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ARTICLE *in* ENVIRONMENTAL SCIENCE AND TECHNOLOGY · APRIL 1993

Impact Factor: 5.33 · DOI: 10.1021/es00041a017

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Environ. Sci. Technol. 1993, 27, 725-731

Estimation of Gibbs Free Energies of Formation for Polychlorinated Biphenyls

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Gibbs free energies of formation for gas, subcooled liquid, and aqueous solution phases were estimated for all 209 polychlorinated biphenyl (PCB) congeners at 298.15 K and 100 000 Pa. A literature search was conducted to locate experimental data or predicted data for PCBs. Where other data were not available, the standard-state enthalpies of formation of the gas and absolute standard-state entropies of the gas were estimated using the NIST Structures and Properties Database and Estimation Program based on Benson's group additivity method. Resultant Gibbs free energies of formation in aqueous solution, as well as all intermediate quantities used in their calculation, are tabulated. Implications of the data relative to dechlorination are briefly discussed.

Introduction

Bioremediation techniques for polluted sediments and aquifers include degradation of toxic compounds by anaerobic microbes. The metabolic system of a microbe is characterized by a continuous input and output of matter and energy. Each cell has a system that transforms chemical and physical energy into biologically useful energy. The potential of any compound to serve as an energy source for an anaerobic microbe depends upon the Gibbs free energy of formation of the compound (*1*, *2*).

Polychlorinated biphenyl (PCB) congeners are environmentally significant halogenated aromatic compounds that could be a source of energy for anaerobic microorganisms by serving as electron acceptors (*3*). In a related study, estimates were made of the Gibbs free energy of formation values for series of halogenated compounds such as chlorobenzenes, chlorobenzoates, and chlorophenols. The results showed that reductive dehalogenation reactions, with these compounds serving as electron acceptors, potentially provide the organisms with sufficient energy to sustain their growth (*2*). A similar analysis of the situation for PCBs has been impossible so far due to a lack of Gibbs free energy values for PCBs. The present study was carried out to fill this void.

Calculation of Gibbs free energy of formation in aqueous solution requires standard-state enthalpy of formation of the ideal gas phase of the PCB, absolute standard-state entropy of the ideal gas phase, vapor pressure, and aqueous solubility. As for many organic chemicals of environmental relevance such as PCBs, these data are not readily available for the following reasons: (1) relatively few of the 209 PCB congeners have been synthesized in sufficient quantities that thermodynamic and physical property determinations have been possible and (2) the extremely low vapor pressures and aqueous solubilities of PCBs make these determinations experimentally demanding, resulting in some erroneous data (*4*).

Efforts to overcome the obstacles mentioned above have led to a variety of rules, correlations, and methods to use in calculating thermodynamic and physical property data for PCBs (*5*–*17*). The purpose of this study was to use the available experimental data and predictive techniques to estimate the Gibbs free energies of formation in aqueous solution for all 209 PCB congeners at standard temperature 298.15 K and pressure 100 000 Pa. A comprehensive table, even of limited accuracy, should be useful in preliminary exploration of environmental alternatives.

Method

The standard-state Gibbs free energy of formation of the ideal gaseous phase PCB, $\Delta_f G°_g$, was calculated by the equation (*18*)

$$\Delta_f G°_g = \Delta_f H°_g - T[S°_g - \sum(\nu_i S_i°_g)] \quad (1)$$

where $\Delta_f H°_g$ is the standard-state enthalpy of formation of the gas, T is the temperature of interest (298.15 K), $S°_g$ is the absolute standard-state entropy of the gas, ν_i is the stoichiometric coefficient of element i, and $S_i°_g$ is the absolute entropy of element i in its standard reference state. $S_i°_g$ values used for carbon, hydrogen, and chlorine were 5.74 ± 0.047, 65.34 ± 0.00369 and 111.54 ± 0.0045 J/mol·K. They were obtained from the JANAF tables and the reported uncertainties are average values (*18*).

Experimental values for $\Delta_f H°_g$ were found in the literature (*19*) for 2,2′-dichlorobiphenyl and 4,4′-dichlorobiphenyl. $S°_g$ values based on calculations from a molecular partition function or interpretation of experimental data were available for 2 chlorobiphenyl, 4 chlorobiphenyl, and 4,4′-dichlorobiphenyl (*20*). In addition, an estimation of these two properties based on the indicated experimental data was available for all the mono-, di-, and trichlorinated biphenyls (*20*).

For the remaining 170 compounds (tetra-, penta-, hexa-, hepta-, octa-, nona-, and decachlorinated biphenyls), $\Delta_f H°_g$ and $S°_g$ values were estimated by Benson's group additivity method using the NIST Structures and Properties Database and Estimation Program (*21*). To improve the predictions from Benson's method, additional correction terms beyond those indicated in the standard method were incorporated using the available experimental data as guidelines. A biphenyl enthalpy correction of 0.9 kJ/mol and an entropy correction of −9.7 J/mol·K were used. In addition, an enthalpy correction of 6.7 kJ/mol and an entropy correction of −10.7 J/mol·K were used to account for the steric hindrance encountered whenever a chlorine was attached in one or more of the following positions: 2,2′,6, and 6′. Chlorines in these positions distort the bond angles between the biphenyl rings, resulting in a sizable energy effect and the need for a correction term.

The standard-state Gibbs free energy of formation of the condensed phase, $\Delta_f G°_{cond}$, at 298.15 K was calculated

0013-936X/93/0927-0725$04.00/0

Table I. Gibbs Free Energies of Formation and Data for PCB Congeners at 298.15 K and 100 000 Pa

no.[a]	structure	VP[b] (Pa)	aq sol[c] (mol/m^3)	$\Delta_f H°_g$[d] (kJ/mol)	$S°_g$[e] (J/mol·K)	$\Delta_f G°_g$[f] (kJ/mol)	$\Delta_f G°_l$[g] (kJ/mol)	$\Delta_f G°_{aq}$[h] (kJ/mol)
				Biphenyl				
		2.03	1.48E-01[i]	182	392.7	280.1	253.3	275.2
				Monochlorobiphenyls				
1	2	9.26E-01	3.21E-02	159	423.1	262.7	234.0	259.6
2	3	3.62E-01	2.50E-02	154	434.7	253.8	222.7	249.0
3	4	3.20E-01	2.45E-02	152	426.5	255.0	223.6	250.0
				Dichlorobiphenyls				
4	2,2′	4.24E-01	7.60E-03	128	448.0	237.7	207.0	236.3
5	2,3	1.51E-01	7.62E-03	136	448.9	245.7	212.5	241.7
6	2,3′	1.65E-01	5.97E-03	129	458.2	235.9	202.9	232.7
7	2,4	1.75E-01	5.87E-03	129	449.6	238.4	205.5	235.4
8	2,4′	1.47E-01	5.89E-03	129	449.8	238.4	205.1	235.0
9	2,5	1.98E-01	5.96E-03	129	450.6	238.1	205.5	235.4
10	2,6	3.65E-01	7.64E-03	129	440.2	241.2	210.2	239.4
11	3,3′	6.46E-02	4.74E-03	122	464.1	227.4	192.1	222.5
12	3,4	5.32E-02	5.53E-03	129	460.3	235.7	199.9	229.9
13	3,4′	5.72E-02	4.65E-03	122	461.3	228.3	192.7	223.1
14	3,5	7.85E-02	4.71E-03	122	456.7	229.6	194.8	225.2
15	4,4′	5.08E-02	4.57E-03	121	446.7	231.3	195.4	225.9
				Trichlorobiphenyls				
16	2,2′,3	6.90E-02	1.96E-03	107	480.2	220.2	185.0	217.6
17	2,2′,4	8.00E-02	1.53E-03	99.6	480.2	213.1	178.3	211.5
18	2,2′,5	9.04E-02	1.56E-03	99.6	480.2	213.1	178.6	211.7
19	2,2′,6	1.67E-01	1.34E-03	99.6	478.2	213.7	180.7	214.2
20	2,3,3′	2.70E-02	1.56E-03	107	481.8	219.7	182.2	215.4
21	2,3,4	2.70E-02	1.82E-03	116	476.1	231.0	193.5	226.3
22	2,3,4′	2.39E-02	1.54E-03	107	476.1	221.4	183.6	216.8
23	2,3,5	4.02E-02	1.56E-03	107	476.1	221.4	184.9	218.1
24	2,3,6	8.70E-02	1.97E-03	107	472.4	222.5	187.9	220.5
25	2,3′,4	3.13E-02	1.23E-03	99.6	481.8	212.6	175.5	209.2
26	2,3′,5	3.53E-02	1.24E-03	99.6	481.8	212.6	175.8	209.5
27	2,3′,6	6.53E-02	1.57E-03	99.6	472.4	215.4	180.1	213.2
28	2,4,4′	2.77E-02	1.21E-03	99.6	476.1	214.3	176.9	210.6
29	2,4,5	3.66E-02	1.45E-03	107	476.1	221.4	184.7	218.0
30	2,4,6	9.46E-02	1.54E-03	99.6	466.7	217.1	182.7	215.9
31	2,4′,5	3.13E-02	1.23E-03	99.6	476.1	214.3	177.2	210.9
32	2,4′,6	5.78E-02	1.55E-03	99.6	466.7	217.1	181.5	214.7
33	2′,3,4	2.43E-02	1.44E-03	107	481.8	219.7	182.0	215.3
34	2′,3,5	3.60E-02	1.24E-03	99.6	476.1	214.3	177.5	211.2
35	3,3′,4	9.49E-03	1.17E-03	100	490.5	210.4	170.3	204.2
36	3,3′,5	1.41E-02	1.01E-03	92.9	484.7	205.0	165.9	200.2
37	3,4,4′	8.41E-03	1.15E-03	100	484.7	212.2	171.8	205.7
38	3,4,5	1.04E-02	1.37E-03	110	478.9	223.5	183.6	217.1
39	3,4′,5	1.25E-02	9.88E-04	92.9	478.9	206.8	167.4	201.6
				Tetrachlorobiphenyls				
40	2,2′,3,3′	1.12E-02	5.53E-04	87.1	507.1	206.3	166.7	202.4
41	2,2′,3,4	1.24E-02	5.14E-04	87.1	513.0	204.6	165.2	201.1
42	2,2′,3,4′	1.31E-02	4.42E-04	77.9	513.0	195.4	156.1	192.4
43	2,2′,3,5	1.83E-02	4.47E-04	77.9	513.0	195.4	156.9	193.2
44	2,2′,3,5′	1.47E-02	4.48E-04	77.9	513.0	195.4	156.4	192.6
45	2,2′,3,6	3.98E-02	3.94E-04	77.9	513.0	195.4	158.9	195.4
46	2,2′,3,6′	2.72E-02	3.89E-04	77.9	507.1	197.2	159.7	196.3
47	2,2′,4,4′	1.51E-02	3.53E-04	68.7	507.1	188.0	149.0	185.9
48	2,2′,4,5	1.67E-02	4.16E-04	77.9	513.0	195.4	156.7	193.2
49	2,2′,4,5′	1.70E-02	3.58E-04	68.7	513.0	186.2	147.6	184.4
50	2,2′,4,6	4.33E-02	3.15E-04	68.7	507.1	188.0	151.6	188.7
51	2,2′,4,6′	3.15E-02	3.12E-04	68.7	507.1	188.0	150.8	188.0
52	2,2′,5,5′	1.93E-02	3.62E-04	68.7	507.1	188.0	149.6	186.4
53	2,2′,5,6′	3.56E-02	3.16E-04	68.7	507.1	188.0	151.1	188.2
54	2,2′,6,6′	6.59E-02	3.49E-04	68.7	495.8	191.3	156.0	192.9
55	2,3,3′,4	4.81E-03	3.17E-04	87.1	513.0	204.6	162.8	199.9
56	2,3,3′,4′	3.96E-03	4.19E-04	87.1	513.0	204.6	162.4	198.8
57	2,3,3′,5	7.18E-03	3.63E-04	77.9	513.0	195.4	154.6	191.4
58	2,3,3′,5′	5.85E-03	3.63E-04	77.9	507.1	197.2	155.9	192.6
59	2,3,3′,6	1.55E-02	4.49E-04	77.9	513.0	195.4	156.5	192.8
60	2,3,4,4′	4.27E-03	4.13E-04	87.1	507.1	206.4	164.3	200.7
61	2,3,4,5	5.58E-03	4.86E-04	96.3	507.1	215.6	174.2	210.2
62	2,3,4,6	1.58E-02	5.17E-04	87.1	507.1	206.4	167.5	203.4
63	2,3,4′,5	6.36E-03	3.59E-04	77.9	507.1	197.2	156.1	192.9
64	2,3,4′,6	1.38E-02	4.44E-04	77.9	507.1	197.2	158.0	194.3
65	2,3,5,6	1.51E-02	5.56E-04	87.1	501.7	208.0	169.0	204.7

Table I. (Continued)

no.[a]	structure	VP[b] (Pa)	aq sol[c] (mol/m^3)	$\Delta_f H°_g$[d] (kJ/mol)	$S°_g$[e] (J/mol·K)	$\Delta_f G°_g$[f] (kJ/mol)	$\Delta_f G°_l$[g] (kJ/mol)	$\Delta_f G°_{aq}$[h] (kJ/mol)
				Tetrachlorobiphenyls				
66	2,3′,4,4′	4.59E-03	3.35E-04	77.9	513.0	195.4	153.5	190.5
67	2,3′,4,5	6.55E-03	3.38E-04	77.9	513.0	195.4	154.4	191.3
68	2,3′,4,5′	6.79E-03	2.91E-04	68.7	507.1	188.0	147.0	184.3
69	2,3′,4,6	1.69E-02	3.59E-04	68.7	507.1	188.0	149.3	186.1
70	2,3′,4′,5	5.19E-03	3.39E-04	77.9	513.0	195.4	153.8	190.8
71	2,3′,4′,6	9.59E-03	4.20E-04	77.9	507.1	197.2	157.1	193.5
72	2,3′,5,5′	7.66E-03	2.95E-04	68.7	507.1	188.0	147.3	184.6
73	2,3′,5′,6	1.42E-02	3.64E-04	68.7	501.7	189.6	150.5	187.2
74	2,4,4′,5	5.80E-03	3.35E-04	77.9	507.1	197.2	155.9	192.8
75	2,4,4′,6	1.50E-02	3.55E-04	68.7	501.7	189.6	150.6	187.4
76	2′,3,4,5	4.76E-03	3.92E-04	87.1	507.1	206.4	164.6	201.1
77	3,3′,4,4′	1.40E-03	3.19E-04	80.4	517.9	196.4	151.6	188.7
78	3,3′,4,5	1.86E-03	3.23E-04	80.4	517.9	196.4	152.3	189.4
79	3,3′,4,5′	2.07E-03	2.79E-04	71.2	517.9	187.2	143.4	180.8
80	3,3′,5,5′	3.05E-03	2.44E-04	62.0	506.6	181.4	138.5	176.2
81	3,4,4′,5	1.65E-03	3.18E-04	80.4	512.5	198.1	153.6	190.7
				Pentachlorobiphenyls				
82	2,2′,3,3′,4	2.01E-03	1.60E-04	66.6	543.9	188.7	144.7	183.5
83	2,2′,3,3′,5	2.99E-03	1.41E-04	57.4	543.9	179.5	136.5	175.6
84	2,2′,3,3′,6	6.48E-03	1.25E-04	57.4	543.9	179.5	138.4	177.8
85	2,2′,3,4,4′	2.33E-03	1.31E-04	57.4	543.9	179.5	135.9	175.2
86	2,2′,3,4,5	1.28E-02	1.52E-04	66.6	543.9	188.7	149.3	188.2
87	2,2′,3,4,5′	2.62E-03	1.32E-04	57.4	543.9	179.5	136.2	175.4
88	2,2′,3,4,6	1.61E-02	1.18E-04	57.4	543.9	179.5	140.7	180.2
89	2,2′,3,4,6′	4.85E-03	1.17E-04	57.4	538.1	181.1	139.5	179.0
90	2,2′,3,4′,5	3.48E-03	1.15E-04	48.2	543.9	170.3	127.7	167.3
91	2,2′,3,4′,6	7.52E-03	1.03E-04	48.2	543.9	170.3	129.6	169.5
92	2,2′,3,5,5′	3.92E-03	1.16E-04	48.2	543.9	170.3	128.0	167.6
93	2,2′,3,5,6	1.51E-02	1.26E-04	57.4	538.1	181.2	142.3	181.6
94	2,2′,3,5,6′	7.24E-03	1.03E-04	48.2	538.1	172.0	131.2	171.1
95	2,2′,3,5′,6	8.49E-03	1.03E-04	48.2	543.9	170.3	129.9	169.8
96	2,2′,3,6,6′	1.57E-02	1.13E-04	48.2	538.1	172.0	133.2	172.8
97	2,2′,3′,4,5	2.73E-03	1.32E-04	57.4	543.9	179.5	136.3	175.5
98	2,2′,3′,4,6	7.05E-03	1.02E-04	48.2	538.1	172.0	131.2	171.1
99	2,2′,4,4′,5	3.16E-03	1.08E-04	48.2	543.9	170.3	127.4	167.2
100	2,2′,4,4′,6	8.18E-03	8.41E-05	39.0	538.1	162.8	122.3	162.7
101	2,2′,4,5,5′	3.58E-03	1.09E-04	48.2	543.9	170.3	127.8	167.5
102	2,2′,4,5,6′	6.61E-03	9.63E-05	48.2	538.1	172.0	131.0	171.1
103	2,2′,4,5′,6	9.23E-03	8.43E-05	39.0	538.1	162.8	122.6	163.0
104	2,2′,4,6,6′	1.70E-02	9.20E-05	39.0	532.2	164.5	125.9	166.1
105	2,3,3′,4,4′	7.07E-04	1.24E-04	66.6	543.9	188.7	142.1	181.6
106	2,3,3′,4,5	5.00E-03	1.26E-04	66.6	543.9	188.7	147.0	186.4
107	2,3,3′,4′,5	1.05E-03	1.10E-04	57.4	543.9	179.5	133.9	173.6
108	2,3,3′,4,5′	1.04E-03	1.09E-04	57.4	538.1	181.2	135.6	175.4
109	2,3,3′,4,6	6.30E-03	1.33E-04	57.4	543.9	179.5	138.4	177.6
110	2,3,3′,4′,6	2.28E-03	1.33E-04	57.4	543.9	179.5	135.8	175.1
111	2,3,3′,5,5′	1.56E-03	9.64E-05	48.2	538.1	172.0	127.4	167.5
112	2,3,3′,5,6	5.91E-03	1.42E-04	57.4	538.1	181.2	139.9	179.0
113	2,3,3′,5′,6	3.37E-03	1.17E-04	48.2	538.1	172.0	129.4	168.9
114	2,3,4,4′,5	4.43E-03	1.24E-04	66.6	538.1	190.4	148.4	187.8
115	2,3,4,4′,6	5.58E-03	1.31E-04	57.4	538.1	181.2	139.8	179.1
116	2,3,4,5,6	3.41E-03	1.86E-04	75.8	532.2	201.3	158.7	197.1
117	2,3,4′,5,6	5.23E-03	1.40E-04	57.4	532.2	182.9	141.4	180.5
118	2,3′,4,4′,5	9.62E-04	1.03E-04	57.4	543.9	179.5	133.7	173.6
119	2,3′,4,4′,6	2.48E-03	1.08E-04	48.2	538.1	172.0	128.6	168.4
120	2,3′,4,5,5′	1.42E-03	9.05E-05	48.2	538.1	172.0	127.2	167.4
121	2,3′,4,5′,6	3.68E-03	9.54E-05	39.0	532.2	164.5	122.1	162.2
122	2′,3,3′,4,5	7.76E-04	1.25E-04	66.6	538.1	190.4	144.1	183.5
123	2′,3,4,4′,5	9.01E-04	1.02E-04	57.4	538.1	181.2	135.3	175.2
124	2′,3,4,5,5′	1.01E-03	1.03E-04	57.4	538.1	181.2	135.6	175.5
125	2′,3,4,5,6′	1.87E-03	1.25E-04	57.4	532.2	182.9	138.8	178.2
126	3,3′,4,4′,5	2.74E-04	9.84E-05	59.9	548.9	180.5	131.6	171.6
127	3,3′,4,5,5′	4.04E-04	8.72E-05	50.7	543.0	173.0	125.1	165.4
				Hexachlorobiphenyls				
128	2,2′,3,3′,4,4′	3.59E-04	5.23E-05	46.1	569.0	174.4	126.2	167.8
129	2,2′,3,3′,4,5	2.08E-03	5.27E-05	46.1	574.9	172.7	128.8	170.4
130	2,2′,3,3′,4,5′	5.35E-04	4.65E-05	36.9	574.9	163.5	116.3	158.1
131	2,2′,3,3′,4,6	2.62E-03	4.18E-05	36.9	574.9	163.5	120.2	162.3
132	2,2′,3,3′,4,6′	1.16E-03	4.14E-05	36.9	574.9	163.5	118.2	160.3
133	2,2′,3,3′,5,5′	7.98E-04	4.14E-05	27.7	569.0	156.0	109.8	152.0
134	2,2′,3,3′,5,6	2.46E-03	4.43E-05	36.9	569.0	165.2	121.8	163.8

Table I. (Continued)

no.[a]	structure	VP[b] (Pa)	aq sol[c] (mol/m^3)	$\Delta_f H°_g$[d] (kJ/mol)	$S°_g$[e] (J/mol·K)	$\Delta_f G°_g$[f] (kJ/mol)	$\Delta_f G°_l$[g] (kJ/mol)	$\Delta_f G°_{aq}$[h] (kJ/mol)
				Hexachlorobiphenyls				
135	2,2′,3,3′,5,6′	1.73E-03	3.69E-05	27.7	574.9	154.3	110.0	152.4
136	2,2′,3,3′,6,6′	3.74E-03	4.01E-05	27.7	569.0	156.0	113.7	155.9
137	2,2′,3,4,4′,5	2.41E-03	4.39E-05	36.9	574.9	163.5	120.0	162.0
138	2,2′,3,4,4′,5′	4.87E-04	4.40E-05	36.9	574.9	163.5	116.1	158.0
139	2,2′,3,4,4′,6	3.05E-03	3.50E-05	27.7	574.9	154.3	111.4	154.0
140	2,2′,3,4,4′,6′	1.26E-03	3.46E-05	27.7	569.0	156.0	110.9	153.5
141	2,2′,3,4,5,5′	2.73E-03	4.43E-05	36.9	574.9	163.5	120.3	162.3
142	2,2′,3,4,5,6	3.41E-03	4.75E-05	46.1	569.0	174.4	131.8	173.6
143	2,2′,3,4,5,6′	5.05E-03	3.96E-05	36.9	569.0	165.2	123.6	165.8
144	2,2′,3,4,5′,6	3.45E-03	3.50E-05	27.7	574.8	154.3	111.7	154.3
145	2,2′,3,4,6,6′	6.36E-03	3.79E-05	27.7	569.0	156.0	115.0	157.3
146	2,2′,3,4′,5,5′	7.28E-04	3.92E-05	27.7	574.9	154.3	107.8	150.1
147	2,2′,3,4′,5,6	2.86E-03	3.70E-05	27.7	569.0	156.0	113.0	155.4
148	2,2′,3,4′,5,6′	1.87E-03	3.10E-05	18.5	569.0	146.8	102.7	145.6
149	2,2′,3,4′,5′,6	1.57E-03	3.51E-05	27.7	574.9	154.3	109.8	152.3
150	2,2′,3,4′,6,6′	4.07E-03	3.36E-05	18.5	569.0	146.8	104.7	147.3
151	2,2′,3,5,5′,6	3.22E-03	3.71E-05	27.7	569.0	156.0	113.3	155.7
152	2,2′,3,5,6,6′	5.96E-03	4.02E-05	27.7	563.2	157.8	116.6	158.8
153	2,2′,4,4′,5,5′	6.63E-04	3.70E-05	27.7	569.0	156.0	109.4	151.8
154	2,2′,4,4′,5,6′	1.71E-03	2.93E-05	18.5	569.0	146.8	102.5	145.5
155	2,2′,4,4′,6,6′	4.43E-03	2.81E-05	9.27	557.3	141.1	99.1	142.2
156	2,3,3′,4,4′,5	7.34E-04	4.20E-05	46.1	574.9	126.3	168.4	157
157	2,3,3′,4,4′,5′	1.39E-04	4.20E-05	46.1	569.0	174.4	123.9	166.0
158	2,3,3′,4,4′,6	9.26E-04	4.41E-05	36.9	574.9	163.5	117.6	159.6
159	2,3,3′,4,5,5′	1.08E-03	3.74E-05	36.9	569.0	165.2	119.8	162.2
160	2,3,3′,4,5,6	1.33E-03	5.30E-05	46.1	569.0	174.4	129.5	171.0
161	2,3,3′,4,5′,6	1.37E-03	3.92E-05	27.7	569.0	156.0	111.2	153.4
162	2,3,3′,4′,5,5′	2.07E-04	3.75E-05	36.9	569.0	165.2	115.7	158.1
163	2,3,3′,4′,5,6	8.67E-04	4.68E-05	36.9	569.0	165.2	119.2	161.1
164	2,3,3′,4′,5′,6	4.48E-04	4.46E-05	36.9	569.0	165.2	117.6	159.5
165	2,3,3′,5,5′,6	1.29E-03	4.16E-05	27.7	563.2	157.8	112.8	154.9
166	2,3,4,4′,5,6	1.18E-03	5.25E-05	46.1	563.2	176.2	130.9	172.5
167	2,3′,4,4′,5,5′	1.88E-04	3.54E-05	36.9	569.0	165.2	115.4	158.0
168	2,3′,4,4′,5′,6	4.87E-04	3.71E-05	27.7	563.2	157.8	110.3	152.8
169	3,3′,4,4′,5,5′	5.36E-05	3.41E-05	39.4	568.1	168.0	115.1	157.7
				Heptachlorobiphenyls				
170	2,2′,3,3′,4,4′,5	3.72E-04	1.94E-05	25.6	605.4	156.9	108.8	152.8
171	2,2′,3,3′,4,4′,6	4.69E-04	1.58E-05	16.39	605.4	147.7	100.1	144.6
172	2,2′,3,3′,4,5,5′	5.55E-04	1.74E-05	16.39	605.4	147.7	100.5	144.8
173	2,2′,3,3′,4,5,6	5.55E-04	1.85E-05	25.6	600.0	158.5	111.4	155.5
174	2,2′,3,3′,4,5,6′	1.21E-03	1.58E-05	16.39	605.4	147.7	102.5	147.0
175	2,2′,3,3′,4,5′,6	7.00E-04	1.41E-05	7.18	605.4	138.4	91.9	136.7
176	2,2′,3,3′,4,6,6′	1.53E-03	1.52E-05	7.18	605.4	138.4	93.8	138.4
177	2,2′,3,3′,4′,5,6	4.40E-04	1.66E-05	16.39	600.0	149.3	101.6	146.0
178	2,2′,3,3′,5,5′,6	6.57E-04	1.49E-05	7.18	600.0	140.1	93.4	138.0
179	2,2′,3,3′,5,6,6′	1.42E-03	1.60E-05	16.39	605.4	147.7	102.9	147.4
180	2,2′,3,4,4′,5,5′	5.06E-04	1.66E-05	7.18	600.0	140.1	92.7	137.1
181	2,2′,3,4,4′,5,6	6.44E-04	1.58E-05	16.39	600.0	149.3	102.5	147.1
182	2,2′,3,4,4′,5,6′	1.31E-03	1.35E-05	7.18	600.0	140.1	95.1	140.0
183	2,2′,3,4,4′,5′,6	6.38E-04	1.35E-05	7.18	605.4	138.4	91.7	136.6
184	2,2′,3,4,4′,6,6′	1.65E-03	1.30E-05	−2.02	600.0	130.9	86.4	131.5
185	2,2′,3,4,5,5′,6	7.28E-04	1.58E-05	16.39	600.0	149.3	102.8	147.4
186	2,2′,3,4,5,6,6′	1.35E-03	1.70E-05	16.39	594.1	151.0	106.1	150.4
187	2,2′,3,4′,5,5′,6	5.98E-04	1.42E-05	7.18	600.0	140.1	93.1	137.9
188	2,2′,3,4′,5,6,6′	1.55E-03	1.36E-05	−2.0	594.1	132.6	88.0	132.9
189	2,3,3′,4,4′,5,5′	1.44E-04	1.60E-05	25.6	600.0	158.5	108.0	152.5
190	2,3,3′,4,4′,5,6	1.96E-04	1.94E-05	25.6	600.0	158.5	108.8	152.8
191	2,3,3′,4,4′,5′,6	2.89E-04	1.67E-05	16.39	600.0	149.3	100.5	144.9
192	2,3,3′,4,5,5′,6	2.89E-04	1.75E-05	16.39	594.1	151.0	102.3	146.6
193	2,3,3′,4′,5,5′,8	1.70E-04	1.76E-05	16.39	594.1	151.0	101.0	145.2
				Octachlorobiphenyls				
194	2,2′,3,3′,4,4′,5,5′	3.86E-04	8.13E-06	5.09	630.5	142.6	94.6	140.8
195	2,2′,3,3′,4,4′,5,6	9.92E-05	7.77E-06	5.09	630.5	142.6	91.3	137.5
196	2,2′,3,3′,4,4′,5′,6	4.87E-04	6.77E-04	−4.1	636.4	131.7	84.3	130.9
197	2,2′,3,3′,4,4′,6,6′	6.15E-04	6.54E-06	−13.3	630.5	124.3	77.4	124.1
198	2,2′,3,3′,4,5,5′,6	1.48E-04	7.06E-06	−4.1	630.5	133.5	83.1	129.6
199	2,2′,3,3′,4,5,6,6′	3.20E-04	7.51E-06	−4.1	630.5	133.5	85.0	131.3
200	2,2′,3,3′,4,5′,6,6′	4.56E-04	6.81E-06	−13.3	630.5	124.3	76.6	123.3
201	2,2′,3,3′,4′,5,5′,6	4.56E-04	7.07E-06	−4.1	630.5	133.5	85.8	132.4
202	2,2′,3,3′,5,5′,6,6′	5.40E-04	7.12E-06	−13.3	619.2	127.6	80.4	126.9
203	2,2′,3,4,4′,5,5′,6	1.35E-04	6.77E-06	−4.1	630.5	133.5	82.8	129.5

Table I. (Continued)

no.[a]	structure	VP[b] (Pa)	aq sol[c] (mol/m³)	$\Delta_f H°_g$[d] (kJ/mol)	$S°_g$[e] (J/mol·K)	$\Delta_f G°_g$[f] (kJ/mol)	$\Delta_f G°_l$[g] (kJ/mol)	$\Delta_f G°_{aq}$[h] (kJ/mol)
				Octachlorobiphenyls				
204	2,2′,3,4,4′,5,6,6′	3.49E-04	6.54E-06	−13.3	624.7	126.0	77.7	124.4
205	2,3,3′,4,4′,5,5′,6	3.84E-05	0.15E-06	5.09	624.7	144.4	90.6	136.8
				Nonachlorobiphenyls				
206	2,2′,3,3′,4,4′,5,5′,6	1.03E-04	3.72E-06	−15.4	661.5	126.7	75.4	123.5
207	2,2′,3,3′,4,4′,5,6,6′	1.30E-04	3.61E-06	−24.6	661.5	117.5	66.8	115.0
208	2,2′,3,3′,4,5,5′,6,6′	1.22E-04	3.74E-06	−24.6	655.6	119.2	68.4	116.5
				Decachlorobiphenyl				
209	2,2′,3,3′,4,4′,5,5′,6,6′	2.75E-05	2.19E-06	−35.9	680.7	114.2	59.7	109.1

[a] Reference 29. [b] Reference 6; all subcooled liquid values, average uncertainty ±75%. [c] Aqueous solubility (*6*); all subcooled liquid values, average uncertainty ±96%. [d] First 39 values refs 19 and 20, otherwise ref 21; average uncertainty ±2.09 kJ/mol (*13*). [e] First 39 values refs 19 and 20, otherwise ref 20; average uncertainty ±1.25 J/mol·K (*13*). [f] Average uncertainty ±2.1 kJ/mol. [g] Subcooled liquid, average uncertainty ±2.8 kJ/mol. [h] Average uncertainty ±3.7 kJ/mol. [i] Values expressed as xE-0y are $x \times 10^{-y}$.

by the equation

$$\Delta_f G°_{cond} = \Delta_f G°_g + RT \ln (P/P°) \quad (2)$$

where R is the ideal gas constant, P is the vapor pressure of the condensed phase, and $P°$ is the standard-state pressure (100 000 Pa).

Use of this equation assumes that vapor pressures are less than 304 kPa and that the compound is not chemically associated in the vapor phase. Both assumptions apply to PCBs.

The literature provided a variety of PCB vapor pressure values (*4–7, 12, 22–24*). For the purposes of completeness, consistency, and validity, we chose to use the subcooled liquid values determined by Burkhard et al. (*6*). This choice results in $\Delta_f G°_l$ for the subcooled liquid phase.

The change from condensed phase to an ideal solution of PCB in water at unit molality and standard temperature and pressure was estimated as recommended by Denbigh (*25*) using the equation

$$\Delta_f G^{\square}_{soln} = \Delta_f G°_{cond} - RT \ln \left(\gamma_i \frac{m_{i_{cond}}}{m°_i} \right) \quad (3)$$

where $\Delta_f G^{\square}_{soln}$ is the standard-state Gibbs free energy of formation of the ideal solution at unit molality, γ_i is the activity coefficient of the solute, $m_{i_{cond}}$ is the molality of the condensed phase solute, and $m°_i$ is the standard-state molality (1 mol of PCB/kg of H_2O).

Since we are dealing with weak solutions, we assume γ_i equals 1 and convert aqueous solubility to molality by assuming the solution is water only.

As in the case of vapor pressures, the literature provided a variety of aqueous solubilities (*4, 6, 9–11, 15–17, 22, 26, 27*). For the reasons stated before, we chose to use all subcooled liquid values determined by Burkhard et al. (*6*).

Results and Discussion

Table I shows the estimated Gibbs free energies of formation in aqueous solution for all 209 PCB congeners and the intermediate results used in the calculations. The free-energy values in aqueous solution are the items of greatest interest for environmental purposes and the ultimate aim of this table.

There were no literature values for $\Delta_f G^{\square}_{aq}$ in aqueous solution against which to compare the values in Table I. Of course agreement with the very limited data available for $\Delta_f H°_g$ and $S°_g$ was good as these data were utilized to construct the correction factors.

The estimated values for $\Delta_f G°_g$ as an ideal gas for mono-, di-, and trichlorinated biphenyls from ref 20 are compared to the values from the corrected Benson's method in Table II. The average absolute difference for the available 39 compounds is 1.04 kJ/mol, which represents a 1.78% average. This compares satisfactorily with the average uncertainty reported by Benson for his method of 2.1 kJ/mol (*13*). However, since the comparison here is between two sets of estimated values, there is no assurance as to the true accuracy of either set of values. Since the values in ref 20 have a wide acceptance, they are used in Table I for the first 39 compounds. For the remaining 170 compounds, the corrected Benson method was employed. Sources of other intermediate values utilized to give values of the desired $\Delta_f G^{\square}_{aq}$ in aqueous solution are listed in Table I.

Uncertainty analysis for Table I was performed by the method of equal effects (*28*). Each input quantity had an associated average uncertainty as reported in the literature. Uncertainties for calculated quantities involve uncertainty contributions from all appropriate input quantities. The average uncertainty for $\Delta_f G^{\square}_{aq}$ in aqueous solution was calculated to be 3.7 kJ/mol. The uncertainty results are also included in Table I footnotes. With the indicated level of uncertainty, any small differences between isomers have to be viewed with skepticism.

A comparison of the Gibbs free energy of formation of substrates and products in aqueous solution allows an estimation of the amount of energy that becomes available during a dechlorination reaction (*1, 2*). Using the data listed in Table I, such calculations indicate that, with hydrogen as the electron donor under standard conditions, the energy available from reductive dechlorination of PCBs ranges between 145 and 168 kJ per dechlorination reaction. Under environmentally relevant hydrogen partial pressures of 100 Pa, these values drop to 128 and 151 kJ per dechlorination reaction; but this amount of energy is still more than enough to theoretically allow microorganisms to grow with hydrogen as an electron donor and PCBs as electron acceptors. Whether such organisms actually exist will of course depend on the evolution of enzymatic mechanisms that can capture this energy efficiently enough. Recently it has been shown that microorganisms

Table II. Comparison of TRC (*20*) and Corrected Benson Predictions for Ideal Gas Gibbs Free Energy of Formation

no.[a]	structure	$\Delta_f G°_g$ (kJ/mol) TRC[b]	corrected Benson	diff
		Monochloribiphenyls		
1	2	262.7	262.9	0.2
2	3	253.8	253.0	−0.8
3	4	255.0	254.6	−0.4
		Dichlorobiphenyls		
4	2,2′	237.7	237.7	0.0
5	2,3	245.7	246.9	0.2
6	2,3′	235.9	236.0	0.1
7	2,4	238.4	237.7	−0.7
8	2,4	238.4	237.7	−0.7
9	2,5	238.1	237.7	−0.4
10	2,6	241.2	239.5	−1.7
11	3,3′	227.4	227.8	0.4
12	3,4	235.7	237.0	0.3
13	3,4′	228.3	227.8	−0.5
14	3,5	229.6	229.6	0.0
15	4,4′	231.3	231.3	0.0
		Trichlorobiphenyls		
16	2,2′,3	220.2	220.4	0.2
17	2,2′,4	213.1	210.8	−2.3
18	2,2′,5	213.1	210.8	−2.3
19	2,2′,6	213.7	212.5	−1.2
20	2,3,3′	219.7	220.4	0.7
21	2,3,4	231.0	231.0	0.0
22	2,3,4′	221.4	222.2	0.8
23	2,3,5	221.4	222.2	0.8
24	2,3,6	222.5	222.2	−0.3
25	2,3′,4	212.6	210.8	−1.8
26	2,3′,5	212.6	210.8	−1.8
27	2,3′,6	215.4	212.5	−2.9
28	2,4,4′	214.3	212.5	−1.8
29	2,4,5	221.4	222.2	0.8
30	2,4,6	217.1	214.3	−2.8
31	2,4′,5	214.3	212.5	−1.8
32	2,4′,6	217.1	214.3	−2.8
33	2′,3,4	219.7	220.4	0.7
34	2′,3,5	214.3	212.5	−1.8
35	3,3′,4	210.4	210.5	0.1
36	3,3′,5	205.0	202.6	−3.4
37	3,4,4′	212.2	212.3	0.1
38	3,4,5	223.5	222.8	−0.7
39	3,4′,5	206.8	204.4	−2.4
abs av diff				1.04

[a] Reference 29. [b] Reference 20.

exist that can catalyze the reductive dechlorination of many of the highly chlorinated PCBs (*30*). Whether these organisms indeed benefit from these reactions is not clear, but the fact that it is possible to enrich for this activity suggests that this may indeed be the case.

Registry numbers supplied by the authors: Biphenyl, 92-52-4; 2-CB, 2051-60-7; 3-CB, 2051-61-8; 4-CB, 2051-62-9; 2,2′-CB, 13029-08-8; 2,3-CB, 16605-91-7; 2,3′-CB, 25569-80-6; 2,4-CB, 33284-50-3; 2,4′-CB, 34883-43-7; 2,5-CB, 34883-39-1; 2,6-CB, 33146-45-1; 3,3′-CB, 2050-67-1; 3,4-CB, 2974-92-7; 3,4′-CB, 2974-90-5; 3,5-CB, 34883-41-5; 4,4′-CB, 2050-68-2; 2,2′,3-CB, 38444-78-9; 2,2′,4-CB, 37680-66-3; 2,2′-,5-CB, 37680-65-2; 2,2′,6-CB, 38444-73-4; 2,3,3′-CB, 38444-84-7; 2,3,4-CB, 55702-46-0; 2,3,4′-CB, 38444-85-8; 2,3,5-CB, 55720-44-0; 2,3,6-CB, 58702-45-9; 2,3′,4-CB, 55712-37-3; 2,3′,5-CB, 38444-81-4; 2,3′,6-CB, 38444-76-7; 2,4,4′-CB, 7012-37-5; 2,4,5-CB, 15862-07-4; 2,4,6-CB, 35693-92-6; 2,4′,5-CB, 16606-02-3; 2,4′,6-CB, 38444-77-8; 2′,3,4-CB, 38444-86-9; 2′,3,5-CB, 37680-68-5; 3,3′,4-CB, 37680-69-6; 3,3′,5-CB, 38444-87-0; 3,4,4′-CB, 38444-90-5; 3,4,5-CB, 53555-66-1; 3,4′,5-CB, 38444-88-1; 2,2′,3,3′-CB, 38444-93-8; 2,2′,3,4-CB, 52663-59-9; 2,2′,3,4′-CB, 36559-22-5; 2,2′,3,5-CB, 70362-46-8; 2,2′,3,5′-CB, 41464-39-5; 2,2′,3,6-CB, 70362-45-7; 2,2′,3,6′-CB, 41464-47-5; 2,2′,4,4′-CB, 2437-79-8; 2,2′,4,5-CB, 70362-47-9; 2,2′,4,5′-CB, 41464-40-8; 2,2′,4,6-CB, 62796-65-8; 2,2′,4,6′-CB, 65194-04-7; 2,2′,5,5′-CB, 35693-99-3; 2,2′,5,6′-CB, 41464-41-9; 2,2′,6,6′-CB, 15968-05-5; 2,3,3′,4-CB, 74338-24-2; 2,3,3′,4′-CB, 41464-43-1; 2,3,3′,5-CB, 70424-67-8; 2,3,3′,5′-CB, 41464-49-7; 2,3,3′,6-CB, 74472-33-6; 2,3,4,4′-CB, 33025-41-1; 2,3,4,5-CB, 33284-53-6; 2,3,4,6-CB, 54230-23-7; 2,3,4′,5-CB, 74472-35-8; 2,3,4′,6-CB, 52663-58-8; 2,3,5,6-CB, 33284-54-7; 2,3′,4,4′-CB, 32598-10-0; 2,3′,4,5-CB, 73575-53-8; 2,3′,4,5′-CB, 73575-52-7; 2,3′,4,6-CB, 60233-24-1; 2,3′,4′,5-CB, 32598-11-1; 2,3′,4′,6-CB, 41464-46-4; 2,3′,5,5′-CB, 41464-42-0; 2,3′,5′,6-CB, 74338-23-1; 2,4,4′,5-CB, 32690-93-0; 2,4,4′,6-CB, 32598-12-2; 2′,3,4,5-CB, 70362-48-0; 3,3′,4,4′-CB, 32598-13-3; 3,3′,4,5-CB, 70362-49-1; 3,3′,4,5′-CB, 41464-48-6; 3,3′,5,5′-CB, 33284-52-5; 3,4,4′,5-CB, 70362-50-4; 2,2′,3,3′,4-CB, 52663-62-4; 2,2′,3,3′,5-CB, 60145-20-2; 2,2′,3,3′,6-CB, 52663-60-2; 2,2′,3,4,4′-CB, 65510-45-4; 2,2′,3,4,5-CB, 55312-69-1; 2,2′-,3,4,5′-CB, 38380-02-8; 2,2′,3,4,6-CB, 55215-17-3; 2,2′,3,4,6′-CB, 73575-57-2; 2,2′,3,4′,5-CB, 68194-07-0; 2,2′,3,4′,6-CB, 58194-05-8; 2,2′,3,5,5′-CB, 52663-61-3; 2,2′,3,5,6-CB, 73575-56-1; 2,2′,3,5,6′-CB, 73575-55-0; 2,2′,3,5′,6-CB, 38379-99-6; 2,2′,3,6,6′-CB, 73575-54-9; 2,2′,3′,4,5-CB, 41464-51-1; 2,2′,3′,4,6-CB, 60233-25-2; 2,2′,4,4′,5-CB, 38380-01-7; 2,2′,4,4′,6-CB, 39485-83-1; 2,2′,4,5,5′-CB, 37680-73-2; 2,2′,4,5,6′-CB, 68194-06-9; 2,2′,4,5′,6-CB, 60145-21-3; 2,2′,4,6,6′-CB, 56558-16-8; 2,3,3′,4,4′-CB, 32598-14-4; 2,3,3′,4,5-CB, 70424-69-0; 2,3,3′,4′,5-CB, 70424-68-9; 2,3,3′,4,5′-CB, 70362-41-3; 2,3,3′,4,6-CB, 74472-35-8; 2,3,3′,4′,6-CB, 38380-03-9; 2,3,3′,5,5′-CB, 39635-32-0; 2,3,3′,5,6-CB, 74472-36-9; 2,3,3′,5′,6-CB, 68194-10-5; 2,3,4,4′,5-CB, 74472-37-0; 2,3,4,4′,6-CB, 74472-38-1; 2,3,4,5,6-CB, 18259-05-7; 2,3,4′,5,6-CB, 68194-11-6; 2,3′,4,4′,5-CB, 31508-00-6; 2,3′,4,4′,6-CB, 56558-17-9; 2,3′,4,5,5′-CB, 68194-12-7; 2,3′,4,5′,6-CB, 56558-18-0; 2′,3,3′,4,5-CB, 76842-07-4; 2′,3,4,4′,5-CB, 65510-44-3; 2′,3,4,5,5′-CB, 70424-70-3; 2′,3,4,5,6′-CB, 74472-39-2; 3,3′,4,4′,5-CB, 57465-28-8; 3,3′,4,5,5′-CB, 39635-33-1; 2,2′,3,3′,4,4′-CB, 38380-07-3; 2,2′,3,3′,4,5-CB, 55215-18-4; 2,2′,3,3′,4,5′-CB, 52663-66-8; 2,2′,3,3′,4,6-CB, 61798-70-7; 2,2′,3,3′,4,6′-CB, 38380-05-1; 2,2′,3,3′,5,5′-CB, 35694-04-3; 2,2′,3,3′,5,6-CB, 52704-70-8; 2,2′,3,3′,5,6′-CB, 52744-13-5; 2,2′,3,3′,6,6′-CB, 38411-22-2; 2,2′,3,4,4′,5-CB, 35694-06-5; 2,2′,3,4,4′,5′-CB, 35065-28-2; 2,2′,3,4,4′,6-CB, 56030-56-9; 2,2′,3,4,4′,6′-CB, 59291-64-4; 2,2′,3,4,5,5′-CB, 52712-04-6; 2,2′,3,4,5,6-CB, 41411-61-4; 2,2′,3,4,5,6′-CB, 68194-15-0; 2,2′,3,4,5′,6-CB, 68194-14-9; 2,2′,3,4,6,6′-CB, 74472-40-5; 2,2′,3,4′,5,5′-CB, 51908-16-8; 2,2′,3,4′,5,6-CB, 68194-13-8; 2,2′,3,4′,5,6′-CB, 74472-42-7; 2,2′,3,4′,5′,6-CB, 38380-04-0; 2,2′,3,4′,6,6′-CB, 68194-08-1; 2,2′,3,5,5′,6-CB, 52663-63-5; 2,2′,3,5,6,6′-CB, 68194-09-2; 2,2′,4,4′,5,5′-CB, 35065-27-1; 2,2′,4,4′,5,6′-CB, 60145-22-4; 2,2′,4,4′,6,6′-CB, 33979-03-2; 2,3,3′,4,4′,5-CB, 38380-08-4; 2,3,3′,4,4′,5′-CB, 69782-90-7; 2,3,3′,4,4′,6-CB, 74472-42-7; 2,3,3′,4,5,5′-CB, 39635-35-3; 2,3,3′,4,5,6-CB, 41411-62-5; 2,3,3′,4,5′,6-CB, 74472-43-8; 2,3,3′,4′,5,5′-CB, 39635-34-2; 2,3,3′,4′,5,6-CB, 74472-44-9; 2,3,3′,4′,5′,6-CB, 74472-45-0; 2,3,3′,5,5′,6-CB, 74472-46-1; 2,3,4,4′,5,6-CB, 41411-63-6; 2,3′,4,4′,5,5′-CB, 52663-72-6; 2,3′,4,4′,5′,6-CB, 59291-65-5; 3,3′,4,4′,5,5′-CB, 32774-16-6; 2,2′,3,3′,4,4′,5-CB, 35065-30-6; 2,2′,3,3′,4,4′,6-CB, 52663-71-5; 2,2′,3,3′,4,5,5′-CB, 52663-

74-8; 2,2',3,3',4,5,6-CB, 68194-16-1; 2,2',3,3',4,5,6'-CB, 38411-25-5; 2,2',3,3',4,5',6-CB, 40186-70-7; 2,2',3,3',4,6,6'-CB, 52663-65-7; 2,2',3,3',4',5,6-CB, 52663-70-4; 2,2',3,3',5,5',6-CB, 52663-67-9; 2,2',3,3',5,6,6'-CB, 52663-64-6; 2,2',3,4,4',5,5'-CB, 35065-29-3; 2,2',3,4,4',5,6-CB, 74472-47-2; 2,2',3,4,4',5,6'-CB, 60145-23-5; 2,2',3,4,4',5',6-CB, 52663-69-1; 2,2',3,4,4',6,6'-CB, 74472-48-3; 2,2',3,4,5,5',6-CB, 52712-05-7; 2,2',3,4,5,6,6'-CB, 74472-49-4; 2,2',3,4',5,5',6-CB, 52663-68-0; 2,2',3,4',5,6,6'-CB, 74487-85-7; 2,3,3',4,4',5,5'-CB, 39635-31-9; 2,3,3',4,4',5,6-CB, 41411-64-7; 2,3,3',4,4',5',6-CB, 74472-50-7; 2,3,3',4,5,5',6-CB, 74472-51-8; 2,3,3',4',5,5',6-CB, 69782-91-8; 2,2',3,3',4,4',5,5'-CB, 35694-08-7; 2,2',3,3',4,4',5,6-CB, 52663-78-2; 2,2',3,3',4,4',5',6-CB, 42740-50-1; 2,2',3,3',4,4',6,6'-CB, 33091-17-7; 2,2',3,3',4,5,5',6-CB, 68194-17-2; 2,2',3,3',4,5,6,6'-CB, 52663-73-7; 2,2',3,3',4,5',6,6'-CB, 40186-71-8; 2,2',3,3',4',5,5',6-CB, 52663-75-9; 2,2',3,3',5,5',6,6'-CB, 2136-99-4; 2,2',3,4,4',5,5',6-CB, 52663-76-0; 2,2',3,4,4',5,6,6'-CB, 74472-52-9; 2,3,3',4,4',5,5',6-CB, 74472-53-0; 2,2',3,3',4,4',5,5',6-CB, 40186-72-9; 2,2',3,3',4,4',5,6,6'-CB, 52663-79-3; 2,2',3,3',4,5,5',6,6'-CB, 52663-77-1; 2,2',3,3',4,4',5,5',6,6'-CB, 2051-24-3.

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Received for review August 17, 1992. Revised manuscript received December 23, 1992. Accepted December 28, 1992.