Determination of the Composition of the Commercial PCBs: Kanechlor, Clophen, Aroclor, Chlorofen, and Sovol, by HRGC-HRMS

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1. Introduction.

The risks PCBs present to the environment and human health are well documented. The contribution of coplanar PCBs to the TEQ value of certain environmental samples may equal, or exceed, that of the 2378-substituted PCDDs and PCDFs. PCBs in the environment may originate from previous industrial use of these compounds or from the products of combustion 1.2.33.

This paper presents basic information on the composition of commercial PCBs.

HRGC-HRMS analysis⁴⁾ was performed on a number of commercial PCB samples; Kanechlor (Japan), Clophen (Germany), Aroclor (USA), Chlorofen (Poland), Sovol (Rusia). Information was obtained on individual PCB congeners, as well as the relative abundance of each congener group. Additionally, levels of coplanar PCB were determined separately after an HPLC carbon column clean-up.

2. Materials and Methods.

Aroclor was purchased from Supelco(USA) and Kanchlor formulation from GL Science in Japan. Clophen, Chlorofen and Sovol formulation were a gift from Dr. Kannan, Institute of Marine Research, University of Kiel, Germany.

PCB standard solutions containing both native and ¹³C-labeled internal standards were obtained from Cambridge Isotope Laboratories and Accu Standard Inc.(USA).

Individual congener and congener group analyses were performed on a 10ppm solution of each PCB sample after the addition of ¹³C-labeled internal standards. Coplanar PCB analysis was preceded by an HPLC carbon, or aluminium oxide, chromatographic step to separate the coplanar PCBs.

HRGC-HRMS was performed on a KRATOS Concept 32 MS with a Shimadzu GC 14A fitted with a DB-5 (60m, 0.32mm, 0.25µm) capillary column. The MS was operated at a resolution >12,000 in an attempt to reduce the interference of fragment ions from higher chlorinated PCBs with lower chlorinated congeners. Two ions were monitored for each congener group and isotope ratios were compared to the theoretical values. Individual congeners were identified by comparison to reference standard solutions and published data^{4,5)}.

3. Results and Discussion.

Figure 1 shows homologue profile of the commercial PCBs analysed on a weight % basis. Also

ANA (po)

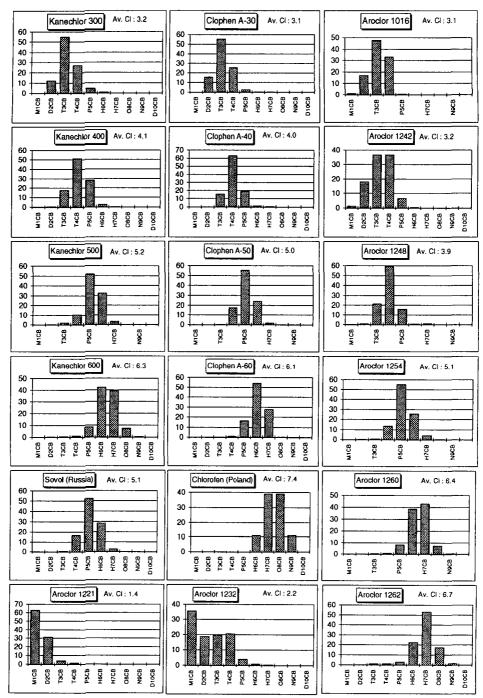


Figure 1. Homologue Profiles of Commercial PCB Samples.
(All data are on a weight % basis)

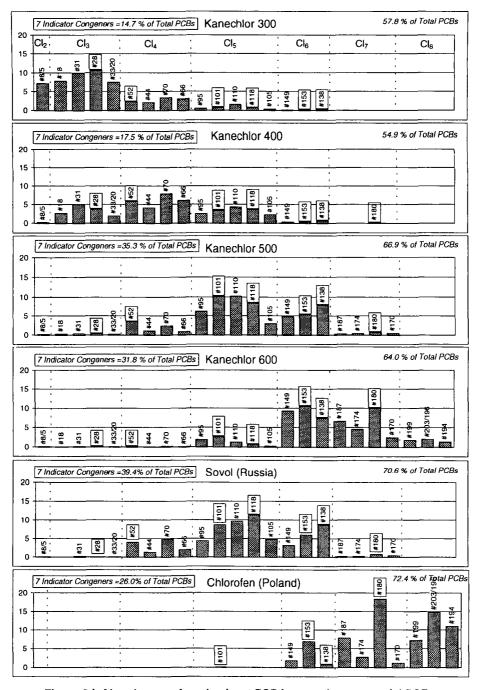


Figure 2-i. Abundances of predominant PCB isomers in commercial PCBs.

(Data are on a weight per cent basis)

ANA (po)

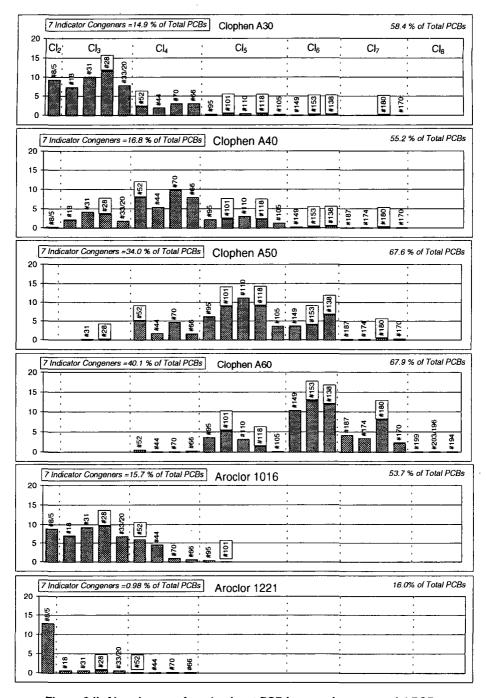


Figure 2-ii. Abundances of predominant PCB isomers in commercial PCBs.

(Data are on a weight per cent basis)

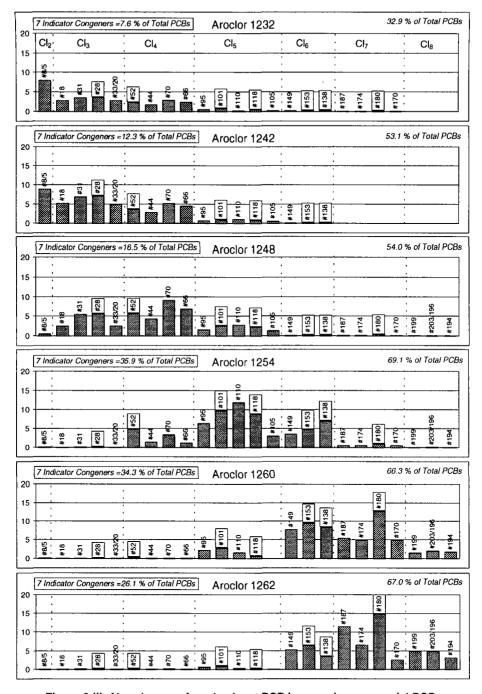


Figure 2-iii. Abundances of predominant PCB isomers in commercial PCBs.

(Data are on a weight per cent basis)

ANA (po)

shown is the average number of chlorine per molecule calculated after converting the data to molar basis. From these data it can be seen that certain of the PCB samples posses similar homologue profiles and a similar average chlorine content.

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Kanechlor 300 ≈ Clophen30 ≈ Aroclor1016

Kanechlor 400 ≈ Clophen40 ≈ Aroclor1248

Kanechlor 500 ≈ Clophen50 ≈ Aroclor1254 ≈ Sovol

Kanechlor 600 ≈ Clophen60 ≈ Aroclor1260
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The samples with the highest chlorine content are Aroclor 1262 and Chlorofen (highest) with Arochlor 1221 and 1232 exhibiting the lowest chlorine contents. The data for are in general agreement with that published previously^{5,6,7)}.

Figure 2 shows individual abundances of 24 predominant PCB congeners (IUPAC number given and dotted line indicates different levels of chlorination) in the commercial PCBs. The congeners shown for all samples are those chosen previously⁴⁾ as characteristic of a Kanechlor mixture (KC-300,400,500,600=1:1:1:1 wt. basis). These 24 congeners represent between 16% to 73% of the total PCBs in each sample.

The indicator congeners shown by a boxed IUPAC number are designated for waste oil analysis in the Netherlands(all 7) and Germany(6; #118 is excluded). These 7 congeners account for 0.98% to 40% of the total PCBs in each sample analysed.

Because of the low degree of chlorination in Aroclors 1221 and 1232, the congeners shown are not representative of these samples. If these samples are excluded, the proportion of the total PCBs accounted for by the 24 and 7 displayed congeners rises to 53% to 73%, and 12% to 40%, respectively.

Acknowledgment

A gift of Sovol, Chlorofen and Clophens from Dr. N. Kannan of the Institute of Marine Research, University of Kiel, Germany is gratefully acknowledged.

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