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Henry's Law Constants for Eleven Polychlorinated Biphenyls at 20 °C

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Henry's law constants for 11 polychlorinated biphenyls (PCBs) were measured using a gas purge system at 20 °C. The studied PCB congeners ranged from 2,4,4′-trichlorobiphenyl to 2,2′,3,4,4′,5,5′-heptachlorobiphenyl, spanning a range of hydrophobicities and solubilities, and including four mono-, and seven di-ortho-chlorinated compounds. For four PCBs, Henry's law constants have not been published before. These are 2,3,5,6-tetrachlorobiphenyl, 2,3,4,5,6-pentachlorobiphenyl, 2,2′,3,4,4′,5-hexachlorobiphenyl, and 2,3,3′,4,4′,5-hexachlorobiphenyl. For the lower chlorinated PCBs, the values are in agreement with available literature data. The values for the higher chlorinated PCBs agreed well with other partitioning data for PCBs and are lower than most available literature data. The measured Henry's law constants decreased with increasing hydrophobicity and showed a high correlation with the number and position of the chlorine atoms. The methods used are suitable for measuring reliable Henry's law constants and also for the higher chlorinated PCB congeners.

Introduction

Physical−chemical data such as the water solubility and partitioning data (including the Henry's law constants) are used as input for environmental risk assessments and fate and transport models. Besides the use of Henry's law constant (*H*) for the prediction of the environmental behavior of compounds, this property is also used in studies of desorption kinetics and partition coefficients of organic compounds in sediment−water systems. In these studies, a gas purge method has been employed.[1−6] This method uses the dynamics of water−air exchange to induce desorption of compounds from sediments or suspended particles. Interpretation of this type of experiments requires reliable values for the Henry's law coefficients of the studied compounds.

The quality of physical−chemical data is not always easy to judge.[7−10] One of the ways to judge whether a data set is of good quality is to verify whether the obtained data are consistent with other properties.[9−11] Values for *H*, for example, are related to vapor pressure, solubility in water and 1-octanol, the 1-octanol−water partition coefficient, and the 1-octanol−air partition coefficient. Especially for the heavier PCBs, disagreement exists on the quality of some of the published data sets for *H*.[9]

The reliable determination of Henry's law constants for compounds such as PCBs can be problematic for several reasons. First, measurements using compounds with very low water solubilities (ng/L range) require a careful preparation of aqueous solutions. Second, the higher chlorinated PCBs have low Henry's law constants. This means special requirements for the test system to measure Henry's law constants are needed, such as the use of a dynamic air−water exchange in which the purged compounds are trapped and concentrated. Also, sorption of hydrophobic compounds to the glass wall can influence the results of these type of experiments. The setup of experiments (i.e., equilibration time of prepared solutions, fraction of compounds purged from the solution) should therefore be carefully chosen.

The preparation of aqueous solutions of sparingly soluble compounds can be done in different ways. Using a carrier solvent is one of them, but this has the disadvantage of influencing the compound's solubility in water. Methods based on the generator column technique are the methods of choice for sparingly soluble compounds.[12] For the determination of Henry's law constants several methods are in use. The advantage of using a dynamic system for this type of measurements, such as the gas purge system, is that detection problems will not occur because the compounds in the gas phase are concentrated on an adsorbent.

The aim of this study was to establish Henry's law constants for a broad range of PCB congeners and to find a relationship between *H* and molecular descriptors, using established methods for measuring *H* and preparing aqueous solutions. In the present paper, we report the experimental determination of Henry's law constants for 11 PCB congeners that present a range in solubility and hydrophobicity and include both mono-ortho and di-ortho congeners. The compounds were chosen to span a range of congeners with different chlorination patterns. The range consisted of three- through hepta-chlorinated congeners, containing symmetrical congeners, and congeners with all chlorines on one of the two aromatic rings. It included four congeners with one chlorine in the ortho position and seven congeners with two chlorines in the ortho position. This set of congeners includes four compounds for which at present no measured Henry's law constants are available in the literature.

Experimental Section

Chemicals. The PCB congeners used in this study were obtained from Promochem (C. N. Schmidt, Amsterdam, The Netherlands). The studied compounds are listed in Table 1, together with some relevant physical−chemical properties. The solvents acetone, *n*-hexane, and isooctane were all nanograde quality and were also obtained from Promochem. Methanol

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Table 1. Measured Water Concentrations and Relevant Physicochemical Properties of the PCB Congeners Studied

compound	$N_{\text{ortho}-\text{Cl}}$	aqueous solubility μmol/L	log K_{OW}	aqueous concentration at $t = 0$ μmol/L
PCB-28 (2,4,4′)	1	0.421[a]	5.66[a]	0.131 ± 0.014
PCB-52 (2,2′5,5′)	2	0.341[a]	5.91[a]	0.103 ± 0.017
PCB-65 (2,3,5,6)	2	0.0147−0.342[b]		0.027 ± 0.002
PCB-105 (2,3,3′,4,4′)	1	0.0179[a]	6.82[a]	0.0054 ± 0.0012
PCB-116 (2,3,4,5,6)	2	0.0123−0.0613[b]	6.754[c]	0.020 ± 0.003
PCB-118 (2,3′,4,4′,5)	1	0.027[a]	6.69[a]	0.0071 ± 0.0013
PCB-137 (2,2′,3,4,4′,5)	2	0.0011−0.002[b]		0.00064 ± 0.00013
PCB-138 (2,2′,3,4,4′,5′)	2	0.0052[a]	7.22[a]	0.0023 ± 0.0003
PCB-153 (2,2′4,4′,5,5′)	2	0.0077[a]	6.87[a]	0.0020 ± 0.0003
PCB-156 (2,3,3′,4,4′,5)	1	0.0011−0.002[b]		0.0014 ± 0.0003
PCB-180 (2,2′,3,4,4′,5,5′)	2	0.0011−0.0051[b]	7.16[a]	0.00115 ± 0.00018

[a] From ref 10 using compiled data measured at 20 °C and using the selected value (termed FAV) for log K_{OW} (25 °C). [b] Individual values or range for PCB isomer group from ref 24. [c] From ref 25.

(absolute quality), hydrochloric acid (Titrisol), and potassium monohydrogen phosphate (analyzed quality) were obtained from J. T. Baker (Deventer, The Netherlands). Tenax TA (60−80 mesh) was obtained from Chrompack (Middelburg, The Netherlands). Chromosorb G-acid washed (45−60 mesh) was obtained from Serva (Brunschwig Chemie, Amsterdam, The Netherlands). The Tenax, Chromosorb, and glass wool were all washed with *n*-hexane and dried before use.

Preparation of Aqueous Solutions. All glassware used in the experiments was rinsed with detergent (Extran MA 02 neutral, Merck, Amsterdam, The Netherlands) and cleaned with Milli-Q water and acetone. The bottles were dried at 105 °C. The 5- and 10-L bottles that were used for the preparation of the aqueous solutions and the bottles used for the purge experiments were also cleaned with *n*-hexane and dried with a nitrogen stream prior to use. PCB congeners were added to Chromosorb by mixing 1 g of Chromosorb with 5 mL of a PCB solution in methanol or isooctane (concentration in the spike solutions was around 0.1 mg/mL for each congener). After mixing, the organic solvents were evaporated under a nitrogen stream. The Chromosorb was further air-dried at 105 °C.

The spiked Chromosorb was added to 5 or 10 L of buffered Milli-Q water as a modification of the generator column method. The water contained 0.6 g of K_2HPO_4 per 5 L of Milli-Q water and was brought to a pH of 6.4 with HCl. The solution is also used when studying sediment−water distributions with the same experimental system because its composition is thought to be representative for surface water composition in freshwater systems in The Netherlands. The salt concentration in the artificial freshwater of 10^{-3} M will lower the solubility of PCBs with less than 0.5 %;[13] this has a negligible influence on *H*.

The solution containing the Chromosorb was gently mixed with a stirring bar for 1 week. After being mixed, a small film was visible at the surface of the water. This film was removed by suction with vacuum. Aqueous concentrations that were determined before the start of a gas purge experiment are also listed in Table 1. These were all at or below reported solubilities (Table 1).

Gas Purge Technique. The gas purge system that was used to determine the Henry's law constants has been described earlier.[14] In short, the system consists of two 1-L thermostated flasks. The flasks have double walls through which water with a constant temperature flows to keep the solutions inside the purge vessel at the desired temperature (20.0 ± 0.1 °C). The first flask contained Milli-Q water through which compressed air passes from a capillary with a glass filter (flow rate 500 mL/min). Wetting the gas prevented volume reduction in the second flask. No measurable volume reduction occurred during the experiments. Before the wetted gas entered the second flask, the gas was cleaned by passing it through a glass column filled with Tenax (5 mm i.d. containing 0.12 g of Tenax). The second flask contained the test solution with PCBs. A metal stirring bar was used to mix the gas bubbles with the solution. The PCBs that were stripped from the solution were trapped on a Tenax column. The trapping efficiency of the Tenax was tested by passing the gas through a second Tenax trap. One trap appeared to be sufficient.

During the experiment, the Tenax traps were changed five times. For the solution containing the lower chlorinated compounds, traps were exchanged at 15-min intervals; for the higher chlorinated compounds, traps were exchanged at 90-min intervals. During the experiment the gas flow rate was checked 20 times with a soap bubble meter. After the experiment was terminated, the concentration in the solution was measured again to construct mass balances from the measured concentrations in the solution and the amounts measured on the Tenax columns.

Chemical Analyses. PCBs in the aqueous solutions were extracted by shaking 10 mL of the solution with 2 mL of *n*-hexane for 2 h. After shaking, the solutions were separated, and the *n*-hexane was analyzed for its PCB contents using gas chromatography. The Tenax columns were rinsed with *n*-hexane using around 10 mL of solvent. After volume reduction, the *n*-hexane was analyzed using gas chromatography. The extraction efficiency of Tenax was tested for the PCB congeners 28, 65, 118, 138, 153, and 180 by adding known amounts of the congeners dissolved in methanol; then Tenax was suspended in water and was dried after shaking the suspension for 3 h. Glass colums were filled with Tenax and eluted with hexane as described above. The recovery of PCBs spiked to Tenax was 94−121 %.

All extracts were analyzed on a Hewlett-Packard 5890 gas chromatograph, equipped with a ^{63}Ni electron capture detector. The column used was a fused silica CP sil 8cb for PCBs from Chrompack (length 50 m, i.d. 0.25 mm). Helium passed through the column with a flow rate of 1 mL/min. The temperature of the injector was 225 °C, and the detector temperature was 300 °C. An amount of 2 μL was splitless injected and eluted using the following temperature program: 2 min at 60 °C, raising to 140 °C with 10 °C/min, raising to 240 °C with 5 °C/min, and stable for 35 min at 240 °C. Data analysis was done with the HP3365 Chemstation using external standards.

Data Handling. The concentration in water (C_{W}) was measured at the start of a purge experiment. For all other time intervals C_{W} was calculated from the cumulative amount that was trapped on Tenax by

$$C_{\text{W}}(t) = C_{\text{W}}(t = 0) - \frac{\sum M_{\text{Tenax}}}{V} \tag{1}$$

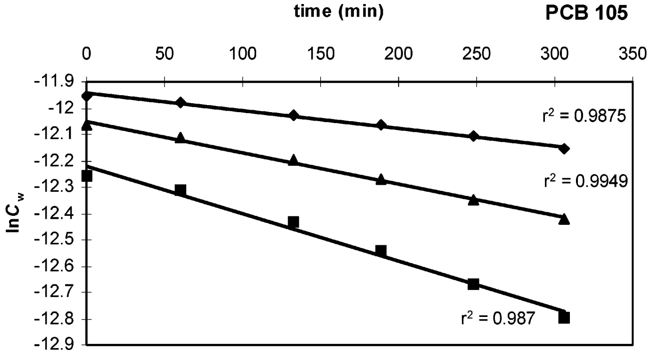

Figure 1. Examples of the measured decrease of C_W with purge time (triplicate), and the linear regressions used for the calculation of H.

where $C_W(t)$ = concentration in water at time t (μg/L); $C_W(t = 0)$ = measured concentration in water at time $t = 0$ (μg/L); M_{Tenax} = cumulative mass trapped on Tenax (μg); and V = volume of water in the purge vessel (L).

Henry's law constants (H) in each experiment were determined from the linear regression of ln C_W versus time. Each experiment consisted of five measurements. The slope of the regression line is the volatilization rate constant (k_{vl}). From k_{vl} (in h^{-1}) the dimensionless Henry's law constant (H') can be calculated with

$$k_{vl} = \frac{F \times H'}{V} \tag{2}$$

where k_{vl} = volatilization rate constant (h^{-1}); F = flow of gas (L/h); V = volume of water in the purge vessel (L); and H' = Henry's law constant (dimensionless air−water partition coefficient) (−). H (in Pa·m^3 mol^{-1}) is calculated from

$$H = H' \times R \times T \tag{3}$$

where H = Henry's law constant (Pa·m^3·mol^{-1}); H' = Henry's law constant (dimensionless air−water partition coefficient) (−); R = gas constant: 8.314 Pa·m^3·mol^{-1}·K^{-1}; and T = experimental temperature (K).

Mass Balances. For each purge experiment, a mass balance check was performed. This was done by measuring the concentration in the purge vessel after termination of the purge experiments. The mass balance was calculated from

$$\text{mass balance (\%)} = \frac{C(t = 0)}{\sum M_{Tenax}/V + C_{end}} \tag{4}$$

where $C(t = 0)$ = measured concentration at $t = 0$ (μg/L); $\sum M_{Tenax}$ = summed masses accumulated on Tenax (μg); V = volume of water in the purge vessel (L); C_{end} = measured concentration at the end of an experiment (μg/L). The mass balances calculated from eq 4 were 85 ± 10 % (n = 16) for all studied compounds.

Results and Discussion

Comparability of H with Literature Values. The Henry's law constants for the 11 chlorobiphenyls studied are given in Table 2.

Each individual value for H was obtained from the linear regression of ln C_W versus time. The linear regressions yielded straight lines with r^2 ranging from 0.97 to 0.998. Each line consisted of five data points. Examples of these linear regressions are shown in Figure 1 for PCB-105. Each value for H is the average of three to six separate purge experiments; the individual values for H and their standard deviations are presented in Table 2. The results of an F test for each regression to obtain H from the measured decrease of ln C_W with time showed that in all cases the significance was ≤ 0.01 (for PCBs with up to 5 chlorines the significance was ≤ 6.0×10^{-5}). The standard deviation of the slope was for all experiments much higher than the standard deviation of the intercept.

Although many data compilations of H for PCBs exist,[15−18] we restricted our comparison with literature values in Table 2 to those references that published experimentally determined values of H using comparable methods and that studied the same compounds. A second source of data was the publication by Li et al.,[10] who critically selected and evaluated physical chemical property data for polychlorinated biphenyls. The values for H that we obtained are comparable to those reported by other authors.[10,14,19,21−22] Only for the higher chlorinated compounds, our data are lower than those reported by Bamford et al.,[22] but agree with those published by others.

Although our average values for H seem to show a much higher variation than those published by Bamford et al.,[22] this actually is not the case. The data from Bamford et al. were all calculated from air and water pairs collected over the duration of one purge experiment that consisted of five measurement intervals. Their relative standard deviations were all less than 15 %, but this does not give an indication of the variability between replicate purge experiments. Our data were obtained the same way, but this was done in three to six replicates. The variation of H values in one purge experiment is shown to be equally low because r^2-values for the linear regression of ln C_W versus time were high (0.92 to 0.99), see also the examples in Figure 1. This leads to standard deviations in the determination of H within one purge experiment that in most cases are very comparable to those reported by Bamford et al.[22]

According to a recent comment[9] on the reliability of measured values for H, it was indicated that for the higher chlorinated biphenyls reported values for H do not always agree with other physical properties. Values for H tend to be too high, but those obtained by Murphy et al.[21] were considered to be the most in agreement with other published partitioning data.[9] One of the reasons given in the comment[9] was that for higher chlorinated PCBs the adsorption of compounds to the air bubbles could have resulted in volatilization rates that were too high, leading to an overestimation of the Henry's law constants. Although the authors[26] agree with the comment that the reported data are higher than those reported by Murphy et al.,[21] they point out that their data are in agreement with other literature values. They disagree with PCB enrichment at the bubble interface because their data set is consistent with values predicted from vapor pressure and solubility. Our data set also does not show the higher values of H for higher chlorinated PCBs that are expected when an enrichment of higher chlorinated PCBs at the bubble interface would occur.

For the data set presented in this paper, the reported values are in close agreement with the data obtained by Murphy et al.,[21] with the exception of PCB-180, where our value was an order of magnitude lower. For the higher chlorinated biphenyls (five or more chlorines), our values deviate most from other reported values for H; our values are mostly lower than those reported by Bamford et al.[22] This is in agreement with a recent comment in which it was stated that reported values for H for higher chlorinated compounds tend to be too high.[9]

Relation of H with Number of Chlorines and ortho-Chlorine Substitution. Bamford et al.[22] observed an increase of H with the number of ortho-chlorines but no strong relationship between H and molecular weight (which is determined by the number

Table 2. Measured Henry's Law Constants and Standard Deviations at 20 °C and Literature Data for 11 PCB Congeners

compound	$N_{\text{ortho-Cl}}$	average Henry's law constant Pa·m^3·mol^{-1}	individual Henry's law constants Pa·m^3·mol^{-1}	literature data at 20 °C, unless indicated otherwise Pa·m^3·mol^{-1}
PCB-28 (2,4,4′)	1	28.1 ± 1.9 (n = 3)	26.0 ± 0.9 29.6 ± 1.1 28.7 ± 1.7	26.75;[21] 27.18 ± 0.19 at 18 °C;[22] 21 ± 2;[14] 20 at 25 °C;[19] 30.2 at 25 °C[10]
PCB-52 (2,2′,5,5′)	2	24 ± 4 (n = 3)	19.3 ± 1.1 26.6 ± 1.7 26 ± 2	24.12;[21] 22.56 ± 0.23 at 18 °C;[22]; 16.4 ± 4;[14] 34.1 ± 2.7 at 25 °C;[20] 20 at 25 °C[19] 25.1 at 25 °C[10]
PCB-65 (2,3,5,6)	2	40 ± 3 (n = 3)	36.3 ± 1.0 43.0 ± 1.9 39.3 ± 0.9	no data available
PCB-105 (2,3,3′,4,4′)	1	5.5 ± 2.3 (n = 3)	3.4 ± 0.4 8.0 ± 0.9 5.1 ± 0.4	15.73 ± 0.44 at 18 °C;[22] 13.8 at 25 °C[10]
PCB-116 (2,3,4,5,6)	2	34 ± 3 (n = 3)	34 ± 4 36 ± 3 31 ± 2	no data available
PCB-118 (2,3′,4,4′,5)	1	7.8 ± 2.3 (n = 3)	6.2 ± 0.4 10.4 ± 0.7 6.8 ± 0.3	8.61;[21] 21.79 ± 0.44 at 18 °C;[22] 14.45 at 25 °C[10]
PCB-137 (2,2′,3,4,4′,5)	2	12 ± 7 (n = 6)	24 ± 7 3.48 ± 0.13 14 ± 2 7.2 ± 0.8 13 ± 3 12 ± 3	no data available
PCB-138 (2,2′,3,4,4′,5′)	2	9 ± 5 (n = 5)	12 ± 2 5.63 ± 0.15 17 ± 4 8.3 ± 1.7 4.1 ± 0.8	7.60;[21] 18.68 ± 0.49 at 18 °C;[22] 2.1 at 25 °C;[19] 30.2 at 25 °C[10]
PCB-153 (2,2′,4,4′,5,5′)	2	15 ± 7 (n = 5)	27 ± 8 8 ± 3 15 ± 3 14 ± 2 12 ± 1.9	10.03;[21] 27.2 ± 0.58 at 18 °C;[22] 2.33 at 25 °C;[19] 13.4 ± 1.1 at 25 °C;[10] 20.0 at 25 °C[10]
PCB-156 (2,3,3′,4,4′,5)	1	3.1 ± 1.3 (n = 6)	4.2 ± 0.6 4.8 ± 0.3 3.2 ± 0.8 0.97 ± 0.10 2.5 ± 0.3 2.9 ± 0.5	no data available
PCB-180 (2,2′,3,4,4′,5,5′)	2	2.2 ± 1.0 (n = 6)	3.3 ± 0.5 0.65 ± 0.08 3.3 ± 0.7 1.5 ± 0.2 2.0 ± 0.3 2.4 ± 0.5	53.0;[21] 8.96 ± 0.20 at 18 °C;[22] 1.01 at 25 °C;[19] 8.5 at 25 °C[10]

of chlorines). Brunner et al.[19] did observe a relationship between H and molecular weight: H decreases with increasing number of chlorines. They noted variability within groups of constant chlorine number that could to some extent be explained if the number of chlorine atoms in ortho position was taken into account.

The number of ortho-chlorines has been shown to increase the value for H.[10,19,20] Brunner et al.[19] found the following relation: $\log H = 2.00 - 0.32$ (number of chlorines) $+ 0.18$ (number of ortho-chlorines) ($r^2 = 0.957$, $n = 58$), in which H was calculated from their value for K, which represents the dimensionless gas−water partition coefficient H' using our eq 3. Although our data set consisted of only 11 measurements, a similar relationship was found: $\log H = 1.94 - 0.32$ (number of chlorines) $+ 0.48$ (number of ortho-chlorines), ($r^2 = 0.91$, $n = 11$). The relationship between log H, number of chlorines, and number of ortho-chlorines is presented in Figure 2. This figure presents the average of all measured values for H for each congener as a function of the number of chlorines. Solid circles indicate congeners with one ortho-chlorine; congeners with two ortho-chlorines are indicated by solid squares. The observed relationship of H with number of chlorines and ortho-chlorine substitution has also been reported for the aqueous solubility of PCBs[12] and the vapor pressures of PCBs.[23]

The data set presented here confirms earlier observations that the number of chlorines and the number of ortho-chlorines influences Henry's law constants for polychlorinated biphenyls. The measurement method provides reliable Henry's law constants. Henry's law constants were measured for 2,3,5,6-

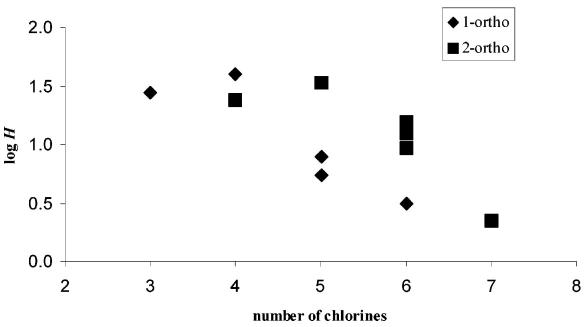

Figure 2. Influence of number of chlorines and number of ortho-chlorines on Henry's law constants (H) for 11 polychlorinated biphenyls; each marker indicates the average H for one PCB congener.

tetrachlorobiphenyl (PCB-65), 2,3,4,5,6-pentachlorobiphenyl (PCB-116), 2,2′,3,4,4′,5-hexachlorobiphenyl (PCB-137), and 2,3,3,4,4′,5-hexachlorobiphenyl (PCB-156), four PCBs for which no measured values exist at this moment. Data presented for the higher chlorinated biphenyls are lower than those reported by various research groups. This is in agreement with the recent discussion by Goss et al.[9] that for higher chlorinated biphenyls much lower values for H than reported in the literature so far are more consistent with other partitioning data.

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