

Review of Polychlorinated Biphenyl Congener Monitoring Methods

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Technical Update, October 2006

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ABSTRACT

A recent review of the trends in measurement, regulation, and use of PCB congener data by showed that the majority of PCB analyses conducted on environmental samples are still reported as total PCBs or as Aroclors using EPA Method 8082 or equivalent. However, increasingly, congener-specific analyses are being used for risk assessment, some NPDES permit monitoring, and for environmental forensic analyses. This technical update presents an overview of the current state of the art in PCB analysis, particularly for determining individual PCB congeners in environmental samples. Also, the relationship between the analytical capabilities of the methods and the objectives of the study are discussed.

There is still no single routine method for the analysis of all 209 PCB congeners. The commonly available analytical methods for PCB congener analysis remain EPA Method 8082, EPA Method 680, and EPA Method 1668A. For very low-concentration samples and complex matrices, EPA Method 1668A is the preferred method of analysis though it is substantially more expensive than other methods. Methods 8082 and 680, or their equivalents, are less expensive options and frequently can meet project-specific data quality objectives when conducted by an experienced laboratory.

CONTENTS

1 BACKGROUND	1-1
Scope and Objectives	1-1
Summary of PCB Chemistry and Production	1-1
Congeners	1-2
Applications of Congener-Specific PCB Analysis	1-4
2 MEASUREMENT OF PCBS AND PCB CONGENERS	2-1
Overview	2-1
Detailed Descriptions of PCB Congener Analytical Methods	2-2
GC/ECD	2-2
GC/LRMS	2-5
GC/HRMS	2-5
Other PCB Congener Methods	2-6
GC/TOFMS	2-6
GC x GC	2-6
<i>3</i> SUMMARY	3-1
Planning a PCB Congener Analysis Program	3-2
4 REFERENCES	4-1
A CAS NUMBERS FOR PCB AROCLORS AND HOMOLOGS	A-1
B IUPAC NUMBERS AND CAS NUMBERS OF ALL PCB CONGENERS	B-1

1 BACKGROUND

Scope and Objectives

EPRI and others have investigated sampling and analytical methods for polychlorinated biphenyl (PCB) congeners. Recognizing that none of the studies was comprehensive, and that sampling and analytical methods develop over time, a review of the state-of-the-art in congener-specific sampling and analysis for PCBs was conducted. This technical update summarizes the state-of-the-art in congener-specific monitoring.

An earlier report by EPRI, titled "Congeners-Specific Measurement and Leaching of PCBs," discussed the measurement issues associated with PCB congeners (EPRI 2002). Since the time of that report, some incremental improvements in congener methods and analytical equipment have been reported; however, the basic methodology being used has changed little. This technical update expands on the earlier discussions regarding the current state of the art in PCB analysis, the quality control issues, and the appropriate applications for each method. Also, the relationship between analytical capabilities and trends in congener usage are discussed.

The basis of this report was a review of recent literature on PCB congener analysis methods. The objective of this study was to elucidate PCB congener-specific measurement issues and trends.

Summary of PCB Chemistry and Production

PCBs are members of a family of man-made chemicals with a unique set of physical and chemical properties. Because of those properties, PCBs were used in a large number of industrial, commercial and consumer products until commercial production of PCBs stopped in the 1970s. PCB issues remain an important concern of utility companies because of their widespread use in electrical equipment, their resistance to decomposition in the environment, their potential toxicity, and the extensive regulations governing their production, use and disposal (EPRI 1999, EPRI 2000).

PCBs were produced commercially in the United States by the Monsanto Corporation for about 50 years between the late 1920s and the 1970s and sold as mixtures under the registered trade name of **Aroclor**®. Aroclors are made up of individual PCB compounds, of which there are 209 (referred to as congeners). Each PCB Aroclor mixture was made using specific combinations of some of the 209 PCB congeners and had a four-number code to identify it from the other PCB Aroclors. The first two numbers of the four-number Aroclor codes started with 12 (meaning that it was a PCB mixture) and ended with two numbers which identified the amount of chlorine in the overall mixture. For example, Aroclor 1242 indicated a mixture of PCBs that had 42% chlorine by weight. Table 1-1 provides some basic PCB terms and definitions.

Term	Definition
Total PCBs	The sum of all PCB compounds (congeners) in a sample
Aroclor	Trade name (Monsanto) for a series of commercial PCB mixtures marketed in the United States
Askarel	A non-flammable, chlorinated dielectric fluid
Congener	One of 209 PCB compounds
Homolog	One of the 10 degrees of chlorination of PCBs (e.g. monochloro biphenyls are all PCB congeners with one chlorine atom attached)

Table 1-1PCB Terms and Definitions

In the early 1970s, Monsanto started producing one additional PCB mixture, named Aroclor 1016, which did not use the same code as the other PCB Aroclors. This Aroclor mixture was made from PCBs and contained about 41 to 42% chlorine, similar to the chlorine content of Aroclor 1242. However, the combination of individual PCBs in Aroclor 1016 was different from that used in Aroclor 1242 (Erickson, 1997).

Congeners

As stated above, PCB Aroclors are made up of individual chlorinated biphenyl molecules called congeners. The biphenyl backbone consists of two benzene rings connected with a single bond. Each individual PCB congener is named by using the numbers identifying the positions of the attached chlorine atoms followed by the level of chlorination (**Error! Reference source not found.**). By specifying both the numbers and locations of the chlorine atoms attached to the biphenyl molecule in this consistent manner, all 209 individual PCB compounds can be uniquely identified.

All PCB congeners have the same basic chemical structure, but the locations and amounts of attached chlorine atoms are different, as shown in **Error! Reference source not found.** PCB congeners are separated into 10 groups (referred to as **homologs**), with each group composed of PCB congeners having the same number of attached chlorine atoms. For example, all PCB congeners containing two attached chlorine atoms are dichlorobiphenyl homologs. A list of names and Chemical Abstracts Service (CAS) numbers for PCB Aroclors and PCB homologs is provided in Appendix A. A list of International Union of Pure and Applied Chemistry (IUPAC) numbers and CAS numbers for all 209 PCB congeners is provided in Appendix B.

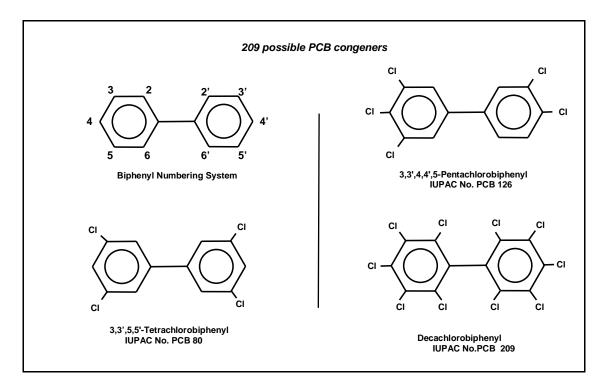


Figure 1-1 PCB Congener Structure and IUPAC Naming Conventions

PCB congeners differ in physical and chemical properties as well as toxicity. Therefore, evaluation of PCB transport, fate, risk, and some remediation alternatives has required the increased use of PCB congener assessment. In addition, analysis of PCB congeners is becoming a more common request of regulatory agencies for monitoring programs including total maximum daily loads (TMDL) and as part of National Pollutant Discharge Elimination System (NPDES) monitoring programs. Until recently the analysis of PCBs in environmental samples has been most commonly performed by identifying PCBs and determining their concentrations by comparison to Aroclor standard materials. Analysis for congeners has been performed on a much less frequent and project specific basis.

The identification and quantification of specific PCB compounds can be critical, particularly with respect to potential toxicity of PCB-contaminated media. As shown in Table 1-2, the congeners most abundant in Aroclors and in the environment, as well as the congeners with the highest toxicity, are quite well known.

Table 1-2PCB Congeners of Concern

	Highest Toxicity and Abundance		Abundant in Aroclors (>4%)		Potential for Toxicity
77	87	4	99	18	37
128	99	8	101	44	81
169	101	18	110	49	114
105	153	28	118	52	119
118	180	31	138	70	123
128	183	42	149	74	157
138	194	52	153	151	158
156	-	53	180	177	167
170	_	70	185	187	168
_	_	91	-	199	189

Table 1-3 summarizes the relationship between PCB Aroclors and congeners.

Table 1-3Relationships between Congeners and Aroclors

Each Aroclor has a unique distribution of congeners	Not all congeners are present in each Aroclor; some are not present in any Aroclor
Different congeners have different human and ecological toxicities	Therefore, different Aroclors have different toxicities based on the amounts of toxic and non-toxic congeners in them
	Solubility, volatility, biodegradation depend on degree of chlorination and chemical structure
Congeners have different transport and fate properties	Therefore, different Aroclors behave differently in the environment

Applications of Congener-Specific PCB Analysis

A recent review of the trends in measurement, regulation, and usage of PCB congener data by EPRI showed that the majority of PCB analyses conducted on environmental samples are still reported as total PCBs or as Aroclors. This is because the PCB cleanup and disposal regulations require PCB data to be reported and evaluated in those units.

However, increasingly, congener-specific analyses are being used for risk assessment, especially for sediments and biota, and for ultra low level analysis of certain waste waters. In addition, congener-specific analysis increasingly is being used to try to identify the sources of PCBs in

complex matrices. There are several reasons for the expanded use of congener analysis as discussed in the next few paragraphs.

PCB cleanup criteria and risk factors generally are based on total PCBs or total Aroclor concentrations. Therefore, there is a driving force to produce accurate total PCBs or Aroclor concentrations. In practice, it can be difficult to produce accurate PCB results in complex matrices such as sediments, mixed wastes, and tissues using conventional EPA methods for a variety of reasons. For example, when multiple PCB Aroclors are present in a sample, the reported concentration of each Aroclor and the reported total PCB concentration is always an estimate because there are common PCB congeners in the various Aroclors. It is difficult to correct for mixture effects. Also, environmental weathering or selective absorption by organisms can alter the PCB Aroclor composition and thus bias the concentrations determined by multipeak calibrations. For these and other reasons, toxicologists and risk assessors believe that risk assessments and cleanup criteria based on individual compounds or the sum of individual compound concentrations is more reliable and accurate.

Because of requirements of the Clean Water Act, some NPDES permits have very low allowable discharge levels (in some cases no PCB discharge is allowed). To achieve these very low detection levels, EPA developed a complex analytical method (number 1668A) based on state of the art laboratory instrumentation. This method determines total PCBs in a water sample as the sum of congeners.

Much of the early work on the environmental transport and fate of PCBs was done with Aroclors, ignoring the changes in Aroclor composition that occur during dissolution, volatilization, degradation and other processes. Most of the recent study of the environmental chemistry of PCBs has focused on congener-specific transport and fate. The application of the more recent scientific data necessitates that site-specific data be congener-based so that it can be compared and evaluated relative to recent published information.

Similarly, the early work on the toxicity of PCBs was based on Aroclor type and concentrations. Much recent work has focused on the health and ecological effects of individual congeners. Therefore, site-specific data must include congener concentrations so that risk calculations based on congeners can be conducted.

Finally, some environmental forensic chemists have used small differences in congener patterns to separate impacts from two or more releases of the same PCB Aroclor. This might be used for allocating liability among PCB sources or for finding and mitigating individual sources of PCBs. These studies often involve the collection and analysis of many samples, the evaluation of the data using multivariate methods, and mapping of the data using GIS systems. The US Navy states the following in reference to using congeners for source identification (NAVFAC 2006):

"Forensic studies (to distinguish age, nature, and location of PCB releases) require analysis of a long set of PCB congeners because changes in the distribution of specific congener concentrations are informative. Low method detection limits may also be necessary to characterize remote or old PCB releases, and minor but informative congeners."

A summary of the rationales and uses of PCB congener data is provided in Table 1-4.

Table 1-4Summary of Rationales and Applications of PCB Congeners

Risk assessment	More accurate determination of toxic congeners gives a better estimation of risk
Achieve lower detection limits	Certain monitoring programs require very low level determination of PCBs not achievable by conventional analysis methods
Overcome matrix interferences and multiple Aroclors	For complex samples, total PCBs determined by summing congener concentrations can provide more accurate results
Correct for Aroclor pattern degradation	Congener analysis is not susceptible to the calibration variations associated with using Aroclors as analytical standards
PCB source identification	Congener data can help to identify sources of PCBs at a site for liability determination or remediation planning
New technology effect	Some project planners/managers choose congener analysis because of a perception that more complex is better whether or not it is needed

2 MEASUREMENT OF PCBS AND PCB CONGENERS

Overview

The methods of PCB analysis have improved and become more sophisticated in the years since Jensen first detected PCBs in environmental samples in 1966 (New Scientist ,1966, Jensen, 1972). Nevertheless, the generation of quality PCB data still is problematic for several reasons (Erickson, 1997, Shifrin, 1998, Wait, 1999).

Because PCBs in the environment are nearly always mixtures derived from Aroclors, their concentrations can be reported as total PCBs, PCB Aroclor concentrations, individual PCB congener concentrations, or as PCB homolog group concentrations. For many years, the commonly used methods for PCB analysis were relatively simple. However, the methods for determining PCBs have become more sophisticated over the past 2 decades as more environmental and health studies have focused on individual congeners and as the required detection limits for some applications have decreased.

There are several methods for the analysis of PCBs, however those based on gas chromatography (GC) are the most widely used by far. Among the GC methods there are low resolution methods and high resolution methods. Low resolution GC methods are capable of resolving some of the PCB congeners in each Aroclor mixture. A distinctive pattern of several GC peaks is obtained for each Aroclor and calibration curves can be developed based on the relationships between Aroclor concentration and some measure of GC response. Thus, they are appropriate for determining PCB Aroclor concentrations and total PCBs in relatively simple samples. Low resolution methods are rarely used currently, except for some field screening and other applications where rapid analysis is required.

High resolution GC methods are capable of resolving many more congeners in each Aroclor mixture. Therefore, they are appropriate for determining Aroclor concentrations and some congener concentrations in more complex samples. **Error! Reference source not found.** illustrates this progression of PCB analysis methods from low to high resolution. In the modern high resolution chromatogram, dozens of individual compounds can be identified and their concentrations determined.

Only the highest resolution methods are capable of determining the concentrations of most of the 209 PCB congeners. Within these congener-specific methods are GC methods having varying levels of resolution, sensitivity, and cost. The cost of these analyses also varies from inexpensive to very expensive as the sophistication of the method increases.

Detailed Descriptions of PCB Congener Analytical Methods

PCBs can be measured using several approaches, including gas chromatography, thin layer chromatography, spectrophotometry, and specialized mass spectrometric methods. An extensive list of PCB methods is provided by Erickson (Erickson 1997). Many of the methods listed in Erickson are not discussed in this EPRI report because they either cannot provide congener-specific data or are not commonly used.

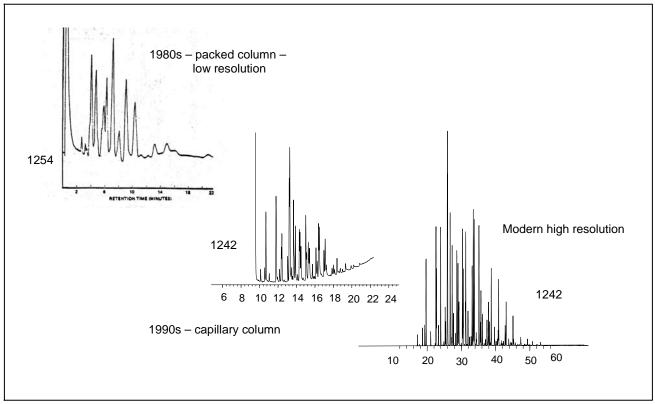


Figure 2-1 The Progression of Increasing Resolution as PCB Methods Became more Advanced

The analysis of PCB congeners requires the use of high resolution methods. As indicated above, there are various GC-based methods available for congener analysis with varying levels of resolution, sensitivity, cost and commercial availability. A detailed description of the three major techniques for PCB congener determination, as well as brief descriptions of some trends in PCB analysis is provided in the following subsections.

GC/ECD

The most common PCB method used by commercial laboratories for groundwater, surface water, non-aqueous phase liquids (NAPLs), and solids is EPA Method 8082 (EPA 1996). This method replaced the previously used EPA PCB Method 8080 in 1996. Technically, EPA Method 8082 is an analytical method only and does not include sample preparation or cleanups. It is part of a compendium of methods known commonly as EPA SW-846 Methods (EPA 1996). This compendium includes multiple and interchangeable method modules for the sample preparation

and cleanup steps which precede the analysis. Thus, any of a number of sample preparation procedures and sample cleanup procedures can be used for EPA Method 8082.

The analysis of PCBs by US EPA SW846 method 8082 uses a gas chromatograph with a high resolution capillary GC column and an electron capture detector to detect PCBs. This technique has been used for years to determine the concentration of PCBs in samples generally reported as Aroclors and total PCBs determined by summing the concentrations of Aroclors detected. Aroclors are identified based on pattern comparison to reference standards and quantitated using 3-5 individual peaks in the chromatograms.

EPA Method 8082 also has been verified for detection of 19 individual congeners and modifications to the method have been documented for up to 77 congeners (EPRI 2002) and 110 congeners (Restek 2005). Individual congeners are identified based on analytical retention time. Since some congeners coelute when using standard analytical columns, the use of multiple columns and analytical runs are often required to differentiate coeluting congeners, and some congeners cannot be quantitated individually. Analyses using ECD also can be biased by interfering compounds present in the sample matrix that make identification and quantitation uncertain. Because of the potential for interferences from non-PCB compounds, it is very important that appropriate cleanup procedures are used by the laboratory prior to analysis by GC/ECD.

Some laboratories have expanded the usability of EPA method 8082 for congeners analysis beyond the original set identified in the SW 846 method (Table 2-1). All 209 congeners cannot be individually resolved in complex matrices and mixtures in a single analysis. However, using two or more different analytical columns and multiple analytical runs, most of the 209 PCB congeners can be determined by GC/ECD. The advantage of GC/ECD for PCB congeners is the selectivity and sensitivity of the instrument for chlorinated compounds. Using GC/ECD can be supplemented, where concentrations are high enough, by analyzing the sample by GC/MS to confirm the identification of the individual congeners.

The estimated method detection limits (EMDLs) presented in the published methods are determined in water free from matrix interferences. No EMDLs are provided in EPA 8082 for individual PCB congeners. However, the EMDLs for chlorinated pesticides by a similar EPA method are about 0.5 μ g/L. However, some laboratories have adjusted the sample size, calibration range, and cleanup criteria to lower detection limits.

IUPAC No.		Congener	IUPAC No.		Congener	
1		2-chlorobiphenyl	87		2,2',3,4,5'-pentachlorobiphenyl	
2		3-chlorobiphenyl	81	W*	^c 3,4,4',5-tetrachlorobiphenyl	
3		4-chlorobiphenyl	77	W*	3,3',4,4'-tetrachlorobiphenyl	
4		2,2'-dichlorobiphenyl	110		2,3,3',4',6-pentachlorobiphenyl	
6		2,3'-dichlorobiphenyl	154		2,2',4,4',5,6'-hexachlorobiphenyl	
8	N	2,4'-dichlorobiphenyl	151	2,2',3,5,5',6-hexachlorobiphenyl		
5	N	2,3-dichlorobiphenyl	123	W*	2',3,4,4',5-pentachlorobiphenyl	

 Table 2-1

 Congener Lists Reported by EPRI (EPRI 2002) and EPA Method 8082

IUPAC No.		Congener	IUPAC No.		Congener
11		3,3'-dichlorobiphenyl	149		2,2',3,4',5',6-hexachlorobiphenyl
18	Ν	2,2',5-trichlorobiphenyl	118	WN*	2,3',4,4',5-pentachlorobiphenyl
15		4,4'-dichlorobiphenyl	106		2,3,3',4,5-pentachlorobiphenyl
32		2,4',6-trichlorobiphenyl	114	W*	2,3,4,4',5-pentachlorobiphenyl
34		2',3,5-trichlorobiphenyl	188		2,2',3,4',5,6,6'-heptachlorobiphenyl
29		2,4,5-trichlorobiphenyl	153		2,2',4,4',5,5'-hexachlorobiphenyl
26		2,3',5-trichlorobiphenyl	105	WN*	2,3,3',4,4'-pentachlorobiphenyl
25		2,3',4-trichlorobiphenyl	138		2,2',3,4,4',5'-hexachlorobiphenyl
31		2,4',5-trichlorobiphenyl	163		2,3,3',4',5,6-hexachlorobiphenyl
50		2,2',4,6-tetrachlorobiphenyl	126	W*	3,3',4,4',5-pentachlorobiphenyl
28	Ν	2,4,4'-trichlorobiphenyl	187		2,2',3,4',5,5',6-heptachlorobiphenyl
33		2',3,4-trichlorobiphenyl	182		2,2',3,4,4',5,6'-heptachlorobiphenyl
20		2,3,3'-trichlorobiphenyl	183		2,2',3,4,4',5',6-heptachlorobiphenyl
69		2,3',4,6-tetrachlorobiphenyl	128	Ν	2,2',3,3',4,4'-hexachlorobiphenyl
52	Ν	2,2',5,5'-tetrachlorobiphenyl	167	W*	2,3',4,4',5,5'-hexachlorobiphenyl
49		2,2',4,5'-tetrachlorobiphenyl	202		2,2',3,3',5,5',6,6'-octachlorobiphenyl
48		2,2',4,5-tetrachlorobiphenyl	156	W*	2,3,3',4,4',5-hexachlorobiphenyl
104		2,2',4,6,6'-pentachlorobiphenyl	157	W*	2,3,3',4,4',5'-hexachlorobiphenyl
44	Ν	2,2',3,5'-tetrachlorobiphenyl	201		2,2',3,3',4,5,5',6'-octachlorobiphenyl
37		3,4,4'-trichlorobiphenyl	180		2,2',3,4,4',5,5'-heptachlorobiphenyl
72		2,3',5,5'-tetrachlorobiphenyl	200		2,2',3,3',4,5',6,6'-octachlorobiphenyl
40		2,2',3,3'-tetrachlorobiphenyl	169	W*	3,3',4,4',5,5'-hexachlorobiphenyl
100		2,2',4,4',6-pentachlorobiphenyl	170		2,2',3,3',4,4',5-heptachlorobiphenyl
74		2,4,4',5-tetrachlorobiphenyl	189	W*	2,3,3',4,4',5,5'-heptachlorobiphenyl
70		2,3',4',5-tetrachlorobiphenyl	208		2,2',3,3',4,5,5',6,6'-nonachlorobiphenyl
80		3,3',5,5'-tetrachlorobiphenyl	195		2,2',3,3',4,4',5,6-octachlorobiphenyl
66	Ν	2,3',4,4'-tetrachlorobiphenyl	207		2,2',3,3',4,4',5,6,6'-nonachlorobiphenyl
93		2,2',3,5,6-pentachlorobiphenyl	194		2,2',3,3',4,4',5,5'-octachlorobiphenyl
95		2,2',3,5',6-pentachlorobiphenyl	206		2,2',3,3',4,4',5,5',6-nonachlorobiphenyl
55		2,3,3',4-tetrachlorobiphenyl	209		decachlorobiphenyl
101	Ν	2,2',4,5,5'-pentachlorobiphenyl			
119	*	2,3',4,4',6-pentachlorobiphenyl			
152		2,2',3,5,6,6'-hexachlorobiphenyl			

Table 2-1 (continued) Congener Lists Reported by EPRI (EPRI 2002) and EPA Method 8082

* - potentially toxic PCB Congeners
 W – PCB congeners of concern identified by the World Health Organization (WHO)
 N – PCB congeners of concern identified by the National Oceanographic and Atmospheric Association (NOAA)
 Bold – EPA 8082 congeners

GC/LRMS

PCBs can also be analyzed using GC with a low resolution mass spectrometer (GC/LRMS). This is the instrumentation combination found in most commercial environmental laboratories. The analysis is based on EPA method 680 (Gebhart, 1985). Samples are analyzed using gas chromatography with a low resolution mass spectrometer operated in scan or selected ion monitoring (SIM) mode. The use of a GC/LRMS eliminates some of the resolution problems encountered with GC/ECD because of the selectivity of the mass spectrometer. However, the mass spectrometer is not generally as sensitive for chlorinated compounds compared to analysis using a GC/ECD. To achieve lower sample reporting limits the operation of the mass spectrometer is frequently done using SIM. The use of SIM with a GC/LRMS focuses the instrument to monitoring only for a select set of ions for PCB congeners eliminating some analytical interference and increasing the instrument sensitivity. Another capability of the GC/MS method is to determine the concentrations of PCB homolog groups in samples which cannot be done by GC/ECD.

Samples can be prepared as noted above for GC/ECD. The use of GC/LRMS can also be used in conjunction with GC/ECD as a confirmatory method for congener identification, especially with complex matrices and mixtures.

Recent developments in GC/LRMS analyses of PCB congeners have been small and incremental. The greater pneumatics of new GCs and the improved sensitivity of new LRMS models have produced better congener separations and somewhat lower detectable levels over just a few years ago. Some new GC columns are available that effectively separate some congener pairs that previously could not be separated. All PCB congeners are now available at high purity and several commercial mixtures of PCB congeners are now available. These advances have greatly improved the comparability of PCB congener data generated by different laboratories.

GC/HRMS

The most technically advanced and sensitive analytical method available for PCB congener analysis is EPA method 1668 (EPA 2000). The method specifies the use of high resolution GC with high resolution mass spectrometry (GC/HRMS). EPA method 1668A was developed to analyze most of the 209 PCB congeners and achieve very low detection limits. In December 1999, EPA released Method 1668A, a modification of EPA Method 1668 designed for aqueous, solid, tissue, and multi-phase matrices (EPA 2000). Although Method 1668 specified only the method of analysis, the modified method includes procedures for sample preparation, cleanup, and analysis. In addition, the method was expanded to include the determination of over 150 PCB congeners, including the toxic PCB congeners designated by the World Health Organization (WHO 1993) and methods for estimating the PCB homolog group concentrations. More importantly, Method 1668A adopted methods from PCB researchers for the isolation of the most toxic PCB congeners (IUPAC 77, 126, and 169) with an EMDL of 5 pg/L for IUPAC 126.

Method 1668A specifies the following sample preparation scheme. Aqueous samples are prepared by solid phase, separatory funnel, or continuous liquid:liquid extraction. Solid samples are extracted using a Soxhlet/Dean-Stark (SDS) extractor. Some samples also require back extraction with acid and base prior to cleanup. Extract cleanup options include GPC, required for all soils, high pressure liquid chromatography (HPLC), and column chromatography using silica gel, Carbopak/Celite, or Florisil. This method is ideally suited for risk assessment and any

projects which require the identification and quantitation of specific PCB congeners at low levels and in complex matrices.

Other PCB Congener Methods

There are several other methods available for PCB analysis, however most are not applicable to congener-specific analysis. For example, EPA Method 4020 determines total PCBs by enzyme immunoassay. While similar methods are valuable for soil screening, they do not have the specificity or sensitivity needed for congener-specific measurement.

Another trend in PCB measurement is fast analysis methods. For example, several portable gas chromatographs are available, and have been improved over models available just a few years ago, that can detect PCBs with analysis times of just a few minutes. Also, portable mass spectrometers have become available that detect PCBs quickly. Finally, bench-top instrument modifications and special software now allow for PCB determinations in just a few minutes. However, all of these methods report PCBs as total PCBs or PCBs as Aroclors. None have the resolution or sensitivity needed for congener analysis.

GC/TOFMS

GC-Time of Flight Mass Spectrometry (TOFMS) uses the separation capabilities of gas chromatography and TOFMS to separate out the different PCB congeners. TOFMS separates ions based on their charge/mass ratios and the differences in time it takes for the ions to travel across a distance. Heavier ions will take longer to travel than lighter ions providing the basis for identification. Since ions will have different travel times the compounds can be separated using this technique in addition to the GC separation. TOFMS instruments are capable of acquiring data much faster than standard quadrupole mass spectrometers. This faster data acquisition allows for the deconvoluting of compounds with retention times on the order of 100's of milliseconds providing higher resolution than standard GC/MS.

Some research laboratories and some commercial laboratories have GC/TOFMA instruments. These instruments are used for conducting EPA Method 1668 or equivalent and result in reduced turnaround time and cost.

GC x GC

GCxGC is a gas chromatographic method that uses two analytical columns set up in tandem to provide a more detailed analysis of samples for PCB congeners. The two columns with different phases and separation capabilities can be used to resolve PCB congeners that are not separated by a single column. Whereas two or more analyses for PCB congeners may be required to resolve the coeluting compounds using conventional GC/ECD or GC/LRMS, the GCxGC technique allows for the two columns to be used in a single analysis. The columns are connected using a modulator that can collect the effluent of the first analytical column and periodically injects the sample into the second analytical column. The effluent of the resulting chromatograms is such that specialized software is required to resolve the two-dimensional responses based on algorithms. The identification of the individual congeners is determined by the multi dimensional response time plot. This method is still in the early stages of development and not used in the commercial environmental laboratory industry. The method also requires

specialized modifications to standard GC instrumentation and the use of the noted software to resolve the data.

3 SUMMARY

Table 2 1

There is still no single routine method for the analysis of all 209 PCB congeners. The commonly available analytical methods for PCB congener analysis remain GC/ECD (EPA Method 8082), GC/LRMS (EPA 680) and GC/HRMS (EPA 1668A). For very low-concentration samples and complex matrices, GC/HRMS is the preferred method of analysis though it is substantially more expensive than other methods. GC/ECD and GC/LRMS are less expensive options and frequently can meet project-specific data quality objectives when conducted by an experienced laboratory. With all methods, rigorous sample extraction and cleanups may be needed to remove non-PCB materials from the extracts. At present, it is most important to identify the data needs, develop a target compound list and associated data quality objectives, and then identify a method that will meet those criteria.

A comparison of the available methods for PCBs is provided in Table 3-1.

Comparison of Methods for PCB Analysis and Determination of PCB Congeners i	n Soil and Water
Samples	

Method Reference	Instrument	Congeners detectable ¹	Detection Limits Aqueous ²	Detection Limits Solid ²	Cost per Sample Range ^³
EPA 4020	Enzyme immunoassay	none	200 ng/L	50 - 500 μg/kg	\$20 - \$40 ⁴
EPA SW 846 8082	GC/ECD	Varies: 19 to >140	0.1 - 10 ng/L	0.01 - 1 μg/kg	\$100 - \$250
EPA 680	GC/LRMS	Not all 209	100 – 1,000 ng/L	10 – 100 µg/kg	\$250 - \$350
EPA 680	GC/LRMS -SIM	Not all 209	10 –100 ng/L	1 – 10 µg/kg	\$250 - \$500
EPA 1668A	GC/HRMS	Almost all 209	0.1 – 1.0 ng/L	0.01 -0.1 µg/kg	\$850 - \$1,500

1 – The development of new GC columns has allowed more congeners to be detected without interferences. The actual congeners measured depends on project-specific requirements.

2 – Detection limits achievable depends on several factors, including the specific instrumentation used, the sample size, and matrix. The detection limits in this table were estimated from various sources (ATSDR 2000)

3 - Costs are estimates based on a limited survey of commercial laboratories.

4 – EPA Method 4020 typically is conducted in the field. The cost is for the test kits only and does not include the labor of conducting the test.

Planning a PCB Congener Analysis Program

Prior to sending samples to the laboratory for PCB congener analysis, the following steps should be taken at a minimum:

- Determine why congener analysis is being conducted
- If congener analysis is required for regulatory purposes, determine if a specific method (e.g., EPA 1668A) is required by the agency or program or permit
- Determine what congeners must be reported
- Determine the congener detection limits required,
- Determine whether reporting of Aroclors and/or homolog groups is required in addition to congeners, and
- Determine the quality control measures, frequencies, and criteria needed to meet data usability

The appropriate testing procedure can be determined once the purpose and scope of the work have been thoroughly described.

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A CAS NUMBERS FOR PCB AROCLORS AND HOMOLOGS

PCBs in General

CAS Number 1336-36-3

PCB Aroclors

Aroclor (Unspecified)	12767-79-2
Aroclor 1016	12674-11-2
Aroclor 1221	11104-28-2
Aroclor 1232	11141-16-5
Aroclor 1242	53469-21-9
Aroclor 1248	12672-29-6
Aroclor 1252	89577-78-6
Aroclor 1254	11097-69-1
Aroclor 1260	11096-82-5
Aroclor 1262	37324-23-5
Aroclor 1268	11100-14-4

PCB Homologs^a

Monochlorbiphenyl - (MCB)	27323-18-8
Dichlorobiphenyl - (DCB)	25512-42-9
Trichlorobiphenyl - (TrCB)	25323-68-6
Tetrachlorobiphenyl - (TCB)	26914-33-0
Pentachlorobiphenyl - (PeCB)	25429-29-2
Hexachlorobiphenyl - (HxCB)	26601-64-9
Heptachlorobiphenyl - (HpCB)	28655-71-2
Octachlorobiphenyl - (OCB)	55722-26-4
Nonachlorobiphenyl - (NCB)	53742-07-7

^a Decachlorobiphenyl (DeCB) is not listed because it is a congener. It is listed in Table B-2.

B IUPAC NUMBERS AND CAS NUMBERS OF ALL PCB CONGENERS

IUPAC Number	Name	CAS Number
PCB 1	2-Chlorobiphenyl	2051-60-7
PCB 2	3-Chlorobiphenyl	2051-61-8
PCB 3	4-Chlorobiphenyl	2051-62-9
PCB 4	2,2'-Dichlorobiphenyl	13029-08-8
PCB 5	2,3-Dichlorobiphenyl	16605-91-7
PCB 6	2,3'-Dichlorobiphenyl	25569-80-6
PCB 7	2,4-Dichlorobiphenyl	33284-50-3
PCB 8	2,4'-Dichlorobiphenyl	34883-43-7
PCB 9	2,5-Dichlorobiphenyl	34883-39-1
PCB 10	2,6-Dichlorobiphenyl	33146-45-1
PCB 11	3,3'-Dichlorobiphenyl	2050-67-1
PCB 12	3,4-Dichlorobiphenyl	2974-92-7
PCB 13	3,4'-Dichlorobiphenyl	2974-90-5
PCB 14	3,5-Dichlorobiphenyl	34883-41-5
PCB 15	4,4'-Dichlorobiphenyl	2050-68-2
PCB 16	2,2',3-Trichlorobiphenyl	38444-78-9
PCB 17	2,2',4-Trichlorobiphenyl	37680-66-3
PCB 18	2,2',5-Trichlorobiphenyl	37680-65-2
PCB 19	2,2',6-Trichlorobiphenyl	38444-73-4
PCB 20	2,3,3'-Trichlorobiphenyl	38444-84-7
PCB 21	2,3,4-Trichlorobiphenyl	55702-46-0
PCB 22	2,3,4'-Trichlorobiphenyl	38444-85-8
PCB 23	2,3,5-Trichlorobiphenyl	55720-44-0
PCB 24	2,3,6-Trichlorobiphenyl	55702-45-9
PCB 25	2,3',4-Trichlorobiphenyl	55712-37-3
PCB 26	2,3',5-Trichlorobiphenyl	38444-81-4
PCB 27	2,3',6-Trichlorobiphenyl	38444-76-7
PCB 28	2,4,4'-Trichlorobiphenyl	7012-37-5

IUPAC Number	Name	CAS Number
PCB 29	2,4,5-Trichlorobiphenyl	15862-07-4
PCB 30	2,4,6-Trichlorobiphenyl	35693-92-6
PCB 31	2,4',5-Trichlorobiphenyl	16606-02-3
PCB 32	2,4',6-Trichlorobiphenyl	38444-77-8
PCB 33	2,3',4'-Trichlorobiphenyl	38444-86-9
PCB 34	2,3',5'-Trichlorobiphenyl	37680-68-5
PCB 35	3,3',4-Trichlorobiphenyl	37680-69-6
PCB 36	3,3',5-Trichlorobiphenyl	38444-87-0
PCB 37	3,4,4'-Trichlorobiphenyl	38444-90-5
PCB 38	3,4,5-Trichlorobiphenyl	53555-66-1
PCB 39	3,4',5-Trichlorobiphenyl	38444-88-1
PCB 40	2,2',3,3'-Tetrachlorobiphenyl	38444-93-8
PCB 41	2,2',3,4-Tetrachlorobiphenyl	52663-59-9
PCB 42	2,2',3,4'-Tetrachlorobiphenyl	36559-22-5
PCB 43	2,2',3,5-Tetrachlorobiphenyl	70362-46-8
PCB 44	2,2',3,5'-Tetrachlorobiphenyl	41464-39-5
PCB 45	2,2',3,6-Tetrachlorobiphenyl	70362-45-7
PCB 46	2,2',3,6'-Tetrachlorobiphenyl	41464-47-5
PCB 47	2,2',4,4'-Tetrachlorobiphenyl	2437-79-8
PCB 48	2,2',4,5-Tetrachlorobiphenyl	70362-47-9
PCB 49	2,2',4,5'-Tetrachlorobiphenyl	41464-40-8
PCB 50	2,2',4,6-Tetrachlorobiphenyl	62796-65-0
PCB 51	2,2',4,6'-Tetrachlorobiphenyl	68194-04-7
PCB 52	2,2',5,5'-Tetrachlorobiphenyl	35693-99-3
PCB 53	2,2',5,6'-Tetrachlorobiphenyl	41464-41-9
PCB 54	2,2',6,6'-Tetrachlorobiphenyl	15968-05-5
PCB 55	2,3,3',4-Tetrachlorobiphenyl	74338-24-2
PCB 56	2,3,3',4'-Tetrachlorobiphenyl	41464-43-1
PCB 57	2,3,3',5-Tetrachlorobiphenyl	70424-67-8
PCB 58	2,3,3',5'-Tetrachlorobiphenyl	41464-49-7
PCB 59	2,3,3',6-Tetrachlorobiphenyl	74472-33-6
PCB 60	2,3,4,4'-Tetrachlorobiphenyl	33025-41-1
PCB 61	2,3,4,5-Tetrachlorobiphenyl	33284-53-6
PCB 62	2,3,4,6-Tetrachlorobiphenyl	54230-22-7

IUPAC Number	Name	CAS Number
PCB 63	2,3,4',5-Tetrachlorobiphenyl	74472-34-7
PCB 64	2,3,4',6-Tetrachlorobiphenyl	52663-58-8
PCB 65	2,3,5,6-Tetrachlorobiphenyl	33284-54-7
PCB 66	2,3',4,4'-Tetrachlorobiphenyl	32598-10-0
PCB 67	2,3',4,5-Tetrachlorobiphenyl	73575-53-8
PCB 68	2,3',4,5'-Tetrachlorobiphenyl	73575-52-7
PCB 69	2,3',4,6-Tetrachlorobiphenyl	60233-24-1
PCB 70	2,3',4',5-Tetrachlorobiphenyl	32598-11-1
PCB 71	2,3',4',6-Tetrachlorobiphenyl	41464-46-4
PCB 72	2,3',5,5'-Tetrachlorobiphenyl	41464-42-0
PCB 73	2,3',5',6-Tetrachlorobiphenyl	74338-23-1
PCB 74	2,4,4',5-Tetrachlorobiphenyl	32690-93-0
PCB 75	2,4,4',6-Tetrachlorobiphenyl	32598-12-2
PCB 76	2,3',4',5'-Tetrachlorobiphenyl	70362-48-0
<i>PCB</i> 77	3,3',4,4'-Tetrachlorobiphenyl	32598-13-3
PCB 78	3,3',4,5-Tetrachlorobiphenyl	70362-49-1
PCB 79	3,3',4,5'-Tetrachlorobiphenyl	41464-48-6
PCB 80	3,3',5,5'-Tetrachlorobiphenyl	33284-52-5
PCB 81	3,4,4',5-Tetrachlorobiphenyl	70362-50-4
PCB 82	2,2',3,3',4-Pentachlorobiphenyl	52663-62-4
PCB 83	2,2',3,3',5-Pentachlorobiphenyl	60145-20-2
PCB 84	2,2',3,3',6-Pentachlorobiphenyl	52663-60-2
PCB 85	2,2',3,4,4'-Pentachlorobiphenyl	65510-45-4
PCB 86	2,2',3,4,5-Pentachlorobiphenyl	55312-69-1
PCB 87	2,2',3,4,5'-Pentachlorobiphenyl	38380-02-8
PCB 88	2,2',3,4,6-Pentachlorobiphenyl	55215-17-3
PCB 89	2,2',3,4,6'-Pentachlorobiphenyl	73575-57-2
PCB 90	2,2',3,4',5-Pentachlorobiphenyl	68194-07-0
PCB 91	2,2',3,4',6-Pentachlorobiphenyl	68194-05-8
PCB 92	2,2',3,5,5'-Pentachlorobiphenyl	52663-61-3
PCB 93	2,2',3,5,6-Pentachlorobiphenyl	73575-56-1
PCB 94	2,2',3,5,6'-Pentachlorobiphenyl	73575-55-0
PCB 95	2,2',3,5',6-Pentachlorobiphenyl	38379-99-6
PCB 96	2,2',3,6,6'-Pentachlorobiphenyl	73575-54-9

IUPAC Number	Name	CAS Number
PCB 97	2,2',3,4',5'-Pentachlorobiphenyl	41464-51-1
PCB 98	2,2',3,4',6'-Pentachlorobiphenyl	60233-25-2
PCB 99	2,2',4,4',5-Pentachlorobiphenyl	38380-01-7
PCB 100	2,2',4,4',6-Pentachlorobiphenyl	39485-83-1
PCB 101	2,2',4,5,5'-Pentachlorobiphenyl	37680-73-2
PCB 102	2,2',4,5,6'-Pentachlorobiphenyl	68194-06-9
PCB 103	2,2',4,5',6-Pentachlorobiphenyl	60145-21-3
PCB 104	2,2',4,6,6'-Pentachlorobiphenyl	56558-16-8
PCB 105	2,3,3',4,4'-Pentachlorobiphenyl	32598-14-4
PCB 106	2,3,3',4,5-Pentachlorobiphenyl	70424-69-0
PCB 107	2,3,3',4',5-Pentachlorobiphenyl	70424-68-9
PCB 108	2,3,3',4,5'-Pentachlorobiphenyl	70362-41-3
PCB 109	2,3,3',4,6-Pentachlorobiphenyl	74472-35-8
PCB 110	2,3,3',4',6-Pentachlorobiphenyl	38380-03-9
PCB 111	2,3,3',5,5'-Pentachlorobiphenyl	39635-32-0
PCB 112	2,3,3',5,6-Pentachlorobiphenyl	74472-36-9
PCB 113	2,3,3',5',6-Pentachlorobiphenyl	68194-10-5
PCB 114	2,3,4,4',5-Pentachlorobiphenyl	74472-37-0
PCB 115	2,3,4,4',6-Pentachlorobiphenyl	74472-38-1
PCB 116	2,3,4,5,6-Pentachlorobiphenyl	18259-05-7
PCB 117	2,3,4',5,6-Pentachlorobiphenyl	68194-11-6
PCB 118	2,3',4,4',5-Pentachlorobiphenyl	31508-00-6
PCB 119	2,3',4,4',6-Pentachlorobiphenyl	56558-17-9
PCB 120	2,3',4,5,5'-Pentachlorobiphenyl	68194-12-7
PCB 121	2,3',4,5',6-Pentachlorobiphenyl	56558-18-0
PCB 122	2,3,3',4',5'-Pentachlorobiphenyl	76842-07-4
PCB 123	2,3',4,4',5'-Pentachlorobiphenyl	65510-44-3
PCB 124	2,3',4',5,5'-Pentachlorobiphenyl	70424-70-3
PCB 125	2,3',4',5',6-Pentachlorobiphenyl	74472-39-2
PCB 126	3,3',4,4',5-Pentachlorobiphenyl	57465-28-8
PCB 127	3,3',4,5,5'-Pentachlorobiphenyl	39635-33-1
PCB 128	2,2',3,3',4,4'-Hexachlorobiphenyl	38380-07-3
PCB 129	2,2',3,3',4,5-Hexachlorobiphenyl	55215-18-4
PCB 130	2,2',3,3',4,5'-Hexachlorobiphenyl	52663-66-8

IUPAC Number	Name	CAS Number
PCB 131	2,2',3,3',4,6-Hexachlorobiphenyl	61798-70-7
PCB 132	2,2',3,3',4,6'-Hexachlorobiphenyl	38380-05-1
PCB 133	2,2',3,3',5,5'-Hexachlorobiphenyl	35694-04-3
PCB 134	2,2',3,3',5,6-Hexachlorobiphenyl	52704-70-8
PCB 135	2,2',3,3',5,6'-Hexachlorobiphenyl	52744-13-5
PCB 136	2,2',3,3',6,6'-Hexachlorobiphenyl	38411-22-2
PCB 137	2,2',3,4,4',5-Hexachlorobiphenyl	35694-06-5
PCB 138	2,2',3,4,4',5'-Hexachlorobiphenyl	35065-28-2
PCB 139	2,2',3,4,4',6-Hexachlorobiphenyl	56030-56-9
PCB 140	2,2',3,4,4',6'-Hexachlorobiphenyl	59291-64-4
PCB 141	2,2',3,4,5,5'-Hexachlorobiphenyl	52712-04-6
PCB 142	2,2',3,4,5,6-Hexachlorobiphenyl	41411-61-4
PCB 143	2,2',3,4,5,6'-Hexachlorobiphenyl	68194-15-0
PCB 144	2,2',3,4,5',6-Hexachlorobiphenyl	68194-14-9
PCB 145	2,2',3,4,6,6'-Hexachlorobiphenyl	74472-40-5
PCB 146	2,2',3,4',5,5'-Hexachlorobiphenyl	51908-16-8
PCB 147	2,2',3,4',5,6-Hexachlorobiphenyl	68194-13-8
PCB 148	2,2',3,4',5,6'-Hexachlorobiphenyl	74472-41-6
PCB 149	2,2',3,4',5',6-Hexachlorobiphenyl	38380-04-0
PCB 150	2,2',3,4',6,6'-Hexachlorobiphenyl	68194-08-1
PCB 151	2,2',3,5,5',6-Hexachlorobiphenyl	52663-63-5
PCB 152	2,2',3,5,6,6'-Hexachlorobiphenyl	68194-09-2
PCB 153	2,2',4,4',5,5'-Hexachlorobiphenyl	35065-27-1
PCB 154	2,2',4,4',5,6'-Hexachlorobiphenyl	60145-22-4
PCB 155	2,2',4,4',6,6'-Hexachlorobiphenyl	33979-03-2
PCB 156	2,3,3',4,4',5-Hexachlorobiphenyl	38380-08-4
PCB 157	2,3,3',4,4',5'-Hexachlorobiphenyl	69782-90-7
PCB 158	2,3,3',4,4',6-Hexachlorobiphenyl	74472-42-7
PCB 159	2,3,3',4,5,5'-Hexachlorobiphenyl	39635-35-3
PCB 160	2,3,3',4,5,6-Hexachlorobiphenyl	41411-62-5
PCB 161	2,3,3',4,5',6-Hexachlorobiphenyl	74472-43-8
PCB 162	2,3,3',4',5,5'-Hexachlorobiphenyl	39635-34-2
PCB 163	2,3,3',4',5,6-Hexachlorobiphenyl	74472-44-9
PCB 164	2,3,3',4',5',6-Hexachlorobiphenyl	74472-45-0

IUPAC Number	Name	CAS Number
PCB 165	2,3,3',5,5',6-Hexachlorobiphenyl	74472-46-1
PCB 166	2,3,4,4',5,6-Hexachlorobiphenyl	41411-63-6
PCB 167	2,3',4,4',5,5'-Hexachlorobiphenyl	52663-72-6
PCB 168	2,3',4,4',5',6-Hexachlorobiphenyl	59291-65-5
PCB 169	3,3',4,4',5,5'-Hexachlorobiphenyl	32774-16-6
PCB 170	2,2',3,3',4,4',5-Heptachlorobiphenyl	35065-30-6
PCB 171	2,2',3,3',4,4',6-Heptachlorobiphenyl	52663-71-5
PCB 172	2,2',3,3',4,5,5'-Heptachlorobiphenyl	52663-74-8
PCB 173	2,2',3,3',4,5,6-Heptachlorobiphenyl	68194-16-1
PCB 174	2,2',3,3',4,5,6'-Heptachlorobiphenyl	38411-25-5
PCB 175	2,2',3,3',4,5',6-Heptachlorobiphenyl	40186-70-7
PCB 176	2,2',3,3',4,6,6'-Heptachlorobiphenyl	52663-65-7
PCB 177	2,2',3,3',4,5',6'-Heptachlorobiphenyl	52663-70-4
PCB 178	2,2',3,3',5,5',6-Heptachlorobiphenyl	52663-67-9
PCB 179	2,2',3,3',5,6,6'-Heptachlorobiphenyl	52663-64-6
PCB 180	2,2',3,4,4',5,5'-Heptachlorobiphenyl	35065-29-3
PCB 181	2,2',3,4,4',5,6-Heptachlorobiphenyl	74472-47-2
PCB 182	2,2',3,4,4',5,6'-Heptachlorobiphenyl	60145-23-5
PCB 183	2,2',3,4,4',5',6-Heptachlorobiphenyl	52663-69-1
PCB 184	2,2',3,4,4',6,6'-Heptachlorobiphenyl	74472-48-3
PCB 185	2,2',3,4,5,5',6-Heptachlorobiphenyl	52712-05-7
PCB 186	2,2',3,4,5,6,6'-Heptachlorobiphenyl	74472-49-4
PCB 187	2,2',3,4',5,5',6-Heptachlorobiphenyl	52663-68-0
PCB 188	2,2',3,4',5,6,6'-Heptachlorobiphenyl	74487-85-7
PCB 189	2,3,3',4,4',5,5'-Heptachlorobiphenyl	39635-31-9
PCB 190	2,3,3',4,4',5,6-Heptachlorobiphenyl	41411-64-7
PCB 191	2,3,3',4,4',5',6-Heptachlorobiphenyl	74472-50-7
PCB 192	2,3,3',4,5,5',6-Heptachlorobiphenyl	74472-51-8
PCB 193	2,3,3',4',5,5',6-Heptachlorobiphenyl	69782-91-8
PCB 194	2,2',3,3',4,4',5,5'- Octachlorobiphenyl	35694-08-7
PCB 195	2,2',3,3',4,4',5,6- Octachlorobiphenyl	52663-78-2
PCB 196	2,2',3,3',4,4',5,6'- Octachlorobiphenyl	42740-50-1
PCB 197	2,2',3,3',4,4',6,6'- Octachlorobiphenyl	33091-17-7
PCB 198	2,2',3,3',4,5,5',6- Octachlorobiphenyl	68194-17-2

IUPAC Number	Name	CAS Number
PCB 199	2,2',3,3',4,5,5',6'- Octachlorobiphenyl	52663-75-9
PCB 200	2,2',3,3',4,5,6,6'- Octachlorobiphenyl	52663-73-7
PCB 201	2,2',3,3',4,5',6,6'- Octachlorobiphenyl	40186-71-8
PCB 202	2,2',3,3',5,5',6,6'- Octachlorobiphenyl	2136-99-4
PCB 203	2,2',3,4,4',5,5',6- Octachlorobiphenyl	52663-76-0
PCB 204	2,2',3,4,4',5,6,6'- Octachlorobiphenyl	74472-52-9
PCB 205	2,3,3',4,4',5,5',6- Octachlorobiphenyl	74472-53-0
PCB 206	2,2',3,3',4,4',5,5',6- Nonachlorobiphenyl	40186-72-9
PCB 207	2,2',3,3',4,4',5,6,6'- Nonachlorobiphenyl	52663-79-3
PCB 208	2,2',3,3',4,5,5',6,6'- Nonachlorobiphenyl	52663-77-1
PCB 209	Decachlorobiphenyl	2051-24-3

Shown in italics are the 12 EPA-designated dioxin-like congeners; those that resemble 2,3,7,8-tetrachlorodibenzo-p-dioxin in structure and toxicity.

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