





Aroclors, Homologs and Congeners – An Evaluation of the Options for PCB Analysis and a Comparison of the Interpretive Value

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Polychlorinated Biphenyls - PCBs







- Most commonly known for use in transformers as dielectric fluids
- Also used in hydraulic fluids, lubricants, as plasticizers and in caulking compounds
- Primary manufacturer was Monsanto product given the trade name Aroclor
- Aroclor nomenclature indicated the average % chlorine in the mixture
 - i.e. Aroclor 1254 = approx 54% chlorine

Why are they important?







- PCBs bioaccumulate
- WHO (World Health Organization) has determined that some of the 209, ones referred to as "dioxin-like" PCBs, dl-PCBs, or coplanar PCBs, may be anticipated to cause cancer
- People can be exposed to PCBs through breathing in contaminated air, consuming contaminated food, and by skin contact with old electrical equipment that contains PCBs.

Polychlorinated Biphenyls - PCBs







PCBs can be grouped or identified by three common descriptions;

- Aroclor a mixture of up to one hundred different congeners, grouped together based on an average percent weight chlorine basis
- Homolog congeners of the same chlorination level. There are 10 chlorination groupings
- Congener any of the individual chlorinated biphenyl compounds of which 209 are possible

Polychlorinated Biphenyls - Aroclors







- The most common analysis technique is GC/ECD, SW-846 Method 8082
- Identifies and quantifies PCBs as an Aroclor

Aroclor 1016 Aroclor 1221 Aroclor 1232

Aroclor 1242 Aroclor 1248 Aroclor 1254

Aroclor 1260 Aroclor 1262

- Limits are typically in the ug/kg and ug/l range
- Technique is prone to interferences

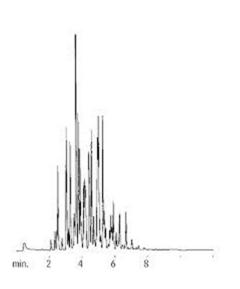
Environmental

Polychlorinated Biphenyls - Aroclors

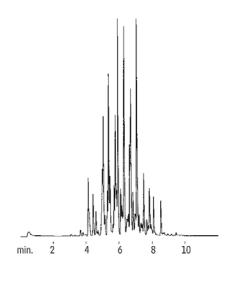




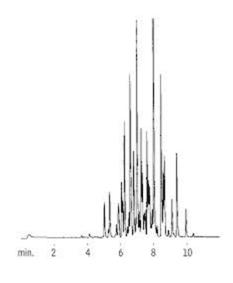




Aroclor 1242



Aroclor 1254



Aroclor 1260

Polychlorinated Biphenyls - Aroclors







- Each Aroclor mix consists of dozens of congeners
- Congeners with the same number of chlorines on the biphenyl ring are called homologs
- For example, Aroclor1254 contains;

1% Trichlorobiphenyls

15% Tetrachlorobiphenyls

53% Pentachlorobiphenyls

26% Hexachlorobiphenyls

4% Heptachlorobiphenyls

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Why are they important?







- Everything you know about Aroclor PCBs applies in some part to PCB Congeners
- Not all PCB congeners are found in Aroclors
- Approximately 130 of the 209 congeners are detected in Aroclors
- Congeners are also categorized by the number of chlorines substituted on the biphenyl ring
- These categories are called homolog groups or isomer groups

Polychlorinated Biphenyls - Homologs







Homologs can be characterized by EPA Method 680 or EPA Method 1668.

EPA Method 680

- Gas Chromatography/Mass Spectrometry (low resolution)
- Can be operated full scan or selected ion monitoring (SIM)
- Therefore, sensitivities similar to what you have with 8270
 - 0.1 ug/l for the lower chlorination homologs
 - 0.3-0.5 ug/l for the higher chlorination homologs

Low/single digit ug/kg for soils/solids

Polychlorinated Biphenyls - Homologs







Nine congeners are used to "characterize" the homolog groups

PCB 1 Monochlorobiphenyls

PCB 5 Dichlorobiphenyls

PCB 29 Trichlorobiphenyls

PCB 50 Tetrachlorobiphenyls

PCB 87 Pentachlorobiphenyls

PCB 154 Hexachlorobiphenyls

PCB 188 Heptachlorobiphenyls

PCB 200 Octachlorobiphenyls

PCB 209 Nona- and decachlorobiphenyl

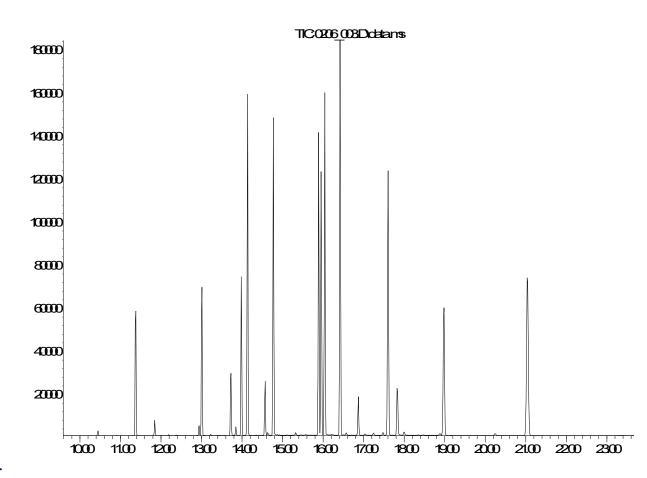
Total Ion Chromatogram of 680 CCAL







Abundance



Time->

Polychlorinated biphenyls - Homologs







- Quantitation is achieved with internal standard calibration using deuterated PAHs, like 8270
- Homolog group is determined by summing the areas of all peaks within a given retention time, that have the same mass
- Even though a select few congeners are used for the calibration response, data does not yield congener information
- Results will consist of a value for each of the homolog groups and a sum of the homolog groups for a PCB total

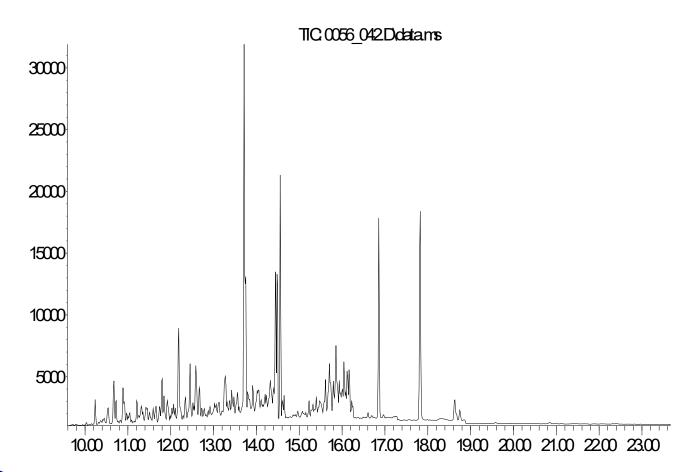
TIC of Typical Sample







Abundance



Time->

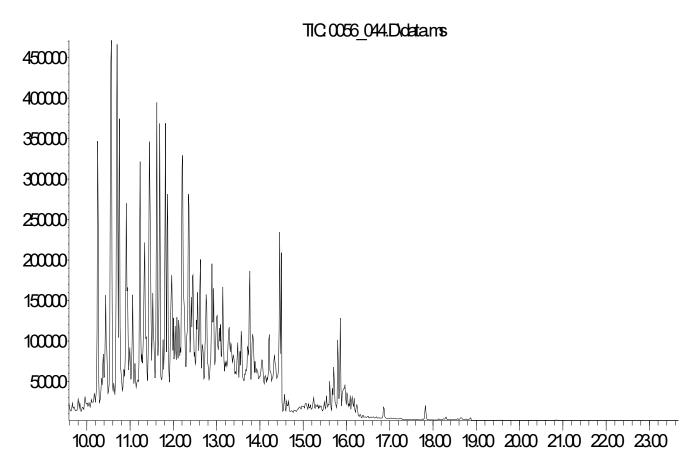
TIC of Contaminated Sample







Abundance



Time->



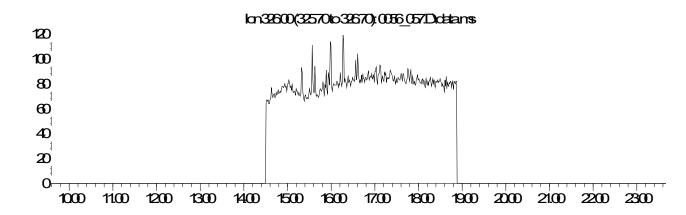
Extracted Ion for Pentachlorobiphenyl



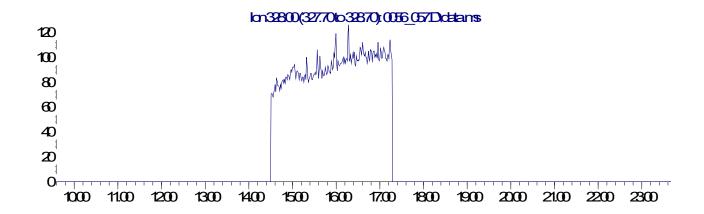




Aburdance



Time-> Abundance



Tine->



What are PCB Congeners?

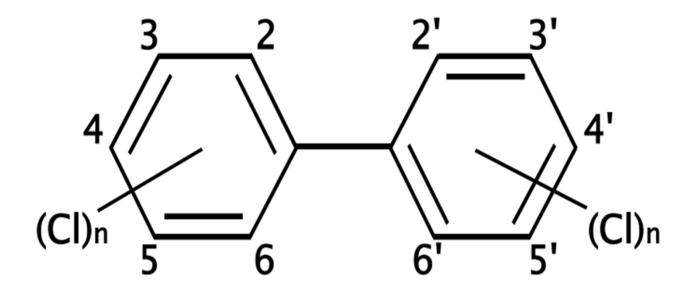






A congener is a specific chlorine substitution pattern on a biphenyl ring.

There are a total of 209 possible substitution patterns ranging from 1 chlorine up to 10 chlorines



Polychlorinated Biphenyls – Congeners







- To monitor and analyze for the more toxic congeners, High Resolution Mass Spectrometry (HRMS) is employed
- EPA Method 1668

HRGC/HRMS

Capillary column to resolve many of the congeners

Special clean-up techniques

Reporting limits of ng/kg and pg/l

Polychlorinated Biphenyls – Congeners







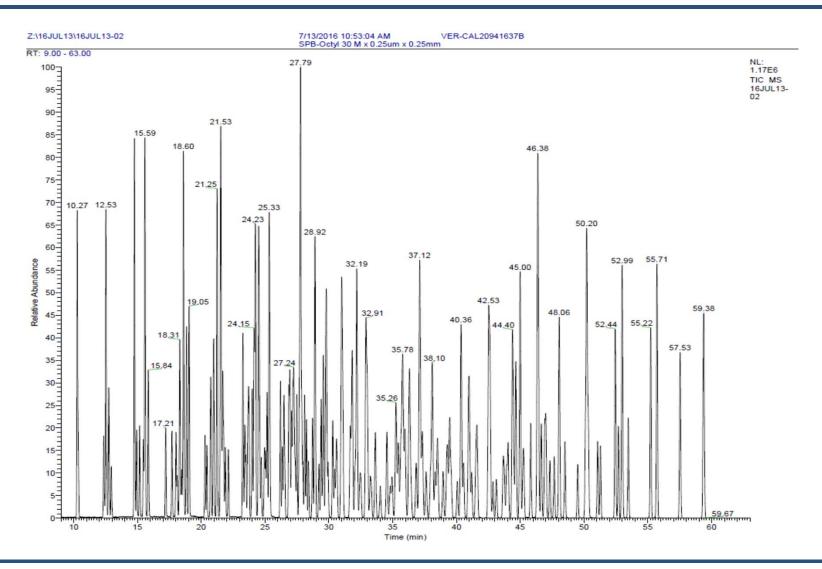
- Able to calibrate for all 209 congeners
- Calibration is also mostly internal standard except that the compounds used as internal standards are isotopically labeled PCB congeners
- Able to differentiate between congeners that are constituents of Aroclors and those that are not.
- Able to differentiate contribution of dl-PCBs from total PCB content

Calibration Standard with 209 Congeners









Example Data – PCB15







16JUL06-02 printed 7/6/2016 13:46 Sample VER-CAL209416378 / PCBCS209-0 Inst ID: DF19780-16JUL06 / Client:



Lancaster Laboratories

Chromatogram RT: 13.61 - 23.61 SM: 5G RT: 18.61 NL: 100-1.82E5 14.77 15.60 17.21 m/z=224.00-224.00 MS 50 16JUL06-02 19.23 16.44 Relative Abundance NL: RT: 18.61 2.82E5 14.77 15.60 m/z=17.21 222.00-222.00 MS 16JUL06-02 16.56 14.09 19.18 14.76 15.58 NL: RT: 18.60 100-4.17E5 m/z=236.04-50 236.04 MS 16JUL06-02 19.59 16.13 17.16 15 20 22 23 16 21 14 17 18 19 Time (min)

Entry: N2PCB15 IS: L2PCB15



Polychlorinated Biphenyls – Congeners







- Can do fingerprinting of PCB sources based on ratios and relative amounts of the individual congeners
- Comparison of Aroclor based PCB congeners versus presence of non-Aroclor based PCB congeners
- Homolog results determined by summing of individual congeners that make up each chlorination level.
- Total PCB concentration as well as special case congeners quantified.

Special Case Congeners







Dioxin-like PCBs (12)

- PCB77
- PCB81
- PCB105
- PCB114
- PCB118
- PCB123
- PCB126
- PCB156
- PCB157
- PCB167
- PCB169
- PCB189

Indicator PCBs (6)

- PCB28
- PCB52
- PCB101
- PCB138
- PCB153
- PCB180

Questions







