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Compilation of Henry’s law constants for water as solvent, version 3.99e

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Abstract. Many atmospheric chemicals occur in the gas phase as well as in liquid cloud droplets and aerosol particles. Therefore, it is necessary to understand the distribution between the phases. According to Henry’s law, the equilibrium ratio between the abundances in the gas phase and in the aqueous phase is constant for a dilute solution. Henry’s law constants of trace gases of potential importance in environmental chemistry have been collected and converted into a uniform format. The compilation contains 17092 values of Henry’s law constants for 4628 species, collected from 672 references. It is also available on the internet at http://www.henrys-law.org.

1 Introduction

Henry’s law is named after the English chemist William Henry, who studied the topic in the early 19th century. In his publication about the quantity of gases absorbed by water (Henry, 1803), he described the results of his experiments:

> ~~“~~[. . .] water takes up, of gas condensed by one, two, or more additional atmospheres, a quantity which, ordinarily compressed, would be equal to twice, thrice, &c. the volume absorbed under the common pressure of the atmosphere. ~~”~~

In other words, the amount of dissolved gas is proportional to its partial pressure in the gas phase. The proportionality factor is called the Henry’s law constant. In atmospheric chemistry, these constants are needed to describe the distribution of trace species between the air and liquid cloud droplets or aerosol particles. In another area of environmental research, the constants are needed to calculate the vaporization of chemicals from rivers and during waste water treatment (e.g. Shen, 1982; Hawthorne et al., 1985; David et al., 2000).

Section 2 provides theoretical background about Henry’s law and commonly used quantities and units. In Sect. 3, the compilation of Henry’s law constants is described in detail. Additional information can be found in the electronic supplement, which is described in Sect. 4.

2 Theoretical background

This publication tries to follow the recommendations of the International Union of Pure and Applied Chemistry (IUPAC) as far as possible. General recommendations for physical chemistry have been published in the so-called “Green Book” by Mills et al. (1993). In addition, there are also the more specific articles about atmospheric chemistry by Calvert (1990) and about solubility by ~~and~~ Gamsjäger et al. (2008, 2010). In accordance with the Green Book, the name “Henry’s law constant” is used here throughout the text, not “Henry’s law coefficient”. IUPAC recommendations for terminology, symbols, and units of Henry’s law constants are described in the following sections.

2.1 Fundamental types of Henry’s law constants

There are many variants of Henry’s law constants which can all be classified into two fundamental types: One possibility is to put the aqueous phase into the numerator and the gas phase into the denominator, i.e., define the constant as the quotient A/G. Here, A and G are quantities describing the equilibrium composition (at infinite dilution) of the aqueous phase and the gas phase, respectively. Alternatively, the Henry’s law constant can be defined as the quotient G/A, which results in the inverse value. There is no advantage or disadvantage in using one or the other, the two types exist purely for historical reasons. Unfortunately, the name “Henry’s law constant” is used for both types. Therefore, statements like "a large Henry's law constant" are meaningless unless the type is specified. Especially the dimensionless constants (see Sects. 2.4.2 and 2.5.3) are very error-prone because their type cannot be deduced from the unit. In order to have a consistent terminology, I recommend the name "Henry's law solubility constant" (or "Henry solubility" for conciseness) when refering to A/G. When refering to G/A, the name "Henry's law volatility constant" (or "Henry volatility") is used.

2.2 Variants of Henry's law constants

For both of the fundamental types described in the previous section, there are several variants. This results from the multiplicity of quantities that can be chosen to describe the composition of the two phases. Typical choices for the aqueous phase are molar concentration (c_a), molality (b), and molar mixing ratio (x). For the gas phase, molar concentration (c_g) and partial pressure (p) are often used. Note, however, that it is not possible to use the gas-phase mixing ratio (y). At a given gas-phase mixing ratio, the aqueous-phase concentration c_a depends on the total pressure and thus the ratio y/c_a is not a constant.

There are numerous combinations of these quantities. The most frequently used variants of Henry solubilities and Henry volatilities are presented in Sects. 2.4 and 2.5, respectively. Conversion factors between them are shown in ~~Tabs.~~Tables **??**, **??**, and **??**. More detailed information about the conversion between different units and definitions of Henry's law constants can be found in Sander (1999) or Sazonov and Shaw (2006).

2.3 Symbols

In the current literature, a plethora of different symbols is used for the Henry's law constants. Several symbols are used for the same variant, and sometimes the same symbol is used for different variants. However, for this work a consistent terminology is indispensable. For Henry's law solubility constants, I follow the IUPAC recommendation for atmospheric chemistry by Calvert (1990) and use the symbol H. ~~For~~ Choosing a suitable symbol for Henry's law volatility constants ~~, the symbol k_H is used as recommended in~~ is more difficult. Although the IUPAC Green Book by Mills et al. (1993) recommends the symbol k_H with a lower case letter k, this symbol is hardly used in the literature at all. A major disadvantage is the internal inconsistency with other IUPAC recommendations: Normally, the lower case letter k describes rate constants, whereas the upper case letter K describes equilibrium constants (Mills et al., 1993). Considering this problem, I decided to use and recommend the symbol K_H with an upper case letter K.

To specify the exact variant of the Henry's law constant, two superscripts are used. They refer to the numerator and the denominator of the definition. For example, H^{cp} refers to the Henry solubility defined as c/p.

If H refers to standard conditions (~~$T^\ominus = 298.15$~~ $T^\ominus = 298.15$ K) it will be denoted as $H^\ominus$.

A summary of the symbols is shown in ~~Tab.~~Table **??**.

2.4 Henry's law solubility constants *H*

2.4.1 Henry solubility defined via concentration (H^{cp})

Atmospheric chemists often define the Henry solubility as:

$$H^{cp} \overset{\text{def}}{=} c_\mathrm{a}/p. \tag{1}$$

Here, c_a is the concentration of a species in the aqueous phase and p is the partial pressure of that species in the gas phase under equilibrium conditions.

The SI unit for H^{cp} is $\mathrm{mol\,(m^3\,Pa)^{-1}}$. However, often the unit $\mathrm{M\,atm^{-1}}$ is used since c_a is usually expressed in M ($1\,\mathrm{M}$ ~~=~~ $= 1\,\mathrm{mol\,dm^{-3}}$) and p in atm ($1\,\mathrm{atm}$ ~~= 101325~~ $= 101\,325\,\mathrm{Pa}$).

2.4.2 The dimensionless Henry solubility H^{cc}

The Henry solubility can also be expressed as the dimensionless ratio between the aqueous-phase concentration c_a of a species and its gas-phase concentration c_g:

$$H^{cc} \overset{\text{def}}{=} c_\mathrm{a}/c_\mathrm{g} = H^{cp} \times RT, \tag{2}$$

where R ~~= gas constant~~ = gas constant (see Table **??**) and T ~~=~~ = temperature.

Sometimes, this dimensionless constant is called the "water-air partitioning coefficient" ~~K_WA~~K_WA. It is closely related to the various, slightly different definitions of the "Ostwald coefficient" L, as discussed by Battino (1984).

2.4.3 Henry solubility defined via aqueous-phase mixing ratio (H^{xp})

Another Henry's law solubility constant is:

$$H^{xp} \overset{\text{def}}{=} x/p. \tag{3}$$

Here, x is the molar mixing ratio in the aqueous phase. For a dilute, aqueous solution the conversion between x and c_a is:

$$c_\mathrm{a} \approx x \frac{\varrho_\mathrm{H_2O}}{M_\mathrm{H_2O}}, \tag{4}$$

where $\varrho_\mathrm{H_2O}$ ~~=~~ = density of water and $M_\mathrm{H_2O}$ ~~=~~ = molar mass of water. Thus:

$$H^{xp} \approx \frac{M_\mathrm{H_2O}}{\varrho_\mathrm{H_2O}} \times H^{cp}. \tag{5}$$

The SI unit for H^{xp} is $\mathrm{Pa^{-1}}$. However, $\mathrm{atm^{-1}}$ is still frequently used.

2.4.4 Henry solubility defined via molality (H^{bp})

~~There are some advantages~~ It can be advantageous to describe the aqueous phase in terms of molality instead of concentration. The molality of a solution does not change with T since it refers to the *mass* of the solvent. In contrast, the concentration c does change with T, since the density of a solution and thus its volume are temperature-dependent. Defining the aqueous-phase composition via molality has the advantage that any temperature dependence of the Henry's law constant is a true solubility phenomenon and not introduced indirectly via a density change of the solution. Using molality, the Henry solubility can be defined as:

$$H^{bp} \stackrel{\text{def}}{=} b/p. \tag{6}$$

Here, b is used as the symbol for molality (instead of m) to avoid confusion with the symbol m for mass. The SI unit for H^{bp} is $\text{mol}\,(\text{kg Pa})^{-1}$. There is no simple way to calculate H^{cp} from H^{bp} since the conversion between concentration c_a and molality b involves ~~all~~ *all* solutes of a solution. For a solution with a total of n solutes with indices ~~$i = 1, \ldots, n$~~ $i = 1, \ldots, n$, the conversion is:

$$c_\text{a} = \frac{b\varrho}{1 + \sum_{i=1}^{n} b_i M_i}, \tag{7}$$

where ϱ ~~=~~ = density of the solution, and M ~~=~~ = molar mass. Here, b is identical to one of the b_i in the denominator. If there is only one solute, Eq. (7) simplifies to:

$$c_\text{a} = \cancel{\frac{b\varrho}{1+bM}} \frac{b\varrho}{1+bM}. \tag{8}$$

Henry's law is only valid for dilute solutions where $bM \ll 1$ and $\varrho \approx \varrho_{\text{H}_2\text{O}}$. In this case the conversion reduces further to:

$$c_\text{a} \approx b\varrho_{\text{H}_2\text{O}} \tag{9}$$

and thus:

$$H^{bp} \approx H^{cp}/\varrho_{\text{H}_2\text{O}}. \tag{10}$$

~~The molality of a solution does not change with T since it refers to the massof the solvent. In contrast, the concentration c does change with T, since the density of a solution and thus its volume are temperature-dependent. Defining the aqueous-phase composition via the molality b has the advantage that any temperature dependence of H^{bp} is a true solubility phenomenon and not introduced indirectly via a density change of the solution.~~

2.5 Henry's law volatility constants ~~k_H~~ K_H

2.5.1 The Henry volatility defined via concentration (~~k_H^{pc}~~ K_H^{pc})

A common way to define a Henry volatility is dividing the partial pressure by the aqueous-phase concentration:

$$K_\text{H}^{pc} \stackrel{\text{def}}{=} p/c_\text{a} = 1/H^{cp}. \tag{11}$$

The SI unit for ~~k_H^{pc} is~~ K_H^{pc} is $\text{Pa m}^3\,\text{mol}^{-1}$.

2.5.2 The Henry volatility defined via aqueous-phase mixing ratio (~~k_H^{px}~~ K_H^{px})

Another Henry volatility is:

$$K_\text{H}^{px} \stackrel{\text{def}}{=} p/x = 1/H^{xp}. \tag{12}$$

The SI unit for ~~k_H^{px}~~ K_H^{px} is Pa. However, atm is still frequently used.

2.5.3 The dimensionless Henry volatility ~~k_H^{cc}~~ K_H^{cc}

The Henry volatility can also be expressed as the dimensionless ratio between the gas-phase concentration c_g of a species and its aqueous-phase concentration c_a:

$$K_\text{H}^{cc} \stackrel{\text{def}}{=} c_\text{g}/c_\text{a} = 1/H^{cc}. \tag{13}$$

~~Sometimes~~In chemical engineering, this dimensionless constant is sometimes called the "air-water partitioning coefficient" ~~K_AW~~ K_AW.

2.5.4 The dimensionless Bunsen coefficient α

According to Sazonov and Shaw (2006), the dimensionless Bunsen coefficient α is defined as: "The volume of saturating gas, reduced to 273.15 K and 1 bar, which is absorbed by unit volume of pure solvent at the temperature of measurement and partial pressure of 1 bar". If the gas is ideal, the pressure cancels out, and the conversion to H^{cp} simply is:

$$H^{cp} = \cancel{\alpha \times \frac{1}{RT^\text{STP}}} \alpha \times \frac{1}{RT^\text{STP}} \tag{14}$$

with ~~T^STP =~~ T^STP = 273.15 K. Note, that according to this definition, the conversion factor is ~~not~~ *not* temperature-dependent! Independent of the temperature that the Bunsen coefficient refers to, 273.15 K is always used for the conversion. The Bunsen coefficient has been used mainly in the older literature.

2.5.5 The Kuenen coefficient S

According to Sazonov and Shaw (2006), the Kuenen coefficient S is defined as: "The volume of saturating gas, reduced to 273.15~~-~~K and 1~~-~~bar, which is dissolved by unit mass of pure solvent at the temperature of measurement and partial pressure 1~~-~~bar". If the gas is ideal, the relation to H^{cp} is:

$$H^{cp} = \underline{S \times \frac{\varrho}{RT^{\mathrm{STP}}}}\, S \times \frac{\varrho}{RT^{\mathrm{STP}}}, \qquad (15)$$

where ϱ is the density of the solvent and ~~$T^{\mathrm{STP}} =$~~ $T^{\mathrm{STP}} =$ 273.15~~-~~K. The SI unit for S is $\mathrm{m^3\,kg^{-1}}$. The Kuenen coefficient has been used mainly in the older literature. IUPAC considers it to be obsolete (Gamsjäger et al., 2010).

2.6 Temperature dependence of Henry's law constants

The temperature dependence of equilibrium constants can generally be described with the van't Hoff equation (e.g. Atkins, 1986). It also applies to Henry's law constants:

$$\frac{\mathrm{d}\ln H}{\mathrm{d}(1/T)} = \underline{\frac{-\Delta_{\mathrm{soln}}H}{R}}\, \frac{-\Delta_{\mathrm{sol}}H}{R}, \qquad (16)$$

where ~~$\Delta_{\mathrm{soln}}H =$~~ $\Delta_{\mathrm{sol}}H =$ enthalpy of dissolution. ~~Integrating the~~ Note that here, the letter H in the symbol $\Delta_{\mathrm{sol}}H$ refers to enthalpy and is not related to the letter H for Henry's law constants. Integrating the above equation leads to:

$$H(T) = A \times \exp\left(\frac{B}{T}\right) \qquad (17)$$

with the parameters A and B. When reporting H as a function of these parameters, it is important to present sufficient significant digits of B because H depends exponentially on it. Alternatively, one can create an expression based on $H^\ominus$ at the reference temperature $T^\ominus$ ~~=~~ = 298.15~~-~~K:

$$H(T) = H^\ominus \times \exp\left(\underline{\frac{-\Delta_{\mathrm{soln}}H}{R}}\, \frac{-\Delta_{\mathrm{sol}}H}{R}\left(\frac{1}{T} - \frac{1}{T^\ominus}\right)\right). \qquad (18)$$

~~Here, $H^\ominus = A \times \exp(B/T^\ominus)$ and $\Delta_{\mathrm{soln}}H/R = -B$~~

Here, $H^\ominus = A \times \exp(B/T^\ominus)$ and $\Delta_{\mathrm{sol}}H/R = -B$. In this work, the values $H^\ominus$ and ~~$\Delta_{\mathrm{soln}}H/R$~~ $\Delta_{\mathrm{sol}}H/R$ are tabulated.

The van't Hoff equation in this form is only valid for a limited temperature range in which ~~$\Delta_{\mathrm{soln}}H$~~ $\Delta_{\mathrm{sol}}H$ does not change much with temperature. To cover a larger temperature range, in which ~~$\Delta_{\mathrm{soln}}H$~~ $\Delta_{\mathrm{sol}}H$ cannot be considered constant anymore, different empirical ~~ways~~ methods can be used. Often, the temperature dependence $\mathrm{d}\ln H/\mathrm{d}(1/T)$ is expressed as the sum of several terms. Then, the analytical derivative is simply the sum of the derivatives of the individual terms. For example, Wilhelm et al. (1977) use the formula:

$$\ln H = A + B \times \left(\frac{T}{\mathrm{K}}\right)^{-1} + C \times \ln\left(\frac{T}{\mathrm{K}}\right) + D \times \left(\frac{T}{\mathrm{K}}\right). \qquad (19)$$

Using the derivatives from ~~Tab.~~Table **??**, the temperature dependence of this expression can be calculated as:

$$\frac{\mathrm{d}\ln H}{\mathrm{d}(1/T)} = 0 + B - C \times \left(\frac{T}{\mathrm{K}}\right) - D \times \left(\frac{T}{\mathrm{K}}\right)^2. \qquad (20)$$

Note that the temperature dependences for H^{cp} and H^{cc} are different since the conversion factor between them includes the temperature:

$$\begin{aligned} H^{cp} &= H^{cc}/(RT) \\ \Leftrightarrow \ln H^{cp} &= \ln H^{cc} + \ln(1/R) + \ln(1/T) \\ \Rightarrow \frac{\mathrm{d}\ln H^{cp}}{\mathrm{d}(1/T)} &= \frac{\mathrm{d}\ln H^{cc}}{\mathrm{d}(1/T)} + \frac{\mathrm{d}\ln(1/T)}{\mathrm{d}(1/T)} \\ &= \frac{\mathrm{d}\ln H^{cc}}{\mathrm{d}(1/T)} + T. \qquad (21) \end{aligned}$$

2.7 Effective Henry's law solubility constants H_{eff}

The Henry's law constants mentioned so far do not consider any chemical equilibria in the aqueous phase. This type is called the "intrinsic" (or "physical") Henry's law constant. For example, the intrinsic Henry's law constant of methanal can be defined as:

$$H^{cp} = \frac{c(\mathrm{HCHO})}{p(\mathrm{HCHO})} \qquad (22)$$

In aqueous solution, methanal is almost completely hydrated:

$$\mathrm{HCHO + H_2O \rightleftharpoons H_2C(OH)_2} \qquad (23)$$

The total concentration of dissolved methanal is:

$$c_{\mathrm{tot}} = c(\mathrm{HCHO}) + c(\mathrm{H_2C(OH)_2}) \qquad (24)$$

Taking this equilibrium into account, an effective Henry's law constant H_{eff} can be defined:

$$H_{\mathrm{eff}} = \frac{c_{\mathrm{tot}}}{p(\mathrm{HCHO})} = \frac{c(\mathrm{HCHO}) + c(\mathrm{H_2C(OH)_2})}{p(\mathrm{HCHO})} \qquad (25)$$

For acids and bases, the effective Henry's law constant is not a useful quantity because it depends on the pH of the solution (Sander, 1999). In order to obtain a pH-independent constant, the product of the intrinsic Henry's law constant H^{cp} and the acidity constant K_A is often used for strong acids, e.g., for HCl:

$$H' = H^{cp} \times K_A = \frac{c(H^+) \times c(Cl^-)}{p(HCl)} \qquad (26)$$

Although H' is usually also called a Henry's law constant, it should be noted that it is a different quantity and it has different units than H^{cp}.

2.8 Dependence of Henry's law constants on ionic strength

Values of Henry's law constants for aqueous solutions depend on the composition of the solution. In general, the solubility of a gas decreases with increasing salinity ~~. This so-called~~ ("salting out"). However, a "salting in" effect has also been observed, e.g., for glyoxal (Kampf et al., 2013; Kurtén et al., 2014). The ionic strength effect can be described with the Sechenov ~~parameter~~(also transliterated "Setschenow") equation (Setschenow, 1889). There are many alternative ways to define ~~such a parameter. An equationbased on the molality of the solution is preferred.~~ the Sechenov equation, depending on how the aqueous-phase composition is described (based on concentration, molality, or molar fraction) and which variant of the Henry's law constants is used. Using the preferred quantity molality (see Sander (1999) for details), the equation becomes:

$$\log\left(\frac{H_0^{bp}}{H^{bp}}\right) = k_s \times b(\text{salt}) \qquad (27)$$

where H_0^{bp} = Henry's law constant in pure water, H^{bp} = Henry's law constant in the salt solution, k_s = molality-based Sechenov constant, and $b(\text{salt})$ = molality of the salt.

Since the atmosphere contains very dilute cloud droplets as well as highly concentrated aerosols, adequate values of Henry's law constants should be used. Unfortunately, Sechenov parameters are unknown for many species. A ~~short~~ list of some available data is presented in Sect. 3.2.4. ~~For more details, see .~~

3 Values of Henry's law constants

3.1 The data compilation

The ~~data compilation~~ compilation of Henry's law constants is presented in ~~Tab. ??~~Table ??, and it is also available online at http://www.henrys-law.org. It contains Henry's law constants for inorganic and organic species of potential importance in environmental chemistry. Most data were measured at ambient conditions (~~about~~ between 20 °C and 25 °C and 1 atm). Data at high temperatures are excluded or (if possible) extrapolated to $T^\ominus$ ~~=~~ = 298.15 K. All data ~~refers~~ refer to aqueous solutions; octanol and other solvents are not included. ~~Most~~ The constants refer to pure water as solvent ~~, however, some data for sea water are also included.~~

~~The current compilation is based on version 3, which is still available at . The collection has been expanded substantially (from 2288 to constants and from 913 to species). In addition, all values have been recalculated. Due to different precision and rounding errors, the last digit of the Henry's law constants has changed in a few cases. Also, a few more publications from the grey literature could be obtained.In these cases, the original data are used now instead of those cited by others.In a few cases, this also resulted in slightly different values~~unless noted otherwise (e.g., sea water).

Inorganic substances are sorted according to the elements they contain. The order chosen is: O, H, N, F, Cl, Br, I, S, rare gases, others. ~~Organic substances (i.e.everything with carbon,~~ Compounds with several of these elements are put into the last of the applicable sections. For example, nitryl chloride which contains O, N and Cl, is listed in the Cl section. Carbon-containing compounds (including CO and CO_2) are sorted somewhat arbitrarily by increasing chain length and complexity. Hetero atoms (O, N, F, Cl, Br, I, ~~and~~ S, P, etc.) are sorted in the same order as for inorganic compounds. The table contains the following groups of species:

The first column of the table shows the systematic name, the chemical formula, trivial names (if any), and the CAS registry number (in square brackets).

The column labeled ~~"~~“H^{cp}~~"~~” contains the Henry's law solubility constants as defined in Eq. (1), rounded to two significant digits and given in the unit $\mathrm{mol/(m^3\,Pa)}$.

The column labeled ~~"~~“$\mathrm{d}\ln H/\mathrm{d}(1/T)$~~"~~” contains the temperature dependence of the Henry solubility as defined in Eq. (18), rounded to two significant digits and given in the unit K. If the term ~~$\Delta_{soln}H$~~ $\Delta_{sol}H$ is temperature-dependent, the value of $\mathrm{d}\ln H/\mathrm{d}(1/T)$ is calculated at $T^\ominus$ ~~=~~ = 298.15 K.

For each table entry the column labeled ~~'type'~~ “type” denotes how the Henry's law constant was obtained in the given reference. Literature reviews are usually most reliable, followed by original publications of experimental determinations of H. Other data has to be treated more carefully. The types listed here are roughly ordered by decreasing reliability:

"L" The cited paper is a ~~literature~~ ~~review.~~ *literature* review.

"M" Original publication of a ~~measured~~ ~~value.~~ ~~Vapor~~ *measured* value.

"V" *Vapor* pressure of the pure substance divided by aqueous solubility (sometimes called "VP/AS").

"R" The cited paper presents a ~~recalculation~~ *recalculation* of previously published material (e.g. extrapolation to a different temperature or concentration range). ~~Thermodynamical calculation ($\Delta_{\mathrm{soln}}G = -RT\ln H$~~

“T” *Thermodynamical* calculation ($\Delta_{\mathrm{sol}}G = -RT\ln H$, see Sander (1999) for details).

“X” The original paper was not available for this study. The data listed here was found in a secondary source.

“C” The paper is a ~~citation~~ *citation* of a reference which I could not obtain (e.g. personal communication, Ph.D. theses, internal papers etc.).

“Q” The value is an estimate obtained with the “~~quantitative~~ *quantitative* structure property relationship” (QSPR) method, see Staudinger and Roberts (1996) for details~~).~~ .

“E” The value is an ~~estimate~~*estimate*. Estimates are only listed if no reliable measurements are available for that compound.

“?” The cited paper doesn’t clearly state how the value was obtained.

“W” The value is probably wrong.

In some cases there might be good agreement between different authors. However, if the original work they refer to is not known one has to be careful when evaluating the reliability. It is possible that they were recalculating data from the same source. The similarity in that case would not be due to independent investigations. The table in the pdf of this document has been hyperlinked to the appropriate notes, and to the NIST Chemistry WebBook from the CAS numbers.

~~When viewing this pdf online, it is possible to click on the CAS registry number to open the web page about this species from the NIST Chemistry WebBook~~The version number of the current compilation is 3.99e. Based upon version 3 (still available at http://www.henrys-law.org), the list has been expanded substantially (from 2288 to 17092 constants and from 913 to 4628 species). In addition, all values have been recalculated using a system of Fortran90 modules. Due to different precision and rounding errors, the last digit of the Henry’s law constants has changed in a few cases. Also, a ~~click on the number of a note in the table will lead you to the corresponding note~~few more articles could be obtained from the grey literature (academic publications not formally published). In these cases, the original data are used now instead of those cited by others. In a few cases, this also resulted in slightly different values.

3.2 Further sources of information

3.2.1 Review articles

Several reviews about Henry’s law have been published, starting with Markham and Kobe (1941), up to more recent publications such as Wilhelm et al. (1977), Mackay and Shiu (1981), Staudinger and Roberts (1996), Staudinger and Roberts (2001), Fogg and Sangster (2003), and Sander et al. (2011). Practical guidance on the use of Henry’s law has been published by Smith and Harvey (2007).

Experimental methods to obtain Henry’s law constants as well as indirect (theoretical) methods have been described and compared by ~~various authors~~several authors. Only a brief summary of some articles is given here. For details, the reader is referred to the original publications: Battino and Clever (1966) [miscellaneous methods, partially of historical interest], ~~including~~ Betterton (1992) [head-space method, bubble column method, thermodynamic cycles, calculation from vapor pressure and solubility, linear correlations], ~~,~~ Turner et al. (1996) [static methods, mechanical recirculation methods, separate measurement of solubility and pure species vapor pressure, ebulliometry, perturbation chromatography], Staudinger and Roberts (1996) [batch air stripping, concurrent flow technique, Equilibrium Partitioning in Closed Systems (EPICS), calculation via Quantitative Property Property Relationships (QPPR), Quantitative Structure Property Relationships (QSPR), UNIversal quasichemical Functional group Activity Coefficients (UNIFAC)], Brennan et al. (1998) ~~,~~[comparison of predictive methods], Sander (1999) ~~,~~ ~~and~~ [QPPR, QSPR, thermodynamic calculations], and Fogg and Sangster (2003) ~~.~~[miscellaneous methods].

3.2.2 Internet

On the internet, the following pages provide Henry’s law constants:

- The NIST Chemistry WebBook at http://webbook.nist.gov/chemistry.
- The Pesticide Properties Database (PPD) at http://www.ars.usda.gov/Services/docs.htm?docid=14199.
- The Screening Information Datasets (SIDS) of the United Nations Environment Programme (UNEP) at http://www.chem.unep.ch/irptc/sids/OECDSIDS/INDEXCHEMIC.htm provide data sets including Henry’s law constants for many species.
- A program to calculate Henry’s law constants is available at http://www.epa.gov/opptintr/exposure/pubs/episuitedl.htm.
- Vapor-liquid equilibrium data from the “Dortmund Data Bank” at http://www.ddbst.com/en/EED/VLE/VLEindex.php.
- The GSI chemical properties database at http://www.gsi-net.com/en/publications/gsi-chemical-database.html.

- The Hazardous Substances Data Bank (HSDB), included in the toxnet database at http://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm.
- Effective Henry's law constants calculated by Hodzic et al. (2014) are available at https://www2.acd.ucar.edu/modeling/gecko.

3.2.3 QSPR

Several publications apply the "Quantitative structure property relationship" (QSPR) method to obtain theoretical predictions for Henry's law constants: Pierotti et al. (1959), Deno and Berkheimer (1960), Nirmalakhandan and Speece (1988b), Dunnivant and Elzerman (1988), Brunner et al. (1990), Sukuzi et al. (1992), Russell et al. (1992), Sukuzi et al. (1992), Brennan et al. (1998), English and Carroll (2001), Dearden and Schüürmann (2003), Yaffe et al. (2003), Kühne et al. (2005), Modarresi et al. (2007), Raventos-Duran et al. (2010).

3.2.4 Salt solutions

Some information about Henry's law constants for salt solutions (Sechenov ~~coefficients~~constants, see Sect. 2.8) can be found in these publications: McDevit and Long (1952) [benzene], Gordon and Thorne (1967a) and Gordon and Thorne (1967b) [naphthalene], Meadows and Spedding (1974) [CO], Zafiriou and McFarland (1980) [NO], Przyjazny et al. (1983) ~~,~~[organic sulfur compounds], Hunter-Smith et al. (1983) [halocarbons], Almeida et al. (1983) [naphthols], Sanemasa et al. (1984) [benzene, alkylbenzenes], Dacey et al. (1984) [dimethyl sulfide], Wisegarver and Cline (1985) [chlorofluorocarbons], Johnson and Harrison (1986) ~~,~~[OCS], Zhou and Mopper (1990) [aldehydes, ketones], Kames and Schurath (1992) ~~,~~[organic nitrates], Benkelberg et al. (1995) [propanone, ethanal, ethane nitrile], De Bruyn et al. (1995b) ~~,~~[organic sulfur compounds], Moore et al. (1995) ~~,~~[halogenated methanes], Dewulf et al. (1995) [halocarbons, aromatics], Wong and Wang (1997) ~~,~~[dimethyl sulfide], Xie et al. (1997) [organic compounds], ~~,~~ Peng and Wan (1998) [halocarbons, aromatics], Moore (2000) [halocarbons], Ni et al. (2000) [organic compounds], Bullock and Teja (2003) ~~,~~[methanol], Endo et al. (2012) [alkanals, alkanones, nitroalkanes, alkylbenzenes, fluorinated alcohols, additional compounds with various polar functional groups], Yu and Yu (2013) [theoretical predictions], and Wang et al. (2014) [38 organic compounds].

4 The electronic supplement

The ~~electronic supplement, available at ,~~ Supplement contains several files with additional information about the compiled Henry's law constants. It includes a `README` file with a detailed description. Here, only a short summary is given:

- The files `henry_*.f90` are the Fortran 90 code that was used to convert the values from the original publications to the uniform format with the unit $\mathrm{mol/(m^3\,Pa)}$. The code and the comments in the code can be used to double-check that the conversion was done correctly.
- If the original publications contained measurements at different temperatures, the fortran code often contains all individual data points, not just the regression line that was used to show the temperature dependence in ~~Tab.~~Table **??**. In addition, the supplement contains plots showing the data points as well as the regression lines according to Eq. (18).
- If the Henry's law constants are needed in electronic form, it is cumbersome to extract them from the pdf of this article. Therefore, the supplement contains declarations of the Henry's law constants (H^{cp}, H^{cc}, H^{xp}, H^{bp}, ~~k_H^{pc}, k_H^{px}, k_H^{cc}~~K_H^{pc}, K_H^{px}, K_H^{cc}, and α) in Fortran 90 syntax.

5 Summary and outlook

A comprehensive compilation of Henry's law constants has been presented. The collection, which is also available at http://www.henrys-law.org, will be continously maintained, updated and extended in the future. If necessary, errata will also be posted on this web page. In addition to providing a source of information, I hope that this work will help to identify gaps in our current knowledge and stimulate research projects. In particular, it seems that even for some well-known chemicals like HCl, Br_2, and BrCl, there is a large uncertainty in the value of the Henry's law constants. I always welcome information about new measurements of Henry's law constants to be included in the table.

The Supplement related to this article is available online at doi:10.5194/acp-0-1-2015-supplement.

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Staffelbach, J. Staudinger, J. St-Pierre, G. Tyndall, J. Überfeld, C. Verlinde, R. Vogt, P. Warneck, and J. C. Wheeler. The CAS registry number is a registered trademark of the American Chemical Society. The service charges for this open access publication have been covered by the Max Planck Society.