

# 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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# 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.<sup>1</sup> 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 de-

cachlorobiphenyl. It is only recently<sup>2</sup> 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.<sup>3</sup> 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.<sup>4</sup> For example, appreciable concentrations are found in the soils, sediments, waters, biota, atmosphere, and precipitation in the Great Lakes Basin.<sup>5-9</sup> The biological and human health effects of PCB's have been reviewed recently.<sup>8</sup>

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 composition of some commercial PCB products (Ref. 1)

| Chlorobiphenyl                                 | Aroclor type or grade |      |      |      |      |      | Kanechloors |        |        | Pencloors |     |
|------------------------------------------------|-----------------------|------|------|------|------|------|-------------|--------|--------|-----------|-----|
|                                                | 1016                  | 1221 | 1232 | 1242 | 1248 | 1254 | 1260        | KC-300 | KC-400 | KC-500    | DK  |
| C <sub>12</sub> H <sub>10</sub>                | 0.1                   | 11   | 6    | 0.1  | -    | 0.1  | -           | -      | -      | -         | -   |
| C <sub>12</sub> H <sub>9</sub> Cl              | 1                     | 51   | 26   | 1    | -    | 0.1  | -           | -      | -      | -         | -   |
| C <sub>12</sub> H <sub>8</sub> Cl <sub>2</sub> | 20                    | 32   | 29   | 16   | 2    | 0.5  | -           | 17     | 3      | -         | -   |
| C <sub>12</sub> H <sub>7</sub> Cl <sub>3</sub> | 57                    | 4    | 24   | 49   | 18   | 1    | -           | 60     | 33     | 5         | -   |
| C <sub>12</sub> H <sub>6</sub> Cl <sub>4</sub> | 21                    | 2    | 15   | 25   | 40   | 21   | -           | 23     | 44     | 27        | -   |
| C <sub>12</sub> H <sub>5</sub> Cl <sub>5</sub> | 1                     | 0.5  | 0.5  | 8    | 36   | 48   | 12          | 0.6    | 16     | 55        | -   |
| C <sub>12</sub> H <sub>4</sub> Cl <sub>6</sub> | 0.1                   | -    | -    | 1    | 4    | 23   | 38          | -      | 5      | 13        | -   |
| C <sub>12</sub> H <sub>3</sub> Cl <sub>7</sub> | -                     | -    | -    | 0.1  | -    | 6    | 41          | -      | -      | -         | -   |
| C <sub>12</sub> H <sub>2</sub> Cl <sub>8</sub> | -                     | -    | -    | -    | -    | -    | 8           | -      | -      | -         | -   |
| C <sub>12</sub> HCl <sub>9</sub>               | -                     | -    | -    | -    | -    | -    | 1           | -      | -      | -         | -   |
| C <sub>12</sub> Cl <sub>10</sub>               | -                     | -    | -    | -    | -    | -    | -           | -      | -      | -         | 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 en-

vironmental 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<sub>ow</sub>*), 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<sub>ow</sub>* 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<sub>ow</sub>* 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.<sup>6</sup>

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<sup>5,10</sup> 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

$$H = p_s/c_s = p_L/c_L. \quad (2.1)$$

Prausnitz<sup>12</sup> 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

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

where  $\Delta S_{fus}$  is the entropy of fusion. It follows that

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

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.*,<sup>13</sup> or estimated from Walden's rule as reviewed by Yalkowsky<sup>14</sup> as 56.5 J/mol K, thus  $\Delta S_{fus}/R$  is 6.79. The dimensionless air-water partition coefficient  $H'$  is given as<sup>15</sup>

$$H' = H/RT. \quad (2.4)$$

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

$$K_{OW} = c_{OW}/c_{WO}, \quad (2.5)$$

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.<sup>13,16-19</sup> Mackay *et al.*<sup>16</sup> and Banerjee *et al.*<sup>17</sup> 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.*,<sup>13</sup> it has been observed that the product  $Q$  varies as a function of molar volume  $v$  (cm<sup>3</sup>/mol) approximately as follows<sup>20</sup>:

$$\log Q = 3.89 - 0.0048v. \quad (2.6)$$

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<sup>21</sup> 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.*<sup>22</sup> Also given in Table 2 are chlorine number, molecular mass, melting point,<sup>3</sup> normal boiling point,<sup>23</sup> entropy of fusion,<sup>13</sup> fugacity ratio calculated from Eq. (2.2), and the molecular descriptors of molar volume at the normal boiling point calculated by the LaBas method,<sup>24</sup> and total molecular surface areas reported by Mackay *et al.*<sup>25</sup>

The reported entropies of fusion  $\Delta S_{fus}$  range from 41.0 to 69.5 J/mol K, with an average of 56.5 J/mol K and show no systematic variation with chlorine number. It is suspected that some of the reported  $\Delta S_{fus}$  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.*<sup>26</sup> 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<sup>3</sup>, but for comparison between congeners, use of the amount-of-substance solubility  $c$  expressed in mol/m<sup>3</sup>, 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.<br><i>n</i> <sup>a</sup> | Cl No.<br><i>N</i> | MW    | MP,K <sup>b</sup> | lit <sup>c</sup> | BP,K<br>calc'd <sup>d</sup> | Molar vol.<br><i>V<sub>m</sub></i> <sup>e</sup><br>cm <sup>3</sup> /mol | Total surface <sup>f</sup><br>area, Å <sup>2</sup> | Fugacity ratio <sup>f</sup><br><i>F</i> | Entropy of fusion <sup>g</sup><br><i>ΔS<sub>fus</sub></i> , 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'-                 | 5                                  | 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.<br><i>n</i> <sup>a</sup> | Cl No.<br><i>N</i> | MW    | MP,K <sup>b</sup> | BP,K<br>lit <sup>c</sup> | BP,K<br>calc'd <sup>d</sup> | Molar vol.<br><i>V<sub>m</sub></i> <sup>e</sup><br>cm <sup>3</sup> /mol | Total surface <sup>f</sup><br>area, Å <sup>2</sup> | Fugacity ratio <sup>f</sup><br><i>F</i> | Entropy of fusion <sup>g</sup><br><i>ΔS<sub>fus</sub></i> , 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                  | 395.3 | 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                                   | -                                                                   |

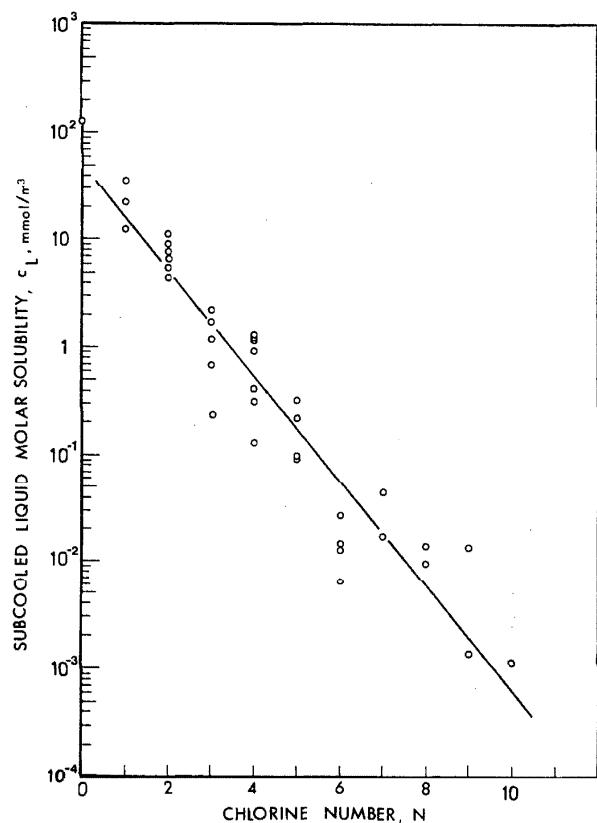
<sup>a</sup>IUPAC or congener number, Ref. 21.<sup>b</sup>Ref. 3.<sup>c</sup>Ref. 23.<sup>d</sup>Calculated values, Ref. 26.<sup>e</sup>Le Bas method, Ref. 24.<sup>f</sup>Ref. 25.<sup>g</sup>Refs. 23 and 69.

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

| Congener<br>No. | <i>S</i> , g/m <sup>3</sup> | Ref.    | <i>S</i> , g/m <sup>3</sup> | Selected values                             |                                             | Congener<br>No. | <i>S</i> , g/m <sup>3</sup> | Ref. | Selected values                             |                                             |              |
|-----------------|-----------------------------|---------|-----------------------------|---------------------------------------------|---------------------------------------------|-----------------|-----------------------------|------|---------------------------------------------|---------------------------------------------|--------------|
|                 |                             |         |                             | <i>c</i> <sub>S</sub> , mmol/m <sup>3</sup> | <i>c</i> <sub>L</sub> , mmol/m <sup>3</sup> |                 |                             |      | <i>c</i> <sub>S</sub> , mmol/m <sup>3</sup> | <i>c</i> <sub>L</sub> , mmol/m <sup>3</sup> |              |
| 0               | 7.48                        | 27      | 7.0 ± 0.5                   | 45.39 ± 3.24                                | 129.7 ± 9.263                               | 9               | 1.94                        | 13   | 2.0 ± 0.10                                  | 8.96 ± 0.45                                 | 9.0 ± 0.5    |
|                 | 7.08                        | 28      |                             |                                             |                                             |                 | 0.58                        | 35   |                                             |                                             |              |
|                 | 5.94                        | 29      |                             |                                             |                                             |                 | 2.09                        | 16   |                                             |                                             |              |
|                 | 3.87                        | 30      |                             |                                             |                                             |                 | 0.587                       | 19   |                                             |                                             |              |
|                 | 7.45                        | 31      |                             |                                             |                                             | 10              | 1.39                        | 13   | 1.40 ± 0.010                                | 6.28 ± 0.045                                | 7.84 ± 0.53  |
|                 | 7.0                         | 32      |                             |                                             |                                             | 15              | 0.062                       | 40   | 0.060 ± 0.02                                | 0.269 ± 0.09                                | 4.56 ± 1.53  |
|                 | 7.50                        | 33      |                             |                                             |                                             |                 | 0.056                       | 35   |                                             |                                             |              |
|                 | 6.71                        | 13      |                             |                                             |                                             |                 | 0.080                       | 3,34 |                                             |                                             |              |
|                 | 7.455                       | 16      |                             |                                             |                                             |                 | 0.046                       | 37   |                                             |                                             |              |
|                 | 7.21                        | 19      |                             |                                             |                                             |                 | 0.104                       | 16   |                                             |                                             |              |
|                 | 6.80                        | 50      |                             |                                             |                                             | 18              | 0.248                       | 39   | 0.40 ± 0.20                                 | 1.55 ± 0.78                                 | 2.39 ± 1.20  |
| 1               | 5.90                        | 3,34    | 5.50 ± 0.5                  | 29.5 ± 2.6                                  | 35.7 ± 3.26                                 |                 | 0.060                       | 19   |                                             |                                             |              |
|                 | 4.13                        | 35      |                             |                                             |                                             |                 | 0.065                       | 36   |                                             |                                             |              |
|                 | 5.06                        | 13      |                             |                                             |                                             | 28              | 0.085                       | 34   | 0.16 ± 0.1                                  | 0.62 ± 0.39                                 | 1.28 ± 0.81  |
|                 | 5.76                        | 16      |                             |                                             |                                             |                 | 0.260                       | 35   |                                             |                                             |              |
|                 | 2.73                        | 19      |                             |                                             |                                             |                 | 0.266                       | 16   |                                             |                                             |              |
|                 | 7.80                        | 50      |                             |                                             |                                             |                 | 0.148                       | 19   |                                             |                                             |              |
| 2               | 1.30                        | 35      | 2.5 ± 1.2                   | 13.25 ± 6.4                                 | 13.2 ± 6.4                                  | 29              | 0.092                       | 35   | 0.140 ± 0.05                                | 0.54 ± 0.19                                 | 1.81 ± 0.53  |
|                 | 3.50                        | 3,34    |                             |                                             |                                             |                 | 0.142                       | 36   |                                             |                                             |              |
|                 | 6.22                        | 16      |                             |                                             |                                             |                 | 0.163                       | 13   |                                             |                                             |              |
|                 | 1.84                        | 19      |                             |                                             |                                             |                 | 0.119                       | 41   |                                             |                                             |              |
|                 | 1.20                        | 50      |                             |                                             |                                             |                 | 0.193                       | 16   |                                             |                                             |              |
| 3               | 1.17                        | 3,34,36 | 1.2 ± 0.3                   | 6.36 ± 1.59                                 | 21.3 ± 5.3                                  |                 | 0.097                       | 19   |                                             |                                             |              |
|                 | 0.90                        | 35      |                             |                                             |                                             | 30              | 0.226                       | 13   | 0.20 ± 0.03                                 | 0.78 ± 0.12                                 | 1.82 ± 0.27  |
|                 | 1.87                        | 16      |                             |                                             |                                             | 33              | 0.078                       | 3,34 | 0.080 ± 0.02                                | 0.31 ± 0.078                                | 0.59 ± 0.17  |
|                 | 1.30                        | 37      |                             |                                             |                                             |                 | 0.291                       | 16   |                                             |                                             |              |
|                 | 0.824                       | 19      |                             |                                             |                                             |                 | 0.795                       | 19   |                                             |                                             |              |
|                 | 1.41                        | 38      |                             |                                             |                                             | 37              | 0.0152                      | 35   | 0.015 ± 0.010                               | 0.0582 ± 0.039                              | 0.024 ± 0.17 |
|                 | 1.20                        | 36      |                             |                                             |                                             |                 | 0.135                       | 16   |                                             |                                             |              |
| 4               | 1.50                        | 3,34    | 1.0 ± 0.2                   | 4.48 ± 0.90                                 | 10.14 ± 0.25                                |                 | 0.0152                      | 19   |                                             |                                             |              |
|                 | 0.79                        | 35      |                             |                                             |                                             | 40              | 0.034                       | 3,34 | 0.030 ± 0.004                               | 0.103 ± 0.014                               | 0.91 ± 0.13  |
|                 | 1.00                        | 16      |                             |                                             |                                             |                 | 0.026                       | 16   |                                             |                                             |              |
|                 | 0.997                       | 19      |                             |                                             |                                             |                 | 0.030                       | 19   |                                             |                                             |              |
| 7               | 1.40                        | 34      | 1.25 ± 0.15                 | 5.60 ± 0.67                                 | 5.51 ± 0.67                                 | 44              | 0.0170                      | 3,34 | 0.10 ± 0.05                                 | 0.342 ± 0.17                                | 0.565 ± 2.83 |
|                 | 1.13                        | 37      |                             |                                             |                                             |                 | 0.080                       | 37   |                                             |                                             |              |
|                 | 2.03                        | 16      |                             |                                             |                                             |                 | 0.121                       | 16   |                                             |                                             |              |
|                 | 1.408                       | 19      |                             |                                             |                                             |                 | 0.172                       | 19   |                                             |                                             |              |
| 8               | 0.637                       | 39      | 1.0 ± 0.4                   | 4.48 ± 1.79                                 | 6.73 ± 2.73                                 | 47              | 0.068                       | 3,34 | 0.090 ± 0.030                               | 0.308 ± 0.103                               | 1.15 ± 0.38  |
|                 | 1.88                        | 3,34    |                             |                                             |                                             |                 | 0.115                       | 16   |                                             |                                             |              |
|                 | 0.62                        | 35      |                             |                                             |                                             |                 | 0.067                       | 19   |                                             |                                             |              |
|                 | 1.33                        | 16      |                             |                                             |                                             |                 |                             |      |                                             |                                             |              |
|                 | 0.706                       | 19      |                             |                                             |                                             |                 |                             |      |                                             |                                             |              |

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

| Congener No. | Ref.     | <i>S</i> , g/m <sup>3</sup> | <i>S</i> , g/m <sup>3</sup> | Selected values                            |                                            | Congener No. | Ref.       | <i>S</i> , g/m <sup>3</sup> | <i>S</i> , g/m <sup>3</sup> | Selected values                            |                                            |  |
|--------------|----------|-----------------------------|-----------------------------|--------------------------------------------|--------------------------------------------|--------------|------------|-----------------------------|-----------------------------|--------------------------------------------|--------------------------------------------|--|
|              |          |                             |                             | <i>c<sub>s</sub></i> , mmol/m <sup>3</sup> | <i>c<sub>L</sub></i> , mmol/m <sup>3</sup> |              |            |                             |                             | <i>c<sub>s</sub></i> , mmol/m <sup>3</sup> | <i>c<sub>L</sub></i> , mmol/m <sup>3</sup> |  |
| 49           | 0.0164   | 13                          | 0.016±0.005                 | 0.055±0.0017                               | 0.133±0.032                                | 129          | 0.00085    | 35                          | 0.00060±0.0004              | 0.00166±0.0011                             | 0.00651±0.00482                            |  |
| 52           | 0.00601  | 42                          | 0.030±0.020                 | 0.103±0.068                                | 0.42±0.28                                  |              | 0.000581   | 16                          |                             |                                            |                                            |  |
|              | 0.0265   | 39                          |                             |                                            |                                            |              | 0.000906   | 19                          |                             |                                            |                                            |  |
|              | 0.046    | 3,34                        |                             |                                            |                                            | 134          | 0.00091    | 35                          | 0.00040±0.00040             | 0.00111±0.0011                             | 0.0061±0.0061                              |  |
|              | 0.0365   | 36                          |                             |                                            |                                            |              | 0.000399   | 16                          |                             |                                            |                                            |  |
|              | 0.041    | 16                          |                             |                                            |                                            |              | 0.000906   | 19                          |                             |                                            |                                            |  |
|              | 0.0184   | 19                          |                             |                                            |                                            | 136          | 0.00098    | 41                          | 0.00080±0.0002              | 0.00222±0.00056                            | 0.016±0.0042                               |  |
| 61           | 0.0192   | 35                          | 0.020±0.020                 | 0.0685±0.068                               | 0.314±0.32                                 |              | 0.000603   | 13                          |                             |                                            |                                            |  |
|              | 0.0209   | 39                          |                             |                                            |                                            |              | 0.00451    | 69                          |                             |                                            |                                            |  |
|              | 0.0099   | 37                          |                             |                                            |                                            |              | 0.00210    | 71                          |                             |                                            |                                            |  |
|              | 0.0525   | 16                          |                             |                                            |                                            | 153          | 0.00105    | 42                          | 0.0010±0.00040              | 0.0028±0.0011                              | 0.0164±0.00325                             |  |
|              | 0.0193   | 19                          |                             |                                            |                                            |              | 0.0088     | 3,34                        |                             |                                            |                                            |  |
| 66           | 0.058    | 3,34                        | 0.040±0.030                 | 0.137±0.103                                | 1.30±1.0                                   |              | 0.0012     | 35                          |                             |                                            |                                            |  |
|              | 0.017    | 16                          |                             |                                            |                                            |              | 0.00995    | 39                          |                             |                                            |                                            |  |
|              | 0.060    | 19                          |                             |                                            |                                            |              | 0.00278    | 16                          |                             |                                            |                                            |  |
|              |          |                             |                             |                                            |                                            |              | 0.00131    | 19                          |                             |                                            |                                            |  |
| 70           | 0.041    | 3,34                        | 0.041±0.010                 | 0.140±0.034                                | 0.85±0.21                                  | 155          | 0.00090    | 34                          | 0.00070±0.0002              | 0.0019±0.00055                             | 0.015±0.0040                               |  |
| 77           | 0.175    | 3,34                        | 0.001±0.001                 | 0.00342±0.0034                             | 0.117±0.12                                 |              | 0.00041    | 13                          |                             |                                            |                                            |  |
|              | 0.00075  | 35                          |                             |                                            |                                            |              | 0.0000204  | 16                          |                             |                                            |                                            |  |
|              | 0.0174   | 16                          |                             |                                            |                                            |              | 0.00091    | 19                          |                             |                                            |                                            |  |
|              | 0.0114   | 19                          |                             |                                            |                                            | 163          | 0.00531    | 36                          | 0.0050±0.002                | 0.0139±0.0055                              | 0.059±0.021                                |  |
|              | 0.000569 | 69                          |                             |                                            |                                            |              | 0.00624    | 41                          | 0.0020±0.0010               | 0.00506±0.0025                             | 0.046±0.025                                |  |
|              | 0.00301  | 71                          |                             |                                            |                                            |              | 0.00217    | 13                          |                             |                                            |                                            |  |
| 86           | 0.0098   | 35                          | 0.020±0.010                 | 0.0613±0.031                               | 0.0337±0.19                                | 185          | 0.00047    | 35                          | 0.00046±0.00020             | 0.00114±0.00051                            | 0.019±0.008                                |  |
|              | 0.0349   | 36                          |                             |                                            |                                            |              | 0.000402   | 16                          |                             |                                            |                                            |  |
|              | 0.0133   | 16                          |                             |                                            |                                            |              | 0.000475   | 19                          |                             |                                            |                                            |  |
|              | 0.0099   | 19                          |                             |                                            |                                            | 194          | 0.0072     | 3,34                        | 0.00020±0.00010             | 0.00047±0.00023                            | 0.001±0.0005                               |  |
| 87           | 0.0045   | 35                          | 0.0040±0.002                | 0.0123±0.031                               | 0.093±0.043                                |              | 0.000272   | 35                          |                             |                                            |                                            |  |
|              | 0.022    | 3,34                        |                             |                                            |                                            |              | 0.000101   | 16                          |                             |                                            |                                            |  |
|              | 0.0086   | 16                          |                             |                                            |                                            |              | 0.00150    | 19                          |                             |                                            |                                            |  |
|              | 0.0101   | 19                          |                             |                                            |                                            | 202          | 0.00018    | 35                          | 0.00030±0.00010             | 0.00070±0.00023                            | 0.016±0.005                                |  |
| 101          | 0.0103   | 39                          | 0.010±0.010                 | 0.0306±0.0306                              | 0.100±0.10                                 |              | 0.000098   | 16                          |                             |                                            |                                            |  |
|              | 0.010    | 40                          |                             |                                            |                                            |              | 0.000179   | 19                          |                             |                                            |                                            |  |
|              | 0.00424  | 42                          |                             |                                            |                                            |              | 0.000147   | 69                          |                             |                                            |                                            |  |
|              | 0.0042   | 35                          |                             |                                            |                                            |              | 0.00017    | 71                          |                             |                                            |                                            |  |
|              | 0.031    | 3,34                        |                             |                                            |                                            | 206          | 0.000112   | 35                          | 0.00011±0.00030             | 0.00024±0.00055                            | 0.0146±0.0030                              |  |
|              | 0.0194   | 13                          |                             |                                            |                                            |              | 0.000012   | 16                          |                             |                                            |                                            |  |
|              | 0.0163   | 16                          |                             |                                            |                                            |              | 0.00011    | 19                          |                             |                                            |                                            |  |
|              | 0.0130   | 19                          |                             |                                            |                                            |              | 0.0000255  | 69                          |                             |                                            |                                            |  |
|              | 0.0154   | 69                          |                             |                                            |                                            |              | 0.0000315  | 71                          |                             |                                            |                                            |  |
|              | 0.0115   | 71                          |                             |                                            |                                            | 208          | 0.000018   | 13                          | 0.000018±0.000010           | 0.000038±0.000022                          | 0.0014±0.00070                             |  |
| 116          | 0.0068   | 35                          | 0.0080±0.0020               | 0.0145±0.0061                              | 0.233±0.057                                | 209          | 0.000015   | 35                          | 0.0000012                   | 0.0000024                                  | 0.0014±0.00060                             |  |
|              | 0.0207   | 41                          |                             |                                            |                                            |              | 0.00000743 | 13                          | ± 0.000005                  | ± 0.000001                                 |                                            |  |
|              | 0.00548  | 13                          |                             |                                            |                                            |              | 0.0000004  | 16                          |                             |                                            |                                            |  |
|              | 0.00904  | 16                          |                             |                                            |                                            |              | 0.00049    | 19                          |                             |                                            |                                            |  |
|              | 0.00682  | 19                          |                             |                                            |                                            |              | 0.0000065  | 69                          |                             |                                            |                                            |  |
| 128          | 0.00044  | 35                          | 0.00060±0.00040             | 0.00166±0.0011                             | 0.029±0.021                                |              | 0.0000041  | 71                          |                             |                                            |                                            |  |
|              | 0.00099  | 41                          |                             |                                            |                                            |              | 0.015      | 3,34                        |                             |                                            |                                            |  |
|              | 0.000285 | 13                          |                             |                                            |                                            |              |            |                             |                             |                                            |                                            |  |
|              | 0.000132 | 16                          |                             |                                            |                                            |              |            |                             |                             |                                            |                                            |  |
|              | 0.00044  | 19                          |                             |                                            |                                            |              |            |                             |                             |                                            |                                            |  |

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

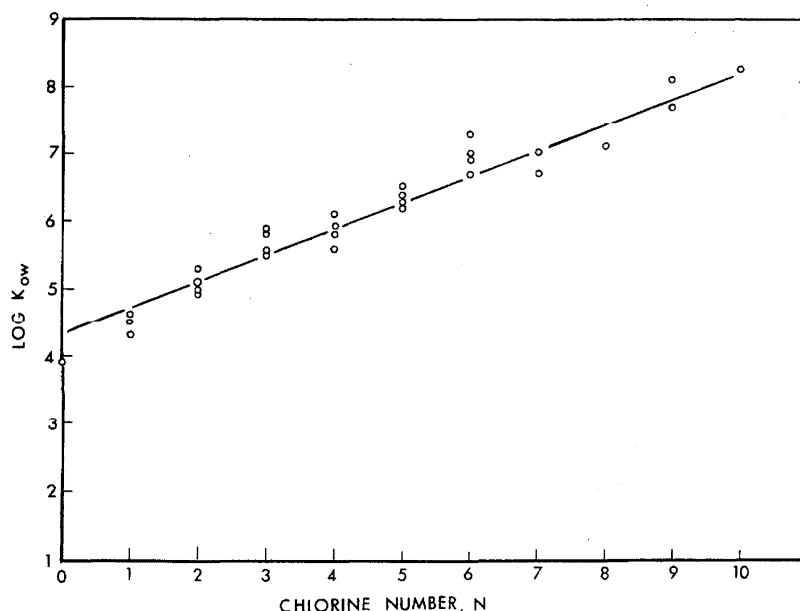
single value was selected by taking into account the accuracy of the method. In some cases information from other tables and other structurally similar congeners influenced the choice of the selected value of its error range. Figure 1 is a plot of  $\log c_L$  versus chlorine number.

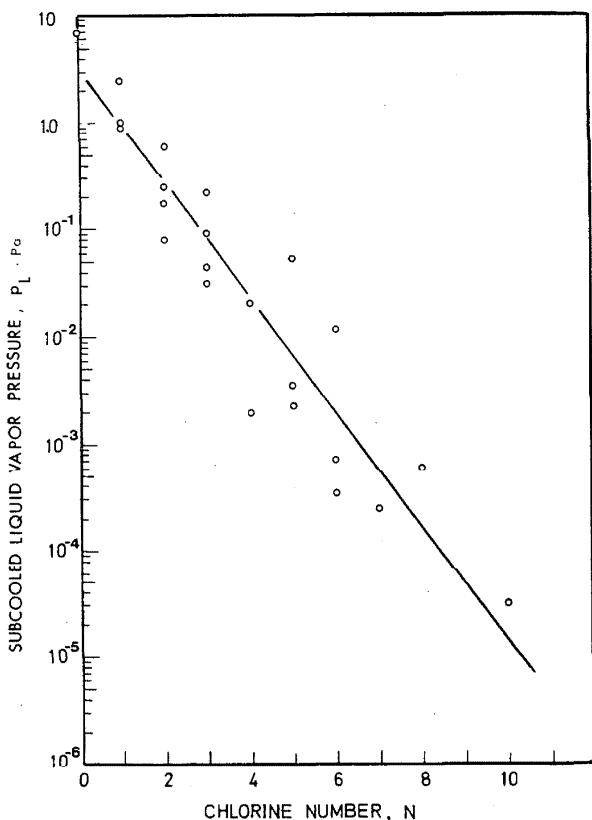
Table 4 gives reported experimental values for octanol-water partition coefficient and selected values with estimated error range. The method of experimental determination is also indicated. The product  $Q$  of  $K_{OW}$  and  $c_L$  is also given. As discussed earlier  $Q$  can be regarded as a pseudosolubility 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<sup>3</sup>/mol and show no systematic trend with chlorine number. The experimental determinations, largely of Murphy *et al.*<sup>64</sup> and Giam *et al.*<sup>65</sup> 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<sup>59</sup> and Westcott *et al.*<sup>66,67</sup> when combined with the solubilities. The average  $H$  value is 48 Pa m<sup>3</sup>/mol. Second, the  $Q$  values tend to fall with increase in chlorine number from approximately 1000 mol/m<sup>3</sup> for biphenyl to approximately 150 mol/m<sup>3</sup> for deca-chlorobiphenyl. 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<sup>3</sup> while  $c_L$  in Eq. (3.1) has units of mol/m<sup>3</sup>.

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.*<sup>70,71</sup> have calculated the vapor pressure, aqueous solubility, and Henry's law constants for all 209 congeners from some experimental data for PCB's.<sup>13,64-67</sup> 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 Kow | Method   | Ref.  | Selected value | Q     | Congener No. | log Kow | Method   | Ref. | Selected value | Q     |
|--------------|---------|----------|-------|----------------|-------|--------------|---------|----------|------|----------------|-------|
| 0            | 4.09    | SF       | 43,44 | 3.90 ± 0.20    | 1030  | 8            | 5.10    | SF       | 53   | 5.10 ± 0.40    | 847.3 |
|              | 4.10    | TLC      | 45    |                |       |              | 5.14    | Gen.col. | 46   |                |       |
|              | 4.04    | HPLC     | 17    |                |       |              | 4.47    | HPLC     | 47   |                |       |
|              | 3.89    | Gen.col. | 46    |                |       |              | 5.10    | calc.    | 47   |                |       |
|              | 3.76    | Gen.col. | 13    |                |       |              | 5.32    | calc.    | 19   |                |       |
|              | 3.70    | HPLC     | 46    |                |       |              | 5.51    | calc.    | 46   |                |       |
|              | 3.79    | HPLC     | 47    |                |       |              | 5.20    | calc.    | 50   |                |       |
|              | 3.75    | HPLC     | 48    |                |       |              |         |          |      |                |       |
|              | 3.79    | calc.    | 19    |                |       | 9            | 5.18    | TLC      | 45   | 5.10 ± 0.20    | 1127  |
|              | 4.03    | calc.    | 49    |                |       |              | 5.16    | Gen.col. | 13   |                |       |
|              | 4.14    | calc.    | 16    |                |       |              | 4.67    | HPLC     | 47   |                |       |
|              |         |          |       |                |       |              | 5.30    | calc.    | 47   |                |       |
| 1            | 4.54    | SF       | 51    | 4.30 ± 0.50    | 712   | 10           | 4.93    | Gen.col. | 13   | 5.00 ± 0.20    | 783.5 |
|              | 4.51    | SF       | 53    |                |       |              | 4.05    | HPLC     | 47   |                |       |
|              | 4.59    | SF       | 45    |                |       |              | 5.31    | calc.    | 47   |                |       |
|              | 4.56    | TLC      | 45    |                |       |              |         |          |      |                |       |
|              | 4.38    | Gen.col. | 46    |                |       | 11           | 5.30    | SF       | 45   | 5.30 ± 0.10    | -     |
|              | 4.50    | Gen.col. | 13    |                |       |              | 5.34    | TLC      | 45   |                |       |
|              | 3.75    | HPLC     | 46    |                |       |              |         |          |      |                |       |
|              | 3.90    | HPLC     | 47    |                |       | 12           | 5.29    | Gen.col. | 46   | 5.30 ± 0.20    | -     |
|              | 4.60    | calc.    | 47    |                |       |              | 5.10    | HPLC     | 46   |                |       |
|              | 4.56    | calc.    | 19    |                |       |              | 5.51    | calc.    | 46   |                |       |
|              | 4.80    | calc.    | 46    |                |       |              |         |          |      |                |       |
|              | 4.72    | calc.    | 50    |                |       | 14           | 5.37    | SF       | 45   | 5.40 ± 0.20    | -     |
| 2            | 4.95    | SF       | 51    | 4.60 ± 0.30    | 527   | 15           | 5.58    | SF       | 40   | 5.30 ± 0.20    | 901   |
|              | 4.71    | SF       | 45    |                |       |              | 5.36    | SF       | 45   |                |       |
|              | 4.72    | TLC      | 45    |                |       |              | 5.28    | TLC      | 45   |                |       |
|              | 4.58    | Gen.col. | 46    |                |       |              | 5.33    | Gen.col. | 46   |                |       |
|              | 4.35    | HPLC     | 48    |                |       |              | 4.92    | HPLC     | 46   |                |       |
|              | 4.42    | HPLC     | 47    |                |       |              | 4.82    | HPLC     | 47   |                |       |
|              | 4.56    | calc.    | 19    |                |       |              | 5.32    | calc.    | 19   |                |       |
|              | 4.80    | calc.    | 46    |                |       |              | 5.51    | calc.    | 46   |                |       |
| 3            | 4.61    | SF       | 45    | 4.50 ± 0.30    | 669   |              | 5.57    | calc.    | 47   |                |       |
|              | 4.69    | TLC      | 46    |                |       |              | 4.77    | calc.    | 50   |                |       |
|              | 4.49    | Gen.col. | 46    |                |       |              |         |          |      |                |       |
|              | 4.34    | HPLC     | 46    |                |       | 16           | 4.15    | HPLC     | 47   | 5.60 ± 0.40    | -     |
|              | 4.40    | HPLC     | 47    |                |       |              | 5.31    | calc.    | 47   |                |       |
|              | 4.56    | calc.    | 19    |                |       |              |         |          |      |                |       |
|              | 4.80    | calc.    | 46    |                |       | 17           | 4.60    | HPLC     | 47   | 5.60 ± 0.10    | -     |
|              | 4.40    | calc.    | 47    |                |       |              | 5.76    | calc.    | 47   |                |       |
|              | 4.34    | calc.    | 50    |                |       |              |         |          |      |                |       |
| 4            | 5.00    | SF       | 45    | 4.9 ± 0.50     | 805.5 | 18           | 5.64    | TLC      | 45   | 5.60 ± 0.10    | 949.8 |
|              | 5.02    | TLC      | 45    |                |       |              | 5.60    | Gen.col. | 46   |                |       |
|              | 4.90    | Gen.col. | 46    |                |       |              | 4.34    | HPLC     | 46   |                |       |
|              | 3.55    | HPLC     | 46    |                |       |              | 4.39    | HPLC     | 47   |                |       |
|              | 3.63    | HPLC     | 47    |                |       |              | 5.55    | calc.    | 47   |                |       |
|              | 4.89    | calc.    | 47    |                |       |              | 6.00    | calc.    | 19   |                |       |
|              | 4.0     | HPLC     | 52    |                |       |              | 6.22    | SF       | 44   |                |       |
|              | 5.32    | calc.    | 19    |                |       |              | 5.63    | calc.    | 50   |                |       |
|              | 5.51    | calc.    | 46    |                |       |              |         |          |      |                |       |
|              | 4.96    | calc.    | 50    |                |       | 19           | 4.52    | Gen.col. | 46   | 5.60 ± 0.60    | -     |
|              |         |          |       |                |       |              | 5.67    | calc.    | 46   |                |       |
|              |         |          |       |                |       |              | 3.73    | HPLC     | 47   |                |       |
| 6            | 4.39    | HPLC     | 47    | 4.8 ± 0.30     | -     |              | 5.48    | calc.    | 47   |                |       |
|              | 5.02    | HPLC     | 47    |                |       |              |         |          |      |                |       |
| 7            | 5.15    | TLC      | 45    | 5.0 ± 0.30     | 551   | 20           | 4.99    | HPLC     | 47   | 5.60 ± 0.50    | -     |
|              | 4.67    | HPLC     | 47    |                |       |              | 5.57    | calc.    | 47   |                |       |
|              | 5.30    | calc.    | 47    |                |       |              |         |          |      |                |       |
|              | 5.23    | calc.    | 19    |                |       | 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 | $Q$   | Congener No. | $\log K_{ow}$                        | Method                                  | Ref.                       | Selected value | $Q$ |
|--------------|--------------------------------------------------------------|------------------------------------------------------------------------|----------------------------------------------|----------------|-------|--------------|--------------------------------------|-----------------------------------------|----------------------------|----------------|-----|
| 22           | 4.84<br>5.42                                                 | HPLC<br>calc.                                                          | 47<br>47                                     | 5.60 ± 0.50    | -     | 47           | 5.27<br>6.29<br>6.67<br>5.68<br>6.44 | HPLC<br>calc.<br>calc.<br>HPLC<br>calc. | 47<br>47<br>19<br>52<br>50 | 5.90 ± 0.30    | 914 |
| 24           | 4.52<br>5.67                                                 | HPLC<br>calc.                                                          | 47<br>47                                     | 5.50 ± 0.50    | -     |              |                                      |                                         |                            |                |     |
| 26           | 5.18<br>5.76                                                 | HPLC<br>calc.                                                          | 47<br>47                                     | 5.50 ± 0.50    | -     | 49           | 5.20<br>6.22                         | HPLC<br>calc.                           | 47<br>47                   | 6.10 ± 0.20    | 167 |
| 28           | 5.74<br>6.00<br>5.62<br>5.11<br>5.69                         | TLC<br>calc.<br>SF<br>HPLC<br>calc.                                    | 45<br>19<br>52<br>47<br>47                   | 5.80 ± 0.20    | 809.6 | 52           | 6.26<br>5.07<br>6.09<br>6.67<br>6.12 | TLC<br>HPLC<br>calc.<br>calc.<br>calc.  | 45<br>47<br>47<br>19<br>50 | 6.10 ± 0.20    | 529 |
| 29           | 5.77<br>5.81<br>5.51<br>5.86<br>5.67<br>6.25<br>5.99<br>6.22 | TLC<br>Gen.col.<br>Gen.col.<br>HPLC<br>HPLC<br>calc.<br>calc.<br>calc. | 45<br>46<br>13<br>46<br>47<br>47<br>19<br>46 | 5.60 ± 0.30    | 721   | 54           | 5.94                                 | TLC                                     | 45                         | 5.90 ± 0.20    | -   |
|              |                                                              |                                                                        |                                              |                |       | 60           | 5.33<br>5.84                         | HPLC<br>calc.                           | 47<br>47                   | 5.90 ± 0.30    | -   |
|              |                                                              |                                                                        |                                              |                |       | 61           | 6.39<br>5.72<br>6.74                 | TLC<br>Gen.col.<br>calc.                | 45<br>13<br>19             | 5.90 ± 0.30    | 250 |
| 30           | 5.47                                                         | Gen.col.                                                               | 13                                           | 5.50 ± 0.20    | 575   | 66           | 5.80<br>6.31<br>6.67                 | HPLC<br>calc.<br>calc.                  | 47<br>47<br>19             | 5.80 ± 0.30    | 821 |
| 31           | 5.77<br>5.79                                                 | TLC<br>Gen.col.                                                        | 45<br>46                                     | 5.70 ± 0.20    | -     | 70           | 6.39<br>5.72<br>6.23<br>5.95<br>6.67 | TLC<br>HPLC<br>calc.<br>HPLC<br>calc.   | 45<br>47<br>47<br>51<br>19 | 5.90 ± 0.30    | -   |
| 32           | 4.60<br>5.75                                                 | HPLC<br>calc.                                                          | 47<br>47                                     | 5.80 ± 0.30    | 433.3 | 74           | 6.16<br>6.67                         | HPLC<br>calc.                           | 47<br>19, 47               | 6.10 ± 0.30    | -   |
| 33           | 6.00<br>6.10                                                 | calc.<br>calc.                                                         | 19<br>50                                     | 5.80 ± 0.30    |       | 77           | 6.52<br>6.67<br>5.62<br>5.62         | TLC<br>calc.<br>HPLC<br>calc.           | 45<br>19<br>47<br>47       | 6.10 ± 0.40    | 368 |
| 36           | 4.15<br>4.15                                                 | HPLC<br>calc.                                                          | 47<br>47                                     | 5.70 ± 0.50    |       |              |                                      |                                         |                            |                |     |
| 37           | 5.90<br>4.54<br>6.00<br>5.56                                 | TLC<br>HPLC<br>calc.<br>calc.                                          | 45<br>47<br>19<br>47                         | 5.90 ± 0.20    | 189.2 | 80           | 6.58                                 | TLC                                     | 45                         | 6.10 ± 0.40    | -   |
|              |                                                              |                                                                        |                                              |                |       | 84           | 4.73<br>6.04                         | HPLC<br>calc.                           | 47<br>47                   | 6.10 ± 0.40    | -   |
| 40           | 4.54<br>5.56<br>6.67                                         | HPLC<br>calc.<br>calc.                                                 | 47<br>47<br>19                               | 5.60 ± 0.30    | 363   | 85           | 5.69<br>6.61                         | HPLC<br>calc.                           | 47<br>47                   | 6.20 ± 0.40    | -   |
| 41           | 5.09<br>6.11                                                 | HPLC<br>calc.                                                          | 48<br>47                                     | 6.00 ± 0.30    |       | 86           | 6.38<br>7.49                         | calc.<br>calc.                          | 46<br>19                   | 6.20 ± 0.40    | 534 |
| 44           | 4.79<br>5.81<br>6.67                                         | HPLC<br>HPLC<br>calc.                                                  | 47<br>47<br>19                               | 6.00 ± 0.30    | 565   |              |                                      |                                         |                            |                |     |

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

| Congener No. | $\log K_{ow}$ | Method    | Ref. | Selected value  | $Q$   | Congener No. | $\log K_{ow}$ | Method    | Ref. | Selected value  | $Q$   |
|--------------|---------------|-----------|------|-----------------|-------|--------------|---------------|-----------|------|-----------------|-------|
| 87           | 6.85          | TLC       | 45   | $6.50 \pm 0.40$ | 293   | 135          | 5.94          | HPLC      | 47   | $7.30 \pm 0.60$ | -     |
|              | 5.45          | HPLC      | 47   |                 |       |              | 7.15          | calc.     | 47   |                 |       |
|              | 6.37          | calc.     | 47   |                 |       | 136          | 6.81          | Gen. col. | 46   | $6.70 \pm 0.20$ | 80.7  |
|              | 7.43          | calc.     | 19   |                 |       |              | 6.63          | Gen. col. | 13   |                 |       |
| 88           | 7.51          | calc.     | 19   | $6.50 \pm 0.40$ | 629   |              | 4.91          | HPLC      | 47   |                 |       |
|              | 6.31          | calc.     | 47   | $6.30 \pm 0.50$ | -     |              | 6.51          | calc.     | 47   |                 |       |
| 91           | 4.94          | HPLC      | 47   | $6.50 \pm 0.50$ | -     | 137          | 6.89          | HPLC      | 47   | $7.0 \pm 0.60$  | -     |
|              | 6.31          | calc.     | 47   |                 |       |              | 7.71          | calc.     | 47   |                 |       |
| 92           | 6.05          | HPLC      | 47   | $6.50 \pm 0.50$ | -     | 138          | 6.62          | HPLC      | 47   | $7.00 \pm 0.50$ | -     |
|              | 6.97          | calc.     | 47   |                 |       |              | 7.44          | calc.     | 47   |                 |       |
| 95           | 5.18          | HPLC      | 47   | $6.40 \pm 0.50$ | -     | 149          | 6.14          | HPLC      | 47   | $6.80 \pm 0.50$ | -     |
|              | 6.55          | calc.     | 47   |                 |       |              | 7.28          | calc.     | 47   |                 |       |
| 97           | 5.75          | HPLC      | 47   | $6.50 \pm 0.50$ | -     | 153          | 5.72          | SF        | 40   | $6.90 \pm 0.20$ | 130   |
|              | 6.67          | calc.     | 47   |                 |       |              | 7.44          | TLC       | 45   |                 |       |
| 99           | 6.29          | HPLC      | 47   | $6.60 \pm 0.60$ | -     |              | 6.90          | Gen. col. | 46   |                 |       |
|              | 7.21          | calc.     | 47   |                 |       |              | 6.93          | HPLC      | 47   |                 |       |
| 101          | 6.11          | SF        | 40   | $6.40 \pm 0.50$ | 47.8  |              | 7.75          | calc.     | 47   |                 |       |
|              | 6.85          | TLC       | 45   |                 |       |              | 8.18          | calc.     | 19   |                 |       |
|              | 6.50          | Gen. col. | 46   |                 |       |              | 8.35          | calc.     | 46   |                 |       |
|              | 5.92          | Gen. col. | 13   |                 |       |              | 8.06          | calc.     |      |                 |       |
|              | 7.64          | HPLC      | 46   |                 |       | 155          | 7.12          | TLC       | 45   | $7.00 \pm 0.40$ | 147   |
|              | 6.15          | HPLC      | 47   |                 |       |              | 8.18          | calc.     | 19   |                 |       |
|              | 6.44          | HPLC      | 48   |                 |       | 165          | 6.57          | HPLC      | 47   | $7.00 \pm 0.50$ | -     |
|              | 6.42          | HPLC      | 54   |                 |       |              | 7.37          | calc.     | 47   |                 |       |
|              | 7.07          | calc.     | 47   |                 |       | 171          | 6.68          | Gen. col. | 13   | $6.70 \pm 0.40$ | 232.2 |
|              | 7.43          | calc.     | 19   |                 |       |              |               |           |      |                 |       |
|              | 7.24          | calc.     | 47   |                 |       | 179          | 6.77          | HPLC      | 47   | $7.00 \pm 0.50$ | -     |
|              |               |           |      |                 |       |              | 8.13          | calc.     | 47   |                 |       |
| 116          | 6.85          | TLC       | 45   | $6.30 \pm 0.30$ | 464.5 | 185          | 7.93          | TLC       | 45   | $7.00 \pm 0.50$ | 191   |
|              | 6.30          | Gen. col. | 13   |                 |       |              | 8.94          | calc.     | 19   |                 |       |
|              | 7.49          | calc.     | 19   |                 |       | 194          | 8.68          | TLC       | 45   | $7.10 \pm 0.50$ | 124   |
|              |               |           |      |                 |       |              | 9.69          | calc.     | 19   |                 |       |
| 118          | 6.66          | HPLC      | 47   | $6.40 \pm 0.30$ | -     | 202          | 8.42          | TLC       | 45   | $7.10 \pm 0.20$ | 198   |
|              | 7.12          | calc.     | 47   |                 |       |              | 7.14          | Gen. col. | 46   |                 |       |
| 120          | 5.22          | HPLC      | 47   | $6.30 \pm 0.30$ | -     |              | 7.11          | Gen. col. | 13   |                 |       |
|              | 5.68          | calc.     | 47   |                 |       |              | 9.69          | calc.     | 19   |                 |       |
|              |               |           |      |                 |       |              | 9.77          | calc.     | 46   |                 |       |
| 128          | 7.44          | TLC       | 45   | $7.00 \pm 0.30$ | 286   | 205          | 9.14          | TLC       | 45   | $7.20 \pm 1.0$  | 231   |
|              | 6.98          | Gen. col. | 13   |                 |       |              | 10.44         | calc.     | 19   |                 |       |
|              | 6.14          | HPLC      | 47   |                 |       | 208          | 8.16          | Gen. col. | 13   | $8.16 \pm 0.10$ | 203   |
|              | 6.96          | HPLC      | 47   |                 |       |              |               |           |      |                 |       |
|              | 8.18          | calc.     | 19   |                 |       | 209          | 9.60          | TLC       | 45   | $8.26 \pm 0.20$ | 262   |
|              | 7.75          | calc.     | 47   |                 |       |              | 8.26          | Gen. col. | 13   |                 |       |
| 129          | 6.50          | HPLC      | 47   | $7.30 \pm 0.50$ | 130   |              | 8.20          | Gen. col. | 46   |                 |       |
|              | 7.32          | calc.     | 47   |                 |       |              | 11.20         | calc.     | 19   |                 |       |
|              | 8.26          | calc.     | 19   |                 |       |              | 11.19         | calc.     | 46   |                 |       |
| 130          | 6.57          | HPLC      | 47   | $7.30 \pm 0.50$ |       |              |               |           |      |                 |       |
|              | 7.39          | calc.     | 47   |                 |       |              |               |           |      |                 |       |
| 134          | 8.18          | calc.     | 19   | $7.30 \pm 0.50$ | 122   |              |               |           |      |                 |       |

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<br>No.<br><i>n</i> | Vapor pressure, Pa   |                      | Ref.   | Henry's law<br>constants<br><i>H</i> , Pa m <sup>3</sup> /mol | Ref. | Selected values      |                      |                                                        |
|-----------------------------|----------------------|----------------------|--------|---------------------------------------------------------------|------|----------------------|----------------------|--------------------------------------------------------|
|                             | <i>P<sub>s</sub></i> | <i>P<sub>L</sub></i> |        |                                                               |      | <i>P<sub>s</sub></i> | <i>P<sub>L</sub></i> | <i>H</i> = <i>p<sub>L</sub></i> / <i>c<sub>L</sub></i> |
| 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 ± 0.09          | 0.90 ± 0.30          | 43 ± 15                                                |
|                             |                      | 1.41                 | 23     |                                                               |      |                      |                      |                                                        |
|                             | 0.172                | 0.57*                | 61     |                                                               |      |                      |                      |                                                        |
|                             |                      | 0.92                 | 59     |                                                               |      |                      |                      |                                                        |
|                             |                      | 0.94                 | 59     |                                                               |      |                      |                      |                                                        |
|                             | 0.175                |                      | 60     |                                                               |      |                      |                      |                                                        |
| 4                           | 0.35                 | 0.82*                | 57     | 22.29                                                         | 64   | 0.26 ± 0.13          | 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     |                                                               |      | 0.10 ± 0.10          | 20 ± 20              |                                                        |
|                             |                      | 0.0775               | 73     |                                                               |      |                      |                      |                                                        |
| 11                          | 0.0267               | 0.029*               | 66     |                                                               |      | 0.09 ± 0.03          |                      |                                                        |
|                             |                      | 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<br>No.<br><i>n</i> | Vapor pressure, Pa    |                       | Ref. | Henry's law<br>constants<br><i>H</i> , Pa m <sup>3</sup> /mol | Ref. | Selected values       |                       |                                                          |
|-----------------------------|-----------------------|-----------------------|------|---------------------------------------------------------------|------|-----------------------|-----------------------|----------------------------------------------------------|
|                             | <i>p</i> <sub>s</sub> | <i>p</i> <sub>L</sub> |      |                                                               |      | <i>p</i> <sub>s</sub> | <i>p</i> <sub>L</sub> | <i>H</i> = <i>p</i> <sub>L</sub> / <i>c</i> <sub>L</sub> |
| 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<br>No.<br><i>n</i> | Vapor pressure, Pa          |                                        | Ref.                 | Henry's law<br>constants<br><i>H</i> , Pa m <sup>3</sup> /mol | Ref. | Selected values                |                       |                                                          |
|-----------------------------|-----------------------------|----------------------------------------|----------------------|---------------------------------------------------------------|------|--------------------------------|-----------------------|----------------------------------------------------------|
|                             | <i>p</i> <sub>s</sub>       | <i>p</i> <sub>L</sub>                  |                      |                                                               |      | <i>p</i> <sub>s</sub>          | <i>p</i> <sub>L</sub> | <i>H</i> = <i>p</i> <sub>L</sub> / <i>c</i> <sub>L</sub> |
| 53                          | 0.0273                      | 59                                     | 30.40                | 64                                                            |      |                                |                       | 30±15                                                    |
| 66                          |                             |                                        |                      | 84.20                                                         | 64   |                                |                       | 84±42                                                    |
| 70                          | 0.0054<br>0.0064<br>0.00769 | 59<br>59<br>70                         | 20.26                | 64                                                            |      | 0.006±0.001                    |                       | 20±15                                                    |
| 77                          | 0.0022<br>0.0020            | 59<br>59                               |                      |                                                               |      | 0.002±0.002                    |                       | 1.7±1.7                                                  |
| 82                          |                             |                                        | 20.27                | 64                                                            |      |                                |                       | 20±15                                                    |
| 86                          | 0.0093                      | 0.051*                                 | 57                   |                                                               |      | 0.051±0.025                    |                       | 151±76                                                   |
| 87                          | 0.0023<br>0.00141           | 59<br>70                               | 33.44                | 64                                                            |      | 0.0023±0.005                   |                       | 25±10                                                    |
| 99                          | 0.0029                      | 59                                     |                      |                                                               |      |                                |                       |                                                          |
| 101                         | 0.0012<br>0.00096           | 0.0039*<br>0.0031*<br>0.0034<br>0.0040 | 66<br>67<br>59<br>59 | 11.46-35.46                                                   | 66   | 0.0011±0.0002<br>0.0035±0.0005 |                       | 35±10                                                    |
| 105                         | 0.00087<br>0.00094          | 59<br>59                               |                      |                                                               |      | 0.00090±<br>.00005             |                       |                                                          |
| 118                         | 0.0012                      | 59                                     | 40.53                | 64                                                            |      |                                |                       |                                                          |
| 128                         | 0.00034<br>5.08E-5          | 59<br>70                               | 50.66                | 64                                                            |      | 0.00034±<br>.00001             |                       | 12±6                                                     |
| 134                         | 0.000146                    | 70                                     | 57.76                | 64                                                            |      |                                |                       |                                                          |
| 138                         | 0.000506<br>0.000565        | 59<br>59                               | 48.64                | 64                                                            |      | 0.0005±<br>.0002               |                       | 82±40                                                    |
| 141                         |                             |                                        | 40.53                | 64                                                            |      | 0.0005±<br>.002                |                       | 40±20                                                    |
| 144                         |                             |                                        | 60.80                | 64                                                            |      |                                |                       | 60±30                                                    |
| 147                         | 0.0012<br>0.00183           | 59<br>59                               |                      |                                                               |      |                                |                       |                                                          |

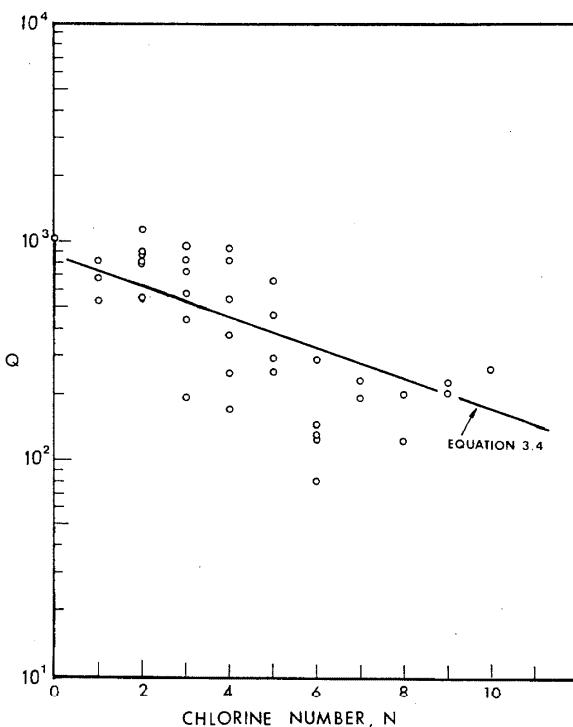
TABLE 5. Vapor pressure and Henry's law constants for PCB congeners at 25 °C — Continued

| Congener<br>No.<br><i>n</i> | Vapor pressure, Pa    |                       | Ref.  | Henry's law<br>constants<br><i>H</i> , Pa m <sup>3</sup> /mol | Ref. | Selected values       |                       |                                                          |
|-----------------------------|-----------------------|-----------------------|-------|---------------------------------------------------------------|------|-----------------------|-----------------------|----------------------------------------------------------|
|                             | <i>p</i> <sub>S</sub> | <i>p</i> <sub>L</sub> |       |                                                               |      | <i>p</i> <sub>S</sub> | <i>p</i> <sub>L</sub> | <i>H</i> = <i>p</i> <sub>L</sub> / <i>c</i> <sub>L</sub> |
| 149                         | 0.00112               | 59                    | 30.40 | 64                                                            |      | 0.0015±<br>.0005      |                       | 30±15                                                    |
|                             | 0.0018                | 59                    |       |                                                               |      |                       |                       |                                                          |
| 151                         |                       |                       | 30.40 | 64                                                            |      |                       |                       | 30±15                                                    |
| 153                         | 0.00058               | 59                    | 35.46 | 64                                                            |      | 0.0007±<br>.00002     |                       | 43±20                                                    |
|                             | 0.00072               | 59                    |       |                                                               |      |                       |                       |                                                          |
|                             | 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±<br>.00005    |                       | 5.4±2.0                                                  |
|                             | 0.00030               | 59                    |       |                                                               |      |                       |                       |                                                          |
| 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±<br>.0003      |                       | 37±20                                                    |
| 209                         | 5.17E-8               | 3.04E-5*              | 60    |                                                               |      | 0.00003±<br>.000015   |                       | 21±10                                                    |
|                             |                       | 1.39E-6               | 59    |                                                               |      |                       |                       |                                                          |
|                             |                       | 1.40E-5               | 68    |                                                               |      |                       |                       |                                                          |

\* calculated *p*<sub>L</sub> from *p*<sub>S</sub> using fugacity ratio *F* in Table 2.

TABLE 6. Summary of selected values of PCB congeners

| Congener<br>No. | Cl<br>No. | MW    | MP,K  | F       | S, g/m <sup>3</sup> |          | c <sub>S</sub><br>mmol/m <sup>3</sup> | c <sub>L</sub><br>mmol/m <sup>3</sup> | log K <sub>ow</sub> | Q         | P <sub>s</sub> , Pa | P <sub>L</sub> , Pa | H<br>Pa m <sup>3</sup> /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                                   | 129.5               | 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   | 0.0595  | 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 <sup>3</sup>                                        |
| $c_L$            | subcooled liquid solubility in water mol/m <sup>3</sup> or mmol/m <sup>3</sup> |
| $c_s$            | solid solubility in water, mol/m <sup>3</sup> or mmol/m <sup>3</sup>           |
| $c_{wo}$         | solubility in water saturated with octanol, mol/m <sup>3</sup>                 |
| $c_{ow}$         | solubility in octanol saturated with water, mol/m <sup>3</sup>                 |
| $H$              | Henry's law constant, Pa m <sup>3</sup> /mol                                   |
| $H'$             | dimensionless Henry's law constant                                             |
| $\Delta H_{fus}$ | 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                                                    |
| $\Delta S_{fus}$ | entropy of fusion, J/mol K                                                     |
| $S$              | aqueous solubility, g/m <sup>3</sup>                                           |
| $T$              | system temperature, K                                                          |
| $T_M$            | normal melting point, K                                                        |
| $v$              | molar volume, m <sup>3</sup> /mol or cm <sup>3</sup> /mol                      |

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