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# Henry's Law Constants of Organic Compounds in Water and *n*-Octane at $T = 293.2$ K

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Henry's law constants at $T = 293.2$ K are reported for several halogenated ethanols and acetones, 3-pentanone, cyclopentanone, and 1,3-dioxane in water and for a larger number of alcohols, ketones, ethers and esters, benzene, pyridine, pentane, and cyclopentane in octane. The instrument and handling technique were validated by comparison with literature data for acetone, ethanol, and methanol from $T = (273.2$ to $303.2)$ K.

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## Introduction

The solubilities of gases in liquids have significance in applications ranging from uptake by the biological systems, syntheses involving gaseous reactants, and removal of atmospheric pollutants by dissolution in rain droplets, aerosols, or surface waters.

The present study was associated with work on the atmospheric fate of a range of organic compounds. Several extensive reviews[1,2] and compilations[3−7] of Henry's law constants are available; however, values for several compounds of interest were not found in the literature. Thus, we report Henry's law constants for several organic compounds in water at $T = 293.2$ K. In addition, we report values for a larger group of organic compounds in octane, also at $T = 293.2$ K.

As a test of the instrument and handling method, the Henry's law constants of acetone, methanol, and ethanol in water were measured for $T = (278.2$ to $303.2)$ K and compared with literature values.

## Experimental Section

Distilled water was used throughout. The sources and purities of the other compounds used are listed in Table 1. These were used without further purification, but where possible, the vapor pressures of the solutes were compared to literature values;[8] the agreement was always within 0.15 kPa.

The vacuum line had two sections, one for outgassing of liquids and solution preparation and the second for pressure measurements. Greaseless taps (J. Youngs, PCJ/5) and taps (J. Youngs, POR/10) were used throughout.

All liquids were outgassed using a system similar to that described by Battino and Evans.[9] The section of the vacuum line used for outgassing was fitted with a cold trap, cooled with liquid nitrogen, a water-cooled condenser, to which the flask containing the liquid was connected, a Pirani gauge (Edwards APF-L-16-AL, 1.3 Pa to 1.3 kPa), and connectors to which the flasks for solution preparation could be connected. All components were connected to the line through vacuum taps and could be isolated from the line.

Flasks containing liquids to be outgassed were attached to the condenser and stirred vigorously, using a magnetic stirrer, with the condenser isolated from the vacuum line. The outgassing section of the line was isolated from the rest of the system, and the tap connecting the condenser to the line was opened briefly. The condenser reduced the amount of vapor released into the line, and any vapor released was frozen in the liquid nitrogen cooled trap. The line was re-evacuated and the procedure repeated. If the liquid was outgassed, no air would be released, and there would be no change in the line pressure once the vapor released had been frozen in the trap. Thus the liquid was considered to be outgassed if there was no change in pressure for two successive cycles of the outgassing procedure.

**Table 1. Sources and Purities of Organic Compounds Used**

| material | stated purity | supplier |
|---|---|---|
| octane | > 99 % | Sigma-Aldrich |
| acetone | 99.5 % | WVR Prolabo |
| fluoroacetone | 99 % | Sigma-Aldrich |
| 1,1-dichloroacetone | 98 % | Sigma-Aldrich |
| cyclopentanone | > 99 % | Sigma-Aldrich |
| pentanone | 90 % | Sigma-Aldrich |
| cyclopentane | 95 % | Sigma-Aldrich |
| pentane | 99 % | Sigma-Aldrich |
| tetrahydrofuran | 99.9 % | Riedel-de Haën |
| 1,4-dioxane | 99 % | Sigma-Aldrich |
| 1,3-dioxane | 97 % | Sigma-Aldrich |
| ethyl formate | 97 % | Sigma-Aldrich |
| ethyl acetate | 99.8 % | Sigma-Aldrich |
| methyl acetate | 99.5 % | Sigma-Aldrich |
| diethyl ether | 99.5 % | Riedel-de Haën |
| 1,2-dimethoxyethane | 98 % | Sigma-Aldrich |
| ethylvinyl ether | 99 % | Sigma-Aldrich |
| propylvinyl ether | 99 % | Sigma-Aldrich |
| $CF_3CH_2OCH_3$ | 99 % | Fluorochem |
| $CF_3CF_2CH_2OCH_3$ | 97 % | Fluorochem |
| $CF_3CH_2OCH_2CF_3$ | 99 % | Fluorochem |
| pyridine | > 99.9 % | Sigma-Aldrich |
| benzene | > 99.9 % | Sigma-Aldrich |
| methanol | 99.9 % | Alkem Chemica |
| ethanol | 99 % | Merck |
| fluoroethanol | 95 % | Sigma-Aldrich |
| difluoroethanol | 95 % | Sigma-Aldrich |
| dichloroethanol | 98 % | Sigma-Aldrich |

Outgassed liquids were stored in pear-shaped flasks with a nominal volume of 100 $cm^3$ fitted with a greaseless tap with the high vacuum side of the tap connected to the flask. The liquids were transferred from the outgassing apparatus by distillation, with the receiver flask cooled with liquid nitrogen. Liquids were generally stored attached to the line,

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**Table 2. Experimental Henry's Law Constants[a] of Acetone, Methanol, and Ethanol in Water at $T = (278.2 \text{ to } 303.2)$ K**

| | $K_H$/kPa | | |
|---|---|---|---|
| $T$/K | acetone | methanol | ethanol |
| 276.2 | $3._6 \cdot 10$; ref 11 | | |
| 278.2 | $(5._6 \pm 1) \cdot 10$ | $7._5 \pm 0.3$ | $6._5 \pm 0.9$ |
| | | $7._2$[12] | $6._3$[12] |
| 279.2 | $4._8 \cdot 10$; ref 11 | | |
| 283.2 | $(7._5 \pm 1) \cdot 10$ | $8._7 \pm 1$ | $10 \pm 1$ |
| | $6._1 \cdot 10$; ref 11 | $10._3$[12] | $9._6$[12] |
| 288.2 | $(1.0 \pm 0.1) \cdot 10^2$ | $13 \pm 1$ | $13 \pm 4$ |
| | $7._4 \cdot 10$; ref 11 | $14._6$[12] | $14._5$[12] |
| 293.2 | $(1.3 \pm 0.1) \cdot 10^2$ | $20 \pm 3$ | $20 \pm 3$ |
| | $1.4_0 \cdot 10^2$; ref 1 | $20._2$[12] | $21._3$[12] |
| | $1.4_0 \cdot 10^2$; ref 11 | $20._8$[13] | $20._5$[13] |
| 298.2 | $(1.7 \pm 0.1) \cdot 10^2$ | $26 \pm 4$ | $26 \pm 2$ |
| | $1.7_3 \cdot 10^2$; ref 1 | $26._7$[3] | $26._5$[3] |
| | $2.0_0 \cdot 10^2$; ref 11 | $27._7$[12] | $30._7$[12] |
| | $1.8_5 \cdot 10^2$; ref 13 | $26._7$[15] | $26._4$[15] |
| | $2.0_8 \cdot 10^2$; ref 14 | $27._3$[16] | $25._5$[16] |
| | $1.7_3 \cdot 10^2$; ref 15 | $27._6$[21] | $25._7$[21] |
| | $2.0_0 \cdot 10^2$; ref 16 | | |
| | $1.4_8 \cdot 10^2$; ref 17 | | |
| | $1.6_3 \cdot 10^2$; ref 18 | | |
| | $1.9_2 \cdot 10^2$; ref 19 | | |
| | $2.0_8 \cdot 10^2$; ref 20 | | |
| | $1.7_3 \cdot 10^2$; ref 21 | | |
| 303.2 | $(2.1 \pm 0.4) \cdot 10^2$ | $32 \pm 5$ | $33 \pm 3$ |
| | | $37._4$[12] | $43._5$[12] |

[a] Uncertainties shown for $K_H$ are 95 % confidence limits. The uncertainty in $T$ was 0.05 K.

**Table 3. Experimental Henry's Law Constants of Organic Compounds[a] in Water at $T$/K = 293.2**

| compound | $K_H$/kPa | compound | $K_H$/kPa |
|---|---|---|---|
| 2-fluoroethanol | $(1.2 \pm 0.2) \cdot 10^2$ | fluoroacetone | $(1.2 \pm 0.1) \cdot 10^2$ |
| 2,2-difluoroethanol | $(6 \pm 2) \cdot 10$ | 1,1-dichloroacetone | $(1.7 \pm 0.1) \cdot 10^2$ |
| 2,2-dichloroethanol | $(1._5 \pm 1) \cdot 10^2$ | 3-pentanone | $(2.6 \pm 0.3) \cdot 10^2$ |
| 1,2-dimethoxyethane | $(2.6 \pm 0.1) \cdot 10$ | cyclopentanone | $(2.0 \pm 0.3) \cdot 10$ |
| | | 1,3-dioxane | $(3.0 \pm 0.2) \cdot 10$ |

[a] Uncertainties shown for $K_H$ are 95 % confidence limits. The uncertainty in $T$ was 0.05 K.

although the cell design allowed them to be detached and stored separately.

To carry out a series of measurements, the sample flask was evacuated, closed, and then weighed. It was then attached to the handling line and cooled with liquid nitrogen, and outgassed solvent was distilled into the flask. It was then closed, allowed to warm to room temperature, and reweighed. The uncertainties in the weights were ± 0.0003 g.

The flask was then attached to the measurement line, which was evacuated while the sample reached thermal equilibrium. The measurement line was then isolated, the cell opened, and the pressure of the solvent measured; this provided a sensitive test of solvent purity. The sample was allowed to equilibrate for 15 min, and the pressure was read and then reread at 5 min intervals until there was no measurable change with time. Where measurements were made at a series of temperatures, the temperature was then adjusted and the process repeated. The sample flask was then cooled with liquid nitrogen to ensure that all of the sample was retained and then closed and removed from the line. The flask was warmed to room temperature and reweighed.

The solute was added by distillation. Thus, the flask was reattached to the sample handling line and refrozen in liquid nitrogen. A sample of degassed solute was distilled into the flask which was then closed, warmed, and reweighed. It was then reattached to the measurement line and pressure measured as described above. This process could be repeated several times, but in the present study, only two solutions were made for each solvent sample. This reduced cumulative errors. In all cases at least two sets of solutions were prepared in this way.

Pressure measurements were made using an absolute Bourdon tube gauge (Texas Instruments 145-01, (0 to 101.3) kPa, calibration traceable to the NBS, with precision of 9 Pa). Experience has shown that the Bourdon tube is sensitive to water vapor, and so the gauge was separated from the cell by a differential Baratron gauge (MKS PDR-C-1B ± 1.3 kPa). Pressure measurements were made by approximately zeroing the differential gauge by introducing dry air into the line connecting it to the Bourdon tube. Thus, the pressure measured was that read from the Bourdon tube corrected for any nonzero reading on the differential gauge. The uncertainties in the pressure readings were ± 0.02 kPa.

The temperature of the sample was controlled by placing the sample flask in a double-walled container with water circulated through the jacket from a circulating water bath (Julabo F34). Thermal contact between the jacket and the cell was provided by filling the container with water and stirring this, using a magnetic stirrer. This system allowed both reasonably rapid changes in solution temperature and easy removal of the sample flask from the measurement line. All temperature measurements were made using a digital thermometer (Dostmann P555 ± 0.01 K), immersed in the water in contact with the cell. The uncertainties of the temperature measurements were ± 0.05 K, and the stability of the temperature was better than ± 0.01 K.

This arrangement did not allow temperature control of the upper part of the measurement line or of the differential gauge. The system was tested by measuring the vapor pressure of water at different temperatures, and it was found that the measured pressures agreed with the literature as long as the sample temperature was less than that of the gauge. At higher sample temperatures condensation occurred in the gauge, and the measurements became inaccurate.

To avoid this problem, heated air was passed over the gauge and upper measurement line. The air was directed onto the system by a ducting system fitted with a fan and three resistors (300 W) fitted with heat exchangers. The air temperature was controlled using a contact thermometer fitted into the ducting. It was found that pressure readings were stable and corresponded to the literature vapor pressure, provided the gauge and upper measurement line were (3 to 10) degrees above the temperature of the liquid. Measurements were made with the gauge and upper part of the measurement line 5° above the sample temperature.

Inevitably, the outgassing of the liquids was time-consuming, but solution preparation was surprisingly straightforward. One significant advantage of the system, that became apparent once the system for preventing condensation had been developed, is that measurements over a range of temperatures could be made relatively quickly, typically two or three temperatures per hour.

## Results and Discussion

In all cases the measured pressures varied linearly with the solute mole fraction, indicating that the concentrations were sufficiently low that solute−solute interactions were negligible. In this case it can be assumed that the solvent

**Table 4. Experimental Henry's Law Constants of Organic Compounds[a] in *n*-Octane at $T$/K = 293.2**

| compound | $K_H$/kPa | compound | $K_H$/kPa |
|---|---|---|---|
| ethanol | $(2.8 \pm 0.1)\cdot 10$ | pyridine | $(1.6 \pm 0.2)\cdot 10$ |
| 2-difluoroethanol | $(8.1 \pm 0.2)\cdot 10$ | benzene | $(1.8_8 \pm 0.05)\cdot 10$ |
| 2,2-dichloroethanol | $(1.6_4 \pm 0.08)\cdot 10^2$ | tetrahydrofuran | $(2.7 \pm 0.2)\cdot 10$ |
| acetone | $(91.7 \pm 0.1)\cdot 10^2$ | 1,4-dioxane | $(1.8 \pm 0.2)\cdot 10$ |
| fluoroacetone | $(3.5 \pm 0.4)\cdot 10$ | 1,3-dioxane | $(2.2 \pm 0.2)\cdot 10$ |
| 1,1-dichloroacetone | $(4.4 \pm 0.3)\cdot 10$ | diethyl ether | $(6.9 \pm 0.7)\cdot 10$ |
| 3-pentanone | $(1.0 \pm 0.1)\cdot 10$ | 1,2-dimethoxyethane | $(1.4 \pm 0.1)\cdot 10$ |
| cyclopentanone | $7.3 \pm 0.3$ | 1,1,1,2,2-pentafluoro-3-methoxypropane | $(8.3 \pm 0.6)\cdot 10^2$ |
| methyl acetate | $(8._5 \pm 1)\cdot 10$ | ethylvinyl ether | $(7.2 \pm 0.3)\cdot 10$ |
| ethyl acetate | $(2.6 \pm 0.1)\cdot 10$ | propylvinyl ether | $(2.4 \pm 0.2)\cdot 10$ |
| ethyl formate | $(7._9 \pm 6)\cdot 10$ | pentane | $(4.8 \pm 0.3)\cdot 10$ |
|  |  | cyclopentane | $(3.6 \pm 0.1)\cdot 10$ |

[a] Uncertainties shown for $K_H$ are 95 % confidence limits. The uncertainty in $T$ was 0.05 K.

obeys Raoult's law so that the vapor pressure of the solute, $p_2$, is given by:

$$p_2 = p - x_1 p_1^{\mathrm{o}} \tag{1}$$

where $p$ is the measured pressure and $x_1$ and $p_1^{\mathrm{o}}$ are the mole fraction and vapor pressure of the solvent. The experimental Henry's law constants are shown in Tables 2 to 4 along with literature data where this is available.

The measurement and handling systems were tested by measurements of acetone, methanol, and ethanol in water in the range of $T$ = (273.2 to 303.2) K. The agreement between the measured $K_H$ values and those reported for these in the literature is excellent. As is clear from Table 2, there is a considerable body of data for acetone; in the case of methanol and ethanol, Dohnal et al.[10] have reviewed the $K_H$ and limiting activity coefficients of methanol and ethanol in water and provide a recommended equation for the calculation of $K_H$ as a function of temperature, including the range of temperatures considered here.

A stringent test of the data comes from the determination of the enthalpy of solvation, $\Delta_{\mathrm{solv}}H°$, of the solute from the temperature dependence of the Henry's law constant. Thus, following the Clausius−Clapeyron equation:

$$\ln K_{\mathrm{H}} = -\frac{\Delta_{\mathrm{solv}}H^{\mathrm{o}}}{RT} + C \tag{2}$$

where $C$ is an integration constant and a plot of ln $K_H$ against $T^{-1}$ yields a straight line with a slope equal to $-\Delta_{\mathrm{solv}}H°/R$. Figure 1 shows the plots for acetone, ethanol, and methanol, respectively, and the $\Delta_{\mathrm{solv}}H°$ values are listed in Table 5 along with values calculated from the temperature dependences reported by Staudinger and Roberts[7] and Dohnal et al.[10]

The enthalpies of solvation can be calculated independently from the enthalpies of vaporization, $\Delta_{\mathrm{vap}}H°$, and limiting enthalpies of solution, $\Delta_{\mathrm{soln}}H°$, of the solute. Thus:

$$\Delta_{\mathrm{solv}}H^{\mathrm{o}} = \Delta_{\mathrm{soln}}H^{\mathrm{o}} - \Delta_{\mathrm{vap}}H^{\mathrm{o}} \tag{3}$$

The $\Delta_{\mathrm{soln}}H°$ data are only available at 298.2 K, and so the $\Delta_{\mathrm{solv}}H°$ are calculated at this temperature. However, there is no significant curvature in the plots in Figure 1 so that the values calculated from the $K_H$ data are effectively averaged over the temperate interval.

Because condensation at the differential gauge had affected the measurements, $\Delta_{\mathrm{solv}}H°$ was also calculated only using the data for $T$ = (273.2 to 293.2) K. There is no significant difference between the values calculated over the different temperature ranges, and so we can conclude that the heating system for the upper part of the measurement line and the differential gauge worked satisfactorily.

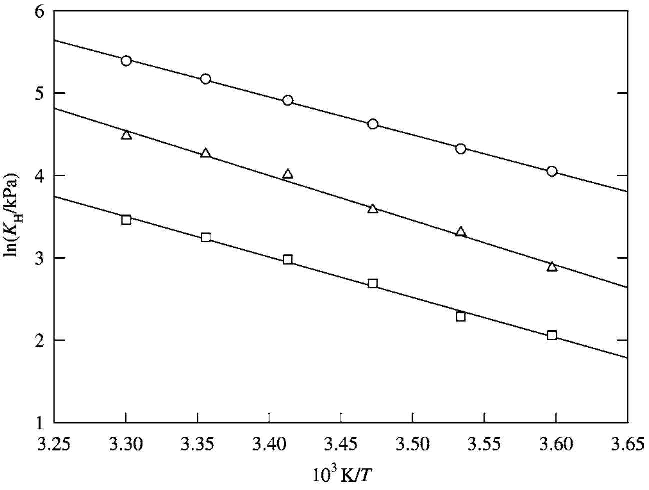

**Figure 1.** Plot of ln($K_H$/kPa) against $10^3$ K/$T$ for: ○, acetone; △, ethanol; and □, methanol. (Note: ethanol values are offset by one unit for clarity.)

**Table 5. Comparison of Solvation Enthalpies from the Temperature Dependence of the Henry's Law Constant and from Enthalpies of Solution and Vaporization at $T$ = 298.2 K**

|  | acetone | methanol | ethanol |
|---|---|---|---|
| $\Delta_{\mathrm{soln}}H°$/kJ·mol$^{-1}$ | −10.0[22] | −7.3[23] | −10.2[24] |
| $\Delta_{\mathrm{vap}}H°$/kJ·mol$^{-1}$ | 31.0[25] | 37.4[25] | 42.3[25] |
| $\Delta_{\mathrm{soln}}H° - \Delta_{\mathrm{vap}}H°$/kJ·mol$^{-1}$ | −41.0 | −44.7 | −52.5 |
| $\Delta_{\mathrm{solv}}H°$/kJ·mol$^{-1}$[a] | −37 ± 1 | −44 ± 6 | −46 ± 3 |
|  | (−38 ± 1) | (−44 ± 15) | (−49 ± 6) |
|  |  | −46.1[b] | −54.0[b] |
|  | −37.6[c] | −41.0[c] | −52.7[c] |

[a] Values in parentheses calculated using the data for $T$ = (278.2 to 293.2) K (see text). Uncertainties shown are 95 % confidence limits. [b] Calculated from the recommended data of Dohnal et al.[12] [c] Calculated from the temperature dependences reported by Staudinger and Roberts.[7]

Enthalpies calculated from pressure data are extremely sensitive to the precisions of the pressure data; for example, the $K_H$ values for methanol and ethanol are the same within their 95 % confidence limits. The $\Delta_{\mathrm{solv}}H°$ values calculated from them differ by 4 kJ·mol$^{-1}$, although of course they agree within their 95 % confidence limits.

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