APPENDIX A

Table A-1 Systematic Numbering of PCB congeners introduced by Ballschmiter and Zell and accepted by IUPAC[2]

BZ No.[a]	Compound	CAS No.	BZ No.[a]	Compound	CAS No.
	Biphenyl	92-52-4	38	3,4,5	53555-66-1
	MonoCB	27323-18-8	39	3,4′,5	38444-88-1
1	2	2051-60-7		TetraCB	26914-33-0
2	3	2051-61-8	40	2,2′,3,3′	38444-93-8
3	4	2051-62-9	41	2,2′,3,4	52663-59-9
	DiCB	25512-42-9	42	2,2′,3,4′	36559-22-5
4	2,2′	13029-08-8	43	2,2′,3,5	70362-46-8
5	2,3	16605-91-7	44	2,2′,3,5′	41464-39-5
6	2,3′	25569-80-6	45	2,2′,3,6	70362-45-7
7	2,4	33284-50-3	46	2,2′,3,6′	41464-47-5
8	2,4′	34883-43-7	47	2,2′,4,4′	2437-79-8
9	2,5	34883-39-1	48	2,2′,4,5	70362-47-9
10	2,6	33146-45-1	49	2,2′,4,5′	41464-40-8
11	3,3′	2050-67-1	50	2,2′,4,6	62796-65-8
12	3,4	2974-92-7	51	2,2′,4,6′	65194-04-7
13	3,4′	2974-90-5	52	2,2′,5,5′	35693-99-3
14	3,5	34883-41-5	53	2,2′,5,6′	41464-41-9
15	4,4′	2050-68-2	54	2,2′,6,6′	15968-05-5
	TriCB	25323-68-6	55	2,3,3′,4	74338-24-2
16	2,2′,3	38444-78-9	56	2,3,3′,4′	41464-43-1
17	2,2′,4	37680-66-3	57	2,3,3′,5	70424-67-8
18	2,2′,5	37680-65-2	58	2,3,3′,5′	41464-49-7
19	2,2′,6	38444-73-4	59	2,3,3′,6	74472-33-6
20	2,3,3′	38444-84-7	60	2,3,4,4′	33025-41-1
21	2,3,4	55702-46-0	61	2,3,4,5	33284-53-6
22	2,3,4′	38444-85-8	62	2,3,4,6	54230-23-7
23	2,3,5	55720-44-0	63	2,3,4′,5	74472-35-8
24	2,3,6	58702-45-9	64	2,3,4′,6	52663-58-8
25	2,3′,4	55712-37-3	65	2,3,5,6	33284-54-7
26	2,3′,5	38444-81-4	66	2,3′,4,4′	32598-10-0
27	2,3′,6	38444-76-7	67	2,3′,4,5	73575-53-8
28	2,4,4′	7012-37-5	68	2,3′,4,5′	73575-52-7
29	2,4,5	15862-07-4	69	2,3′,4,6	60233-24-1
30	2,4,6	35693-92-6	70	2,3′,4′,5	32598-11-1
31	2,4′,5	16606-02-3	71	2,3′,4′,6	41464-46-4
32	2,4′,6	38444-77-8	72	2,4′,5,5′	41464-42-0
33	2′,3,4	38444-86-9	73	2,3′,5′,6	74338-23-1
34	2′,3,5	37680-68-5	74	2,4,4′,5	32690-93-0
35	3,3′,4	37680-69-6	75	2,4,4′,6	32598-12-2
36	3,3′,5	38444-87-0	76	2′,3,4,5	70362-48-0
37	3,4,4′	38444-90-5	77	3,3′,4,4′	32598-13-3

Table A-1 (continued)

BZ No.[a]	Compound	CAS No.	BZ No.[a]	Compound	CAS No.
78	3,3′,4,5	70362-49-1	134	2,2′,3,3′,5,6	52704-70-8
79	3,3′,4,5′	41464-48-6	135	2,2′,3,3′,5,6′	52744-13-5
80	3,3′,5,5′	33284-52-5	136	2,2′,3,3′,6,6′	38411-22-2
81	3,4,4′,5	70362-50-4	137	2,2′,3,4,4′,5	35694-06-5
	PentaCB	25429-29-2	138	2,2′,3,4,4′,5′	35065-28-2
82	2,2′,3,3′,4	52663-62-4	139	2,2′,3,4,4′,6	56030-56-9
83	2,2′,3,3′,5	60145-20-2	140	2,2′,3,4,4′,6′	59291-64-4
84	2,2′,3,3′,6	52663-60-2	141	2,2′,3,4,5,5′	52712-04-6
85	2,2′,3,4,4′	65510-45-4	142	2,2′,3,4,5,6	41411-61-4
86	2,2′,3,4,5	55312-69-1	143	2,2′,3,4,5,6′	68194-15-0
87	2,2′,3,4,5′	38380-02-8	144	2,2′,3,4,5′,6	68194-14-9
88	2,2′,3,4,6	55215-17-3	145	2,2′,3,4,6,6′	74472-40-5
89	2,2′,3,4,6′	73575-57-2	146	2,2′,3,4′,5,5′	51908-16-8
90	2,2′,3,4′,5	68194-07-0	147	2,2′,3,4′,5,6	68194-13-8
91	2,2′,3,4′,6	58194-05-8	148	2,2′,3,4′,5,6′	74472-42-7
92	2,2′,3,5,5′	52663-61-3	149	2,2′,3,4′,5′,6	38380-04-0
93	2,2′,3,5,6	73575-56-1	150	2,2′,3,4′,6,6′	68194-08-1
94	2,2′,3,5,6′	73575-55-0	151	2,2′,3,5,5′,6	52663-63-5
95	2,2′,3,5′,6	38379-99-6	152	2,2′,3,5,6,6′	68194-09-2
96	2,2′,3,6,6′	73575-54-9	153	2,2′,4,4′,5,5′	35065-27-1
97	2,2′,3′,4,5	41464-51-1	154	2,2′,4,4′,5,6′	60145-22-4
98	2,2′,3′,4,6	60233-25-2	155	2,2′,4,4′,6,6′	33979-03-2
99	2,2′,4,4′,5	38380-01-7	156	2,3,3′,4,4′,5	38380-08-4
100	2,2′,4,4′,6	39485-83-1	157	2,3,3′,4,4′,5′	69782-90-7
101	2,2′,4,5,5′	37680-73-2	158	2,3,3′,4,4′,6	74472-42-7
102	2,2′,4,5,6′	68194-06-9	159	2,3,3′,4,5,5′	39635-35-3
103	2,2′,4,5′,6	60145-21-3	160	2,3,3′,4,5,6	41411-62-5
104	2,2′,4,6,6′	56558-16-8	161	2,3,3′,4,5′,6	74472-43-8
105	2,3,3′,4,4′	32598-14-4	162	2,3,3′,4′,5,5′	39635-34-2
106	2,3,3′,4,5	70424-69-0	163	2,3,3′,4′,5,6	74472-44-9
107	2,3,3′,4′,5	70424-68-9	164	2,3,3′,4′,5′,6	74472-45-0
108	2,3,3′,4,5′	70362-41-3	165	2,3,3′,5,5′,6	74472-46-1
109	2,3,3′,4,6	74472-35-8	166	2,3,4,4′,5,6	41411-63-6
110	2,3,3′,4′,6	38380-03-9	167	2,3′,4,4′,5,5′	52663-72-6
111	2,3,3′,5,5′	39635-32-0	168	2,3′,4,4′,5′,6	59291-65-5
112	2,3,3′,5,6	74472-36-9	169	3,3′,4,4′,5,5′	32774-16-6
113	2,3,3′,5′,6	68194-10-5		HeptaCB	28655-71-2
114	2,3,4,4′,5	74472-37-0	170	2,2′,3,3′,4,4′,5	35065-30-6
115	2,3,4,4′,6	74472-38-1	171	2,2′,3,3′,4,4′,6	52663-71-5
116	2,3,4,5,6	18259-05-7	172	2,2′,3,3′,4,5,5′	52663-74-8
117	2,3,4′,5,6	68194-11-6	173	2,2′,3,3′,4,5,6	68194-16-1
118	2,3′,4,4′,5	31508-00-6	174	2,2′,3,3′,4,5,6′	38411-25-5
119	2,3′,4,4′,6	56558-17-9	175	2,2′,3,3′,4,5′,6	40186-70-7
120	2,3′,4,5,5′	68194-12-7	176	2,2′,3,3′,4,6,6′	52663-65-7
121	2,3′,4,5′,6	56558-18-0	177	2,2′,3,3′,4′,5,6	52663-70-4
122	2′,3,3′,4,5	76842-07-4	178	2,2′,3,3′,5,5′,6	52663-67-9
123	2′,3,4,4′,5	65510-44-3	179	2,2′,3,3′,5,6,6′	52663-64-6
124	2′,3,4,5,5′	70424-70-3	180	2,2′,3,4,4′,5,5′	35065-29-3
125	2′,3,4,5,6′	74472-39-2	181	2,2′,3,4,4′,5,6	74472-47-2
126	3,3′,4,4′,5	57465-28-8	182	2,2′,3,4,4′,5,6′	60145-23-5
127	3,3′,4,5,5′	39635-33-1	183	2,2′,3,4,4′,5′,6	52663-69-1
	HexaCB	26601-64-9	184	2,2′,3,4,4′,6,6′	74472-48-3
128	2,2′,3,3′,4,4′	38380-07-3	185	2,2′,3,4,5,5′,6	52712-05-7
129	2,2′,3,3′,4,5	55215-18-4	186	2,2′,3,4,5,6,6′	74472-49-4
130	2,2′,3,3′,4,5′	52663-66-8	187	2,2′,3,4′,5,5′,6	52663-68-0
131	2,2′,3,3′,4,6	61798-70-7	188	2,2′,3,4′,5,6,6′	74487-85-7
132	2,2′,3,3′,4,6′	38380-05-1	189	2,3,3′,4,4′,5,5′	39635-31-9
133	2,2′,3,3′,5,5′	35694-04-3	190	2,3,3′,4,4′,5,6	41411-64-7

Table A-1 (continued)

BZ No.[a]	Compound	CAS No.	BZ No.[a]	Compound	CAS No.
191	2,3,3′,4,4′,5′,6	74472-50-7	201	2,2′,3,3′,4,5′,6,6′[c]	40186-71-8
192	2,3,3′,4,5,5′,6	74472-51-8	202	2,2′,3,3′,5,5′,6,6′	2136-99-4
193	2,3,3′,4′,5,5′,6	69782-91-8	203	2,2′,3,4,4′,5,5′,6	52663-76-0
	OctaCB	31472-83-0[b]	204	2,2′,3,4,4′,5,6,6′	74472-52-9
194	2,2′,3,3′,4,4′,5,5′	35694-08-7	205	2,3,3′,4,4′,5,5′,6	74472-53-0
195	2,2′,3,3′,4,4′,5,6	52663-78-2		**NonaCB**	53742-07-7
196	2,2′,3,3′,4,4′,5,6′	42740-50-1	206	2,2′,3,3′,4,4′,5,5′,6	40186-72-9
197	2,2′,3,3′,4,4′,6,6′	33091-17-7	207	2,2′,3,3′,4,4′,5,6,6′	52663-79-3
198	2,2′,3,3′,4,5,5′,6	68194-17-2	208	2,2′,3,3′,4,5,5′,6,6′	52663-77-1
199	2,2′,3,3′,4,5,5′,6′[c]	52663-75-9		**DecaCB**	2051-24-3
200	2,2′,3,3′,4,5,6,6′[c]	52663-73-7	209	2,2′,3,3′,4,4′,5,5′,6,6′	2051-24-3

[a] Data from Ballschmiter and Zell (1980). Eleven congeners (Nos. 33, 34, 76, 98, 122, 123, 124, 125, 177, 196, and 201) have different chemical Ballschmiter and IUPAC numbers, as noted by Guitart et al. (1991).

[b] Four chlorines on each ring at unspecified locations.

[c] Revised numbering sequence as noted by Schulte and Malisch (1983).

APPENDIX B

Limit of Detection (LOD) Calculation[104]

Limit of detection was calculated from the Linear Least Squares' Line procedure.

$y = a + bx$ (B-1)

y = instrument signals

x = normally are concentrations

a = intercept

b = slope of the straight line

$Y_L = Y_B + k S_B$ (B-2)

Y_L = lowest detectable instrument signals

Y_B = blank signal

$\cong$ intercept, a

k = consant depending on definition such as k = 3, 1.5 or 10 According to IUPAC, in calculation of LOD, k = 3 was used and in this work this value was used.

S_B = blank signal standard deviation

$\cong S_{y/x}$

$S_{y/x}$ can be calculated from the equation

$S_{y/x} = \{\Sigma(Y_i - \hat{Y}_i)^2/(n-2)\}^{1/2}$ (B-3)

Y_i = response value from the instrument corresponding to the individual x - values

$\hat{Y}i$ = value of y on the calculated regression line corresponding to the individual x-values

n = number of points on the calibration line

From equation (B-2) and (B-3)

$Y_L = a + 3 S_{y/x}$ (B-4)

Thus the concentration at limit of detection (C_L) can be calculated by using the equation (B-6)

$$Y_L = a + bC_L \qquad \text{(B-5)}$$

Thus

$$a + 3\,S_{y/x} = a + b\,C_L$$

$$C_L = 3S_{y/x}/b \qquad \text{(B-6)}$$

PCBs No. 10 on HP-608 column at 0.5-7 μg l^{-1} was used as an example in calculation of LOD. The linear regression equation is Y = 258 + 2117.5x

Concentration (μg l^{-1})	Y_i	$\hat{Y}_i$	$\lvert Y_i - \hat{Y}_i \rvert$	$\lvert Y_i - \hat{Y}_i \rvert^2$
0.5	1197	1317	120	14340
1	2200	2376	176	30800
3	7037	6611	426	181476
5	1090.8	10846	62	3844
7	14887	15081	194	37636
			$\sum\lvert Yi - \hat{Y}i\rvert^2$	268096

$$S_{y/x} = [268096/(5-2)]^{1/2}$$

$$= 299$$

$$C_L = (3 \times 299)/2117.5$$

$$= 0.42\ \mu g\ l^{-1}$$

VITA

Name	Mr. Nitirat Chimnoi
Date of Birth	July 7, 1972
Academic status	High school certificate holder from Rattanathibate school, Nonthaburi, 1989
	B. S. (Chemistry) degree holder from Kasetsart University, 1993
Employment	Scientist, Chulabhorn Research Institute, Bangkok, 1993 to present
Practical Experience	MS and GC/MS trainee at Finnigan MAT, Bremen, Germany, February, 1995 to June, 1995