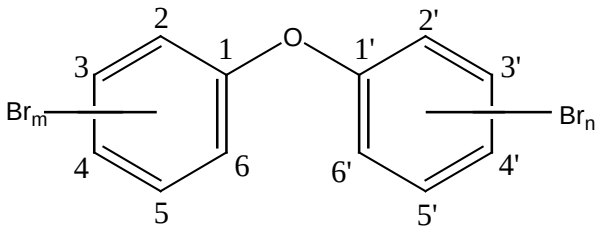
4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

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 to 10

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 or triBDE 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 or diBDE homologs contains 12 isomers. The numbering system for PBDEs is also shown above. The structures of representative 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 ~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 2002a).

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'-tetraBDE may be referred to as BDE 47 in this document. The identities of several PBDE congeners are shown in Table 4-1 (WHO 1994a, 1994b).

In the United States, Albemarle Corporation and Great Lakes Chemical Corporation previously marketed mixtures of PBDEs under trade names (e.g., DE-60F, DE-61, DE-62, DE-71, for pentaBDE mixtures; DE-79 for octaBDE mixtures; and DE 83R, Saytex 102E for decaBDE mixtures). The Great Lakes Corporation merged with Crompton Chemical Corporation and was renamed Chemtura, which produced decaBDE under the brand names AZUB DB-40, AZUB DB-65, AZUB 2DA-65, and AZUB 3DA-65 (EPA 2010). There were 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 decaBDEs are listed in Table 4-2 (WHO 1994a). La Guardia et al. (2006) published detailed congener composition profiles of penta-, octa-, and decaBDE flame retardant mixtures; 39 discrete PBDEs were found in the six commercial products evaluated by GC/MS electron ionization (EI) and electron-capture negative ionization (ECNI).

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

Table 4-1. Chemical Identity of Polybrominated Diphenyl Ether (PBDE) Congeners[a]

IUPAC Number[b]	Compound/substituents	CAS number[c]
	Biphenyl	92-52-4
	MonoBDE	101-55-3
1	2	
2	3	
3	4	
	DiBDE	2050-47-7
4	2,2’	
5	2,3	
6	2,3’	
7	2,4	
8	2,4’	
9	2,5	
10	2,6	
11	3,3’	
12	3,4	
13	3,4’	
14	3,5	
15	4,4’	
	TriBDE	49690-94-0
16	2,2’,3	
17	2,2’,4	
18	2,2’,5	
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	
27	2,3’,6	
28	2,4,4’	
29	2,4,5	
30	2,4,6	
31	2,4’,5	
32	2,4’,6	
33	2’,3,4	
34	2’,3,5	
35	3,3’,4	
36	3,3’,5	
37	3,4,4’	
38	3,4,5	
39	3,4’,5	

Table 4-1. Chemical Identity of Polybrominated Diphenyl Ether (PBDE) Congeners[a]

IUPAC Number[b]	Compound/substituents	CAS number[c]
	TetraBDE	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'	
48	2,2’,4,5	
49	2,2’,4,5'	
50	2,2’,4,6	
51	2,2’,4,6'	
52	2,2’,5,5'	
53	2,2’,5,6'	
54	2,2’,6,6'	
55	2,3,3’,4	
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	
62	2,3,4,6	
63	2,3,4’,5	
64	2,3,4’,6	
65	2,3,5,6	
66	2,3’,4,4’	
67	2,3’,4,5	
68	2,3’,4,5’	
69	2,3’,4,6	
70	2,3’,4’,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	
76	2’,3,4,5	
77	3,3’,4,4’	
78	3,3’,4,5	
79	3,3’,4,5’	
80	3,3’,5,5’	
81	3,4,4’,5	

Table 4-1. Chemical Identity of Polybrominated Diphenyl Ether (PBDE) Congeners[a]

IUPAC Number[b]	Compound/substituents	CAS number[c]
	PentaBDE	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	
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	
96	2,2’,3,6,6’	
97	2,2’,3’,4,5	
98	2,2’,3’,4,6	
99	2,2’,4,4’,5	
100	2,2’,4,4’,6	
101	2,2’,4,5,5’	
102	2,2’,4,5,6’	
103	2,2’,4,5’,6	
104	2,2’,4,6,6’	
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	
115	2,3,4,4’,6	
116	2,3,4,5,6	
117	2,3,4’,5,6	
118	2,3’,4,4’,5	
119	2,3’,4,4’,6	
120	2,3’,4,5,5’	
121	2,3’,4,5’,6	
122	2’,3,3’,4,5	
123	2’,3,4,4’,5	
124	2’,3,4,5,5’	
125	2’,3,4,5,6’	
126	3,3’,4,4’,5	
127	3,3’,4,5,5’	

Table 4-1. Chemical Identity of Polybrominated Diphenyl Ether (PBDE) Congeners[a]

IUPAC Number[b]	Compound/substituents	CAS number[c]
	HexaBDE	36483-60-0
128	2,2’,3,3’,4,4’	
129	2,2’3,3’,4,5	
130	2,2’,3,3’,4,5’	
131	2,2’,3,3’,4,6	
132	2,2’,3,3’,4,6’	
133	2,2’,3,3’,5,5’	
134	2,2’,3,3’,5,6	
135	2,2’,3,3’,5,6’	
136	2,2’,3,3’,6,6’	
137	2,2’,3,4,4’,5	
138	2,2’,3,4,4’,5’	
139	2,2’,3,4,4’,6	
140	2,2’,3,4,4’,6’	
141	2,2’,3,4,5,5’	
142	2,2’,3,4,5,6	
143	2,2’,3,4,5,6’	
144	2,2’,3,4,5’,6	
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	
150	2,2’,3,4’,5,6’	
151	2,2’,3,5,5’,6	
152	2,2’,3,5,6,6’	
153	2,2’,4,4’,5,5’	
154	2,2’,4,4’,5,6’	
155	2,2’,4,4’,6,6’	
156	2,3,3’,4,4’,5	
157	2,3,3’,4,4’,5’	
158	2,3,3’,4,4’,6	
159	2,3,3’,4,5,5’	
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	
165	2,3,3’,5,5’,6	
166	2,3,4,4’,5,6	
167	2,3’,4,4’,5,5’	
168	2,3’,4,4’,5’,6	
169	3,3’,4,4’,5,5’	

Table 4-1. Chemical Identity of Polybrominated Diphenyl Ether (PBDE) Congeners[a]

IUPAC Number[b]	Compound/substituents	CAS number[c]
	HeptaBDE	68928-80-3
170	2,2',3,3',4,4',5	
171	2,2',3,3',4,4',6	
172	2,2',3,3',4,5,5'	
173	2,2',3,3',4,5,6	
174	2,2',3,3',4,5,6'	
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	
179	2,2',3,3',5,6,6'	
180	2,2',3,4,4',5,5'	
181	2,2',3,4,4',5,6	
182	2,2',3,4,4',5,6'	
183	2,2',3,4,4',5',6	
184	2,2',3,4,4',6,6'	
185	2,2',3,4,5,5',6	
186	2,2',3,4,5,6,6'	
187	2,2',3,4',5,5',6	
188	2,2',3,4',5,6,6'	
189	2,3,3',4,4',5,5'	
190	2,3,3',4,4',5,6	
191	2,3,3',4,4',5',6	
192	2,3,3',4,5,5',6	
193	2,3,3',4',5,5',6	
	OctaBDE	32536-52-0
194	2,2',3,3',4,4',5,5'	
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'	
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'	
201	2,2',3,3',4,5',6,6'	
202	2,2',3,3',5,5',6,6'	
203	2,2',3,4,4',5,5',6	
204	2,2',3,4,4',5,6,6'	
205	2,3,3',4,4',5,5',6	
	NonaBDE	63936-56-1
206	2,2',3,3',4,4',5,5',6	
207	2,2',3,3',4,4',5,6,6'	
208	2,2',3,3',4,5,5',6,6'	

Table 4-1. Chemical Identity of Polybrominated Diphenyl Ether (PBDE) Congeners[a]

IUPAC Number[b]	Compound/substituents	CAS number[c]
	DecaBDE	1163-19-5
209	2,2',3,3',4,4',5,5',6,6'	

[a]WHO 1994a
[b]Ballschmiter and Zell 1980
[c]No CAS numbers were identified for the individual PBDE congeners.

BDE = brominated diphenyl ether; CAS = Chemical Abstracts Service; IUPAC = International Union of Pure and Applied Chemistry

Table 4-2. Chemical Identity of Technical Polybrominated Diphenyl Ethers (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 79-8DE; 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 82-0DE; 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; RTECS = Registry of Toxic Effects of Chemical Substances

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	=	OcBDE	=	octaBDE
nonabromodiphenyl ether	=	NoBDE	=	nonaBDE
decabromodiphenyl ether	=	DeBDE	=	decaBDE

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information found in the literature regarding the physical and chemical properties of selected technical PBDE mixtures is presented in Table 4-3. Recent information regarding the vapor pressure, water solubility, Henry's Law constant, and log K_{ow} of some PBDE congeners is presented in Table 4-4.

Commercially available product mixtures of PBDEs (see Table 4-2) are not pure substances, but instead are mixtures of congeners. For example, the commercial mixture pentaBDE denotes the main component of the mixture contains the pentaBDE homolog. However, the commercial pentaBDE mixture actually contains tetraBDE (24–38%) and pentaBDE (50–62%) homologs with small amounts of hexaBDE (4–8%) and trace amounts of triBDE (0–1%) homologs. In this document, the commercial mixture of pentabromodiphenyl ether 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 PBDEs with only five bromine atoms (see Section 4.1). Commercial octaBDE is a mixture of hexa-, hepta-, octa-, and nonaBDE homologs with trace amounts of decaBDE (i.e., BDE 209). In this document, the commercial mixture of octabromodiphenyl ether 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 PBDEs with only eight bromine atoms (see Section 4.1). The composition of commercial decabromodiphenyl ether is 97% of the decaBDE (i.e., BDE 209); the remainder is nonaBDE homologs and trace amounts of octaBDE homologs (WHO 1994a). In this document, commercial decabromodiphenyl ether may be called "the commercial decaBDE mixture,"

Table 4-3. Physical and Chemical Properties of Technical Polybrominated Diphenyl Ether (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]	No data
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[e]	5.92–6.22[e]	6.80[e]
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[f]
Henry's Law constant (atm-m^3/mole)	$1.2x10^{-5}$[g]; $1.2x10^{-6}$[e]; $3.5x10^{-6}$[f]	$7.5x10^{-8}$[e]; $2.6x10^{-7}$[e]	$1.62x10^{-6}$[g]; $1.93x10^{-8}$[d]; $1.2x10^{-8}$[e]; $4.4x10^{-8}$[e]
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 4-3. Physical and Chemical Properties of Technical Polybrominated Diphenyl Ether (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,f]	None[c]	No data

[a]WHO 1994a
[b]ENVIRON 2003a
[c]ENVIRON 2003b
[d]EU 2001
[e]Estimated values were calculated using EPIWIN v4.10 (EPA 2014e).
[f]Hardy 2002a
[g]Estimated value was calculated using vapor pressure and water solubility values in table.

Table 4-4. Physical and Chemical Properties of Some Polybrominated Diphenyl Ether (PBDE) Congeners

Congener	Vapor pressure (mm Hg)[a,b]	Water solubility (µg/L)[a]	Henry's Law constant (atm m^3/mol)[a]	Log K_{ow}[c]	Log K_{OA}[d]
BDE 3	$1.94x10^{-3}$	–	–	–	–
BDE 15	$1.30x10^{-4}$	130	$2.07254x10^{-4}$	–	–
BDE 17	–	–	–	5.74	9.30
BDE 28	$1.64x10^{-5}$	70	$5.03331x10^{-5}$	5.94	9.50
BDE 47	$1.40x10^{-6}$	15	$1.48038x10^{-5}$	6.81	10.53
BDE 66	$9.15x10^{-7}$	18	$4.93461x10^{-6}$	–	10.82
BDE 77	$5.09x10^{-7}$	6	$1.18431x10^{-5}$	–	10.87
BDE 85	$7.40x10^{-8}$	6	$1.08562x10^{-6}$	–	11.66
BDE 99	$1.32x10^{-7}$	9	$2.26992x10^{-6}$	7.32	11.31
BDE 100	$2.15x10^{-7}$	40	$6.80977x10^{-7}$	7.24	11.13
BDE 138	$1.19x10^{-8}$	–	–	–	–
BDE 153	$1.57x10^{-8}$	1	$6.61238x10^{-7}$	7.90	11.82
BDE 154	$2.85x10^{-8}$	1	$2.36862x10^{-6}$	7.82	11.92
BDE 183	$3.51x10^{-9}$	2	$7.30323x10^{-8}$	8.27	11.96
BDE 190	$2.12x10^{-9}$	–	–	–	–

[a]Tittlemier et al. 2002.
[b]Liquid sub-cooled vapor pressures.
[c]Braekevelt et al. 2003.
[d]Harner 2001.

– = no data reported; BDE = brominated diphenyl ether

"technical decaBDE," or "technical DeBDE" which represents 97% BDE 209 congener with 3% nona- and octaBDE homolog impurities. The compositions of commercial product mixtures of PBDEs (e.g., technical penta-, octa-, and decaBDE) are given in Table 4-5.

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 2002a). The commercial decaBDE product has been analyzed for trace quantities of 15 2,3,7,8-substituted PBDDs and 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 no measurable quantities of PBDDs/PBDFs, there are some materials that have reported quantifiable concentrations 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 PBDFs 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 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. 1989, 1990; Lenoir et al. 1994). However, studies performed in the late 1980s may have suffered from analytical methods that could not differentiate between PBDDs/PBDFs formed (e.g., 2,3,7,8-substituted congeners) and decaBDE, which might have artificially elevated the concentrations of PBDEs detected (Hamm et al. 2001).

Table 4-5. Typical Congener Composition of Penta-, Octa-, and Deca-Brominated Diphenyl Ether (BDE)

Congener (weight percentage)	PentaBDE	OctaBDE	DecaBDE
BDE 47	25–37%		
BDE 99	35–50%		
BDE 100	6–10%		
BDE 153	3–5%	5–10%	
BDE 154	2–4%	1–5%	
BDE 183		40%	
BDE 196		8%	
BDE 197		21%	
BDE 203		5–35%	
BDE 206			2.2%
BDE 207		7%	0.24%
BDE 208		10%	0.06%
BDE 209			97%

Source: EPA 2010