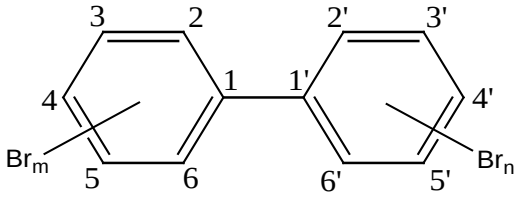
4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Polybrominated Biphenyls. PBBs are a class of structurally similar brominated hydrocarbons in which 2–10 bromine atoms are attached to the biphenyl molecule. Monobrominated structures (i.e., one bromine atom attached to the molecule) are often included when describing PBBs. The general chemical structure of PBBs is shown below:



where m + n = 1–10

It can be seen from the structure that a large number of brominated compounds are possible. The 209 possible compounds for PBBs are called "congeners". However, the number of PBB congeners that actually exist in commercial PBB mixtures is much less compared to polychlorinated biphenyls (PCBs). Typically, only a subset of the 209 possible congeners is observed for PBBs. PBBs can be categorized by degree of bromination. The term "homolog" is used to refer to all PBBs with the same number of bromines (e.g., tribromobiphenyls). Based on the number of bromine substituents, there are 10 homologous groups of PBBs (monobrominated through decabrominated). Each homologous group contains one or more congeners. The mono-, di-, tri-, tetra-, penta-, hexa-, hepta-, octa-, nona-, and decabromo congeners can exist in 3, 12, 24, 42, 46, 42, 24, 12, 3, and 1 forms, respectively. Homologs with different substitution patterns are referred to as isomers. For example, the group of dibromobiphenyl homologs contains 12 isomers. The numbering system for PBBs 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. In a PBB molecule, the benzene rings can rotate around the bond connecting them; the two extreme configurations are planar (the two benzene rings are in the same plane; dihedral angle=0°) and nonplanar (the two benzene rings are in perpendicular planes to each other; dihedral angle=90°). 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 bromine atoms forces the benzene rings to adopt a configuration with a larger dihedral angle or a nonplanar configuration. The benzene rings of non-*ortho* substituted PBBs, as well as mono-*ortho* substituted PBBs, may assume a small dihedral angle (in which the dihedral angle is small, but >0°) or "near" planar configuration. These

molecules 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 nonplanar congeners (Hardy 2002a).

Like PCBs, the 209 congeners for PBBs are arranged in ascending numerical order using a numbering system developed by Ballschmiter and Zell (1980) that follows the IUPAC rules of substituent characterization of biphenyls. The resulting numbers assigned by Ballschmiter and Zell (which are also referred to as congener, IUPAC, or BZ numbers) are widely used for identifying individual congeners of PBBs. For example, the PBB congener, 2,2',4,4',5,5'-hexabromobiphenyl, may be referred to as BB 153 in this document. The identities of several PBB congeners are shown in Table 4-1 (WHO 1994a, 1994b).

Michigan Chemical Corporation, the major producer of PBBs from 1970 to 1976, marketed mixtures of PBBs under the trade name FireMaster (e.g., BP-6 and FF-1). However, the FireMaster trade name has also been used for other brominated flame retardants using different numerical designations. Other former producers of PBBs in the United States included White Chemical Corporation (Bayonne, New Jersey) and Hexcel Corporation (Sayreville, New Jersey), which both produced technical mixtures of octabromobiphenyl and decabromobiphenyl until 1979. The trade names of some commercial PBB mixtures formerly produced in other countries are: Berk Corporation, Great Britain (e.g., BerkFlam, Flammex); Chemische Fabrik Kalk, Germany (e.g., Bromkal); and Ugine Kuhlmann (now Atofina in France) (e.g., Adine).

The chemical identities of hexabromobiphenyl, octabromobiphenyl, decabromobiphenyl (BB 209), and BB 153, the most abundant congener in commercial FireMaster FF-1 and FireMaster BP-6, are listed in Table 4-2.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information found in the literature regarding the physical and chemical properties of hexabromobiphenyl, octabromobiphenyl, decabromobiphenyl, and BB 153 is presented in Table 4-3. The data for the properties listed in Table 4-3 may not be reliable because products of questionable purity were used by earlier investigators to derive them. For example, the water solubility of hexabromobiphenyl (Neufeld et al. 1977) was reported to be the same as that of FireMaster FF-1 (Getty et al. 1977), although FireMaster FF-1 contained only 84.4% (Robertson et al. 1983b) hexabrominated biphenyls. However, recent physical and chemical property data have been reported for hexabromobiphenyl in Tittlemier et al. (2002).

Table 4-1. Chemical Identity of Polybrominated Biphenyl (PBB) Congeners

IUPAC No.[a]	Compound/ substituents	CAS No.[b]
	Biphenyl	92-52-4
	Monobromo-	26264-10-8
1	2	2052-07-7
2	3	2113-57-7
3	4	92-66-0
	Dibromo-	27479-65-8
4	2,2’	13029-09-9
5	2,3	115245-06-2
6	2,3’	49602-90-6
7	2,4	53592-10-2
8	2,4’	49602-91-7
9	2,5	57422-77-2
10	2,6	59080-32-9
11	3,3’	16400-51-4
12	3,4	60108-72-7
13	3,4’	57186-90-0
14	3,5	16372-96-6
15	4,4’	92-86-4
	Tribromobiphenyl	51202-79-0
16	2,2’,3	
17	2,2’,4	
18	2,2’,5	59080-34-1
19	2,2’,6	
20	2,3,3’	
21	2,3,4	
22	2,3,4’	
23	2,3,5	
24	2,3,6	
25	2,3’,4	
26	2,3’,5	59080-35-2
27	2,3’,6	
28	2,4,4’	6430-90-6
29	2,4,5	115245-07-3
30	2,4,6	59080-33-0
31	2,4’,5	59080-36-3
32	2,4’,6	64258-03-3
33	2’,3,4	
34	2’,3,5	
35	3,3’,4	
36	3,3’,5	
37	3,4,4’	6683-35-8

Table 4-1. Chemical Identity of Polybrominated Biphenyl (PBB) Congeners

IUPAC No.[a]	Compound/ substituents	CAS No.[b]
38	3,4,5	115245-08-4
39	3,4’,5	72416-87-6
	Tetrabromobiphenyl	40088-45-7
40	2,2’,3,3’	
41	2,2’,3,4	
42	2,2’,3,4’	
43	2,2’,3,5	
44	2,2’,4,5’	
45	2,2’,3,6	
46	2,2’,3,6’	
47	2,2’,4,4'	66115-57-9
48	2,2’,4,5	
49	2,2’,4,5'	60044-24-8
50	2,2’,4,6	
51	2,2’,4,6'	97038-95-4
52	2,2’,5,5'	59080-37-4
53	2,2’,5,6'	60044-25-9
54	2,2’,6,6'	97038-96-5
55	2,3,3’,4	97038-99-8
56	2,3,3’,4’	
57	2,3,3’,5	
58	2,3,3’,5’	
59	2,3,3’,6	
60	2,3,4,4’	
61	2,3,4,5	115245-09-5
62	2,3,4,6	115245-10-8
63	2,3,4’,5	
64	2,3,4’,6	
65	2,3,5,6	
66	2,3’,4,4’	84303-45-7
67	2,3’,4,5	
68	2,3’,4,5’	
69	2,3’,4,6	
70	2,3’,4’,5	59080-38-5
71	2,3’,4’,6	
72	2,3’,5,5’	
73	2,3’,5’,6	
74	2,4,4’,5	
75	2,4,4’,6	64258-02-2
76	2’,3,4,5	
77	3,3’,4,4’	77102-82-0
78	3,3’,4,5	

Table 4-1. Chemical Identity of Polybrominated Biphenyl (PBB) Congeners

IUPAC No.[a]	Compound/ substituents	CAS No.[b]
79	3,3',4,5'	97038-98-7
80	3,3',5,5'	16400-50-3
81	3,4,4',5	59589-92-3
	Pentabromobiphenyl	56307-79-0
82	2,2',3,3',4	
83	2,2',3,3',5	
84	2,2',3,3',6	
85	2,2',3,4,4'	
86	2,2',3,4,5	
87	2,2',3,4,5'	
88	2,2',3,4,6	77910-04-4
89	2,2',3,4,6'	
90	2,2',3,4',5	
91	2,2',3,4',6	
92	2,2',3,5,5'	
93	2,2',3,5,6	
94	2,2',3,5,6'	
95	2,2',3,5',6	88700-05-4
96	2,2',3,6,6'	
97	2,2',3',4,5	
98	2,2',3',4,6	
99	2,2',4,4',5	81397-99-1
100	2,2',4,4',6	97038-97-6
101	2,2',4,5,5'	67888-96-4
102	2,2',4,5,6'	80274-92-6
103	2,2',4,5',6	59080-39-6
104	2,2',4,6,6'	97063-75-7
105	2,3,3',4,4'	
106	2,3,3',4,5	
107	2,3,3',4',5	
108	2,3,3',4,5'	
109	2,3,3',4,6	
110	2,3,3',4',6	
111	2,3,3',5,5'	
112	2,3,3',5,6	
113	2,3,3',5',6	
114	2,3,4,4',5	96551-70-1
115	2,3,4,4',6	
116	2,3,4,5,6	38421-62-4
117	2,3,4',5,6	
118	2,3',4,4',5	6788-97-5
119	2,3',4,4',6	86029-64-3

Table 4-1. Chemical Identity of Polybrominated Biphenyl (PBB) Congeners

IUPAC No.[a]	Compound/ substituents	CAS No.[b]
120	2,3',4,5,5'	80407-70-1
121	2,3',4,5',6	
122	2',3,3',4,5	
123	2',3,4,4',5	74114-77-5
124	2',3,4,5,5'	
125	2',3,4,5,6'	
126	3,3',4,4',5	84303-46-8
127	3,3',4,5,5'	81902-33-2
	Hexabromobiphenyl	36355-01-8
128	2,2',3,3',4,4'	82865-89-2
129	2,2'3,3',4,5	
130	2,2',3,3',4,5'	82865-90-5
131	2,2',3,3',4,6	
132	2,2',3,3',4,6'	119264-50-5
133	2,2',3,3',5,5'	55066-76-7
134	2,2',3,3',5,6	
135	2,2',3,3',5,6'	119264-51-6
136	2,2',3,3',6,6'	
137	2,2',3,4,4',5	81381-52-4
138	2,2',3,4,4',5'	67888-98-6
139	2,2',3,4,4',6	
140	2,2',3,4,4',6'	
141	2,2',3,4,5,5'	120991-47-1
142	2,2',3,4,5,6	
143	2,2',3,4,5,6'	
144	2,2',3,4,5',6	119264-52-7
145	2,2',3,4,6,6'	
146	2,2',3,4',5,5'	
147	2,2',3,4',5,6	
148	2,2',3,4',5,6'	
149	2,2',3,4',5',6	69278-59-7
150	2,2',3,4',5,6'	93261-83-7
151	2,2',3,5,5',6	119264-53-8
152	2,2',3,5,6,6'	
153	2,2',4,4',5,5'	59080-40-9
154	2,2',4,4',5,6'	36402-15-0
155	2,2',4,4',6,6'	59261-08-4
156	2,3,3',4,4',5	77607-09-1
157	2,3,3',4,4',5'	84303-47-9
158	2,3,3',4,4',6	
159	2,3,3',4,5,5'	120991-48-2
160	2,3,3',4,5,6	

Table 4-1. Chemical Identity of Polybrominated Biphenyl (PBB) Congeners

IUPAC No.[a]	Compound/ substituents	CAS No.[b]
161	2,3,3',4,5',6	
162	2,3,3',4',5,5'	
163	2,3,3',4',5,6	
164	2,3,3',4',5',6	82865-91-5
165	2,3,3',5,5',6	
166	2,3,4,4',5,6	
167	2,3',4,4',5,5'	67888-99-7
168	2,3',4,4',5',6	84303-48-0
169	3,3',4,4',5,5'	60044-26-0
	Heptabromobiphenyl	35194-78-6
170	2,2',3,3',4,4',5	69278-60-0
171	2,2',3,3',4,4',6	
172	2,2',3,3',4,5,5'	82865-92-7
173	2,2',3,3',4,5,6	
174	2,2',3,3',4,5,6'	88700-04-3
175	2,2',3,3',4,5',6	
176	2,2',3,3',4,6,6'	
177	2,2',3,3',4',5,6	
178	2,2',3,3',5,5',6	119264-54-9
179	2,2',3,3',5,6,6'	
180	2,2',3,4,4',5,5'	67733-52-2
181	2,2',3,4,4',5,6	
182	2,2',3,4,4',5,6'	119264-55-0
183	2,2',3,4,4',5',6	
184	2,2',3,4,4',6,6'	119264-56-1
185	2,2',3,4,5,5',6	
186	2,2',3,4,5,6,6'	119264-57-2
187	2,2',3,4',5,5',6	84303-49-1
188	2,2',3,4',5,6,6'	119264-58-3
189	2,3,3',4,4',5,5'	88700-06-5
190	2,3,3',4,4',5,6	79682-25-0
191	2,3,3',4,4',5',6	
192	2,3,3',4,5,5',6	
193	2,3,3',4',5,5',6	
	Octabromobiphenyl	27858-07-7
194	2,2',3,3',4,4',5,5'	67889-00-3
195	2,2',3,3',4,4',5,6	
196	2,2',3,3',4,4',5',6	
197	2,2',3,3',4,4',6,6'	119264-59-4
198	2,2',3,3',4,5,5',6	
199	2,2',3,3',4,5,6,6'	
200	2,2',3,3',4,5,6,6'	119264-60-7

Table 4-1. Chemical Identity of Polybrominated Biphenyl (PBB) Congeners

IUPAC No.[a]	Compound/ substituents	CAS No.[b]
201	2,2',3,3',4,5',6,6'	69887-11-2
202	2,2',3,3',5,5',6,6'	59080-41-0
203	2,2',3,4,4',5,5',6	
204	2,2',3,4,4',5,6,6'	119264-61-8
205	2,3,3',4,4',5,5',6	
	Nonabromobiphenyl	27753-52-2
206	2,2',3,3',4,4',5,5',6	69278-62-2
207	2,2',3,3',4,4',5,6,6'	119264-62-9
208	2,2',3,3',4,5,5',6,6'	119264-63-0
	Decabromobiphenyl	13654-09-6
209	2,2',3,3',4,4',5,5',6,6'	13654-09-6

[a]Ballschmiter and Zell 1980
[b]Not all PBBs have been assigned CAS numbers
[c]WHO 1994b

Table 4-2. Chemical Identity of Selected PBBs[a]

Characteristic	Hexabromo-biphenyl	Octabromo-biphenyl	Decabromo-biphenyl	2,2',4,4'5,5'-Hexa-bromobiphenyl
Synonym(s)	FireMaster BP-6[b]; FireMaster FF-1[b]	Bromkal 80[b]	Flammex B 10[b]; Adine 0102[b]; Berkflam B 10[b]	2,2',4,4'5,5'hexa-bromo-1,1'-biphenyl
Registered trade name(s)	FireMaster BP-6; FireMaster FF-1	Bromkal 80	Flammex B 10; Adine 0102; Berkflam B 10	None
Chemical formula	$C_{12}H_4Br_6$	$C_{12}H_2Br_8$	$C_{12}Br_{10}$	$C_{12}H_4Br_6$
Chemical structure				
Identification numbers:				
CAS registry	59536-65-1 (BP-6); 67774-32-7 (FF-1); 36355-01-8 (hexa-bromo mixture)	27858-07-7 (octo-bromo mixture) 61288-13-9 (Bromkal 80)	13654-09-6 (pure and technical)	59080-40-9
NIOSH RTECS	LK 5060000 (BP-6); LK 5065000 (FF-1)	DV 570000 (octa-bromo mixture)	No data	No data
EPA hazardous waste	No data	No data	No data	No data
OHM/TADS	No data	No data	No data	No data
DOT/UN/NA/IMCO shipping	No data	No data	No data	No data
HSDB	No data	No data	No data	2913
NCI	No data	No data	No data	No data

[a]All information obtained from IARC (1986) except where noted.
[b]These are mixtures of compounds, and their compositions are given in the text.

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; RTECS = Registry of Toxic Effects of Chemical Substances

Table 4-3. Physical and Chemical Properties of Selected PBBs[a]

Property	Hexabromobiphenyl	Octabromobiphenyl	Decabromobiphenyl	2,2',4,4',5,5'-Hexabromobiphenyl
Molecular weight	627.4	785.2	943.1	627.4
Color	White	White	White	White
Physical state	Solid	Solid	Solid	Solid
Melting point	72 °C	200–250 °C; 365–367 °C[b] (for industrial product)	380–386 °C	No data
Boiling point	No data	No data	No data	No data
Density	No data	No data	No data	No data
Odor	No data	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	11 µg/L; 3 µg/L[c]	20–30 µg/L	Insoluble	11 µg/L[d]
Organic solvent(s)	Soluble in acetone, benzene	Soluble in methylene chloride, benzene	Moderately soluble in chlorobenzene, o-xylene	Acetone (6 weight percent); benzene (75 weight percent)[c]
Partition coefficients:				
Log K_{ow}	6.39[e]	5.53	8.58[f]	9.10 (estimated)[d]
Log K_{oc}	3.33–3.87[g]	No data	No data	5.088[d]
Vapor pressure	5.2×10^{-8} mmHg at 25 °C[h]; 5.6×10^{-6} mm Hg (liquid sub-cooled)[c]	7×10^{-11} mmHg at 28 °C[i]	No data	7.6×10^{-5} mm Hg at 90 °C[d]
Henry's law constant	3.9×10^{-6} atm-m^3/mol[j]; 1.38×10^{-6} atm-m^3/mol[c]	No data	No data	5.7×10^{-3} atm-m^3/mol[d]
Autoignition temperature	No data	No data	No data	No data
Flashpoint	No data	No data	No data	No data
Flammability limits	No data	No data	No data	No data
Conversion factors	Since these compounds exist in the particle phase in the ambient atmosphere, the concentrations in air are expressed in weight per unit volume of the air.			
Explosive limits	No data	No data	No data	No data

[a]All information obtained from IARC (1978) and Norris et al. (1973) unless otherwise noted.
[b]Sundstrom et al. 1976b
[c]Tittlemier et al. 2002
[d]Hardy (2002a)
[e]Doucette and Andren 1988
[f]The values for 2,2'4,4'6,6'- and 2,2',3,3',4,4'-hexabromobiphenyl are given as 7.20 (Chessells et al. 1992) and 8.09 (Anliker et al. 1988), respectively.
[g]Estimated from the Freundlich adsorption constants given by Jacobs et al. (1978).
[h]Jacobs et al. 1976
[i]Waritz et al. 1977
[j]Estimated from the ratio of vapor pressure and water solubility.

Of the 209 possible congeners of PBBs, only about 42 have been synthesized in pure form even on a laboratory scale (Sundstrom et al. 1976b). The PBBs produced for commercial use were mixtures of PBBs with other non-PBB impurities. The technical products were FireMaster BP-6, FireMaster FF-1, Bromkal 80, and Flammex B 10 (or Adine 0102 or Berkflam B 10) (IARC 1986). FireMaster FF-1, a white powder, was made by grinding brown flakes of FireMaster BP-6 and adding 2% calcium silicate as an anticaking agent (Fries 1985b). The exact composition of FireMaster BP-6 or FireMaster FF-1 seems to have varied between and within batches (Sundstrom et al. 1976a). Table 4-4 provides the concentrations of the PBB congeners in FireMaster FF-1 and FireMaster BP-6.

An interesting feature of commercial FireMaster FF-1 and FireMaster BP-6 is that they contain >50% of the congener BB 153. The second most abundant congener is 2,2',3,4,4',5,5'-heptabromobiphenyl (BB 180). A detailed analysis of FireMaster BP-6 (lot 7062) was able to separate 22 congeners of PBBs that included four tri, five tetra, three penta, seven hexa, and three hepta congeners of PBBs (Robertson et al. 1983b, 1984b). The coplanar and toxic congeners 3,3',4,4'-tetra-, 3,3',4,4',5-penta-, and 3,3',4,4',5,5'-hexabrominated biphenyls were found at abundances of 0.159, 0.079, and 0.294%, respectively (Orti et al. 1983; Robertson et al. 1983b). In addition to the 22 congeners, other investigators have identified 2,2',3,3',4,4',5,6'-octa-, 2,2',3,3',4,4',5,5'-octa-, 2,2',3,3',4,4',5,5',6-nona-, and decabromobiphenyl in commercial PBBs (Moore et al. 1978). Other impurities detected in FireMaster FF-1 and FireMaster BP-6 were tetra-, penta-, and hexabromonaphthalene (Di Carlo et al. 1978); however, at a detection limit of 0.5 ppm, brominated dioxins and dibenzofurans were not detected in commercial FireMaster FF-1 or FireMaster BP-6 (Hass et al. 1978).

Commercial octabromobiphenyl (Bromkal 80) contained at least four compounds. Assays of two commercial octabromobiphenyls showed the following compositions: 1.0–1.8% heptabromobiphenyl, 33.0–45.2% octabromobiphenyl, 47.4–60.0% nonabromobiphenyl, and 5.7–6.0% decabromobiphenyl (Norris et al. 1973; Waritz et al. 1977). Notably, the major component of commercial octabromobiphenyl was nonabromobiphenyl, and not octabromobiphenyl. Commercial decabromobiphenyl (Flammex B 10) contained 96.8% decabromobiphenyl, 2.9% nonabromobiphenyl, and 0.3% octabromobiphenyl (Di Carlo et al. 1978).

Pyrolysis of FireMaster BP-6 in the temperature range of 600–900 °C in the absence of oxygen produced bromobenzenes and brominated biphenyls as key products, but no brominated dioxins and dibenzofurans (Thoma and Hutzinger 1987; Thoma et al. 1987). Thermolysis of FireMaster BP-6 between 400 and

Table 4-4. Identified PBB Congeners in FireMaster® BP-6 and FireMaster® FF-1

IUPAC No.[a]	Structure	Percent composition of FireMaster BP-6	Percent composition of FireMaster FF-1	References
Dibromobiphenyls				
4	2,2'-	0.020		Moore et al. 1979
Tribromobiphenyls				
18	2,2',5-	0.050		Robertson et al. 1984b
26	2,3',5-	0.024		
31	2,4',5-	0.015		
37	3,4,4'-	0.021		
Tetrabromobiphenyls				
49	2,2',4,5'-	0.025		
52	2,2',5,5'-	0.052		
66	2,3',4,4'-	0.028		
70	2,3',4',5-	0.017		
77	3,3',4,4'-		<0.080	Orti et al. 1983
		0.159		Robertson et al. 1984b
Pentabromobiphenyls				
95	2,2',3,5',6-	0.020		Orti et al. 1983
99	2,2',4,4',5-		<0.08	
101	2,2',4,5,5'-	2.69		Robertson et al. 1984b
		4.50	3.70	Aust et al. 1981
			1.54	Orti et al. 1983
		2.60		Krüger 1988
118	2,3',4,4',5-	2.94		Robertson et al. 1984b
			0.70	Robertson et al. 1984b
		3.20		Krüger 1988
126	3,3',4,4',5-		<0.01	
		0.079		Robertson et al. 1984b
Hexabromobiphenyls				
132	2,2'3,3',4,6'-	1		Krüger 1988
138	2,2',3,4,4',5'-	12.3		Robertson et al. 1984b
		12	8.6	Aust et al. 1981
			5.23	Orti et al. 1983
		10.6		Krüger 1988
149	2,2',3,4',5',6-	2.24		Robertson et al. 1984b
		1.40	1.30	Aust et al. 1981
			0.78	Orti et al. 1983
153	2,2',4,4',5,5'-	53.9		Robertson et al. 1984b
		47.8	47.1	Aust et al. 1981
		55.2		Orti et al. 1983
		58.5		Krüger 1988

Table 4-4. Identified PBB Congeners in FireMaster® BP-6 and FireMaster® FF-1

IUPAC No.[a]	Structure	Percent composition of FireMaster BP-6	Percent composition of FireMaster FF-1	References
155	2,2'4,4',6,6'-	0.5		
156	2,3,3',4,4',5-	0.980		Robertson et al. 1984b
		5.0		Aust et al. 1981
		0.37		Orti et al. 1983
		1.0		Krüger 1988
157	2,3,3',4,4',5'-	0.05		Orti et al. 1983
		0.526		Robertson et al. 1984b
		0.5`		Krüger 1988
167	2,3',4,4',5,5'-	5.5	3.3	Aust et al. 1981
		3.37		Orti et al. 1983
		<0.3		
		7.95		Robertson et al. 1984b
		5.5		Krüger 1988
169	3,3',4,4',5,5'-	0.294		Robertson et al. 1984b
Heptabromobiphenyls				
170	2,2',3,3',4,4',5-	0.256		
		1.1	1.5	Aust et al. 1981
		1.66		Orti et al. 1983
		2.4		Krüger 1988
172	2,2',3,3',4,5,5'-	<0.30		Orti et al. 1983
174	2,2',3,3',4,5,6'-	0.24		
178	2,2',3,3',5,5',6-	0.3		Krüger 1988
180	2,2',3,4,4',5,5'	6.97		Robertson et al. 1984b
			24.7	Aust et al. 1981
			23.5	Orti et al. 1983
187	2,2',3,4',5,5',6-	0.392		Robertson et al. 1984b
			1.0	Krüger 1988
189	2,3,3',4,4',5,5'-		0.51	Orti et al. 1983
Octabromobiphenyls				
194	2,2',3,3',4,4',5,5'-	0.9	2.4	Aust et al. 1981
			1.65	Orti et al. 1983
196	2,2',3,3',4,4',5,6'-			Moore et al. 1980
201	2,2',3,3',4,5,5',6'-			Orti et al. 1983
203	2,2',3,4,4',5,5',6-			

Source: WHO 1994b

[a]Ballschmiter and Zell 1980

600 °C in the presence of air produced 2,3,7,8-tetrabromodibenzofuran in the percent (1%=10 g/kg) range (Rappe and Buser 1980). Pyrolysis of FireMaster BP-6 in an open quartz tube at 800 °C produced 0.48–1.49 g/kg 2,3,7,8-TCDD equivalent levels of polybrominated dibenzofurans (Zacharewski et al. 1988). FireMaster BP-6 hydrolyzed when refluxed with 2% potassium hydroxide in ethanol, but the possible rate of PBB hydrolysis under much milder environmental conditions remains unknown (Pomerantz et al. 1978).

Hexabromonapthalene has been identified as a toxic contaminant of Firemaster BP-6 or FF-1 at concentration levels of approximately 150 ppm (Birnbaum et al. 1983). Previously reported to be a single compound, hexabromonapthalene was shown to be a 60:40 mixture of 1,2,3,4,6,7-hexabromonaphthalene and 2,3,4,5,6,7-hexabromonaphthalene.