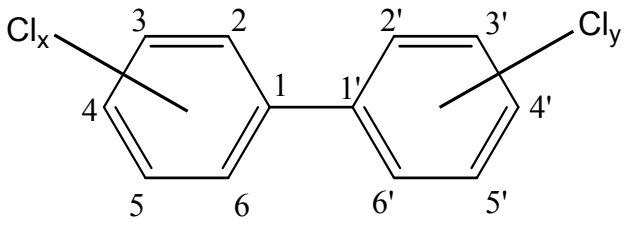
4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

PCBs are a class of chemical compounds in which 2–10 chlorine atoms are attached to the biphenyl molecule. Monochlorinated biphenyls (i.e., one chlorine atom attached to the biphenyl molecule) are often included when describing PCBs. The general chemical structure of chlorinated biphenyls is shown below.



It can be seen from the structure that a large number of chlorinated compounds are possible. The 209 possible compounds are called congeners. PCBs can also be categorized by degree of chlorination. The term "homolog" is used to refer to all PCBs with the same number of chlorines (e.g., trichloro-biphenyls). Homologs with different substitution patterns are referred to as isomers. For example, the dichlorophenyl homolog contains 12 isomers.

The numbering system for the PCBs is also shown above. Positions 2, 2', 6, and 6' are called ortho positions, positions 3, 3', 5, and 5' are called meta positions, and positions 4 and 4' are called para positions. The benzene rings can rotate around the bond connecting them; the two extreme configurations are planar (the two benzene rings in the same plane) and the nonplanar in which the benzene rings are at a 90E angle to each other. The degree of planarity is largely determined by the number of substitutions in the ortho positions. The replacement of hydrogen atoms in the ortho positions with larger chlorine atoms forces the benzene rings to rotate out of the planar configuration. The benzene rings of non-*ortho* substituted PCBs, as well as mono-*ortho* substituted PCBs, may assume a planar configuration and are referred to as planar or coplanar congeners; the benzene rings of other congeners cannot assume a planar or coplanar configuration and are referred to as non-planar congeners.

Monsanto Corporation, the major U.S. producer of PCBs from 1930 to 1977, marketed mixtures of PCBs under the trade name Aroclor. The Aroclors are identified by a four-digit numbering code in which the

first two digits indicate the type of mixture and the last two digits indicate the approximate chlorine content by weight percent. Thus, Aroclor 1242 is a chlorinated biphenyl mixture of varying amounts of mono- through heptachlorinated homologs with an average chlorine content of 42%. The exception to this code is Aroclor 1016, which contains mono- through hexachlorinated homologs with an average chlorine content of 41% (Hutzinger et al. 1974).

The trade names of some commercial PCB mixtures manufactured in other countries are Clophen (Germany), Fenclor (Italy), Kanechlor (Japan), and Phenoclor (France) (De Voogt and Brinkman 1989). The composition of commercial Clophen A-60 and Phenoclor DP-6 is similar to Aroclor 1260; that of Kanechlor 500 is similar to Aroclor 1254. Fenclor contains 100% decachlorobiphenyl (De Voogt and Brinkman 1989). The chemical identity of the Aroclors is summarized in Table 4-1. The identity of the 209 PCB congeners is shown in Table 4-2. The congeners are arranged in ascending numerical order using a numbering system developed by Ballschmiter and Zell (1980) that follow the IUPAC rules of substituent characterization in biphenyls. The resulting PCB numbers, also referred to as congener, IUPAC, or BZ numbers, are widely used for identifying individual congeners.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Physical and chemical properties of the Aroclors are summarized in Table 4-3. An important property of PCBs is their general inertness; they resist both acids and alkalis and have thermal stability. This made them useful in a wide variety of applications, including dielectric fluids in transformers and capacitors, heat transfer fluids, and lubricants (Afghan and Chau 1989). In general, PCBs are relatively insoluble in water, and the solubility decreases with increased chlorination (see Table 4-3). PCBs are also freely soluble in nonpolar organic solvents and biological lipids (EPA 1980b). PCBs are combustible liquids, and the products of combustion may be more hazardous than the material itself. By-products of combustion include hydrogen chloride, polychlorinated dibenzodioxins (PCDDs), and polychlorinated dibenzofurans (PCDFs) (NFPA 1994).

The approximate weight percent of chlorobiphenyls in some commercial Aroclors is summarized in Table 4-4, and the congener composition of Aroclors is shown in Table 4-5. The congener composition of commercial PCBs may vary from lot to lot even in products from the same manufacturer. In addition, no two descriptions of commercial PCB mixtures, even from the same lot or a manufactured product, are identical because of slight differences in the conditions of the chlorination process or the use of different analysis procedures. For example, a late production Aroclor 1254 lot (Aroclor 1254 “Late”), with greatly

Table 4-1. Chemical Identity of Selected Technical Polychlorinated Biphenyls or Aroclors[a,b]

Characteristic	Aroclor 1016	Aroclor 1221	Aroclor 1232	Aroclor 1242	Aroclor 1248
Synonym(s)	PCB-1016; Polychlorinated biphenyl mixture with 41.5% chlorine	PCB-1221; Polychlorinated biphenyl mixture with 21% chlorine	PCB-1232; Polychlorinated biphenyl mixture with 32% chlorine	PCB-1242; Polychlorinated biphenyl mixture with 41.5% chlorine	PCB-1248; Polychlorinated biphenyl mixture with 48% chlorine
Registered trade name(s)	Aroclor[c]	Aroclor	Aroclor	Aroclor	Aroclor
Chemical formula	See Table 4-4	See Table 4-4	See Table 4-4	See Table 4-4	See Table 4-4
Chemical structure	See Section 4.1	See Section 4.1	See Section 4.1	See Section 4.1	See Section 4.1
Identification numbers:					
CAS registry	12674-11-2	11104-28-2	11141-16-5	53469-21-9	12672-29-6
NIOSH RTECS	TQ1351000	TQ1352000	TQ1354000	TQ1356000	TQ1358000
EPA hazardous waste[d]	3502[e]	3502[e]	3502[e]	3502[e]	3502[e]
OHM/TADS	8500400[f]	8500401[f]	8500402[f]	8500403[f]	8500404[f]
DOT/UN/NA/IMCO shipping	UN2315/IMO9.2[g]	UN2315/IMO9.2[g]	UN2315/IMO9.2[g]	UN2315/IMO9.2[g]	UN2315/IMO9.2[g]
HSDB	6352[g]	6353[g]	6354[g]	6355[g]	6356[g]
NCI	No data	No data	No data	No data	No data

Table 4-1. Chemical Identity of Selected Technical Polychlorinated Biphenyls or Aroclors [a,b] (*continued*)

Characteristic	Aroclor 1254	Aroclor 1260	Aroclor 1262	Aroclor 1268
Synonym(s)	PCB-1254; Polychlorinated biphenyl mixture with 54% chlorine	PCB-1260; Polychlorinated biphenyl mixture with 60% chlorine	PCB-1262; Polychlorinated biphenyl mixture with 61.5–62.5% chlorine	PCB-1268; Polychlorinated biphenyl mixture with 68% chlorine
Registered trade name(s)	Aroclor	Aroclor	Aroclor	Aroclor
Chemical formula	See Table 4-4	See Table 4-4	See Table 4-4	See Table 4-4
Chemical structure	See Section 4.1	See Section 4.1	See Section 4.1	See Section 4.1
Identification numbers:				
CAS registry	11097-69-1	11096-82-5	37324-23-5	11100-14-4
NIOSH RTECS	TQ1360000	TQ1362000	TQ1364000[h]	No data
EPA hazardous waste[d]	3502[e]	3502[e]	No data	No data
OHM/TADS	8500405[f]	8500406[f]	No data	No data
DOT/UN/NA/IMO shipping	UN2315/IMO9.2[g]	UN2315/IMO9.2[g]	UN2315[h]	UN2315[h]
HSDB	6357[g]	1822[g]	No data	No data
NCI	C02664[i]	No data	No data	No data

[a]All information obtained from SANSS 1990 and Hutzinger et al. 1974 except where noted.
[b]Chemical names used are those currently indexed by the Chemical Abstracts Service.
[c]Aroclor is the trade name for chlorinated biphenyls made by Monsanto Chemical Company.
[d]Designation prior to May 19, 1980.
[e]EPA 1980a
[f]EPA-NIH 1990
[g]HSDB 2000
[h]Chemfinder 2000
[i]NIOSH 1987a

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; PCB = polychlorinated biphenyl; RTECS = Registry of Toxic Effects of Chemical Substances

Table 4-2. Chemical Identity of Polychlorinated Biphenyl Congeners and Homologs

PCB No.[a]	Structure	CAS No.[b]
	Biphenyl	92-52-4
	Monochlorobiphenyl	27323-18-8
1	2	2051-60-7
2	3	2051-61-8
3	4	2051-62-9
	Dichlorobiphenyl	25512-42-9
4	2,2N	13029-08-8
5	2,3	16605-91-7
6	2,3N	25569-80-6
7	2,4	33284-50-3
8	2,4N	34883-43-7
9	2,5	34883-39-1
10	2,6	33146-45-1
11	3,3N	2050-67-1
12	3,4	2974-92-7
13	3,4N	2974-90-5
14	3,5	34883-41-5
15	4,4N	2050-68-2
	Trichlorobiphenyl	25323-68-6
16	2,2N,3	38444-78-9
17	2,2N,4	37680-66-3
18	2,2N,5	37680-65-2
19	2,2N,6	38444-73-4
20	2,3,3N	38444-84-7
21	2,3,4	55702-46-0
22	2,3,4N	38444-85-8
23	2,3,5	55720-44-0
24	2,3,6	55702-45-9
25	2,3N,4	55712-37-3
26	2,3N,5	38444-81-4
27	2,3 N,6	38444-76-7
28	2,4,4N	7012-37-5
29	2,4,5	15862-07-4
30	2,4,6	35693-92-6
31	2,4N,5	16606-02-3
32	2,4N,6	38444-77-8
33	2N,3,4	38444-86-9

Table 4-2. Chemical Identity of Polychlorinated Biphenyl Congeners and Homologs *(continued)*

PCB No.[a]	Structure	CAS No.[b]
34	2N,3,5	37680-68-5
35	3,3N,4	37680-69-6
36	3,3N,5	38444-87-0
37	3,4,4N	38444-90-5
38	3,4,5	53555-66-1
39	3,4N,5	38444-88-1
	Tetrachlorobiphenyl	26914-33-0
40	2,2N,3,3N	38444-93-8
41	2,2N,3,4	52663-59-9
42	2,2N,3,4N	36559-22-5
43	2,2N,3,5	70362-46-8
44	2,2N,3,5N	41464-39-5
45	2,2N,3,6	70362-45-7
46	2,2N,3,6N	41464-47-5
47	2,2N,4,4N	2437-79-8
48	2,2N,4,5	70362-47-9
49	2,2N,4,5N	41464-40-8
50	2,2N,4,6	62796-65-0
51	2,2N,4,6N	68194-04-7
52	2,2N,5,5N	35693-99-3
53	2,2N,5,6N	41464-41-9
54	2,2N,6,6N	15968-05-5
55	2,3,3N,4	74338-24-2
56	2,3,3N,4N	41464-43-1
57	2,3,3N,5	70424-67-8
58	2,3,3N,5N	41464-49-7
59	2,3,3N,6	74472-33-6
60	2,3,4,4N	33025-41-1
61	2,3,4,5	33284-53-6
62	2,3,4,6	54230-22-7
63	2,3,4N,5	74472-35-8
64	2,3,4N,6	52663-58-8
65	2,3,5,6	33284-54-7
66	2,3N,4,4N	32598-10-0
67	2,3N,4,5	73575-53-8
68	2,3N,4,5N	73575-52-7
69	2,3N,4,6	60233-24-1
70	2,3N,4N,5	32598-11-1
71	2,3N,4N,6	41464-46-4

Table 4-2. Chemical Identity of Polychlorinated Biphenyl Congeners and Homologs *(continued)*

PCB No.[a]	Structure	CAS No.[b]
72	2,3N,5,5N	41464-42-0
73	2,3N,5N,6	74338-23-1
74	2,4,4N,5	32690-93-0
75	2,4,4N,6	32598-12-2
76	2N,3,4,5	70362-48-0
77	3,3N,4,4N	32598-13-3
78	3,3N,4,5	70362-49-1
79	3,3N,4,5N	41464-48-6
80	3,3N,5,5N	33284-52-5
81	3,4,4N,5	70362-50-4
	Pentachlorobiphenyl	25429-29-2
82	2,2N,3,3N,4	52663-62-4
83	2,2N,3,3N,5	60145-20-2
84	2,2N,3,3N,6	52663-60-2
85	2,2N,3,4,4N	65510-45-4
86	2,2N,3,4,5	55312-69-1
87	2,2N,3,4,5N	38380-02-8
88	2,2N,3,4,6	55215-17-3
89	2,2N,3,4,6N	73575-57-2
90	2,2N,3,4N,5	68194-07-0
91	2,2N,3,4N,6	68194-05-8
92	2,2N,3,5,5N	52663-61-3
93	2,2N,3,5,6	73575-56-1
94	2,2N,3,5,6N	73575-55-0
95	2,2N,3,5N,6	38379-99-6
96	2,2N,3,6,6N	73575-54-9
97	2,2N,3N,4,5	41464-51-1
98	2,2N,3N,4,6	60233-25-2
99	2,2N,4,4N,5	38380-01-7
100	2,2N,4N,4N,6	39485-83-1
101	2,2N,4,5,5N	37680-73-2
102	2,2N,4,5,6N	68194-06-9
103	2,2N,4,5N,6	60145-21-3
104	2,2N,4,6,6N	56558-16-8
105	2,3,3N,4,4N	32598-14-4
106	2,3,3N,4,5	70424-69-0
107	2,3,3N,4N,5	70424-68-9
108	2,3,3N,4,5N	70362-41-3
109	2,3,3N,4,6	74472-35-8

Table 4-2. Chemical Identity of Polychlorinated Biphenyl Congeners and Homologs *(continued)*

PCB No.[a]	Structure	CAS No.[b]
110	2,3,3N,4N,6	38380-03-9
111	2,3,3N,5,5N	39635-32-0
112	2,3,3N,5,6	74472-36-9
113	2,3,3N,5N,6	68194-10-5
114	2,3,4,4N,5	74472-37-0
115	2,3,4,4N,6	74472-38-1
116	2,3,4,5,6	18259-05-7
117	2,3,4N,5,6	68194-11-6
118	2,3N,4,4N,5	31508-00-6
119	2,3N,4,4N,6	56558-17-9
120	2,3N,4,5,5N	68194-12-7
121	2,3N,4,5N,6	56558-18-0
122	2N,3,3N,4,5	76842-07-4
123	2N,3,4,4N,5	65510-44-3
124	2N,3,4,5,5N	70424-70-3
125	2N,3,4,5,6N	74472-39-2
126	3,3N,4,4N,5	57465-28-8
127	3,3N,4,5,5N	39635-33-1
	Hexachlorobiphenyl	26601-64-9
128	2,2N,3,3N,4,4N	38380-07-3
129	2,2N,3,3N,4,5	55215-18-4
130	2,2N,3,3N,4,5N	52663-66-8
131	2,2N,3,3N,4,6	61798-70-7
132	2,2N,3,3N,4,6N	38380-05-1
133	2,2N,3,3N,5,5N	35694-04-3
134	2,2N,3,3N,5,6	52704-70-8
135	2,2N,3,3N,5,6N	52744-13-5
136	2,2N,3,3N,6,6N	38411-22-2
137	2,2N,3,4,4N,5	35694-06-5
138	2,2N,3,4,4N,5N	35065-28-2
139	2,2N,3,4,4N,6	56030-56-9
140	2,2N,3,4,4N,6N	59291-64-4
141	2,2N,3,4,5,5N	52712-04-6
142	2,2N,3,4,5,6	41411-61-4
143	2,2N,3,4,5,6N	68194-15-0
144	2,2N,3,4,5N,6	68194-14-9
145	2,2N,3,4N,6,6N	74472-40-5
146	2,2N,3,4N,5,5N	51908-16-8
147	2,2N,3,4N,5,6	68194-13-8

Table 4-2. Chemical Identity of Polychlorinated Biphenyl Congeners and Homologs *(continued)*

PCB No.[a]	Structure	CAS No.[b]
148	2,2N,3,4N,5,6N	74472-41-6
149	2,2N,3,4N,5N,6	38380-04-0
150	2,2N,3,4N,5,6N	68194-08-1
151	2,2N,3,5,5N,6	52663-63-5
152	2,2N,3,5,6,6N	68194-09-2
153	2,2N,4,4N,5,5N	35065-27-1
154	2,2N,4,4N,5,6N	60145-22-4
155	2,2N,4,4N,6,6N	33979-03-2
156	2,3,3N,4,4N,5	38380-08-4
157	2,3,3N,4,4N,5N	69782-90-7
158	2,3,3N,4,4N,6	74472-42-7
159	2,3,3N,4,5,5N	39635-35-3
160	2,3,3N,4,5,6	41411-62-5
161	2,3,3N,4,5N,6	74472-43-8
162	2,3,3N,4N,5,5N	39635-34-2
163	2,3,3N,4N,5,6	74472-44-9
164	2,3,3N,4N,5N,6	74472-45-0
165	2,3,3N,5,5N,6	74472-46-1
166	2,3,4,4N,5,6	41411-63-6
167	2,3N,4,4N,5,5N	52663-72-6
168	2,3N,4,4N,5N,6	59291-65-5
169	3,3N,4,4N,5,5N	32774-16-6
	Heptachlorobiphenyl	28655-71-2
170	2,2N,3,3N,4,4N,5	35065-30-6
171	2,2N,3,3N,4,4N,6	52663-71-5
172	2,2N,3,3N,4,5,5N	52663-74-8
173	2,2N,3,3N,4,5,6	68194-16-1
174	2,2N,3,3N,4,5,6N	38411-25-5
175	2,2N,3,3N,4,5N,6	40186-70-7
176	2,2N,3,3N,4,6,6N	52663-65-7
177	2,2N,3,3N,4N,5,6	52663-70-4
178	2,2N,3,3N,5,5N,6,	52663-67-9
179	2,2N,3,3N,5,6,6N	52663-64-6
180	2,2N,3,4,4N,5,5N	35065-29-3
181	2,2N,3,4,4N,5,6	74472-47-2
182	2,2N,3,4,4N,5,6N	60145-23-5
183	2,2N,3,4,4N,5N,6	52663-69-1
184	2,2N,3,4,4N,6,6N	74472-48-3
185	2,2N,3,4,5,5N,6	52712-05-7

Table 4-2. Chemical Identity of Polychlorinated Biphenyl Congeners and Homologs *(continued)*

PCB No.[a]	Structure	CAS No.[b]
186	2,2N,3,4,5,6,6N	74472-49-4
187	2,2N,3,4N,5,5N,6	52663-68-0
188	2,2N,3,4N,5,6,6N	74487-85-7
189	2,3,3N,4,4N,5,5N	39635-31-9
190	2,3,3N,4,4N,5,6	41411-64-7
191	2,3,3N,4,4N,5N,6	74472-50-7
192	2,3,3N,4,5,5N,6	74472-51-8
193	2,3,3N,4N,5,5N,6	69782-91-8
	Octachlorobiphenyl	31472-83-0
194	2,2N,3,3N,4,4N,5,5N	35694-08-7
195	2,2N,3,3N,4,4N,5,6	52663-78-2
196	2,2N,3,3N,4,4N,5,6N	42740-50-1
197	2,2N,3,3N,4,4N,6,6N	33091-17-7
198	2,2N,3,3N,4,5,5N,6	68194-17-2
199	2,2N,3,3N,4,5,5N,6N	52663-75-9
200	2,2N,3,3N,4,5,6,6N	52663-73-7
201	2,2N,3,3N,4,5N,6,6N	40186-71-8
202	2,2N,3,3N,5,5N,6,6N	2136-99-4
203	2,2N,3,4,4N,5,5N,6	52663-76-0
204	2,2N,3,4,4N,5,6,6N	74472-52-9
205	2,3,3N,4,4N,5,5N,6	74472-53-0
	Nonachlorobiphenyl	53742-07-7
206	2,2N,3,3N,4,4N,5,5N,6	40186-72-9
207	2,2N,3,3N,4,4N,5,6,6N	52663-79-3
208	2,2N,3,3N,4,5,5N,6,6N	52663-77-1
	Decachlorobiphenyl	2051-24-3
209	2,2N,3,3N,4,4N,5,5N,6,6N	2051-24-3

[a]Ballschmiter and Zell 1980, also referred to as BZ number
[b]Erickson 1986

Table 4-3. Physical and Chemical Properties of Some Aroclors[a]

Property	Aroclor 1016	Aroclor 1221	Aroclor 1232	Aroclor 1242
Molecular weight[b]	257.9[c]	200.7[c]	232.2[c]	266.5[c]
Color	Clear	Clear	Clear	Clear
Physical state	Oil	Oil	Oil	Oil
Melting point, EC	No data	1[d]	No data	No data
Boiling point, EC	325–356	275–320	290–325	325–366
Density, g/cm^3 at 25 EC	1.37	1.18	1.26	1.38
Odor	No data	No data	No data	Mild hydrocarbon[d]
Odor threshold:				
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data
Solubility:				
Water, mg/L	0.42 (25 EC)[e]	0.59 (24 EC)[f]	0.45 (25 EC)	0.24[c]; 0.34 (25 EC)[e] 0.10 (24 EC)[f]
Organic solvent(s)	Very soluble[g]	Very soluble[g]	Very soluble[g]	Very soluble[g]
Partition coefficients:				
Log K_{ow}[h]	5.6	4.7	5.1	5.6
Log K_{oc}	No data	No data	No data	No data
Vapor pressure, mm Hg at 25 EC	$4x10^{-4}$ [c]	$6.7x10^{-3}$ [c]	$4.06x10^{-3}$ [c]	$4.06x10^{-4}$ [c]
Henry's law constant, atm-m^3/mol at 25 EC[i]	$2.9x10^{-4}$	$3.5x10^{-3}$	No data	$5.2x10^{-4}$
Autoignition temperature	No data	No data	No data	No data
Flashpoint, EC (Cleveland open cup)	170	141–150	152–154	176–180
Flammability limits, EC	None to boiling point	176	328	None to boiling point
Conversion factors				
Air (25 EC)[j]	1 mg/m^3=0.095 ppm	1 mg/m^3=0.12 ppm	1 mg/m^3=0.105 ppm	1 mg/m^3=0.092 ppm
Explosive limits	No data	No data	No data	No data

Table 4-3. Physical and Chemical Properties of Some Aroclors[a] *(continued)*

Property	Aroclor 1254	Aroclor 1260	Aroclor 1262	Aroclor 1268
Molecular weight[b]	328[c]	357.7[c]	389	453
Color	Light yellow	Light yellow	No data	Clear[k]
Physical state	Viscous liquid	Sticky resin	No data	Viscous liquid[k]
Melting point	No data	No data	No data	No data
Boiling point, EC	365–390	385–420	390–425	435–450
Density, g/cm^3 at 25 EC	1.54	1.62	1.64	1.81
Odor	Mild hydrocarbon[d]	No data	No data	No data
Odor threshold:				
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data
Solubility:				
Water, mg/L	0.012[c]; 0.057 (24 EC)	0.0027[c];0.08 (24 EC)[f]	0.052 (24 EC)[f]	0.300 (24 EC)[f]
Organic solvent(s)	Very soluble[g]	Very soluble[g]	No data	Soluble
Partition coefficients:				
Log K_{ow}	6.5	6.8	No data	No data
Log K_{oc}	No data	No data	No data	No data
Vapor pressure, mm Hg at 25 EC	7.71x10^{-5} [c]	4.05x10^{-5} [c]	No data	No data
Henry's law constant, atm-m^3/mol at 25 EC[i]	2.0x10^{-3}	4.6x10^{-3}	No data	No data
Autoignition temperature	No data	No data	No data	No data
Flashpoint EC (Cleveland open cup)	No data	No data	195E C	195E C

Table 4-3. Physical and Chemical Properties of Some Aroclors[a] *(continued)*

Property	Aroclor 1254	Aroclor 1260	Aroclor 1262	Aroclor 1268
Flammability limits, EC	None to boiling point	None to boiling point	None to boiling point	None to boiling point
Conversion factors, Air (25 EC)[j]	1 mg/m^3=0.075 ppm	1 mg/m^3=0.065 ppm	1 mg/m^3=0.061 ppm	1 mg/m^3=0.052 ppm
Explosive limits	No data	No data	No data	No data

[a]All information obtained from Monsanto Chemical Company 1985 and Hutzinger et al. 1974 unless otherwise noted.
[b]Average weight from Table 3-3.
[c]EPA 1979h; data on temperature not available.
[d]NIOSH 1997
[e]Paris et al. 1978
[f]Hollifield 1979
[g]EPA 1985b
[h]These log K_{ow} values represent an average value for the major components of the individual Aroclor. Experimental values for the individual components were obtained from Hansch and Leo 1985.
[i]These Henry's law constants were estimated by dividing the vapor pressure by the water solubility. The first water solubility given in this table was used for the calculation. The resulting estimated Henry's law constant is only an average for the entire mixture; the individual chlorobiphenyl isomers vary significantly from the average. Burkhard et al. (1985) estimated the following Henry's law constants (atm-m^3/mol) for various Aroclors at 25 EC: 1221 (2.28×10^{-4}), 1242 (3.43×10^{-4}), 1248 (4.4×10^{-4}), 1254 (2.83×10^{-4}), and 1260 (4.15×10^{-4}).
[j]These air conversion factors were calculated by using the average molecular weight and ideal gas law.
[k]Chemical Health and Safety Data; National Toxicology Program (http://ntp-server.niehs.nih.gov)

Table 4-4. Approximate Weight Percent of PCB Homologs in Some Aroclors

Homolog	Aroclor 1016[a]	Aroclor 1221[b]	Aroclor 1232[c]	Aroclor 1242[d]	Aroclor 1248[e]
$C_{12}H_9Cl$	0.70	60.06	27.55	0.75	0.07
$C_{12}H_8Cl_2$	17.53	33.38	26.83	15.04	1.55
$C_{12}H_7Cl_3$	54.67	4.22	25.64	44.91	21.27
$C_{12}H_6Cl_4$	22.07	1.15	10.58	20.16	32.77
$C_{12}H_5Cl_5$	5.07	1.23	9.39	18.85	42.92
$C_{12}H_4Cl_6$	Not detected	Not detected	0.21	0.31	1.64
$C_{12}H_3Cl_7$	Not detected	Not detected	0.03	Not detected	0.02
$C_{12}H_2Cl_8$	Not detected	Not detected	Not detected	Not detected	Not detected
$C_{12}H_1Cl_9$	Not detected	Not detected	Not detected	Not detected	Not detected
Average molecular mass	262	206	240	272	300

Empirical Formula	Aroclor 1254[f]	Aroclor 1254[g]	Aroclor 1260[d]	Aroclor 1262[h]	Aroclor 1268
$C_{12}H_9Cl$	0.02	Not detected	0.02	0.02	No data
$C_{12}H_8Cl_2$	0.09	0.24	0.08	0.27	No data
$C_{12}H_7Cl_3$	0.39	1.26	0.21	0.98	No data
$C_{12}H_6Cl_4$	4.86	10.25	0.35	0.49	No data
$C_{12}H_5Cl_5$	71.44	59.12	8.74	3.35	No data
$C_{12}H_4Cl_6$	21.97	26.76	43.35	26.43	No data
$C_{12}H_3Cl_7$	1.36	2.66	38.54	48.48	No data
$C_{12}H_2Cl_8$	Not detected	0.04	8.27	19.69	No data
$C_{12}H_1Cl_9$	0.04	0.04	0.70	1.65	No data
Average molecular mass	334	334	378	395	453

Source: Frame et al. (1996)

[a]Lot A2 Aroclor 1016
[b]Lot A1 Aroclor 1221
[c]Lot A1.5 Aroclor 1232
[d]Mean of three Lots
[e]Lot A3.5 Aroclor 1248
[f]Lot A4 Aroclor 1254 (Monsanto Lot KI-02-6024) from abnormal late production (1974–1977)
[g]Lot G4 Aroclor 1254 (GE/118-peak analytical standard)
[h]Lot A6 Aroclor 1262

Table 4-5. Polychlorinated Biphenyl Congener Compositions (in Weight Percent)[a] in Aroclors[b]

		Aroclor						
PCB No.	Chlorine positions	1016[c]	1242[d]	1248[e]	1248[f]	1254[g] "Late"	1254[h]	1260[i]
1	2	0.52	0.54	0.05	0.02	0.02	—	0.02
2	3	0.02	0.03	—	—	—	—	—
3	4	0.15	0.18	0.01	—	—	—	—
4	2,2N	3.62	3.08	0.32	0.04	0.02	0.06	0.02
5	2,3	0.17	0.14	0.00	—	—	—	—
6	2,3N	1.64	1.43	0.13	0.00	0.01	0.02	0.01
7	2,4	0.29	0.26	0.02	—	—	—	—
8	2,4N	8.29	7.05	0.81	0.26	0.05	0.13	0.04
9	2,5	0.58	0.50	0.04	—	—	—	—
10	2,6	0.23	0.20	—	—	—	—	—
11	3,3N	—	—	—	—	—	—	—
12	3,4	0.07	0.06	—	—	—	—	—
13	3,4N	0.24	0.22	0.02	—	—	—	—
14	3,5	—	—	—	—	—	—	—
15	4,4N	2.40	2.10	0.22	0.06	0.01	0.03	0.01
16	2,2N,3	3.88	3.14	1.04	0.71	0.02	0.09	0.01
17	2,2N,4	3.98	3.13	1.05	0.93	0.02	0.08	0.02
18	2,2N,5	10.86	8.53	4.29	3.29	0.08	0.25	0.05
19	2,2N,6	0.99	0.80	0.22	0.14	—	—	—
20	2,3,3N	0.88	0.72	0.14	0.08	—	—	—
21	2,3,4	NM	NM	—	—	—	—	—
22	2,3,4N	3.50	2.84	1.33	1.38	0.02	0.04	0.01
23	2,3,5	0.01	0.01	—	0.00	—	—	—
24	2,3,6	0.16	0.13	0.01	—	—	—	—
25	2,3N,4	0.72	0.59	0.11	0.04	—	—	—
26	2,3N,5	1.57	1.28	0.40	0.23	—	0.03	—
27	2,3,6	0.51	0.41	0.12	0.07	—	—	—
28	2,4,4N	8.50	6.86	3.59	5.57	0.06	0.19	0.03
29	2,4,5	0.10	0.08	0.00	0.01	—	—	—
30	2,4,6	0.00	—	—	—	—	—	—
31	2,4N,5	9.32	7.34	5.07	5.47	0.11	0.28	0.04
32	2,4N,6	2.37	1.90	0.88	0.93	0.01	0.05	0.01
33	2N,3,4	6.21	5.01	2.23	2.21	0.05	0.16	0.03

Table 4-5. Polychlorinated Biphenyl Congener Compositions (in Weight Percent)[a] in Aroclors[b] *(continued)*

		Aroclor						
PCB No.	Chlorine positions	1016[c]	1242[d]	1248[e]	1248[f]	1254[g] "Late"	1254[h]	1260[i]
34	2N,3,5	0.03	0.02	0.00	0.00	—	—	—
35	3,3N,4	0.05	0.08	0.00	—	—	—	—
36	3,3N,5	—	—	—	—	—	—	—
37	3,4,4N	1.02	2.03	0.79	0.95	0.01	0.07	0.01
38	3,4,5	—	—	—	—	—	—	—
39	3,4N,5	—	—	—	—	—	—	—
40	2,2N,3,3N	0.58	0.76	1.13	0.92	0.15	0.12	—
41	2,2N,3,4	0.76	0.68	0.77	0.75	0.02	0.01	—
42	2,2N,3,4N	1.59	1.19	1.67	1.79	0.09	0.15	0.01
43	2,2N,3,5	0.28	0.18	0.30	0.19	—	—	—
44	2,2N,3,5N	4.47	3.55	6.31	5.09	0.67	2.31	0.03
45	2,2N,3,6	1.23	0.89	1.09	0.91	0.02	0.05	—
46	2,2N,3,6N	0.49	0.36	0.47	0.39	—	—	—
47	2,2N,4,4N	1.26	0.93	1.49	2.41	0.07	0.14	—
48	2,2N,4,5	1.61	1.18	1.66	1.54	0.05	0.12	—
49	2,2N,4,5N	3.35	2.53	4.12	4.17	0.26	1.10	0.01
50	2,2N,4,6	0.01	0.00	—	—	—	—	—
51	2,2N,4,6N	0.32	0.23	0.30	0.31	—	—	—
52	2,2N,5,5N	4.63	3.53	6.93	5.58	0.83	5.38	0.24
53	2,2N,5,6N	0.95	0.71	1.05	0.88	0.04	0.12	—
54	2,2N,6,6N	0.01	0.01	—	0.01	—	—	—
55	2,3,3N,4	—	0.10	0.06	0.05	—	—	—
56	2,3,3N,4N	0.07	1.81	3.16	3.19	1.70	0.55	0.02
57	2,3,3N,5	0.01	0.02	0.02	0.02	—	—	—
58	2,3,3N,5N	—	—	—	—	—	—	—
59	2,3,3N,6	0.41	0.32	0.37	0.23	0.01	0.02	—
60	2,3,4,4N	0.04	1.18	1.85	2.67	0.95	0.18	0.04
61	2,3,4,5	—	—	—	—	—	—	—
62	2,3,4,6	—	—	—	—	—	—	—
63	2,3,4N,5	0.06	0.12	0.17	0.19	0.07	0.02	—
64	2,3,4N,6	1.87	1.70	3.01	3.32	0.36	0.59	0.01
65	2,3,5,6	—	—	—	—	—	—	—
66	2,3N,4,4N	0.39	3.39	5.84	7.22	3.56	1.01	0.02
67	2,3N,4,5	0.06	0.16	0.13	0.10	0.01	—	—

Table 4-5. Polychlorinated Biphenyl Congener Compositions (in Weight Percent)[a] in Aroclors[b] *(continued)*

		Aroclor						
PCB No.	Chlorine positions	1016[c]	1242[d]	1248[e]	1248[f]	1254[g] "Late"	1254[h]	1260[i]
68	2,3N,4,5N	—	—	—	—	—	—	—
69	2,3N,4,6	0.00	—	—	—	—	—	—
70	2,3N,4N,5	0.59	3.73	7.28	7.39	6.83	3.49	0.04
71	2,3N,4N,6	1.16	1.03	1.67	1.86	0.11	0.15	0.01
72	2,3N,5,5N	0.00	0.01	0.02	0.01	—	—	—
73	2,3N,5N,6	0.00	0.00	—	—	—	—	—
74	2,4,4N,5	0.33	1.81	3.14	4.67	2.19	0.84	0.05
75	2,4,4N,6	0.06	0.04	0.08	0.08	—	—	—
76	2N,3,4,5	—	0.08	0.13	0.13	0.03	0.02	—
77	3,3N,4,4N	—	0.31	0.41	0.52	0.20	0.03	—
78	3,3N,4,5	—	—	—	—	—	—	—
79	3,3N,4,5N	—	—	—	—	—	—	—
80	3,3N,5,5N	—	—	—	—	—	—	—
81	3,4,4N,5	—	0.01	0.01	0.02	0.00	—	—
82	2,2N,3,3N,4	—	0.26	0.81	0.62	1.53	1.11	—
83	2,2N,3,3N,5	—	0.11	0.26	0.20	0.56	0.48	0.01
84	2,2N,3,3N,6	0.05	0.41	1.26	0.91	1.58	2.32	0.11
85	2,2N,3,4,4N	—	0.31	0.98	1.14	2.49	1.28	0.01
86	2,2N,3,4,5	—	0.03	0.11	0.09	0.10	0.06	—
87	2,2N,3,4,5N	—	0.46	1.45	1.11	3.41	3.99	0.41
88	2,2N,3,4,6	—	0.00	0.02	0.02	—	—	—
89	2,2N,3,4,6N	—	0.09	0.20	0.17	0.11	0.09	—
90	2,2N,3,4N,5	—	—	NM	NM	NM	NM	—
91	2,2N,3,4N,6	0.06	0.21	0.63	0.56	0.53	0.93	0.01
92	2,2N,3,5,5N	—	0.09	0.38	0.25	0.57	1.29	0.30
93	2,2N,3,5,6	—	0.00	0.04	0.03	—	—	—
94	2,2N,3,5,6N	—	0.01	0.03	0.02	0.01	0.02	—
95	2,2N,3,5N,6	0.31	0.61	1.96	1.43	1.84	6.25	2.45
96	2,2N,3,6,6N	0.04	0.03	0.08	0.06	0.01	0.04	—
97	2,2N,3N,4,5	—	0.38	1.22	0.97	2.78	2.62	0.09
98	2,2N,3N,4,6	—	—	—	—	—	—	—
99	2,2N,3N,4N,5	0.01	0.46	1.47	1.81	4.53	3.02	0.04
100	2,2N,4N,4N,6	—	—	—	—	—	—	—
101	2,2N,4,5,5N	0.04	0.69	2.22	1.89	5.49	8.02	3.13

Table 4-5. Polychlorinated Biphenyl Congener Compositions (in Weight Percent)[a] in Aroclors[b] *(continued)*

		Aroclor						
PCB No.	Chlorine positions	1016[c]	1242[d]	1248[e]	1248[f]	1254[g] "Late"	1254[h]	1260[i]
102	2,2N,4,5,6N	0.04	0.07	0.19	0.17	0.09	0.15	—
103	2,2N,4,5N,6	—	—	0.02	0.01	—	0.03	—
104	2,2N,4,6,6N	—	—	—	—	—	—	—
105	2,3,3N,4,4N	0.00	0.47	1.60	1.45	7.37	2.99	0.22
106	2,3,3N,4,5	—	—	—	—	—	—	—
107	2,3,3N,4N,5	—	—	—	—	—	—	—
108	2,3,3N,4,5N	—	—	—	—	—	—	—
109	2,3,3N,4,6	—	0.06	0.18	0.13	0.78	0.37	0.01
110	2,3,3N,4N,6	—	0.83	2.97	2.55	8.42	9.29	1.33
111	2,3,3N,5,5N	—	—	—	—	—	—	—
112	2,3,3N,5,6	—	—	—	—	—	—	—
113	2,3,3N,5N,6	—	—	—	—	0.01	—	—
114	2,3,4,4N,5	—	0.04	0.12	0.12	0.50	0.18	—
115	2,3,4,4N,6	—	0.04	0.11	0.11	0.37	0.20	—
116	2,3,4,5,6	—	—	—	—	—	—	—
117	2,3,4N,5,6	—	0.03	0.09	0.10	0.19	0.23	—
118	2,3N,4,4N,5	—	0.66	2.29	2.35	13.59	7.35	0.48
119	2,3N,4,4N,6	—	—	0.06	0.06	0.12	0.08	—
120	2,3N,4,5,5N	—	—	—	—	—	—	—
121	2,3N,4,5N,6	—	—	—	—	—	—	—
122	2N,3,3N,4,5	—	0.01	0.06	0.05	0.25	0.10	—
123	2N,3,4,4N,5	—	0.03	0.07	0.08	0.32	0.15	—
124	2N,3,4,5,5N	—	0.03	0.10	0.07	0.47	0.29	0.01
125	2N,3,4,5,6N	—	0.02	0.04	0.03	0.03	0.02	—
126	3,3N,4,4N,5	—	—	0.00	0.00	0.02	0.00	—
127	3,3N,4,5,5N	—	—	—	—	—	—	—
128	2,2N,3,3N,4,4N	—	0.02	0.12	0.08	1.71	1.42	0.53
129	2,2N,3,3N,4,5	—	—	0.02		0.39	0.38	0.14
130	2,2N,3,3N,4,5N	—	—	0.04	0.01	0.50	0.60	0.22
131	2,2N,3,3N,4,6	—	—	—	—	0.14	0.19	0.07
132	2,2N,3,3N,4,6N	—	0.04	0.15	0.14	1.50	2.29	2.90
133	2,2N,3,3N,5,5N	—	—	—	—	—	0.11	0.07
134	2,2N,3,3N,5,6	—	—	—	0.01	0.20	0.37	0.34
135	2,2N,3,3N,5,6N	—	—	0.04	0.04	0.28	0.61	1.08

Table 4-5. Polychlorinated Biphenyl Congener Compositions (in Weight Percent)[a] in Aroclors[b] *(continued)*

		Aroclor						
PCB No.	Chlorine positions	1016[c]	1242[d]	1248[e]	1248[f]	1254[g] "Late"	1254[h]	1260[i]
136	2,2N,3,3N,6,6N	—	—	0.05	0.06	0.24	0.70	1.46
137	2,2N,3,4,4N,5	—	—	0.03	0.02	0.52	0.42	0.02
138	2,2N,3,4,4N,5N	—	0.10	0.38	0.41	5.95	5.80	6.54
139	2,2N,3,4,4N,6	—	—	—	—	0.14	0.15	—
140	2,2N,3,4,4N,6N	—	—	—	—	—	—	—
141	2,2N,3,4,5,5N	—	0.01	0.07	0.09	0.69	0.98	2.62
142	2,2N,3,4,5,6	—	—	—	—	—	—	—
143	2,2N,3,4,5,6N	—	—	—	—	—	—	—
144	2,2N,3,4,5N,6	—	—	—	0.01	0.12	0.24	0.61
145	2,2N,3,4N,6,6N	—	—	—	—	—	—	—
146	2,2N,3,4N,5,5N	—	—	0.04	0.05	0.45	0.67	1.15
147	2,2N,3,4N,5,6	—	—	—	—	0.02	0.10	—
148	2,2N,3,4N,5,6N	—	—	—	—	—	—	—
149	2,2N,3,4N,5N,6	—	0.06	0.24	0.33	1.82	3.65	8.75
150	2,2N,3,4N,5,6N	—	—	—	—	—	—	—
151	2,2N,3,5,5N,6	—	—	0.04	0.08	0.22	0.69	3.04
152	2,2N,3,5,6,6N	—	—	—	—	—	—	—
153	2,2N,4,4N,5,5N	—	0.06	0.23	0.43	3.29	3.77	9.39
154	2,2N,4,4N,5,6N	—	—	—	—	0.02	0.04	—
155	2,2N,4,4N,6,6N	—	—	—	—	—	—	—
156	2,3,3N,4,4N,5	—	0.01	0.06	0.04	1.13	0.82	0.52
157	2,3,3N,4,4N,5N	—	—	0.01	0.00	0.30	0.19	0.02
158	2,3,3N,4,4N,6	—	0.01	0.04	0.04	0.90	0.81	0.58
159	2,3,3N,4,5,5N	—	—	—	—	—	—	—
160	2,3,3N,4,5,6	—	—	—	—	—	—	—
161	2,3,3N,4,5N,6	—	—	—	—	—	—	—
162	2,3,3N,4N,5,5N	—	—	—	—	—	—	—
163	2,3,3N,4N,5,6	—	0.01	0.06	0.08	0.70	1.03	2.42
164	2,3,3N,4N,5N,6	—	—	0.02	0.03	0.31	0.40	0.69
165	2,3,3N,5,5N,6	—	—	—	—	—	—	—
166	2,3,4,4N,5,6	—	—	—	—	0.05	0.05	—
167	2,3N,4,4N,5,5N	—	—	0.01	0.01	0.35	0.27	0.19
168	2,3N,4,4N,5N,6	—	—	—	—	—	—	—
169	3,3N,4,4N,5,5N	—	—	—	—	—	—	—

Table 4-5. Polychlorinated Biphenyl Congener Compositions (in Weight Percent)[a] in Aroclors[b] *(continued)*

		Aroclor						
PCB No.	Chlorine positions	1016[c]	1242[d]	1248[e]	1248[f]	1254[g] "Late"	1254[h]	1260[i]
170	2,2N,3,3N,4,4N,5	—	—	—	0.08	0.35	0.52	4.11
171	2,2N,3,3N,4,4N,6	—	—	—	—	0.08	0.14	1.11
172	2,2N,3,3N,4,5,5N	—	—	—	—	0.03	0.07	0.70
173	2,2N,3,3N,4,5,6	—	—	—	—	—	—	0.10
174	2,2N,3,3N,4,5,6N	—	—	—	0.08	0.14	0.34	4.96
175	2,2N,3,3N,4,5N,6	—	—	—	—	—	—	0.17
176	2,2N,3,3N,4,6,6N	—	—	—	—	0.01	0.04	0.59
177	2,2N,3,3N,4N,5,6	—	—	—	0.03	0.08	0.20	2.57
178	2,2N,3,3N,5,5N,6,	—	—	—	—	—	0.03	0.83
179	2,2N,3,3N,5,6,6N	—	—	—	0.02	0.02	0.10	2.03
180	2,2N,3,4,4N,5,5N	—	—	0.02	0.21	0.42	0.67	11.38
181	2,2N,3,4,4N,5,6	—	—	—	—	—	—	0.01
182	2,2N,3,4,4N,5,6N	—	—	—	—	—	—	—
183	2,2N,3,4,4N,5N,6	—	—	—	0.06	0.09	0.18	2.41
184	2,2N,3,4,4N,6,6N	—	—	—	—	—	—	—
185	2,2N,3,4,5,5N,6	—	—	—	—	—	—	0.55
186	2,2N,3,4,5,6,6N	—	—	—	—	—	—	—
187	2,2N,3,4N,5,5N,6	—	—	—	0.09	0.09	0.25	5.40
188	2,2N,3,4N,5,6,6N	—	—	—	—	—	—	—
189	2,3,3N,4,4N,5,5N	—	—	—	—	0.01	0.01	0.10
190	2,3,3N,4,4N,5,6	—	—	—	—	0.05	0.07	0.82
191	2,3,3N,4,4N,5N,6	—	—	—	—	—	—	0.17
192	2,3,3N,4,5,5N,6	—	—	—	—	—	—	—
193	2,3,3N,4N,5,5N,6	—	—	—	—	—	0.03	0.53
194	2,2N,3,3N,4,4N,5,5N	—	—	—	—	—	0.01	2.07
195	2,2N,3,3N,4,4N,5,6	—	—	—	—	—	—	0.84
196	2,2N,3,3N,4,4N,5,6N	—	—	—	—	—	—	1.09
197	2,2N,3,3N,4,4N,6,6N	—	—	—	—	—	—	0.07
198	2,2N,3,3N,4,5,5N,6	—	—	—	—	—	—	0.10
199	2,2N,3,3N,4,5,5N,6N	—	—	—	—	—	0.01	1.78
200	2,2N,3,3N,4,5,6,6N	—	—	—	—	—	—	0.25
201	2,2N,3,3N,4,5N,6,6N	—	—	—	—	—	—	0.24
202	2,2N,3,3N,5,5N,6,6N	—	—	—	—	—	—	0.33
203	2,2N,3,4,4N,5,5N,6	—	—	—	—	—	0.02	1.40

Table 4-5. Polychlorinated Biphenyl Congener Compositions (in Weight Percent)[a] in Aroclors[b] *(continued)*

		Aroclor						
PCB No.	Chlorine positions	1016[c]	1242[d]	1248[e]	1248[f]	1254[g] "Late"	1254[h]	1260[i]
204	2,2N,3,4,4N,5,6,6N	—	—	—	—	—	—	—
205	2,3,3N,4,4N,5,5N,6	—	—	—	—	—	—	0.10
206	2,2N,3,3N,4,4N,5,5N,6	—	—	—	—	0.03	0.03	0.53
207	2,2N,3,3N,4,4N,5,6,6N	—	—	—	—	—	—	0.05
208	2,2N,3,3N,4,5,5N,6,6N	—	—	—	—	0.01	0.01	0.13
209	2,2N,3,3N,4,4N,5,5N,6,6N	—	—	—	—	—	—	NM
Sum of weight percents =		100.0	100.0	100.2	100.2	100.2	100.4	100.3

[a]Weight percent values in table are biased high with respect to mole percent values (not calculated).
[b]Source: Frame et al. (1996)
[c]Lot A2 Aroclor 1016
[d]Mean of three Lots of Aroclor 1242
[e]Lot A3.5 Aroclor 1248
[f]Lot G3.5 Aroclor 1248
[g]Lot A4 Aroclor 1254 (Monsanto Lot KI-02-6024) from abnormal late production (1974–1977)
[h]Lot G4 Aroclor 1254 (GE/118-peak analytical standard)
[i]Mean of three Lots of Aroclor 1260

NM = congener not measured, but present at trace level.

increased levels of the high TEF (i.e., 2,3,7,8-tetrachlorodibenzo-*p*-dioxin ("dioxin") Equivalency Factor; "T" often defined as "toxic") chlorobiphenyls, were produced from 1974 to 1977 (see Section 5.1).

The pyrolysis of technical-grade PCB mixtures produces several PCDFs (Rappe et al. 1979; Schecter and Charles 1991). PCDFs are also produced during the commercial production and handling of PCBs. The amount of PCDFs formed depends upon the manufacturing conditions. The concentrations of PCDF impurities in various commercial Aroclors are shown in Table 4-6. The impurities 2,3,7,8-tetrachlorodibenzofuran and 2,3,4,7,8-pentachlorodibenzofuran were found at concentrations of 0.33 and 0.83 ppm, respectively, in Aroclor 1248; and at 0.11 and 0.12 ppm, respectively, in Aroclor 1254 (Van den Berg et al. 1985). Concentrations of PCDFs in commercial PCB mixtures including Clophen A-60, Phenoclor DP-6, and Kanechlor 400 have been reported (De Voogt and Brinkman 1989).

Physical properties such as solubility, vapor pressure, and Henry's law constant have been reported for individual congeners (Dunnivant and Elzerman 1988; Dunnivant et al. 1992; Falconer and Bidleman 1994; Murphy et al. 1987; Sabljic and Güsten 1989). Physical and chemical properties for several PCB congeners are presented in Table 4-7 (Bidelman 1984; Dunnivant et al. 1992; Erikson 1986; Hansch and Leo 1979; Hutsinger et al. 1974; Mackay et al. 1992; Murray and Andren 1991; Yalkowsky et al. 1983). Experimentally determined log K_{ow} values for 19 congeners and an estimation method for the determination of log K_{ow} values of other PCB congeners are also available (Sabljic et al. 1993). The congeners reported are important due to their toxicity or because they occur in higher concentrations in the environment.

Table 4-6. Concentrations of Chlorinated Dibenzofurans (CDFs) in Commercial Polychlorinated Biphenyl Mixtures[a]

PCB	Tetra-CDF	Penta-CDF	Hexa-CDF	Total (PCDFs)[b]
Aroclor 1016 (1977)	Not detected	Not detected	Not detected	–
Aroclor 1016	Not detected	Not detected	Not detected	–
Aroclor 1242	0.07	0.03	0.003	0.15
Aroclor 1242	0.07	0.03	0.003	0.15
Aroclor 1242	2.3	2.2	Not detected	4.5
Aroclor 1254 (1969)	0.1	0.2	1.4	1.7
Aroclor 1254 (1970)	0.2	0.4	0.9	1.5
Aroclor 1254	0.02	0.2	0.4–0.6	0.8
Aroclor 1254	0.1	3.6	1.9	5.6
Aroclor 1260 (1969)	0.1	3.6	1.9	5.6
Aroclor 1260 (Lot AK3)	0.2	0.3	0.3	0.8
Aroclor 1260	0.3	1.0	1.1	3.8[b]
Aroclor 1260	0.8	0.9	0.5	2.2
Clopen A-60	1.4	5.0	2.2	8.6
Phenoclor DP-6	0.7	10.0	2.9	13.6
Kanechlor 400	–	–	–	. 20.0

Source: Adapted from de Voogt and Brinkman 1989

[a]in µg/g
[b]Total includes quantities of tri-CDF and hepta-CDF isomers that were analyzed.

CDF = chlorodibenzofuran; PCDFs = polychlorinated dibenzofurans

Table 4-7. Physical and Chemical Properties of Several Congeners of Polychlorinated Biphenyls

Property	PCB 77	PCB 138	PCB 153	PCB 169	PCB 180
Molecular weight	291.98[a]	360.9[b]	360.88[b]	360.86[a]	395.32[b]
Molecular formula	$C_{12}H_6Cl_4$[b]	$C_{12}H_4Cl_6$[b]	$C_{12}H_4Cl_6$[b]	$C_{12}H_4Cl_6$[b]	$C_{12}H_3Cl_7$[b]
Melting point EC	173[c]	78.5–80[c]	103–104[c]	201–202[c]	109–110[b]
Boiling point EC	360 (calc.)[b]	400 (calc.)[b]	No data	No data	240–280 (20 mmHg)[b]
Density g/cm^3 at 25 EC	1.2024 (20 EC)[b]	No data	No data	No data	No data
Odor	No data	No data	No data	No data	No data
Solubility:					
Water mg/L	0.175 ppm[c]; 0.00055[e]	0.0159–0.0159 (calc.)[b]	0.00091 ppm[d]; 0.00086[e]	0.000036–0.01230 (calc.)[b]	0.00031–0.00656 (calc.)[b]; 0.00023[e]
Organic solvents	–	–	–	–	–
Partition coefficients:					
Log K_{ow}	6.04–6.63[b]	6.50–7.44 (calc.)[b]	8.35[e]; 6.72[b]	7.408[b]	6.70–7.21 (calc.)[b]
Log K_{oc}	4.41–5.75[b]	5.21–7.3[b]	4.75–7.68[b]	6.60[b]	5.78–6.9[b]
Vapor pressure mm Hg at 25 EC	$4.4x10^{-7}$ [d]	$4.0x10^{-6}$ [f]	$3.80x10^{-7}$ [f] $9.0x10^{-7}$ [d]	$4.02x10^{-7}$ [b]	–
Henry's law constant atm-m^3/mol at 25 EC	$0.43x10^{-4}$ [g] $0.94x10^{-4}$ [i] $0.83x10^{-4}$ [e]	$1.07x10^{-4}$ [h] $0.21x10^{-4}$ [b]	2.78 (10^4)[g] 1.32 (10^4)[i] 1.31 (10^4)[e]	$0.15x10^{-4}$ [b] $0.59x10^{-4}$ [b]	$1.07x10^{-4}$ [e]
Explosive limits	No data	No data	No data	No data	No data

[a]HSDB 2000
[b]Yalkowsky et al. 1983
[c]Hutsinger et al. 1974
[d]Mackay et al. 1992
[e]Dunnivant et al. 1992
[f]Erikson 1986
[g]Hansch and Leo 1995
[h]Bidelman 1984
[i]Murray and Andren 1991