The IUPAC-NIST Solubility Data Series: A guide to preparation and use of compilations and evaluations (IUPAC Technical Report)*,§

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Abstract: The IUPAC-NIST Solubility Data Series (SDS) is an ongoing project that provides comprehensive reviews of published data for solubilities of gases, liquids, and solids in liquids or solids. Data are compiled in a uniform format, evaluated, and, where data from independent sources agree sufficiently, recommended values are proposed. This paper is a guide to the SDS and is intended for the benefit of both those who use the SDS as a source of critically evaluated solubility data and who prepare compilations and evaluations for future volumes. A major portion of this paper presents terminology and nomenclature currently recommended by IUPAC and other international bodies and relates these to obsolete forms that appear in the older solubility literature. In addition, this paper presents a detailed guide to the criteria and procedures used in data compilation, evaluation, and presentation and considers special features of solubility in gas + liquid, liquid + liquid, and solid + liquid systems. In the past, much of this information was included in introductory sections of individual volumes of the SDS. However, to eliminate repetitive publication, this information has been collected, updated, and expanded for separate publication here.

Keywords: data compilation; data evaluation; IUPAC Analytical Chemistry Division; phase equilibria; solubility; Solubility Data Series; solubility terminology and nomenclature; solution equilibria.

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INTRODUCTION

The Solubility Data Series (SDS) was conceived by the late Prof. A. S. Kertes with the aim of providing a comprehensive review of published data for solubility of gases, liquids, and solids in liquids or solids. As an ongoing IUPAC project, the SDS exhaustively compiles and critically evaluates experimentally determined solubility data from the primary chemical literature. Between 1979 and 2009, the project has produced 87 volumes, each of which presents data for a chemically related group of systems. Data are compiled in a uniform format. The data for each system are evaluated and, where data from independent sources agree sufficiently, recommended values are proposed. This paper is a guide to the SDS and is intended for the benefit of both those who use the SDS as a source of critically evaluated solubility data and those who prepare compilations and evaluations for future volumes. Individuals interested in participating in volume preparation should contact the authors of this paper or consult the IUPAC web site for further information.

Solubility data have long been widely used in chemistry and an array of related fields of science and engineering for many different purposes. For some intended purposes, highly precise data are required; for others, order-of-magnitude estimates are perfectly satisfactory. Because the SDS addresses an audience with diverse needs for data precision, all data of whatever precision are compiled unless there is strong reason to believe that experimental shortcomings or other mistakes render a report unreliable. The essential criterion for data to be recommended in the SDS is that two or more independent data sets (i.e., from separate and independent laboratories) agree within their experimental error. It is every user's responsibility to determine whether the precision and reliability of recommended data are suitable for the intended purpose.

Solubility measurements have been reported in the chemical literature since the earliest days of chemistry. One of the tasks of the SDS is facilitating comparisons of data by converting various measurements to consistent units expressed in unambiguous and accepted terminology. A major portion of this paper presents terminology and nomenclature currently recommended by IUPAC and other international bodies and relates these to obsolete forms that appear in the older solubility literature.

The first volume of the SDS was published in 1979. Organization, reviewing, and editing of the Series was handled by the IUPAC Solubility Data Commission (V.8) until 2002, when, along with reorganization of IUPAC committees, these functions were transferred to the Subcommittee on Solubility and Equilibrium Data (SSED) of Division V (Analytical Chemistry) of IUPAC. Until 1996, volumes in the series were published in hard-cover book format. In 1998, publication was assumed by the *Journal of Physical and Chemical Reference Data* (*JPCRD*) published by the American Institute of Physics for the National Institute of Standards and Technology (NIST). During the 30-year life of the SDS, great advances have been made in the preparation and dissemination of electronic databases. Selected parts of the SDS are currently available from the NIST web site, and SDS volumes published as *JPCRD* articles are available in searchable electronic form (portable document format, pdf). The history of the SDS and the people and organizations that have produced it are detailed elsewhere [1–3].

A feature of each volume (or technical paper, when published in *JPCRD*) has been an introduction to one of solubility of gases in liquids, or liquids in liquids, or solids in liquids, as appropriate to the subject matter. While these introductions were revised periodically, their repetitive nature led to the decision that a single introduction be prepared for publication as an IUPAC Technical Report and simultaneously as a paper in *JPCRD* [4]. In that way, reference could be made to these publications and repetition could be eliminated. This Technical Report provides up-to-date requirements for formatting

data and compilation sheets, as well as for terminology, symbols, and units, for use by both authors preparing contributions to the SDS and users. Updated versions in this guide supersede all materials in the previous introductions. The guidelines are consistent with those for publication in *JPCRD* [4].

RECOMMENDED TERMS AND SYMBOLS FOR EXPRESSION OF SOLUBILITY

Terms and symbols used in describing solubility phenomena have undergone significant changes since publication of the first volume of the SDS. These changes involve more precise definitions of a number of terms and a systematic application of quantity calculus, as described in [5] and, in latest form, in [6,7]. The current list of symbols is compatible with [6,7], although in ref. [7] a number of changes and corrections have been made to definitions listed in [8].

Terms and symbols involving composition of mixtures and solutions are of primary importance in compilations and evaluations of solubility, and these are summarized in Tables 1–7 in the next section, reproduced (with some modifications) from [5] with the permission of IUPAC, copyright © 2003.

Recommended quantities, symbols, and units for quantitative expression of solubilities

Table 1 Basic quantities used in definitions related to solubility.

Name	Symbol	Definition	SI units	Notes
solubility (general)	s	See [6,7]	various	1
mass	m	SI base unit	kg	2
amount of substance	n	SI base unit	mol	
volume	V	SI derived unit	m^3	3
molar volume	V_m	$V_{m,B} = V/n_B$	$m^3\ mol^{-1}$	4
partial molar volume of B	V_B	$V_B = (\partial V/\partial n_B)_{T, p, n_{j \neq B}}$	$m^3\ mol^{-1}$	5
stoichiometric number of an ion i	v_i		1	
sum of stoichiometric numbers of ions in a salt	v	$v = v_+ + v_-$	1	6
charge number of ion i	z_i		1	
partial pressure (of gas B)	p_B	$p_B = y_B p$	$N\ m^{-2} = Pa$	7

Notes:
1. Subscripts *x*, *m*, *c*, etc. may be added to the symbol *s* for solubility, giving corresponding new terms *solubility (mole fraction basis)*, *solubility (molality basis)*, *solubility (amount concentration basis)*, etc. (see subsequent tables), in analogy with recommendations in [6,7] for quantities such as activity coefficients.
2. The symbol *m* for mass should not be confused with the same symbol for molality in Table 4.
3. Litre, L or l, is an acceptable unit for volume.
4. For pure substance B. For a mixture, the mean molar volume is $\overline{V}_m = V/n$ where *n* is the total amount of all components in the mixture.
5. For entities B. In the SDS, the *C* thermodynamic components are labeled $i = 1, 2, 3,…, C$.
6. For a salt $M_{v+}X_{v-}$.
7. For gas B; y_B is the mole fraction of B in the vapor phase, and *p* is the total pressure.

Table 2 Quantities used to describe solubilities based on **mass**.

Name	Symbol	Definition	SI units	Notes and references
mass fraction	w	$w_B = m_B / \sum_{i=1}^{C} m_i$	1	1
solute mass fraction	w_s	$w_{s,B} = m_B / \sum_{i=1}^{p_s} m_i$	1	2
solvent mass fraction	w_v	$w_{v,A} = w_A / \sum_{i=p_s+1}^{p} w_i$	1	3
mass ratio	ζ	$\zeta_{A,B} = m_A/m_B$	1	

Notes:
1. For entities B; summation is over all entities, total number p. The entities may be thermodynamic components labeled $i = 1, 2, 3,…, C$.
2. Summation is over all solute components p_s.
3. Summation is over all solvent components $p_v = p - p_s$.

Table 3 Quantities used to describe solubilities based on **amount of substance**.

Name	Symbol	Definition	SI units	Notes
mole fraction, amount-of-substance fraction, amount fraction	x, y	$x_B = n_B / \sum_{i=1}^{C} n_i$	1	1
ionic (species) mole (amount) fraction of salt	x_+, x_-	$x_{+B} = \dfrac{v_{+B} x_B}{1 + \sum_{i=1}^{p}(v_i - 1)x_i}$ $x_{-B} = \dfrac{v_{-B} x_{+B}}{v_{+B}}$	1	2
ionic (species) mole (amount) fraction of solvent	x'_A	$x'_A = \dfrac{x_A}{1 + \sum_{i=1}^{p_s}(v_i - 1)x_i}$	1	2
solute mole (amount) fraction	x_s	$x_{s,B} = x_B / \sum_{i=1}^{p_s} x_i$	1	3
solvent mole (amount) fraction	x_v	$x_{v,A} = x_A / \sum_{i=p_s+1}^{p} x_i$	1	4
mole (amount) ratio	r	$r_{A,B} = n_A/n_B$	1	

Notes:
1. For entities B; summation is over all entities, total number p. The entities may be thermodynamic components labeled $i = 1, 2, 3,…, C$. Symbol x is usually used for components in condensed phases, y for those in gaseous phases. The entities may also be particular assumed species in the system. Thus the nature of the species must be specified.

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Table 3 (*Continued*).

2. These quantities are special forms of mole fractions for ionic species, are generalizations of those given in Robinson and Stokes [9], pp. 31–32, and refer to a mixture of p_s binary salts i, each of which ionizes completely, and a mixture of p_v non-electrolytes j, of which some may be solvent components. B refers to any one of the p_s electrolytes, and A is substance $p_s + 1$ of the p_v non-electrolyte species. The sum of the ionic amount fractions of salts and solvents (electrolytes and non-electrolytes) is unity, so that $C = p_s + p_v$. For a single solvent,

$$x'_A = \frac{x_A}{1 + \sum_{i=1}^{p_s}(v_i - 1)x_i}$$

so that

$$\sum_{i=1}^{p_s}(x_{+i} + x_{-i}) + x'_A = 1$$

The quantities are used in formulation of solubility equations for electrolytes, in defining activity coefficients of salts, and in tabulation of salt effects on the solubility of gases. The concept can be applied to systems containing only non-ionic species, where the term *species (mole) amount fraction* is appropriate.
3. Summation is over all solute components, p_s in number. Where these quantities are used in representations of phase diagrams, they are often called *Jänecke solute fractions*.
4. Summation is over all solvent components $p_v = p - p_s$.

Table 4 Quantities used to describe solubility based on **mass** and **amount of substance**.

Name	Symbol	Definition	SI units	Notes
molality	m	$m_B = n_B / \sum_{i=p_s+1}^{p} n_i M_i$	mol kg^{-1}	1
aquamolality	$m^{(C)}$	$m_B^{(C)} = m_B \bar{M} / M_C$	mol kg^{-1}	2

Notes:
1. For a solute B in a mixed solvent containing $p - p_s$ solvent components, where M_i is the molar mass of solvent component i. The *standard molality* is usually taken as $m^{\ominus} = 1$ mol kg^{-1}.
2. For a solute B either in pure solvent A or a mixed solvent with components A, C. Component C is a reference component, usually ordinary water, but any other solvent reference component may be chosen, when the term used is *solvomolality*. The average molar mass of the mixed solvent is:

$$\bar{M} = x_{v,A}M_A + (1 - x_{v,A})M_C$$

with $x_{v,A}$ the solvent mole fraction of component A. See [5] for the history and uses of this term.

Table 5 Quantities used to describe solubility based on **volume** alone, or on **mass** or **amount of substance** and **volume**.

Name	Symbol	Definition	SI units	Notes
volume fraction	φ	$\varphi_B = x_B V_{m,B}^* / \sum_{j=1}^{C} x_j V_{m,j}^*$	1	1,2
solvent volume fraction	$\varphi_{v,A}$	$\varphi_{v,A} = \varphi_A / \sum_{i=p_s+1}^{p} \varphi_i$	1	1
mass concentration, mass density	ρ, γ	$\rho_B = m_B/V$	kg m^{-3}	2
amount concentration, amount-of-substance concentration	c	$c_B = n_B/V = $ [solute]	mol m^{-3}	2,3

Notes:
1. The true volume fraction of component i is $c_i V_i$. Lack of knowledge of partial molar volumes has led to the convention that volume fractions are calculated in terms of the molar volumes of the pure components, V_m^*.
2. For a solute B in a mixed solvent.
3. Both symbols c_B and [formula of solute B] are used. The *standard amount concentration* is given the symbol $c^\ominus$, and is usually 1 mol dm^{-3}. To avoid ambiguity, the term *concentration* should not be used as a general term for the *composition* of a solution or mixture; e.g., "the composition in terms of mole fraction", not "the concentration in terms of mole fraction".

Table 6 Quantities used in specifying conditions under which solubility is measured or in interpretation of solubility.

Name	Symbol	Definition	SI units	Notes
ionic strength (molality basis)	I_m	$I_m = \frac{1}{2}\sum_i m_i z_i^2$	mol kg^{-1}	1
ionic strength (amount concentration basis)	I_c	$I_c = \frac{1}{2}\sum_i c_i z_i^2$	mol m^{-3}	1
salinity	S	See note 2	1	2
chlorinity	w_{Cl}	See note 2	1	2
mass density	ρ, γ	$\rho = m/V$	kg m^{-3}	3
relative (mass) density	d	$d = \rho/\rho^\ominus$	1	4
Henry's law constant	k_H	$k_{H,B} = \lim_{x_B \to 0} (f_B / x_B) = (\partial f_B / \partial x_B)_{x_B=0}$	Pa = N m^{-2}	5
solubility product, solubility constant	K_s, $K_s^\ominus$	$K_s = (\nu_\pm \gamma_\pm m/m^\ominus)^\nu \exp(-\nu M_w \sum m \varphi_m)$	1	6

Notes:
1. The summations are over all ionic substances. For a solution containing a single completely ionized salt B with ions of charges z_+, z_-, the definitions become:
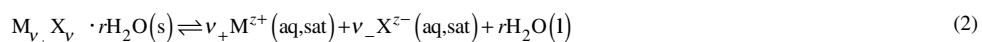
$$I_m = (1/2)|z_+z_-|\nu_B m_B \quad I_c = (1/2)|z_+z_-|\nu_B c_B \tag{1}$$

2. Used in reporting the composition of seawater. *Salinity*, S, is the mass of dissolved salts in sea water, brackish water, brine, or other saline solution divided by the mass of the solution. *Chlorinity*, w_{Cl}, is the mass of dissolved halides (reported as chloride) in sea water, brackish water, brine, or other saline solution divided by the mass of the solution. See [7] for further discussion of these terms.

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Table 6 *(Continued).*

3.   *m* is the total mass of the system. Mass density is equal to the total mass concentration. The term *density* may be used where there is no confusion with other quantities such as energy density, etc.

4.   The ratio of the mass density of a mixture at Celsius temperature *t*, pressure *p* to the mass density $\rho^{\ominus}$ of a reference substance at temperature *t'* pressure *p'*. For liquid solutions, the reference substance is often water at 4 °C, 0.1 MPa. (In some cases, 1 atm is used instead of 0.1 MPa.) The older term *specific gravity* is discouraged.

5.   For a gas B. For discussion of various forms of the Henry's law constant, see [7]. For gases that react with the solvent, care must be taken to distinguish between *stoichiometric* Henry's law constants and *species* Henry's law constants. Very often, the stoichiometric coefficient is tabulated. For example, gaseous carbon dioxide dissolves in aqueous solution and partially hydrolyzes to produce hydrogen carbonate, carbonate and hydrogen ions. The stoichiometric Henry's law constant is calculated from the total amount fraction or molality of dissolved CO_2, while the species constant is calculated from the actual amount fraction or molality of CO_2 as derived from calculations based on the equilibrium constants for formation of hydrogen carbonate and carbonate ions.

6.   The definition is for a hydrated salt B (in the absence of added electrolyte with one or more common ions) that dissociates completely in water:

$$M_{v_+} X_{v_-} \cdot rH_2O(s) \rightleftharpoons v_+ M^{z+}(aq,sat) + v_- X^{z-}(aq,sat) + rH_2O(l) \tag{2}$$

where $\gamma_{\pm}$ is the mean activity coefficient and φ_m the osmotic coefficient (both on the molality basis), and M_w is the molar mass of water.

     Analogous solubility products may be defined using amount fractions, with the corresponding activity and osmotic coefficients. A definition based on amount concentrations is difficult because of lack of a simple and consistent definition of the corresponding osmotic coefficient. For the distinction between *solubility product* and *solubility constant*, see [7].

Table 7 contains formulae for conversions between pairs of the most frequently encountered quantities used to describe solubility. The formulae are given for multicomponent systems, with simple directions for use with two-component systems.

Table 7 Interconversions between quantities used as measures of solubility for C-component systems containing $C-1$ solutes i and single solvent C (the last component in the list). ρ, density of solution; M_i, molar mass of substance i. For two-component systems, set summations to zero.

	x_B	w_B	m_B	c_B
$x_B =$	x_B	$\dfrac{1}{1+\dfrac{M_B}{M_C}\left(\dfrac{1}{w_B}-1+\sum\limits_{j\neq B}^{C-1}\left(\dfrac{M_C}{M_j}-1\right)\dfrac{w_j}{w_B}\right)}$	$\dfrac{1}{1+\dfrac{1}{m_B M_C}+\sum\limits_{j\neq B}^{C-1}\dfrac{m_i}{m_B}}$	$\dfrac{1}{1+\dfrac{1}{M_C}\left(\dfrac{\rho}{c_B}-M_B\right)+\sum\limits_{j\neq B}^{C-1}\dfrac{c_i}{c_B}\left(1-\dfrac{M_j}{M_C}\right)}$
$w_B =$	$\dfrac{1}{1+\dfrac{M_C}{M_B}\left(\dfrac{1}{x_B}-1+\sum\limits_{j\neq B}^{C-1}\left(\dfrac{M_j}{M_C}-1\right)\dfrac{x_j}{x_B}\right)}$	w_B	$\dfrac{1}{1+\dfrac{1}{m_B M_B}\left(1+\sum\limits_{j\neq B}^{C-1}m_j M_j\right)}$	$\dfrac{c_B M_B}{\rho}$
$m_B =$	$\dfrac{1}{M_C\left(\dfrac{1}{x_B}-1-\sum\limits_{j\neq B}^{C-1}\dfrac{x_j}{x_B}\right)}$	$\dfrac{1}{M_B\left(\dfrac{1}{w_B}-1+\sum\limits_{j\neq B}^{C-1}\dfrac{w_j}{w_B}\right)}$	m_B	$\dfrac{1}{\dfrac{1}{c_B}\left(\rho-\sum\limits_{j\neq B}^{C-1}c_j M_j\right)-M_B}$
$c_B =$	$\dfrac{\rho}{M_B+M_C\left(\dfrac{1}{x_B}-1+\sum\limits_{j\neq B}^{C-1}\left(\dfrac{M_j}{M_C}-1\right)\dfrac{x_j}{x_B}\right)}$	$\dfrac{\rho w_B}{M_B}$	$\dfrac{\rho}{\dfrac{1}{m_B}\left(1+\sum\limits_{j\neq B}^{C-1}m_j M_j\right)+M_B}$	c_B

LIST OF TERMS AND SYMBOLS NOT RECOMMENDED

Table 8 Terms that are considered obsolete for use in the SDS and their replacements.

Obsolete term	Replace by	Notes
g per 100 g solution	mass fraction, w_B	1,2
mass%	mass fraction, w_B	1,2
mol%	mole fraction, x_B	1,3
molarity	amount-of-substance concentration, amount concentration, c_B	
molar, M or ᴍ	mol dm^{-3} (or mol l^{-1})	
molal, m	mol kg^{-1}	
number of moles	amount of substance	
number of moles of B	amount of B	4
overbar for partial quantities, e.g., $\overline{V}_B$	Use V_B, e.g., restrict overbar to indicate an average, except in special cases where the overbar is necessary to distinguish the symbol for volume.	

Notes:
1. B in all entries refers to substance B.
2. For column headings in a table, use 100 w_B instead of mass%.
3. For column headings in a table, use 100 x_B instead of mol%.
4. The name or symbol of the substance replaces "substance". Do not use "amount of substance of B" but rather "amount of B".

SPECIAL CONSIDERATIONS FOR GAS + LIQUID SYSTEMS

Basic thermodynamics

For a solute gas B that does not react with the solvent A, both components are present in each phase, and equality of the chemical potentials of B in the gas and vapor phases gives [10]:

$$\mu_B^v = \mu_B^{v,\ominus}(T) + RT \ln\left[f_B(T, p_{A,s})/p^\ominus \right] = \mu_B^l = \mu_B^{l,\ominus}(T, p_{A,s}) + RT \ln\left[\gamma_B(T, p_{A,s}) x_B \right] \tag{3}$$

where f is the fugacity, $p_{A,s}$ the saturation vapor pressure of A, and the liquid phase activity coefficients γ_i are referenced to Henry's law on the mole fraction scale; i.e., the activity coefficient approaches zero at infinite dilution of solute. This equation leads directly to the solubility of gas B at the saturation pressure:

$$\ln x_B = \ln\left[f_B(T, p_{A,s})/\gamma_{x,B} k_H(T, p_{A,s}) \right] \tag{4}$$

where k_H is the Henry's law constant (Table 6) at the saturation pressure:

$$\ln\left[k_H(T, p_{A,s})/p^\ominus \right] = \frac{\mu_B^l(T, p_{A,s}) - \mu_B^v(T, p_{A,s})}{RT} \tag{5a}$$

and for the dependence on temperature (with T_r a reference temperature):

$$\ln\left[k_H\left(T,p_{A,s}\right)/p^{\ominus}\right]=\ln\left[k_H\left(T_r,p_{A,s}\right)/p^{\ominus}\right]-\int_{T_r}^{T}\frac{\Delta_{sln}H^{\ominus}\left(T,p_{A,s}\right)}{R}d\left(\frac{1}{T}\right) \tag{5b}$$

The enthalpy term is thus the difference between the partial molar enthalpy of B at infinite dilution and the molar enthalpy of an ideal gas, both at the saturation pressure of the solvent. An equivalent deduction based on fugacities and an extensive discussion of solubilities of gases are given by Wilhelm [11,12].

For accurate work, the Henry's law constant is evaluated using a plot based on the formula in Table 6 and the activity coefficients are estimated after correction to a constant reference pressure using the Poynting correction [11]. The solubility then follows from eq. 4, and is reported ideally as the mole fraction of dissolved gas at standard partial pressure and the saturation pressure of the solvent [12]. Most work discussed in the SDS is for low-pressure gases, those for which corrections for non-ideal behavior are made using a virial expansion including the second and third virial coefficients, and activity coefficients are assumed to be independent of pressure.

For the dependence of solubility on temperature, several empirical equations have been used; see [11,13]. With the solubility expressed as the mole fraction of solute at standard partial pressure and at the saturation pressure of the solvent, the left-hand side of eq. 5 becomes simply $-\ln x_B$. A common representation of solubility is then given by the Clarke–Glew equation [11,13] as derived in [14]:

$$\ln x_B = A + B\left(T_r/T\right) + C\ln\left(T/T_r\right) + D\left(T/T_r\right) \tag{6}$$

where A, B, C, D are empirical constants and T_r is a reference temperature, chosen preferably as the value roughly in the middle of the observed range of temperatures. For an ideal system, the constants in this and other empirical equations can be related to thermodynamic thermal quantities [13–15]. Two points should be kept in mind: (1) the coefficients derived from a least-squares analysis are highly correlated, so that addition of successive terms alters the values of preceding terms, rendering any thermodynamic values uncertain; and (2) for a non-ideal system, if the experimental data follow an equation of this form, since the ideal part determines the form of the equation, it follows that the non-ideal part also has the same form of temperature dependence.

Alternative measures of solubility

While most modern works report solubility of a gas in a liquid as the mole fraction of dissolved gas under specific conditions of temperature and pressure, as described above, experimental methods traditionally determined volumes of dissolved gas as the primary quantity. This led to various measures of solubility based on volume as follows. The definitions are derived mainly from [16,17], but with corrections.

absorption coefficient, β (in gas solubility)
Now essentially obsolete. For a gas B absorbed by liquid A, the volume of gas, $V_B^g(T^{\ominus}, p^{\ominus})$, absorbed by a mass of pure solvent A, $m_A^{1,*}$, where V_B^g has been reduced to standard conditions of temperature (usually $T^{\ominus} = 273.15$ K) and total pressure, usually either $p^{\ominus} = 100$ kPa (1 bar) or 101.325 kPa = 1 atm:

$$\beta_B = \left[V_B^g\left(T^{\ominus},p^{\ominus}\right)/V_A^{1,*}\right]_{eq} = \alpha_B\left(1-p_A/p^{\ominus}\right) \tag{7}$$

Because the volume of gas must be reduced to standard conditions, which requires knowledge of the appropriate equation of state, this coefficient is most useful for total pressures near the standard value.

This absorption coefficient is the Bunsen coefficient, α, in terms of the total pressure of the gaseous mixture of A and B rather than partial pressure of B alone. The Bunsen coefficient has been called an absorption coefficient.

Ostwald coefficient, L

Four definitions have been used:

1. Ostwald's original definition [17,18]: Volume of gas, V^g, absorbed at equilibrium divided by the volume of the pure absorbing liquid, $V^{1,*}$, at a specified temperature and total pressure. For a gas B absorbed by liquid A,

$$L_{V,B}^0 = \left(V_B^g / V_A^{1,*}\right)_{eq} \tag{8}$$

2. Based on solution volume [17,19]: Volume of gas, V^g, absorbed by a volume of saturated liquid, V^1, at a specified temperature and total pressure. For a gas B absorbed by liquid A,

$$L_{V,B} = \left(V_B^g / V^1\right)_{eq} \tag{9}$$

3. Based on amount concentration [11,17,19–21]: Concentration of absorbed gas in the liquid phase divided by concentration of gas in the vapor phase. For a gas B absorbed by liquid A,

$$L_{c,B} = \left(c_B^1 / c_B^g\right)_{eq} \tag{10}$$

4. Based on infinitely dilute amount concentration [17,19–21]: Concentration of absorbed gas in the liquid phase divided by concentration of gas in the vapor phase, extrapolated to infinite dilution of absorbed gas. For a gas B absorbed by liquid A,

$$L_{c,B}^\infty = \lim_{c_B^1 \to 0} \left(c_B^1 / c_B^g\right)_{eq} \tag{11}$$

Ostwald referred to definition 1 as the solubility of a gas. All definitions refer to absorbed gases that can be removed from the liquid by lowering the total pressure or increasing the temperature. Thus, gases that react with the solvent, such as HCl(g) or SO_2(g), are excluded.

For mole fractions of absorbed gas less than about 0.01, the definitions all give numerical results within experimental error. In reporting experimental data, especially for gases of higher solubility, it is important to specify which definition is being used [17].

For definition 3, an amount n_B^g of gas from the gas phase is absorbed by the liquid phase, so that

$$L_{c,B} = \left(c_B^1 / c_B^g\right)_{eq} = \left(V_B^g / V_B^1\right)_{eq} \tag{12}$$

so that definitions 2 and 3 are identical.

If the gas is ideal ($p_B V_B^g = n_B RT$), the liquid is incompressible, and the ideal Henry's law ($p_B = k_H x_B$) holds,

$$L_{V,B} = \alpha_B \left(T / T^{\ominus}\right) \tag{13}$$

For a rigorous relation between Henry's law constant and the Ostwald coefficient (definition 3), see [11,22].

Bunsen coefficient, α

Measure of gas solubility, now essentially obsolete. For a gas B absorbed by liquid A, the volume of gas, $V_B^g(T^\ominus, p_B^\ominus)$, absorbed by a volume of pure solvent A, $V_A^{1,*}$, where V_B^g has been reduced to standard conditions of temperature (usually $T^\ominus = 273.15$ K) and partial pressure, usually either $p_B^\ominus = 100$ kPa (1 bar) or 101.325 kPa (1 atm):

$$\alpha_B = \left[V_B^g\left(T^\ominus, p_B^\ominus\right) / V_A^{1,*} \right]_{eq} \tag{14}$$

Because the volume of gas must be reduced to standard conditions, which requires knowledge of the appropriate equation of state, this coefficient is most useful for total pressures near the standard value. If the gas is ideal ($p_B V_B^g = n_B RT$), the liquid is incompressible, and the ideal Henry's law ($p_B = k_H x_B$) holds:

$$\alpha_B = \left[V_B^g\left(T^\ominus, p_B^\ominus\right) / V_A^{1,*} \right]_{eq} = \left(\frac{V_B^g\left(T, p\right)}{V_A^{1,*}} \right)\left(\frac{T^\ominus}{T} \right)_{eq} = L_{v,B}\left(T^\ominus / T\right) \tag{15}$$

Kuenen (Künen) coefficient, S

Now essentially obsolete. For a gas B absorbed by liquid A, the volume of gas, $V_B^g(T^\ominus, p^\ominus)$, absorbed by a mass of pure solvent A, $m_A^{1,*}$, where V_B^g has been reduced to standard conditions of temperature (usually $T^\ominus = 273.15$ K) and total pressure, usually either $p^\ominus = 100$ kPa (1 bar) or 101.325 kPa (1 atm):

$$S_B = \left[V_B^g\left(T^\ominus, p^\ominus\right) / m_A^{1,*} \right]_{eq} \tag{16}$$

Because the volume of gas must be reduced to standard conditions, which requires knowledge of the appropriate equation of state, this coefficient is most useful for total pressures near the standard value.

The Kuenen coefficient is proportional to the molality. If the gas is ideal, the liquid is incompressible, and the ideal Henry's law holds:

$$S_B = \left[V_B^g\left(T^\ominus, p_B^\ominus\right) / m_A^{1,*} \right]_{eq} = \alpha_B V_{m,A}^{1,*} / M_A \tag{17}$$

where M_A is the molar mass and $V_{m,A}$ the molar volume of the solvent.

Relation of mole fraction solubility to various coefficients

For an ideal gas dissolved in an incompressible liquid, and where the ideal Henry's law ($p_B = k_H x_B$) holds, the solubility of the gas (as a mole fraction in the liquid phase) is related to the absorption, Ostwald, Bunsen, and Kuenen coefficients by:

$$
\begin{aligned}
x_B &= \frac{1}{1 + \dfrac{RT^\ominus}{p^\ominus V_{m,A}^{1,*} \beta_B}} = \frac{1}{1 + \dfrac{RT}{p^\ominus V_{m,A}^{1,*} L_{v,B}}} \\[2ex]
&= \frac{1}{1 + \dfrac{RT^\ominus}{p^\ominus V_{m,A}^{1,*} \alpha_B}} = \frac{1}{1 + \dfrac{RT^\ominus}{p^\ominus M_A S_B}}
\end{aligned}
\tag{18}
$$

For other conversions between the above definitions and conversions between Ostwald and Bunsen coefficients, see [13].

Salt effects: Sechenov (Setschenow, Сеченов) equation [5,7,16]

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

$$\lg(s_o/s) = k_s I_s \tag{19}$$

where s_o, s are the solubilities of non-electrolyte 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.

Other composition variables in place of ionic strength and Napierian instead of common logarithms can be used; see [7,16]. Salt effects can also be analyzed by use of Pitzer equations, e.g., in [23]. See section on solid + liquid systems. Positive values of the Sechenov parameter correspond to the commonly observed salting-out effect; negative values to the less common salting-in effect.

SPECIAL CONSIDERATIONS FOR LIQUID + LIQUID SYSTEMS

In principle, binary solubility of a liquid in a liquid implies the occurrence of two conjugate liquid phases in equilibrium at a given temperature and pressure. Commonly among studied systems, one component is water and the other an organic liquid. For example, in the system heptane + water [24], the solubility of heptane in the water-rich phase at $T = 298$ K is $x_1 = 5.3 \times 10^{-7}$, while the solubility of water in the conjugate heptane-rich phase is $x_2 = 6.0 \times 10^{-4}$. For this system, as with many others, data do not extend to the critical solution temperature, as is the case in other systems such as methanol + cyclohexane [25]. In studies where monitoring of water pollution is of major importance, the phase of interest is the water-rich phase, and the critical solution point is of minor interest. In other cases, the conjugate, organic-rich phase is of interest. For instance, when ethanol, which is hygroscopic, is blended into hydrocarbon motor fuels, it is highly desirable for water to not form a separate phase during storage. Here again, the critical solution point is of minor interest.

For solubility data at temperatures far from the critical solution temperature, fitting equations of the form of the Clarke–Glew equation or other empirical equation (discussed in the previous section) are adequate for many purposes. For solubility data that extend to, or close to, the critical solution temperature, another approach based on modern critical solution theory is indicated, with a fitting equation of the form:

$$x_B = x_{cB} \pm \left(B_1/2\right)|\theta|^{\beta} \pm \left(B_2/2\right)|\theta|^{\beta+w} + A_1|\theta| \pm \left(B_3/2\right)|\theta|^{\beta+2w} + A_2|\theta|^{1-\alpha w}$$
$$|\theta| = 1 - T/T_c \tag{20}$$

where subscript c indicates the critical value, $\beta = 0.329$ is the critical index, $\alpha = 0.11$, $w = 0.5$ (first Wegner correction), and B_1, B_2, B_3, A_1, A_2 are empirical constants. The absolute sign on θ takes care of cases where T_c is a lower critical solution temperature. The ± sign refers to both branches of the co-existence curve. Note that the second term of this equation determines the overall shape of the coexistence curve, and should always be given as the leading term; subsequent terms should be used successively in fitting procedures in the order given. An extensive discussion of this fitting equation, including how to extract reliable values of both the critical solution temperature and composition from experimental data, is given in [25].

Phase diagrams (e.g., temperature vs. composition for binary systems) are often used to present a graphical overview of solubility.

SPECIAL CONSIDERATIONS FOR SOLID + LIQUID SYSTEMS

Several types of fitting equation have been used in the SDS to analyze the dependence of solubility on temperature and, in multicomponent systems, on composition. The equations are based on the solubility product K_s, but only systems at constant pressure are discussed here. See specialized books on phase equilibria for more complex systems and higher-component systems.

Phase diagrams (e.g., temperature vs. composition phase diagrams for binary systems; triangular diagrams, showing mass or mole fractions along solubility curves in ternary systems; triangular prismatic phase diagrams for ternary systems to show both composition and temperature dependence) are often used to present a graphical overview of solubility.

Dependence on temperature

The approach described below provides a rapid and reliable way of comparing data that exist over the complete range of composition of the system. Extensive examples are found in [26] for electrolyte systems. The basis of the method is to construct an equation with a right-hand side which has a rigorous interpretation, and can usually be expressed in a suitable analytical form (with reference temperature and composition the melting point of a pure solid phase), and a left-hand side in which mole fractions are used to construct a function $Y(T)$ that describes the composition change along the solubility curve. The examples below are illustrative of common types.

Binary non-electrolyte solid + liquid system with compound formation

This type of system includes many binary intermetallic systems as well as non-electrolytes. For a binary non-electrolyte system of a solid binary compound $B \cdot rA$ dissolved in A with complete dissociation:

$$B \cdot rA(s) \rightleftharpoons B(sln) + rA(sln) \tag{21}$$

$$-\Delta_{sln}G^{\ominus}(T)/RT = \ln K_s = \ln\left(a_B a_A^r\right) \tag{22}$$

where a_i is the (relative) activity of i. Use mole fractions as composition variables, and symmetrical activity coefficients $f_i = 1$ at $x_i = 1$ to find:

$$-\Delta_{sln}G^{\ominus}(T)/RT = \ln\left(x_B x_A^r f_B f_A^r\right) \tag{23}$$

Subtract eq. 23 at $T = T_{fus}$ [the congruent melting or fusion point of the binary compound, where $x_B = 1/(1 + r)$] from eq. 23 at T. Since the left side of the resulting equation depends on T only,

$$Y_B(T) = \ln\left[\frac{x_B\left(1 - x_B\right)^r\left(1 + r\right)^{1+r}}{r^r}\right] = -\int_{T_{fus}}^{T}\frac{\Delta_{sln}H^{\ominus}}{R}\,d\left(\frac{1}{T}\right) - \ln\left[\left(\frac{f_B}{f_B^*}\right)\left(\frac{f_A}{f_A^*}\right)^r\right] \tag{24}$$

where the enthalpy term is the standard enthalpy of solution (or fusion), referred to the standard states of pure supercooled or superheated liquid components A and B and pure binary compound (designated by *) at the given temperature:
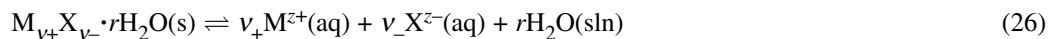
$$\Delta_{sln}H^{\ominus} = H_B^{\ominus} + rH_A^{\ominus} - H_{B \cdot rA}^* \tag{25}$$

The temperature and composition of the binary solid (or pure solid, when $r = 0$) serve as a reference point for the solubility curve. The enthalpy term may be represented by a Clarke–Glew type of

equation, or any other suitable equation that fits the data. Equation 24 gives $Y_B = 0$ and slope $dT/dx_B = 0$ at the congruent melting point (stable or metastable) of the binary compound.

Binary electrolyte solid + liquid system with compound formation

The general solubility equilibrium discussed in this section is:

$$M_{\nu+}X_{\nu-}\cdot rH_2O(s) \rightleftharpoons \nu_+M^{z+}(aq) + \nu_-X^{z-}(aq) + rH_2O(sln) \qquad (26)$$

i.e., a solid salt hydrate that dissociates completely into its constituent ions and water on dissolution. The solubility product is (writing w for H_2O):

$$-\Delta_{sln}G^{\ominus}\left(T\right)/RT = \ln K_s = \ln\left(a_M^{\nu+} a_X^{\nu-} a_w^r\right) \qquad (27)$$

For the ionic system, ionic (species) mole fractions x_+, x_-, x'_w [7] are used, where B is the anhydrous salt $M_{\nu+}X_{\nu-}$:

$$x_+ = \frac{\nu_+ x_B}{1+\left(\nu-1\right)x_B}; \quad x_- = \frac{\nu_- x_B}{1+\left(\nu-1\right)x_B}; \quad x'_w = \frac{1-x_B}{1+\left(\nu-1\right)x_B} \qquad (28)$$

along with symmetrical activity coefficients, to give:

$$-\Delta_{sln}G^{\ominus}\left(T\right)/RT = \ln\left(x_+^{\nu+} x_-^{\nu-} f_{\pm}^{\nu} f_w^r\right) \qquad (29)$$

where $\nu = \nu_+ + \nu_-$ and $f_{\pm}^{\nu} = f_+^{\nu+} f_-^{\nu-}$. The standard state refers to the solid in its state at the particular T and p, pure water, and pure supercooled liquid salt under the same conditions.

The deduction then proceeds using the same method as for eq. 24, to give:

$$Y_B\left(T\right) = \ln\left\{\frac{x_B^{\nu}\left(1-x_B\right)^r\left(\nu+r\right)^{\nu+r}}{r^r\left[1+\left(\nu-1\right)x_B\right]^{\nu+r}}\right\} = -\int_{T_{fus}}^{T}\frac{\Delta_{sln}H^{\ominus}}{R}d\left(\frac{1}{T}\right) - \ln\left[\left(\frac{f_B}{f_B^*}\right)\left(\frac{f_A}{f_A^*}\right)^r\right] \qquad (30)$$

where the enthalpy term is of the same form as eq. 25. While the constants in the left-hand logarithmic term in eq. 30 can be omitted in constructing an empirical fitting equation, it is recommended to retain them for consistency, especially in systems where several hydrates exist as well as the pure component.

For an anhydrous salt, set $r = 0$ and $r^r = 1$. Equation 30 gives $Y_B = 0$ and slope $dT/dx_B = 0$ at the congruent melting point, T_{fus}, (stable or metastable) of the salt or salt hydrate where $x_B = 1/(1 + r)$.

In [26], application of the ionic mole fraction equations is described for the pressure dependence of solubility and the vapor pressure of saturated solutions.

The solubility of ice is of importance in many binary aqueous electrolyte systems. The appropriate function Y_B can be derived from eq. 30 by setting $\nu = 0$, $r = 1$, except in the term in square brackets in the denominator. The enthalpy term is the enthalpy of fusion of ice at the given T and x_B along the ice solubility curve.

In all cases discussed above, the term containing $\Delta_{sln}H$, when expanded in a Taylor series about T_{fus}, gives an expression of the general form of the Clarke–Glew equation, for both ideal and non-ideal systems.

The enthalpy and heat capacity of fusion at the freezing point of water are known accurately, and a special equation has been derived for this case; see [26].

Ionic mole fractions have also been used to analyze solubility in ternary systems [27].

The equation analogous to eq. 30 in terms of molality is:

$$Y_B(T) = v \ln\left(\gamma_{m,B} m_B r M_A / \gamma_{m,B}^*\right) - v\left(r\phi_{m,B} m_B M_A - \phi_{m,B}^*\right) = -\int_{T_{fus}}^{T} \frac{\Delta_{fus}H^{\ominus}}{R} d\left(\frac{1}{T}\right) \tag{31}$$

where the molality at the composition of the solid phase is $1/rM_A$ and ϕ_m is the osmotic coefficient (based on molality). Note that eq. 31 applies to liquid phases with molality up to the order of that of the hydrated salt. It does not apply to an anhydrous salt phase, where the molality becomes infinite. However, the equation is useful for analysis of solubility under these conditions, and facilitates use of semi-empirical theories of electrolyte solutions, such as that of Pitzer and co-workers, summarized and reviewed extensively in [26,27]. Note that the enthalpy term still involves both fusion and dissociation, but the standard states are different than those in eq. 25: the pure solid and pure water at a particular T, p remain as standard states, but that for the salt is the partial molar enthalpy at infinite dilution. While the activity coefficient terms in eq. 31 may be transferred to the right-hand side, the osmotic terms cannot, as they contain the molality in an explicit form. Equation 31 is thus best suited for cases where $r = 0$.
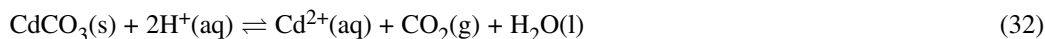
Dependence on composition

The solubility product, K_s, (see Table 6) is used to describe dependence of solubility on composition, where again Pitzer equations are useful for expression of the activity and osmotic coefficients.

The Pitzer equations for activity and osmotic coefficients [28,29] use a standardized form of the Debye–Hückel term describing electrostatic interactions between ions, and add a virial series of terms that depend on ionic strength and account for short-range forces between ions of unlike charge at higher molality. Values of the important Debye–Hückel parameters require accurate knowledge of the static dielectric constant of water, which can be found in [30]. An example of the use of Pitzer equations in the SDS is found in [31] for copper halides and pseudo-halides, and a detailed description of their application to a solubility problem is found in [32] for the system ($FeSO_4$ + H_2SO_4 + H_2O).

Specific ionic interaction theory (SIT) applied to solubility equilibria

The solubility product of *sparingly* soluble ionic solids provides information on their Gibbs energy of formation. These solubility products are usually determined in aqueous solutions containing an inert electrolyte in order to keep activity coefficients of reacting species constant. To obtain standard solubility constants valid at ionic strength $I_m = 0$ mol kg^{-1}, it is recommended to extrapolate experimental solubility constants using the Brønsted–Guggenheim–Scatchard SIT model. This method is comprehensively described in Appendix B of the OECD NEA volumes on chemical thermodynamics [33]. In each volume, the selected interaction coefficients have been listed. The special notation for solubility products is derived from the symbols used for stability constants; see [34,35] for a full explanation.

The solubility constant of cadmium carbonate, otavite, has, for example, been determined in an ionic medium containing non-complexing sodium perchlorate of an ionic strength I_m in excess of the interacting ionic species.

$$CdCO_3(s) + 2H^+(aq) \rightleftharpoons Cd^{2+}(aq) + CO_2(g) + H_2O(l) \tag{32}$$

According to the SIT model, there is a linear relationship between the measured logarithmic solubility constants lg*K_{ps0} and the ionic strength I_m of the background 1:1 electrolyte. For the sub- and superscripts on the symbol for solubility constant, p indicates that a gas is involved in the equilibrium, 0 that the central metal ion has no ligands, and * that a proton is involved in the equilibrium.

$$\lg{}^* K_{ps0} + \lg \gamma\left(\mathrm{Cd}^{2+}\right) - 2\lg \gamma\left(\mathrm{H}^+\right) + \lg a\left(\mathrm{H}_2\mathrm{O}\right) = \lg{}^* K_{ps0}^{\ominus} \tag{33a}$$

$$\lg{}^* K_{ps0} - \Delta z^2 D + \lg a\left(\mathrm{H}_2\mathrm{O}\right) = \lg{}^* K_{ps0}^{\ominus} - \Delta \varepsilon\, I_m \tag{33b}$$

The reaction interaction coefficient is $\Delta\varepsilon = \varepsilon(\mathrm{Cd}^{2+}, \mathrm{ClO}_4^-) - 2\varepsilon(\mathrm{H}^+, \mathrm{ClO}_4^-)$. The ionic charge is z. Thus, $\Delta z^2 = 2$ and $D = \dfrac{A\sqrt{I_m}}{1 + B\sqrt{I_m}}$, where $A = 0.509\ \mathrm{kg}^{1/2}\ \mathrm{mol}^{-1/2}$, $B = 1.5\ \mathrm{kg}^{1/2}\ \mathrm{mol}^{-1/2}$ at 25 °C. The solubility constant $\lg{}^* K_{ps0}^{\ominus}$ at $I_m = 0$ and the reaction interaction coefficient $\Delta\varepsilon$ can be obtained as intercept and slope, respectively, of a linear least-squares fit to the data.

Constrained solubility equilibria involving solid solutions

At atmospheric pressure and ambient temperatures, mixed crystals such as magnesium calcites $\mathrm{Ca}_{(1-x)}\mathrm{Mg}_x\mathrm{CO}_3$ or strontiobarites $\mathrm{Ba}_{(1-x)}\mathrm{Sr}_x\mathrm{SO}_4$ may dissolve congruently in aqueous solutions. This phenomenon has been called "stoichiometric saturation" [36]. From the thermodynamic point of view, stoichiometric saturation is a constrained (metastable) solubility equilibrium [37]. Recently, the implications of these constrained solubility equilibria for nuclear waste management have been discussed comprehensively [38].

COMPILATIONS AND EVALUATIONS

The formats for the compilations and critical evaluations have been modified in the transition of the SDS from a monograph series to journal publication. The following description reflects current (2010) practice.

The structure and order of presentation in all SDS volumes published in *JPCRD* is as follows. The title page with the abstract and keywords is followed by the table of contents, list of tables, list of figures, the authors' preface to the volume, critical evaluations, compilations, and cumulative references containing all the references cited in the preface and the original publications cited in the critical evaluations and compilations in the same order as they appear in the preface, critical evaluations, and compilations. References in the compilations that relate to publications for syntheses of materials, experimental methods and procedures, and details on apparatus are not cited in the cumulative references; they are given in parentheses within the body of the text of the compilations.

A compilation is a summary of experimental determination of solubility reported in the primary chemical literature for a particular chemical system of two or more components. The format used for the compilations is, for the most part, self-explanatory; it contains all experimental data and methods exactly as reported in the original publication. Normally, a compilation is divided into sections headed in boldface type, with detailed contents described below.

Based on a review of all the data in the compilations, the evaluator's task is to assess the reliability and quality of the data, to estimate errors where necessary, and to classify data as described below. Critical evaluations are only prepared where two or more compiled independent measurements of solubility for a given system at similar conditions of temperature and pressure are available. The evaluation takes the form of a summary in which all the data supplied in the compilations have been critically reviewed. Details on the structures of compilations and critical evaluations follow below.

Compilations

Components: Each component of the system being compiled is listed according to IUPAC name, formula, and Chemical Abstracts (CA) Registry Number. The CA name is also included if this differs from the IUPAC name, as are trivial names, if appropriate. Chemical formula is given according to:

Inorganic compounds: The name is determined by the principles of naming in the IUPAC "Red Book" [39]; first, the accepted trivial name, second, the systematic name (additive or substitutive nomenclature as needed). Then the CASSI (Chemical Abstracts Service Source Index) name, and last the CASSI number is given.

Organic compounds: The name is determined by the principles of naming in the IUPAC "Blue Book" [40]; first, the retained name (if available), second, the systematic name (additive or substitutive nomenclature as needed). Then the CASSI name, and last the CASSI number. For compounds whose systematic name is too complex for general use (such as many biomolecules and pharmaceuticals), the INN (International Nonproprietary Name) [41] is given.

Polymers: The name is determined by the principles of naming in the IUPAC "Purple Book" [42], which is compatible with [6,39,40].

Components are ordered in a given compilation according to:

- saturating components;
- non-saturating components according to chemical families based on the IUPAC 18-column periodic table; within carbon compounds, according to increasing carbon number;
- solvents according to chemical families based on the IUPAC 18-column periodic table; within carbon compounds, according to increasing carbon number.

In each class, ordering follows the 18-column IUPAC periodic table. The same order is followed in arranging compilations within a given volume.

Original measurements: References are abbreviated in the forms given by CASSI. Names originally in other than roman alphabets are given as transliterated by CA. In the case of multiple entries (e.g., translations), an asterisk indicates the publication used for compilation of the data.

Variables: Ranges of temperature, pressure, etc. are indicated here.

Prepared by: The names of all compilers are given here.

Experimental values: Components are described as (1), (2), etc., as defined in *Components*. Data are reported in the units used in the original publication, with the exception that modern names for units and quantities are used; see Tables 1–8. Usually, only one type of value (e.g., mass fraction or its equivalent) is found in the original paper. Generally, where necessary, the compiler converts reported results to consistent units (often mole fractions) chosen by the volume editor to facilitate evaluation and other comparisons. Data produced in this way are identified by the word "(compiler)" and the sources of any ancillary data used (e.g., atomic weights, densities) are noted. Temperatures are expressed as $t/°C$, $t/°F$, or T/K as in the original; if necessary, conversions to T/K are made, sometimes in the compilations, and always in the critical evaluation. However, the author's units are expressed according to IUPAC recommendations as far as possible. Errors in calculations, fitting equations, etc. are noted, and where possible corrected. Material inserted by the compiler is identified by the word "compiler". Details of smoothing equations (with limits) are included if they are present in the original publication and if the temperature or pressure ranges are wide enough to justify this procedure and if the compiler finds that the equations are consistent with the data. The precision of the original data is preserved when derived quantities are calculated, if necessary by the inclusion of one additional significant figure. In some cases, compilers note that numerical data have been obtained from published graphs using digitizing techniques. In these cases, the precision of the data may be determined by the quality of the original graph and the limitations of the digitizing technique.

Method: The apparatus and procedure are described briefly. Abbreviations used in CA are often used here to save space, reference being made to sources for further details if these are cited in the original paper.

Source and purity of materials: For each component, referred to as (1), (2), etc., the following information (in this order and in abbreviated form) is provided if available in the original paper: source and specified method of preparation; properties; degree of purity.

Estimated error: If estimated errors were omitted by the original authors, and if relevant information is available, the compilers have attempted to estimate errors (identified by "(compiler)") from the internal consistency of data and type of apparatus used. Methods used by the compilers for estimating and reporting errors are based on the latest edition of the *VIM* [43] and the *GUM* [44]. Helpful hints are to be found in Ku [45].

Comments and/or additional data: Compilations may include this section, in which short comments relevant to the general nature of the work or additional experimental and thermodynamic data are included which are judged by the compiler to be of value to the reader.

Evaluations

Where two or more compiled independent measurements of solubility for a given system at similar conditions of temperature and pressure exist, an evaluation is prepared. The evaluator's task is to assess the reliability and quality of the data, to estimate errors where necessary, and to classify data as described below. The evaluation takes the form of a summary in which all the data supplied by the compiler have been critically reviewed. There are three sections of a typical evaluation and these are described below.

Components: The format is the same as for compilations.

Evaluator: Name and affiliation of the evaluator(s) and the date up to which the literature was checked are given.

Critical evaluation:

(a) Critical text. The evaluator checks that the compiled data are correct, assesses their reliability and quality, estimates errors where necessary, and recommends numerical values based on all the published data (including theses, reports, and patents) for each given system. Thus, the evaluator reviews the merits or shortcomings of the various data. Only published data are considered. Documented rejection of some published data may occur at this stage, and the corresponding compilations may be removed, at the discretion of the evaluator and volume editor.

Occasionally, it is not clear why two groups of workers obtained very different but internally consistent sets of results at the same temperature and pressure, although both sets were obtained by reliable methods. In such cases, a decisive assessment may not be possible.

Some solubility data have been published in a smoothed form. Such data are particularly difficult to evaluate, and unless specifically discussed by the authors, the estimated error on such values can be regarded only as an "informed guess".

Many high-pressure solubility data have been obtained in a more general study of high-pressure vapor–liquid equilibrium. In such cases, a note is included to indicate that additional vapor–liquid equilibrium data are given in the source. Since the evaluation is for the compiled data, it is possible that the solubility data are given a classification which is better than that which would be given for the complete vapor–liquid data (or vice versa). As an example, it is difficult to determine coexisting liquid and vapor compositions near the critical point of a mixture using some common experimental techniques that yield accurate high-pressure solubility data.

(b) Fitting equations. If the use of a smoothing equation is justifiable, the evaluator may provide an equation representing the solubility as a function of the variables reported in the compilations, stating the limits within which it should be used. Least-squares analyses are described concisely in [46]. For confidence limits, consult [47].

(c) Graphical summary. In addition to (b) above, graphical summaries are often given. Generally, experimental data are shown as points (using separate symbols for each compilation, if appropriate) and smooth curves for fitting equations. Care is taken to accurately represent the applicable range of any fitting equation by limiting the curve shown.

(d) Classification of values. Based on all available information and professional judgement, the evaluator attempts to evaluate compiled data according to quality. Four data categories are generally used: *recommended*, *tentative*, *doubtful*, and *rejected*. Data are *recommended* if the results of at least two independent groups are available and they are in good agreement, and if the evaluator has no doubt as to the adequacy and reliability of the applied experimental and computational procedures. Data are reported as *tentative* if only one set of measurements is available, or if the evaluator considers some aspect of the computational or experimental method as mildly undesirable but estimates that it should cause only minor errors. Data are considered *doubtful* if the evaluator considers some aspect of the computational or experimental method as undesirable but still considers the data to have some value where the order of magnitude of the solubility is needed. Data determined by an inadequate method or under ill-defined conditions are *rejected*. However, references to these data are included in the evaluation together with a comment by the evaluator as to the reason for their rejection. In some older SDS volumes, data were sometimes classified as *best*. This term was undefined, but was probably synonymous with *recommended* as defined above. The classification *best* is no longer used.

Data classifications are made based on degree of agreement between sets of independent data relative to the experimental error in each set. Thus, the degree of precision implied by a particular classification is not uniform over all systems evaluated.

(e) References. All pertinent references, including all those publications appearing in the accompanying compilations and those which, by virtue of their poor precision, have been rejected and not compiled are given here in the usual format as superscripts. As described above, the full bibliographic references are given in the cumulative references in the same order as cited in the preface, critical evaluations, and compilations.

(f) Units. While the original data may be reported in the units used by the investigators, the final recommended values are reported in SI units when the data can be accurately converted.

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