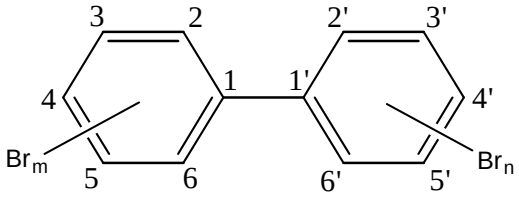
6. CHEMICAL AND PHYSICAL INFORMATION

6.1 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

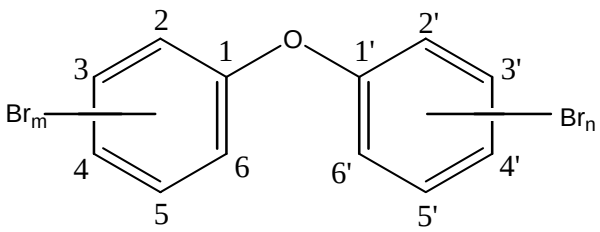
molecules are referred to as planar or coplanar congeners. The benzene rings of other congeners cannot assume a planar or coplanar configuration and are referred to as nonplanar congeners (Hardy 2002).

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 6-1 (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 6-2.

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



where m + n = 1–10

Table 6-1. Chemical Identity of Polybrominated Biphenyl (PBB) and Polybrominated Diphenyl Ether (PBDE) Congeners

IUPAC No.[a]	Compound/ substituents	CAS No.[b]	
		Brominated biphenyls (BB)[c]	Brominated diphenyl ethers (BDE)[d]
	Biphenyl	92-52-4	92-52-4
	Monobromo-	26264-10-8	101-55-3
1	2	2052-07-7	
2	3	2113-57-7	
3	4	92-66-0	
	Dibromo-	27479-65-8	2050-47-7
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	49690-94-0
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		

Table 6-1. Chemical Identity of Polybrominated Biphenyl (PBB) and Polybrominated Diphenyl Ether (PBDE) Congeners

IUPAC No.[a]	Compound/ substituents	CAS No.[b]	
		Brominated biphenyls (BB)[c]	Brominated diphenyl ethers (BDE)[d]
36	3,3',5		
37	3,4,4'	6683-35-8	
38	3,4,5	115245-08-4	
39	3,4',5	72416-87-6	
	Tetrabromobiphenyl	40088-45-7	40088-47-9
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		

Table 6-1. Chemical Identity of Polybrominated Biphenyl (PBB) and Polybrominated Diphenyl Ether (PBDE) Congeners

IUPAC No.[a]	Compound/ substituents	CAS No.[b]	
		Brominated biphenyls (BB)[c]	Brominated diphenyl ethers (BDE)[d]
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		
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	32534-81-9
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		

Table 6-1. Chemical Identity of Polybrominated Biphenyl (PBB) and Polybrominated Diphenyl Ether (PBDE) Congeners

IUPAC No.[a]	Compound/ substituents	CAS No.[b]	
		Brominated biphenyls (BB)[c]	Brominated diphenyl ethers (BDE)[d]
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	
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	36483-60-0
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'		

Table 6-1. Chemical Identity of Polybrominated Biphenyl (PBB) and Polybrominated Diphenyl Ether (PBDE) Congeners

IUPAC No.[a]	Compound/ substituents	CAS No.[b]	
		Brominated biphenyls (BB)[c]	Brominated diphenyl ethers (BDE)[d]
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		
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	68928-80-3
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		

Table 6-1. Chemical Identity of Polybrominated Biphenyl (PBB) and Polybrominated Diphenyl Ether (PBDE) Congeners

IUPAC No.[a]	Compound/ substituents	CAS No.[b]	
		Brominated biphenyls (BB)[c]	Brominated diphenyl ethers (BDE)[d]
192	2,3,3',4,5,5',6		
193	2,3,3',4',5,5',6		
	Octabromobiphenyl	27858-07-7	32536-52-0
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	
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	63936-56-1
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	1163-19-5
209	2,2',3,3',4,4',5,5',6,6'	13654-09-6	1163-19-5

[a]Ballschmiter and Zell 1980
[b]Not all PBBs have been assigned CAS numbers; with the exception of BDE 209, no CAS numbers were identified for the PBDE class.
[c]WHO 1994b
[d]WHO 1994a

Table 6-2. 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

It can be seen from the structure that a large number of brominated compounds are possible. The 209 possible compounds for PBDEs are called “congeners”. However, the number of PBDE congeners that actually exist in commercial PBDE mixtures are much less compared to PCBs. Typically, only a subset of the 209 possible congeners is observed for PBDEs. PBDEs can also be categorized by degree of bromination. The term “homolog” is used to refer to all PBDEs with the same number of bromines (e.g., tribromodiphenyl ether refers to PBDEs containing only three bromine atoms). Based on the number of bromine substituents, there are 10 homologous groups of PBDEs (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 dibromodiphenyl ether homologs contains 12 isomers. The numbering system for PBDEs is also shown above. The structures of representative PBB and PBDE molecules appear similar when drawn in one dimension. However, there are important three-dimensional differences in their structures due to the ether linkage and location/number of halogen atoms. The *ortho* positions of the aromatic rings must be nonhalogen-substituted for a diphenyl ether molecule to assume a planar or near planar configuration. Halogen substitution of the diphenyl ether molecule in the *ortho* position (2,2’,6,6’) will force the aromatic rings orthogonal to one another (e.g., the phenyl rings will be positioned in space with a dihedral angle >0°). This is particularly evident for decabromodiphenyl ether, which is predicted to have a dihedral angle of ca. 90° and a high barrier to rotation around the ether linkage preventing this molecule from assuming a planar configuration. The benzene rings of non-*ortho* substituted PBDEs 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 (Hardy 2002).

Like PCBs, the 209 congeners for PBDEs 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 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 PBDEs. For example, the PBDE congener, 2,2',4,4'-tetrabromodiphenyl ether may be referred to as BDE 47 in this document. The identities of several PBDE congeners are shown in Table 6-1 (WHO 1994a, 1994b).

In the United States, Albemarle Corporation and Great Lakes Chemical Corporation market mixtures of PBDEs under trade names (e.g., DE-60F, DE-61, DE-62, and DE-71 for pentaBDE mixtures; DE-79 for octaBDE mixtures; and DE 83R, Saytex 102E for decaBDE mixtures). There are also several trade

names used by producers from Europe and Japan for the BDE mixtures. The chemical identities of commercial mixtures of penta-, octa-, and decabromodiphenyl ethers are listed in Table 6-3 (WHO 1994a).

Various synonyms and abbreviations for PBDEs exist in the literature and are shown below:

polybrominated biphenyl ethers	=	Polybromobiphenyl ethers	=	PBBE
polybrominated biphenyl oxides	=	Polybromobiphenyl oxides	=	PBBEs
polybrominated diphenyl ethers	=	Polybromodiphenyl ethers	=	PBDEs or PBDPEs
polybrominated diphenyl oxides	=	Polybromodiphenyl oxides	=	PBDOs or PBDPOs

For consistency in this document, polybrominated diphenyl ethers or PBDEs will be used to identify this class of chemicals. The PBDE homologs are abbreviated as follows in this document:

dibromodiphenyl ether	=	DiBDE	=	diBDE
tribromodiphenyl ether	=	TrBDE	=	triBDE
tetrabromodiphenyl ether	=	TeBDE	=	tetraBDE
pentabromodiphenyl ether	=	PeBDE	=	pentaBDE
hexabromodiphenyl ether	=	HxBDE	=	hexaBDE
heptabromodiphenyl ether	=	HpBDE	=	heptaBDE
octabromodiphenyl ether	=	OBDE	=	octaBDE
nonabromodiphenyl ether	=	NoBDE	=	nonaBDE
decabromodiphenyl ether	=	DeBDE	=	decaBDE

6.2 PHYSICAL AND CHEMICAL PROPERTIES

Polybrominated Biphenyls. Information found in the literature regarding the physical and chemical properties of hexabromobiphenyl, octabromobiphenyl, decabromobiphenyl, and BB 153 is presented in Table 6-4. The data for the properties listed in Table 6-4 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).

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

Table 6-3. Chemical Identity of Technical PBDEs

Characteristic	Pentabromodiphenyl ether	Octabromodiphenyl ether	Decabromodiphenyl ether
Synonym(s)	Pentabromodiphenyl ether; pentabromodiphenyl oxide; pentabromobiphenyl oxide; benzene, 1,1-oxybis, pentabromo derivative	Octabromodiphenyl ether; Octabromodiphenyl oxide; octabromobiphenyl oxide; benzene, octabromo derivative; phenyl ether, octabromo derivative	Decabromodiphenyl ether; decabromodiphenyl oxide; decabromobiphenyl oxide; benzene, 1,1'-oxybis(2,3,5,6,-penta-bromo-) ether, bis-(pentabromophenyl);
Registered trade name	DE 71; Bromkal 70-5 DE; FR 1205/1215; Bromkal 70; Bromkal G1; Pentabromprop; Tardex 50; Tardex 50 L; Saytex 115	Bromkal 7908DE; DE 79; FR 143; Tardex 80; FR 1208; Adine 404; Saytex 111	FR-300 BA; DE-83-RTM; Saytex 102; Saytex 102E; FR-1210; Adine 505; AFR 1021; Berkflam B10E; BR55N; Bromkal 81; Bromkal 82-ODE; Bromkal 83-10 DE; Caliban F/R-P 39P; Caliban F/R-P 44; Chemflam 011; DE 83; DP 10F; EB 10FP; EBR 700; Flame Cut BR 100; FR P-39; BR 100; FR 330BA; FR P-39; FRP 53; FR-PE; FR-PE(H); Planelon DB 100; Tardex 100; NC-1085; HFO-102; Hexcel PF1; Phoscon Br-250
Chemical formula	$C_{12}H_{10-y}Br_yO$ where y=4–6	$C_{12}H_{10-y}Br_yO$ where y=6–9	$C_{12}Br_{10}O$
Chemical structure			
Identification numbers:			
CAS registry	32534-81-9	32536-52-0	1163-19-5
NIOSH RTECS	No data	No data	No data
EPA hazardous waste	No data	No data	No data
OHM/TADS	No data	No data	No data
DOT/UN/IMCO shipping	No data	No data	No data
HSDB	7109	7110	2911
NCI	No data	No data	No data

Source: WHO 1994a

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; PBB = polybrominated biphenyl; RTECS = Registry of Toxic Effects of Chemical Substances

Table 6-4. 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; 367–367 °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. 1976
[c]Tittlemier et al. 2002
[d]Hardy (2002)
[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.

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 6-5 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 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

Table 6-5. 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. 1984
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. 1984
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. 1984
		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. 1984
			0.70	Robertson et al. 1984
		3.20		Krüger 1988
126	3,3',4,4',5-		<0.01	
		0.079		Robertson et al. 1984
Hexabromobiphenyls				
132	2,2'3,3',4,6'-	1		Krüger 1988
138	2,2',3,4,4',5'-	12.3		Robertson et al. 1984
		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. 1984
		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. 1984
		47.8	47.1	Aust et al. 1981
		55.2		Orti et al. 1983
		58.5		Krüger 1988

Table 6-5. Identified PBB Congeners in FireMaster® BP-6 and FireMaster® FF-1

IUPAC No.[a]	Structure	Percent composition of		References
		FireMaster BP-6	FireMaster FF-1	
155	2,2'4,4',6,6'-	0.5		
156	2,3,3',4,4',5-	0.980		Robertson et al. 1984
		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. 1984
		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. 1984
		5.5		Krüger 1988
169	3,3',4,4',5,5'-	0.294		Robertson et al. 1984
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. 1984
			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. 1984
			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

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.

Polybrominated Diphenyl Ethers. Information found in the literature regarding the physical and chemical properties of selected technical PBDE mixtures is presented in Table 6-6. Recent information regarding the vapor pressure, water solubility, Henry's Law constant, and log K_{ow} of some PBDE congeners is presented in Table 6-7.

Commercially available product mixtures of PBDEs (see Table 6-3) are not pure substances, but instead are mixtures of congeners. For example, the commercial mixture pentabromodiphenyl ether denotes the main component of the mixture contains the pentabromodiphenyl ether homolog. However, the commercial pentaBDE mixture actually contains tetrabromodiphenyl ether (24–38%) and pentabromodiphenyl ether (50–62%) homologs with small amounts of hexabromodiphenyl ether (4–8%) and trace amounts of tribromodiphenyl ether (0–1%) homologs. In this document, the commercial mixture of pentaBDE may be called "the commercial pentaBDE mixture," "technical pentaBDE," or "technical PeBDE" to distinguish this mixture of homologs from the pentaBDE homolog which refers to polybrominated diphenyl ethers with only five bromine atoms (see Section 6.1). Commercial octabromodiphenyl ether is a mixture of hexa-, hepta-, octa-, and nonabrominated diphenyl ether homologs with trace amounts of decabromodiphenyl ether (i.e., BDE 209). In this document, the commercial mixture of octaBDE may be called "the commercial octaBDE mixture," "technical octaBDE," or "technical OBDE" to distinguish this mixture of different homologs from the octaBDE homolog, which refers to polybrominated diphenyl ethers with only eight bromine atoms (see Section 6.1). The composition of commercial decabromodiphenyl ether is 97% of the decabromodiphenyl ether (i.e., BDE 209); the remainder is nonabromodiphenyl ether homologs and trace amounts of octabromodiphenyl ether homologs (WHO 1994a). In this document, commercial decabromodiphenyl ether may be called "the commercial decaBDE mixture," "technical decaBDE," or "technical DeBDE" which represents 97% BDE 209 congener with 3% nona- and octaBDE homolog impurities. The composition of commercial octaBDE (e.g., DE-79) is <10% of nonaBDE, <33% of octaBDE, <45% of heptaBDE, and <12% of hexaBDE (i.e., 2% of BDE 154 and 14% of BDE 153)

Table 6-6. Physical and Chemical Properties of Technical PBDE Mixtures

Property	Pentabromodiphenyl ether	Octabromodiphenyl ether	Decabromodiphenyl ether
Molecular weight	Mixture	Mixture	959.22[a]
Color	Clear, amber to pale yellow[a]	Off-white[a]	Off-white[a]
Physical state	Highly viscous liquid	Powder	Powder[a]
Melting point	-7 to -3 °C (commercial)[b]	85–89 °C (commercial)[c]; 200 °C (range, 167–257)[a]; 79–87 °C[a]; 170–220 °C[a]	290–306 °C[a]
Boiling point	>300 °C (decomposition starts above 200 °C)[a,b]	Decomposes at >330 °C (commercial)[c]	Decomposes at >320, >400, and 425 °C[a]
Density (g/mL)	2.28 at 25 °C[a]; 2.25–2.28[b]	2.76[a]; 2.8 (commercial)[c]	3.0[a]; 3.25[a]
Odor	No data	Faint[a]	Odorless[a]
Odor threshold:			
Water	No data	No data	Not applicable
Air	No data	No data	Not applicable
Solubility:			
Water	13.3 µg/L (commercial)[b,d]; 2.4 µg/L (pentabromodiphenyl ether component)[b]; 10.9 µg/L (tetrabromodiphenyl ether component)[b]	<1 ppb at 25 °C (commercial)[c]; 1.98 µg/L (heptabromodiphenyl ether component)[c]	<0.1 µg/L[g]
Organic solvent(s)	10 g/kg methanol; miscible in toluene[d]	acetone (20 g/L); benzene (200 g/L); methanol (2 g/L) all at 25 °C[a]	acetone (0.05%), benzene (0.48%), methylene bromide (0.42%), xylene (0.87%), and toluene (0.2%)[e]
Partition coefficients:			
Log K_{ow}	6.64–6.97[d]; 6.57 (commercial)[b]	6.29 (commercial)[c]	6.265[e]
Log K_{oc}	4.89-5.10[f]	5.92-6.22[f]	6.80[f]
Vapor pressure	$2.2x10^{-7}$–$5.5x10^{-7}$ mm Hg at 25 °C[d]; $3.5x10^{-7}$ mm Hg (commercial)[b]	$9.0x10^{-10}$–$1.7x10^{-9}$ mm Hg at 25 °C[d]; $4.9x10^{-8}$ mm Hg at 21 °C (commercial)[c]	$3.2x10^{-8}$ mm Hg[g]; $3.47x10^{-8}$ mm Hg[e]
Henry's Law constant (atm-m^3/mole)	$1.2x10^{-5h}$; $1.2x10^{-6f}$; $3.5x10^{-6f}$	$7.5x10^{-8f}$; $2.6x10^{-7f}$	$1.62x10^{-6h}$; $1.93x10^{-8d}$; $1.2x10^{-8f}$; $4.4x10^{-8f}$
Autoignition temperature	Decomposes above 200 °C[b,d]	Decomposes above 330 °C (commercial)[c]	Not applicable[a]
Flashpoint	No data	No data	None
Flammability limits	Not applicable (flame retardant)[b,d]	Not applicable (flame retardant)[c]	Non-flammable[a]

Table 6-6. Physical and Chemical Properties of Technical PBDE Mixtures

Property	Pentabromodiphenyl ether	Octabromodiphenyl ether	Decabromodiphenyl ether
Conversion factors	1 ppm=23.48 mg/m^3 at 20 °C[d]	No data	No data
Explosive limits	None[b,g]	None[c]	No data

[a] WHO 1994a
[b] ENVIRON 2003a
[c] ENVIRON 2003b
[d] EU 2001
[e] American Chemistry Council 2002
[f] Estimated values were calculated using EPIWIN v3.10 (EPA 2001).
[g] Hardy 2002
[h] Estimate value was calculated using vapor pressure and water solubility values in table.

Table 6-7. Physical and Chemical Properties of Some PBDE Congeners[a,b]

Congener	Vapor pressure (mm Hg)[a,c]	Water solubility (µg/L)[a]	Henry's Law constant (atm m^3/mol)[a]	Log K_{ow}[b]
BDE-3	$1.94x10^{-3}$	–	–	–
BDE-15	$1.30x10^{-4}$	130	$2.07254x10^{-4}$	–
BDE-17	–	–	–	5.74
BDE-28	$1.64x10^{-5}$	70	$5.03331x10^{-5}$	5.94
BDE-47	$1.40x10^{-6}$	15	$1.48038x10^{-5}$	6.81
BDE-66	$9.15x10^{-7}$	18	$4.93461x10^{-6}$	–
BDE-77	$5.09x10^{-7}$	6	$1.18431x10^{-5}$	–
BDE-85	$7.40x10^{-8}$	6	$1.08562x10^{-6}$	–
BDE-99	$1.32x10^{-7}$	9	$2.26992x10^{-6}$	7.32
BDE-100	$2.15x10^{-7}$	40	$6.80977x10^{-7}$	7.24
BDE-138	$1.19x10^{-8}$	–	–	–
BDE-153	$1.57x10^{-8}$	1	$6.61238x10^{-7}$	7.90
BDE-154	$2.85x10^{-8}$	1	$2.36862x10^{-6}$	7.82
BDE-183	$3.51x10^{-9}$	2	$7.30323x10^{-8}$	8.27
BDE-190	$2.12x10^{-9}$	–	–	–

[a]Tittlemier et al. 2002
[b]Braekvelt et al. 2003
[c]liquid sub-cooled vapor pressures

– = No data reported; BDE = brominated diphenyl ether

(ENVIRON 2003b). The composition of commercial pentaBDE (e.g., DE-71) is 4–12% of hexaBDE (i.e., 4% BDE 154 and 6% BDE 153), 50–62% of pentaBDE (i.e., 8% of BDE 100, 43% of BDE 99), 24–38% of tetraBDE (i.e., <1% of BDE 66, <1% of BDE 49, 28% of BDE 47), and 0–1% of triBDE (i.e., >1% of BDE 28/33) (ENVIRON 2003b). The compositions of commercial product mixtures of PBDEs (e.g., technical penta-, octa-, and decaBDE) are given in Table 6-8. The chemical composition of commercial pentaBDE product has been shown to vary over the past 10–20 years and between different commercial products (ENVIRON 2003a).

Trace analysis of these commercial mixtures for 15-different 2,3,7,8-substituted brominate dibenzo-*p*-dioxins and dibenzofurans revealed no detectable amounts of these substances (Hardy 2002). The commercial decaBDE product has been analyzed for trace quantities of 15 2,3,7,8-substituted polybrominated-*p*-dibenzodioxins (PBDDs) and polybrominated dibenzofurans (PBDFs). None of the analytes were present at or above the quantization limits established under an EPA test rule (BFRIP 2002). While in today's commercial PBDE samples, there are not measurable quantities of PBDDs/PBDFs, there are some materials that have reported quantifiable levels of these contaminants. For example, hexabromodibenzofurans have been detected in commercial decaBDE mixtures at concentrations as high as 200 µg/kg. In other PBDE mixtures (e.g., tetra- to hexaBDEs), the sum of tetra-, penta-, and hexabromodibenzofurans were reported at a concentrations of 8,000 µg/kg. In addition, tetra- and pentabromo- *p*-dibenzodioxins have been measured in commercial decaBDE at concentrations of 0.05 and 0.35 µg/kg, respectively (WHO 1998).

When pyrolyzed up to 900 °C, PBDEs may produce PBDFs and PBDDs (Buser 1986; EU 2001). The amount of PCDFs and PBDDs formed depends upon the conditions of pyrolysis. For example, 2,3,7,8-tetrabromodibenzofuran in ppm concentrations can be generated during pyrolysis of decabromodiphenyl ether (decaBDE) in the temperature range of 400–700 °C (Bieniek et al. 1989). PBDFs may also be produced during the pyrolysis of polymers containing PBDEs as flame retardants (Brenner and Knies 1993; Dumler et al. 1989a, 1990; Lenoir et al. 1994). However, studies performed in the late 1980's may have suffered from analytical methods that could not differentiate between PBDD/Fs formed (e.g., 2,3,7,8-substituted congeners) and decaBDE which might have artificially elevate levels of PBDFs detected (Ranken et al. 1994).

Table 6-8. Composition of Commercial Brominated Diphenyl Ethers

		Great Lakes				
		Commercial pentaBDE product		Commercial octaBDE product		Commercial decaBDE product
BDE homologue group	BDE congener[a]	2002	Late 1970s – early 1980s	2002	Late 1970s – early 1980s	2002
		DE-71b	Product	DE-79b	Product	DE-83R and DE-83b
DecaBDE (1 congener)	BDE-209	–	0.8	<0.70%	1.6%	>98%
NonaBDE (3 congeners)	–	–	0.2	<10%	13.0%	–
OctaBDE (12 congeners)	–	–	0.3	<33%	30.7%	–
HeptaBDE (24 congeners)	–	–	2.6	<45%	45.1%	–
HexaBDE (42 congeners)		4–12%	13.3	<12%	8.5%	–
	BDE-154	(4%)		(2%)		
	BDE-153	(6%)		(14%)		
PentaBDE (46 congeners)		50–62%	58.1	<0.50%	1.1%	–
	BDE-100	(8%)		(ND)		
	BDE-99	(43%)		(<1%)		
	BDE-85	(–)		(–)		
TetraBDE (42 congeners)		24–38%	24.6	–	–	–
	BDE-66	(<1%)		(ND)		
	BDE-49	(<1%)		(ND)		
	BDE-47	(28%)		(<1%)		
TriBDE (24 congeners)		0–1%	–	–	–	–
	BDE-28/33	(>1%)		(ND)		

Source: ENVIRON 2003b

aIUPAC numbering system
bAs currently produced

– = Data not reported; ( ) = % concentration of congener; BDE = bromodiphenyl ether; ND = Not detected