Gas Chromatography and Mass Spectrometry of Polychlorinated Terphenyls (Aroclor 5460)[1,2]

by

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Polychlorinated terphenyls (PCT's) are chemically similar to polychlorinated biphenyls (PCB's), chlorinated naphthalenes (CN's) and chlorinated insecticides and have been found in environmental samples(ZITKO et al. 1972, VILLENEUVE et al. 1973). The effects of ingestion of the PCT mixture Aroclor 5460 on experimental animals have been reported (ADDISON et al. 1972, ALLEN and NORBACK 1973). This paper presents gas chromatographic-mass spectral (GC-MS) data of the analysis of a PCT mixture, Aroclor 5460 (Monsanto), including the number of chlorines per molecule for the GC-separated components.

INSTRUMENTAL CONDITIONS

A Finnigan 1015C GC-MS system was used with a 183 cm x 2 mm id glass column packed with 3% OV-210 on 100/120 mesh Gas Chrom Q (fluidized). The column conditions were: column temperature, 225° C isothermal; injector temperature, 273° C; flow rate 25 ml/min helium at ambient temperature. The conditions used for mass spectrometry were: manifold temperature, 140° C; ion source pressure, 10^{-6} torr; filament current, 500 μA; electron voltage, 70 eV; electron multiplier, 2.9 kV. One second scans were made from 14 m/e to 650 m/e.

Materials

Aroclor 5460 was dissolved in hexane at a concentration of 625 μg/μl for GC-MS analysis.

RESULTS AND DISCUSSION

Aroclor 5460 was separated into 15 major peaks as shown in Figure 1. The chlorine content of peaks 1 through 14 as determined from mass spectral data is shown in Table 1. The concentration of

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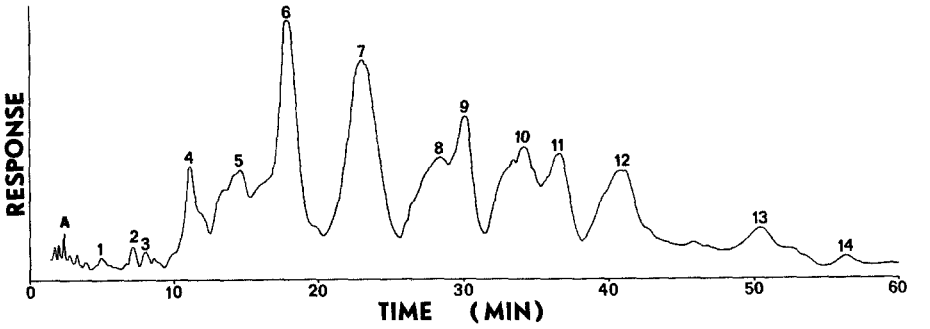

Figure 1. Gas-Liquid Chromatogram of Aroclor 5460 (Total Ionization Detector).

TABLE 1

Chlorine content and parent ion of peaks 1 through 14 of Aroclor 5460.

Peak Number	No. Chlorine Atoms/Molecule	m/e Parent Ion
1	5	400
2,3	6	434
4,5	7	468
5,6	8	502
6-11	9	536
10-13	10	570
14	11	604

a number of minor components was too low to permit mass spectral analysis. The mass spectra of peak A (Figure 1) suggests that it is a PCB with seven chlorines per molecule, the parent ion having a mass of 392. The mass spectra for peaks 1 and 14 were weak due to the low concentration of these compounds in the Aroclor 5460 mixture. The parent ions for these peaks correspond to those for PCT's containing five and eleven chlorine atoms per molecule, respectively (Table 1). A semi-logarithmic plot of the retention time of these peaks versus the chlorine atoms per molecule, further supports their identity.

Rote and Morris (1973) using a unit resolution, computer-controlled GC-MS system and isotopic abundance ratios, calculated the theoretical probability of the occurrence of ions of different masses in the molecular clusters for PCB's, CN's and PCT's. Table 2 shows the masses of the ions they calculated to be most abundant for each PCT of a given chlorine content. The mass spectral analysis of Aroclor 5460 shows good agreement between the data obtained and that presented by Rote and Morris (1973). An exception

was peak 1 with five chlorine atoms per molecule for which the parent ion at m/e 400 and the M+2 ion at m/e 402 appeared to be of equal intensity, (Table 2). This finding could, however, be due to the low concentration of the component available for analysis.

TABLE 2

Comparison of the masses of the most abundant ions predicted by Rote and Morris (1973) to the observed ion intensities for the penta- through undecachloroterphenyls of Aroclor 5460.

Peak No.	No. Chlorine Atoms/Molecule	m/e of most abundant ion predicted by Rote and Morris (1973)	m/e of most intense ion observed
1	5	402	400 and 402
2,3	6	436	436
4,5	7	470	470
5,6	8	506	506
6-11	9	540	540
10-13	10	574	574
14	11	608	608

Gas chromatographic-mass spectral analysis of Aroclor 5460 made it possible to separate and identify the penta- through undecachloroterphenyls on the basis of their GC retention times and mass spectra. PCT's with higher levels of chlorination, if they exist, were not resolved under the conditions employed.

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