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Henry's Law Constants of Some Aromatic Aldehydes and Ketones Measured by an Internal Standard Method

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Dimensionless Henry's law constants k_H (air—water partition coefficients) for a series of aromatic aldehydes and ketones were measured by using an internal standard method. It was demonstrated that the technique works well for both liquid and solid species. The k_H values of these compounds, which usually are difficult to be determined experimentally, are in the order of 10^{-6} to 10^{-3}. The measurements were carried out under atmospheric pressure and at various temperatures [(273 to 298) K]. The temperature dependence of k_H was also studied, and the van't Hoff parameters were calculated. All the data are reported with the corresponding standard deviations and uncertainties at the 95 % confidence level. The theoretical dipole moments in the gas phase were computed by utilizing Cerius^2 molecular modeling software to justify the discrepancies among the k_H values of the isomers. These calculations exhibit linear relationships between the dipole moment and k_H within each isomer series.

Introduction

The dimensionless Henry's law constants, k_H, or air—water partition coefficients are important parameters of organic compounds with applications in environmental study, health science, and chemical processing. The knowledge of k_H values is essential to predict the transport of harmful organic species in the environment and assess the corresponding risks. Vapor pressure and aqueous solubility of pure components have been extensively used to estimate k_H.[1] In addition to direct measurement of the substrate concentrations in both gas and liquid phases at equilibrium, various techniques have been applied to determine k_H experimentally in either static[2,3] or dynamic systems.[4,5] However, the reported methods have disadvantages,[6,7] and accurate measurements of Henry's law constants for compounds having extremely low k_H values are rare in the literature.

Due to the difficulties in experimental determination of low k_H, the Henry's law constants of many aromatic aldehydes and ketones are usually calculated by computer using various theoretical models.[8,9] These data are the intrinsic Henry's law constants k_H*,[5,10] which can be defined by eq 1

$$k_H^* = [\mathrm{RR'CO}]_g / [\mathrm{RR'CO}]_{aq} \qquad (1)$$

where $[\mathrm{RR'CO}]_g$ and $[\mathrm{RR'CO}]_{aq}$ are the concentrations of the carbonyls in the gas and the aqueous phase at thermodynamic equilibrium, respectively. The k_H^* values are less applicable in the real world because aldehydes and ketones are subject to reversible hydration upon dissolution to give *gem*-diols. Comparatively, the apparent dimensionless Henry's law constants k_H defined by eq 2 are more useful for modeling the behavior of toxic chemicals in the environment

$$k_H = [\mathrm{RR'CO}]_g / ([\mathrm{RR'C(OH)_2}] + [\mathrm{RR'CO}]_{aq}) \qquad (2)$$

where $[\mathrm{RR'C(OH)_2}]$ is the concentration of the *gem*-diols.[5,10] The relationship between k_H^* and k_H can be expressed by eq 3

$$k_H^* = (1 + K_{hyd}) k_H \qquad (3)$$

where K_{hyd} is the hydration constant of the carbonyls.[5,10]

In the present paper, we report the experimental determination of the apparent dimensionless Henry's law constant k_H for a series of aromatic aldehydes and ketones by using the recently developed internal standard method.[7] The approach is elegantly simple as the knowledge of many experimental variables is not required and random errors such as those associated with gas chromatographic (GC) injection volumes can be minimized. The technique works well for both liquid and solid compounds that have k_H values in the order of 10^{-6} to 10^{-3}. The Henry's law constants in units of $\mathrm{Pa \cdot m^3 \cdot mol^{-1}}$ can be simply obtained by multiplying k_H by RT (R = 8.314 $\mathrm{Pa \cdot m^3 \cdot mol^{-1} \cdot K^{-1}}$). The results were compared with the available literature data and correlated to the theoretical dipole moments. Additionally, the temperature dependence of k_H, which follows the van't Hoff relationship, was also studied.

Theory

A mixture containing similar amounts of the analyte (A) and the internal standard (I) is used to prepare the dilute standard (organic solvent) and aqueous solutions. The aqueous solution is placed in a closed system to reach the thermodynamic equilibrium, and the headspace samples as well as the standard solution are subject to GC analysis. The dimensionless Henry's law constant of the analyte ($k_{H,A}$) can be calculated by eq 4

$$k_{H,A} = \frac{R_1}{R_2} \cdot k_{H,I} \qquad (4)$$

where R_1 and R_2 are the GC peak area ratios (analyte-to-internal standard) for the headspace and the standard solution, respectively, and $k_{H,I}$ is the known dimensionless Henry's law constant of the internal standard. The detailed derivation can be found in the literature.[7] The exact knowledge of the substrate concentrations, the GC injection volumes, as well as the gas and the liquid phase volumes in the closed system is not required in this approach, which gives it advantages over previously

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Table 1. Dimensionless Henry's Law Constants k_H of Benzaldehyde, Acetophenone, and Phenol at Different Temperatures T

	$k_H \cdot 10^5$					
compound	T/K = 278	T/K = 283	T/K = 288	T/K = 293	T/K = 298	lit. T/K = 298
benzaldehyde[a]	24	35	50	74	125	109[b], 112[c]
SD	4	5	7	11	14	
95 % CL[d]	5	6	9	14	17	
acetophenone	5.6	8.1	13	19	35	37[e], 43[c], 44[f]
SD	0.9	1.2	2	3	4	
95 % CL	1.1	1.5	3	4	5	
phenol	0.18	0.32	0.60	1.1	1.7	1.3[c], 1.4[g]
SD	0.04	0.06	0.11	0.2	0.3	
95 % CL	0.05	0.07	0.14	0.3	0.4	

[a] Allen et al.[17] [b] Betterton et al.[5] [c] Yaffe et al.[9] [d] Uncertainty at the 95 % confidence level. [e] Betterton.[10] [f] Nirmalakhandan et al.[8] [g] Rochester et al.[18]

Table 2. Dimensionless Henry's Law Constants k_H of Some Aromatic Aldehydes and Ketones at Different Temperatures T

	$k_H \cdot 10^5$					
compound	T/K = 278	T/K = 283	T/K = 288	T/K = 293	T/K = 298	lit. T/K = 298
salicylaldehyde	9.1	12	19	25	38	NA[a]
SD	1.6	2	3	4	5	
95 % CL	2.0	3	4	5	6	
2-methylbenzaldehyde	27	39	57	85	136	NA
SD	5	6	8	13	15	
95 % CL	6	7	10	16	19	
3-methylbenzaldehyde	23	34	48	73	126	NA
SD	4	5	7	11	14	
95 % CL	5	6	9	14	17	
4-methylbenzaldehyde	15	22	31	47	83	78[b]
SD	3	3	5	7	10	
95 % CL	4	4	6	9	12	
2-methoxybenzaldehyde[c]	0.50	0.89	1.3	2.2	4.3	NA
SD	0.09	0.14	0.2	0.4	0.5	
95% CL	0.11	0.17	0.3	0.5	0.6	
3-methoxybenzaldehyde[c]	1.0	1.9	2.7	4.3	8.6	NA
SD	0.2	0.3	0.4	0.7	1.0	
95 % CL	0.3	0.4	0.5	0.9	1.2	
4-methoxybenzaldehyde[c]	0.21	0.40	0.62	0.99	1.7	NA
SD	0.04	0.07	0.10	0.16	0.2	
95 % CL	0.05	0.09	0.12	0.20	0.3	
propiophenone	6.7	11	14	26	43	54[d]
SD	1.3	2	2	4	6	
95 % CL	1.6	3	3	5	7	
2′-methylacetophenone	9.1	15	21	33	56	NA
SD	1.7	2	3	5	7	
95 % CL	2.1	3	4	6	9	
3′-methylacetophenone	4.5	7.3	11	16	28	NA
SD	0.8	1.2	2	3	4	
95 % CL	1.0	1.5	3	4	5	
4′-methylacetophenone	3.4	5.1	7.3	14	24	35[b]
SD	0.6	0.8	1.2	2	4	
95 % CL	0.7	1.0	1.5	3	5	
2′-methoxyacetophenone[c]	0.25	0.50	0.72	1.3	2.5	NA
SD	0.05	0.08	0.12	0.2	0.3	
95 % CL	0.06	0.10	0.15	0.3	0.4	
3′-methoxyacetophenone[c]	0.23	0.44	0.64	1.1	2.3	NA
SD	0.05	0.07	0.11	0.2	0.3	
95 % CL	0.06	0.09	0.14	0.3	0.4	
2′-hydroxyacetophenone	5.8	9.2	15	24	41	NA
SD	1.1	1.4	2	4	5	
95 % CL	1.4	1.7	3	5	6	

[a] NA = no data available. [b] Nirmalakhandan et al.[8] [c] Data were determined by using MSD. All the others were measured by FID. [d] Yaffe et al.[9]

reported methods. The limitation of this method is that it only works for compounds having low k_H values, and the accuracy of $k_{H,A}$ is dependent upon that of $k_{H,I}$.

Experimental Section

Materials. All chemicals of high purity were used without further purification. Pentane (98 %) was obtained from Fisher Scientific and used as the solvent for the standard solutions. Acetophenone (99 %), benzaldehyde (99+ %), 2′-methoxyacetophenone (99 %), and phenol (99 %) were purchased from Sigma-Aldrich. All the other aromatic aldehydes and ketones were supplied by Alfa Aesar as the following: 2-methylbenzaldehyde (98 %), 3-methylbenzaldehyde (97 %), 4-methylbenzaldehyde (98 %), 2-methoxybenzaldehyde (98 %), 3-methoxybenzaldehyde (98 %), 4-methoxybenzaldehyde (98 %), 2′-methylacetophenone (97 %), 3′-methylacetophenone (97 %), 4′-methylacetophenone (96 %), 3′-methoxyacetophenone (97 %), 2′-hydroxyacetophenone (97 %), propiophenone (99 %), and salicylaldehyde (99 %). The in-house deionized water was used to prepare the dilute aqueous solutions.

Table 3. Dipole Moments μ in the Gas Phase Computed by Cerius^2 for Selected Isomers

	μ/Cm		
compound	*ortho*	*meta*	*para*
methylbenzaldehydes	4.33	4.40	4.74
methoxybenzaldehydes	4.63	3.27	5.95
methylacetophenones	2.80	3.55	3.89
methoxyacetophenones	3.98	5.07	NC[a]

[a] NC = not computed.

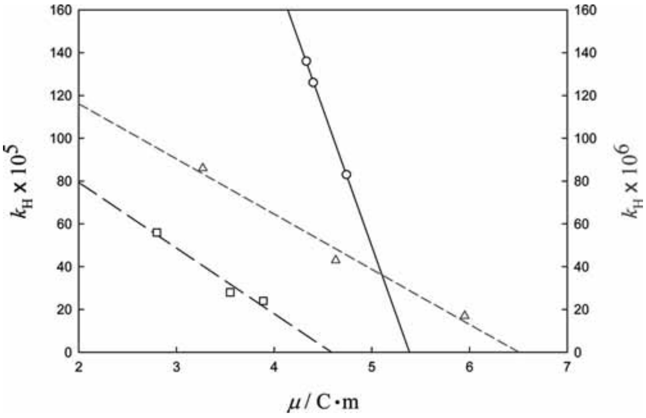

Figure 1. Correlation between dimensionless Henry's law constant k_H and dipole moment μ for a series of isomers at 298 K: ○, methylbenzaldehydes ($r^2 = 0.9997$, $\sigma = 7.3 \cdot 10^{-6}$); □, methylacetophenones ($r^2 = 0.9625$, $\sigma = 4.8 \cdot 10^{-5}$); △, methoxybenzaldehydes ($r^2 = 0.9825$, $\sigma = 6.5 \cdot 10^{-6}$).

Equipment. An Agilent Technologies model 6890N gas chromatograph equipped with both a flame ionization detector (FID) and a model 5973N mass selective detector (MSD) was used to quantify the compounds in the headspace samples and in the standard solution. The GC injectors were in the splitless mode, and the analytes were separated either on a 60 m × 0.25 mm (i.d.) capillary column (SA-WAX, Sigma-Aldrich) with carbowax as the stationary phase for FID or on a 30 m × 0.25 mm (i.d.) capillary column (HP-5MS, Agilent Technologies) with a stationary phase of poly(phenylmethylsiloxane) for MSD. The GC oven temperature was kept at 140 °C isothermal for the analysis using FID or initially held at 60 °C for 3 min and ramped at 8 °C per minute to 200 °C for the analysis using MSD. A toluene solution containing 5 % volume fraction of dimethyldichlorosilane was used to chemically deactivate the entire inside surface of the 40 mL sample vials (Supelco) to prevent the adsorption of the analytes. After the addition of the dilute aqueous solutions, the vials were capped with silicone/poly(tetrafluoroethylene)-faced septa and holed screw caps (Supelco) and kept in an open water bath, of which the temperature was controlled by a BIO-RAD cooling module refrigerated water circulator. A 500 μL gastight, valve-locking microsyringe (model 500 R-V-GT, Scientific Glass Engineering) was used to withdraw the headspace samples and inject them into the GC. Various Eppendorf micropipettes were used to prepare the solutions.

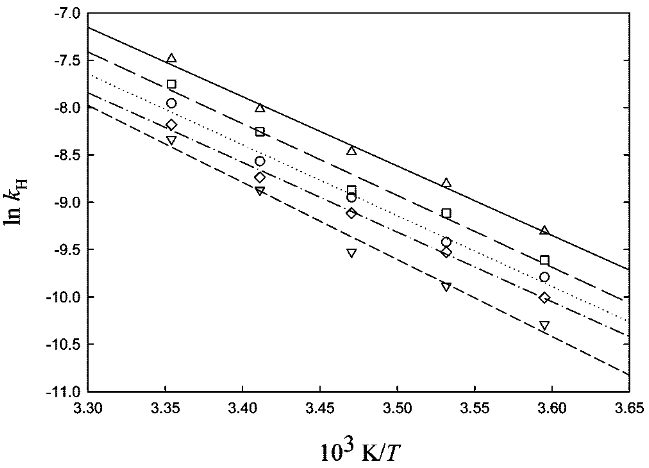

Figure 2. van't Hoff plots for selected aromatic ketones in the temperature range of (278 to 298) K: ○, acetophenone; □, propiophenone; △, 2′-methylacetophenone; ◇, 3′-methylacetophenone; ▽, 4′-methylacetophenone.

Sample Preparation and Analysis. Benzaldehyde was used as the internal standard for all the measurements. Equal volumes of the substrates and benzaldehyde were mixed in appropriate combinations so that they could be separated by GC. For the determination of k_H for phenol, which is a solid, the substrate was dissolved in an equal molar amount of benzaldehyde to make the mixture. The dilute standard solution was prepared by adding 1 μL of the mixture to approximately 25 mL of pentane. An appropriate amount (50 μL to 150 μL) of the mixture was added to 250 mL of water to prepare the dilute aqueous solution. The aqueous concentrations of each analyte were in the range of approximately (100 to 180) ppm, which was well below the corresponding solubilities[11,12] and low enough to obey Henry's law.[1,13] Additionally, the interactions among the analytes should be trivial and not affect the k_H values.

Aliquots of the dilute aqueous solution were transferred into the sample vials, which were then placed in the water bath with the temperature kept at (278 to 298) K. The headspace-to-liquid volume ratios were maintained at less than 1. At least 1 h[13] was allowed for the establishment of thermodynamic equilibrium in the vials. Both the headspace samples and the standard solution were analyzed by either GC or GC–MS. The injection volumes were 200 μL for the headspace samples and 1 μL for the standard solution, respectively. The FID and MSD responses were examined to be linear throughout the concentration range of the samples.[14] All measurements were conducted under atmospheric pressure at 1 atm.

Molecular Modeling. The molecular modeling of each compound was conducted by using the commercially available Cerius^2 software package (version 4.10, Accelrys) running on a Silicon Graphics four processor Tesro workstation. The molecules were constructed in the 3D sketcher module, and the partial charges were calculated by utilizing the Charge Equilibration technique.[15] The molecules were taken through several cycles of minimization and molecular dynamics under NPT conditions utilizing the COMPASS force field[16] prior to the calculation of dipole moments.

Results and Discussion

The dimensionless Henry's law constants of acetophenone and phenol were measured by using benzaldehyde[17] as the internal standard to validate the method. As the k_H value decreases, MSD must be used instead of FID to detect the signals for the headspace samples. Consequently, the k_H values of acetophenone and phenol at five different temperatures were determined by FID and MSD, respectively. The relative standard deviation (RSD) was usually less than 3 % for the measurements of R_2. The RSD associated with R_1 was often less than 5 % for $k_H > 10^{-5}$ but could be up to 10 % if k_H values are in the order of 10^{-6}. These deviations are acceptable when compared with the

Table 4. van't Hoff Parameters *A* and *B* and Standard Enthalpy and Entropy of the Phase Change (Liquid to Gas) $\Delta H°$, $\Delta S°$

compound	A/K	B	$\Delta H°$/kJ·mol^{-1}	$\Delta S°$/J·K^{-1}·mol^{-1}	r^2	σ
salicylaldehyde	−5954 ± 296[a]	12.06 ± 1.03	49.5 ± 2.5	100.3 ± 8.6	0.9926	0.057
2-methylbenzaldehyde	−6648 ± 267	15.64 ± 0.93	55.3 ± 2.2	130.0 ± 7.7	0.9952	0.051
3-methylbenzaldehyde	−6897 ± 426	16.37 ± 1.48	57.3 ± 3.5	136.1 ± 12.3	0.9887	0.081
4-methylbenzaldehyde	−6920 ± 478	16.02 ± 1.66	57.5 ± 4.0	133.2 ± 13.8	0.9859	0.091
2-methoxybenzaldehyde	−8627 ± 511	18.79 ± 1.77	71.7 ± 4.2	156.2 ± 14.7	0.9896	0.097
3-methoxybenzaldehyde	−8485 ± 576	19.00 ± 2.00	70.5 ± 4.8	158.0 ± 16.6	0.9864	0.110
4-methoxybenzaldehyde	−8444 ± 278	17.32 ± 0.96	70.2 ± 2.3	144.0 ± 8.0	0.9968	0.053
acetophenone	−7480 ± 462	17.04 ± 1.61	62.2 ± 3.8	141.7 ± 13.4	0.9887	0.088
propiophenone	−7581 ± 591	17.60 ± 2.05	63.0 ± 4.9	146.3 ± 17.0	0.9821	0.113
2′-methylacetophenone	−7329 ± 342	17.03 ± 1.19	60.9 ± 2.8	141.6 ± 9.9	0.9935	0.065
3′-methylacetophenone	−7361 ± 313	16.45 ± 1.09	61.2 ± 2.6	136.8 ± 9.1	0.9946	0.060
4′-methylacetophenone	−8140 ± 615	18.88 ± 2.14	67.7 ± 5.1	157.0 ± 17.8	0.9831	0.117
2′-methoxyacetophenone	−9217 ± 509	20.25 ± 1.77	76.6 ± 4.2	168.4 ± 14.7	0.9909	0.097
3′-methoxyacetophenone	−9146 ± 611	19.89 ± 2.12	76.0 ± 5.1	165.4 ± 17.6	0.9868	0.116
2′-hydroxyacetophenone	−8072 ± 209	19.23 ± 0.73	67.1 ± 1.7	159.9 ± 6.1	0.9980	0.040
phenol	−9503 ± 255	20.94 ± 0.89	79.0 ± 2.1	174.1 ± 7.4	0.9978	0.049

[a] The number following the symbol ± is the standard error.

various reported methods. The standard deviations (SD) of $k_{\mathrm{H,A}}$ (S_{A}) were calculated by the deviation propagation equation

$$\frac{S_{\mathrm{A}}}{k_{\mathrm{H,A}}} = \sqrt{\left(\frac{S_1}{R_1}\right)^2 + \left(\frac{S_2}{R_2}\right)^2 + \left(\frac{S_{\mathrm{I}}}{k_{\mathrm{H,I}}}\right)^2} \qquad (5)$$

where S_1, S_2, and S_{I} are the standard deviations for R_1, R_2, and $k_{\mathrm{H,I}}$, respectively. The corresponding estimated uncertainties at the 95 % confidence level were also computed, and all the data are presented in Table 1 along with the reported values for benzaldehyde.[17] The results at 298 K were found to be in good agreement with the literature values by running *t* tests, as shown in the Appendix. However, the RSD of the Henry's law constants for all analytes are fairly large due to the high RSD values of $k_{\mathrm{H,I}}$,[17] and so are the uncertainties.

The determination of k_{H} for the other 14 aromatic aldehydes and ketones was carried out by using either FID or MSD (for acetophenones and benzaldehydes with a methoxy substituent). The experimental k_{H} data at different temperatures are summarized in Table 2 with the corresponding standard deviations and uncertainties at the 95 % confidence level. Most of these k_{H} values have not been previously measured or computed. The result for 4-methylbenzaldehyde at 298 K matches fairly well with the literature data, as demonstrated by the statistical analysis in the Appendix. However, there are slight discrepancies existing for propiophenone and 4′-methylacetophenone in comparison with the calculated theoretical k_{H}. One possible explanation lies in the fact that the conjugated aromatic ketones can have resonance structures which would cause them to be more hydrophilic, as proposed by Betterton.[10] Consequently, these compounds will have lower k_{H} values than expected. Further research needs to be done to explore this behavior. Additionally, it may be noted that the computed literature k_{H} could be actually $k_{\mathrm{H}}{}^*$, which should be different from the experimental k_{H} as shown by eq 3.

There are also discrepancies in k_{H} among the isomeric acetophenones and benzaldehydes with either methyl or methoxy substituents. The differences could be explained by the polarities of the compounds as the more polar species will have stronger interaction with water molecules and thus give lower k_{H} data. Cerius^2 molecular modeling software was used to calculate the theoretical dipole moments of the isomers in the gas phase, and the results are shown in Table 3. The calculated dipole moments for a series of isomers exhibit high linear relationships with the corresponding k_{H} at 298 K, as depicted by Figure 1. All the squares of the correlation coefficient (r^2) values are greater than 0.96, and the standard deviations of the fitted data (σ) are also given for Figure 1. The linearity is observed at other temperatures as well. However, this kind of correlation is less predictive among nonisomeric compounds as many other factors may affect the Henry's law constant.

Efforts were made to determine the dimensionless Henry's law constants of 3-hydroxybenzaldehyde and 4-hydroxybenzaldehyde by using GC–MS. However, the predicted k_{H} values for the hydroxybenzaldehydes are in the order of 10^{-7}.[8] Both compounds are also solids and have low solubilities in water. Consequently, the amount of the substrates partitioning into the gas phase would be too low to be detected by MSD, which resulted in unsuccessful measurements.

The Henry's law constants usually increase with an increase in temperature. If the pressure is kept constant, the temperature dependence of the dimensionless Henry's law constant follows the van't Hoff relationship

$$\ln k_{\mathrm{H}} = -\left(\frac{\Delta H°}{R}\right)\frac{1}{T} + \left(\frac{\Delta S°}{R}\right) \qquad (6)$$

where T is the temperature and $\Delta H°$ and $\Delta S°$ are the standard enthalpy and entropy, respectively, of the phase change (liquid to gas) for the substrate. The equation may be expressed more simply as

$$\ln k_{\mathrm{H}} = \frac{A}{T} + B \qquad (7)$$

The parameters A and B can be readily obtained by plotting $\ln k_{\mathrm{H}}$ as the function of $1/T$.

The van't Hoff plots of $\ln k_{\mathrm{H}}$ versus $1/T$ for acetophenone, propiophenone, and methylacetophenones, as shown in Figure 2, exhibit a high degree of linearity. The temperature dependence of k_{H} was evaluated for all the other compounds examined in this study. Linear regression of the van't Hoff plot was used to calculate A and B. In each case, the r^2 value is greater than 0.98. The standard errors associated with the van't Hoff parameters were obtained by regression analysis at the 95 % confidence level using the LINEST function in Microsoft Excel. Additionally, the values of $\Delta H°$ and $\Delta S°$ were computed for each compound, and the results including r^2 and σ are summarized in Table 4.

Conclusions

Dimensionless Henry's law constants k_{H} at temperatures of (278 to 298) K were measured for phenol and 15 selected

Table 5. *t* Values for Comparison of k_H at 298 K

compound	$k_H \cdot 10^5$ (this study)	$k_H \cdot 10^5$ (lit.)	*t*
acetophenone	35	37	1.12
		43	4.47
		44	5.03
phenol	1.7	1.3	2.98
		1.4	2.24
4-methylbenzaldehyde	83	78	1.12
propiophenone	43	54	4.10
4′-methylacetophenone	24	35	6.15

aromatic aldehydes and ketones by using the internal standard method. It was demonstrated that the technique worked well for both liquid and solid compounds with k_H values in the order of 10^{-6} to 10^{-3}. The accuracy of the data is acceptable, as evidenced by comparison with the available literature values. However, the corresponding standard deviations and the 95 % confidence intervals are largely affected by that of the internal standard (benzaldehyde). It can be predicted that the majority of the compounds explored in this study would stay in the water body in the environment as pollutants. The k_H data for the isomeric aldehydes and ketones are highly correlated to the corresponding theoretical dipole moments. The temperature dependence of k_H, which follows the van't Hoff relationship, was also examined for all the substrates. The thermodynamic parameters were calculated by linear regression analysis. Most of the data presented in this paper have not been previously reported.

Appendix

Comparison of Experimental and Literature Data. The literature k_H values at 298 K in Table 1 and Table 2 are computed theoretical data or experimentally measured results, of which either the standard deviations or the number of measurements (N) are not available. Consequently, only the simple t test is used to compare the k_H obtained in this study with the literature data. Assuming the mean of the experimental k_H is $\bar{x}$, the literature k_H is the true value x_t, the standard deviation is s, and N is equal to 5 for the measurements, the t values can be calculated by

$$t = \frac{|\bar{x} - x_t|}{s}\sqrt{N} \tag{8}$$

and the results are given in Table 5.The critical value of t at the 99 % confidence level is 4.60, which is higher than most of the test values of t. Thus, it can be concluded that there is no significant difference between the measured and the literature data at the 99 % confidence level. The few exceptions have been briefly discussed in the text.

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