10], methanol-cyclohexane

80. monotectoid reaction

Isothermal reversible reaction of a solid *phase* α_1 which is transformed into two different solid phases α_2 and β during the cooling of a system. In a binary system:

 $\alpha_1 \rightleftharpoons \alpha_2 + \beta$

where the forward arrow indicates the direction of cooling. The equilibrium process occurs along the monotectoid line at the monotectoid temperature. The monotectoid composition and temperature, isobaric invariants of the system, define the monotectoid point, which lies between the compositions of phases β and α_2 .

Note: Derived from Greek, meaning "resembling a monotectic".

Example: system Al-Zn [10] Modified from [1].

81. multicomponent system

See higher-order system

82. mutual solubility

in a¹ In a system of two or more liquid or solid *components*, solubility of all components in all phases.

Note. If mutual solubility is limited over a range of temperature and composition, the liquids or solids are said to exhibit *partial miscibility* and the system possesses a *miscibility gap*.

83. non-saturating solute

Solute which forms an unsaturated solution.

Note. Together with the term *saturating solute* used to distinguish among solutes in *ternary* and *higher-order systems*

84. number concentration, C

Number of entities of a constituent in a *mixture* divided by the volume of the mixture.

See also *amount*.

85. osmotic coefficient φ_x , φ_m Factor to correct for non-ideal behavior of the *solvent* in a *solution*. (a) *Amount fraction* basis. For solvent A,

 $\varphi_{\rm x,A} = (\mu_{\rm A} - \mu^*_{\rm A})/RT \ln x_{\rm A}$

where μ^*_A is the standard chemical potential of A, i.e., the chemical potential of pure liquid A. (b) *Molality* basis. For a solvent A in a solution of total molality $\sum m_B$,

$$\varphi_{\rm m,A} = (\mu^*_{\rm A} - \mu_{\rm A})/RTM_{\rm A}\Sigma m_{\rm B}$$

where M_A is the molar mass of the solvent.

Note 1: The coefficient φ_x was previously called the rational osmotic coefficient.

Note 2: For a single salt with sum of stoichiometric coefficients of its ions v and molality $m_{\rm B}$, $\varphi_{\rm m,A} = (\mu^*_{\rm A} - \mu_{\rm A})/vRTM_{\rm A}m_{\rm B}$

From [2].

86. Ostwald coefficient, *L*

Volume V^{g} of an amount n_{B}^{l} of a dissolved gas calculated at given temperature *T* and pressure *p* divided by the volume of the dissolving liquid of volume V^{l} and containing an amount n_{A} of *solvent* at the same temperature *T* and pressure *p*.

Par

Note 1: There are two Ostwald coefficients, depending on whether the liquid is the *equilibrium solution* or the pure liquid, with mathematical definitions:

Ostwald coefficient, solution reference $L_{\rm B} = V^{\rm g}(T, p, n_{\rm B}^{\rm l}) / V^{\rm l}(T, p, n_{\rm A}, n_{\rm B}^{\rm l}) = c_{\rm B}^{\rm l} / c_{\rm B}^{\rm g}$ Ostwald coefficient, pure solvent reference $L_{\rm B}^{*} = V^{\rm g}(T, p, n_{\rm B}^{\rm l}) / V^{\rm l}(T, p, n_{\rm A})$

Note 2: The relations between the *molality* $m_B(p^e)$ or *amount fraction* $x_B(p^e)$ of dissolved gas and the Ostwald coefficients are:

$$\frac{1}{x_{\rm B}} = 1 + \frac{1}{m_{\rm B}(p)M_{\rm A}} = 1 + \frac{RTZ_{\rm B}}{V_{\rm A}p_{\rm B}L_{\rm B}}$$
$$\frac{1}{x_{\rm B}} = 1 + \frac{1}{m_{\rm B}(p)M_{\rm A}} = 1 + \frac{RTZ_{\rm B}}{pV_{\rm mA}L_{\rm B}^*}$$

where $V_{\rm A}$, $V_{\rm m,A}$ are the respective partial molar volume and molar volume of the solvent and $Z_{\rm B}$ is the compression factor of the gas.

Note 3: A discussion of the Ostwald coefficient from a historical perspective is available [16]

Note 4: The Ostwald coefficient and the related quantities for expression of gas solubility; absorption coefficient, Bunsen coefficient, and Kuenen coefficient appear frequently in the older literature of gas solubility determination. However, the modern practice, recommended here, is to express gas solubility as molality, amount fraction or amount ratio.

87. Ostwald ripening

from Growth of larger crystals from those of smaller size which have a lower *solubility* than the larger ones.

[1]

88. partial miscibility

See *mutual solubility*.

89. partial pressure

For a *mixture* of gases the contribution by a gaseous *constituent* B to the total pressure.

Partial pressure $p_{\rm B} = y_{\rm B}p$, where $y_{\rm B}$ is the *amount fraction* of constituent B and p is the total artial pressu pressure.

Note: In real (non-ideal) gases there is a difficulty about defining partial pressure. [1], [2]

90. percent, % One part in a hundred parts.

Example: The amount fraction $x = 2.8 \times 10^{-2} = 2.8 \%$ [1]

91. peritectic reaction incongruent reaction.

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Isothermal, reversible reaction between two phases, a liquid and a solid, that results, on cooling of a binary, ternary or higher-order system in one, two, ... (n - 1), where n is the number of *components*) new solid *phases*. For example, in a binary system

 $1 + \alpha \Rightarrow \beta$

where the forward arrow indicates the direction of cooling. The *equilibrium* process occurs along the peritectic line, characterized by the peritectic temperature. The peritectic composition and temperature, isobaric invariants of the system, define the peritectic point, which lies between the compositions of phases 1 and α .

Note: Derived from Greek, peri- = around and -tektos = fusible.

Example: alloy system Cu-Zn [10], salt-water system Na₂SO₄-H₂O

92. peritectoid reaction

metatectoid reaction

Isothermal, reversible reaction in the solid state, that, on cooling of a binary, ternary, or higherorder system, results in one, two, ... (n-1) new solid phases. For a binary system:

 $\alpha + \gamma \Rightarrow \beta$

where the forward arrow indicates the direction of cooling. The equilibrium process occurs at the peritectoid point, characterized by the peritectoid line at the peritectoid temperature. The peritectoid composition and temperature, isobaric invariants of the system, define the peritectoid point, which lies between the compositions of phases α and β .

Note 1: Derived from Greek, meaning "resembling a peritectic".

Note 2: metatectoid, meaning "resembling a metatectic", is not acceptable as synonym for peritectoid.

Example: systems Al-Cu [10], hexacosane (n-C₂₆H₅₄) – octacosane (n-C₂₈H₅₈)

Modified from [1].

93. peritonic reaction

transition (reaction)

Isothermal (or isobaric), isoplethic reaction, especially in *ternary systems*, where a pure compound and its binary compound, or two binary compounds containing one ionic component (of an ionic compound) or one neutral *component* (of a binary compound) in common, or a binary and a ternary compound with one or more components in common, exist in equilibrium with saturated liquid. The equilibrium process is, for example:

AX·
$$p$$
H₂O(s) + B^{z+}(aq, sat) + ($q - p$)H₂O(l) = BX· q H₂O(s) + A^{z+}(aq, sat)
from a combination of eutonic and peritectic.

Note: Named from a combination of eutonic and peritectic.

IUPAC

Example: system KCl-MgCl₂-H₂O

94. permil, ‰ per mille permille promille One part in a thousand parts or $1000 \times (\text{mass fraction})$ or g kg⁻¹. See also salinity

95. phase

System or portion of a system which is uniform in chemical composition and physical state.

Note: At *equilibrium* all intensive variables (temperature, pressure, electric field, magnetic induction, chemical potential etc.) are uniform within a phase. Modified from [1].

96. phase diagram

Graphical representation of chemical *equilibrium* by points, lines, and surfaces in unary, *binary*, ternary, and higher-order systems containing two or more phases.

97. phase rule

Gibbs' phase rule

Relation connecting number of possible stable phases P in an equilibrium system with the number of *components*, C, and the number of degrees of freedom, F, i.e., the number of variables that can be assigned free values:

$$F = C + 2 - P$$

Note 1: The phase rule as stated holds under the conditions: (a) negligible surface contributions (unless the curvature is constant); (b) uniform normal pressure is the only external force; (c) Interphase surfaces are deformable, heat-conducting and permeable to all components.

Note 2: Sometimes the Phase Rule is written as v = (C - r) + 2 - P where r is the number of chemical reactions which can take place in the system. This form requires that C be the number of species assumed for the system, rather than the number of components.

Note 3: For the phase rule in the presence of surface phases see [17]. Modified from [1, 17]

98. plait point

See critical solution point.

99. polythermal method

See synthetic method

100. precipitation

The sedimentation of a solid material (a precipitate) from a liquid solution in which the material is present in amounts greater than its *solubility* in the liquid. [1]

101. primary data

Data reported in peer reviewed scientific reports of original research which allow an assessment of data quality.

Note: Primary data are distinguished from secondary data appearing in reviews, handbooks, compendia, etc. which hold the possibility of error and bias through transcription error, incomplete coverage of the primary literature, etc.

102. Raoult's Law

See *Henry's law*

103. reciprocal salt system

System containing n ionic species and a single solvent, Because of electrical neutrality, the system has *n* components.

Note 1: Notation for reciprocal salt systems specifies all ionic species. For example:

$$K^+$$
, $Na^+ \parallel Cl^-$, $NO_3^- - H_2O$

denotes a four-component (quaternary) reciprocal salt system.

Note 2: In this example, the solution may become saturated with respect to any one of KCl, NaCl, KNO₃, NaNO₃ or their hydrates.

Note 3: Ternary systems containing a common ion can be considered as a limiting case of this class of system, where there is only one cation or anion. For example:

$$Na^{+}, Zn^{2+} \parallel SO_4^{2-} - H_2O$$

104. retrograde solubility

(1) Solubility that decreases with an increase in conditions such as temperature or added *component*, where an increase is expected as the usual case.

(2) In ternary liquid systems with *coexisting phases*, where the *critical solution point* is not a maximum on a ternary diagram, under specific conditions it is possible to pass from a homogeneous mixture in which the composition of a given component is greater than that of the critical mixture to a heterogeneous mixture and back to a homogeneous mixture by altering the relative amounts of the two other components. [18]

105. salinity, S

(a) Conventional salinity, S_T: mass of total salt (in all forms) divided by mass of saline solution. (b) Relative to *chlorinity*: S = 1.80655 Cl in seawater and brackish waters.

Note 1. Used in describing composition of saline solutions, e.g., seawater, brackish waters and brines.

Note 2: Usual unit for this mass fraction is permil. See also *chlorinity*. [6]

106. salt effect (in solubility)

Change in *solubility* of a *solute* in aqueous solution on addition of a salt that does not possess a common ion with the original solute.

Note: If the solubility increases on addition of a salt, the addition is said to cause salting-in; if the opposite, it causes salting-out.

See also Sechenov equation

107. saturated solution

Solution which has the same concentration of a solute as one that is in equilibrium with undissolved solute at specified values of temperature and pressure.

Note: Ternary and higher-order systems can be saturated with respect to one component while being unsaturated with respect to another. Modified from [1].

108. saturating solute

Solute which forms a saturated solution.

Note: Together with the term *non-saturating solute* used to distinguish among solutes in *ternary* and *higher-order systems*

109. saturation State of a saturated solution. Modified from [1].

110. saturation vapor pressure

The pressure exerted by a pure substance (at a given temperature) in a system containing only the vapor and condensed *phase* (liquid or solid) of the substance.

[1]

111. scaling equation

Dimensionless equation representing *mutual solubilities* in a number of chemically-related liquid systems. Each mutual solubility is subtracted from the solubility at the *critical solution point* and the temperature is divided by the *critical solution temperature*.

112. Schreinemakers' method

See *wet residue method*

113. Sechenov equation

Expression of the salt effect that relates the change in solubility of a nonelectrolyte (e.g., gas or organic liquid) to increasing *ionic strength* of aqueous solutions,



where s_0 , s are the solubilities of nonelectrolyte in pure water and saline solution, respectively, K_s the Sechenov parameter (an empirical proportionality constant), and I_s the ionic strength of the saline solution.

Note: Positive values of the Sechenov parameter correspond to the commonly observed saltingout effect; negative values to the less common salting-in effect. [5]

114. Sieverts' law

Solubility of a diatomic gas in a molten metal is proportional to the square root of the partial pressure.

115. smoothing equation

See *fitting* equation

116. solid mixture

See *mixture*

117. solid solution

See solution

118. solubility *s*

The analytical composition of a *mixture* or *solution* which is *saturated* with one of the *components* of the mixture or solution, expressed in terms of the proportion of the designated component in the designated mixture or solution.

Note 1: The definition refers to *constituents* B; i.e., s_B .

Note 2: Solubility may be expressed in any units corresponding to quantities that denote relative composition, such as *mass, number or amount concentration, molality, amount (mole) fraction, mole ratio*, etc.

Note 3: The mixture or solution may involve any physical state: solid, liquid, gas, vapor, supercritical fluid.

Note 4: The term solubility is also often used in a more general sense to refer to processes and phenomena related to *dissolution*.

119. solubility constant

Generalization of *solubility product* to include the undissociated salt or uncharged cation-anion pair as *solute* and, as well, reaction between *solution* species and the cation or anion of the solid salt.

Note 1: The solubility constant can also be considered as relating to a solubility *equilibrium* as described under *solubility product* plus one or more simultaneous homogeneous equilibria in solution.

Note 2: Examples and specialized notation for solubility constants are described in [19-23]. See also *solubility product*.

120. solubility parameter, δ

Parameter used in predicting the *solubility* of non-electrolytes (including polymers) in a given *solvent*. For a substance B:

$$\delta_{\rm B} = \left(\Delta_{\rm vap} E_{\rm m,B} / V_{\rm m,B}\right)^{1/2}$$

where $\Delta_{\text{vap}} E_{\text{m}}$ is the molar energy of vaporization at zero pressure and V_{m} is the molar volume [24].

Note 1: For a substance of low molecular weight, the value of the solubility parameter can be estimated most reliably from the enthalpy of vaporization and the molar volume.

Note 2: The solubility of a substance B can be related to the square of the difference between the solubility parameters for supercooled liquid B and solvent at a given temperature, with appropriate allowances for entropy of mixing. Thus a value can be estimated from the solubility of the solid in a series of solvents of known solubility parameter. For a polymer, it is usually taken to be the value of the solubility parameter of the solvent producing the solution with maximum intrinsic viscosity or maximum swelling of a network of the polymer. See [24] for the original definition, theory, and extensive examples.

Note 3: The SI units are $Pa^{1/2} = J^{1/2} m^{-3/2}$, but units used frequently are $(\mu Pa)^{1/2} = (J \text{ cm}^{-3})^{1/2}$ or (cal cm⁻³)^{1/2}, where 1 $(J \text{ cm}^{-3})^{1/2} \approx 2.045$ (cal cm⁻³)^{1/2}. Modified from [1, 24].

121. solubility product, K_s

Equilibrium constant for the *dissolution* process of an ionic solid or an addition compound that dissociate completely in *solution*; for example:

$$\mathbf{M}_{\nu_{+}} \mathbf{X}_{\nu_{-}} \cdot r\mathbf{H}_{2}\mathbf{O}(\mathbf{s}) \rightleftharpoons \nu_{+} \mathbf{M}^{z_{+}} (\mathbf{aq}, \mathbf{sat}) + \nu_{-} \mathbf{X}^{z_{-}} (\mathbf{aq}, \mathbf{sat}) + r\mathbf{H}_{2}\mathbf{O}(\mathbf{l})$$

where a hydrated ionic solid (mole ratio water/salt = r) has been shown as a common occurrence of a combined ionic solid and addition compound. The equilibrium constant is::

or

 $K_{\rm s} = a_{\perp}^{\nu_+} a_{\perp}^{\nu_-} a_{\rm w}^{\nu_-}$

 $K_s = (\gamma_{\pm}/m^{\circ})^{\nu} (m_{+})^{\nu_{+}} (m_{-})^{\nu_{-}} \exp(-rM_w \sum_i m_i \varphi_m)$ where a_+ , a_- and a_w are the respective cation, anion and water activities, $v = v_+ + v_-$ is the sum of the stoichiometric numbers and z_+ , z_- the charge numbers of the cation and anion, *m molality*, γ_{\pm} the mean ionic *activity coefficient* (referenced to molality), $m^{\circ} = 1 \mod \text{kg}^{-1}$ the standard molality, M_w the molar mass of water and φ_m the *osmotic coefficient* (referenced to molality). The summation is over all species in solution.

Note 1: For the special case where there is no common cation or anion and no reaction with solution species and the cation or anion of the salt to form, e.g., an acid, base or complex ion in the solution:

$$K_{\rm s} = (\nu_{\pm} \gamma_{\pm} m / m^{\rm o})^{\nu} \exp(-r \nu M_{\rm w} m \varphi_{\rm m})$$

where $v_{\pm} = (v_{+}^{\nu+}v_{-}^{\nu-})^{1/\nu}$ and *m* is the stoichiometric molality of the anhydrous salt, with $m_{+} = v_{+}m$, $m_{-} = v_{-}m$.

Note 2: For the special case where common anions, molality m_X , with balancing cations of molality $m_{\rm N}$, exist in solution, but there is no reaction with solution species and the cation or anion of the salt:

 $K_{\rm s} = (\gamma_{+}/m^{\rm o})^{\nu}m_{+}^{\nu}(\nu_{-}m+m_{\rm x})^{\nu_{-}}\exp[-rM_{\rm w}(\nu m+m_{\rm N}+m_{\rm x})\varphi_{m}]$

See also solubility constant. Modified from [1]

122. solubilization

Process or agent that increases *solubility* or the rate of *dissolution* of a *solute*.

Note: Sometimes used loosely to include agents such as surfactants which hold a *component* in micelles or colloidal suspension rather than in solution.

123. solute

Minor component of a *solution* which is regarded as having been dissolved by the *solvent*. Modified from [1].

124. solute amount (mass) fraction

See Jänecke coordinates.

125. solution

Liquid or solid *phase* containing more than one substance, when, for convenience, one (or more) of the substances, called the *solvent*, is treated differently from the other substances, called solutes.

Note 1: When the sum of the *amount fractions* of the solutes is small compared with unity, the solution is called a dilute solution.

Note 2: A superscript ∞ attached to the symbol for a property of a solution denotes the property in the limit of *infinite dilution*.

See mixture. [2, 15] **126. solvent** Major *component* of a *solution* which is regarded as having dissolved the *solute*. Modified from [1].

127. solvent amount (mass) fraction

Amount or mass fraction of a solvent in a solution containing s solute constituents and p - ssolvent constituents. For a solvent A:

$$x_{v,A} = x_A / \sum_{i=s+1}^{p} x_i$$
, where $\sum_{i=1}^{p} x_i = \sum_{i=1}^{s} x_i + \sum_{i=s+1}^{p} x_i = 1$

and the summation is over all solvent substances, p - s in number.

See also Jänecke coordinates. [5]

128. solvent volume fraction, $\varphi_{\rm v}$

For a solvent A, volume fraction of A divided by the sum of the volume fractions of solvent in a solution containing both p solvents and s solutes:

$$\varphi_{\mathbf{v},\mathbf{B}} = \varphi_{\mathbf{B}} / \sum_{j=s+1}^{p} \varphi_{j}$$

where the summation is over the p - s solvent *components*.

Note: Used to express solvent composition for a system containing a solute in a mixed solvent.

See also volume fraction.

[5]

129. species amount (mole) fraction

See ionic amount (mole) fraction

130. spinodal curve

Boundary of separation between *metastable* and unstable *phases* on a temperature-composition or pressure-composition *phase diagram* for a liquid or solid *system* of two or more *components*. From [8]

131. standard concentration

Chosen value of amount concentration.

Note: In principle one may choose any value for the standard concentration, although the choice must be specified. The most common choice for standard concentration is $c^{\theta} = 1 \mod \text{dm}^{-3}$, which is universally accepted.

Modified from [1] and [2].

132. standard molality, m^{Θ} , m° , b^{Θ} , b° Chosen value of *molality*.

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Note: In principle one may choose any value for the standard molality, although the choice must be specified. The most common choice for standard molality is $m^{\theta} = 1 \mod \lg^{-1}$, which is universally accepted.

Modified from [1] and [2].

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133. standard pressure, p^{θ} , p^{0}

Chosen value of pressure.

Note: In principle one may choose any value for the standard pressure, although the choice must be specified. In practice, the most common choice is $p^{\circ} = 0.1$ MPa = 100 kPa (= 1 bar). The value for $p^{\bullet} = 100$ kPa, is the IUPAC recommendation since 1982, and is recommended for tabulating thermodynamic data. Prior to 1982 the standard pressure was usually taken to be $p^{\theta} =$ 101 325 Pa (= 1 atm, called the *standard atmosphere*). In any case, the value for p^{θ} should be specified. The conversion of values corresponding to different p° is described in [25-27]. The newer value of p° , 100 kPa is sometimes called the standard state pressure.

Modified from [1] and [2]

134. standard state

State of a system chosen as standard for reference by convention. Three standard states are recognized:

For a gas *phase* it is the (hypothetical) state of the pure substance in the gaseous phase at the standard pressure $p = p^{\Theta}$, assuming ideal behavior.

For a pure phase, or a *mixture*, or a *solvent* in the liquid or solid state it is the state of the pure substance in the liquid or solid phase at the standard pressure $p = p^{\theta}$.

For a solute in solution it is the (hypothetical) state of solute at the standard molality m^{Θ} , standard pressure p^{Θ} or standard concentration c^{Θ} and exhibiting infinitely dilute solution behavior.

[1]

135. supercritical fluid

State of a compound, mixture or element above its critical pressure (p_c) and critical temperature ALL ON $(T_{\rm c})$.

[1]

136. supersaturated solution

Solution which has a greater concentration of a *solute* than one that is in *equilibrium* with undissolved solute at specified values of temperature and pressure.

See also saturated solution, unsaturated solution.

137. supersaturation

State of a *supersaturated solution*. Modified from [1].

138. syntectic reaction

Isothermal reversible reaction of two liquid *phases* l_1 , l_2 which are transformed into a solid phase α during the cooling of a *system*. For a binary system:

 $l_1 + l_2 \Rightarrow \alpha$

where the forward arrow indicates the direction of cooling. The equilibrium reaction occurs along the syntectic line, characterized by the syntectic temperature. The syntectic composition and temperature, isobaric invariants of the system, define the syntectic point, which lies between the composition of the two liquid phases.

Note 1: Derived from Greek, meaning "melting together".

Example: system K-Zn [10]

Note 2: Occasionally a similar reaction takes place in the subsolidus region. Quite appropriately it is called syntectoid reaction.

139. synthetic method

Class of experimental procedures for *solubility* determination in which a *solution* of known composition is prepared. Two major subclasses are recognized. In the isothermal method one liquid *component* is titrated with a second liquid component at constant temperature until persistent turbidity is observed (i.e., to the *cloud point*). In the polythermal method a *mixture* of known composition is heated above its solution temperature and monitored visually during cooling until turbidity (the cloud point) is observed.

140. system

Arbitrarily defined part of the universe, regardless of form or size.

Note: In the context of *solubility* phenomena a system contains two or more *components* whose solubility is of interest. Modified from [1].

141. ternary diagram

Gibbs' triangular representation

Triangular plot (usually an equilateral or right-angled triangle) whose vertices represent the pure *components* of a *ternary system* at constant temperature and pressure. Any point within the triangle represents the composition in terms of the two independent amount (or mass) fractions. Lines parallel to the sides of the triangle represent constant proportions of the respective components (isopleths).

Note 1: In an *isobaric* diagram, an axis perpendicular to the plane of the triangle may be added to represent temperature.

Note 2: In addition, any triangle of any shape within the main triangle can be used to obtain the composition of the system represented by a point within the triangle in terms of the compositions represented by its vertices.

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142. ternary system

System containing three components.

143. thermodynamic component

See *component*

144. tie-line

connodal, conodal Straight line connecting *phases* in *equilibrium* on a *phase diagram*. [24]

145. transition point

See peritonic point.

146. unsaturated solution

Solution which has a lower concentration of a solute than one that is in equilibrium with undissolved solute at specified values of temperature and pressure.

147. unsaturation

State of an *unsaturated solution*.

148. upper critical solution temperature

See critical solution point

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149. Van der Waals' equations

See Gibbs-Konovalov equations

150. volume fraction, φ

Volume of a *constituent* of a *mixture* divided by the sum of volumes of all constituents prior to mixing. For a substance B:

$$\varphi_{\mathbf{B}} = x_{\mathbf{B}} V_{\mathbf{m},\mathbf{B}}^* / \sum_{j=1}^{C} x_j V_{\mathbf{m},j}^*$$

where $V_{m_i}^*$ is the molar volume of the pure constituent *j*.

See also *solvent volume fraction*. Extended from [1].

151. wet residue method

Schreinemakers' method, initial complex method

Method for determining composition of a solid *phase* in a *ternary system* at constant temperature and pressure by analysis of the total mixture of solid and liquid in *equilibrium*.

Note 1: The method relies on the fact that the wet residue lies on the *tie-line* connecting the solid phase and the *saturated* liquid phase. Equally well, the initial mixture of solid and liquid used in the *solubility* experiment can be used, when it is referred to as the "initial complex" method. In either case, two or more tie-lines intersect at the composition of the solid phase.

Note 2: The method is generally more reliable than isolation and analysis of the solid phase, especially when the solid phase is a hydrate. [29, 30]

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4. QUANTITIES, SYMBOLS and UNITS USED IN THIS GLOSSARY

4.1 Quantities, symbols and units

Entries in the table are consistent with terminology, symbols and units given in [2, 4].

Name	Symbol	Definition	SI Unit	Notes
absorption	β^*	$\beta_{\rm B}^* = V^{\rm g}(T, p_{\rm A} + p_{\rm B} = p^{\rm e}, n_{\rm B}^{\rm l}) / V^{\rm l}(T, p^{\rm e}, n_{\rm A})$	1	
coefficient				
(in gas solubility)				
activity coefficient,	f	$RT \ln (x_{\rm B}f_{\rm B}) = \mu_{\rm B} (T, p, x) - \mu_{\rm B}^* (T, p)$	1	
amount fraction				
basis				
activity coefficient,	2,	$RT \ln(\gamma - m / m^{e}) = \mu - \mu^{e} = \lim_{n \to \infty} \left[\mu - RT \ln(m / m^{e}) \right]$	1	
molality basis		$m_{\mathrm{m},\mathrm{B}} \to 0^{1/2} \mathrm{m}^{-1} $		
activity coefficient			1	
at infinite dilution	1 3	$\ln f_{\mu}^{\infty} = \lim \left(\frac{\mu_{\rm B} - \mu_{\rm B}}{1 - \ln x_{\rm B}} - \ln x_{\rm B} \right)$		
at minite anation		$x_{\rm B} \rightarrow 0$ RT		
amount	<i>c</i> , <i>U</i>	$c_{\rm B} = [\text{species B}] = n_{\rm B}/V$	mol m ⁻³	
concentration	[species], (
	М			
amount (mole)	x	C	1	
fraction		$x_{\rm B} = n_{\rm B} / \sum n_i$		
amount of substance	n	(SI base unit)		
amount ratio	r	$r_{12} = n_1 / n_2$	I	
Bunsen coefficient,	α^{*}	$\alpha_{\rm B}^{*} = V^{\rm g}(T^{\rm e}, p^{\rm e}, n_{\rm B}^{\rm h}) / V^{\rm h}(T, p^{\rm e}, n_{\rm A})$	1	
pure solvent basis				
Bunsen coefficient,	α	$\alpha_{\rm B} = V^{\rm g}(T^{\rm e}, p^{\rm e}, n_{\rm B}^{\rm -1}) / V^{\rm t}(T, p^{\rm e}, n_{\rm A}, n_{\rm B}^{\rm -1})$	1	
solution basis		Gro C		
chemical potential	μ	$\mu_{\rm B} = (\partial G / \partial n_{\rm B})_{T, n, n, p}$	J mol ⁻¹	
compression factor.	Ζ	$Z_{\rm B} = pV_{\rm m B} / RT$	1	
compressibility				
factor				
(molar) energy of	$\Delta_{\rm vap}E_{\rm m}$	$\Delta_{\rm vap} E_{\rm m} = E_{\rm m}^{\rm g} - E_{\rm m}^{\rm l}$	J mol ⁻¹	
vaporization				
(molar) enthalpy	H _m	H/n	J mol ⁻¹	
(molar) entropy	S _m	S/n	J K ⁻¹ mol ⁻¹	
Gibbs energy	G	G = H - TS	J	
Kuenen coefficient,	S^*	$S_{\rm B}^{*} = V^{\rm g}(T^{\rm o}, p^{\rm o}, n_{\rm B}^{\rm l}) / m^{\rm l}(T, p^{\rm o}, n_{\rm A})$	m ^s kg ⁻¹	
pure solvent basis				
Kuenen coefficient,	S	$S_{\rm B} = V^{\rm g}(T^{\rm e}, p^{\rm e}, n_{\rm B}^{\rm i}) / m^{\rm i}(T, p^{\rm e}, n_{\rm A}, n_{\rm B}^{\rm i})$	m kg	
solution basis			<u> </u>	
mass	т	(SI base unit)	kg ()	6
mass concentration	γ, ρ	$\rho_{\rm B} = m_{\rm B} / V$	kg m	\bigcirc

mass fraction	142	C	1	
	W	$w_{\rm B} = m_{\rm B} / \sum_{i}^{\infty} m_{i}$	1	
		i=1		
molality	<i>m</i> , <i>b</i>	$m_{\rm B} = n_{\rm B} / M_{\rm A} (n - \sum_{\rm B} n_{\rm B})$		
molar mass	М	$M_{\rm A} = m_{\rm A} / n_{\rm A} \ (= {\rm mass} / {\rm amount})$	kg mol ⁻¹	
number density of entities, number	С	$C_{\rm B} = N_{\rm B} / V$	m ⁻³	
concentration				
osmotic coefficient, amount fraction basis	φ_{x}	$\varphi_{\rm x,A} = (\mu_{\rm A} - \mu^*_{\rm A})/RT \ln x_{\rm A}$	1	
osmotic coefficient, molality basis	$\varphi_{ m m}$	$\varphi_{\mathrm{m,A}} = (\mu_{\mathrm{A}}^* - \mu_{\mathrm{A}})/RTM_{\mathrm{A}}\Sigma m_{\mathrm{B}}$	1	
Ostwald coefficient, pure solvent basis	L^*	$L_{\rm B}^{*} = V^{\rm g}(T, p, n_{\rm B}^{\rm l}) / V^{\rm l}(T, p, n_{\rm A})$	1	
Ostwald coefficient, solution basis	L	$L_{\rm B} = V^{\rm g}(T, p, n_{\rm B}^{\rm l}) / V^{\rm l}(T, p, n_{\rm A}, n_{\rm B}^{\rm l}) = c^{\rm l}_{\rm B} / c^{\rm g}_{\rm B}$	1	
partial molar enthalpy	HB	$H_{\rm B} = (\partial H / \partial n_{\rm B})_{T, p, n_i \neq n_{\rm B}}$	J mol ⁻¹	
partial molar entropy	S _B	$S_{\rm B} = (\partial S / \partial n_{\rm B})_{T, p, n_i \neq n_{\rm B}}$	J K ⁻¹ mol ⁻¹	
partial molar volume	V _B	$V_{\rm B} = (\partial V / \partial n_{\rm B})_{T, p, n_{\rm isB}}$	m ³ mol ⁻¹	
pressure	р	(normal force) / area	Ра	
solubility	S	composition of saturated solution or mixture	(various)	
solubility parameter	δ	$\delta_{\mathrm{B}} = (\Delta_{\mathrm{vap}} E_{\mathrm{m,B}} / V_{\mathrm{m,B}})^{1/2}$	$Pa^{1/2}$	
solute amount fraction; Jänecke amount fraction	x _s	$x_{s, B} = x_B / \sum_{i=1}^{s} x_i$	1	
solvent amount fraction	x _v	$x_{v,A} = x_A / \sum_{i=s+1}^{p} x_i$	1	
stoichiometric number (of a salt)	v	$v = v_+ + v$	1	
temperature (Celsius)	<i>θ</i> , <i>t</i>	$\theta / {}^{\circ}\text{C} = T / \text{K} - 273.15$	°C	
temperature, thermodynamic	Т	(SI base unit)	ĸ	
volume	V	9	m ⁻³	
volume fraction	φ	$\varphi_{\rm B} = x_{\rm B} V_{\rm m, B}^* / \sum_{j=1}^{C} x_j V_{{\rm m},j}^*$		<u>^</u>

4.2 Subscripts and superscripts

4.2.1 Subscripts

- А general constituent, usually solvent
- В general constituent
- m molar (divided by amount of substance)
- vaporization vap
- 1, 2 general constituent

4.2.2 Superscripts

vapor g liquid pure substance

 $\theta, 0$ x