A Critical Review of Aqueous Solubilities, Vapor Pressures, Henry's Law Constants, and Octanol–Water Partition Coefficients of the Polychlorinated Biphenyls

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Relationships between the environmentally relevant physical chemical properties of the polychlorinated biphenyls, namely, aqueous solubility, vapor pressure, Henry's law constant, and octanol–water partition coefficient are discussed. Reported experimental data are tabulated and critically reviewed. Recommended values are given for 42 of the 209 congeners; however, procedures are suggested for estimating the properties of the other congeners. Properties of mixtures are not treated.

Key words: critically reviewed data; Henry's law constant; octanol–water partition coefficient; polychlorinated biphenyl (PCB); PCB, solubility; vapor pressure.

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1. Introduction

The polychlorinated biphenyls (PCB's) are a group of xenobiotic chemicals first manufactured commercially about 1930 and which were widely used as transformer coolants, dielectric fluids, solvents, and flame retardants until restrictions on their use were introduced in the early 1970s.[1] Of the approximately 570 000 000 kg sold in the U.S. as of 1975, some 68 000 000 kg were estimated to be mobile in the environment and some 130 000 000 kg were in landfills or equipment dumps. There are 209 possible chlorinated biphenyls ranging from the three monochlorobiphenyls to decachlorobiphenyl. It is only recently[2] that all 209 congeners have been individually synthesized and characterized.

The characteristic properties of the PCB's are hydrophobicity or lipophilicity (i.e., large octanol–water partition coefficient and low aqueous solubility), relatively low vapor pressure, and extreme resistance to chemical reaction.[3] These properties result in persistence in the environment, a tendency to accumulate in biota and in sediments, and the ability to be transported through the atmosphere to regions remote from source discharges.[4] For example, appreciable concentrations are found in the soils, sediments, waters, biota, atmosphere, and precipitation in the Great Lakes Basin.[5–9] The biological and human health effects of PCB's have been reviewed recently.[8]

The industrial chemical products are mixtures of numerous congeners separated by distillation into defined boiling ranges. For example, the Aroclors manufactured by Monsanto were marketed in seven grades designated by a four digit number, the first two (usually 12, but in one case

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TABLE 1. Approximate percent compositon of some commercial PCB products (Ref. 1)

	Aroclor type or grade							Kanechlors			Penclors
Chlorobiphenyl	1016	1221	1232	1242	1248	1254	1260	KC-300	KC-400	KC-500	DK
$C_{12}H_{10}$	0.1	11	6	0.1	-	0.1	-	-	-	-	-
$C_{12}H_9Cl$	1	51	26	1	-	0.1	-	-	-	-	-
$C_{12}H_8Cl_2$	20	32	29	16	2	0.5	-	17	3	-	-
$C_{12}H_7Cl_3$	57	4	24	49	18	1	-	60	33	5	-
$C_{12}H_6Cl_4$	21	2	15	25	40	21	-	23	44	27	-
$C_{12}H_5Cl_5$	1	0.5	0.5	8	36	48	12	0.6	16	55	-
$C_{12}H_4Cl_6$	0.1	-	-	1	4	23	38	-	5	13	-
$C_{12}H_3Cl_7$	-	-	-	0.1	-	6	41	-	-	-	-
$C_{12}H_2Cl_8$	-	-	-	-	-	-	8	-	-	-	-
$C_{12}HCl_9$	-	-	-	-	-	-	1	-	-	-	-
$C_{12}Cl_{10}$	-	-	-	-	-	-	-	-	-	-	100

10) designating the carbon number and the last two (e.g., 42) designating the mass percentage of chlorine.

Table 1 (Ref. 1) gives the approximate percentage composition of the Aroclors. At least nine other trade designations have been used in various countries by various manufacturers.

The presence of such a large number of congeners renders chemical analysis and reporting very difficult. A common practice has been to report environmental concentration in terms of an Aroclor grade equivalent, but this practice is imprecise because the environmental distribution of congeners differs from the commercial grade distribution. It is likely that there is differential transport, reaction, and accumulation between congeners. Further, to elucidate the environmental transport and transformations of a mixture requires that the mixture be assigned properties such as a unique solubility or vapor pressure. Such an assignment is fundamentally erroneous because a mixture does not have unique phase equilibrium physical chemical properties. The reported measured solubilities or vapor pressures can only be regarded as some average of the properties of the individual PCB congeners.

It has become increasingly accepted that the only rigorous method of addressing the problem of calculating the environmental fate of the PCB's is to obtain properties for all the congeners and treat each congener separately. Unfortunately, relatively few congeners have been synthesized in sufficient quantities that property determinations have been possible. Further, these determinations are experimentally demanding and many erroneous data exist. There is, however, a tendency for the congeners to have properties which vary systematically with chlorine number, thus the properties of one congener can be estimated from those of another. This estimation requires that all available property data be gathered, critically reviewed, and "best" values assigned. The assigned values of solubility (c), octanol–water partition coefficient (K_{ow}), vapor pressure (p), and Henry's law constants (H) should be internally consistent. For example, H, is equal to p/c, and c and K_{ow} are related inversely. Typically, substitution of one chlorine atom for a hydrogen causes p and c to fall by a factor of 3 to 4, K_{ow} to rise by a similar factor, while H remains relatively constant. This enables estimates to be made of properties of one chlorine number group from another. The congener properties depend not only on chlorine number, but on the configuration. It is thus desirable to develop "rules" for estimating properties as a function of chlorine arrangement as well as chlorine number. This is presently impossible, but some progress has been

made recently in identifying characteristic groupings which cause, for example, unusually large K_{OW} values.[6]

In this study we gather and critically review the available data for PCB congeners and assign selected values where possible. Sufficient data exist for assessing only 42 of the 209 congeners; however, it is hoped that in the future rules or correlation procedures can be developed for estimating the properties of all 209 congeners, at least with sufficient accuracy for the purpose of environmental modeling.

2. Physical Chemical Property Relationships

The various physical chemical properties of PCB's can be related by a series of thermodynamic equations in terms of basic molecular properties. These relationships have been discussed in detail previously[5,10] and will only be summarized here. To describe the behavior of PCB congeners in the environment requires equilibrium partitioning, reaction rate, and transport phenomena information. Here we only consider equilibrium data.

Because PCB's are sparingly soluble in water it can be assumed that the air–water partition coefficient or Henry's law constant H, defined as p/c is independent of concentration for a congener. Here p is the PCB partial pressure in equilibrium with an aqueous solution of concentration c. Applying this relation to a saturated solution of a solid PCB at a defined temperature T gives H equal to p_S/c_S, where p_S is the vapor pressure of the pure solid PCB and c_S is its solubility. Applied to a liquid PCB, H equals p_L/c_L, where p_L is the partial pressure of the water-saturated PCB liquid. Since the solubility of water in liquid PCB is expected to be small, p_L can be assumed to equal the vapor pressure p_L; thus

$$H = p_S/c_S = p_L/c_L. \tag{2.1}$$

Prausuitz[12] applied the Clausius–Clapeyron relation to the solid and liquid forms of a pure substance at a temperature T that is below the melting point T_M to obtain

$$p_L/p_S = \exp[\Delta S_{fus}(T_M/T - 1)/R], \tag{2.2}$$

where ΔS_{fus} is the entropy of fusion. It follows that

$$c_L/c_S = \exp[\Delta S_{fus}(T_M/T - 1)/R]. \tag{2.3}$$

The group p_S/p_L or c_S/c_L is termed the fugacity ratio. The entropy of fusion can be calculated from the experimentally measured enthalpy of fusion as discussed by Miller *et al.*,[13] or estimated from Walden's rule as reviewed by Yalkowsky[14] as 56.5 J/mol K, thus $\Delta S_{fus}/R$ is 6.79. The dimensionless air–water partition coefficient H' is given as[15]

$$H' = H/RT. \tag{2.4}$$

The other important partition property is the octanol–water partition coefficient K_{OW}:

$$K_{OW} = c_{OW}/c_{WO}, \tag{2.5}$$

where c_{OW} is the concentration of the solute in octanol saturated with water and c_{WO} is the concentration of the solute in water saturated with octanol, these concentrations being in equilibrium.

There has been considerable interest in the relationship between the aqueous solubility and octanol–water partition coefficient.[13,16–19] Mackay *et al.*[16] and Banerjee *et al.*[17] have suggested that the product Q of K_{OW} and the subcooled liquid solubility c_L is relatively constant. More recently, based on the measurement of c_L and K_{OW} of a wide range of PCB congeners by Miller *et al.*,[13] it has been observed that the product Q varies as a function of molar volume v (cm^3/mol) approximately as follows[20]:

$$\log Q = 3.89 - 0.0048v. \tag{2.6}$$

Since K_{OW} is the ratio c_{OW}/c_{WO} [Eq. (2.16)] and c_{WO} is approximately equal to the subcooled liquid solubility in water c_L, then Q is approximately equal to c_{OW} or the saturation subcooled liquid solubility of PCB in octanol. Since both PCB and octanol are organic in nature it is likely that this solubility is fairly constant. In reality it should be termed a "pseudosolubility" because the two substances may be miscible.

We use these thermodynamic relationships as constraints or guides when interpreting the reported experimental data, and when selecting recommended values.

3. Physical Chemical Properties

The literature data are reported here in a series of tables as follows.

Table 2 lists the congeners by their chemical name and isomer number following the Ballschmiter and Zell[21] system. In subsequent tables, only the number is given. Biphenyl is assigned number zero. This facilitates comparisons with other tabulations such as that of Mullin *et al.*[22] Also given in Table 2 are chlorine number, molecular mass, melting point,[3] normal boiling point,[23] entropy of fusion,[13] fugacity ratio calculated from Eq. (2.2), and the molecular descriptors of molar volume at the normal boiling point calculated by the LaBas method,[24] and total molecular surface areas reported by Mackay *et al.*[25]

The reported entropies of fusion ΔS_{fus} range from 41.0 to 69.5 J/mol K, with an average of 56.J/mol K and show no systematic variation with chlorine number. It is suspected that some of the reported ΔS_{fus} values may be in error, thus to avoid possibly biasing the data for which values are reported, and in the interest of simplicity, a single value of 56.5 J/mol K (as suggested by Walden's rule) was used to calculate the fugacity value of all congeners. Few congener boiling points are reported, but for illustrative purposes some calculated values are given in Table 2 using the method of Mackay *et al.*[26] These values should be regarded as merely estimates, but they are consistent with the reported Aroclor mixture distillation ranges.

Table 3 gives reported experimental aqueous solubilities for the congeners and calculated subcooled liquid solubilities using the fugacity ratios. In Table 2 solubilities are normally reported in units of mg/L or the equivalent g/m^3, but for comparison between congeners, use of the amount-of-substance solubility c expressed in mol/m^3, is preferable. The solid solubility is a function of molecular size and melting point, but the subcooled liquid solubility is a function only of molecular size; thus the appropriate solubility for comparison is that of the subcooled liquid c_L. In each case a

TABLE 2. Physical properties of some PCB congeners at 25 °C

Congener No.	IUPAC No. n[a]	Cl No. N	MW	MP,K[b]	BP,K lit[c]	BP,K calc'd[d]	Molar vol. V_m[e] cm³/mol	Total surface[f] area, Å²	Fugacity ratio[f] F	Entropy of fusion[g] ΔS_{fus},J/mol K
Biphenyl	0	0	154.2	344	529	529	178	195.2	0.35	51.04
2-chloro	1	1	188.7	307	547	558	205.5	208.4	0.814	50.21
3-	2	1	188.7	298	557	558	205.5	210	1.0	-
4-	3	1	188.7	350.9	564	558	205.5	210	0.3	-
2,2'-dichloro	4	2	223.1	334		585	226.4	224.2	0.44	-
2,3'-	6	2	223.1	oil		585	226.4	226	1.0	-
2,4 -	7	2	223.1	297.4		585	226.4	-	1.0	-
2,4'-	8	2	223.1	316		585	226.4	226	0.66	-
2,5-	9	2	223.1	oil		585	226.4	227.6	1.0	-
2,6-	10	2	223.1	307.9		585	226.4	-	0.80	41.0
3,3'-	11	2	223.1	302		585	226.4	-	0.912	-
3,4-	12	2	223.1	323		585	226.4	-	0.566	-
3,5-	14	2	223.1	304		585	226.4	-	0.872	-
4,4'-	15	2	223.1	422	588-62	585	226.4	227.6	0.059	-
2,2',3-trichloro	16	3	257.5	301		610	247.3	-	0.934	-
2,2',4-	17	3	257.5			610	247.3	-	-	-
2,2',5-	18	3	257.5	317		610	247.3	242	0.65	-
2,2',6-	19	3	257.5	-		610	247.3	-	-	-
2,3,3'-	20	3	257.5	-		610	247.3	-	-	-
2,3,4'-	22	3	257.5	346		610	247.3	-	0.335	-
2,3,5-	23	3	257.5	314		610	247.3	-	0.694	-
2,3,6-	24	3	257.5	-		610	247.3	-	-	-
2,4,4'-	28	3	257.5	330		610	247.3	243.6	0.484	-
2,4,5-	29	3	257.5	351		610	247.3	241.6	0.30	65.52
2,4,6-	30	3	257.5	335.5		610	247.3	-	0.427	49.37
2,4',5-	31	3	257.5	340		610	247.3	-	0.384	-
2,4',6-	32	3	257.5	-		610	247.3	-	-	-
2',3,4-	33	3	257.5	333		610	247.3	241.6	0.452	-
3,3',5-	36	3	257.5	-		610	247.3	-	-	-
3,4,4'-	37	3	257.5	360		610	247.3	243.2	0.244	-
2,2',3,3'-tetrachloro	40	4	292.0	394		633	268.2	255.6	0.113	-
2,2',3,4-	41	4	292.0			633	268.2	-	-	-
2,2',3,5'-	44	4	292.0	320		633	268.2	257.6	0.608	-
2,2',4,4'-	47	4	292.0	356		633	268.2	259.6	0.268	-
2,2'4,5-	48	4	292.0	339.1		633	268.2	-	0.393	69.40
2,2',4,5'-	49	4	292.0	337		633	268.2	-	0.411	-
2,2',5,5'-	52	4	292.0	360		633	268.2	259.6	0.243	-
2,2'6,6'-	54	4	292.0			633	268.2	-		
2,3,4,4'-	60	4	292.0	415		633	268.2	-	0.0695	-
2,3,4,5-	61	4	292.0	365		633	268.2	255.2	0.218	69.45
2,3',4,4'-	66	4	292.0	397		633	268.2	259.2	0.105	-
2,3',4',5-	70	4	292.0	377		633	268.2	259.2	0.165	-
2,4,4',5-	74	4	292.0	398		633	268.2	-	0.102	-
3,3',4,4'-	77	4	292.0	453		633	268.2	258.8	0.029	85.35
3,3',5,5'-	80	4	292.0	437		633	268.2	-	0.0421	-

TABLE 2. Physical properties of some PCB congeners at 25 °C — Continued

Congener No.	IUPAC No. n[a]	Cl No. N	MW	MP,K[b]	BP,K lit[c]	BP,K calc'd[d]	Molar vol. V_m[e] cm³/mol	Total surface[f] area, Å²	Fugacity ratio[f] F	Entropy of fusion[g] ΔS_{fus},J/mol K
2,2'3,3',5-pentachloro	83	5	326.4			654	289.1	-	-	-
2,2',3,3',6-	84	5	326.4			654	289.1	-	-	-
2,2',3,4,4'-	85	5	326.4			654	289.1	-	-	-
2,2',3,4,5-	86	5	326.4	373		654	289.1	271.2	0.182	-
2,2',3,4,5'-	87	5	326.4	387		654	289.1	273.6	0.138	-
2,2',3,4,6-	88	5	326.4	373		654	289.1	271.6	-	-
2,2',3,4',6-	91	5	326.4			654	289.1	-	-	-
2,2',3,5,5'-	92	5	326.4			654	289.1	-	-	-
2,2',3,5',6-	95	5	326.4			654	289.1	-	-	-
2,2',3',4,5-	97	5	326.4	354		654	289.1	-	0.279	53.77
2,2',4,5,5'-	101	5	326.4	349.5		654	289.1	269.2	0.318	53.6
2,3,4,5,6-	116	5	326.4	397		654	289.1	269.2	0.105	53.81
2,3',4,4',5-	118	5	326.4	378		654	289.1	-	0.190	-
2,3',4,5,5'-	120	5	326.4	350		654	289.1	275.2	0.306	-
2,2',3,3',4,4'-hexa	128	6	360.9	423		673	310	286.8	0.058	68.62
2,2',3,3',4,5-	129	6	360.9	358		673	310	286.8	0.256	-
2,2',3,3',4,5'-	130	6	360.9			673	310	-	-	-
2,2',3,3',5,6-	134	6	360.9	373		673	310	287.2	0.181	-
2,2',3,3',5,6'-	135	6	360.9			673	310	-	-	-
2,2',3,3',6,6'-	136	6	360.9	387		673	310	-	0.138	54.81
2,2',3,4,4',5-	137	6	360.9	350		673	310	-	0.306	-
2,2',3,4,4',5'-	138	6	360.9	352		673	310			-
2,2',3,4',5',6-	149	6	360.9	oil		673	310	-	1.0	-
2,2',4,4',5,5'-	153	6	360.9	376		673	310	290.8	0.170	-
2,2',4,4',6,6'-	155	6	360.9	387		673	310	291.5	0.131	45.19
2,3,3',4,4',5-	156	6	360.9			673	310	-	-	-
2,3,3',4,4',5'-	157	6	360.9			673	310		-	-
2,3,3',4,4',6-	158	6	360.9			673	310	-	-	-
2,3,3',4',5,6-	163	6	360.9	361.2		673	310	-	0.237	-
2,3,3',5,5',6-	165	6	360.9			673	310	-	-	-
2,2',3,3',4,4',6-hepta	171	7	395.3	395.4		690	330.9	-	0.109	51.05
2,2',3,3',5,6,6'-	179	7	395.3			690	330.9	-	-	-
2,2',3,4,4',5',6-	183	7	395.3			690	330.9	-	-	-
2,2',3,4,5,5',6-	185	7	359.3	422		690	330.9	302.8	0.059	-
2,2',3,4',5,5',6-	187	7	395.3			690	330.9	-	-	-
2,2',3,3',4,4',5,5'-	194	8	429.8	432		705	351.8	317.9	0.047	-
2,2',3,3',5,5',6,6'-	202	8	429.8	435		705	351.8	318.7	0.044	52.74
2,2',3,3',4,4',5,5',6-	206	9	464.2	479		718	372.7	331.9	0.016	84.09
2,2',3,3',4,5,5',6,6'-	208	9	464.2	455.8		718	372.7	-	0.028	49.74
Deca-	209	10	498.7	578.9		729	393.6	345.9	0.0017	49.37

[a]IUPAC or congener number, Ref. 21.
[b]Ref. 3.
[c]Ref. 23.
[d]Calculated values, Ref. 26.
[e]Le Bas method, Ref. 24.
[f]Ref. 25.
[g]Refs. 23 and 69.

TABLE 3. Aqueous solubility of PCB congeners at 25 °C

Congener No.	S, g/m^3	Ref.	Selected values S, g/m^3	c_S, mmol/m^3	c_L, mmol/m^3
0	7.48	27	7.0 ± 0.5	45.39± 3.24	129.7±9.263
	7.08	28			
	5.94	29			
	3.87	30			
	7.45	31			
	7.0	32			
	7.50	33			
	6.71	13			
	7.455	16			
	7.21	19			
	6.80	50			
1	5.90	3,34	5.50 ± 0.5	29.5±2.6	35.7±3.26
	4.13	35			
	5.06	13			
	5.76	16			
	2.73	19			
	7.80	50			
2	1.30	35	2.5±1.2	13.25±6.4	13.2±6.4
	3.50	3,34			
	6.22	16			
	1.84	19			
	1.20	50			
3	1.17	3,34,36	1.2±0.3	6.36±1.59	21.3±5.3
	0.90	35			
	1.87	16			
	1.30	37			
	0.824	19			
	1.41	38			
	1.20	36			
4	1.50	3,34	1.0±0.2	4.48± 0.90	10.14±0.25
	0.79	35			
	1.00	16			
	0.997	19			
7	1.40	34	1.25±0.15	5.60± 0.67	5.51±0.67
	1.13	37			
	2.03	16			
	1.408	19			
8	0.637	39	1.0±0.4	4.48±1.79	6.73±2.73
	1.88	3,34			
	0.62	35			
	1.33	16			
	0.706	19			
9	1.94	13	2.0±0.10	8.96±0.45	9.0±0.5
	0.58	35			
	2.09	16			
	0.587	19			
10	1.39	13	1.40±0.010	6.28±0.045	7.84±0.53
15	0.062	40	0.060±0.02	0.269±0.09	4.56±1.53
	0.056	35			
	0.080	3,34			
	0.046	37			
	0.104	16			
	0.060	19			
	0.065	36			
18	0.248	39	0.40±0.20	1.55±0.78	2.39±1.20
	0.64	35			
	0.407	16			
	0.135	19			
28	0.085	34	0.16±0.1	0.62±0.39	1.28±0.81
	0.260	35			
	0.266	16			
	0.148	19			
29	0.092	35	0.140±0.05	0.54±0.19	1.81±0.63
	0.142	36			
	0.163	13			
	0.119	41			
	0.193	16			
	0.097	19			
30	0.226	13	0.20±0.03	0.78±0.12	1.82±0.27
33	0.078	3,34	0.080±0.02	0.31±0.078	0.69±0.17
	0.291	16			
	0.796	19			
37	0.0152	35	0.015±0.010	0.0582±0.039	0.024±0.17
	0.135	16			
	0.0152	19			
40	0.034	3,34	0.030±0.004	0.103±0.014	0.91±0.13
	0.026	16			
	0.030	19			
44	0.0170	3,34	0.10±0.05	0.342±0.17	0.565±2.83
	0.080	37			
	0.121	16			
	0.172	19			
47	0.068	3,34	0.090±0.030	0.308±0.103	1.15±0.38
	0.115	16			
	0.067	19			

TABLE 3. Aqueous solubility of PCB congeners at 25 °C — Continued

Congener No.	S, g/m^3	Ref.	Selected values S, g/m^3	c_S, mmol/m^3	c_L, mmol/m^3
49	0.0164	13	0.016±0.005	0.055±0.0017	0.133±0.032
	0.00601	42			
52	0.0265	39	0.030±0.020	0.103±0.068	0.42±0.28
	0.046	3,34			
	0.0365	36			
	0.041	16			
	0.0184	19			
61	0.0192	35	0.020±0.020	0.0685±0.068	0.314±0.32
	0.0209	39			
	0.0099	37			
	0.0525	16			
	0.0193	19			
66	0.058	3,34	0.040±0.030	0.137±0.103	1.30±1.0
	0.017	16			
	0.060	19			
70	0.041	3,34	0.041±0.010	0.140±0.034	0.85±0.21
77	0.175	3,34	0.001±0.001	0.00342±.0034	0.117±0.12
	0.00075	35			
	0.0174	16			
	0.0114	19			
	0.000569	69			
	0.00301	71			
86	0.0098	35	0.020±0.010	0.0613±0.031	0.0337±0.19
	0.0349	36			
	0.0133	16			
	0.0099	19			
87	0.0045	35	0.0040±.002	0.0123±0.031	0.093±.043
	0.022	3,34			
	0.0086	16			
	0.0101	19			
88	0.012	35	0.012±0.001	0.0368±0.0031	0.202±0.02
101	0.0103	39	0.010±.010	0.0306±0.0306	0.100±0.10
	0.010	40			
	0.00424	42			
	0.0042	35			
	0.031	3,34			
	0.0194	13			
	0.0163	16			
	0.0130	19			
	0.0154	69			
	0.0115	71			
116	0.0068	35	0.0080±0.0020	0.0145±0.0061	0.233±.057
	0.0207	41			
	0.00548	13			
	0.00904	16			
	0.00682	19			
128	0.00044	35	0.00060±.00040	0.00166±0.0011	0.029±0.021
	0.00099	41			
	0.000285	13			
	0.000132	16			
	0.00044	19			
129	0.00085	35	0.00060±.0004	0.00166±0.0011	0.00651±.00482
	0.000581	16			
	0.000906	19			
134	0.00091	35	0.00040±.00040	0.00111±0.0011	0.0061±0.0061
	0.000399	16			
	0.000906	19			
136	0.00099	41	0.00080±.0002	0.00222±0.00056	0.016±0.0042
	0.000603	13			
	0.00451	69			
	0.00210	71			
153	0.00105	42	0.0010±.00040	0.0028±0.0011	0.0164±.00325
	0.0088	3,34			
	0.0012	35			
	0.00995	39			
	0.00278	16			
	0.00131	19			
155	0.00090	34	0.00070±.0002	0.0019±.00055	0.015±0.0040
	0.00041	13			
	0.0000204	16			
	0.00091	19			
163	0.00531	36	0.0050±0.002	0.0139±0.0055	0.059±0.021
171	0.00624	41	0.0020±0.0010	0.00506±.0025	0.046±0.025
	0.00217	13			
185	0.00047	35	0.00046±.00020	0.00114±.00051	0.019±0.008
	0.000402	16			
	0.000475	19			
194	0.0072	3,34	0.00020±.00010	0.00047±.00023	0.001±0.0005
	0.000272	35			
	0.000101	16			
	0.00150	19			
202	0.00018	35	0.00030±.00010	0.00070±.00023	0.016±0.005
	0.000393	13			
	0.000088	16			
	0.000179	19			
	0.000147	69			
	0.00017	71			
206	0.000112	35	0.00011±.000030	0.00024±.000065	0.0146±.0030
	0.000012	16			
	0.00011	19			
	0.0000255	69			
	0.0000315	71			
208	*0.000018*	13	*0.000018±.0000010*	*0.000038±.000022*	*0.0014±0.00070*
209	0.000016	35	0.0000012	0.0000024	0.0014±0.00060
	0.00000743	13	± 0.0000005	± 0.000001	
	0.0000004	16			
	0.00049	19			
	0.0000065	69			
	0.0000041	71			
	0.015	3,34			

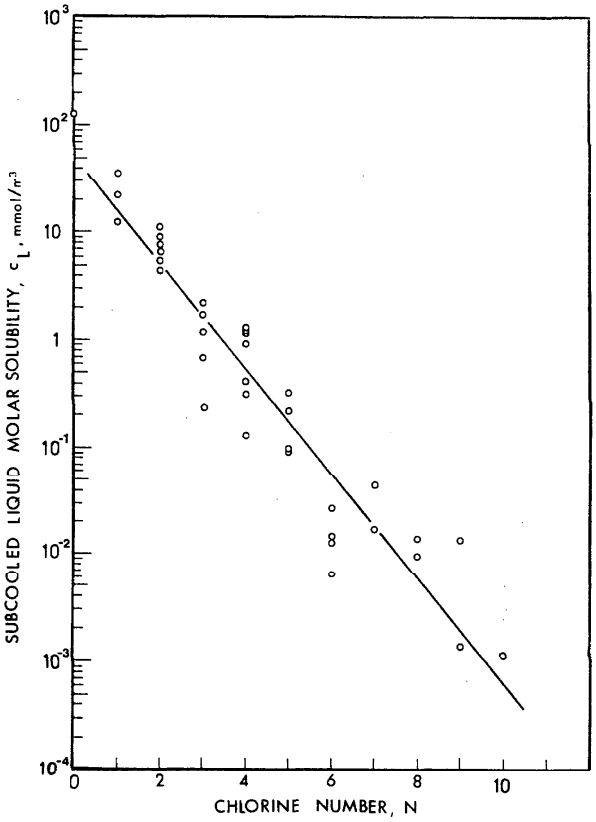

FIG. 1. Plot of log c_L vs chlorine number.

single value was selected by taking into account the accuracy of the method. In some cases information from other tables and other structurally similar congeners influenced the choice of the selected value of its error range. Figure 1 is a plot of log c_L versus chlorine number.

Table 4 gives reported experimental values for octanol–water partition coefficient and selected values with estimated error range. The method of experimental determination is also indicated. The product Q of K_{OW} and c_L is also given. As discussed earlier Q can be regarded as a pseudosolubility in octanol. It is expected that Q should vary systematically with chlorine number; thus when an outlying value was obtained from the selected c_L and K_{OW}, both were re-examined, and in some cases an adjustment to either or both was made, or the error limits were increased. The trend in log K_{OW} with chlorine number is illustrated in Fig. 2.

Table 5 gives vapor pressure and Henry's law constant data in similar format to Tables 3 and 4. The selected values of c_L, and p_L and H reported in Tables 3 and 5 are in each case consistent, i.e., H is equated to p_L/c_L or to p_S/c_S. Forcing this consistency influenced the choice of the values of solubility, vapor pressure, and H. Figure 3 is a plot of log p_L versus chlorine number.

Complete c_S, c_L, K_{OW}, p_S, p_L, and H data are reported for 26 congeners, including biphenyl; and c_S, c_L, and K_{OW} data are reported for another 16 congeners in Table 6.

The data displays two striking features. First, the Henry's law constants principally lie in the range of 20 to 100 Pa m^3/mol and show no systematic trend with chlorine number. The experimental determinations, largely of Murphy *et al.*[64] and Giam *et al.*[65] support this conclusion, as do

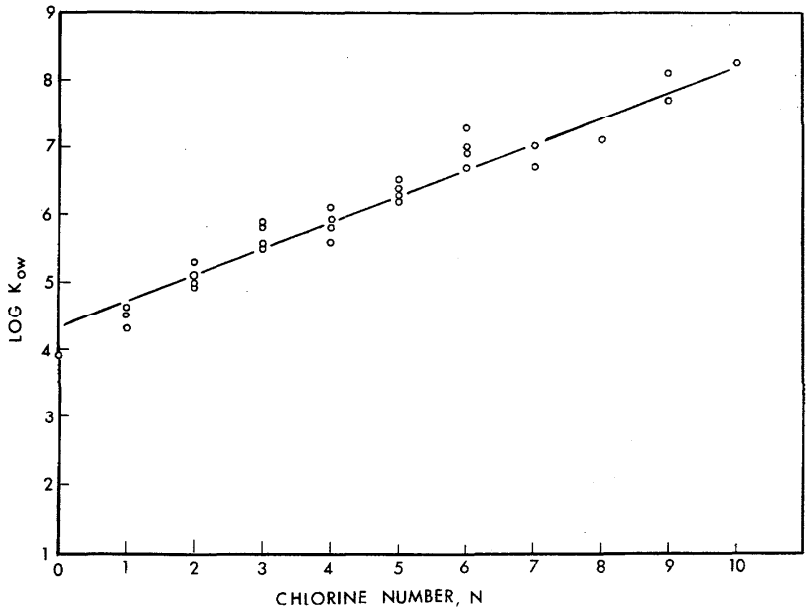

FIG. 2. Plot of log K_{OW} vs chlorine number.

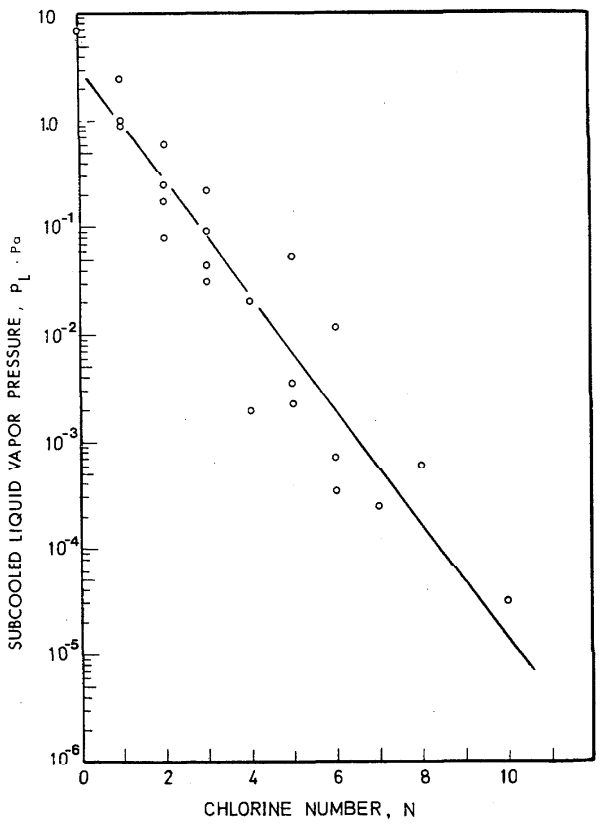

FIG. 3. Plot of log p_L vs chlorine number.

the reported vapor pressures of Bidleman[59] and Westcott *et al.*[66,67] when combined with the solubilities. The average H value is 48 Pa m^3/mol. Second, the Q values tend to fall with increase in chlorine number from approximately 1000 mol/m^3 for biphenyl to approximately 150 mol/m^3 for decachlorobiphenyl. This is illustrated in Fig. 4.

Some congeners shown in Table 6 have outlying H values, notably Nos. 18, 77, 86, 155, and 171. It is not known if this is a real effect or if there is error in the measurements. It is suggested that these values be used with caution.

Simple approximate correlations for mean isomer values of c_L, p_L, and K_{OW} as a function of chlorine number can thus be proposed, but it must be emphasized that there is evidence for variation in all three quantities as a function of chlorine configuration for a given set of isomers. This variation is rarely more than a factor of 3 from the mean isomer value. It is thus possible for a trichlorobiphenyl to have a lower solubility c_L than a tetrachlorobiphenyl, but such cases are exceptional. The correlations with chlorine number N, which are also shown as lines in Figs. 1–4, were determined by linear regression and are

$$\log c_L = -1.40 - 0.47N (c_L \text{ in mol/m}^3), \quad (3.1)$$

$$\log p_L = +0.28 - 0.55N (p_L \text{ in Pa}), \quad (3.2)$$

$$\log K_{OW} = 4.33 + 0.40N, \quad (3.3)$$

$$\log Q = 2.90 - 0.07N = \log c_L + \log K_{OW}, \quad (3.4)$$

$$\log H = 1.68 - 0.08N = \log p_L - \log c_L. \quad (3.5)$$

Equation (3.4) was obtained by adding Eqs. (3.1) and (3.3) and not by regression of the Q data. It should be noted that the tables and figures express c in mmol/m^3 while c_L in Eq. (3.1) has units of mol/m^3.

These correlations should be used only to give approximate values of the PCB properties. They could also be used to estimate the properties of PCB mixtures if ideality (Raoult's law) is assumed to apply.

The use of chlorine number as a molecular descriptor is the simplest available correlating technique. It is likely that molecular volume and surface area are better descriptors and that it may be possible to correlate the different solubilities and octanol–water partition coefficients of isomers by these descriptors. At this stage the data available are insufficient to permit such more detailed analyses.

Recently Burkhard *et al.*[70,71] have calculated the vapor pressure, aqueous solubility, and Henry's law constants for all 209 congeners from some experimental data for PCB's.[13,64–67] Since these were computer generated results rather than experimentally determined values, they were not included in this discussion; however, that compilation is an additional valuable source of estimated PCB properties.

Finally, it should be noted that there are few data for the higher chlorine number congeners, there are considerable discrepancies between reported values, and accurate measurements require exceptional care. It is conceivable that a consistent bias exists in the available measurements. The selected values presented here should be used with appropriate caution.

TABLE 4. Octanol-water partition coefficients (log K_{ow}) for PCB congeners

Congener No.	log K_{ow}	Method	Ref.	Selected value	Q
0	4.09	SF	43,44	3.90 ± 0.20	1030
	4.10	TLC	45		
	4.04	HPLC	17		
	3.89	Gen.col.	46		
	3.76	Gen col.	13		
	3.70	HPLC	46		
	3.79	HPLC	47		
	3.75	HPLC	48		
	3.79	calc.	19		
	4.03	calc.	49		
	4.14	calc.	16		
1	4.54	SF	51	4.30 ± 0.50	712
	4.51	SF	53		
	4.59	SF	45		
	4.56	TLC	45		
	4.38	Gen.col.	46		
	4.50	Gen.col.	13		
	3.75	HPLC	46		
	3.90	HPLC	47		
	4.60	calc.	47		
	4.56	calc.	19		
	4.80	calc.	46		
	4.72	calc.	50		
2	4.95	SF	51	4.60 ± 0.30	527
	4.71	SF	45		
	4.72	TLC	45		
	4.58	Gen.col.	46		
	4.35	HPLC	48		
	4.42	HPLC	47		
	4.56	calc.	19		
	4.80	calc.	46		
3	4.61	SF	45	4.50 ± 0.30	669
	4.69	TLC	46		
	4.49	Gen.col.	46		
	4.34	HPLC	46		
	4.40	HPLC	47		
	4.56	calc.	19		
	4.80	calc.	46		
	4.40	calc.	47		
	4.34	calc.	50		
4	5.00	SF	45	4.9 ± 0.50	805.5
	5.02	TLC	45		
	4.90	Gen.col.	46		
	3.55	HPLC	46		
	3.63	HPLC	47		
	4.89	calc.	47		
	4.0	HPLC	52		
	5.32	calc.	19		
	5.51	calc.	46		
	4.96	calc.	50		
6	4.39	HPLC	47	4.8 ± 0.30	-
	5.02	HPLC	47		
7	5.15	TLC	45	5.0 ± 0.30	551
	4.67	HPLC	47		
	5.30	calc.	47		
	5.23	calc.	19		
8	5.10	SF	53	5.10 ± 0.40	847.3
	5.14	Gen.col.	46		
	4.47	HPLC	47		
	5.10	calc.	47		
	5.32	calc.	19		
	5.51	calc.	46		
	5.20	calc.	50		
9	5.18	TLC	45	5.10 ± 0.20	1127
	5.16	Gen.col.	13		
	4.67	HPLC	47		
	5.30	calc.	47		
10	4.93	Gen.col.	13	5.00 ± 0.20	783.5
	4.05	HPLC	47		
	5.31	calc	47		
11	5.30	SF	45	5.30 ± 0.10	-
	5.34	TLC	45		
12	5.29	Gen.col.	46	5.30 ± 0.20	-
	5.10	HPLC	46		
	5.51	calc.	46		
14	5.37	SF	45	5.40 ± 0.20	-
15	5.58	SF	40	5.30 ± 0.20	901
	5.36	SF	45		
	5.28	TLC	45		
	5.33	Gen.col.	46		
	4.92	HPLC	46		
	4.82	HPLC	47		
	5.32	calc.	19		
	5.51	calc.	46		
	5.57	calc.	47		
	4.77	calc.	50		
16	4.15	HPLC	47	5.60 ± 0.40	-
	5.31	calc.	47		
17	4.60	HPLC	47	5.60 ± 0.10	-
	5.76	calc.	47		
18	5.64	TLC	45	5.60 ± 0.10	949.8
	5.60	Gen.col.	46		
	4.34	HPLC	46		
	4.39	HPLC	47		
	5.55	calc.	47		
	6.00	calc.	19		
	6.22	SF	44		
	5.63	calc.	50		
19	4.52	Gen.col.	46	5.60 ± 0.60	-
	5.67	calc.	46		
	3.73	HPLC	47		
	5.48	calc	47		
20	4.99	HPLC	47	5.60 ± 0.50	-
	5.57	calc.	47		
21	6.00	calc.	19		

TABLE 4. Octanol-water partition coefficients (log K_{ow}) for PCB congeners — Continued

Congener No.	log K_{ow}	Method	Ref.	Selected value	Q
22	4.84	HPLC	47	5.60 ± 0.50	-
	5.42	calc.	47		
24	4.52	HPLC	47	5.50 ± 0.50	-
	5.67	calc.	47		
26	5.18	HPLC	47	5.50 ± 0.50	-
	5.76	calc.	47		
28	5.74	TLC	45	5.80 ± 0.20	809.6
	6.00	calc.	19		
	5.62	SF	52		
	5.11	HPLC	47		
	5.69	calc.	47		
29	5.77	TLC	45	5.60 ± 0.30	721
	5.81	Gen.col.	46		
	5.51	Gen.col.	13		
	5.86	HPLC	46		
	5.67	HPLC	47		
	6.25	calc.	47		
	5.99	calc.	19		
	6.22	calc.	46		
30	5.47	Gen.col.	13	5.50 ± 0.20	575
31	5.77	TLC	45	5.70 ± 0.20	-
	5.79	Gen.col.	46		
	5.30	HPLC	46		
	5.11	HPLC	47		
	5.69	calc.	47		
	6.22	calc.	46		
32	4.60	HPLC	47	5.80 ± 0.30	433.3
	5.75	calc.	47		
33	6.00	calc.	19	5.80 ± 0.30	
	6.10	calc.	50		
36	4.15	HPLC	47	5.70 ± 0.50	
	4.15	calc.	47		
37	5.90	TLC	45	5.90 ± 0.20	189.2
	4.54	HPLC	47		
	6.00	calc.	19		
	5.56	calc.	47		
40	4.54	HPLC	47	5.60 ± 0.30	363
	5.56	calc.	47		
	6.67	calc.	19		
41	5.09	HPLC	48	6.00 ± 0.30	
	6.11	calc.	47		
44	4.79	HPLC	47	6.00 ± 0.30	565
	5.81	HPLC	47		
	6.67	calc.	19		
47	5.27	HPLC	47	5.90 ± 0.30	914
	6.29	calc.	47		
	6.67	calc.	19		
	5.68	HPLC	52		
	6.44	calc.	50		
49	5.20	HPLC	47	6.10 ± 0.20	167
	6.22	calc.	47		
52	6.26	TLC	45	6.10 ± 0.20	529
	5.07	HPLC	47		
	6.09	calc.	47		
	6.67	calc.	19		
	6.12	calc.	50		
54	5.94	TLC	45	5.90 ± 0.20	-
60	5.33	HPLC	47	5.90 ± 0.30	-
	5.84	calc.	47		
61	6.39	TLC	45	5.90 ± 0.30	250
	5.72	Gen.col.	13		
	6.74	calc.	19		
66	5.80	HPLC	47	5.80 ± 0.30	821
	6.31	calc.	47		
	6.67	calc.	19		
70	6.39	TLC	45	5.90 ± 0.30	-
	5.72	HPLC	47		
	6.23	calc.	47		
	5.95	HPLC	51		
	6.67	calc.	19		
74	6.16	HPLC	47	6.10 ± 0.30	-
	6.67	calc.	19,47		
77	6.52	TLC	45	6.10 ± 0.40	368
	6.67	calc.	19		
	5.62	HPLC	47		
	5.62	calc.	47		
80	6.58	TLC	45	6.10 ± 0.40	-
84	4.73	HPLC	47	6.10 ± 0.40	-
	6.04	calc.	47		
85	5.69	HPLC	47	6.20 ± 0.40	-
	6.61	calc.	47		
86	6.38	calc.	46	6.20 ± 0.40	534
	7.49	calc.	19		

TABLE 4. Octanol-water partition coefficients (log K_{ow}) for PCB congeners — Continued

Congener No.	log K_{ow}	Method	Ref.	Selected value	Q
87	6.85	TLC	45	6.50 ± 0.40	293
	5.45	HPLC	47		
	6.37	calc.	47		
	7.43	calc.	19		
88	7.51	calc.	19	6.50 ± 0.40	629
91	4.94	HPLC	47	6.30 ± 0.50	-
	6.31	calc.	47		
92	6.05	HPLC	47	6.50 ± 0.50	-
	6.97	calc.	47		
95	5.18	HPLC	47	6.40 ± 0.50	-
	6.55	calc.	47		
97	5.75	HPLC	47	6.60 ± 0.50	-
	6.67	calc.	47		
99	6.29	HPLC	47	6.60 ± 0.60	-
	7.21	calc.	47		
101	6.11	SF	40	6.40 ± 0.50	47.8
	6.85	TLC	45		
	6.50	Gen.col.	46		
	5.92	Gen.col.	13		
	7.64	HPLC	46		
	6.15	HPLC	47		
	6.44	HPLC	48		
	6.42	HPLC	54		
	7.07	calc.	47		
	7.43	calc.	19		
	7.24	calc.	47		
116	6.85	TLC	45	6.30 ± 0.30	464.5
	6.30	Gen.col.	13		
	7.49	calc.	19		
118	6.66	HPLC	47	6.40 ± 0.30	-
	7.12	calc.	47		
120	5.22	HPLC	47	6.30 ± 0.30	
	5.68	calc.	47		-
128	7.44	TLC	45	7.00 ± 0.30	286
	6.98	Gen.col.	13		
	6.14	HPLC	47		
	6.96	HPLC	47		
	8.18	calc.	19		
	7.75	calc.	47		
129	6.50	HPLC	47	7.30 ± 0.50	130
	7.32	calc.	47		
	8.26	calc.	19		
130	6.57	HPLC	47	7.30 ± 0.50	
	7.39	calc.	47		
134	8.18	calc.	19	7.30 ± 0.50	122
135	5.94	HPLC	47	7.30 ± 0.60	-
	7.15	calc.	47		
136	6.81	Gen.col.	46	6.70 ± 0.20	80.7
	6.63	Gen.col.	13		
	4.91	HPLC	47		
	6.51	calc.	47		
137	6.89	HPLC	47	7.0 ± 0.60	-
	7.71	calc.	47		
138	6.62	HPLC	47	7.00 ± 0.50	-
	7.44	calc.	47		
149	6.14	HPLC	47	6.80 ± 0.50	-
	7.28	calc.	47		
153	6.72	SF	40	6.90 ± 0.20	130
	7.44	TLC	45		
	6.90	Gen.col.	46		
	6.93	HPLC	47		
	7.75	calc.	47		
	8.18	calc.	19		
	8.35	calc.	46		
	8.06	calc.			
155	7.12	TLC	45	7.00 ± 0.40	147
	8.18	calc.	19		
165	6.57	HPLC	47	7.00 ± 0.50	-
	7.37	calc.	47		
171	6.68	Gen.col.	13	6.70 ± 0.40	232.2
179	6.77	HPLC	47	7.00 ± 0.60	-
	8.13	calc.	47		
185	7.93	TLC	45	7.00 ± 0.50	191
	8.94	calc.	19		
194	8.68	TLC	45	7.10 ± 0.50	124
	9.69	calc.	19		
202	8.42	TLC	45	7.10 ± 0.20	198
	7.14	Gen.col.	46		
	7.11	Gen.col.	13		
	9.69	calc.	19		
	9.77	calc.	46		
206	9.14	TLC	45	7.20 ± 1.0	231
	10.44	calc.	19		
208	8.16	Gen.col.	13	8.16 ± 0.10	203
209	9.60	TLC	45	8.26 ± 0.20	262
	8.26	Gen.col.	13		
	8.20	Gen.col.	46		
	11.20	calc.	19		
	11.19	calc.	46		

SF shake flask.
TLC thin layer chromatography.
Gen. col. generator column.
HPLC high pressure liquid chromatography.
calc. calculated value.

TABLE 5. Vapor pressure and Henry's law constants for PCB congeners at 25 °C

Congener No. n	Vapor pressure, Pa p_S	p_L	Ref.	Henry's law constants H, Pa m³/mol	Ref.	Selected values p_S	p_L	$H = p_L/c_L$
0	1.40	3.71*	55	41.34	61	2.43 ±0.1	6.9±0.7	53.5±6.0
	0.58	1.66*	56	30.40	11			
	1.33	3.80*	57	66.27	62			
		7.55	58					
		3.92	23					
	1.27	3.63*	50					
		7.05	59					
		6.22	59					
	1.15	3.29*	60					
	1.01		70					
	1.80		70					
1	1.12	1.38*	50,57	74.58	62	2.04±0.6	2.5±0.6	70±20
		1.84	23					
		1.89	59					
		2.56	59					
	1.53		72					
2		0.98	59	62.11	62		1.0±0.05	76±30
		1.01	59					
	0.723		23					
3	0.60	2.00*	50,57	58.06	62	0.27±.09	0.90±.30	43±15
		1.41	23					
	0.172	0.57*	61					
		0.92	59					
		0.94	59					
	0.175		60					
4	0.36	0.82*	57	22.29	64	0.26±.13	0.60±0.3	59±20
	0.133	0.30*	63					
	0.279		70					
6				21.28	64			40±20
7		0.184	59				0.25±0.7	45±15
		0.321	59					
8	0.279		70	96.66	64			90±20
9		0.184	19				0.18±.18	20±20
	0.0775		73					
11	0.0267	0.029*	66				0.09±.03	
		0.086	59					
		0.095	59					
	0.0258		70					

TABLE 5. Vapor pressure and Henry's law constants for PCB congeners at 25 °C — Continued

Congener No. n	Vapor pressure, Pa p_S	p_L	Ref.	Henry's law constants H, Pa m^3/mol	Ref.	Selected values p_S	p_L	$H = p_L/c_L$
15	0.00253	0.043*	63				0.08±.03	17±6.0
		0.071	59					
		0.084	59					
	0.0090		70					
16				81.77	65			80±30
18	0.267	0.4120*	57	101.50	65	0.14±.07	0.22±0.11	92±40
	0.012	0.0185*	50	20.06				
	0.0897		70					
20				81.77	65			82±40
29		0.044	59			0.13±.03	0.044±.01	24±15
30		0.0306	23			0.038±.25	0.09±0.06	50±25
		0.0950	59					
		0.1440	59					
	0.0124		73					
31		0.034	59	94.13	65	0.015±.004	0.04±0.01	55±40
		0.047	59	20.26	64			
33	0.0133	0.030*	66	39.52		0.014±.004	0.03±0.01	44±20
			67	15.20	64			
	0.0046		73					
37				84.21	65			84±40
40		0.0098	59				0.02±.02	22±22
44				79.24	65			50±30
				24.32	64			
47	0.0115		50				0.02±.01	17±10
	0.0101		70					
49	0.00113		70	20.27	64			20±20
50				76.80	65			77±40
52	0.104	0.4280*	57	14.1-53.7	67	0.005±.002	0.002±.001	48±24
	0.00493	0.0203*	50	22.29	64			
	0.0071	0.0292*	66					
	0.00253	0.0104*	67					
		0.0159	59					
		0.0229	59					
	0.00427		70					

TABLE 5. Vapor pressure and Henry's law constants for PCB congeners at 25 °C — Continued

Congener No. n	Vapor pressure, Pa p_S	p_L	Ref.	Henry's law constants H,Pa m^3/mol	Ref.	Selected values p_S	p_L	$H = p_L/c_L$
53		0.0273	59	30.40	64			30±15
66				84.20	64			84±42
70		0.0054	59	20.26	64		0.006±0.001	20±15
		0.0064	59					
	0.00769		70					
77		0.0022	59				0.002±.0002	1.7±1.7
		0.0020	59					
82				20.27	64			20±15
86	0.0093	0.051*	57				0.051±.025	151±76
87		0.0023	59	33.44	64		0.0023±.005	25±10
	0.00141		70					
99		0.0029	59					
101	0.0012	0.0039*	66			0.0011±.0002	0.0035±.0005	35±10
	0.00096	0.0031*	67	11.46-35.46	66			
		0.0034	59					
		0.0040	59					
105		0.00087	59				0.00090±	
		0.00094	59				.00005	
118		0.0012	59	40.53	64			
128		0.00034	59	50.66	64		0.00034±	12±6
	5.08E-5		70				0.0001	
134	0.000146		70	57.76	64			
138		0.000506	59	48.64	64		0.0005±	82±40
		0.000565	59				.0002	
141				40.53	64		0.0005±	40±20
							.002	
144				60.80	64		-	60±30
147		0.0012	59					
		0.00183	59					

TABLE 5. Vapor pressure and Henry's law constants for PCB congeners at 25 °C — Continued

Congener No. n	Vapor pressure, Pa p_S	p_L	Ref.	Henry's law constants H,Pa m^3/mol	Ref.	Selected values p_S	p_L	$H = p_L/c_L$
149		0.00112	59	30.40	64		0.0015±	30±15
		0.0018	59				.0005	
151				30.40	64			30±15
153		0.00068	59	35.46	64		0.0007±	43±20
		0.00072	59				.00002	
	0.000457		70					
155	0.0016	0.0122*	66			0.0016±.0001	0.012±.001	818±40
	0.00173		67					
156		0.000215	59	88.15	64			88±40
157				58.77	64			60±20
158				64.85	64			65±20
170		0.000084	59					
171		0.00019	59				0.00025±	5.4±2.0
		0.00030	59				.00005	
180		0.00013	59					
		0.000129	59					
183				63.84	64			
187		3.05E-4	59					
202	2.83E-5	6.43E-4*	60				0.0006±	37±20
							0.0003	
209	5.17E-8	3.04E-5*	60				0.00003±	21±10
		1.39E-6	59				0.000015	
		1.40E-5	68					

* calculated p_L from p_S using fugacity ratio F in Table 2.

TABLE 6. Summary of selected values of PCB congeners

Congener No.	Cl No.	MW	MP,K	F	S, g/m^3	c_S mmol/m^3	c_L mmol/m^3	log K_{OW}	Q	p_{S_s}, Pa	p_{L_s}, Pa	H Pa m^3/mol
0	0	154.2	344	0.352	7.0	45.39	129.7	3.9	1030	2.43	6.9	53.5
1	1	188.7	307	0.817	5.5	29.15	35.66	4.3	711.6	2.04	2.5	70.1
2	1	188.7	298.1	1.0	2.5	13.25	13.24	4.6	527	1.0	1.0	75.55
3	1	188.7	350.9	0.301	1.2	6.36	21.15	4.5	668.7	0.271	0.90	42.56
4	2	223.1	334	0.442	1.0	4.48	10.14	4.9	805.5	0.265	0.6	59.17
7	2	223.1	297.4	1.0	1.25	5.6	5.51	5.0	550.8	0.254	0.25	45.39
8	2	223.1	316	0.666	1.0	4.48	6.73	5.1	847.3	0.279		
9	2	223.1	298.1	1.0	2.0	8.96	8.95	5.1	1127	0.18	0.18	20.1
10	2	223.1	307.9	0.801	1.4	6.28	7.84	5.0	783.5			
15	2	223.1	422	0.059	0.06	0.269	4.56	5.3	901	0.0048	0.08	17.0
18	3	257.5	317	0.651	0.4	1.55	2.39	5.6	949.8	0.143	0.22	92.21
28	3	257.5	330	0.484	0.16	0.621	1.28	5.8	809.6			
29	3	257.5	351	0.30	0.14	0.544	1.81	5.6	721.1	0.132	0.044	24.29
30	3	257.5	335.5	0.427	0.2	0.777	1.82	5.5	574.9	0.0384	0.09	49.51
33	3	257.5	333	0.452	0.08	0.311	0.69	5.8	433.4	0.0136	0.003	43.67
37	3	257.5	360	0.244	0.015	0.0582	0.24	5.9	189.2			
40	4	292.0	394	0.113	0.03	0.103	0.91	5.6	362.9	0.00225	0.002	21.94
44	4	292.0	320	0.606	0.1	0.342	0.565	6.0	565			
47	4	292.0	356	0.268	0.09	0.308	1.15	5.9	914.2	0.0054	0.002	17.38
49	4	292.0	337	0.413	0.016	0.0548	0.133	6.1	167			
52	4	292.0	360	0.244	0.03	0.103	0.42	6.1	529	0.0049	0.002	47.59
61	4	292.0	365	0.218	0.02	0.0685	0.314	5.9	249.4			
66	4	292.0	397	0.105	0.04	0.0147	1.30	5.8	821			
77	4	292.0	453	0.0294	0.001	0.0342	1.165	6.5	368.3	0.0000588	0.002	1.72
86	5	326.4	373	0.182	0.02	0.0613	0.337	6.2	534	0.00927	0.051	151.4
87	5	326.4	387	0.132	0.004	0.0123	0.0927	6.5	293.1	0.000304	0.0023	24.81
88	5	326.4	373	0.182	0.012	0.0368	0.202	6.5	639.3			
101	5	326.4	349.5	0.311	0.01	0.0306	0.0986	6.4	247.8	0.00109	0.0035	35.48
116	5	326.4	397	0.105	0.008	0.0145	0.233	6.3	464.5			
128	6	360.9	423	0.0582	0.0006	0.00166	0.0286	7.0	285.5	0.0000198	0.00034	11.91
129	6	360.9	358	0.256	0.0006	0.00166	0.0065	7.3	129.6			
134	6	360.9	373	0.182	0.0004	0.00111	0.0061	7.3	121.6	0.000146		
136	6	360.9	385.2	0.138	0.0008	0.00222	0.0161	6.7	80.7			
153	6	360.9	376	0.17	0.001	0.00277	0.0163	6.9	129.6	0.000119	0.0007	42.9
155	6	360.9	387	0.132	0.0007	0.00194	0.0147	7.0	146.7	0.00159	0.012	817.9
171	7	395.3	395.4	0.109	0.002	0.00506	0.046	6.7	232.2	0.0000273	0.00025	5.4
185	7	395.3	422	0.0596	0.00045	0.00114	0.0191	7.0	191.1			
194	8	429.8	432	0.0474	0.0002	0.00047	0.0098	7.1	123.5			
202	8	429.7	435	0.0443	0.0003	0.00070	0.0158	7.1	198.3	0.0000266	0.0006	38.08
206	9	464.2	479	0.0163	0.00011	0.000237	0.0146	7.2	230.9			
208	9	464.2	455.8	0.0276	1.8E-5	0.000038	0.00141	8.16	203.1			
209	10	498.7	578.9	0.00167	1.2E-6	2.4E-6	0.00144	8.26	262.0	5.0E-8	0.00003	20.84

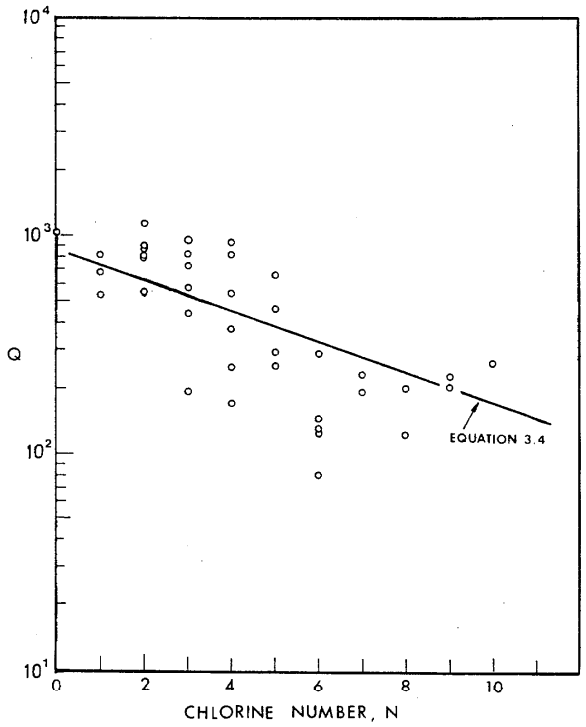

FIG. 4. Plot of log Q vs chlorine number.

4. List of Symbols

c	solubility in water, mol/m^3
c_L	subcooled liquid solubility in water mol/m^3 or mmol/m^3
c_S	solid solubility in water, mol/m^3 or mmol/m^3
c_{WO}	solubility in water saturated with octanol, mol/m^3
c_{OW}	solubility in octanol saturated with water, mol/m^3
H	Henry's law constant, Pa m^3/mol
H'	dimensionless Henry's law constant
ΔH_{fus}	enthalpy of fusion, J/mol
K_{OW}	octanol–water partition coefficient
N	chlorine number
n	congener number
p	pressure, Pa
p_S	solid vapor pressure, Pa
p_L	subcooled liquid vapor pressure, Pa
Q	product of c_L and K_{OW} or pseudosolubility in octanol
R	gas constant, 8.314 J/mol K
ΔS_{fus}	entropy of fusion, J/mol K
S	aqueous solubility, g/m^3
T	system temperature, K
T_M	normal melting point, K
v	molar volume, m^3/mol or cm^3/mol

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