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PHYSICAL, SPECTRAL AND CHROMATOGRAPHIC PROPERTIES OF ALL 209 INDIVIDUAL PCB CONGENERS

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ABSTRACT:

Physical, spectral and chromatographic data for all 209 individual PCB congeners is presented. The individual congeners were synthesized and then isolated and purified. Recent emphasis on the source of the toxicity of commercial PCB formulations has increased the need for a complete set of the PCB congeners. Through the use of two capillary GC columns: 40% octadecyl/ 15% phenyl methyl siloxane and 50% phenyl methyl siloxane, it was possible to separate 201 PCB congeners with only four unresolved pairs. The data compiled in this study for all 209 congeners will aid in the identification of selected individual components of these environmental pollutants. The use of this data also presents the opportunity for the improved quantification of the commercial PCB formulations.

INTRODUCTION:

Polychlorinated biphenyls (PCB'S) have been the subject of a broad spectrum of analytical and environmental studies over the past 25 years. The combination of their widespread use, environmental persistence, and improper disposal has led to ecosystem contamination on a global level (1-4). Of particular interest is the high potential for bioaccumulation of PCB's through the food chain, resulting ultimately in the ingestion of these compounds by humans. PCB residues are frequently found in human blood, adipose tissue and breast milk (5,6). More importantly, several instances of human poisonings via PCB ingestion have been documented (7).

Commercial PCB products (Aroclor™, Chlorphen™, Kannechlor™ and Fenclor™) contain many of the possible PCB congeners; and recent research has focused on the premise that the toxicity of these products can be estimated by the identification and quantification of selected PCB congeners (8-11). The most toxic congeners are those which can adopt a coplanar configuration similar to that of 2,3,7,8-TCDD (10,12). In this regard, the three most toxic PCB congeners studied to date are IUPAC #77, 126 and 169. Additional congeners which possess a partially planar configuration are also of interest, and Yang et al (10) listed 19 such PCB congeners thought to be responsible for biological activity. The chlorine substitution pattern com-

mon to all of these congeners is the lack of chlorines in the ortho positions. This congener-specific toxicological premise has provided the motivation for the development of analytical procedures which yield reliable separations.

This task is made more difficult in "real world" environmental samples by the presence of interfering compounds (e.g. DDT, DDE) which are often present at much higher concentrations than the target compounds. Consequently, two basic approaches have been developed to improve the separation of these multicomponent pollutants. The first approach employs the preparative separation of the extract or mixture followed by analysis using high resolution or multi-dimensional GC. The second approach relies on the direct characterization of the extract or mixture via a congener-specific high resolution GC column (13-15) or multi-dimensional GC (16-18).

Both approaches require the use of accurate, well-characterized spiking, calibration and QC solutions. These solutions contain the appropriate PCB congeners to determine elution patterns, establish response factors, monitor the efficiency of clean-up and recovery procedures. These approaches require all the congeners present in the commercial products and are facilitated by the availability of all 209 PCB congeners.

This report describes the first preparative isolation of all 209 individual PCB congeners from synthetic mixtures subsequently providing the opportunity to determine the physical characteristics of the entire set. Data obtained on these compounds include melting points, high resolution gas chromatography retention indices on two columns of differing selectivity, electron capture detector response factors, matrix isolated FT/IR spectra and electron impact mass spectra.

MATERIALS AND METHODS:

A. *Chemicals:* The 2-,3-, and 4-chloroanilines, 2,6-, 2,5-, 2,4-, 2,3-, 3,5-, and 3,4-dichloroanilines, 2,4,6,-, 2,4,5-, and 2,3,4-trichloroanilines as well as 2,3,5,6- and 2,3,4,5-tetrachloranilines were purchased from Aldrich Chemical Co. Benzene, chlorobenzene, 1,4-, 1,3-, and 1,2-dichlorobenzene, 1,2,4-, 1,2,3-, 1,3,5-trichlorobenzene, 1,2,4,5-tetrachlorobenzene and pentachlorobenzene were purchased from Aldrich Chemical Co. Isoamyl nitrite was obtained from Eastman Organic Chemicals. 2,3,5-, 2,3,6-, 3,4,5-trichloroanilines, 2,3,4,6-tetrachloroaniline, 1,2,3,4- and 1,2,3,5-tetrachlorobenzene were prepared at AccuStandard's laboratories using standard methods.

B. *Synthesis Schemes:* All 209 congeners were synthesized by one or more of the following schemes outlined in Figure 1.

C. *Isolation and Purification:* All reaction products were isolated as

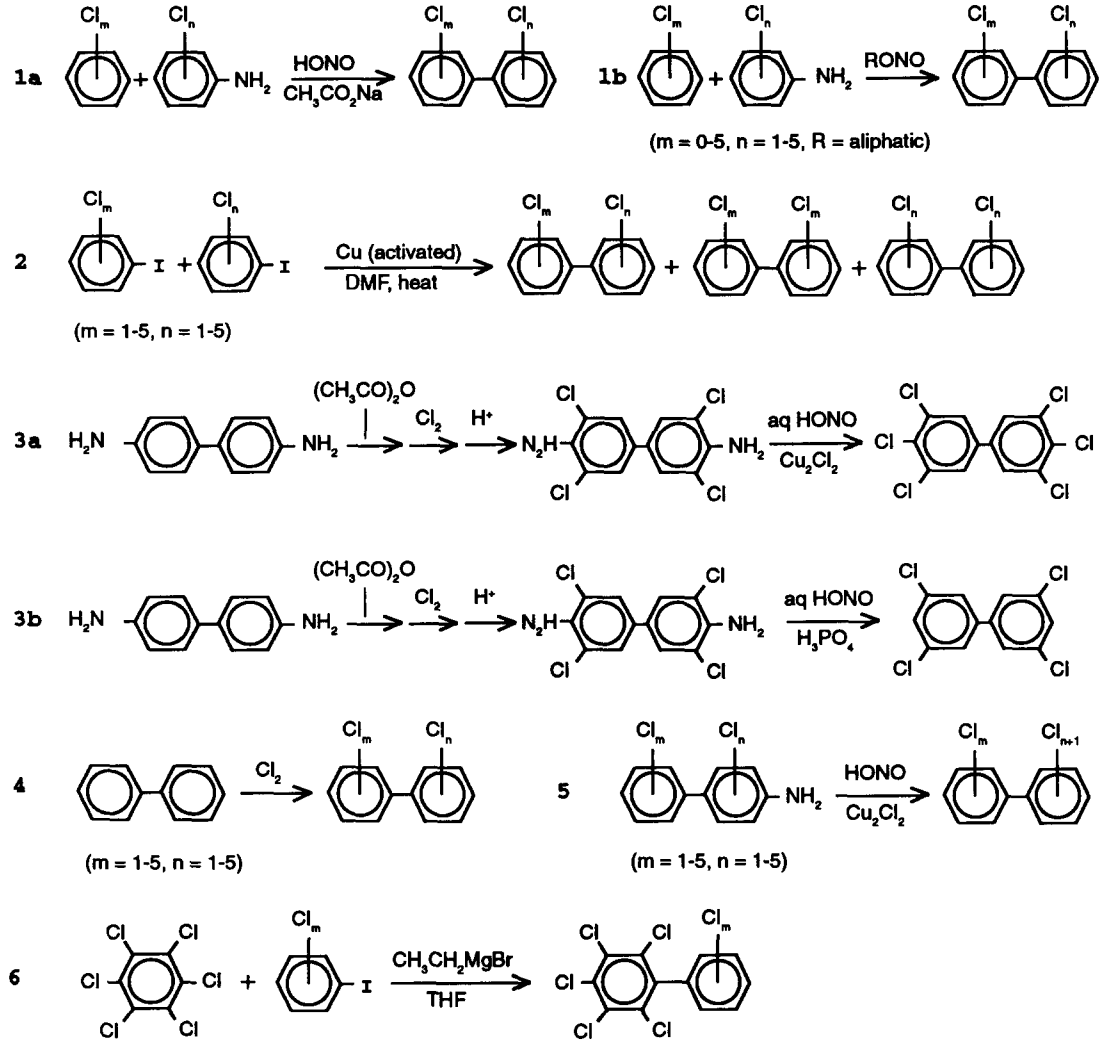

Figure 1. Synthesis schemes for all 209 PCB congeners

1a Gomberg - Bachman reaction
1b Cadogan modification of Gomberg - Bachman reaction
2 Ullman reaction
3a Chlorination of benzidine followed by deamination
3b Chlorination of benzidine followed by Sandmeyer reaction
4 Chlorination
5 Sandmeyer reaction
6 Grignard coupling

the methylene chloride soluble fractions. The residues were distilled and subsequently passed through a column containing one or more of the following adsorbents: silica gel, alumina, Florisil™ and/or charcoal using an appropriate solvent system. The fractions containing the target congeners were stripped to dryness and the residues fractionally crystallized from one or more solvents such as acetone, hexane, methanol or toluene.

D. *Chromatography:* All gas chromatographic runs were performed on a Hewlett Packard 5890 GC equipped with an autosampler, split/splitless injector and a Nickel 63 electron capture detector. Column 1 was a 50M x 0.25mm x 25µm film 40% octadecyl, 15% phenyl substituted methyl siloxane fused silica capillary (Quadrex Corp.). Column 2 was a 25M x 0.25mm x 0.25µm film 50% phenyl substituted methyl siloxane fused silica capillary (Quadrex Corp.). Both columns were operated at 30 psig headpressure using helium as the carrier gas. The oven temperature was programmed from 150°C (2 min.) to 300°C at 5°C/minute, and held at 300°C for 5 minutes. One microlitre (1.0µL) injections were made via the autosampler in the splitless mode. The concentration of each sample was 100 ng/µL. The injector and detector were set at 250°C and 300°C, respectively. The retention times of the PCB congeners were computed relative to octachloronaphthalene (OCN). The response factors (by weight) for the congeners were calculated relative to OCN using values obtained from integrated peak areas.

E. *Gas Chromatography/Mass Spectrometry:* All mass spectra were obtained on a Hewlett Packard model 5890 GC interfaced to a HP 5971A mass selective detector. An autosampler was used to inject 1.0 µL samples of each PCB congener (100 ng/µL concentration). A 25M x 0.25mm x 0.25µm film 5% phenyl substituted methyl siloxane capillary column (Quadrex Corp.) was used to chromatograph all samples. The MSD was controlled by a HP chemstation DOS based software and autotuned using DFTPP as the tuning standard. Electron impact mass spectra were obtained over the range of 50-520 amu.

F. *Matrix Isolated Gas Chromatography/Fourier Transform Infrared Spectrometry:* A Mattson Scientific Matrix-Isolated GC/FT-IR was used to generate the IR spectra. The Cryolect instrument employed a Hewlett Packard model 5890A GC interfaced to a Mattson Sirius model 100 FT-IR spectrometer equipped with a broadband MCT detector and sample chamber. The system was controlled by a Pixel computer. The GC was equipped with a flame ionization detector. The analytical column was a 30M x 0.32mm x 0.25µm film DB-5 (J&W Scientific). The GC oven was programmed from 50°C (1 min) to 120°C at 25°C/min, then to 320°C at 5°C/min, and held at 320°C for 7 minutes. Column head pressure was 10 psig using helium/argon (98.5/1.5%) as the carrier gas. Fifty nanograms of each PCB was injected on-column. The column ef-

fluent was split with 80% going to the Cryolect for spectral analysis and 20% going to the FID for quantitation and measurement of retention times.

G. *Melting points:* All melting points were obtained on a Fisher Johns melting point apparatus. The melting point was determined by rapidly elevating the temperature to a point 20-25°C below the approximate melting point and then raising the temperature at a rate of 1-2°C/minute. The melting points were corrected using melting point standards (Aldrich).

RESULTS AND DISCUSSION:

Synthesis Schemes: The synthesis of all 209 PCB congeners proceeded via the schemes presented in the Materials & Methods Section. Table I lists the specific reaction scheme(s) used in synthesizing each congener.

Table 1. Reaction scheme(s) needed to synthesize each individual PCB congener

BZ#	Compound	Reaction Scheme	BZ#	Compound	Reaction Scheme
1	2-Chlorobiphenyl	1a, 1b	51	2,2',4,6'-Tetrachlorobiphenyl	1a, 1b, 2
2	3-Chlorobiphenyl	1a, 1b	52	2,2',5,5'-Tetrachlorobiphenyl	1a, 1b, 2
3	4-Chlorobiphenyl	1a, 1b	53	2,2',5,6'-Tetrachlorobiphenyl	1a, 1b, 2
4	2,2'-Dichlorobiphenyl	1a, 1b, 2	54	2,2',6,6'-Tetrachlorobiphenyl	1a, 1b, 2
5	2,3-Dichlorobiphenyl	1a, 1b	55	2,3,3',4-Tetrachlorobiphenyl	1a, 1b, 2
6	2,3'-Dichlorobiphenyl	1a, 1b	56	2,3,3',4'-Tetrachlorobiphenyl	1a, 1b, 2
7	2,4-Dichlorobiphenyl	1a, 1b	57	2,3,3',5-Tetrachlorobiphenyl	2
8	2,4'-Dichlorobiphenyl	1b, 2, 5	58	2,3,3',5'-Tetrachlorobiphenyl	1a, 1b
9	2,5-Dichlorobiphenyl	1a, 1b	59	2,3,3',6-Tetrachlorobiphenyl	2
10	2,6-Dichlorobiphenyl	1a, 1b	60	2,3,4,4'-Tetrachlorobiphenyl	1a, 1b
11	3,3'-Dichlorobiphenyl	2	61	2,3,4,5-Tetrachlorobiphenyl	1a, 1b
12	3,4-Dichlorobiphenyl	1a, 1b	62	2,3,4,6-Tetrachlorobiphenyl	1a, 1b
13	3,4'-Dichlorobiphenyl	1a, 1b	63	2,3,4',5-Tetrachlorobiphenyl	2
14	3,5-Dichlorobiphenyl	1a, 1b	64	2,3,4',6-Tetrachlorobiphenyl	1a, 1b, 2
15	4,4'-Dichlorobiphenyl	1a, 1b, 2	65	2,3,5,6-Tetrachlorobiphenyl	1a, 1b
16	2,2',3-Trichlorobiphenyl	1a, 1b	66	2,3',4,4'-Tetrachlorobiphenyl	1a, 1b, 2
17	2,2',4-Trichlorobiphenyl	1a, 1b	67	2,3',4,5-Tetrachlorobiphenyl	1a, 1b, 2
18	2,2',5-Trichlorobiphenyl	1a, 1b	68	2,3',4,5'-Tetrachlorobiphenyl	1a, 1b, 2
19	2,2',6-Trichlorobiphenyl	1a, 1b, 2	69	2,3',4,6-Tetrachlorobiphenyl	1a, 1b
20	2,3,3'-Trichlorobiphenyl	1a, 1b, 2	70	2,3',4',5-Tetrachlorobiphenyl	1a, 1b, 2
21	2,3,4-Trichlorobiphenyl	1a, 1b	71	2,3',4',6-Tetrachlorobiphenyl	1a, 1b
22	2,3,4'-Trichlorobiphenyl	1a, 1b, 2	72	2,3',5,5'-Tetrachlorobiphenyl	1a, 1b, 2
23	2,3,5-Trichlorobiphenyl	1a, 1b	73	2,3',5',6-Tetrachlorobiphenyl	1a, 1b
24	2,3,6-Trichlorobiphenyl	1a, 1b	74	2,4,4',5-Tetrachlorobiphenyl	1a, 1b, 2
25	2,3',4-Trichlorobiphenyl	1a, 1b, 2	75	2,4,4',6-Tetrachlorobiphenyl	1a, 1b
26	2,3',5-Trichlorobiphenyl	1a, 1b, 2	76	2',3,4,5-Tetrachlorobiphenyl	1a, 1b, 2
27	2,3',6-Trichlorobiphenyl	1a, 1b, 2	77	3,3',4,4'-Tetrachlorobiphenyl	1b, 2
28	2,4,4'-Trichlorobiphenyl	1a, 1b, 2, 5	78	3,3',4,5-Tetrachlorobiphenyl	1b
29	2,4,5-Trichlorobiphenyl	1a, 1b	79	3,3',4,5'-Tetrachlorobiphenyl	1a, 1b
30	2,4,6-Trichlorobiphenyl	1a, 1b	80	3,3',5,5'-Tetrachlorobiphenyl	1a, 3a
31	2,4',5-Trichlorobiphenyl	1a, 1b, 2	81	3,4,4',5-Tetrachlorobiphenyl	1a, 1b
32	2,4',6-Trichlorobiphenyl	1a, 1b, 2	82	2,2',3,3',4-Pentachlorobiphenyl	1a, 1b
33	2',3,4-Trichlorobiphenyl	1a, 1b, 2	83	2,2',3,3',5-Pentachlorobiphenyl	1a, 1b
34	2',3,5-Trichlorobiphenyl	1a, 1b, 2	84	2,2',3,3',6-Pentachlorobiphenyl	1a, 1b
35	3,3',4-Trichlorobiphenyl	1a, 1b	85	2,2',3,4,4'-Pentachlorobiphenyl	1a, 1b
36	3,3',5-Trichlorobiphenyl	1a, 1b	86	2,2',3,4,5-Pentachlorobiphenyl	1a, 1b
37	3,4,4'-Trichlorobiphenyl	1a, 1b	87	2,2',3,4,5'-Pentachlorobiphenyl	1a, 1b
38	3,4,5-Trichlorobiphenyl	1a, 1b	88	2,2',3,4,6-Pentachlorobiphenyl	1b, 2
39	3,4',5-Trichlorobiphenyl	1a, 1b	89	2,2',3,4,6'-Pentachlorobiphenyl	1b, 2
40	2,2',3,3'-Tetrachlorobiphenyl	1a, 1b, 2	90	2,2',3,4',5-Pentachlorobiphenyl	1a, 1b
41	2,2',3,4-Tetrachlorobiphenyl	1a, 1b	91	2,2',3,4',6-Pentachlorobiphenyl	1a, 1b, 2
42	2,2',3,4'-Tetrachlorobiphenyl	1a, 1b	92	2,2',3,5,5'-Pentachlorobiphenyl	1a, 1b
43	2,2',3,5-Tetrachlorobiphenyl	1a, 1b	93	2,2',3,5,6-Pentachlorobiphenyl	1b, 2
44	2,2',3,5'-Tetrachlorobiphenyl	1a, 1b	94	2,2',3,5,6'-Pentachlorobiphenyl	1a, 1b, 2
45	2,2',3,6-Tetrachlorobiphenyl	1a, 1b, 2	95	2,2',3,5',6-Pentachlorobiphenyl	1a, 1b
46	2,2',3,6'-Tetrachlorobiphenyl	1a, 1b, 2	96	2,2',3,6,6'-Pentachlorobiphenyl	1a, 1b
47	2,2',4,4'-Tetrachlorobiphenyl	2	97	2,2',3',4,5-Pentachlorobiphenyl	1b, 2
48	2,2',4,5-Tetrachlorobiphenyl	1a, 1b	98	2,2',3',4,6-Pentachlorobiphenyl	1b, 2
49	2,2',4,5'-Tetrachlorobiphenyl	1a, 1b	99	2,2',4,4',5-Pentachlorobiphenyl	1a, 1b
50	2,2',4,6-Tetrachlorobiphenyl	1a, 1b, 2	100	2,2',4,4',6-Pentachlorobiphenyl	1b, 2

Table 1. Reaction scheme(s) needed to synthesize each individual PCB congener (continued)

BZ#	Compound	Reaction Scheme
101	2,2',4,5,5'-Pentachlorobiphenyl	1a, 1b
102	2,2',4,5,6'-Pentachlorobiphenyl	1a, 1b, 2
103	2,2',4,5',6-Pentachlorobiphenyl	1a, 1b, 2
104	2,2',4,6,6'-Pentachlorobiphenyl	1b
105	2,3,3',4,4'-Pentachlorobiphenyl	1a, 1b, 2
106	2,3,3',4,5-Pentachlorobiphenyl	1a, 1b, 2
107	2,3,3',4',5-Pentachlorobiphenyl	1a, 1b, 2
108	2,3,3',4,5'-Pentachlorobiphenyl	1a, 1b, 2
109	2,3,3',4,6-Pentachlorobiphenyl	1a, 1b, 2
110	2,3,3',4',6-Pentachlorobiphenyl	1a, 1b, 2
111	2,3,3',5,5'-Pentachlorobiphenyl	1a, 1b, 2
112	2,3,3',5,6-Pentachlorobiphenyl	1b, 2
113	2,3,3',5',6-Pentachlorobiphenyl	1a, 1b, 2
114	2,3,4,4',5-Pentachlorobiphenyl	1b, 2
115	2,3,4,4',6-Pentachlorobiphenyl	1b, 2
116	2,3,4,5,6-Pentachlorobiphenyl	1a, 1b, 2, 6
117	2,3,4',5,6-Pentachlorobiphenyl	1b, 2
118	2,3',4,4',5-Pentachlorobiphenyl	1a, 1b, 2
119	2,3',4,4',6-Pentachlorobiphenyl	1a, 1b, 2
120	2,3',4,5,5'-Pentachlorobiphenyl	1a, 1b, 2
121	2,3',4,5',6-Pentachlorobiphenyl	1a, 1b, 2
122	2',3,3',4,5-Pentachlorobiphenyl	1a, 1b, 2
123	2',3,4,4',5-Pentachlorobiphenyl	1b, 2
124	2',3,4,5,5'-Pentachlorobiphenyl	1a, 1b, 2
125	2',3,4,5,6'-Pentachlorobiphenyl	1a, 1b
126	3,3',4,4',5-Pentachlorobiphenyl	1a, 1b
127	3,3',4,5,5'-Pentachlorobiphenyl	1a, 1b
128	2,2',3,3',4,4'-Hexachlorobiphenyl	1b, 2
129	2,2',3,3',4,5-Hexachlorobiphenyl	1a, 1b
130	2,2',3,3',4,5'-Hexachlorobiphenyl	1a, 1b, 2
131	2,2',3,3',4,6-Hexachlorobiphenyl	1a, 1b, 2
132	2,2',3,3',4,6'-Hexachlorobiphenyl	1b, 2
133	2,2',3,3',5,5'-Hexachlorobiphenyl	1a, 2
134	2,2',3,3',5,6-Hexachlorobiphenyl	1a, 1b, 2
135	2,2',3,3',5,6'-Hexachlorobiphenyl	1a, 1b
136	2,2',3,3',6,6'-Hexachlorobiphenyl	1b, 2
137	2,2',3,4,4',5-Hexachlorobiphenyl	1a, 1b
138	2,2',3,4,4',5'-Hexachlorobiphenyl	1b
139	2,2',3,4,4',6-Hexachlorobiphenyl	1a, 1b, 2
140	2,2',3,4,4',6'-Hexachlorobiphenyl	1b
141	2,2',3,4,5,5'-Hexachlorobiphenyl	1a, 1b, 2
142	2,2',3,4,5,6-Hexachlorobiphenyl	1a, 1b, 2
143	2,2',3,4,5,6'-Hexachlorobiphenyl	1a, 1b, 2
144	2,2',3,4,5',6-Hexachlorobiphenyl	1a, 1b, 2
145	2,2',3,4,6,6'-Hexachlorobiphenyl	1a, 1b, 2
146	2,2',3,4',5,5'-Hexachlorobiphenyl	1b
147	2,2',3,4',5,6-Hexachlorobiphenyl	1a, 1b
148	2,2',3,4',5,6'-Hexachlorobiphenyl	1b, 2
149	2,2',3,4',5',6-Hexachlorobiphenyl	1b, 2
150	2,2',3,4',6,6'-Hexachlorobiphenyl	1b
151	2,2',3,5,5',6-Hexachlorobiphenyl	1a, 1b, 2
152	2,2',3,5,6,6'-Hexachlorobiphenyl	1a, 1b
153	2,2',4,4',5,5'-Hexachlorobiphenyl	2
154	2,2',4,4',5,6'-Hexachlorobiphenyl	1b
155	2,2',4,4',6,6'-Hexachlorobiphenyl	1b, 2
156	2,3,3',4,4',5-Hexachlorobiphenyl	1b
157	2,3,3',4,4',5'-Hexachlorobiphenyl	1b
158	2,3,3',4,4',6-Hexachlorobiphenyl	1b, 2
159	2,3,3',4,5,5'-Hexachlorobiphenyl	1b
160	2,3,3',4,5,6-Hexachlorobiphenyl	1b, 6
161	2,3,3',4,5',6-Hexachlorobiphenyl	1a, 1b
162	2,3,3',4',5,5'-Hexachlorobiphenyl	1b, 2
163	2,3,3',4',5,6-Hexachlorobiphenyl	1b, 2
164	2,3,3',4',5',6-Hexachlorobiphenyl	1b, 2
165	2,3,3',5,5',6-Hexachlorobiphenyl	1b, 2
166	2,3,4,4',5,6-Hexachlorobiphenyl	1b, 6
167	2,3',4,4',5,5'-Hexachlorobiphenyl	1b
168	2,3',4,4',5',6-Hexachlorobiphenyl	1b, 2
169	3,3',4,4',5,5'-Hexachlorobiphenyl	1b, 2, 3b
170	2,2',3,3',4,4',5-Heptachlorobiphenyl	1b
171	2,2',3,3',4,4',6-Heptachlorobiphenyl	1b
172	2,2',3,3',4,5,5'-Heptachlorobiphenyl	1b
173	2,2',3,3',4,5,6-Heptachlorobiphenyl	1b
174	2,2',3,3',4,5,6'-Heptachlorobiphenyl	1b
175	2,2',3,3',4,5',6-Heptachlorobiphenyl	1b
176	2,2',3,3',4,6,6'-Heptachlorobiphenyl	1b
177	2,2',3,3',4',5,6-Heptachlorobiphenyl	1b, 2
178	2,2',3,3',5,5',6-Heptachlorobiphenyl	1b, 2
179	2,2',3,3',5,6,6'-Heptachlorobiphenyl	1b
180	2,2',3,4,4',5,5'-Heptachlorobiphenyl	1b
181	2,2',3,4,4',5,6-Heptachlorobiphenyl	1a, 1b
182	2,2',3,4,4',5,6'-Heptachlorobiphenyl	1b, 2
183	2,2',3,4,4',5',6-Heptachlorobiphenyl	1b, 2
184	2,2',3,4,4',6,6'-Heptachlorobiphenyl	1b
185	2,2',3,4,5,5',6-Heptachlorobiphenyl	1a, 1b
186	2,2',3,4,5,6,6'-Heptachlorobiphenyl	1a, 1b
187	2,2',3,4',5,5',6-Heptachlorobiphenyl	1b, 2
188	2,2',3,4',5,6,6'-Heptachlorobiphenyl	1b, 2
189	2,3,3',4,4',5,5'-Heptachlorobiphenyl	1a, 1b, 2
190	2,3,3',4,4',5,6-Heptachlorobiphenyl	1a, 6
191	2,3,3',4,4',5',6-Heptachlorobiphenyl	1b, 2
192	2,3,3',4,5,5',6-Heptachlorobiphenyl	1a, 1b, 2
193	2,3,3',4',5,5',6-Heptachlorobiphenyl	1b, 2
194	2,2',3,3',4,4',5,5'-Octachlorobiphenyl	1b, 2
195	2,2',3,3',4,4',5,6-Octachlorobiphenyl	1b, 2
196	2,2',3,3',4,4',5',6-Octachlorobiphenyl	1b, 2
197	2,2',3,3',4,4',6,6'-Octachlorobiphenyl	1b
198	2,2',3,3',4,5,5',6-Octachlorobiphenyl	1b, 2
199	2,2',3,3',4,5,6,6'-Octachlorobiphenyl	1b
200	2,2',3,3',4,5',6,6'-Octachlorobiphenyl	1b
201	2,2',3,3',4,5,5',6'-Octachlorobiphenyl	1b, 2
202	2,2',3,3',5,5',6,6'-Octachlorobiphenyl	1b, 2
203	2,2',3,4,4',5,5',6-Octachlorobiphenyl	1a, 1b, 2
204	2,2',3,4,4',5,6,6'-Octachlorobiphenyl	1b
205	2,3,3',4,4',5,5',6-Octachlorobiphenyl	1b, 2
206	2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl	1b, 2
207	2,2',3,3',4,4',5,6,6'-Nonachlorobiphenyl	1b
208	2,2',3,3',4,5,5',6,6'-Nonachlorobiphenyl	1b
209	2,2',3,3',4,4',5,5',6,6'-Decachlorobiphenyl	4

Gas Chromatographic Data: Octachloronaphthalene (OCN) was chosen as the internal standard for the compilation of relative retention times and relative response factor data. This was done to facilitate a comparison between data from this study and that published by Mullin and co-workers (19). All retention times obtained on the two GC columns used in this study were compiled relative to OCN. The response factors were calculated via a direct comparison of the integrated areas between each specific PCB congener and OCN.

Table II lists the relative retention times and response factors for the 209 PCB congeners compiled on data obtained by using the octadecyl/phenyl substituted siloxane phase column.

Table II. Relative Retention Times and Response Factors for 209 PCB congeners obtained on the octadecyl/phenyl siloxane column

cong. #	relative retention time	relative response factor	cong. #	relative retention time	relative response factor	cong. #	relative retention time	relative response factor	cong. #	relative retention time	relative response factor
1	0.2776	0.0170	54	0.4029	0.1636	106	0.6740	0.8235	158	0.7302	0.8893
2	0.2728	0.0050	55	0.5732	0.1636	107	0.6693	0.6000	159	0.7603	1.0350
3	0.2817	0.0365	56	0.5816	0.5390	108	0.6666	0.7609	160	0.7288	1.0324
4	0.2769	0.0705	57	0.5422	0.4305	109	0.6095	0.7490	161	0.6912	0.8336
5	0.3357	0.3225	58	0.5475	0.4694	110	0.6276	0.5925	162	0.7341	0.7025
6	0.3288	0.1830	59	0.5028	0.4936	111	0.6331	0.5975	163	0.7239	0.6869
7	0.3216	0.3205	60	0.5847	0.7310	112	0.6036	0.5810	164	0.7185	0.6335
8	0.3379	0.1925	61	0.5579	0.8185	113	0.5896	0.4999	165	0.6853	0.6811
9	0.3190	0.2140	62	0.4982	0.7465	114	0.6857	1.0308	166	0.7450	0.9129
10	0.2838	0.2040	63	0.5541	0.4475	115	0.6249	1.5120	167	0.7717	0.6685
11	0.3859	0.5450	64	0.5184	0.5090	116	0.6223	1.1155	168	0.6981	0.5905
12	0.3925	0.1340	65	0.4943	0.5900	117	0.6204	0.6104	169	0.8496	0.6944
13	0.3929	0.0666	66	0.5665	0.4646	118	0.6746	0.4979	170	0.8348	0.8690
14	0.3666	0.1229	67	0.5478	0.8000	119	0.6055	0.5465	171	0.7751	0.6662
15	0.4003	0.0695	68	0.5321	0.8190	120	0.6403	0.5336	172	0.8000	0.8307
16	0.3966	0.2720	69	0.4816	0.3925	121	0.5693	0.5000	173	0.7780	0.8976
17	0.3840	0.2648	70	0.5614	0.4005	122	0.6840	0.5336	174	0.7584	0.6256
18	0.3774	0.1855	71	0.5142	0.4209	123	0.6701	0.5295	175	0.7356	0.6627
19	0.3441	0.1536	72	0.5282	0.3535	124	0.6636	0.5167	176	0.6992	0.4857
20	0.4518	0.4289	73	0.4776	0.3140	125	0.6106	0.4895	177	0.7661	0.6225
21	0.4533	0.6817	74	0.5601	0.4084	126	0.7519	0.4880	178	0.7261	0.7030
22	0.4631	0.5055	75	0.4963	0.4935	127	0.7196	0.5459	179	0.6863	0.7900
23	0.4259	0.4690	76	0.5598	0.3731	128	0.7496	0.8120	180	0.8092	0.8209
24	0.3917	0.4568	77	0.6461	0.2708	129	0.7271	0.6815	181	0.7692	0.9125
25	0.4376	0.4100	78	0.6250	0.3384	130	0.7142	0.6090	182	0.7402	0.6025
26	0.4338	0.2985	79	0.6149	0.2796	131	0.6678	0.6057	183	0.7479	0.6716
27	0.3896	0.1219	80	0.5835	0.3224	132	0.6783	0.5065	184	0.6852	0.4775
28	0.4488	0.4525	81	0.6351	0.3410	133	0.6788	0.5086	185	0.7552	0.9687
29	0.4314	0.3945	82	0.6352	0.5590	134	0.6592	0.4682	186	0.7077	0.7384
30	0.3716	0.4700	83	0.6007	0.4215	135	0.6391	0.3865	187	0.7393	0.5456
31	0.4437	0.3337	84	0.5663	0.3605	136	0.6038	0.3198	188	0.6730	0.3850
32	0.4027	0.3685	85	0.6230	0.5930	137	0.7153	0.7810	189	0.8849	1.0999
33	0.4539	0.3545	86	0.6699	0.5975	138	0.7236	0.6305	190	0.8425	0.9916
34	0.4227	0.2855	87	0.6140	0.5966	139	0.6594	0.6250	191	0.8150	0.8974
35	0.5159	0.1978	88	0.5549	0.5127	140	0.6603	0.4809	192	0.8038	0.8965
36	0.4866	0.1887	89	0.5742	0.3708	141	0.7060	0.7655	193	0.8087	0.8175
37	0.5247	0.1820	90	0.5901	0.4085	142	0.6707	0.8870	194	0.9139	0.9205
38	0.5048	0.3106	91	0.5591	0.3417	143	0.6582	0.5297	195	0.8778	0.7907
39	0.4954	0.1725	92	0.5815	0.3735	144	0.6461	0.5848	196	0.8477	0.7536
40	0.5188	0.4236	93	0.5488	0.3709	145	0.6037	0.4166	197	0.7875	0.6006
41	0.5143	0.5205	94	0.5359	0.2774	146	0.6889	0.4199	198	0.8371	0.7956
42	0.5063	0.4326	95	0.5465	0.3457	147	0.6516	0.4892	199	0.7959	0.7225
43	0.4816	0.3479	96	0.5052	0.2265	148	0.6219	0.3875	200	0.7747	0.5040
44	0.4985	0.3784	97	0.6114	0.3969	149	0.6524	0.3897	201	0.8386	0.7158
45	0.4520	0.0978	98	0.5495	0.3564	150	0.5906	0.3095	202	0.7616	0.4055
46	0.4584	0.2576	99	0.5990	0.3677	151	0.6384	0.4576	203	0.8511	0.8933
47	0.4950	0.3681	100	0.5407	0.5871	152	0.5924	0.3068	204	0.7831	0.6867
48	0.4905	0.3041	101	0.5910	0.3675	153	0.6988	0.4649	205	0.9217	0.9222
49	0.4865	0.2937	102	0.5483	0.2888	154	0.6351	0.3785	206	0.9458	1.0150
50	0.4342	0.2966	103	0.5285	0.3590	155	0.5773	0.3030	207	0.8803	1.3085
51	0.4500	0.2570	104	0.4814	0.2375	156	0.7953	1.0072	208	0.8668	0.8188
52	0.4789	0.2376	105	0.7009	0.8249	157	0.7978	0.8927	209	0.9691	0.8217
53	0.4386	0.2209									

The retention data is further categorized in Table III into subgroups according to the degree of chlorination. A review of these two tables indicates several general trends. The retention times of the congeners increases with the degree of chlorination which is consistent with published

Table III. Relative retention to OCN of congeners subgrouped via chlorine substitution on the octadecyl / phenyl siloxane column

Monochlorobiphenyls

Cong. #	Structure	RRT
1	2-Cl	0.2726
2	2-Cl	0.2728
3	4-Cl	0.2817

Dichlorobiphenyls

Cong. #	Structure	RRT
4	2,2'	0.2769
10	2,6	0.2838
9	2,5	0.3190
7	2,4	0.3216
6	2,3'	0.3288
5	2,3	0.3357
8	2,4'	0.3374
14	3,5	0.3666
11	3,3'	0.3859
12	3,4	0.3925
13	3,4'	0.3929
15	4,4'	0.4003

Trichlorobiphenyls

Cong. #	Structure	RRT
19	2,2',6	0.3441
30	2,4,6	0.3716
18	2,2',5	0.3774
17	2,2',4	0.3840
27	2,3',6	0.3896
24	2,3,6	0.3917
16	2,2',3	0.3966
32	2,4',6	0.4027
34	2',3,5	0.4227
23	2,3,5	0.4259
29	2,4,5	0.4314
22	2,3,4'	0.4631
26	2,3',5	0.4338
25	2,3',4	0.4376
31	2,4',5	0.4437
28	2,4,4'	0.4488
20	2,3,3'	0.4518
21	2,3,4	0.4533
33	2',3,4	0.4539
36	3,3',5	0.4866
39	3,4',5	0.4954
38	3,4,5	0.5048
35	3,3',4	0.5159
37	3,4,4'	0.5247

Tetrachlorobiphenyls

Cong. #	Structure	RRT
54	2,2',6,6'	0.4029
50	2,2',4,6	0.4342
53	2,2',5,6'	0.4386
51	2,2',4,6'	0.4500
45	2,2',3,6	0.4520
46	2,2',3,6'	0.4584
73	2,3',5',6	0.4776
52	2,2',5,5'	0.4789
43	2,2',3,5	0.4816
69	2,3',4,6	0.4816
49	2,2',4,5'	0.4865
48	2,2',4,5	0.4905
47	2,2',4,4'	0.4950
65	2,3,5,6	0.4943
75	2,4,4',6	0.4963
62	2,3,4,6	0.4982

Tetrachlorobiphenyls (con't)

Cong. #	Structure	RRT
44	2,2',3,5'	0.4985
59	2,3,3',6	0.5028
42	2,2',3,4'	0.5063
71	2,3',4',6	0.5142
41	2,2',3,4	0.5143
64	2,3,4',6	0.5184
40	2,2',3,3'	0.5188
72	2,3',5,5'	0.5282
68	2,3',4,5'	0.5321
57	2,3,3',5	0.5422
58	2,3,3',5'	0.5475
67	2,3',4,5	0.5478
63	2,3,4',5	0.5541
61	2,3,4,5	0.5579
76	2',3,4,5	0.5598
74	2,4,4',5	0.5601
70	2,3',4',5	0.5614
66	2,3',4,4'	0.5665
55	2,3,3',4	0.5732
56	2,3,3',4'	0.5816
80	3,3',5,5'	0.5835
60	2,3,4,4'	0.5847
79	3,3',4,5'	0.6149
78	3,3',4,5	0.6250
81	3,4,4',5	0.6351
77	3,3',4,4'	0.6461

Pentachlorobiphenyls

Cong. #	Structure	RRT
104	2,2',4,6,6'	0.4914
96	2,2'3,6,6'	0.5052
103	2,2',4,5',6	0.5285
94	2,2',3,5,6'	0.5359
100	2,2',4,4',6	0.5407
95	2,2',3,5',6	0.5465
102	2,2',4,5,6'	0.5483
93	2,2',3,5,6	0.5488
98	2,2',3',4,6	0.5495
88	2,2',3,4,6	0.5549
91	2,2',3,4',6	0.5591
84	2,2',3,3',6	0.5663
121	2,3',4,5',6	0.5693
89	2,2',3,4,6'	0.5742
92	2,2',3,5,5'	0.5815
113	2,3,3',5',6	0.5896
90	2,2',3,4',5	0.5901
101	2,2',4,5,5'	0.5910
99	2,2',4,4',5	0.5990
83	2,2',3,3',5	0.6007
112	2,3,3',5,6	0.6036
119	2,3',4,4',6	0.6055
109	2,3,3',4,6	0.6095
(IUPAC # 108)		
86	2,2',3,4,5	0.6099
125	2',3,4,5,6'	0.6106
97	2,2',3',4,5	0.6114
87	2,2',3,4,5'	0.6140
117	2,3,4',5,6	0.6204
116	2,3,4,5,6	0.6223
85	2,2',3,4,4'	0.6230
115	2,3,4,4',6	0.6249
110	2,3,3',4',6	0.6276
111	2,3,3',5,5'	0.6331

Pentachlorobiphenyls

Cong. #	Structure	RRT
82	2,2',3,3',4	0.6352
120	2,3',4,5,5'	0.6403
124	2',3,4,5,5'	0.6636
108	2,3,3',4,5'	0.6666
(IUPAC # 107)		
107	2,3,3',4',5	0.6693
(IUPAC # 109)		
123	2',3,4,4',5	0.6701
106	2,3,3',4,5	0.6740
118	2,3',4,4',5	0.6746
122	2',3,3',4,5	0.6840
114	2,3,4,4',5	0.6851
105	2,3,3',4,4'	0.7009
127	3,3',4,5,5'	0.7196
126	3,3',4,4',5	0.7519

Hexachlorobiphenyls

Cong. #	Structure	RRT
155	2,2',4,4',6,6'	0.5773
150	2,2',3,4',6,6'	0.5906
152	2,2',3,5,6,6'	0.5924
145	2,2',3,4,6,6'	0.6037
136	2,2',3,3',6,6'	0.6038
148	2,2',3,4',5,6'	0.6219
154	2,2',4,4',5,6'	0.6351
151	2,2',3,5,5',6	0.6384
135	2,2',3,3',5,6'	0.6391
144	2,2',3,4,5',6	0.6461
147	2,2',3,4',5,6	0.6516
149	2,2',3,4',5',6	0.6524
143	2,2',3,4,5,6'	0.6582
134	2,2',3,3',5,6	0.6592
139	2,2',3,4,4',6	0.6594
140	2,2',3,4,4',6'	0.6603
131	2,2',3,3',4,6	0.6678
142	2,2',3,4,5,6	0.6707
132	2,2',3,3',4,6'	0.6783
133	2,2',3,3',5,5'	0.6788
165	2,3,3',5,5',6	0.6853
146	2,2',3,4',5,5'	0.6889
161	2,3,3',4,5',6	0.6912
168	2,3',4,4',5',6	0.6981
153	2,2',4,4',5,5'	0.6986
141	2,2',3,4,5,5'	0.7060
130	2,2',3,3',4,5'	0.7142
137	2,2',3,4,4',5	0.7153
164	2,3,3',4',5',6	0.7185
138	2,2',3,4,4',5'	0.7236
163	2,3,3',4',5,6	0.7239
129	2,2',3,3',4,5	0.7271
160	2,3,3',4,5,6	0.7288
158	2,3,3',4,4',6	0.7302
166	2,3,4,4',5,6	0.7450
128	2,2',3,3',4,4'	0.7496
159	2,3,3',4,5,5'	0.7603
162	2,3,3',4',5,5'	0.7641
167	2,3',4,4',5,5'	0.7717
156	2,3,3',4,4',5	0.7953
157	2,3,3',4,4',5'	0.7978
169	3,3',4,4',5,5'	0.8460

Heptachlorobiphenyl

Cong. #	Structure	RRT
188	2,2',3,4',5,6,6'	0.6730
184	2,2',3,4,4',6,6'	0.6852
179	2,2',3,3',5,6,6'	0.6863
176	2,2',3,3',4,6,6'	0.6992
186	2,2',3,4,5,6,6'	0.7077
178	2,2',3,3',5,5',6	0.7261
175	2,2',3,3',4,5',6	0.7356
187	2,2',3,4',5,5',6	0.7393
182	2,2',3,4,4',5,6'	0.7402
183	2,2',3,4,4',5',6	0.7479
185	2,2',3,4,5,5',6	0.7552
174	2,2',3,3',4,5,6'	0.7584
181	2,2',3,4,4',5,6	0.7692
177	2,2',3,3',4',5,6	0.7661
171	2,2',3,3',4,4',6	0.7751
173	2,2',3,3',4,5,6	0.7780
172	2,2',3,3',4,5,5'	0.8000
192	2,3,3',4,5,5',6	0.8038
193	2,3,3',4',5,5',6	0.8087
191	2,3,3',4,4',5,6	0.8150
170	2,2',3,3',4,4',5	0.8348
190	2,3,3',4,4',5,6	0.8425
189	2,3,3',4,4',5,5'	0.8849

Octachlorobiphenyls

Cong. #	Structure	RRT
202	2,2',3,3',5,5',6,6'	0.7616
200	2,2',3,3',4,5',6,6'	0.7747
(IUPAC # 201)		
204	2,2',3,4,4',5,6,6'	0.7831
197	2,2',3,3',4,4',6,6'	0.7850
199	2,2',3,3',4,5,6,6'	0.7959
(IUPAC # 200)		
198	2,2',3,3',4,5,5',6	0.8371
201	2,2',3,3',4,4',5',6	0.8386
(IUPAC # 199)		
196	2,2',3,3',4,4',5',6	0.8477
203	2,2',3,4,4',5,5',6	0.8511
195	2,2',3,3',4,4',5,6	0.8778
194	2,2',3,3',4,4',5,5'	0.9139
205	2,3,3',4,4',5,5',6	0.9217

Nonachlorobiphenyls

Cong. #	Structure	RRT
208	2,2',3,3',4,5,5',6,6'	0.8188
207	2,2',3,3',4,4',5,6,6'	0.8803
206	2,2',3,3',4,4',5,5',6	0.9458

Decachlorobiphenyl

Cong. #	Structure	RRT
210	2,2',3,3',4,4',5,5',6,6'	0.9691

Relative retention of congeners to Octachloronaphthalene on C_{18} column

results. Within each subgroup, the ortho-substituted congeners elute first. Within the multichlorinated subgroups (>three chlorines), the congeners which are substituted in the o,o' positions, in most instances, elute before other congeners. These are followed by congeners substituted in the o,m positions. Throughout the congener subgroups, the number of individual congeners which exhibit retention times overlapping into the next higher chlorine substituted grouping follows a gaussian-like distribution. This distribution can be correlated with the substitution pattern of the congeners. Overall, the retention data conforms to the guidelines established and published by Mullin et al (19) and Ballschmitter and co-workers (20).

These guidelines are also applicable to the elution patterns obtained on a 50% phenyl substituted methyl siloxane phase - Tables IV and V. A review of Table IV reveals that with the exception of a few individual congener peak shifts, the elution patterns of the chlorinated subgroups are similar to those obtained on the octadecyl substituent type column. The lack of peak shifting may be attributed to the fact that neither stationary phase used in this study possesses substituent groups containing a strong permanent dipole or a strong electron acceptor. A study using a highly polar stationary phase (78% cyanopropyl substitution) and a trifluoropropyl stationary phase (electron-accepting groups) is on-going; and the results will be published in a future paper.

Tables II and IV also list the relative response factors for the 209 PCB congeners. Duplicate injections of all 209 congeners were made on both the octadecyl/phenyl siloxane and the 50% phenyl siloxane columns in order to ensure reliability of results. Excellent linearity of response for the ECD was established for both columns over a range exceeding that of the target concentration. These response factors were calculated relative to OCN and showed variations of < 4% for the same congener on the same column. OCN response was monitored throughout the study and exhibited a RSD of < 1% for 50 replicate injections.

However, a comparison of the response factors obtained on the octadecyl/phenyl siloxane column versus the 50% phenyl siloxane column for the same congener revealed some considerable variations. This may be a result of the differences in column dimensions, flow rates, retention characteristics as well as the variability of response of the ECD (21). This suggests that attempts at assigning absolute or relative response factors to PCB congeners is highly system dependent and may only be meaningful for identifying chlorine substitution patterns within a specified set of working parameters. In spite of this, the response factors should be useful for corroborating the identification of individual congeners when used in conjunction with retention data.

Table IV. Relative Retention Times and Response Factors for 209 PCB Congeners obtained on the 50% phenyl methyl siloxane column

cong. #	relative retention time	relative response factor	cong. #	relative retention time	relative response factor	cong. #	relative retention time	relative response factor	cong. #	relative retention time	relative response factor
1	0.1541	0.0377	54	0.3667	0.1590	106	0.6476	0.9936	158	0.7236	0.9735
2	0.1906	0.0055	55	0.5412	0.9152	107	0.6414	0.7512	159	0.7443	1.2165
3	0.1959	0.0192	56	0.5573	0.7340	108	0.6416	0.9565	160	0.7189	1.2833
4	0.2176	0.0439	57	0.4861	0.5212	109	0.5721	0.9744	161	0.6629	1.0795
5	0.2659	0.5948	58	0.5024	0.6532	110	0.6150	0.6990	162	0.7555	0.8955
6	0.2565	0.2746	59	0.4651	0.6069	111	0.5832	0.7311	163	0.7204	0.8060
7	0.2368	0.5537	60	0.5541	0.9982	112	0.5694	0.7377	164	0.7237	0.6960
8	0.2637	0.2614	61	0.5014	1.0040	113	0.5565	0.6701	165	0.6600	0.8240
9	0.2376	0.3027	62	0.4323	0.9519	114	0.6635	1.0832	166	0.7364	1.1420
10	0.2137	0.3199	63	0.4991	0.5418	115	0.5873	1.2680	167	0.7645	0.7545
11	0.3114	0.0572	64	0.4773	0.6611	116	0.5810	1.1636	168	0.6728	0.7305
12	0.3184	0.1519	65	0.4314	0.8003	117	0.5864	0.8155	169	0.8714	0.7275
13	0.3214	0.0689	66	0.5217	0.6246	118	0.6487	0.5859	170	0.8669	0.8300
14	0.2749	0.1504	67	0.4907	0.5184	119	0.5626	0.7024	171	0.7885	0.6655
15	0.3325	0.0676	68	0.4675	0.5687	120	0.5915	0.6598	172	0.8072	0.8700
16	0.3496	0.3770	69	0.4121	0.5985	121	0.5061	0.6216	173	0.7986	0.9821
17	0.3162	0.3375	70	0.5186	0.5144	122	0.6750	0.6168	174	0.7758	0.6455
18	0.3160	0.2129	71	0.4776	0.6140	123	0.6421	0.6437	175	0.7259	0.7220
19	0.2922	0.1853	72	0.4642	0.4856	124	0.6365	0.6447	176	0.6969	0.5435
20	0.4002	0.6624	73	0.4229	0.4297	125	0.5889	0.5840	177	0.7829	0.6302
21	0.3918	1.0293	74	0.5038	0.5554	126	0.7531	0.5300	178	0.7196	0.6155
22	0.4114	0.8207	75	0.4248	0.7101	127	0.6944	0.6801	179	0.6874	0.4149
23	0.3439	0.6532	76	0.5155	0.5745	128	0.7709	0.9759	180	0.8164	0.8625
24	0.3282	0.6624	77	0.6298	0.3109	129	0.7354	0.8229	181	0.7681	1.0699
25	0.3676	0.5507	78	0.5900	0.4787	130	0.7137	0.7144	182	0.7267	0.6788
26	0.3664	0.3687	79	0.5736	0.3546	131	0.6622	0.7290	183	0.7379	0.7326
27	0.3301	0.2474	80	0.5168	0.4517	132	0.6890	0.5429	184	0.6502	0.5784
28	0.3781	0.5894	81	0.6078	0.3833	133	0.6544	0.6160	185	0.7589	1.1595
29	0.3487	0.5142	82	0.6372	0.7192	134	0.6577	0.5260	186	0.7092	0.9045
30	0.2824	0.6515	83	0.5804	0.4929	135	0.6280	0.4359	187	0.7324	0.6026
31	0.3774	0.3990	84	0.5608	0.3890	136	0.6034	0.3429	188	0.6414	0.4616
32	0.3431	0.4885	85	0.6030	0.8331	137	0.7030	0.9388	189	0.9119	1.1412
33	0.3977	0.4654	86	0.5850	0.8602	138	0.7216	0.7129	190	0.8667	1.0605
34	0.3486	0.3553	87	0.5991	0.7795	139	0.6305	0.7889	191	0.8285	0.8235
35	0.4664	0.1851	88	0.5169	0.7043	140	0.6388	0.5389	192	0.8069	0.9475
36	0.4141	0.1886	89	0.5607	0.4517	141	0.6974	0.9475	193	0.8249	0.8115
37	0.4798	0.1694	90	0.5465	0.4879	142	0.6571	1.1715	194	0.9570	0.8759
38	0.4399	0.3624	91	0.5278	0.3966	143	0.6527	0.6338	195	0.9216	0.7625
39	0.4279	0.1637	92	0.5415	0.4550	144	0.6234	0.7690	196	0.8718	0.7374
40	0.5020	0.4736	93	0.5129	0.4090	145	0.5812	0.5080	197	0.7882	0.5876
41	0.4803	0.6765	94	0.5019	0.3217	146	0.6635	0.4599	198	0.8575	0.8610
42	0.4660	0.4780	95	0.5220	0.3995	147	0.6264	0.5350	199	0.8206	0.7640
43	0.4279	0.3861	96	0.4844	0.2417	148	0.5785	0.4409	200	0.7778	0.5024
44	0.4641	0.3814	97	0.5868	0.4290	149	0.6395	0.4015	201	0.8635	0.7190
45	0.4146	0.0970	98	0.5095	0.4088	150	0.5574	0.3369	202	0.7653	0.4305
46	0.4318	0.2761	99	0.5527	0.4468	151	0.6190	0.5419	203	0.8688	1.0050
47	0.4315	0.3945	100	0.4772	0.4157	152	0.5739	0.3439	204	0.7735	0.9730
48	0.4331	0.3100	101	0.5492	0.3677	153	0.6729	0.4875	205	0.9627	0.9735
49	0.4302	0.2919	102	0.5117	0.3015	154	0.5902	0.4071	206	0.9944	1.0310
50	0.3660	0.3221	103	0.4726	0.3789	155	0.5106	0.3439	207	0.9033	1.3795
51	0.4000	0.2765	104	0.4380	0.2557	156	0.8041	1.0155	208	0.8917	0.8646
52	0.4280	0.2428	105	0.6995	0.9860	157	0.8151	0.8609	209	1.0140	0.2655
53	0.3964	0.2345									

Table V. Relative etention to OCN of PCB congeners subgrouped via chlorine substitution on the 50% phenyl methyl siloxane column

Monochlorobiphenyls

Cong. #	Structure	RRT
1	2-Cl	0.1541
2	2-Cl	0.1906
3	4-Cl	0.1959

Dichlorobiphenyls

Cong. #	Structure	RRT
10	2,6	0.2137
4	2,2'	0.2176
7	2,4	0.2368
9	2,5	0.2376
6	2,3'	0.2565
8	2,4'	0.2637
5	2,3	0.2659
14	3,5	0.2749
11	3,3'	0.3114
12	3,4	0.3184
13	3,4'	0.3214
15	4,4'	0.3325

Trichlorobiphenyls

Cong. #	Structure	RRT
30	2,4,6	0.2824
19	2,2',6	0.2922
18	2,2',5	0.3160
17	2,2',4	0.3162
24	2,3,6	0.3282
27	2,3',6	0.3301
32	2,4',6	0.3431
23	2,3,5	0.3439
34	2',3,5	0.3486
29	2,4,5	0.3487
16	2,2',3	0.3496
26	2,3',5	0.3664
25	2,3',4	0.3676
31	2,4',5	0.3774
28	2,4,4'	0.3781
21	2,3,4	0.3918
33	2',3,4	0.3977
20	2,3,3'	0.4000
22	2,3,4'	0.4114
36	3,3',5	0.4141
39	3,4',5	0.4279
38	3,4,5	0.4399
35	3,3',4	0.4664
37	3,4,4'	0.4798

Tetrachlorobiphenyls

Cong. #	Structure	RRT
50	2,2',4,6	0.3660
54	2,2',6,6'	0.3667
53	2,2',5,6'	0.3964
51	2,2',4,6'	0.4000
69	2,3',4,6	0.4121
45	2,2',3,6	0.4146
73	2,3',5',6	0.4229
75	2,4,4',6	0.4248
43	2,2',3,5	0.4279
52	2,2',5,5'	0.4280
49	2,2',4,5'	0.4302
65	2,3,5,6	0.4314

Tetrachlorobiphenyls (con't)

Cong. #	Structure	RRT
47	2,2',4,4'	0.4315
46	2,2',3,6'	0.4318
62	2,3,4,6	0.4323
48	2,2',4,5	0.4331
44	2,2',3,5'	0.4641
72	2,3',5,5'	0.4642
59	2,3,3',6	0.4651
42	2,2',3,4'	0.4660
68	2,3',4,5'	0.4675
64	2,3,4',6	0.4773
71	2,3',4',6	0.4776
41	2,2',3,4	0.4803
57	2,3,3',5	0.4861
67	2,3',4,5	0.4907
63	2,3,4',5	0.4991
40	2,2',3,3'	0.5020
61	2,3,4,5	0.5014
58	2,3,3',5'	0.5024
74	2,4,4',5	0.5038
76	2',3,4,5	0.5155
80	3,3',5,5'	0.5168
70	2,3',4',5	0.5186
66	2,3',4,4'	0.5217
55	2,3,3',4	0.5412
60	2,3,4,4'	0.5541
56	2,3,3',4'	0.5573
79	3,3',4,5'	0.5736
78	3,3',4,5	0.5900
81	3,4,4',5	0.6078
77	3,3',4,4'	0.6288

Pentachlorobiphenyls

Cong. #	Structure	RRT
104	2,2',4,6,6'	0.4380
103	2,2',4,5',6	0.4726
100	2,2',4,4',6	0.4772
96	2,2'3,6,6'	0.4844
94	2,2',3,5,6'	0.5019
121	2,3',4,5',6	0.5061
98	2,2',3',4,6	0.5095
102	2,2',4,5,6'	0.5117
93	2,2',3,5,6	0.5129
88	2,2',3,4,6	0.5169
95	2,2',3,5',6	0.5220
91	2,2',3,4',6	0.5278
92	2,2',3,5,5'	0.5415
90	2,2',3,4',5	0.5465
101	2,2',4,5,5'	0.5492
99	2,2,4,4',5	0.5527
113	2,3,3',5',6	0.5565
89	2,2',3,4,6'	0.5607
84	2,2',3,3',6	0.5608
119	2,3',4,4',6	0.5626
112	2,3,3',5,6	0.5694
109	2,3,3',4,6	0.5721
(IUPAC # 108)		
83	2,2',3,3',5	0.5804
116	2,3,4,5,6	0.5810
111	2,3,3',5,5'	0.5832
86	2,2',3,4,5	0.5850

Pentachlorobiphenyls (con't)

Cong. #	Structure	RRT
117	2,3,4',5,6	0.5864
97	2,2',3',4,5	0.5868
115	2,3,4,4',6	0.5873
125	2',3,4,5,6'	0.5889
120	2,3',4,5,5'	0.5915
87	2,2',3,4,5'	0.5991
85	2,2',3,4,4'	0.6030
110	2,3,3',4',6	0.6150
124	2',3,4,5,5'	0.6365
82	2,2',3,3',4	0.6372
107	2,3,3',4',5	0.6414
(IUPAC # 107)		
108	2,3,3',4,5'	0.6416
(IUPAC # 109)		
123	2',3,4,4',5	0.6421
106	2,3,3',4,5	0.6476
118	2,3',4,4',5	0.6487
114	2,3,4,4',5	0.6635
122	2',3,3',4,5	0.6750
127	3,3',4,5,5'	0.6944
105	2,3,3',4,4'	0.6995
126	3,3',4,4',5	0.7531

Hexachlorobiphenyls

Cong. #	Structure	RRT
155	2,2',4,4',6,6'	0.5106
150	2,2',3,4',6,6'	0.5574
152	2,2',3,5,6,6'	0.5739
148	2,2',3,4',5,6'	0.5785
145	2,2',3,4,6,6'	0.5812
154	2,2',4,4',5,6'	0.5902
136	2,2',3,3',6,6'	0.6034
151	2,2',3,5,5',6	0.6190
144	2,2',3,4,5',6	0.6234
147	2,2',3,4',5,6	0.6264
135	2,2',3,3',5,6'	0.6280
139	2,2',3,4,4',6	0.6305
140	2,2',3,4,4',6'	0.6388
149	2,2',3,4',5',6	0.6395
143	2,2',3,4,5,6'	0.6527
133	2,2',3,3',5,5'	0.6544
142	2,2',3,4,5,6	0.6571
134	2,2',3,3',5,6	0.6577
165	2,3,3',5,5',6	0.6600
131	2,2',3,3',4,6	0.6622
161	2,3,3',4,5',6	0.6629
146	2,2',3,4',5,5'	0.6635
168	2,3',4,4',5',6	0.6728
153	2,2',4,4',5,5'	0.6729
132	2,2',3,3',4,6'	0.6890
141	2,2',3,4,5,5'	0.6974
137	2,2',3,4,4',5	0.7030
130	2,2',3,3',4,5'	0.7137
160	2,3,3',4,5,6	0.7189
163	2,3,3',4',5,6	0.7204
158	2,3,3',4,4',6	0.7236
164	2,3,3',4',5',6	0.7237
129	2,2',3,3',4,5	0.7354
166	2,3,4,4',5,6	0.7364
159	2,3,3',4,5,5'	0.7443

Hexachlorobiphenyls (con't)

Cong. #	Structure	RRT
162	2,3,3',4',5,5'	0.7555
167	2,3',4,4',5,5'	0.7645
128	2,2',3,3',4,4'	0.7709
156	2,3,3',4,4',5	0.8041
157	2,3,3',4,4',5'	0.8151
169	3,3',4,4',5,5'	0.8714

Heptachlorobiphenyls

Cong. #	Structure	RRT
188	2,2',3,4',5,6,6'	0.6414
184	2,2',3,4,4',6,6'	0.6502
179	2,2',3,3',5,6,6'	0.6874
176	2,2',3,3',4,6,6'	0.6969
186	2,2',3,4,5,6,6'	0.7092
178	2,2',3,3',5,5',6	0.7196
175	2,2',3,3',4,5',6	0.7259
182	2,2',3,4,4',5,6'	0.7267
187	2,2',3,4',5,5',6	0.7322
183	2,2',3,4,4',5',6	0.7379
185	2,2',3,4,5,5',6	0.7589
181	2,2',3,4,4',5,6	0.7681
174	2,2',3,3',4,5,6'	0.7758
177	2,2',3,3',4',5,6	0.7829
171	2,2',3,3',4,4',6	0.7885
173	2,2',3,3',4,5,6	0.7986
192	2,3,3',4,5,5',6	0.8069
180	2,2',3,4,4',5,5'	0.8164
193	2,3,3',4',5,5',6	0.8249
191	2,3,3',4,4',5',6	0.8285
190	2,3,3',4,4',5,6	0.8667
170	2,2',3,3',4,4',5	0.8669
189	2,3,3',4,4',5,5'	0.9119

Octachlorobiphenyls

Cong. #	Structure	RRT
202	2,2',3,3',5,5',6,6'	0.7653
204	2,2',3,4,4',5,6,6'	0.7735
200	2,2',3,3',4,5',6,6'	0.7778
(IUPAC # 201)		
197	2,2',3,3',4,4',6,6'	0.7882
199	2,2',3,3',4,5,6,6'	0.8206
(IUPAC # 200)		
198	2,2',3,3',4,5,5',6	0.8575
201	2,2',3,3',4,4',5',6	0.8635
(IUPAC # 199)		
203	2,2',3,4,4',5,5',6	0.8688
196	2,2',3,3',4,4',5',6	0.8718
195	2,2',3,3',4,4',5,6	0.9216
194	2,2',3,3',4,4',5,5'	0.9570
205	2,3,3',4,4',5,5',6	0.9627

Nonachlorobiphenyls

Cong. #	Structure	RRT
208	2,2',3,3',4,5,5',6,6'	0.8917
207	2,2',3,3',4,4',5,6,6'	0.9033
206	2,2',3,3',4,4',5,5',6	0.9944

Decachlorobiphenyl

Cong. #	Structure	RRT
210	2,2',3,3',4,4',5,5',6,6'	1.0140

Gas Chromatography/Mass Spectrometry: The mass spectra of PCB's have been studied by numerous investigators (1,22-24), and a number of features have been identified: 1. Ion clusters with the expected chlorine isotope distribution pattern for each subgrouping 2. Prominent odd electron clusters, consisting of the parent ion cluster and those generated by the loss

of an even number of chlorine atoms. 3. Electron clusters generated by the loss of an odd number of chlorine atoms. The relative intensity of these even electron clusters are highly variable and mainly determined by the nature of the ortho substitution in the PCB. 4. Doubly charged ion species which assume appreciable abundance in the mass spectra of the more highly chlorinated PCB's.

To reduce the effect of differences in ionization efficiencies among the PCB isomers, the data was reduced to percentages of the base peak in the parent ion cluster. In comparing congeners having the same degree of chlorination, there are relatively large differences among the M-Cl (M-35) ions compared to the $M-Cl_2$ (M-70) ions. Within an isomer group, PCB's containing three chlorine atoms or two o,o' chlorine atoms were found to have the highest intensity of M-Cl and $M-Cl_2$ ions. The intensity of the M-Cl and $M-Cl_2$ mass peaks of the remaining isomers have a tendency to decrease as follows, four ortho chlorines > two o,o ortho chlorines > one ortho chlorine > no ortho chlorines.

The above trends can be understood in terms of the stabilities of the parent ions and their daughter ions. A key factor in determining the stability of the ions of an isomer group is the steric hindrance resulting from the interaction of ortho chlorine atoms. An increase in the ability of the rings to attain a co-planar configuration increases the amount of resonance stabilization.

PCB's having four ortho chlorines have small M-Cl ions because the steric hindrance is still strong after losing only one chlo-

Figure 2. Ordering of the relative intensities of the M-35 mass spectral peak of the hexachlorobiphenyl isomers by the number of ortho chlorines and the number of meta chlorines adjacent to those ortho chlorines

PCB ISOMER	RELATIVE % M-35	NUMBER OF ORTHO CHLORINES	NUMBER OF ADJACENT ORTHO-META CHLORINES
3,3',4,4',5,5'	0.17	0	0
2,3',4,4',5,5'	0.55		0
2,3,3',4,4',5	0.46	1	1
2,3,3',4,5,5'	0.50		
2,3,3',4',5,5'	0.61		
2,3,3',4,4',5'	0.70		
2,3,3',4,4',6	0.61		1
2,3,4,4',5,6	0.74		2
2,3,3',4',5,6	0.87		2
2,3,3',4,5,6	0.99	2 (O,O)	2
2,3',4,4',5',6	1.07		0
2,3,3',4,5',6	1.26		1
2,3,3',4',5',6	1.35		1
2,3,3',5,5',6	1.71		2
2,2',4,4',5,5'	5.90		0
2,2',3,4,4',5'	11.47		
2,2',3,4,4',5	12.59		
2,2',3,4',5,5'	15.58		1
2,2',3,4,5,5'	18.09	2 (O,O')	
2,2',3,3',4,4'	22.61		
2,2',3,3',4,5	28.93		
2,2',3,3',4,5'	29.02		2
2,2',3,3',5,5'	37.03		
2,2',4,4',5,6'	10.18		0
2,2',3,4,4',6	14.99		
2,2',3,4',5',6	16.78		
2,2',3,4,5',6	18.93		1
2,2',3,4,4',6'	19.72		
2,2',3,4',5,6'	21.74		
2,2',3,4,5,6'	22.06	3	
2,2',3,4',5,6	22.96		
2,2',3,5,5',6	24.69		
2,2',3,4,5,6	26.42		
2,2',3,3',4,6'	28.20		2
2,2',3,3',4,6	29.33		
2,2',3,3',5,6'	29.99		
2,2',3,3',5,6	38.43		3
2,2',4,4',6,6'	1.48		0
2,2',3,4',6,6'	2.10		
2,2',3,4,6,6'	2.55	4	1
2,2',3,3',6,6'	2.87		
2,2',3,5,6,6'	3.04		2

rine, so there is little gain in resonance stabilization. In contrast, PCB's having three ortho chlorines or two o,o' chlorines would be expected to have a gain in resonance stabilization and show a correspondingly larger relative abundance of M-Cl ions. The remaining ortho chlorine combinations exhibit weak M-Cl ions because they are already stabilized and have little driving force to lose a chlorine atom.

PCB's having the same degree of chlorination can be divided into groups having three or four or two o,o' chlorines. The ordering of the relative intensity of the M-Cl ions within each group is apparent. The greater the number of ortho chlorines having an adjacent meta chlorine (i.e. o,m chlorine pair), the greater the intensity of the M-Cl ions. This can be explained by the formation of a chloronium ion (figure 3) which increases the stability of the ion upon losing a chlorine atom.

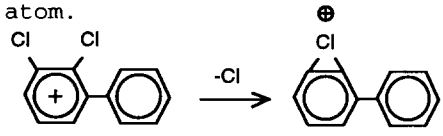

Figure 3. Formation of a chloronium ion leading to the increased stability of the parent PCB ion

This grouping is not seen in PCB's having two o,o chlorines nor in those having one or no ortho chlorines since the energy gained in removing an ortho chlorine is not sufficient to result in the preferential loss of chlorine atoms. The random rearrangement of the Cl substitution pattern due to electron impact which has been noted for the less sterically hindered isomers also destroys the differences among groups (22). The differences in the relative intensity of the M-35 mass spectral peak can help distinguish between PCB isomers on the basis of differences in their ortho substitution. In some cases, where ortho substitution is identical, differences in meta substitution may be of value in distinguishing among isomers.

Matrix Isolated GC/FT-IR: The infrared spectra of PCB congeners and commercial Aroclor products have been studied (25-27). The spectra of all the PCB congeners contain the major absorption bands associated with biphenyl. These bands occur in the regions: 4000-2000 cm^{-1}, C-H stretching; 2000-1250 cm^{-1}, C=C stretching; and 1250-250 cm^{-1}, bending and deformations. Of the three regions, the range from 1200-300 cm^{-1} is the most useful for determining individual congeners.

Matrix isolated FT/IR spectra of all 209 PCB congeners indicate that each congener has its own unique absorption pattern which can be used to identify the individual congener. Table VI is a compilation of the five strongest absorption wavelengths associated with each congener.

Melting Points: Table VII is a compilation of all 209 congeners and lists the melting points obtained for the crystalline congeners. A review of the literature (28-35) provided melting points for approximately one-third of the congeners; and a survey of Table VII reveals that our results are in good agreement with these published values.

Table VI. Selected Matrix Isolated FT/IR absorption bands for all 209 PCB congeners

Congener No.	Absorption Band Intensity Strong → Weak					Congener No.	Absorption Band Intensity Strong → Weak				
1	750.2	699.5	1471.3	1039.9	771.7	73	789.7	1413.7	1568.5	1600.9	811.1
2	756.9	698.7	1477.7	1597.9	1570.6	74	1458.9	1099.1	1088.8	1016.9	830.8
3	1482.4	760.9	1097.6	834	1009.4	75	1099.2	1583.2	1447.5	1544.4	1430.5
4	752.6	762.6	1467.1	1462.1	1064.6	76	757.8	1430.2	1544.8	1378	812.9
5	759.3	699.3	1453.2	1410	1044.9	77	1464.3	1137.1	816.8	1033.6	1363
6	756.3	1463	1467.8	1040	825.2	78	1546.9	1436.9	811.7	1369.9	786.6
7	1469.8	817.4	700	1107.8	825.2	79	806.4	1590.2	1552.9	1481.1	1434
8	757.6	1471.1	830.7	1098.5	1008	80	1559.6	1589.3	805.8	1129.9	1378.6
9	1463	1101	700	766.4	815.5	81	1433.3	1098.8	1543.8	808.7	1373.3
10	1428.3	698	781	761.5	1441.9	82	1439.2	1415.8	791	753.9	1179.2
11	722.5	1597.2	780.3	1468	1566.3	83	1413.3	787.6	1386	1041	1558.3
12	1467.6	761.4	1033.2	1138.3	1139.5	84	1434.2	1044.6	1178.5	812.4	785.3
13	1098.3	803.9	785	1475.7	832.3	85	1440.9	794.7	1108.8	1179	817.2
14	1561.9	761.3	806.5	1596	697.9	86	1409.7	1350.2	759.3	736.9	1178.7
15	1097.4	815.1	1477.7	1488.4	1007.1	87	1444.8	819.3	1101.2	1363.7	1179.7
16	756.7	1411.8	787.7	810.7	1035.8	88	1346.1	1424.4	743	761.8	1570.4
17	1463.9	821.1	758	1590.3	1105.8	89	1430.2	791.7	1435.4	1368.6	778.8
18	758.9	1463.3	1100.9	1019	816.5	90	850.4	1416	819.7	1109.6	1389.7
19	754.9	1431.5	779.8	794.9	1444	91	1438.4	846.7	809.3	1107.8	1178.8
20	781.1	1451.8	1398.6	1561.2	702	92	1475.1	1101	1036.1	832.6	1390.4
21	1444.5	1450.1	700	1364.9	837.2	93	1395	741.5	678.2	1044.2	1166.2
22	1094.9	1452.4	804.2	785.9	1494.2	94	1408.9	794.3	1436.2	1385.8	780.7
23	1414.1	699.4	766.2	1554.3	1121	95	816.2	1033.6	1180.8	1436.6	1098.9
24	1433.9	1181.3	698.5	1385.9	763.5	96	1429.6	796.8	1437.3	1179.6	812.2
25	1463.3	1109.2	836.9	1604	787.6	97	1445.7	1417.9	789.2	1060.4	889.6
26	1458.7	1103.8	1032.2	1464.8	696.6	98	848.7	1431.2	1413.8	1547.3	785.6
27	786	1434.2	1444.3	695.3	1561.6	99	1456.6	1450.6	801	1098.2	1107.3
28	1469.1	1098.7	816.5	738.6	1006.7	100	800	1432.7	1580.1	1098.6	1547.2
29	1458.2	699.8	1092.7	1048.5	1447.1	101	1457.8	1101.2	1075.4	1144.2	1480.7
30	833.1	1544.7	1581.2	698.2	1371.1	102	1438.3	793.1	781	1096.8	1477.8
31	1460.6	1098.2	1499.6	1027	833.1	103	1439.8	851.8	1097.6	818.8	1371.2
32	787.7	1433.7	780.2	1440.1	1114.5	104	1436	1416	836.6	1579.4	795.3
33	1461.9	758.5	1136.4	1035.9	1041.3	105	1443.3	1136.5	1355.6	787.5	1036.2
34	757.4	1562.1	1590.9	809.2	1045.3	106	1412.5	1348.9	1400	698.4	789.3
35	1465.8	737.2	786.5	1138.4	1553.6	107	1480	1138.7	821.4	1415.9	1036.1
36	1561.4	1592.4	807.7	786.2	712	108	806.1	1567.2	1427.2	1357.9	1594.5
37	1466	1098	815.2	1015.2	1376.5	109	704	1343.4	1430.5	1415	824.4
38	1434.7	1546	761.3	1377.6	813.5	110	1435.9	1177.1	1037.4	813.8	1135.9
39	1097	1498.9	1559.2	804.5	827.9	111	1555	1414.6	1377.8	1568.1	809.5
40	1441.6	782.6	1407.2	1420.3	1041.5	112	719	1390.4	1063.6	1165.1	708.3
41	1444.1	1365.9	757	1436.3	1177.6	113	1568.4	814.3	1178.3	1377.5	701.9
42	837.2	1444.5	787	1452	1417.3	114	1413.9	1496.4	1346.7	738.4	1018.4
43	758.9	1412.7	1388.1	1123.5	1557.6	115	1342.6	1419.5	747	1097.6	821.6
44	1450.2	1033.5	1102	788.5	755.3	116	701.5	1351.2	1329.8	1386.4	1372.6
45	1434.7	757	1386.6	1177.6	1440.5	117	1495.6	1059.1	1385.8	677.8	1095.5
46	779.7	1435.5	1412.9	1563.6	811.7	118	1455.2	1094.3	1142.5	1051	824.7
47	1465.7	791.9	1107.4	1588.7	817.8	119	1431	853.4	1447.1	1579.3	1544.9
48	1456.9	1075	760.1	1347.5	735.8	120	1470.3	1565.4	808.9	1430.4	1569.8
49	1459.9	1100.1	1106.7	843.7	1018.3	121	854.7	1596	1564.9	801.3	1372.5
50	757.8	1546.9	1429.9	1582.5	1373.7	122	1430.5	785.9	1544.7	1164.7	817.3
51	1435.5	790.4	820.2	1107.2	780.3	123	1431.3	810.5	1365.7	1483	1110.7
52	1463.5	1102.2	817.9	1456.6	1026.9	124	1433.8	1544.1	817.6	814.3	1102.3
53	1434.4	1444.2	793.7	1099.4	780.5	125	1419.8	790.1	1434.6	817.9	1547.2
54	798.5	1434.2	777.6	1564.3	1084.2	126	1432.6	811.9	1033.8	1144.7	1359.7
55	1446.5	1359.3	789.5	743	1178.3	127	1545.8	808.1	1420.9	1586.1	1416.2
56	1449.3	1036.2	787.1	1136.3	752.2	128	1434.3	1184.9	796.9	1356	817.5
57	1555.3	1414.4	1576.8	1125.9	697	129	1410.5	1348.3	1420	788.6	735.6
58	785.2	1560.1	1387.6	1570.4	1585.3	130	1413	818.1	1390.4	1460.3	1361.9
59	1434.1	1442.7	786.6	709.5	812.6	131	1412.3	1345.9	1425.4	740.1	788.9
60	1447.2	1093.1	816.1	836.2	1363.4	132	1431.8	1181.1	811.7	1365.5	875.9
61	1414.9	1350.4	708.4	766.5	824.5	133	1557.2	1125.9	835.2	1378.2	869
62	1422.8	1345.5	697.9	819.8	770.4	134	735.9	1397	1071.1	1049.4	1167
63	1495.2	1121	830.1	1416.2	1040.2	135	1043.7	1417.2	1181.1	812.3	1369.9
64	1437.1	787.7	1498	1094.7	1181.4	136	1179.4	1430.4	813.5	1049.3	1407.2
65	700.3	1392	1062.8	680.9	1380.2	137	1413.5	1350.8	789.8	1106.6	821.4
66	1463.4	817.9	1107.9	1036.1	777.7	138	1440.9	805.7	1368.1	1054	1180.2
67	1459.1	1453.6	886.5	697.2	789.6	139	1424.4	801.7	1346.6	1108.7	819.6
68	847.5	805.7	1482.6	1569.2	1597	140	1426.5	804.4	859.3	1366.3	1576.3
69	845.3	1446.8	1580.7	1372.1	787.7	141	1421	1348.4	1099.7	1474.6	819.1
70	1460.4	1033.8	1139.8	1105.2	824.2	142	1353.4	742	1329.2	1387.6	690.9
71	789.7	1439.5	1435	781.1	1136.2	143	1404.9	1349	798.3	1436.5	1565
72	1558.3	808.5	1487.9	1104	1569.9	144	1344.6	1433.5	1428.2	1099.1	818
						145	1409.5	1346.6	780.5	796	1572

Table VI. Selected Matrix Isolated FT/IR absorption bands for all 209 PCB congeners (con't)

Congener No.	Absorption Band Intensity Strong → Weak					Congener No.	Absorption Band Intensity Strong → Weak				
146	1470.6	1416.8	1079.3	1146	1389	178	1393.9	1358.8	1095.2	1048.1	1401
147	1400.1	848.2	1482.5	1386.1	1167	179	1062.6	1399.2	813.2	1410.7	1348.4
148	1409.8	857.6	1588.4	1126.7	1371.9	180	1413	1469.7	1353.2	847.2	1066.5
149	1436	1475.5	1181	1049.4	1392.9	181	1330.3	1390.9	803.9	1352.2	1368.6
150	854.3	1430.9	819.1	1549.1	1374.3	182	1406.5	1349.7	800.7	1548.8	1587.2
151	1393.9	1099	1409.5	1045.7	1087.4	183	1424.2	1133.8	1095.6	1350	1357.5
152	1397.6	782	675.6	1436	797.4	184	1413.5	813	1346.9	1569.6	1373.9
153	1449	1455.1	1087.1	1148.2	1048.9	185	1353.6	1330.6	1361.1	1408.6	1098.8
154	1434	818.9	1105.5	1578.6	1083.8	186	1353.8	1363.3	782.4	1328.5	1437.6
155	1577.9	817.1	1419.1	1550	859.3	187	1398.2	1468.4	1389.1	1167.7	908.7
156	1413	1136.5	1343.6	1036.5	773	188	1400.1	859.8	1587.8	1369	672.2
157	1426.7	810.1	1353.9	1167.5	789.4	189	1406.6	817.6	1339.8	771.6	840.3
158	1414.5	1343.5	820.1	1132.2	1037.6	190	1329.8	731.2	1368.4	1350.6	1387.9
159	1404.2	1342.7	809.9	1569.5	1595.2	191	1415	1341.1	1405.7	817.6	1547.8
160	722.1	1328.2	1349.6	1381.7	1366.7	192	1365.7	1327.1	1350	728.1	1569.3
161	1409.5	1567	1341.1	810.1	1595.8	193	1373.2	1167.5	724.2	1401.5	819
162	816.1	1546.2	1413.9	1391.9	1367.7	194	1403.1	1349.9	1181.8	1342	852.3
163	1400.5	1383.9	729.8	1066.6	1479.6	195	1372.9	1328.3	1350.8	806.4	1368
164	1425.9	818.9	1180.2	808.6	1371	196	1402.4	1341.6	1350.8	802.8	1335.7
165	1078.5	724.6	1385.1	1569	812	197	1403.4	814	1564.4	1356.8	1336.2
166	1329.3	1379.4	1353.2	751.4	737.4	198	1360.8	1353.8	1331.1	1401.3	749
167	1431	1066	1471.2	813.3	1553	199	1353.6	1329.2	1411.6	1181.7	1073.9
168	1420.5	1552.1	1367.4	862.3	822.3	200	1403.8	1338	1368.3	685.3	1169
169	1423.1	1538.1	808	1357.3	1529.8	201	1403.3	1338.3	1377.3	1169	745.6
170	1409.5	1181	794.4	1348.4	666.3	202	1406.4	1331.3	1073.6	1169	760.6
171	1419.8	1347	806.2	1177.8	818.3	203	1356.1	1329.6	1333.9	1383.4	1393.5
172	1346	1409.6	1382.6	841	1558.4	204	1365.7	817.8	1353.2	1331.1	1550.1
173	1352.6	737.2	1328	1384.7	1372.7	205	1370	1327.5	1383.9	1327.5	727.3
174	1418.1	1182.4	814.6	1345.5	1380.7	206	1378.4	1354.6	1331.3	1341.5	805.6
175	1407.8	1343	1389.2	823.7	1124.8	207	1374.4	1338	1357.9	818.5	693.6
176	1423.8	1343	1180.6	898.5	813.8	208	1343	1338.9	1409.3	1082.4	691.3
177	1401.7	1378.9	1367	686.7	1166.5	209	1345.5	1328.3	829.4	696.9	760.8

Table VII. Melting points for all crystalline PCB congeners

Cong. No.	Structure	CAS No.	Melting Point °C (Corrected)	Melting Point °C Literature
1	2-Chlorobiphenyl	2051-60-7	30 - 31.5	34 [1], 33 - 34 [31]
2	3-Chlorobiphenyl	2051-61-8	oil	oil [1], 16 - 17 [31]
3	4-Chlorobiphenyl	2051-62-9	76 - 78	77.7 [1], 77 - 78 [31]
4	2,2'-Dichlorobiphenyl	13029-08-8	60 - 61	60.5 [1], 59 - 60 [31]
5	2,3-Dichlorobiphenyl	16605-91-7	oil	27.7 - 28.2 [33]
6	2,3'-Dichlorobiphenyl	25569-80-6	oil	oil [1]
7	2,4-Dichlorobiphenyl	33284-50-3	oil	24.1 - 24.4[33], 24 - 25 [31]
8	2,4'-Dichlorobiphenyl	34883-43-7	44 - 45	46 [1]
9	2,5-Dichlorobiphenyl	34883-39-1	oil	22 - 23 [35]
10	2,6-Dichlorobiphenyl	33146-45-1	35 - 36	35 - 36 [1]
11	3,3'-Dichlorobiphenyl	2050-67-1	29 - 30	29 [1]
12	3,4-Dichlorobiphenyl	2974-92-7	48 - 50	49 - 50 [1], 48 - 49 [33]
13	3,4'-Dichlorobiphenyl	2974-90-5	oil	oil [1]
14	3,5-Dichlorobiphenyl	34883-41-5	32 - 33	36 [1], 31 - 32 [33]
15	4,4'-Dichlorobiphenyl	2050-68-2	150 - 152	149 - 150 [1]
16	2,2',3-Trichlorobiphenyl	38444-78-9	oil	28.1 - 28.8 [33]
17	2,2',4-Trichlorobiphenyl	37680-66-3	oil	
18	2,2',5-Trichlorobiphenyl	37680-65-2	44 - 46	
19	2,2',6-Trichlorobiphenyl	38444-73-4	90 - 92	
20	2,3,3'-Trichlorobiphenyl	38444-84-7	43 - 44.5	
21	2,3,4-Trichlorobiphenyl	55702-46-0	102 - 103	
22	2,3,4'-Trichlorobiphenyl	38444-85-8	72 - 73	73 - 73.2 [33]
23	2,3,5-Trichlorobiphenyl	55720-44-0	39 - 40	41 [1]
24	2,3,6-Trichlorobiphenyl	58702-45-9	56 - 57	
25	2,3',4-Trichlorobiphenyl	55712-37-3	36 - 37	
26	2,3',5-Trichlorobiphenyl	38444-81-4	42 - 43	
27	2,3',6-Trichlorobiphenyl	38444-76-7	oil	
28	2,4,4'-Trichlorobiphenyl	7012-37-5	58 - 59	57 - 58 [1]
29	2,4,5-Trichlorobiphenyl	15862-07-4	77 - 78	78 - 79 [1]
30	2,4,6-Trichlorobiphenyl	35693-92-6	62 - 63	62.5 - 64.5 [1]
31	2,4',5-Trichlorobiphenyl	16606-02-3	64.5 - 65	63.5 - 64.5 [1]
32	2,4',6-Trichlorobiphenyl	38444-77-4	55 - 56	
33	2',3,4-Trichlorobiphenyl	38444-86-9	61 - 62	60.1 - 60.4 [33]
34	2',3,5-Trichlorobiphenyl	37680-68-5	57 - 58	58 [1]
35	3,3',4-Trichlorobiphenyl	37680-69-6	65.5 - 67	

Table VII. Melting points for all crystalline PCB congeners (con't)

Cong. No.	Structure	CAS No.	Melting Point °C (Corrected)	Melting Point °C Literature
36	3,3',5-Trichlorobiphenyl	38444-87-0	78 - 79	
37	3,4,4'-Trichlorobiphenyl	38444-90-5	88 - 90	86.8 - 87.8 [33]
38	3,4,5-Trichlorobiphenyl	53555-66-1	71 - 71.5	
39	3,4',5-Trichlorobiphenyl	38444-88-1	87 - 88	88 [1]
40	2,2',3,3'-Tetrachlorobiphenyl	38444-93-8	123 - 124	121 - 122[27]
41	2,2',3,4-Tetrachlorobiphenyl	52663-59-9	48 - 50	
42	2,2',3,4'-Tetrachlorobiphenyl	36559-22-5	68 - 69	68 - 70 [1], 68.5 70 [2]
43	2,2',3,5-Tetrachlorobiphenyl	70362-46-8	45 - 46	
44	2,2',3,5'-Tetrachlorobiphenyl	41464-39-5	47.5 - 48.5	49 - 50 [28]
45	2,2',3,6-Tetrachlorobiphenyl	70362-45-7	80 - 81	
46	2,2',3,6'-Tetrachlorobiphenyl	41464-47-5	125 - 126	125.5 - 127 [28]
47	2,2',4,4'-Tetrachlorobiphenyl	2437-79-8	45.5 - 46	41 - 42 [1]
48	2,2',4,5-Tetrachlorobiphenyl	70362-47-9	86 - 87	
49	2,2',4,5'-Tetrachlorobiphenyl	41464-40-8	66 - 67	66 - 68.5 [1], 65 - 66.5 [26]
50	2,2',4,6-Tetrachlorobiphenyl	62796-65-8	47 - 48	
51	2,2',4,6'-Tetrachlorobiphenyl	68194-04-7	oil	
52	2,2',5,5'-Tetrachlorobiphenyl	35693-99-3	85.5 - 86.5	86.5 - 87 [1], 85 - 86.5 [26]
53	2,2',5,6'-Tetrachlorobiphenyl	41464-41-9	101 - 103	103 - 104.5 [28]
54	2,2',6,6'-Tetrachlorobiphenyl	15968-05-5	197 -198	198 [1]
55	2,3,3',4-Tetrachlorobiphenyl	74338-24-2	85.5 - 86.5	
56	2,3,3',4'-Tetrachlorobiphenyl	41464-43-1	98 - 99	96 - 97 [28]
57	2,3,3',5-Tetrachlorobiphenyl	70424-67-8	87 - 88	
58	2,3,3',5'-Tetrachlorobiphenyl	41464-49-7	125 - 126	127.5 - 129 [28]
59	2,3,3',6-Tetrachlorobiphenyl	74472-33-6	oil	
60	2,3,4,4'-Tetrachlorobiphenyl	33025-41-1	144.5 - 146.5	142 [1]
61	2,3,4,5-Tetrachlorobiphenyl	33284-53-6	85.5 - 90.5	92 - 92.5 [1], 91 [5]
62	2,3,4,6-Tetrachlorobiphenyl	54230-23-7	78 - 79	
63	2,3,4',5-Tetrachlorobiphenyl	74472-34-7	88 - 90	
64	2,3,4',6-Tetrachlorobiphenyl	52663-58-8	87 - 88	
65	2,3,5,6-Tetrachlorobiphenyl	33284-54-7	76 - 78.5	79 [1]
66	2,3',4,4'-Tetrachlorobiphenyl	32598-10-0	124 - 126	124 [1], 127 - 128 [2]
67	2,3',4,5-Tetrachlorobiphenyl	73557-53-8	62 - 63.5	
68	2,3',4,5'-Tetrachlorobiphenyl	73575-52-7	92 - 93	
69	2,3',4,6-Tetrachlorobiphenyl	60233-24-1	52 - 54	
70	2,3',4',5-Tetrachlorobiphenyl	32598-11-1	104 - 105	104 [1], 104 - 105 [2]
71	2,3',4',6-Tetrachlorobiphenyl	41464-46-4	36 - 37	oil [28]
72	2,3',5,5'-Tetrachlorobiphenyl	41464-42-0	106 - 107.5	105.5 - 106.5 [28]
73	2,3',5',6-Tetrachlorobiphenyl	74338-23-1	70 - 72	
74	2,4,4',5-Tetrachlorobiphenyl	32690-93-0	127 - 129	125 [1]
75	2,4,4',6-Tetrachlorobiphenyl	32598-12-2	62 - 63	
76	2',3,4,5-Tetrachlorobiphenyl	70362-48-0	134 - 135	
77	3,3',4,4'-Tetrachlorobiphenyl	32598-13-3	180 - 181	177 - 178 [28]
78	3,3',4,5-Tetrachlorobiphenyl	70362-49-1	118 - 120	
79	3,3',4,5'-Tetrachlorobiphenyl	41464-48-6	121 - 123	119 - 120 [28]
80	3,3',5,5'-Tetrachlorobiphenyl	33284-52-5	171 - 173	164 [1]
81	3,4,4',5-Tetrachlorobiphenyl	70362-50-4	160 - 163	
82	2,2',3,3',4-Pentachlorobiphenyl	52663-62-4	118 - 120	119 - 120.5 [1]
83	2,2',3,3',5-Pentachlorobiphenyl	60145-20-2	83 - 84	
84	2,2',3,3',6-Pentachlorobiphenyl	52663-60-2	109 - 110	
85	2,2',3,4,4'-Pentachlorobiphenyl	65510-45-4	47.5 - 48.5	
86	2,2',3,4,5-Pentachlorobiphenyl	55312-69-1	85 - 86	
87	2,2',3,4,5'-Pentachlorobiphenyl	38380-02-8	110 - 112	112 - 114 [1]
88	2,2',3,4,6-Pentachlorobiphenyl	55215-17-3	66 - 66.5	
89	2,2',3,4,6'-Pentachlorobiphenyl	73575-57-2	85 - 86	
90	2,2',3,4',5-Pentachlorobiphenyl	68194-07-0	51 - 53	
91	2,2',3,4',6-Pentachlorobiphenyl	68194-05-8	62 - 63	
92	2,2',3,5,5'-Pentachlorobiphenyl	52663-61-3	60 - 61	oil [1]
93	2,2',3,5,6-Pentachlorobiphenyl	73575-56-1	96 - 97.5	
94	2,2',3,5,6'-Pentachlorobiphenyl	73575-55-0	82 - 83	
95	2,2',3,5',6-Pentachlorobiphenyl	38379-99-6	93 - 94	98.5 - 100 [1]
96	2,2',3,6,6'-Pentachlorobiphenyl	73575-54-9	119 - 120	
97	2,2',3',4,5-Pentachlorobiphenyl	41464-51-1	78 - 79	87.5 - 82.5[28]
98	2,2',3',4,6-Pentachlorobiphenyl	60233-25-2	94 - 95	
99	2,2',4,4',5-Pentachlorobiphenyl	38380-01-1	59 - 60	
100	2,2',4,4',6-Pentachlorobiphenyl	39485-83-1	oil	
101	2,2',4,5,5'-Pentachlorobiphenyl	37680-73-2	78 - 79	76 - 77 [28]
102	2,2',4,5,6'-Pentachlorobiphenyl	68194-06-9	71 - 72	
103	2,2',4,5',6-Pentachlorobiphenyl	60145-21-3	69 - 70	
104	2,2',4,6,6'-Pentachlorobiphenyl	56558-16-8	87 - 88	
105	2,3,3',4,4'-Pentachlorobiphenyl	32598-14-4	116.5 - 117.5	117 - 118.5 [28], 101 - 105 [1]
106	2,3,3',4,5-Pentachlorobiphenyl	70424-69-0	85 - 86	
107	2,3,3',4',5-Pentachlorobiphenyl	70424-68-9	96 - 97	
108	2,3,3',4,5'-Pentachlorobiphenyl	70362-41-3	120 - 122	121 - 122 [34]
109	2,3,3',4,6-Pentachlorobiphenyl	74472-35-8	70 - 71	

Table VII. Melting points for all crystalline PCB congeners (con't)

Cong. No.	Structure	CAS No.	Melting Point °C (Corrected)	Melting Point °C Literature
110	2,3,3',4',6-Pentachlorobiphenyl	38380-03-9	53 - 55	oil [1]
111	2,3,3',5,5'-Pentachlorobiphenyl	39635-32-0	107 - 107.5	105 [30]
112	2,3,3',5,6-Pentachlorobiphenyl	74472-36-9	91-93	
113	2,3,3',5',6-Pentachlorobiphenyl	68194-10-5	56 - 57	
114	2,3,4,4',5-Pentachlorobiphenyl	74472-37-0	98 - 99	98 - 99 [1]
115	2,3,4,4',6-Pentachlorobiphenyl	74472-38-1	64.5 - 65	
116	2,3,4,5,6-Pentachlorobiphenyl	18259-05-7	122 - 125	123 [1], 124 - 125 [32]
117	2,3,4',5,6-Pentachlorobiphenyl	68194-11-6	167 - 171	
118	2,3',4,4',5-Pentachlorobiphenyl	31508-00-6	111 - 113	112 - 113 [28]
119	2,3',4,4',6-Pentachlorobiphenyl	56558-17-9	75 - 77	
120	2,3',4,5,5'-Pentachlorobiphenyl	68194-12-7	131 - 133	
121	2,3',4,5',6-Pentachlorobiphenyl	56558-18-0	93 - 94.5	
122	2',3,3',4,5-Pentachlorobiphenyl	76842-07-4	117 - 118	
123	2',3,4,4',5-Pentachlorobiphenyl	65510-44-3	134 - 135	
124	2',3,4,5,5'-Pentachlorobiphenyl	70424-70-3	116 - 117	
125	2',3,4,5,6'-Pentachlorobiphenyl	74472-39-2	126 - 127	
126	3,3',4,4',5-Pentachlorobiphenyl	57465-28-8	160 - 161	
127	3,3',4,5,5'-Pentachlorobiphenyl	39635-33-1	152 - 153	
128	2,2',3,3',4,4'-Hexachlorobiphenyl	38380-07-3	150 - 152	
129	2,2',3,3',4,5-Hexachlorobiphenyl	55215-18-4	102 - 104	
130	2,2',3,3',4,5'-Hexachlorobiphenyl	52663-66-8	114 - 116	
131	2,2',3,3',4,6-Hexachlorobiphenyl	61798-70-7	135 - 137	
132	2,2',3,3',4,6'-Hexachlorobiphenyl	38380-05-1	116 - 118	
133	2,2',3,3',5,5'-Hexachlorobiphenyl	35694-04-3	127 - 128	128 - 129 [1]
134	2,2',3,3',5,6-Hexachlorobiphenyl	52704-70-8	132 - 133	
135	2,2',3,3',5,6'-Hexachlorobiphenyl	52744-13-5	102 - 103	
136	2,2',3,3',6,6'-Hexachlorobiphenyl	38411-22-2	112 - 113.5	114 - 114.5 [1]
137	2,2',3,4,4',5-Hexachlorobiphenyl	35694-06-5	81 - 82	77 - 78 [1], 78.5 - 80 [30]
138	2,2',3,4,4',5'-Hexachlorobiphenyl	35065-28-2	79 - 80	78.5 - 80 [1]
139	2,2',3,4,4',6-Hexachlorobiphenyl	56030-56-9	75.5 - 77	
140	2,2',3,4,4',6'-Hexachlorobiphenyl	59291-64-4	68 - 69	69.5 - 71 [1]
141	2,2',3,4,5,5'-Hexachlorobiphenyl	52712-04-6	88 - 89	
142	2,2',3,4,5,6-Hexachlorobiphenyl	41411-61-4	134 - 135	134 - 137
143	2,2',3,4,5,6'-Hexachlorobiphenyl	68194-15-0	89 - 90	
144	2,2',3,4,5',6-Hexachlorobiphenyl	68194-14-9	72 - 74	
145	2,2',3,4,6,6'-Hexachlorobiphenyl	74472-40-5	136 - 137	
146	2,2',3,4',5,5'-Hexachlorobiphenyl	51908-16-8	88 - 90	
147	2,2',3,4',5,6-Hexachlorobiphenyl	68194-13-8	136 - 138	
148	2,2',3,4',5,6'-Hexachlorobiphenyl	74472-41-6	80.5 - 81	
149	2,2',3,4',5',6-Hexachlorobiphenyl	38380-04-0	78 - 79	oil
150	2,2',3,4',6,6'-Hexachlorobiphenyl	68194-08-1	76 - 77	
151	2,2',3,5,5',6-Hexachlorobiphenyl	52663-63-5	98 - 100	
152	2,2',3,5,6,6'-Hexachlorobiphenyl	68194-09-2	126 - 127	
153	2,2',4,4',5,5'-Hexachlorobiphenyl	35065-27-1	102 - 103.5	103 - 104 [1]
154	2,2',4,4',5,6'-Hexachlorobiphenyl	60145-22-4	68 - 70	
155	2,2',4,4',6,6'-Hexachlorobiphenyl	33979-03-2	111 - 113	112.5 [1], 112 - 113 [31]
156	2,3,3',4,4',5-Hexachlorobiphenyl	38380-08-4	129.5 - 131	
157	2,3,3',4,4',5'-Hexachlorobiphenyl	69782-90-7	161 - 162	
158	2,3,3',4,4',6-Hexachlorobiphenyl	74472-42-7	110 - 112	
159	2,3,3',4,5,5'-Hexachlorobiphenyl	39635-35-3	149 - 150	
160	2,3,3',4,5,6-Hexachlorobiphenyl	41411-62-5	92 - 92.5	97 -100 [1]
161	2,3,3',4,5',6-Hexachlorobiphenyl	74474-43-8	105 - 106	
162	2,3,3',4',5,5'-Hexachlorobiphenyl	39635-34-2	143 - 144	
163	2,3,3',4',5,6-Hexachlorobiphenyl	74472-44-9	121 - 123	
164	2,3,3',4',5',6-Hexachlorobiphenyl	74472-45-0	92 - 94	
165	2,3,3',5,5',6-Hexachlorobiphenyl	74472-46-1	151 - 152	
166	2,3,4,4',5,6-Hexachlorobiphenyl	41411-63-6	164 - 167	160 - 165 [32]
167	2,3',4,4',5,5'-Hexachlorobiphenyl	52663-72-6	125 - 127	
168	2,3',4,4',5',6-Hexachlorobiphenyl	59291-65-5	108.5 - 109.5	110 - 111 [1]
169	3,3',4,4',5,5'-Hexachlorobiphenyl	32774-16-6	208 - 210	201 - 202 [1]
170	2,2',3,3',4,4',5-Heptachlorobiphenyl	35065-30-6	136.5 - 138.5	134.5 - 135.5 [1]
171	2,2',3,3',4,4',6-Heptachlorobiphenyl	52663-71-5	116.5 - 118.5	
172	2,2',3,3',4,5,5'-Heptachlorobiphenyl	52663-74-8	135 - 137	
173	2,2',3,3',4,5,6-Heptachlorobiphenyl	68194-16-1	204 - 205	
174	2,2',3,3',4,5,6'-Heptachlorobiphenyl	38411-25-5	124 - 125	130.5 - 130.7 [1]
175	2,2',3,3',4,5',6-Heptachlorobiphenyl	40186-70-7	121 - 123	
176	2,2',3,3',4,6,6'-Heptachlorobiphenyl	52663-65-7	102 - 103	
177	2,2',3,3',4',5,6-Heptachlorobiphenyl	52663-70-4	152 - 154	
178	2,2',3,3',5,5',6-Heptachlorobiphenyl	52663-67-9	110 - 112	
179	2,2',3,3',5,6,6'-Heptachlorobiphenyl	35065-29-3	129 - 131	
180	2,2',3,4,4',5,5'-Heptachlorobiphenyl	35065-29-3	112.5 - 114	109 - 110 [1]
181	2,2',3,4,4',5,6-Heptachlorobiphenyl	74472-47-2	125 - 126	
182	2,2',3,4,4',5,6'-Heptachlorobiphenyl	60145-23-5	107.5 - 109.5	
183	2,2',3,4,4',5',6-Heptachlorobiphenyl	52663-69-1	93 - 95	

Table VII. Melting points for all crystalline PCB congeners (con't)

Cong. No.	Structure	CAS No.	Melting Point °C (Corrected)	Melting Point °C Literature
184	2,2',3,4,4',6,6'-Heptachlorobiphenyl	74472-48-3	115 - 117	
185	2,2',3,4,5,5',6-Heptachlorobiphenyl	52712-05-7	148 - 150	
186	2,2',3,4,5,6,6'-Heptachlorobiphenyl	74472-49-4	195 - 198	
187	2,2',3,4',5,5',6-Heptachlorobiphenyl	52663-68-0	104 - 105	
188	2,2',3,4',5,6,6'-Heptachlorobiphenyl	74487-85-7	134 - 135	
189	2,3,3',4,4',5,5'-Heptachlorobiphenyl	39635-31-9	162 - 163	
190	2,3,3',4,4',5,6-Heptachlorobiphenyl	41411-64-7	122 - 124	116 - 118 [32]
191	2,3,3',4,4',5',6-Heptachlorobiphenyl	74472-50-7	112.5 - 114.5	
192	2,3,3',4,5,5',6-Heptachlorobiphenyl	74472-51-8	171 - 174	
193	2,3,3',4',5,5',6-Heptachlorobiphenyl	69782-91-8	138 - 141	
194	2,2',3,3',4,4',5,5'-Octachlorobiphenyl	35694-08-7	155 - 157	156 - 157 [1], 159 - 160 [1]
195	2,2',3,3',4,4',5,6-Octachlorobiphenyl	52663-78-2	170 - 172	
196	2,2',3,3',4,4',5',6-Octachlorobiphenyl	42740-50-1	127 - 129 [1]	126 - 128 [1]
197	2,2',3,3',4,4',6,6'-Octachlorobiphenyl	33091-17-7	137 - 139	132 [1]
198	2,2',3,3',4,5,5',6-Octachlorobiphenyl	68194-17-2	195 - 197	
199 (IUPAC #200)	2,2',3,3',4,5,6,6'-Octachlorobiphenyl	52663-73-7	175 - 176	
200 (IUPAC #201)	2,2',3,3',4,5',6,6'-Octachlorobiphenyl	40186-71-8	141 - 143	
201 (IUPAC #199)	2,2',3,3',4,5,5',6'-Octachlorobiphenyl	52663-75-9	157 - 158	
202	2,2',3,3',5,5',6,6'-Octachlorobiphenyl	2136-99-4	157 - 159	161 [1]
203	2,2',3,4,4',5,5',6-Octachlorobiphenyl	52663-76-0	111 - 113	
204	2,2',3,4,4',5,6,6'-Octachlorobiphenyl	74472-52-9	175 - 179	
205	2,3,3',4,4',5,5',6-Octachlorobiphenyl	74472-53-0	197 - 199	
206	2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl	40186-72-9	202 - 204	
207	2,2',3,3',4,4',5,6,6'-Nonachlorobiphenyl	52663-79-3	213 - 215	
208	2,2',3,3',4,5,5',6,6'-Nonachlorobiphenyl	52663-77-1	180 - 181	
209	2,2',3,3',4,4',5,5',6,6'-Decachlorobiphenyl	2051-24-3	318 - 320	305.6, 310 [1]

CONCLUSIONS:

The synthesis and the subsequent compilation of chromatographic, spectral and physical data of all 209 PCB congeners will provide a means for the more accurate identification of biologically active and toxic congeners. In addition to improving the qualitative aspect of PCB analysis, this data will also aid in the quantification of these compounds.

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