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DETERMINATION OF POLYCHLORINATED BIPHENYLS AND ORGANOCHLORINES BY DUAL COLUMN GAS CHROMATOGRAPHY

by

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This paper is dedicated to the memory of

Dr. P. Goulden

A scientist, a colleague, and a friend

MANAGEMENT PERSPECTIVE

A compound (congener) specific analysis for polychlorinated biphenyl (PCB) mixtures in environmental samples was developed for the National Water Quality Laboratory (NWQL) for their routine analytical operations. The method is unique in that dual column chromatography is used. One column, termed the working column, is used for identification and quantitation of the congeners in the sample. The second column is employed to confirm the presence of the congeners. Only when a compound is identified on both columns is its concentration included in the total. The concentration of a particular congener can be checked from the results on both columns to ensure coeluting impurities or negative peaks do not enhance the concentrations. In addition, guard columns are used before the working columns. Preliminary studies show that the method is accurate and precise over the concentration range found in environmental samples. Use of this method reduces the time of analysis and the time required to interpret the chromatograms. Use of the results at the congener level will assist those researchers involved with the fate of particular PCB's in the environment.

Dr. J. Lawrence
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PERSPECTIVE ADMINISTRATIVE

Le Laboratoire national d'analyse de la qualité de l'eau (LNQE) a mis au point une méthode d'analyse pour les mélanges de biphényles polychlorés (BPC) spécifiques à un composé (congénère) d'un des échantillons environnementaux pour leurs travaux analytiques ordinaires. Le caractère particulier de cette méthode est l'utilisation de la chromatographie à colonnes jumelles. Une colonne, appelée colonne de travail, est utilisée pour l'identification et l'analyse quantitative des congénères de l'échantillon. La deuxième colonne est utilisée pour confirmer la présence des congénères. La concentration d'un composé n'est ajoutée au total que si celui-ci est identifié par les deux colonnes. La concentration d'un congénère en particulier peut être vérifiée à partir des résultats des deux colonnes pour vérifier que la coélution des impuretés (ou pics négatifs) n'augmente pas les concentrations. De plus, on peut utiliser des colonnes de purification avant les colonnes de travail. Les études préliminaires montrent que cette méthode est suffisamment exacte et précise pour les plages de concentration observées dans les échantillons de l'environnement. L'utilisation de cette méthode réduit la durée de l'analyse et le temps requis pour l'interprétation des chromatogrammes. L'utilisation des résultats obtenus pour les congénères sera d'un grand secours pour les chercheurs qui étudient le devenir d'isomères particuliers de BPC dans l'environnement.

Dr J. Lawrence

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ABSTRACT

A method has been developed that utilizes dual capillary column gas chromatography with split/splitless injection to determine congener concentrations of polychlorinated biphenyls. A particular congener must be confirmed in the response from both GC columns before it is considered being present in the sample and then the concentration of the congener is included in the total PCB concentration. Prior to establishing the method, the following aspects were checked: reproducibility of the injector; linearity of the detector response to these compounds; influence of guard columns; and the influence of OCs that coelute with the PCBs during the cleanup stages. The positive resolutions of these possible problems showed linear responses of the detectors over a concentration range of 2200 ppb to 40 ppb with reproducibility as measured by the coefficient of variance being 10% or less for each congener. Simultaneously, the method analyses those OCs which are collected in the same fraction during the cleanup stages. Two computer programs were developed, one to determine the means, standard deviation, and other statistical values from the result files of multiple injections of the same solution and the other to provide an output that correlates the results of the analysis from both columns and separates the results into the degree of chlorine substitution on the PCBs. The method provided excellent results when standards were run and was used to analyze environmental samples.

RÉSUMÉ

On a élaboré une méthode utilisant la chromatographie gazeuse à colonnes capillaires jumelles avec ou sans injection partagée pour déterminer les concentrations des congénères des biphényles polychlorés. Il faut confirmer la présence d'un congénère particulier dans la réponse des deux colonnes de CG avant de considérer que celui-ci est présent dans l'échantillon et d'ajouter la concentration de ce congénère à la concentration totale de BPC. Avant le développement de cette méthode, les aspects suivants ont été vérifiés : caractéristiques de reproductibilité de l'injecteur; linéarité de la réponse du détecteur pour ces composés; influence des colonnes de purification et influence des composés organiques qui sont coélués avec les BPC au cours des étapes de purification. La solution de ces problèmes possibles a indiqué des réponses linéaires des détecteurs sur une plage de concentrations de 2200 à 40 parties par milliard,avec une reproductibilité de 10 % ou moins pour chaque congénère, d'après des mesures du coefficient de variance. En même temps, cette méthode permet d'analyser les composés organiques qui sont recueillis dans la même fraction au cours des étapes de purification. Deux programmes d'ordinateur ont été élaborés, un pour calculer la moyenne, l'écart-type et d'autres valeurs statistiques à partir des fichiers des résultats des injections multiples de la même solution et l'autre, pour obtenir des valeurs permettant de corréler les résultats de l'analyse des deux colonnes et de séparer les résultats selon le degré de substitution par le chlore de ces BPC. Cette méthode a fourni d'excellents résultats lors de l'analyse d'étalons et elle a été utilisée pour analyser des échantillons environnementaux.

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1.0 INTRODUCTION

Polychlorobiphenyls (PCBs) are introduced into the environment by Aroclor or like mixtures, which are commercial preparations of PCBs whose designation (e.g., 1221) reflects the percent of chlorine in the formulation. There are a maximum number of 209 PCBs ranging from mono chlorine substitution to ten chlorine atoms substituted in the ten available ring sites with each compound of the 209 being called a congener of the PCB family (the numbering of the PCB congeners is shown in Appendix A). These man-made chemicals have been judged to be deleterious to the environment (National Research Council, 1978) so their ongoing monitoring in environmental samples is a necessity.

At present, routine analytical laboratories are using packed column chromatography and calculating the concentrations of PCBs using the Webb-McCall method (Webb and McCall, 1973) or a variation of this method (Water Quality Methods Manual). The single column methodology is based on the response for Aroclor mixtures rather than individual PCB congeners and does not allow for confirmation of suspected PCB contributors. Also, there is some subjectivity in that method as selecting and ratioing peaks with respect to Aroclor standards requires a high degree of consistency. Our objective was to establish a method that uses dual columns, requires minimum interpretation from the analyst and is based on the contribution of the congeners not their mixtures which could partially weather in the environment thereby yielding biased results. This report describes the successful steps taken to achieve this goal.

2.0 METHODOLOGY

A Hewlett-Packard 5890 gas chromatograph equipped with an HP 7673A auto sampler, a split/splitless injector, dual EC detectors and two HP 3392a integrators was used. The operation of the sampler and

the GC as well as the data collection was controlled by the Laboratory Automated System (LAS) package of the RTE-A software of an HP 1000 computer. Information collected by the computer could be printed out on an HP 2934A printer, plotted on a HP 7550a plotter equipped with the CPLOT software, or stored on tape using an HP 7294ST tape drive unit. The computer is equipped with a FORTRAN compiler. Operating conditions for the gas chromatograph are listed in Table I. Each of the analysis requires about one hour. The LAS software permits the user to enter the retention times and response factors for up to 125 individual peaks in a calibration table. The response factors could be entered by conducting a calibration run or manually after establishing the response factors over a series of concentrations as was done in this work for the organochlorines.

For most sequences of runs, there were initial injections of the solvent (isooctane) blanks and one PCB standard. For the remainder of each sequence, a solvent blank would be injected after every second sample. Care was taken to ensure that vial caps were crimped onto the vials so that they were snug. A cap which was too loose would allow some volatilization of the solvent and a cap too tight would cause a slight vacuum in the vial when the sample is withdrawn. For all injections and samples, the solvent was isooctane (Brudrick and Jackson).

Crosslinked columns for the study were supplied by HIRESCO of Mississauga, Ontario. Two columns were 30 m by 0.25 mm with a liquid phase thickness of 0.25 u. One of these was coated with OV-1 liquid phase and the other with SE-52 liquid phase. A third column was 25 m by 0.255 mm with liquid phase (SE-52) thickness of 0.1 u. Precolumns were supplied by SUPELCO Can. (Toronto, Ontario) and were 1 meter sections of inert fused silica capillary tubing,, 0.33 mm id. These were fastened to the working columns with butt connectors.

Standards for the organochlorines were obtained as authentic samples from E.P.A., Edison, N.J. These included 1,2-, 1,3-, and 1,4-dichlorobenzene. 1,,2,3-, 1,,2,4-, and 1,,2,3-trichlorobenzene, 1,2,3,4-tetrachlorobenzene, pentachloro- and hexachlorobenzene, α-, β-, and γ-lindane, α- and β-chlordane, α- and β-endosulphan, mirex, p,p'-DDT, o,p'-DDE, methoxychlor, p,p'-DDE, o,p'-DOT, endrin, dieldrin,

aldrin, hexachlorobutadiene, octachlorostyrene, photomirex, endrin aldehyde, 1,2-dibromobenzene, 1,2,3-tribromobenzene and 1,2,3,4-tetrabromobenzene.

Aroclor mixtures 1221, 1254 and 1016 were obtained from the U.S., E.P.A. Depository and Aroclor 1262 was obtained from the same source but by way of Beak Consultants of Mississauga, Ontario. Decachlorbiphenyl was also obtained from the U.S., E.P.A. Depository. The mixtures were made up to selected concentrations in isooctane. Our calibration standard was a standard solution of 1000 parts Aroclor 1221, 500 parts of Aroclor 1016, 350 parts of Aroclor 1254 and 300 parts of Aroclor 1264 (Millen et al, 1983). To this mixture, 50 parts of decachlorobiphenyl was added.

Cleaned up sediment samples and standard sediment samples were supplied by the National Water Quality Laboratory and Water Quality Branch, Ontario Region.

3.0 METHOD SET UP

Preliminary work was carried out using single column gas chromatography. First the linearity of the detector response was established by injecting serial dilutions of Aroclor 1262 on an SE-52 column with ten injections of standard at each concentration. The results are presented in Table 2. Each entry is the mean of ten injections and the coefficient of variance (CV) is 5% or less for each entry. These values were obtained using a statistical program we developed for the HP system in the National Water Quality Laboratory (NWQL) and it is listed in Appendix B. This program can provide results in one hour which would require over a week's work using the conventional method of re-entering the data. The values listed in Table 2 indicate that the detector response is linear from 5 ppm to 41 ppt of Aroclor 1262. At moderate retention times of less than 35 minutes, the response is extremely linear as can be judged by examining the values for the concentrations of 5.0, .50 and .05 x 10^{-9} total PCB. A chromatogram of this Aroclor is shown in Fig. 1.

Next, it had to be established if there would be much interference between the peaks for the PCB congeners and those for the

OCs which elute with the PCBs in fraction A (OCAs) of the absorption chromatography cleanup step (Water Quality Methods Manual). The column was changed to one which had an OV-1 liquid phase as it was imperative that two columns of differing polarity be used for this study. The PCB standard was injected as was an OCA mixture, and finally a solution containing the PCBs and the OCAs. These were chromatographed on an OV-1 capillary column equipped with guard column. The results are listed in Table 3. As indicated in this Table, there are three PCB peaks that interfere with three OCA peaks. Two of the PCB peaks are minor contributors to the samples and expected to be minor contributors to any sample analyzed. Preliminary work indicated that the detector response was linear over the range of interest for this column.

The next step was to operate the system in dual column mode. A thin liquid phase SE-52 column was used in conjunction with the OV-1 liquid phase column. Good peak shape was obtained for the PCBs on both columns, as shown in Figs. 2 and 3. Analysis of the results indicate that the samples are split evenly between the two columns. The linearity of detector response was checked using dilutions of the standard over a range of total PCB from 2250 ppm to 24 ppb. Result are listed in Tables 4 and 5. Prior to working on the PCBs, OCs were quantitated with CVs of 5% or less for most of the 32 compounds (Scott and Misunis, 1989). For the PCB analysis, the same degree of reproducibility was expected. Later eluting peaks generally have high CVs, perhaps as the peaks are broader after spending longer times on the column. Also, the same degree of reproducibility is harder to achieve in dual column mode than in single column mode, especially when guard columns are used. Another factor is that in splitless/split injections, the reproducibility is not as good as in split mode (Onuska et al, 1983). The values for the CVs in the Tables are reasonable. At the lowest concentration levels injected, only about one third of the congeners are present in measurable amounts. There is a high degree of reproducibility on both columns with good linearity from 2250 to 24 ppb on both columns as measured by the bulk PCB concentration. The responses for each congener were subjected to a linear regression analysis to obtain the response factor, the correlation coefficient and the statistical minimum concentration (Long and Wineforderdner, 1983)

with the errors noted by (Scott and Misunis (1989). These results are shown in Table 6. The correlation coefficients are above .99 for most of the congeners and minimal detectable concentrations of less than 10^{-13}g.

Once the above steps had been completed, with the linearity, reproducibility, acceptable chromatography, and a reasonable split between the two columns established, a calibration mixture was injected. This had to be done manually, and was injected in triplicate. The precision was better than 3% for the majority of the peaks. The peaks corresponding to the various congeners contained in the calibration standard were assigned the appropriate Ballschmiter number (Ballschmiter and Zell, 1980) for both columns. This is shown in Figs. 4 and 5 and the relative response factor for each contributing congener was placed in the calibration table of the LAS software. The thin phase SE-52 column eluted the peaks earlier than the OV-1 column, and there were more co-eluting peaks on the SE-52 column. Accordingly, the OV-1 column would be the working column and the SE-52 column would be used for confirmation. The retention times and response factors for the OCAs were also entered into the calibration table at this time.

The congeners are numbered 1 to 209 and these numbers also denote the degree of chlorine substitution (these numbers are listed in Appendix A). However, the congeners do not necessarily elute in the same order on both columns and this makes it difficult to match the output for both columns. A program was created which matched peaks from both columns, listed the output as to degree of chlorine substitution and gives the total PCB concentration based on the particular congener being detected on both columns. This program is listed in Appendix C. Other compounds such as the OCAs are also part of the output of this program. For convenience in this report, this program will be referred to as Program 2.

With the relative response factors known for the PCBs, it is quite easy to calibrate the instrument. for the PCBs, this can be done in two ways. The first is to put a known amount of decachlorbiphenyl in each sample. While running Program 2, in one of its modes, the concentration of added decachlorobiphenyl is an input factor and the program automatically scales the results to the response for

decachlorobiphenyl and the response from the detector. The second method is to inject a known concentration of an Aroclor mixture. A value for the total concentration will be obtained from running Program 2. This is divided into the known value and subsequent results can be multiplied by this factor. Of the two methods of calibration, the authors recommend the second for two reasons. The first is that the Aroclor mixture will usually contain several PCB congeners, eluting over a ten minute time span. This will give a more representative response than the one which elutes at the very end of the chromatogram. The second reason is related to the first in that decachlorobiphenyl is the last compound of interest to elute on the chromatogram. From the preliminary work, we have found that those compounds which spend the greatest amount of time in the chromatographic column have the poorest precision. Therefore, calibration using this compound alone may lead to some error.

The computer report lists all PCB congeners detected in the sample on both columns. It is the task of the operator to assess these results. First, only those peaks that are detected on both columns will be considered in the total titled, "Confirmed". On both columns several congeners coelute. If this coelution is the same for both columns there is no problem. However, when there is a difference of coelution for the two columns, the analyst much check the computer result and make the appropriate adjustments. For example, congeners 118 and 149 may coelute on one column (e.g., A) but be separated on the other (e.g., B). Considering that "B" is the working column, the analyst must check that the peak corresponding to congeners 118+149 appear on "A". If this peak is present on "A" and both congeners are present according to the results from the "B" column, the concentration of the peak from congener 149 should be added to the confirmed total. Generally, one will find that the sum for these two congeners will approximate the value derived from the coeluted peaks. There are other instances of this. Another example of what the analyst must look for is an impurity coeluting with a particular congener. When this occurs there is usually a large discrepancy between the concentrations for the congener on the two columns. The analyst will generally subtract the value related to the impurity and include the value from the

confirmation column. The next problem the analyst must examine is large negative peaks, which alter the baseline. Those congeners which are affected will have enhanced concentrations. In this instance, the analyst may wish to exchange values from the confirmation column for those from the working column for those congeners which are affected. Finally, the presence of OCs may interfere with the PCB results and vice versa. Since the elution times are different on both columns for the PCB and OCs, it is simple to assign the correct concentration to the proper compound.

4.0 RESULTS

4.1 Standards

A series of Aroclors and Aroclor mixtures were analyzed using the first method outlined above. This was convenient as the volumes did not have to be adjusted for addition of the decachlorobiphenyl. The results are listed in Table 7. We deemed the agreement between the measured and actual concentrations as very good. Of the four samples listed, only one showed a marked difference. The other three have less than a 6% difference with the known concentration.

4.2 Standard Sediment

Before the method can be used on environmental samples, it must be demonstrated that it can measure PCBs in the presence of possible interferences from a sediment. First, the extract from standard reference sediment was analyzed by the new methodology. Using PCB congener concentrations derived from the results using the OV-1 column a total PCB concentration of 41.02 was calculated. Examination of the chromatogram (Fig. 6) shows that there is negative peak at 22 minutes. As the baseline is automatically tracked to include the minimum of peaks, the negative peaks enhances the contributions of those congeners or other compounds. The chromatogram derived simultaneously from the SE-52 thin liquid phase column (Fig. 7) exhibits a slight negative peak in the same elution range as the OV-1 column. Therefore, the concentrations of the congeners so affected on

the OV-1 results are replaced by those obtained from the SE-52 capillary column results. This is shown in Table 8, and the value for PCBs in the reference is now calculated at 37.4 ppb.

The next step is to add to the extract of a standard representative sediment, an aliquot of the standard PCB solution. Ten aliquots of this were then analyzed on the GC as were ten aliquots of the appropriate dilution of the PCB standard. The results measured as the means of the concentrations, coefficient of variance and retention times are listed in Table 9. These results show that for this sediment, the method reported here does produce reliable results as indicated by the CV values which are, for all congeners, low. In addition, the values about the negative peaks are also reproducible.

4.3 Samples

Previously, three sediment extracts had been analyzed using standard methods used by the NWQL for OCs (Methods Manual, DOE) and a modified Webb-McCall method for gross PCB concentration. The results for the OC analysis are listed in Table 10(a). There is very good agreement between the analysis by both methods, although the chromatographic methods used to obtain the results are not identical. The OCs reported here, elute in the time span anticipated for congeners in Aroclors 1221, 1016, and 1254 on the capillary columns used.

Listed in Table 10(b) are the PCB results. The first entries are the PCB values measured by this method and under these are the values determined previously. For two of the three samples, there is a factor of two difference between our measured values and the previously calculated value. The sample (Sample 3) that had been previously analyzed as having 24 ppb of PCB is actually below the reported detectable amount for that method. Our method produces a value of 54.4 ppb. The sample (Sample 1) that had been analyzed at 146 ppb was analyzed by us and found to contain 318 ppb of PCBs present. However, the chromatogram of this sample, shown in Fig. 8 exhibits a negative peak where many of the tetra- and pentachlorobiphenyls elute. The chromatogram from the other column (SE-52) does not have a negative peak, so for those peaks, the concentration values from the secondary

column are substituted. This produces a total PCB concentration of 279 ppb, 38 ppb lower than our original value. Using a single packed column gives an elution pattern where several congeners coelute. In an actual sample a specific peak may be several congeners or some other compound(s) that elute at that time. The expertise requires that one can detect PCB contributions from other non-PCB coeluters. With the dual column capillary method most of this guess work is removed, and since the method actually expects individual congeners to elute at specific times, interferences with the analysis is diminished. The other major advantage is that negative peaks are frequently found in chromatograms of sediment samples and with the dual columns, both elutants may not be influenced to the same extent, so that a reasonable estimate of the PCB concentration can be attained. Accordingly, the value reported here is probably a closer estimate of the actual PCB concentration in the sample. The value from the third sample agrees for both methods, but in light of what was said above this may be fortuitous. The latter part of Table 10(b) lists the contributing congeners and their concentrations, grouped as per degree of substitution.

5.0 DISCUSSION

The availability of all 209 PCB congeners, (Mullin et al, 1984) make it possible to quantitate and qualify the majority of these compounds using capillary column gas chromatography. Using computer assisted gas chromatography, the analysis is considerably simplified. When using dual column gas chromatography with computer assistance, the results of the analysis of environmental samples are more dependable, as well as a participating congener listing being produced. Although a minimal detectable amount of 40 ppb total PCB is quoted for this work, the individual congeners are detected at considerably lower concentrations.

Using this analysis, the contributions of particular congeners to the total PCB concentration in a sample are obtained. If the result files are catalogued and samples from that particular site are analyzed over a long period of time, the variation of the

particular congeners can be ascertained. Some of the 209 congeners are more reactive than others, and their behaviour can be separated from the others using the congener specific analysis. Also, some congeners are more biologically active than others. A case in point is the effect of hexachlorosubstituted PCBs 136, 155, 153, 128 and 169 on chicks (McKinney et al, 1976). Another study investigated the influence of the planar congeners 15, 37, 77, 81, 126 and 169 to induce AHH (Safe et al, 1985). The four higher congeners only were found to induce AHH and bind to the cytosolic receptor protein. This method permits the analysis of congeners of interest so similar studies in the aquatic medium can be undertaken. Their presence can be readily detected and monitored from site specific samples. The methodology presented here provides a step forward for analyzing aquatic samples for a broad spectrum of compounds.

This concept is important, as it provides the thrust of a research program of which the methodology presented here represents one part. When analyzing environmental samples, often only target compounds are requested. These target compounds represent only a small portion of all peaks present in the resulting chromatogram. The more that computer programs can assist the analyst in identifying peaks from a complicated pattern of peaks, and also identify more peaks from that pattern, the more understanding we will have as to contaminants in the aqueous phase. This added information will benefit researchers and those responsible for managing the aquatic ecosystem.

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TABLE 1

CHROMATOGRAPHIC DETAILS

INSTRUMENT: H.P. 5890 GAS CHROMATOGRAPH
DETECTORS: Dual Electron Capture
INTEGRATORS: H.P. 3390 - 2
AUTOSAMPLER: H.P. 7673

CARRIER GAS: H_2 MAKEUP GAS: Ar:Me (95:5)

COLUMN HEAD PRESSURE: 20 psi

INJECTION: Split/splitless

PURGE TIME: .75 min

INITIAL TEMPERATURE: 80°C INITIAL TIME: 2 min.

FIRST RAMP: 10°C/min FINAL TEMPERATURE: 140°C

FINAL TIME: 0.0 min.

SECOND RAMP: 2°c/min FINAL TEMPERATURE: 245°C

FINAL TIME: 0.0 min.

PEAK WIDTH: 0.060 from 0 to 25 min
0.080 from 25 to 48 min
0.10 from 48 to 60 min

TIME OF RUN : 60.5 min.

TABLE 2

AROCHLOR 1262 DILUTION SERIES

CONGENER NUMBER	Response in Area Units					
	Concentration ($X10^{9}$ g)					
	5.0	2.0	1.0	0.50	0.050	0.041
95+66	1177220	420379	208252	113397	11581	9004
101	1293978	461582	225091	121775	12896	10075
136	1010720	369893	184840	103710	10226	7722
151	3216734	1140210	559779	308696	32959	25126
144+153	1369333	486479	239271	130722	12307	9470
149	5567733	2022980	1010206	564430	64260	50490
146	703551	252637	120618	66521	6649	5131
131	7507100	2703140	1328850	730356	76006	59547
141	4699001	1636860	791515	440599	46175	36101
137+130	799458	291654	143282	79929	8018	6086
138	4902512	1626500	740932	421922	41792	32118
178	1390456		240857	133212	12853	10697
187+182	7354968	2673550	1327810	747434	75865	59846
183	3081945	1055601	497199	275355	27408	21597
185	1119589		176189	99894	10346	7879
174	5707268	1983860	942060	516448	51745	40621
177	2671434	931365	440419	243941	24192	18983
171	2074000	722211		193995	18600	14433
173	663080	239523	115624	66445	6440	4893
204	869838	307141	149548	85809	8360	6539
180	12912446	4446121	2093140	117730	107205	86650
191	675268	243612	117935	68507	6417	5263
170+190	4327333	1377600	608792	322195	32969	25436
201	5459167	1878050	880479	492264	46793	37235
203+196	6384656	2106540	948591	529947	50132	40398
195	2014778	656564	296967	169562	16650	13111
194	4738045	1507380	665903	364363	35392	28321

TABLE 3

COMPARISON OF RESPONSES FROM PCB MIXTURE, ORGANOCHLORINE STANDARD AND THEIR COMBINATION

RETENTION TIME or CONGENER NUMBER	COMBINATION AREA	CV	PCB AREA	CV	OC AREA	CV	
2.65	34826	30			24879	28	
2.82	70220	4.7			67400	4.6	
4.44	36991	4.8			39739	4.0	
4.58	188966	2.5			187353	4.7	
4.82	668435	3.0			644300	3.8	
4.90	29035	16			48763	19	
5.06	12579	6.0			30326	13	
5.17	31641	5.8			12968	6.2	
5.25	38536	4.7			39529	9.1	
5.44	26948	4.6			24463	10	
6.45	67300	2.5			69600	7.8	
7.13	370658	2.3			359695	5.1	
7.80	5980	4.4	6341	13			
8.69	82378	15			80378	3.7	
5+8	70212	16	28610	1.5	49689	3.3	(78299)
13.03	91507	3.5			91097	4.5	
13.75	217518	3.2	4197	5.4	209628	4.8	(213825)
14.57	48758	2.2			48498	3.5	
18	31711	3.3	44323	1.8			
17	17268	3.8	25122	2.1			
16+32	36589	2.7	34573	2.1			
26	4056	5.5	5709	2.6			
31+28	45999	2.1	59945	3.6			
33+53	15902	3.6	31855	3.0			
19.10	68646	1.9			62771	4.1	
22	10050	4.0	14312	2.6			
45	5261	3.8	6570	3.1			
49	17471	4.6	19774	3.2			
21.53	271833	3.6			261538	4.8	
47	20259	23	45688	6.0			
44	27208	3.9	25634	4.1			
42	10897	4.8	14437	4.6			
64+41	21822	6.1	24581	3.9			
40	4917	12	5335	6.1			
24.69	70874	2.5			70456	4.8	
74	8371	4.8	15359	5.1			
70+76	20069	11	37243	4.7			
95+66	56770	5.9	50476	3.8			
91	5913	5.2	4715	4.1			
26.58	60052	3.2			60430	5.0	

TABLE 3 (CONT.)

Rt or #	COMBINATION AREA	CV	PCB AREA	CV	OC AREA	CV	
56+60	10334	6.1	18047	5.3			
84	9105	5.2	5094	4.9			
90	69749	3.7	11117	5.1			
27.71	51554	5.6			61135	5.1	
89	16298	5.8	24066	4.8			
97	12536	6.0	14685	5.2			
29.58	99910	3.9			98174	5.5	
87	24588	6.1	22676	5.6			
136	83272	5.6	8835	3.5	66986	11	(75731)
110	47071	6.1	43861	5.4			
31.24	59380	7.3			60859	9.0	
82	5733	8.1	8591	14			
151	20060	7.1	17691	8.3			
32.16	85188	5.0			75278	7.3	
149+ 118	55692	6.4	45254	5.1			
33.86	215921	5.8			228236	8.9	
141	26560	7.1	24643	6.1			
36.89	83135	9.3			122010	11	
138	57106	9.6	56559	7.4			
178	4934	7.7	5028	3.0			
187+ 182	25144	8.3	23601	6.9			
183	11304	8.6	11171	8.5			
39.56	59315	6.1					
39.89	12113	12			62355	9.6	
174	22018	8.3	21400	8.8	10297	16	
177	11419	9.1	10818	8.2			
42.44	61105	12			70849	16	
180	37217	13	37076	11			
43.88	100144	7.4			105987	10	
170	16840	37	16330	10			
201	9181	11	8890	12			
203	10453	11	9916	11			
195	4008	10	3744	10			
194	7843	18	7487	12			

TABLE 4

PEAK HEIGHTS AND CV'S FOR PCBS
ELUTED FROM OV-1 COLUMN

CONGENER		CONCENTRATION (total ppb impinging on detector)			
RT	#	2250	1125	563	285
8.67	1	94545(1.2)	50710(1.9)	27435(2.5)	15920(13.)
9.89	2	22558(4.9)	16881(8.9)	7253(8.4)	7142(20.)
10.60	4+10	59160(1.9)	32258(2.0)	16986(2.5)	9565(4.8)
11.66	7	100338(2.6)	48024(2.7)	22798(3.2)	12366(2.6)
12.06	6	84628(2.2)	42501(2.4)	20923(2.9)	11482(2.5)
12.30	8+5	308658(2.2)	158024(2.6)	77712(3.1)	42174(2.7)
13.12	13	11053(2.3)	5634(2.6)	2802(3.9)	1533(3.9)
14.14	12	12354(4.0)	6245(3.7)	2994(4.0)	1612(5.4)
14.36	18	122003(2.6)	64177(2.8)	32594(3.0)	18203(3.5)
14.46	17	70162(3.0)	35356(3.1)	17694(2.7)	9913(4.5)
14.90	24+27	12945(4.5)	6453(5.0)	3312(3.4)	1802(5.2)
15.24	16	60854(2.7)	30132(2.7)	14902(3.0)	8231(3.1)
16.22	29	1973(3.6)	945(2.9)		
16.46	26	16918(3.5)	8476(2.9)	4137(3.4)	2273(3.0)
16.56	25	10709(3.4)	5404(2.8)		
16.93	31+28	146218(4.1)	65563(3.5)	29079(3.9)	15694(2.7)
17.49	33	78978(4.0)	38336(3.3)	18380(3.6)	10012(3.3)
17.84	22	41858(4.2)	19942(3.2)	9587(3.4)	5248(2.9)
18.19	45	15872(3.1)	8073(2.9)	4029(2.9)	2182(4.5)
18.64	46	6456(3.1)	3401(4.8)	1633(2.8)	904(5.1)
19.23	52	49839(3.2)	25530(2.8)	12742(3.1)	7014(4.0)
19.49	49	42520(3.5)	21245(2.8)	10468(3.2)	5704(3.7)
19.66	48	19091(3.3)	9413(3.2)	4712(3.2)	
19.74	47	23926(3.5)	11985(2.9)	5977(3.2)	3246(3.2)
20.42	44	56154(3.8)	28347(3.5)	13843(3.7)	8091(4.9)
20.61	42	28779(4.0)	14390(3.4)	7211(3.8)	4122(4.6)
21.21	41+71	56034(4.3)	27053(3.5)	12933(3.6)	7028(3.3)
21.63	40	11602(4.0)	5916(3.1)	2921(3.2)	1590(3.2)
22.44	31	1208(4.5)			
23.01	74	7278(4.8)	3781(4.2)	1821(4.2)	900(4.9)
23.28	70	12543(4.6)	6461(3.5)	3124(4.4)	1712(5.0)
23.58	95	40979(3.7)	20745(3.0)	10391(3.5)	5676(4.2)
23.98	91	2029(3.7)	1036(3.2)		
24.50	60	2229(5.0)	1178(3.8)	561(4.0)	
24.91	84	2838(4.1)	1446(3.5)	707(4.3)	
25.11	89	4229(3.8)	2158(3.7)	1057(4.7)	
25.53	101	37868(4.4)	19103(3.1)	9384(3.8)	5119(3.8)
26.90	97	987(5.3)	515(1.5)4		
27.23	87	4103(5.1)	2123(3.2)	1037(4.8)	566(4.5)
27.69	136	23825(4.0)	12186(3.2)	6153(3.7)	3307(4.3)
27.99	110	12241(4.9)	6296(3.6)	3097(4.7)	1682(3.2)
28.59	82	1822(8.4)			
29.28	151	58029(4.6)	29100(3.6)	14452(4.0)	7883(3.7)
29.54	135	20129(4.4)	10220(3.6)	5130(4.4)	2796(3.8)

TABLE 4 (CONT.)

PEAK HEIGHTS AND CV'S FOR PCBS
ELUTED FROM OV-1 COLUMN

CONCENTRATION (ppb)

RT	CONGENER	2250	1125	563	285
30.14	149+181	27744(4.7)	64792(3.8)	31898(3.9)	17124(3.6)
30.78	134+114	4433(4.9)	2280(4.0)	1124(6.3)	618(15)2
31.35	131	1023(5.6)			
31.94	105+146	33128(5.4)	16660(3.3)	8194(4.3)	4463(3.8)
32.32	153	128550(5.9)	64898(4.0)	30969(4.7)	16499(3.8)
33.18	141	72290(5.5)	36302(3.5)	17872(4.3)	9639(4.0)
33.76	137+130	13161(5.3)	6758(3.3)	3386(3.9)	1807(3.5)
34.16	138	84527(6.8)	41036(4.0)	19633(9.9)	10486(6.7)
34.40	158	8433(6.0)	4436(3.9)	2074(4.5)	
35.30	178	18421(5.4)	9463(3.7)	4685(4.5)	2531(4.1)
35.71	175	3406(5.8)	1726(3.8)	842(4.3)	
35.94	182	114865(6.0)	57933(4.0)	27921(4.9)	14927(4.1)
36.34	183	44797(6.1)	22545(3.9)	11013(4.8)	5955(4.2)
36.69	167	1281(26.)			
37.07	185	12178(6.2)	6433(3.4)	3193(5.1)	1747(3.6)
37.58	174	88473(6.8)	44290(3.9)	21299(5.0)	11378(4.0)
37.87	177	43378(6.6)	22044(3.7)	10751(5.3)	5795(4.0)
38.22	156+171	18204(6.9)	9494(4.1)	4726(5.5)	2531(5.2)
38.57	157	11961(5.8)	6159(4.0)	3087(5.2)	
39.19	173	7978(6.3)	4168(3.5)	2064(4.9)	
39.52	200	9817(6.9)	5257(4.0)	2565(5.6)	1376(5.2)
39.77	172	1963(6.5)	1025(4.6)		
40.03	180	165641(8.5)	81855(4.6)	37251(6.3)	19582(4.8)
40.27	193	9559(7.0)	5017(3.9)	2489(5.9)	
40.57	191	2703(7.2)	1431(4.7)		
40.84	199	8129(6.5)	4275(3.6)	2140(5.3)	1094(6.6)
41.97	170	41411(8.9)	21568(4.3)	10322(6.5)	5628(4.7)
42.18	190	10093(7.7)	5531(4.5)	2728(6.8)	1478(4.7)
43.24	201	51849(8.1)	27335(4.5)	13063(6.1)	7234(4.8)
43.67	203+196	52518(8.5)	27444(4.4)	13229(6.0)	7232(5.0)
44.58		921(9.1)			
45.64	195	14434(8.3)	7850(3.9)	3894(6.6)	2103(5.5)
46.04	207	3148(8.4)	1597(5.5)	794(6.3)	
47.59	194	36074(10.)	19516(5.0)	9443(7.8)	5204(5.8)
48.09	205	1690(8.7)	959(4.5)		
50.77	206	12449(9.8)	7014(5.0)	3476(8.3)	1898(7.1)
53.29	209	90414(11.)	49159(5.1)	24018(8.5)	13041(7.4)

TABLE 4 (CONT.)

PEAK HEIGHTS AND CV'S FOR PCBS
ELUTED FROM OV-1 COLUMN

CONCENTRATION (ppb)

RT	CONGENER	225	113	56	28
8.67	1	12206(2.2)	6378(2.8)	3247(2.8)	1670(1.9)
9.89	2	4884(3.3)	3449(2.0)	5290(26.)	7097(35.)
10.60	4+10	7204(2.7)	3615(2.7)	1780(3.7)	856(5.4)
11.66	7	9089(2.7)	4465(3.4)	2260(3.0)	1185(1.5)
12.06	6	8504(2.6)	4182(3.2)	2093(3.1)	1069(2.6)
12.30	8+5	31107(2.5)	15137(3.2)	7586(2.8)	3954(2.0)
13.12	13	11302(2.5)	5575(3.3)		
14.14	12	1196(4.4)	537(4.1)		
14.36	18	13746(2.7)	6802(3.1)	3383(2.7)	1704(1.9)
14.46	17	7490(2.5)			
14.90	24+27	1341(4.6)	646(5.7)		
15.24	16	6152(3.0)	3017(3.3)	1523(3.0)	761(2.1)
15.31					
16.22	29				
16.46	26	1621(14.)	769(12.)		
16.56	25				
16.93	31+28	11660(3.0)	5578(3.5)	2781(3.6)	1438(3.0)
17.49	33	7492(2.7)	3672(3.5)	1921(2.7)	1037(5.9)
17.84	22	3907(3.1)	1878(4.1)	936(3.9)	
18.19	45	1607(2.5)	787(4.2)		
18.64	46	689(4.9)			
19.23	52	5345(3.5)	2605(3.4)	1330(3.3)	645(3.0)
19.49	49	4315(2.8)	2106(3.4)	1063(4.0)	
19.66	48				
19.74	47	2445(2.6)	1187(3.2)		
20.42	44	6074(3.4)	3328(3.8)		
20.61	42	3030(3.9)	1648(3.1)		
21.21	41+71	5285(2.9)	2594(3.6)	1346(3.7)	689(4.1)
21.63	40	1191(4.1)	568(2.2)5		
22.44	31				
23.01	74	754(4.8)			
23.28	70	1310(4.8)	577(4.2)		
23.58	95	4303(3.1)	2114(3.5)	1021(5.5)	
23.98	91				
24.50	60				
24.91	84				
25.11	89				
25.53	101	3878(3.4)	1881(4.1)	961(3.8)	
26.90	97				
27.23	87				
27.69	136	2494(2.9)	1227(4.2)	601(3.6)	
27.99	110	1270(3.8)	603(4.9)		
28.59	82	SOLVENT			
29.28	151	5936(3.3)	3018(4.0)	1643(4.9)	876(14.)
29.54	135	2117(3.6)	1081(4.6)		
30.14	149+181	12885(3.9)	6368(4.7)	3293(4.5)	1739(6.8)

TABLE 4 (CONC.)

PEAK HEIGHTS AND CV'S FOR PCBS
ELUTED FROM OV-1 COLUMN

RT	CONGENER	CONCENTRATION (ppb) 225	113	56	28
30.78	134+114				
31.35	131				
31.94	105+146	3339(4.0)	1624(5.4)	819(4.0)	
32.32	153	12411(3.8)	6004(5.4)	3077(4.2)	1613(5.8)
33.18	141	7263(3.9)	3614(5.0)	1849(4.2)	653(4.6)
33.76	137+130	1345(3.4)	658(3.7)		
34.16	138	7807(4.6)	3894(8.9)	1963(5.5)	1132(10.)
34.40	158				
35.30	178	1887(4.2)	902(5.1)		
35.71	175				
35.94	182	11205(4.4)	5451(5.6)	2792(4.7)	1465(5.7)
36.34	183	4451(4.7)			
36.69	167				
37.07	185	1297(4.5)	625(5.4)		
37.58	174	8525(4.4)	4211(5.7)		1136(6.2)
37.87	177	4311(4.2)	2112(5.9)	1036(4.3)	569(5.7)
38.22	156+171	1882(4.8)	899(6.9)		
38.57	157	1213(4.4)	600(4.7)		
39.19	173	833(6.1)			
39.52	200	1000(6.0)			
39.77	172				
40.03	180	14380(4.4)	6945(7.3)	3517(5.5)	1976(7.6)
40.27	193				
40.57	191				
40.84	199	794(4.5)			
41.97	170	4200(4.7)	2058(6.7)	962(9.5)	523(8.0)
42.18	190	1113(5.3)7			
43.02	198				
43.24	201	5679(11.)	2700(6.5)	1354(7.4)	843(8.6)
43.67	203+196	5315(5.3)	2642(6.2)	1320(5.5)	756(7.8)
44.58					
45.64	195	1542(5.3)	754(8.7)		
46.04	207				
47.59	194	3791(6.0)	1870(8.7)	924(6.9)	561(11.)
48.09	205				
50.77	206	1354(6.3)	656(8.5)		
53.29	209	9233(6.5)	4774(9.3)	2395(7.2)	3611(10.)

TABLE 5

PEAK HEIGHTS AND CV FOR PCB CONGENERS
ELUTED FROM SE-52 COLUMN

RT	CONGENER #	CONCENTRATION (total ppb impinging on detector) 2250	1125	563	282
9.82	1	72991(1.2)	40262(1.9)	21467(2.6)	12594(3.1)
11.53	3	16998(2.0)	8863(2.6)	4468(3.6)	2474(3.9)
12.28	4+10	48060(1.8)	26878(1.8)	14181(2.6)	8200(3.2)
13.47	7	81912(2.2)	41927(1.9)	20751(2.9)	11722(4.3)
14.02	6	66110(1.9)	35019(1.8)	17764(2.7)	10134(4.1)
14.32	8+5	236508(1.8)	126220(1.9)	63928(3.0)	36282(4.0)
15.45	13		4541(1.9)	2278(2.6)	
16.55	12	9002(3.1)	4638(2.3)	2229(4.5)	1281(6.6)
16.80	18	86988(2.4)	46865(2.1)	24221(3.1)	13851(4.0)
16.89	17	69531(2.5)	36900(2.1)	18789(3.3)	10635(4.9)
17.44	24+27	9899(2.7)	5155(2.5)	2617(3.2)	1397(7.4)
17.96	16+32	69369(2.6)	36012(2.2)	18166(3.2)	10285(4.4)
18.81	29	1940(3.4)	1053(3.2)		
19.21	26	14940(3.1)	7861(1.6)	3922(3.4)	2247(11.)
19.35	25	9080(2.9)	4827(1.9)	2398(3.8)	1383(15.)
19.80	28+31	124364(3.3)	59808(2.3)	28446(4.2)	15814(7.0)
20.48	33	68744(3.1)	34899(2.2)	17318(3.9)	9781(5.8)
21.00	22	34030(3.3)	17266(2.1)	8556(4.1)	4803(7.2)
21.36	45	12948(3.1)	6702(2.4)	3404(3.7)	1884(6.4)
21.93	46	5112(3.0)	2632(2.8)	1338(3.7)	725(2.1)
22.38	52	41854(3.1)	21974(2.1)	11182(3.7)	6293(6.4)
22.67	49	34462(3.0)	17760(2.0)	9019(3.6)	5046(5.2)
22.88	47+48	23731(3.2)	12289(2.3)	6209(3.7)	3466(4.6)
23.55			SOLVENT		
23.86	44	46346(3.2)	24448(2.6)	12203(3.8)	7488(11.)
24.07	42	24730(3.3)	13013(2.4)	6502(4.2)	3896(11.)
24.74	41+71+64	38758(3.5)	19535(2.6)	9800(4.0)	5482(5.2)
25.35	40	10490(3.1)	5437(2.6)	2741(3.7)	1514(4.5)
26.30		957(4.0)			
26.59	74	7413(3.5)	3883(2.6)	1937(4.9)	1095(16.)
26.93	70+76	12605(3.7)	6583(2.4)	3273(4.8)	1830(11.)
27.26	95	130296(11.)	35214(3.0)	18164(2.5)	9328(4.2)
27.74	91	1869(4.0)	955(3.0)		
28.47	56	2447(3.7)	1279(2.5)	635(4.7)	
28.73	84	3555(3.9)	1823(3.1)	915(4.8)	
28.87	89	2456(3.9)	1261(3.5)		
29.18	101	33482(3.6)	17178(3.0)	8719(4.8)	4789(5.5)
29.56	99	682(2.5)			
30.85	97	957(4.5)			
31.28	87	4018(3.7)	2062(2.8)	1039(5.4)	567(7.6)
31.80	136	20052(3.9)		5291(4.5)	2837(6.0)
32.09	110	11938(3.9)		3121(5.2)	1681(7.3)
33.15	151	51796(3.9)	26060(2.9)	13392(5.2)	7185(6.5)
33.52	135	25394(3.4)	13277(3.3)	7102(4.7)	
34.16	149	109615(3.8)	55200(3.1)	28192(5.3)	15192(6.1)

TABLE 5(CONT.)

PEAK HEIGHTS AND CV FOR PCB CONGENERS
ELUTED FROM SE-52 COLUMN

RT	CONGENER #	CONCENTRATION (total ppb impinging on detector) 2250	1125	563	282
34.30	118				
34.94	114	4154(4.4)	2087(3.2)	1044(5.6)	577(6.0)6
35.27	131	1561(4.7)	786(4.0)		
35.79	105+132	13902(4.0)	7090(3.7)	3560(5.8)	1892(6.6)
36.28	153	128887(4.4)	63940(3.5)	31887(5.7)	16862(6.6)
37.33	141	54598(4.3)	27247(3.6)	13900(5.4)	7459(6.5)
37.96	176	11242(4.1)	5678(4.0)	2910(5.1)	1534(6.5)
38.51	138	81578(4.8)	39155(4.2)	19195(6.2)	10076(7.1)
39.30	178	17766(4.5)	9073(4.2)	4783(6.8)	2491(7.4)
39.74	175	3475(4.3)	1753(4.4)	852(6.0)	
40.01	182+187	104669(4.6)	52224(4.7)	26026(6.4)	13689(6.1)
40.41	183	42380(4.7)	211220(4.3)	10673(6.0)	5593(6.8)
40.74	128	4016(4.5)	2060(4.5)	961(7.5)	
40.97	167	1341(4.8)	707(7.8)		
41.22	185	12773(4.6)	6563(4.9)	3343(6.4)	1764(7.8)
41.97	174	81802(4.7)	39670(5.0)	19859(6.3)	10368(5.2)
42.36	177	40322(5.3)	19887(4.8)	10070(6.2)	5265(6.1)
42.70	171	24006(4.5)	12075(4.9)	6136(6.4)	3203(7.1)
43.12		1290(8.1)	627(6.3)		
43.34	157	7672(4.5)	3847(5.2)	1969(6.5)	999(6.4)
43.81	200	10724(4.9)	5488(5.4)	2782(6.6)	1430(5.3)
44.35	180	176379(5.7)	82912(6.2)	39566(7.5)	20058(6.5)
44.55	193	9051(5.0)	4644(6.0)		
44.87	191	2430(5.5)	1259(6.5)		
45.72	199	7605(4.7)	3893(5.7)	1968(7.0)	1027(6.7)
46.74	170	56363(5.9)	27494(6.4)	13466(7.5)	7108(8.0)
47.22	198	2882(5.2)	1857(11.)	744(7.1)	
47.54	201	54262(5.7)	26870(7.0)	13376(7.0)	6994(7.6)
47.95	203	43898(5.5)	21691(7.0)	10833(7.1)	5655(6.4)
49.20		1184(6.0)			
50.36	195	17541(5.8)	9006(7.7)	4586(7.8)	2344(6.8)
50.98	207	2097(6.1)	1102(8.3)		
52.18	194	41480(6.9)	20562(10.)	10298(9.1)	5236(7.0)
52.55	205	1775(8.6)	915(11.)		
55.22	206	12814(8.4)	6651(11.)	3438(9.1)	1721(6.3)
57.69	209	94114(8.4)	46094(13.)		11650(14.)

TABLE 5(CONT.)

PEAK HEIGHTS AND CV FOR PCB CONGENERS
ELUTED FROM SE-52 COLUMN

RT	CONGENER #	CONCENTRATION (total ppb impinging on detector) 225	113	56	28
9.82	1	9146(4.1)	4697(4.2)	2396(3.7)	1371(4.7)
11.53	3		858(8.5)		
12.28	4+10	5888(4.4)	3010(4.6)	1642(5.4)	858(7.0)
13.47	7	8340(3.8)	4141(4.5)	2269(3.5)	1212(5.5)
14.02	6	7247(3.7)	3592(4.6)	1963(4.1)	1040(5.8)
14.32	8+5	26075(3.8)	12959(4.4)	7127(3.5)	3822(5.2)
15.45	13	905(4.2)			
16.55	12	885(3.7)			
16.80	18	10040(3.9)	5013(4.3)	2748(3.9)	1416(6.2)
16.89	17	7737(3.4)	3823(4.9)		
17.44	24+27	985(7.0)			
17.96	16+32	7419(3.6)	3677(4.8)	2030(3.8)	1069(5.1)
18.81	29				
19.21	26	1606(4.7)	760(5.8)		
19.35	25				
19.80	28+31	11429(3.3)	5475(5.4)	3036(3.7)	1677(6.6)
20.48	33	7166(3.0)	3516(5.1)	2061(3.2)	1187(6.8)
21.00	22	3511(3.5)	1650(5.9)	911(5.0)	
21.36	45	1366(3.6)	651(4.0)		
21.93	46	533(1.7)7			
22.38	52	4631(3.4)	2242(5.0)	1210(5.5)	619(5.4)
22.67	49	3678(3.3)	1783(4.9)	955(5.7)	
22.88	47+48	2513(3.7)	1225(5.0)		
23.55		8271(34.)	SOLVENT		
23.86	44	5705(4.8)	2882(5.0)		
24.07	42	2987(5.6)	1477(7.3)		
24.74	41+71+64	4020(3.7)	1937(5.8)		
25.35	40	1096(3.3)			
26.30					
26.59	74	784(4.4)			
26.93	70+76	1336(4.1)	630(5.7)		
27.26	95	3822(3.1)	1854(5.4)	1010(5.2)	
27.74	91				
28.47	56				
28.73	84				
28.87	89				
29.18	101	3556(3.4)	1690(6.0)	938(5.1)	
29.56	99				
30.85	97				
31.28	87				
31.80	136	2117(3.6)	1010(6.3)	552(4.9)	
32.09	110	1259(3.5)	608(9.2)		
33.15	151	5379(4.1)	2589(6.7)	1479(4.2)	845(10.)
33.52	135				
34.16	149	11494(4.2)	5652(6.7)	3291(4.5)	1858(6.6)

TABLE 5(CONC.)

PEAK HEIGHTS AND CV FOR PCB CONGENERS
ELUTED FROM SE-52 COLUMN

RT	CONGENER #	CONCENTRATION (total ppb impinging on detector) 225	113	56	28
34.30	118				
34.94	114				
35.27	131				
35.79	105+132	1417(3.7)	666(6.8)		
36.28	153	12811(4.0)	6091(6.9)	3475(4.9)	1922(7.5)
37.33	141	5573(3.8)	2685(6.1)	1531(5.0)	827(7.6)
37.96	176	1130(4.3)			
38.51	138	7478(5.3)		2016(6.7)	1112(8.1)
39.30	178	1826(4.7)	881(12.)	582(3.4)	
39.74	175				
40.01	182+187	10365(4.8)	4903(7.3)	2838(5.2)	1582(8.0)
40.41	183		1994(7.4)	1143(5.6)	638(7.8)
40.74	128				
40.97	167				
41.22	185	1305(4.1)	619(8.7)		
41.97	174	7897(4.4)	3756(7.8)	2185(5.2)	1233(8.0)
42.36	177	3981(4.3)	1872(7.8)	1075(5.5)	604(8.2)
42.70	171	2399(4.5)	1144(7.0)	653(5.3)	
43.12					
43.34	157	728(4.9)			
43.81	200	1051(7.6)			
44.35	180	15134(4.9)	6963(9.4)	4045(6.2)	
44.55	193				
44.87	191				
45.72	199	747(4.8)			
46.74	170	5365(5.5)	2462(9.3)	1445(6.0)	868(8.0)
47.22	198				
47.54	201	5213(5.4)	2449(8.7)	1430(5.9)	852(9.2)
47.95	203	4198(5.1)	1998(8.4)	1163(6.5)	709(8.2)
49.00					
50.36	195	1758(5.8)	822(9.2)		
50.98	207				
52.18	194	3954(5.7)	1841(9.4)	1080(6.7)	702(8.9)
52.55	205				
55.22	206	1268(6.2)	592(11.)		
57.69	209	8605(6.7)	3957(9.3)	2374(7.2)	3343(8.8)

TABLE 6

RESPONSE FACTORS and MININAL DETECTABLE AMOUNTS
of
PCB CONGENERS

	OV-1			SE-52			
Congener	Slope	Ci@	Cor. Coeff	Slope	Ci@	Cor. Coeff.	No. Points
1	1119.35	1.9	0.9986	1192.29	1.7	0.9980	9
3	2490.35	1.2	0.9570	2175.48	0.15	1.0000	9
4+10	3361.30	0.42	0.9985	971.49	1.46	0.9978	9
7	38448.28	0.03	0.9996	30338.17	0.02	0.9998	9
6	17438.96	0.02	0.9999	12547.94	0.08	0.9993	9
8+5	6726.62	0.31	0.9999	4772.75	0.82	0.9993	6
12	10565.72	0.001	1.0000	6121.63	0.03	0.9997	9
13	4488.00	0.02	0.9999	(5262.86	0.001	1.0000)	5
16	27951.07	0.09	0.9960				9
17	23084.69	0.03	0.9999	21596.34	0.07	0.9993	9
18	13885.44	0.12	0.9995	9179.71	0.19	0.9990	9
(16+)32	27705.32	0.01	0.9999	13470.78	0.06	0.9997	9
22	46854.95	0.01	0.9996	38626.71	0.007	0.9999	8
24+27	19028.37	0.007	0.9999	9881.88	0.02	0.9996	7
25	22785.11	0.005	1.0000	17671.75	0.02	0.9993	5
26	19028.31	0.007	0.9999	15546.47	0.02	0.9995	7
28+31	7759.11	0.50	0.9981	9387.71	0.15	0.9997	9
29	19730.01	0.004	0.9997	17636.36	0.01	0.9988	3
33	15737.34	0.05	0.9998	12884.81	0.04	0.9999	9
40	25774.95	0.004	0.9999	20896.43	0.008	0.9997	6
41+71+65	38490.17	0.005	0.9998	36435.13	0.010	0.9999	7
42	33999.62	0.009	0.9998	30642.48	0.02	0.9994	7
44	19484.73	0.03	0.9998	16982.79	0.060	0.9993	7
45	28837.87	0.005	0.9999	21190.45	0.009	0.9997	9
46	21511.76	0.006	0.9996	16423.18	0.004	0.9998	6
47(+48)	25941.98	0.006	0.9999	12268.82	0.028	0.9997	6
48	22734.14	0.008	1.0000				
49	27925.78	0.008	0.9999	22639.60	0.018	0.9998	8
52	22976.67	0.02	0.9998	19137.44	0.030	0.9995	9
56				14384.55	0.005	0.9997	4
60	4026.98	0.02	0.9995				4
70+76	15708.85	0.009	0.9998	14485.91	0.01	0.9996	7
74	22143.18	0.004	0.9998	21094.29	0.007	0.9996	6
84	16716.64	0.002	0.9999	17756.01	0.003	0.9999	4
87	40938.02	0.002	0.9998	36325.45	0.002	0.9998	5
89	30243.27	0.002	0.9999	15350.00	0.004	0.9999	3
91	33816.65	0.001	0.9999	26700.00	0.001	0.9999	3
95	24491.54	0.043	0.9985	29291.01	0.06	0.9987	8
101	31797.25	0.006	0.9999	25333.58	0.013	0.9998	8
105+132 +164	19709.13	0.009	0.9999	6952.67	0.02	0.9999	7
110	27832.67	0.005	0.9998	23303.90	0.005	0.9998	6
128				28833.46	0.003	0.9998	4
131	39024.99	0.0003	1.0000	39024.99	0.0003	1.000	3
134+114	63100.00	0.001	0.9998				5

TABLE 6 (Cont.)

RESPONSE FACTORS and MININAL DETECTABLE AMOUNTS
of
PCB CONGENERS

	OV-1			SE-52			
Congener	Slope	Ci@	Cor. Coeff	Slope	Ci@	Cor. Coeff.	No. Points
135	28002.13	0.04	0.9994	42003.25	0.02	0.9995	4
136	25074.09	0.008	0.9999	20188.75	0.01	0.9998	8
137+130	62681.45	0.002	0.9999				7
138	42149.52	0.02	0.9998	38490.40	0.02	0.9997	8
141	78597.39	0.004	0.9999	58525.95	0.005	0.9999	9
149+181	9285.25	2.32	0.6210	20413.45	0.03	0.9999	9
151	27756.30	0.09	0.9934	27756.30	0.09	0.9934	9
153	24083.84	0.03	0.9999	21609.99	0.02	1.0000	9
156+171	20723.64	0.01	0.9997	39989.20	0.003	0.9999	8
158	35290.94	0.009	0.9995				
167				44700.00	0.001	0.9995	3
170	16587.54	0.02	0.9998	22386.76	0.02	0.9999	9
172	1963.00	0.05	0.9997				7
173	33189.52	0.007	0.9999				8
174	24370.61	0.001	1.0000	31678.06	0.02	0.9999	9
175	24370.61	0.002	1.0000	18673.41	0.09	0.8718	4
176				37348.56	0.003	0.9999	6
177	55006.57	0.004	0.9999	51546.21	0.003	0.9999	9
178	25600.56	0.007	0.9999	23640.00	0.008	0.9998	8
180	20977.99	0.08	0.9997	30805.79	0.09	0.9994	9
182	73748.28	0.007	0.9999	29277.78	0.012	1.0000	9
183	28691.61	0.01	0.9999	24185.72	0.007	1.0000	8
185	28354.46	0.007	0.9995	29714.72	0.005	0.9998	7
190	42045.80	0.008	0.9988				6
191	90099.95	0.002	0.9994	81000.00	0.001	0.9998	3
193	34114.68	0.009	0.9996	33522.23	0.008	0.9999	3
194				26954.30	0.02	0.9992	8
195	7549.92	0.05	0.9990	7954.67	0.02	0.9998	7
198				17185.21	0.03	0.9869	4
199	45289.17	0.004	0.9996	44715.44	0.002	0.9999	6
200	16131.99	0.02	0.9993	13239.80	0.009	0.9999	6
201				22294.79	0.01	0.9999	9
203+196	19329.89	0.03	0.9997	16720.55	0.01	0.9999	9
205	84500.00	0.002	0.9977	88750.03	0.0007	0.9998	4
206	21250.41	0.02	0.9979	26017.34	0.008	0.9992	7
207	55426.02	0.01	0.9973	52425.04	0.002	0.9996	4
209	6376.69	0.29	0.9989	10655.30	0.12	0.9996	8

@ Statistical Mininum Amount (Long & Winefordner, 1983)

TABLE 7

COMPARISON OF TOTAL PCB CONCENTRATIONS IN STANDARDS

(A) STANDARDS:

	EXPECTED CONCENTRATION (pg/uL injected)	ANALYSED CONCENTRATION (pg/uL injected)
1221	50	58.8
1016	41	40.4
1262	50	42.9
1221+1254+1262 (1:1:1)	200	203.7

TABLE 8

CONCENTRATION OF PCB's IN STANDARD SEDIMENT

Congener	Concentration (ppb)	
	OV-1 Column	SE-52 Column
Di-sub		
11	2.51	
Tri-sub		
18	1.32	
31	5.84	
33	1.78	
Tetra-sub		
45	1.06	
49	1.24	
64	1.26	
70	2.14	
74	1.48	
Penta-sub		
87	(0.66)	0.38
89	3.62	
95	(1.41)	3.55
99	(2.33)	0.01
101	(3.75)	2.27
110	(1.21)	0.15
Hexa-sub		
138	0.83	
153	0.80	
Hepta-sub		
180	7.13	
Total	41.02 (using OV-1 only)	
	37.37 (combining OV-1 and SE-52)	

TABLE 9

CONCENTRATIONS (ng/g) OF PCB'S
ANALYSED IN A SEDIMENT MATRIX

COMPOUND #	OV-1				XE-52	
	PCB STD.	PCB+SED	RT	RT	PCB STD.	PCB+SED
001	27.41(3.2)	27.92(2.1)	8.73	6.98	17.04(4.2)	18.99(4.3)
003	2.97(8.8)	4.03(6.2)	9.97			
004	5.92(3.6)	5.98(2.5)	10.68	8.42	6.09(4.2)	6.56(4.9)
007	0.73(3.8)	0.77(2.7)	11.75	9.11	0.81(6.3)	1.17(3.0)
006	1.47(3.9)	1.56(2.6)	12.15	9.41	1.51(6.6)	1.57(3.2)
005	1.40(4.0)		12.39	9.63		
019						
013	0.49(3.8)	5.44(2.7)	13.21	10.19	0.53(5.9)	2.27(10.)
012	0.21(4.8)	0.34(4.4)				
018+017	2.96(3.9)	3.32(2.7)	14.46	11.06	4.47(5.9)	5.18(5.4)
017	1.09(4.1)	1.11(2.3)				
027	0.19(4.1)	0.17(3.0)	15.00	11.45		
016	0.74(4.1)	0.80(2.3)	15.35	11.77	0.79(7.0)	0.95(7.8)
026	0.28(4.3)	0.38(3.8)	16.58	12.63	0.27(25.)	
031	5.11(5.2)	6.37(2.9)	17.04	13.01	5.79(9.1)	8.25(3.4)
033	1.37(6.4)	1.72(3.0)	17.61	13.45	2.26(7.9)	2.92(2.3)
022	0.40(5.0)	0.48(3.2)	17.98	13.82	0.32(6.7)	0.35(4.4)
045	0.22(6.9)	0.33(11.)	18.30	14.02	0.27(3.7)	0.34(3.0)
046	0.13(4.4)	0.25(7.2)	18.75	14.42	0.13(4.8)	0.18(4.8)
011	0.70(4.5)	1.16(2.7)	19.35	14.83	0.75(8.1)	
049	0.48(4.5)	0.77(2.5)	19.61	15.03	1.27(5.4)	1.43(2.9)
047	0.35(5.0)	0.49(3.0)	19.87			
044	0.91(5.9)	1.27(3.0)	20.54	15.94	0.95(7.3)	
042	0.29(5.6)	0.37(2.8)	20.75			
064	0.72(5.0)	0.98(3.0)	21.34	16.52	0.85(7.8)	1.14(2.9)
040	0.18(8.0)	0.26(3.5)	21.76	16.96	0.17(7.3)	0.22(7.5)
070	0.30(4.1)	0.71(3.5)	23.42	18.27	0.35(12.)	1.54(2.9)
095	0.64(4.1)	0.86(3.1)	23.70	18.48	0.72(7.9)	1.24(2.0)
084	0.07(3.9)		25.05	19.74	0.09(10.)	0.68(2.6)
089	0.05(2.9)	0.05(7.2)	25.24			
101	0.43(4.8)	1.01(9.0)	26.67	20.09	0.55(9.3)	1.00(2.2)
087	0.03(6.0)	0.13(4.8)	27.38	21.81		0.10(2.8)
110	0.18(4.9)	0.39(7.1)	26.67	22.49		0.05(5.1)
082	0.09(20.)	0.14(19.)	28.88			
151	0.72(4.8)	0.76(3.7)	29.42	23.41	0.80(8.4)	0.91(3.1)
135	0.30(4.8)	0.31(4.8)	29.69	23.73	0.35(7.5)	0.42(8.9)
149	1.66(4.9)	1.87(4.2)	30.28	24.31	0.27(8.7)	3.29(3.6)
131	0.02(5.2)	0.02(4.6)	31.28			
105	0.63(5.2)	0.75(4.3)	32.09	25.78	1.06(12.)	1.59(5.1)
153				26.71	1.85(10.)	2.41(2.9)
141	0.35(5.5)	0.37(4.5)	33.33	27.08	0.39(8.9)	2.41(2.9)
138	0.67(12.)	0.77(5.2)	34.32	28.17	0.77(11.)	1.07(4.0)
178	0.30(5.8)	0.22(5.4)	35.45			
187						
183	0.64(6.1)	0.67(5.4)	36.49	29.91	0.78(8.6)	0.96(7.7)

TABLE 9 (CONT.)

CONCENTRATIONS (ng/g) OF PCB'S
ANALYSED FROM A SEDIMENT MATRIX

COMPOUND #	OV-1				XE-52	
	PCB+OCA	PCB+OCA+SED	RT	RT	PCB+OCA	PCB+OCA+SED
185	0.90(6.3)	0.18(5.2)	37.22	30.60	0.18(9.4)	0.30(16.)
174	0.28(6.2)	0.94(5.8)	37.73	31.27	1.08(9.6)	1.28(4.0)
177	0.33(6.5)	0.30(5.9)	38.02	31.65	0.34(9.4)	0.40(4.9)
156	0.33(6.5)	0.37(6.3)	38.38	31.96	0.55(8.4)	0.69(9.4)
157	0.03(5.8)	0.03(6.3)	38.72			
173	0.14(6.2)	0.14(6.2)	39.34	32.57	0.14(9.1)	0.23(14.)
200	0.22(8.2)	0.25(6.7)	39.68	33.10	0.25(11.)	0.35(7.8)
180	31.22(7.7)	34.50(7.1)	40.19	33.59	2.20(12.)	2.86(3.9)
199	0.07(8.2)	0.07(7.1)	41.00	34.28	0.08(22.)	0.08(12.)
170	0.77(7.9)	0.93(7.3)	42.14	35.76	0.89(13.)	1.23(4.6)
190	0.09(7.0)	0.10(7.4)	42.35			
201	0.81(7.9)	0.82(8.0)	43.40	36.56	1.01(10.)	1.17(3.7)
203	0.83(7.6)	0.86(7.4)	43.82	36.94	1.09(11.)	1.28(3.9)
195	0.62(8.8)	0.66(8.8)	45.81	39.15	0.71(11.)	0.87(4.8)
207	0.17(9.6)	0.02(5.6)	46.20			
194	0.37(9.1)	0.40(9.4)	47.76	40.98	0.46(15.)	0.62(6.5)
206	0.17(9.5)	0.20(9.9)	50.93	43.84	0.20(13.)	0.45(16.)
209	2.70(10.)	2.70(11.)	53.45	46.18	3.42(13.)	4.05(6.2)

TABLE 10(a)

CONCENTRATIONS OF ORGANOCHLORINES IN

SEDIMENT SAMPLES (ng/g)

(B) SAMPLES:

	SAMPLE 1		SAMPLE 2		SAMPLE 3	
	Other	This Work	Other	This Work	Other	This Wor
1,4-Dichlorobenzene			9.72			
1,2-Dichlorobenzene			4.90			
1,2.4-Trichlorobenzene	2.30	**1.90**	4.94	**4.98**	1.86	**1.65**
1,2,3,4-Tetrachlorobenz.	2.50	**2.55**	2.99	**3.01**	3.28	**3.50**
Pentachlorobenzene	2.18	**2.29**	3.38	**3.27**	2.53	**2.64**
HCB	6.12	**0.34**	1.45	**1.99**	1.58	
p,p-DDE	3.63	**3.06**	3.49	**4.48**	1.36	**2.66**
p,p-DDT	1.38		2.82	**3.73**	1.46	
Hexachlorobutadiene	1.43					0.29
Mirex	0.68	**0.90**				

TABLE 10(b)

CONCENTRATION OF PCB CONGENERS IN SEDIMENT SAMPLES (ng/g)

	Sample 1		Sample 2	Sample 3
Total PCB	279.5		51.4	54.4
(Other)	146.4		50.6	28.2
Congener			WORKING COLUMN	
Number	OV-1	SE-52	OV-1	OV-1
Di-sub				
11	24.1		5.58	3.20
Tri-sub				
16	3.78			0.30
17	5.70		3.06	1.14
18	16.92		1.74	2.04
22	3.24		0.36	
24	0.24			
26	3.54		0.48	1.14
31	52.02		5.04	6.96
33	11.34		1.44	1.92
Tetra-sub				
40	4.68			
44	27.66			
45	4.86			
46	3.12			
49	14.58		5.64	1.26
64	(21.24)	18.42		1.54
66	(27.90)	12.48		3.60
70	(34.08)	24.78	2.76	2.58
74	(12.48)	8.16	1.38	1.68
Penta-sub				
84	(12.72)	6.30	7.98	8.40
87	3.18		0.78	0.60
99	3.66		1.44	4.50
101	7.08		3.90	3.78
105	4.68			
110	8.34		2.28	1.80
Hexa-sub				
128	1.02		0.90	0.60
138	2.46		1.50	1.14
141	0.30		0.30	0.18
151			0.54	
153	2.18		1.86	1.20
Hepta-sub				
170			1.50	
174	0.36		0.48	
177			0.18	
180			2.04	1.07
Octa-sub				
203	0.33			

APPENDIX A

Ballschmiter and Zell Numbers for all PCB Isomers

APPENDIX A

BALLSCHMITER AND ZELL NUMBERS FOR ALL PCB ISOMERS

#	Substitution Pattern
Monochlorobiphenyls	
1	2
2	3
3	4
Dichlorobiphenyls	
4	2,2'
5	2,3
6	2,3'
7	2,4
8	2,4'
9	2,5
10	2,6
11	3,3'
12	3,4
13	3,4'
14	3,5
15	4,4'
Trichlorobiphenyls	
16	2,2',3
17	2,2',4
18	2,2',5
19	2,2',6
20	2,3,3'
21	2,3,4
22	2,3,4'
23	2,3,5
24	2,3,6
25	2,3',4
26	2,3',5
27	2,3',6
28	2,4,4'
29	2,4,5
30	2,4,6
31	2,4'5
32	2,4',6
33	2',3,4
34	2'3,5
35	3,3',4
36	3,3',5
37	3,4,4'
38	3,4,5
39	3,4',5

#	Substitution Pattern
Tetrachlorobiphenyls	
40	2,2',3,3'
41	2,2',3,4
42	2,2',3,4'
43	2,2',3,5
44	2,2',3,5'
45	2,2',3,6
46	2,2',3,6'
47	2,2',4,4'
48	2,2',4,5
49	2,2',4,5'
50	2,2',4,6
51	2,2',4,6'
52	2,2'5,5'
53	2,2',5,6'
54	2,2',6,6'
55	2,3,3',4
56	2,3,3',4'
57	2,3,3',5
58	2,3,3',5'
59	2,3,3',6
60	2,3,4,4'
61	2,3,4,5
62	2,3,4,6
63	2,3,4',5
64	2,3,4',6
65	2,3,5,6
66	2,3',4,4
67	2,3',4,5
68	2,3',4,5'
69	2,3',4,6
70	2,3',4',5
71	2,3',4',6
72	2,2',5,5'
73	2,3',5',6
74	2,4,4',5
75	2,4,4',6
76	2',3,4,5
77	3,3',4,4'
78	3,3',4,5
79	3,3',4,5'
80	3,3',5,5'
81	3,34,4'5

#	Subsitution Pattern
Pentachlorobiphenyls	
82	2,2',3,3',4
83	2,2',3,3',5
84	2,2',3,3',6
85	2,2',3,4,4'
86	2,2',3,4,5
87	2,2',3,4,5'
88	2,2',3,4,6
89	2,2',3,4,6'
90	2',2,3,4',5
91	2,2',3,4',6
92	2,2',3,5,5'
93	2,2',3,5,6
94	2,2',3,5,6'
95	2,2',3,5',6
96	2,2',3,6,6'
97	2,2',3',4,5
98	2,2',3',4,6
99	2,2',4,4',5
100	2,2',4,4',6
101	2,2',4,5,5'
102	2,2',4,5,6'
103	2,2',4,5',6
104	2,2',4,6,6'
105	2,3,3',4,4'
106	2,3,3',4,5
107	2,3,3',4',5
108	2,3,3',4,5'
109	2,3,3',4,6
110	2,3,3',4',6
111	2,3,3',5,5'
112	2,3,3',5,6
113	2,3,3',5',6
114	2,3,4,4',5
115	2,3,4,4',6
116	2,3,4,5,6
117	2,3,4',5,6
118	2,3',4,4',5
119	2,3',4,4',6
120	2,3',4,5,5'
121	2,3',4,5',6
122	2',3,3',4,5
123	2',3,4,4',5
124	2',3,4,5,5'
125	2',3,4,5,6'
126	3,3',4,4',5
127	3,3',4,5,5'

APPENDIX A (Cont.)

BALLSCHMITER AND ZELL NUMBERS FOR ALL PCB ISOMERS

#	Substitution Pattern
Hexachlorobiphenyls	
128	2,2',3,3',4,4'
129	2,2',3,3',4,5
130	2,2',3,3',4,5'
131	2,2',3,3',4,6
132	2,2',3,3',4,6'
133	2,2',3,3',5,5'
134	2,2',3,3',5,6
135	2,2',3,3',5,6'
136	2,2',3,3',6,6'
137	2,2',3,4,4',5
138	2,2',3,4,4',5'
139	2,2',3,4,4',6
140	2,2',3,4,4',6'
141	2,2',3,4,5,5'
142	2,2',3,4,5,6
143	2,2',3,4,5,6'
144	2,2',3,4,5',6
145	2,2',3,4,6,6'
146	2,2',3,4',5,5'
147	2,2',3,4',5,6
148	2,2',3,4',5,6'
149	2,2',3,4',5',6
150	2,2',3,4',6,6'
151	2,2',3,5,5',6
152	2,2',3,5,6,6'
153	2,2',4,4',5,5'
154	2,2',4,4',5,6'
155	2,2',4,4',6,6'
156	2,3,3',4,4',5
157	2,3,3',4,4',5'
158	2,3,3',4,4',6
159	2,3,3',4,5,5'
160	2,3,3',4,5,6
161	2,3,3',4,5',6
162	2,3,3',4',5,5'
163	2,3,3',4',5,6
164	2,3,3',4,5',6
165	2,3,3',5,5',6
166	2,3,4,4',5,6
167	2,3',4,4',5,5'
168	2,3',4,4',5',6
169	3,3',4,4',5,5'

#	Substitution Pattern
Heptachlorobiphenyls	
170	2,2',3,3',4,4',5
171	2,2',3,3',4,4',6
172	2,2',3,3',4,5,5'
173	2,2',3,3',4,5,6
174	2,2',3,3',4,5,6'
175	2,2',3,3',4,5',6
176	2,2',3,3',4,6,6'
177	2,2',3,3',4',5,6
178	2,2',3,3',5,5',6
179	2,2',3,3',5,6,6'
180	2,2',3,4,4',5,5'
181	2,2',3,4,4',5,6
182	2,2',3,4,4',5,6'
183	2,2',3,4,4',5',6
184	2,2',3,4,4',6,6'
185	2,2',3,4,5,5',6
186	2,2',3,4,5,6,6'
187	2,2',3,4,5,5',6
188	2,2',3,4',5,6,6'
189	2,3,3',4,4',5,5'
190	2,3,3',4,4',5,6
191	2,3,3',4,4',5',6
192	2,3,3',4,5,5',6
193	2,3,3',4',5,5',6
Octachlorobiphenyls	
194	2,2',3,3',4,4',5,5'
195	2,2',3,3',4,4',5,6
196	2,2',3,3',4,4',5,6'
197	2,2',3,3',4,4',6,6'
198	2,2',3,3',4,5,5',6
199	2,2',3,3',4,5,6,6'
200	2,2',3,3',4,5',6,6'
201	2,2',3,3',4,5,5',6'
202	2,2',3,3',5,5',6,6'
203	2,2',3,4,4',5,5',6
204	2,2',3,4,4',5,6,6'
205	2,3,3',4,4',5,5',6
Nonachlorobiphenyls	
206	2,2',3,3',4,4',5,5',6
207	2,2',3,3',4,4',5,6,6'
208	2,2',3,3',4,5,5',6,6'
Decachloropihenyl	
209	2,2',3,3',4,4',5,5',6,6'

APPENDIX B

Fortran 7 Listing of Statistical Program for HP 1000 Computer System

```
      Program STAT1

$include /las/sys/inc.ftn.nolist
$include /las/sys/fields_dl92.ftn.nolist
      Integer*2 Las_OpenFile,NF,RS,
     + Las_CloseFile,Error,DCB(Dcb_Length), Npks,
     + Defined,OpenMode,Unlock,PE,KE,Las_ReadValues,Len,TrimLen
      Integer*4 ValueNameList(2),Lockid,ListName,Buffer(64)
      Character ListPointer*((ListPointerFixedLength)+
     + 2*(ListPointerFieldLength))
      Character FileName*(PathNameLength),FileType*(FileTypeLength),
     +          NFile(15)*36,FullFile*(PathNameLength),LocalName*40,
     +          PathComponent*4,TITLE*63
      Real*4 Value(30,11), Mean(30),Temp(30),
     +   Dot(30), STDEV(30), COEF(30)
      Real C(30)
      REAL*8 MEAN2(30)
      Equivalence  ( Buffer(1),      Npks)
      Common  C,Value
      Logical Btest
      Defined = 0
      FileType='RESULT'
      PathComponent='DL92'

      Write(1,'("ENTER TITLE (up to 63 characters")')
      Read(1,'(A)') TITLE
*****************************************************************
*                     START OF INPUT                            *
*                                                               *
*****************************************************************
      Write(1,'("Number of files to be analysed")')
      Read *,NF
      Write(1,'("Enter Local Name for each of the Files")')
      If (len.eq.0)len=1
         Do  4,J=1,NF
 75      Write(1,'(a,"file name (/E to exit):")') FileType(1:len)
         Read (1,'(a)') NFile(J)
         IF (NFILE(J) .EQ. '/E' )STOP
         Call CaseFold(NFile(J))
         Openmode = 0
         Lockid = 0
         If (Las_OpenFile(DCB,NFile(J),Result,Openmode,Lockid,
     +      Error) .ne. 1) then
         Write(1,'("Error in Opening File, Re-enter Name")')
         Go To 75
        Else
         Call Las_CloseFile(DCB,unlock,error)
         if (error .ne. 0) write (1,'("close File Error",i5)')Error
         End if
   4      Continue
*
```

```
 15    Write(1,'("Number of peaks to be analysed")')
       Read *, PE
       Write(1,'("Enter Retention Times using RETURN KEY")')
       DO 3, I=1,PE
       Read (1,2,err=3)(C(I))
 2     FORMAT (F5.2)
 3     CONTINUE
 60    Write(1,'("ANALYSIS FOR HEIGHT=1:AREA=2:AMOUNT = 3")')
       Write(1,'(" ENTER 1 FOR HEIGHTS,2 FOR AREA, OR 3 FOR AMOUNT")')
       Read*,RS
        Do 1000, J=1,NF
         FullFile = ' '
         LocalName = NFile(J)
          If (Las BuildRootName(LocalName,FileType,FullFile,Error)
     +     .ne. 1) then
           Write(1,'("BuildRootName Error ",i5)') Error
           End if

         if (FileName.eq.' ') stop

        OpenMode=0
        Lockid=0
*****************************************************************
*     OPENING THE FILES ONE BY ONE TO START EXTRACTING          *
*                THE REQUIRED VALUES                            *
*****************************************************************
          If (Las OpenFile(DCB,FullFile,FileType,OpenMode,Lockid,
     +       Error) .ne. 1) then
          Write(1,'("Open Error = ",i5)') Error
          End if
          ValueNameList(1) = F NumberPeaks
          ValueNameList(2) = 0

          If (Las ReadValues(DCB,ValueNameList,Defined,Buffer,
     +        Error) .ne. 1) then
           Write (1,'("Read Values Error = ",i5)') Error
           end if
*            Write(1,'("Number of Peaks = ", i2 )') Npks

           If (Npks .eq. 0) then
           Write(1,'("No Processed Information in Result File")')
           End if
*****************************************************************
*  THE RETRIEVAL OF INFORMATION FROM THE FILES IS DONE IN THIS  *
*    SUBROUTINE                                                 *
*****************************************************************
          Call STATB(DCB,Npks,PE,J,NF,RS)
*****************************************************************
* THE NECESSARY INFORMATION IS BROUGHT BACK TO MAIN PROGRAM THROUGH *
* THE USE OF "COMMON"                                           *
*****************************************************************
*
```

```
            unlock=0
            Call Las CloseFile(DCB.unlock.error)
              if (error.ne.0) write(1,'("Close File Error",i5)') Error
 1000     Continue
*************************************************************
*        START OF THE STATISTICAL PORTION OF THE            *
*              PROGRAM                                      *
*************************************************************
          Do 2000, I=1,PE
             Mean(I) = 0
             Mean2(I) = 0
             DOT(I) = 0
             STDEV(I)= 0
             PP = 0
*            Call VSUM(Mean(I),Value(I,1),PE,NF)
              Do 2005, J=1,NF
               If (Value(I,J) .eq. 0) then
                Goto 2005
                Else
              Mean(I) = Mean(I)+Value(I,J)
              Mean2(I) = Mean2(I)+ Value(I,J)*Value(I,J)
                PP = PP+1
                END IF
 2005           CONTINUE
             Mean(I) = (Mean(I))/PP
*            Call VSAD (-Mean(I),Value(I,1),1,Temp(I),1,NF)
*            Call VDOT(DOT(I),Temp(I),1,Temp(I),1,NF)
             D1 = Mean2(I)/PP
             D2 = Mean(I)*Mean(I)
             DOT(I) =PP*(D1-D2)/(PP-1)
             STDEV(I) = SQRT(DOT(I))
*            DOT = VARIENCE
*            STDEV(I) = SQRT (DOT(I))/(NF-1)
             COEF(I) = (STDEV(I))/(MEAN(I))
             COEF(I) = COEF(I)*100
 2000       END DO
*************************************************************
*    START OF OUTPUTTING THE INFORMATION                    *
*                                                           *
*************************************************************
         Write(6,'(1X,a)') TITLE
         Write(6,16)
  16     Format('0')
          IF(RS.GT.2) THEN
          GO TO 302
          END IF
          If (RS .EQ. 1) then
          Write(6,'(1X,"STATISTICS BASED ON PEAK HEIGHTS")')
          Else
          Write(6,'(1X,"STATISTCIS BASED ON PEAK AREAS")')
          Write(6,16)
*
*
```

```
            End if
            GO TO 303
  302       WRITE(6,'("STATISTICS BASED ON CONCENTRATIONS")')
  303       CONTINUE

            Do 3000, M=1,PE,6
              If (M .le. 6) then
               Write(6,17) (C(I),I=1,6)
   17          Format ('0',19X,6(F5.2,5X))
               Do 2001, J=1,NF
                If (RS.LE. 2) then
                Write(6,18) NFILE(J) (14:28),(Value(I,J),I=1,6)
   18           Format(X,A15,6(1X,F9.2))
                Else
                Write(6,181) NFILE(J) (14:28),(Value(I,J),I=1,6)
  181           Format(X,A15,6(1x,F9.5))
                End if
  2001         End do
               If (RS.LE.2) then
              Write(6,19)'MEAN',(Mean(I),I=1,6)
   19         Format (X,A4,10X,6(F10.2))
              Write(6,20) 'STD. DEV.',(STDEV(I),I=1,6)
   20         Format (X,A9,5X,6(F10.2))
              Write(6,21)'Coeff. Var.',(COEF(I),I=1,6)
   21         Format (X,A11,3X,6(F10.5))
              Else
              Write(6,191)'MEAN',(Mean(I),I=1,6)
  191         Format(X,A11,3X,6(F10.5))
              Write(6,191)'STD. DEV.',(STDEV(I),I=1,6)
              Write(6,191)'COEFF. VAR.',(COEF(I),I=1,6)
              END IF
              I=7
             Else if (M.GT.6.AND.m+6.LT.PE) THEN
               k=M
              Write(6,22) (C(I),I=k,k+6)
   22         Format('0',19X,6(F5.2,5X))
               DO 2002, J=1,NF
                IF (RS.LE.2) THEN
                Write(6,23) NFILE(J) (14:28),(VALUE(I,J), I=k,k+5)
   23           Format(X,A14,6(1X,F9.2))
                ELSE
                WRITE(6,181) NFILE(J) (14:28),(VALUE(I,J),I=k,k+5)
                End if
  2002         END DO
                If (RS.LE.2) Then
                Write(6,24) 'Mean',(Mean(I),I=k,k+5)
   24           Format(X,A4,10X,6(F10.2))
                Write(6,25) 'Std. Dev.',(STDEV(I),I=k,k+5)
   25           Format (X,A9,5X,6(F10.2))
                Write(6,26) 'Coeff. Var.',(COEF(I),I=k,k+5)
   26           Format (X,A11,3X,6(F10.5))
*
*
*
*
*
*
```

```
*
*
*
*
                Else
                Write(6,191) 'Mean',(Mean(I),I=k,k+5)
                Write(6,191) 'Std. Dev.',(STDEV(I),I=k,k+5)
                Write(6,191) 'Coeff. Var.',(COEF(I),I=k,k+5)
                End if
               ELSE
               k=m
               N=PE-k
               Write (6,27)
   27          Format('0')
               Write(6,28) (C(I),I=k,PE)
   28          Format(19x,6(F5.2,5X))
                Do 30, J=1,NF
                IF (RS.LE.2) Then
                Write(6,29) NFILE(J) (14:28),(VALUE(I,J),I=k,PE)
   29           Format(X,A15,6(1X,F9.2))
                ELSE
                 Write(6,181) NFILE(J) (14:28),(VALUE(I,J),I=k,PE)
                END IF
   30           End do
                If (RS.LE.2) then
               Write(6,31) 'Mean',(Mean(I),I=k,PE)
   31          Format(X,A4,10X,6(F10.2))
               Write(6,32) 'Std. Dev.',(STDEV(I),I=k,PE)
   32          Format(X,A9,5X,6(F10.2))
               Write(6,33) 'Coeff. Var.',(COEF(I),I=k,PE)
   33          Format(X,A11,3X,6(F10.5))
                Else
                Write(6,191) 'Mean', (MEAN(I),I=k,PE)
                Write(6,191) 'Std. Dev.',(STDEV(I),I=k,PE)
                Write(6,191) 'Coeff. Var.',(COEF(I),I=k,PE)
                End if

             End if
 3000     End do
*****************************************************************
*            NOW THE FILES CAN BE CHANGED OR RETAINED           *
*            AS WELL AS THE RETENTION TIMES USED                *
*****************************************************************
          WRITE(6,34)
  34      FORMAT('1')
          Write(1,'("DO YOU WISH TO USE THESE FILES AGAIN?")')
          Write(1,'("ENTER 1 FOR YES OR 2 FOR NO")')
          Read*,SY
           If (sy .eq. 2) then
           stop
           end if
          Write(1,'("TO LEAVE FILES UNCHANGED ENTER 0, TO ADD TO ")'
          Write(1,'("TO THE NUMBER OF FILES ENTER 1, AND TO DELETE")
          Write(1,'("FILES ENTER 2, MAX NUMBER OF FILES IS 10")')
          Read*,SY1
*
*
*
*
*
```

```
*
*
      If (SY1 .EQ. 1) then
      Write(1,'("NUMBER OF FILES TO BE ADDED")')
      Read*,SY2
      Write(1,'("ENTER FILE NAMES")')
       Do 6, J=NF+1,NF+SY2
       Write(1,'(a,"FILENAME")') FileType(1:len)
       Read(1,'(a)') NFILE(J)
       Call CaseFold(NFile(J))
6      End do
       NF = NF+SY2
      Else if (SY1 .EQ. 2) then
       Write(1,'("HOW MANY FILES TO BE DELETED")')
       No = 0.0
       Read*,SY3
       Write(1,'("ENTER THE ORDER NUMBER OF THE FILE FROM THE ")')
       Write(1,'("INITIAL ENTRY OF THE FILE NAMES - E.G.3(rd)")')
       Write(1,'("WHEN ASKED")')
        Do 7, S=1,SY3

       Write(1,'("ENTER FILE ORDER #")')
       READ*,J
        Q=J-No
        BB=NF-1
        Do 8,Q  = J-No,BB-No
        NFile(Q) = NFile(Q+1)

          Do I=1,PE
          Value(I,Q) = Value(I,Q+1)
          END DO
8         Continue
          No = No+1
7         Continue
          NF = NF-SY3
       Else
       Continue
      End if
      Write(1,'("DO YOU WISH TO USE THE SAME NUMBER OF PEAKS")')
      Write(1,'("AND RETENTION TIMES?")')
      Write(1,'("ENTER1 FOR YES AND 2 FOR NO")')
      Read*,SSS
       If (SSS.eo.1) then
       Go to 60
       End if
      Go to 15
      End
```

```
          Subroutine STATB(DCB,Npks,PE,N,RE,RS)

$Include  /las/sys/inc.ftn,nolist
$Include /las/sys/fields_d192.ftn,nolist

        Integer*2 Las_OpenList,Las_ReadListValues,Npks,Defined,
     +     Las_CloseList,Error,DCB(Dcb_Length),OpenMode,Unlock,
     +     PE,N,RS
        Integer* 4 ValueNameList(4),LockId,ListName,EntryNumber
        Character ListPointer*((ListPointerFixedLength)+
     +            3*(ListPointerFieldLength))
        Character FileName*(PathNameLength),FileType*(FileTypeLength),
     +            NFile(20)*36,FullFile*(PathNameLength),LocalName*40,
     +            PathComponent*4
        Real*4 Value(30,11),buffer(3),rbuff
        Real C(30),R1(30),R2(30),R3(30),R4(30),A1,A2
        Common C,Value
        Logical Btest
        Defined = 0
        N=N
*****************************************************************
* THE WINDOWS ABOUT THE RETENTION TIMES ARE SET AT .05 MIN.     *
* THIS SHOULD BE LARGE ENOUGH FOR ALL ANALYSIS                  *
*****************************************************************
        Do 6 I=1,PE
           A = 0.05
           R1(I) = C(I) - A
           R2(I) = C(I) + A
           R1(I) = 100*R1(I)
           R1(I) = AINT(R1(I))
           R1(I) = R1(I)/100
           R2(I) = 100*R2(I)
           R2(I) = AINT(R2(I))
           R2(I) = R2(I)/100
   6       Continue

           IF (RS.EQ.3) THEN
            GO TO 10
           END IF

        ListName = L_ProcessedList
        ValueNameList(1) = F_RetentionTime
        ValueNameList(2) = F_Area
        ValueNameList(3) = F_Height
        ValueNameList(4) = 0

         If(Las_OpenList(DCB,ListPointer,ListName,ValueNameList,
     +     Defined,Error) .ne. 1) then
           Write(1,'("OpenListError =",I5)') Error
```

```
            Else if (.not. Btest(Defined,15)) then
            Write(1,'("No Retention Times")')

            Else if ( .not. Btest(Defined,14)) then
            Write(1,'("No Areas")')

            Else if (.not. Btest(Defined,13)) then
            Write(1,'("No Heights")')
            Else
            Endif
*****************************************************************
* THE FILE IS OPEN AND READY TO BE READ. tHE RETENTION          *
* IS CHECKED AS WELL AS THE TYPE OF VALUE WANTED .E.G.          *
* CONCENTRATION. HEIGHT. THE VALUES ARE PLACED IN COMMON        *
*****************************************************************
       Do 7, I=1,PE
          EntryNumber = 1
           Do while (EntryNumber .le. Npks)
            If (Las_ReadListValues(DCB,ListPointer,Buffer,
     +           EntryNumber,Error) .ne. 1) Then
            Write(1,*) 'Error in Read List Values = ',Error
            Entrynumber = Npks
            Go to 8
            Else
    9         D = 100*Buffer(1)
              ST = AINT(D)
              Buffer(1) = ST/100
             End if
             rbuff = 0.0
              If(RS.EQ. 1) then
              rbuff = Buffer(3)
              Else
              rbuff = Buffer(2)
              End if
          VALUE(I,N) = 0.0
            If  (Buffer(1) .lt.R2(I) .and. Buffer(1) .gt.R1(I)) then
                Value (I,N) = rbuff
                 R1(I) = R1(I+1)
                 R2(I) = R2(I+1)
                I=I+1

             Else
            End if
            EntryNumber = EntryNumber + 1
           End do
           IF (I.GT.PE) THEN
           GO TO 8
           END IF
    7     End do
          Go To 8
```

```
   10      ListName = L_Processedlist
           ValueNameList (1) = F_RetentionTime
           ValueNameList (2) = F_Amount
           ValueNameList(3) = 0

           If (Las_OpenList(DCB,ListPointer,ListName,ValueNameList,
     +     Defined,Error) .ne. 1) then
           Write(1,'("Open List Error =",I5)') Error

           Else if (.not. Btest(Defined,15)) then
           Write(1,'("No Retention Times")')

           Else if (.not. Btest(Defined,14)) then
           Write(1,'("No Concentrations")')

           Else
           End if

           Do 11, I=1,PE
           EntryNumber = 1
            Dowhile(EntryNumber .le. Nbks)
           If(Las_ReadListValues(DCB,ListPointer,Buffer,
     +      EntryNumber,Error) .ne.1) Then
           Write(1,*) 'Error in Read List Values = '.Error
            EntryNumber = Nbks
            Go To 8
           Else
            D=100*Buffer(1)
            ST = AINT(D)
            Buffer(1) = ST/100
           End if
           rbuff = 0.0
           rbuff = Buffer(2)
           If (Buffer(1) .lt.R2(I) .and. Buffer(1) .gt. R1(I)) then
            Value(I,N) = rbuff
            R1(I) = R1(I+1)
            R2(I) = R2(I+1)
            I=I+1
            Else
            End if
            EntryNumber = EntryNumber + 1
            End do
            If (I.GT.PE) Then
            Go To 8
            End If
   11       End Do
*****************************************************************
* NOW THE LIST IS CLOSED AND RETURN TO THE MAIN PROGRAM         *

    8      If (Las_CloseList(DCB,ListPointer,Error).ne.1) then
           Write (1,'("Close List Error = ", i5)') Error
           End if
          END
```

APPENDIX C

Fortran 7 Listing of PCB Program for HP 1000 Computer System

```
          Program PCB2

$include /las/sys/inc.ftn,nolist
$include /las/sys/fields_dl92.ftn,nolist
        Integer*2 Las_OpenFile,RS,Las_OpenList,Las_CloseList,
     + Las_CloseFile,Error,DCB(Dcb_Length), Npks,Rbuff(64),
     + Defined,OpenMode,Unlock,Las_ReadValues,Len,TrimLen,inst,
     + X1,X2,X3,X4,X5,X6,X7,X8,X9,x10,bfs,x11,BS,nbrparams,desig
        Integer*4 ValueNameList(7),LockId,ListName,Buffer(2),
     +             EntryNumber,MPKS, BA,BB,BC,XS1,XS2,XS
        Character ListPointer*((ListPointerFixedLength)+
     + 4*(ListPointerFieldLength)),PX*30,SX*30
        Character FileName*(PathNameLength),FileType*(FileTypeLength),
     +            NFile*36,FullFile*(PathNameLength),LocalName*40,
     +            PathComponent*4,TITLE*63,PFILE*36,
     +            BUF(3)*3,PeakName*30,CNAME(150)*30,
     +            DName(125)*30,Result_file(pathnamelength)
        Real*4 ValueA(150),PCB1A,PCB1B,PCB2A,PCB2B,PCB3A,PCB3B,PCB4A,
     +  PCB4B,PCB5A,PCB5B,PCB6A,PCB6B,PCB7A,PCB7B,PCB8A,PCB8B,PCB9A,
     +  PCB9B, VALUEB(125),CB(125),C(150),Amount,Valc(125),CC(125),
     +  x10a,x10b, PCB1C,PCB1D,PCB2C,PCB2D,PCB3C,PCB3D,PCB4C,PCB4D,
     +  PCB5C,PCB5D,PCB6C,PCB6D,PCB7C,PCB7D,PCB8C,PCB8D,PCB9C,PCB9D,
     +  PCB11C,PCB11D
        Real RetentionTime
        Equivalence  ( Buffer(1),      Npks)
        Equivalence  (Rbuff(3), Peakname)
        Equivalence (Rbuff(1), Amount )
        Equivalence (Rbuff(18), Retentiontime)
        Logical Btest,NOSWAP
        Data pcb1a/0./,pcb1b/0./,pcb2a/0./,pcb2b/0./,pcb3a/0./,
     +    pcb3b/0./,pcb4a/0./,pcb4b/0./pcb5a/0./,pcb5b/0./,pcb6a/0./,
     +    pcb6b/0./,pcb7a/0./,pcb7b/0./,pcb8a/0./,pcb9a/0./,pcb9b/0./
        Data x1/0/,x2/0/,x3/0/,x4/0/,x5/0/,x6/0/,x7/0/,x8/0/,x9/0/,
     +       X10/0/,X11/0/
        Defined = 0
        FileType='RESULT'
        PathComponent='DL92'
*****************************************************************************
*      THE FOLLOWING SECTION GETS THE RESULT FILE NAME
*****************************************************************************
        Call Las_Tell(mode,isnt,desc,nbrparams,error)
        I=1

        Call Las_skedgetchar(i,NFile,len,error)
         if (error.ne.0) then
        Write(6,'("Cannot get file because error=",I3)') error
        go to 30
        end if
        Result_file = NFile
           Call CaseFold(NFile)
           Openmode = 0
           Lockid = 0
```

```
*************************************************************************
*       NOW TO BUILD NAME                                               *
*************************************************************************
        FullFile = '    '
        Localname = NFile
         If (Las_BuildRootName(LocalName,Result,FullFile,Error)
     +  .ne. 1) then
          Write(6,'("BuildRootName Error",i5)') Error
          End if
          If (FileName .eq.' ') stop
*************************************************************************
*     OPEN FILE TO EXTRACT THE NECESSARY INFORMATION                    *
*************************************************************************
          OpenMode = 0
          Lockid = 0
         If (Las_OpenFile(DCB,FullFile,FileType,OpenMode,Lockid,
     +       Error) .ne. 1) then
         Write(6,'("Open Error = ",i5)') Error
         End if
         ValueNameList(1) = F_NumberPeaks
         ValueNameList(2) = 0

         If (Las_ReadValues(DCB,ValueNameList,Defined,Buffer,
     +        Error) .ne. 1) then
          Write (6,'("Read Values Error = ",i5)') Error
          end if
             Mpks = Npks
          If (Npks .eq. 0) then
          Write(6,'("No Processed Information in Result File")')
          End if
          If (Las_CloseList(DCB,ListPointer,Error).ne.1)then
          Write(6,'("Close List Error = ",i5)') Error
          End if
          DEFINED = 0
          Listname = L_ProcessedList
          ValueNameList(3) = F_RetentionTime
          ValueNameList(1) = F_Amount
          ValueNameList(2) = F_PeakName
          ValueNameList(4) = 0

         If(Las_OpenList(DCB,ListPointer,ListName,ValueNameList,
     +   Defined,Error).ne.1) then
         Write(6,'("Open List Error =",i4)') Error
         Else if (.not. Btest(Defined,15)) then
         Write(6,'("No A Retention Times")')
         Else if (.not. Btest(Defined,14)) then
         Write(6,'("No A Amounts")')
         Else if (.not. Btest(Defined,13)) then
         Write(6,'("No A Peak Names")')
         Else
         end if
*************************************************************************
*       NOW GET THE DATA FROM A CHANNEL                                 *
```

```
*****************************************************************
*       NOW GET THE DATA FROM A CHANNEL                         *
*****************************************************************
          I=1
          EntryNumber = 1
          Dowhile(EntryNumber.le.Npks)
           If(Las_ReadListValues(DCB,ListPointer,rbuff,
     +        EntryNumber,Error) .ne. 1) Then
           Write(6,*) 'Error in Read List Values =',Error
           Entrynumber = Npks
           Go to 11
            End if
            If (Peakname.eq.'   ') then
            go to 15
            else
            Cname(I)(1:30) = peakname
            C(I) = RetentionTime
            Valuea(I) = Amount
             I=I+1
            end if
 15         Continue
            Cname(I) = '       '
            EntryNumber = EntryNumber + 1
            BA = I
           End do
  11      If(Las CloseList(DCB,ListPointer,Error).ne.1) then
          Write(6,'("Close List Error = ",I4)') Error
          End if
           NPKS = 0

          unlock=0
          Call Las CloseFile(DCB,unlock,error)
            if (error.ne.0) write(6,'("Close File Error",i5)') Error
*****************************************************************
*           NOW SET THE B CHANNEL FILE                          *
*****************************************************************
          PFILE = NFILE

          IF(PFILE(18:18) .EQ. 'A') THEN
          PFILE(18:18) = 'B'
          ELSE
          PFILE(18:18) = 'A'
          END IF
          CALL CASEFOLD(PFILE)

          IF (LAS_OPENFILE(DCB,PFILE,RESULT,OPENMODE,LOCKID,
     +    ERROR) .NE. 1) THEN
          WRITE (6,'("OPEN ERROR = ",I5)') ERROR
          END IF
```

```
      VALUENAMELIST(1) = F_NUMBERPEAKS
      VALUENAMELIST(2) = 0
      DEFINED = 0

      IF (LAS_READVALUES(DCB,VALUENAMELIST,DEFINED,BUFFER,
     +  ERROR) .NE. 1) THEN
      WRITE(6,'("READ VALUES ERROR = ",I5)') ERROR
      END IF

      IF (NPKS .EQ. 0) THEN
      WRITE(6,'("NO PROCESSED INFORMATION")')
      END IF

      IF (LAS_CLOSELIST(DCB,LISTPOINTER,ERROR).NE.1) THEN
      WRITE(6,'("CLOSE LIST ERROR =",I3)') ERROR
      End if

      Defined = 0
      LISTNAME= L_PROCESSEDLIST
      VALUENAMELIST(3) = F_RETENTIONTIME
      VALUENAMELIST(1) = F_AMOUNT
      VALUENAMELIST(2) = F_PEAKNAME
      VALUENAMELIST(4) = 0


      IF (LAS_OPENLIST(DCB,LISTPOINTER,LISTNAME,VALUENAMELIST,
     +  DEFINED,ERROR).NE.1) THEN
      WRITE(6,'("OPEN LIST ERROR = ",I5)')ERROR
      Else if (.not. Btest(Defined,15)) then
       Write(6,'("No B Peak Names")')
      Else if (.not. Btest(Defined,14)) then
       Write(6,'("No B Retention Times")')
      Else if (.not. Btest(Defined,13)) then
       Write(6,'("No B Amounts")')
      Else
      End if

      ENTRYNUMBER =  1
      I=1
       DO WHILE(ENTRYNUMBER .LE. NPKS)
       IF(LAS_READLISTVALUES(DCB,LISTPOINTER,Rbuff,
     +  ENTRYNUMBER,ERROR).NE. 1) THEN
       WRITE(6,*) 'ERROR IN READ LIST VALUES =',ERROR
       ENTRYNUMBER = NPKS
       GO TO 5000

       ELSE
        If (Peakname .EQ. '   ') then
        go to 16
        Else
```

```
            Dname(I)(1:30) = PeakName
            CB(I)= RetentionTime
            ValueB(I) = Amount
            I = I+1
            End if
16          Continue
            Dname(I) = '                '
            ENTRYNUMBER = ENTRYNUMBER + 1
            END IF
            BB = I
            END DO

5000        IF(LAS_CLOSELIST(DCB,LISTPOINTER,ERROR) .NE. 1) THEN
            Write(6,'("Close List Error =",I5)') ERROR
            end if
           CALL LAS_CLOSEFILE(DCB,UNLOCK,ERROR)
           IF (ERROR .NE.0) WRITE(6,'("CLOSE FILE ERROR",I5)')ERROR

          BA = BA-1
          BB= BB-1
*************************************************************************
*      SORT THE COMPOUNDS ACCORDING TO NUMBERS                          *
*************************************************************************
         DO  Q = 1.250
         NOSWAP = .TRUE.
          DO  M=2,BA
           IF(CNAME(M)(1:3) .LT. CNAME(M-1)(1:3)) THEN
           PX='     '
           PX = Cname(M)
           Cname(M) = Cname(M-1)
           Cname(M-1) = PX
           CX = C(M)
           C(M) = C(M-1)
           C(M-1) = CX
           CX = 0.0
           VALUEAX= 0.0
           VALUEAX=VALUEA(M)
           VALUEA(M) = VALUEA(M-1)
           VALUEA(M-1) = VALUEAX
           NOSWAP = .FALSE.
           END IF
           END DO
           IF (NOSWAP) GO TO 692
*          WRITE(1,'("PNAME =",A3)') PNAME(M)
           END DO
  692      CONTINUE
           DO Q = 1,150
           NOSWAP = .TRUE.
            DO M = 2,BB
            IF (DNAME(M)(1:3) .LT. DNAME(M-1)(1:3)) THEN
```

```
            SX = '      '
            SX = Dname(M)
            Dname(M) =Dname(M-1)
            Dname(M-1) = SX
            CBX = CB(M)
            CB(M) = CB(M-1)
            CB(M-1) = CBX
            CX = 0
            VALUEBX = 0
            VALUEBX = VALUEB(M)
            VALUEB(M) =VALUEB(M-1)
            VALUEB(M-1) = VALUEBX
            NO SWAP = .FALSE.
            END IF
            END DO
            IF (NOSWAP) GO TO 693
            END DO
693         CONTINUE

             bfs = 0
*****************************************************************
*  COMPARING NAMES COMMON TO BOTH LISTS AND PUT THEM IN ONE LIST*
*    AS WELL AS THE VALUE AND RETENTION TIME                    *
*****************************************************************

          XS = 0
            Do I=1.BA
              IF(Cname(I)(1:3).gt.'500') then
              bfs = bfs+1
              End if
              Do J = 1,BB
              If(Cname(I)(1:3).eq.Dname(J)(1:3).and.Dname(J)(1:3).gt.
     +        '500') then
              Cname(I)(1:30) = Dname(J)(1:30)
              CC(I) = CB(J)
              Valc(I) = Valueb(J)
              BS = BS+1
              Dname(J)(1:30) = '                              '
              CB(J) = 0.0
              Valueb(J) = 0.0
              go to 200
              end if
              If(Cname(I)(1:3).EQ.Dname(J)(1:3).and.Dname(J)(1:3).lt.
     +        '500') then
              CC(I)= CB(J)
              Cname(I)(16:27) = Dname(J)(5:15)
              Valc(I) = Valueb(J)
              XS=XS+1
              CB(J) = 0.0
              Valueb(J) = 0.0
              Dname(J)(1:30) = '                              '
```

```
              Go to 200
              End if
             End do
200          Continue
            End do
             XS= XS+BS
           Do Q = 1,250
            Do I = 1,BB
            NOSWAP = .TRUE.
       If (DName(I)(1:30) .EQ. '                                        ') then
             Dname(I) = Dname(I+1)
             CB(I) = CB(I+1)
             Valueb(I) = Valueb(I+1)
             Dname(I+1) = '                '
             CB(I+1) = 0.0
             ValueB(I+1) = 0.0
             NOSWAP = .FALSE.
             End if
            End do
            IF (NOSWAP) GO TO 695
            End do
695         CONTINUE
          XS1= BB-XS
*****************************************************************
*  ADD UNMATCHEDCOMPOUNDS FROM B LIST TO A LIST                 *
*****************************************************************
          Do J=1,XS1
           CC(BA+J) = CB(J)
           If (Dname(J)(1:3).gt.'210') then
           Cname(BA+J)(1:30) = Dname(J)(1:30)
           Else
           Cname(BA+J)(1:3) = Dname(J)(1:3)
           Cname(BA+J)(16:27) = Dname(J)(4:15)
           End if
           Valc(BA+J) = Valueb(J)
           CB(J) = 0.0
           Valueb(J) = 0.0
          End do

          XS2 = BA + XS1
*****************************************************************
*  NOW PUT COMPOUNDS IN THEIR NUMERICAL ORDER, PCB'S FIRST      *
*****************************************************************
          DO Q = 1,150
          Noswap = .TRUE.
           Do M = 2,XS2
           If(Cname(M) .lt. Cname(M-1)) then
            PX = Cname(M)
            Cname(M) = Cname(M-1)
            Cname(M-1) = PX
            PX = '                '
```

```
            CX = C(M)
            C(M) = C(M-1)
            C(M-1) = CX
            CX = CB(M)
            CB(M) = CB(M-1)
            CB(M-1) = CX
             CX = CC(M)
             CC(M) = CC(M-1)
             CC(M-1) = CX
            Valuex = ValueA(M)
            ValueA(M) = ValueA(M-1)
            ValueA(M-1) = Valuex
            Valuex = ValueB(M)
            ValueB(M) = ValueB(M-1)
            ValueB(M-1) = Valuex
            Valuex = Valc(M)
            Valc(M)= Valc(M-1)
            Valc(M-1)= Valuex
            SX = '          '
            Noswap = .FALSE.
            End if
            End do
           If (Noswap)  go to 694
          End do
 694      Continue

          Do N= 1,XS2
          if(C(N) .EQ. CB(N)) then
             C(N) = 0.0
             Valuea(N) = 0.0
           Else
             ValueB(N) = Valc(N)
             CB(N) = CC(N)
           End if
           End do
*************************************************************************
*     SORT AS TO DEGREE OF SUBSTITUTION AND DO TWO SUMS: ONE FOR  *
*     CONFIRMED HITS, THE OTHER FOR POSSIBLE PRESENCE             *
*************************************************************************
           DO M = 1,XS2
            IF(CNAME(M)(1:3).GT.'003' ) THEN
             GO TO 521
              END IF
               IF (VALUEA(M).GT.0.0.AND.VALC(M).GT.0.0) THEN
                 PCB1C = PCB1C+VALUEA(M)
                 PCB1D = PCB1D+VALC(M)
                ELSE
                 IF (CNAME(M)(1:3).EQ.CNAME(M)(16:18))THEN
                 PCB1C = PCB1C+VALUEA(M)
                 PCB1D = PCB1D+VALC(M)
```

```
              END IF
              END IF
            PCB1A = PCB1A+VALUEA(M)
            PCB1B = PCB1B+VALC(M)
            X1 = X1 + 1

            GO TO 750
521         IF (CNAME(M)(1:3) .GT.'015') THEN
             GO TO 522
            END IF
              IF (VALUEA(M).GT.0.0.AND.VALC(M).GT.0.0) THEN
              PCB2C=PCB2C+VALUEA(M)
              PCB2D=PCB2D+VALC(M)
              ELSE
               IF(CNAME(M)(1:3).EQ.CNAME(M)(16:18)) THEN
               PCB2C= PCB2C+VALUEA(M)
               PCB2D=PCB2D+VALC(M)
               END IF
               END IF
             PCB2A = PCB2A+VALUEA(M)
             PCB2B = PCB2B+VALC(M)
             X2 = X2 +1

            GO TO 750
522         IF (CNAME(M)(1:3) .GT.'039') THEN
            GO TO 523
            END IF
             IF (VALUEA(M).GT.0.0.AND.VALC(M).GT.0.0) THEN
             PCB3C = PCB3C+VALUEA(M)
             PCB3D = PCB3D+VALC(M)
             ELSE
              IF (CNAME(M)(1:3) .EQ. CNAME(M)(16:18))THEN
              PCB3C = PCB3C+VALUEA(M)
              PCB3D = PCB3D+VALC(M)
              END IF
              END IF
             PCB3A = PCB3A+VALUEA(M)
             PCB3B = PCB3B+VALC(M)
             X3 = X3 + 1

             GO TO 750
523          IF (CNAME(M)(1:3).GT.'081') THEN
             GO TO 524
             END IF
             IF (VALUEA(M).GT.0.0 .AND. VALC(M) .GT.0.0) THEN
              PCB4C = PCB4C+VALUEA(M)
              PCB4D = PCB4D+VALC(M)
             ELSE
               IF (CNAME(M)(1:3) .EQ. CNAME(M)(16:18)) THEN
```

```
                PCB4C=PCB4C+VALUEA(M)
                PCB4D = PCB4D + VALC(M)
                END IF
                END IF
              PCB4A = PCB4A+VALUEA(M)
              PCB4B = PCB4B+VALC(M)
              X4 = X4 + 1

              GO TO 750
524           IF (CNAME(M)(1:3) .GT.'127')THEN
              GO TO 525
              END IF
               IF (VALUEA(M) .GT. 0.0 .AND. VALC(M) .GT.0.0) THEN
               PCB5C = PCB5C+VALUEA(M)
               PCB5D = PCB5D + VALC(M)
               ELSE
               IF (CNAME(M)(1:3) .EQ. CNAME(M)(16:18)) THEN
               PCB5C = PCB5C + VALUEA(M)
               PCB5D = PCB5D + VALC(M)
               END IF
               END IF
              PCB5A = PCB5A+VALUEA(M)
              PCB5B = PCB5B+VALC(M)
              X5 = X5 + 1

              GO TO 750
525           IF (CNAME(M)(1:3) .GT. '169' ) THEN
              GO TO 526
              END IF
               IF (VALUEA(M) .GT. 0.0 .AND. VALC(M) .GT.0.0) THEN
               PCB6C = PCB6C+VALUEA(M)
               PCB6D = PCB6D+VALC(M)
               ELSE
               IF (CNAME(M)(1:3) .EQ. CNAME(M)(16:18)) THEN
               PCB6C = PCB6C+VALUEA(M)
               PCB6D = PCB6D+VALC(M)
               END IF
               END IF
              PCB6A = PCB6A+VALUEA(M)
              PCB6B = PCB6B+VALC(M)
              X6 = X6 + 1

              GO TO 750
526           IF (CNAME(M)(1:3) .GT. '193') THEN
              GO TO 527
              END IF
               IF (VALUEA(M) .GT. 0.0 .AND. VALC(M) .GT. 0.0) THEN
               PCB7C = PCB6C+VALUEA(M)
               PCB7D = PCB7D + VALC(M)
               ELSE
```

```
            IF(CNAME(M)(1:3) .EQ.CNAME(M)(16:18)) THEN
            PCB7C = PCB7C+VALUEA(M)
            PCB7D= PCB7D+VALC(M)
            END IF
            END IF
           PCB7A=PCB7A+VALUEA(M)
           PCB7B= PCB7B +VALC(M)
           X7 = X7 + 1

           GO TO 750
527        IF (CNAME(M)(1:3) .GT. '205') THEN
           GO TO 528
           END IF
           IF (VALUEA(M) .GT.0.0 .AND. VALC(M) .GT. 0.0) THEN
           PCB8C = PCB8C+ VALUEA(M)
           PCB8D = PCB8D+ VALC(M)
           ELSE
            IF(CNAME(M)(1:3) .EQ. CNAME(M)(16:18)) THEN
           PCB8C = PCB8C + VALUEA(M)
           PCB8D = PCB8D + VALC(M)
           END IF
           END IF
           PCB8A = PCB8A+VALUEA(M)
           PCB8B = PCB8B+VALC(M)
           X8 = X8 + 1

           GO TO 750
528        IF (CNAME(M)(1:3) .GT.'208') THEN
           GO TO 529
           END IF
            IF (VALUEA(M).GT.0.0 .AND. VALC(M) .GT. 0.0) THEN
            PCB9C = PCB9C + VALUEA(M)
            PCB9D = PCB9D+ VALC(M)
            ELSE
            IF (CNAME(M)(1:3) .EQ. CNAME(M)(16:18)) THEN
             PCB9C = PCB9C+VALUEA(M)
             PCB9D = PCB9D+ VALC(M)
             END IF
             END IF
           PCB9A = PCB9A+VALUEA(M)
           PCB9B = PCB9B+VALC(M)
           X9 = X9 + 1

           GO TO 750
529         If (Cname(M)(1:3).gt.'209') then
            X11 = X11+1
            Go to 530
            Else
            X10A=Valuea(M)
            X10B=Valc(M)
            End if
530         Continue
```

```
 750          CONTINUE

          END DO
*************************************************************************
*    THE TEDIOUS TASK OF OUTPUTTING                                     *
*************************************************************************
        WRITE(6,'(2X,"ANALYSIS OF PCB s by ISOMER and SUBSTITUTION")')
        WRITE(6,'(2x,"FOR FILES",A27,"and ",A14)') NFILE(1:27),PFILE(14
     +  :27)
  706   FORMAT(1X,A10,A30,X,A5)
        WRITE(6,707)
  707   FORMAT('0')
         If (PCB1A .EQ. 0.0 .and.PCB2B .EQ.0.0) Then
        Write(6,'(2x,"No Mono-Substituted PCBs")')
        Write(6,707)
        Go to 708
        End if
        WRITE(6,'(2X,"MONOSUBSTITUTED PCB S")')
        WRITE(6,707)
        WRITE(6,'(1X,"COMPONENT   CONC.A      CONC.B    RT.A    RT.B   COELUTE
     + COELUTE")')
        WRITE(6,'(45X,"ON A       ON B")')
         DO 717, M=1,X1
        WRITE(6,714) CNAME(M)(1:3),VALUEA(M),VALC(M),C(M),CC(M),
     + CNAME(M)(5:11),CNAME(M)(16:23)
  714   FORMAT(1X,A8,2X,F8.5,2X,F8.5,2X,F5.2,2X,F5.2,3x,A8,2X,A8)
  717    CONTINUE
         WRITE(6,'(2X,"TOTAL CONFIRMED MONO SUBST. ON A =",F8.4)')PCB1C
         WRITE(6,'(2X,"TOTAL CONFIRMED MOMO SUBST. ON B =",F8.4)')PCB1D
         WRITE(6,'(2X,"TOTAL POSSIBLE MONO SUBST. ON A =",F8.4)') PCB1A
         WRITE(6,'(2X,"TOTAL POSSIBLE MONO SUBST. ON B =",F8.4)') PCB1B
         Write(6,707)
  708     X1= X1+1
         If (PCB2A .EQ. 0.0 .and. PCB2B .EQ. 0.0) then
         Write(6,'(2x,"No Di-Substituted PCBs")')
         Go to 709
         End if
         Write(6,707)
         WRITE(6,'(2X,"DISUBSTITUTED PCB S")')
         WRITE(6,707)
        WRITE(6,'(1X,"COMPONENT   CONC.A      CONC.B    RT.A    RT.B    COELUTE
     +  COELUTE")')
        WRITE(6,'(45X,"ON A       ON B")')
          DO 718,M=X1,X1+X2-1
        WRITE(6,714) CNAME(M)(1:3),VALUEA(M),VALC(M),C(M),CC(M),
     +  CNAME(M)(5:11),CNAME(M)(16:23)
  718     CONTINUE
         WRITE(6,'(2X,"TOTAL CONFIRMED DI-SUBST ON A =",F8.4)')PCB2C
         WRITE(6,'(2X,"TOTAL CONFIRMED DI-SUBST ON B =",F8.4)')PCB2D
         WRITE(6,'(2X,"TOTAL POSSIBLE DI-SUBST. ON A =",F8.4)') PCB2A
         WRITE(6,'(2X,"TOTAL POSSIBLE DI-SUBST. ON B =",F8.4)') PCB2B
```

```
      WRITE(6,707)
709   X2 = X1+X2
       If (PCB3A .eq. 0.0 .and. PCB3B .eq.0.0) Then
       Write(6,'(2x,"No Tri-Substituted  PCBs"))')
       Go to 710
       End if
      Write(6,707)
      WRITE(6,'(2X,"TRISUBSTITUTED PCB S")')
      WRITE(6,707)
     WRITE(6,'(1X,"COMPONENT  CONC.A     CONC.B   RT.A   RT.B   COELUTE
    +  COELUTE")')
     WRITE(6,'(45X,"ON A        ON B")')
        DO 719,M=X2,X2+X3-1
     WRITE(6,714) CNAME(M)(1:3),VALUEA(M),VALC(M),C(M),CC(M),
    +  CNAME(M)(5:11),CNAME(M)(16:23)
719    CONTINUE
      WRITE(6,'(2X,"TOTAL CONFIRMED TRI-SUBST ON A=",F8.4)')PCB3C
      WRITE(6,'(2X,"TOTAL CONFIRMED TRI-SUBST ON B=",F8.4)')PCB3D
       WRITE(6,'(2X,"TOTAL POSSIBLE TRI-SUBST. ON A =",F8.4)') PCB3A
       WRITE(6,'(2X,"TOTAL POSSIBLE TRI-SUBST. ON B =",F8.4)') PCB3B
710   X3 = X2+X3
      If(PCB4A .eq.0.0 .and. PCB4B .eq.0.0) then
      Write(6,'(2x,"No Tetra-Substituted PCBs"))')
      Go to 711
      End if
       Write(6,707)
       WRITE(6,'(2X,"TETRASUBSTITUTED PCB S")')
       WRITE(6,707)
     WRITE(6,'(1X,"COMPONENT  CONC.A     CONC.B   RT.A   RT.B  COELUTE
    +  COELUTE")')
     WRITE(6,'(45X,"ON A        ON B")')
       DO 720,M=X3,X3+X4-1
     WRITE(6,714) CNAME(M)(1:3),VALUEA(M),VALC(M),C(M),CC(M),
    +  CNAME(M)(5:11),CNAME(M)(16:23)
720    CONTINUE
     WRITE(6,'(2X,"TOTAL CONFIRMED TETRA-SUBST ON A =",F8.4)')PCB4C
     WRITE(6,'(2X,"TOTAL CONFIRMED TETRA-SUBST ON B =",F8.4)')PCB4D
     WRITE(6,'(2X,"TOTAL POSSIBLE TETRA-SUBST. ON A =",F8.4)') PCB4A
     WRITE(6,'(2X,"TOTAL POSSIBLE TETRA-SUBST. ON B =",F8.4)') PCB4B
      WRITE(6,707)
711    X4 = X3+X4
       If(PCB5A .eq. 0.0 .and. PCB5B .eq. 0.0) then
       Write(6,'(2x,"No Penta-Substituted PCBs"))')
       Go to 712
       End if
       WRITE(6,'(2X,"PENTASUBSTITUTED PCB S")')
       WRITE(6,707)
     WRITE(6,'(1X,"COMPONENT  CONC.A     CONC.B   RT.A   RT.B  COELUTE
    +  COELUTE")')
     WRITE(6,'(45X,"ON A        ON B")')
```

```
        DO 721,M=X4,X4+X5-1
       WRITE(6,714) CNAME(M)(1:3),VALUEA(M),VALC(M),C(M),CC(M),
     +    CNAME(M)(5:11),CNAME(M)(16:23)
721      CONTINUE
      WRITE(6,'(2X,"TOTAL CONFIRMED PENTA-SUBST ON A =",F8.4)')PCB5C
      WRITE(6,'(2X,"TOTAL CONFIRMED PENTA-SUBST ON B =",F8.4)')PCB5D
         WRITE(6,'(2X,"TOTAL POSSIBLE PENTA-SUBST. ON A =",F8.4)') PCB5A
         WRITE(6,'(2X,"TOTAL POSSIBLE PENTA-SUBST. ON B =",F8.4)') PCB5B
        WRITE(6,707)
712      X5 = X4+X5
         If (PCB6A .eq. 0.0 .and. PCB6B .eq.0.0) then
         Write(6,'(2x,"No Hexa-Substituted PCBs")')
         Go to 713
         End if
         WRITE(6,'(2X,"HEXASUBSTITUTED PCB S")')
        WRITE(6,707)
      WRITE(6,'(1X,"COMPONENT  CONC.A     CONC.B   RT.A   RT.B  COELUTE
     +  COELUTE")')
       WRITE(6,'(45X,"ON A        ON B")')
         DO 722,M=X5,X5+X6-1
       WRITE(6,714) CNAME(M)(1:3),VALUEA(M),VALC(M),C(M),CC(M),
     +  CNAME(M)(5:11),CNAME(M)(16:23)
722      CONTINUE
        WRITE(6,'(2X,"TOTAL CONFIRMED HEXA-SUBST ON A =",F8.4)')PCB6C
        WRITE(6,'(2X,"TOTAL CONFIRMED HEXA-SUBST ON B =",F8.4)')PCB6D
        WRITE(6,'(2X,"TOTAL POSSIBLE HEXA-SUBST. ON A =",F8.4)')PCB6A
        WRITE(6,'(2X,"TOTAL POSSIBLE HEXA-SUBST. ON B =",F8.4)')PCB6B
         WRITE(6,707)
713      X6 = X5+X6
         If (PCB7A .eq.0.0 .and. PCB7B .eq.0.0) then
         Write(6,'(2x,"No Hepta-Substituted PCBs")')
         Go to 753
         End if
         WRITE(6,'(2X,"HEPTASUBSTITUTED PCB S")')
           WRITE(6,707)
      WRITE(6,'(1X,"COMPONENT  CONC.A     CONCB.   RT.A   RT.B  COELUTE
     +  COELUTE")')
       WRITE(6,'(6,45X,"ON A        ON B")')
          DO 723,M=X6,X6+X7-1
       WRITE(6,714) CNAME(M)(1:3),VALUEA(M),VALC(M),C(M),CC(M),
     +  CNAME(M)(5:11),CNAME(M)(16:23)
723      CONTINUE
      WRITE(6,'(2X,"TOTAL CONFIRMED HEPTA-SUBST ON A=",F8.4)')PCB7C
      WRITE(6,'(2X,"TOTAL CONFIRMED HEPTA-SUBST ON B=",F8.4)')PCB7D
      WRITE(6,'(2X,"TOTAL POSSIBLE HEPTA-SUBST. ON A =",F8.4)') PCB7A
      WRITE(6,'(2X,"TOTAL POSSIBLE HEPTA-SUBST. ON B =",F8.4)') PCB7B
          WRITE(6,707)
753       X7= X6+X7
          If(PCB8A.eq.0.0 .and. PCB8B.eq.0.0) then
          Write(6,'(2x,"No Octa-Substituted PCBs")')
```

```
          Go to 754
          End if
         WRITE(6,'(2X,"OCTASUBTITUTED PCB S")')
          WRITE(6,707)
        WRITE(6,'(1X,"COMPONENT  CONC.A     CONC.B   RT.A   RT.B  COELUTE
     +  COELUTE")')
        WRITE(6,'(45X,"ON A        ON B")')
          DO 724, M=X7,X7+X8-1
        WRITE(6,714) CNAME(M)(1:3),VALUEA(M),VALC(M),C(M),CC(M),
     +  CNAME(M)(5:11),CNAME(M)(16:23)
 724      CONTINUE
        WRITE(6,'(2X,"TOTAL CONFIRMED OCTA-SUBST ON A =",F8.4)')PCB8C
        WRITE(6,'(2X,"TOTAL CONFIRMED OCTA-SUBST ON B =",F8.4)')PCB8D
        WRITE(6,'(2X,"TOTAL POSSIBLE OCTA-SUBST. ON A =",F8.4)') PCB8A
        WRITE(6,'(2X,"TOTAL POSSIBLE OCTA-SUBST. ON B =",F8.4)') PCB8B
          WRITE(6,707)
 754      X8 = X8+X7
          If (PCB9A .eq.0.0 .and.PCB9B.eq.0.0) then
          Write(6,'(2x,"No Nona(9)-Substituted PCBs")')
          Go to 755
           End if
          WRITE(6,'(2X,"NONA SUBSTITUTED PCB S")')
          WRITE(6,707)
        WRITE(6,'(1X,"COMPONENT  CONC.A     CONC.B   RT.A   RT.B  COELUTE
     +  COELUTE")')
        WRITE(6,'(45X,"ON A        ON B")')
           DO 725,M = X8,X8+X9-1
        WRITE(6,714) CNAME(M)(1:3),VALUEA(M),VALC(M),C(M),CC(M),
     +  CNAME(M)(5:11),CNAME(M)(16:23)
 725      CONTINUE
        WRITE(6,'(2X,"TOTAL CONFIRMED NONA-SUBST ON A =",F8.4)')PCB9C
        WRITE(6,'(2X,"TOTAL CONFIRMED NONA-SUBST ON B =",F8.4)')PCB9D
        WRITE(6,'(2X,"TOTAL POSSIBLE NONA-SUBST. ON A =",F8.4)') PCB9A
        WRITE(6,'(2X,"TOTAL POSSIBLE NONA-SUBST. ON B =",F8.4)') PCB9B
          WRITE(6,707)
          X10 = X8+X9
 755      WRITE(6,707)
          If (Cname(x10)(1:3).eq. '209') then
          WRITE(6,'(3X,"DECA CONC. ON A =",F8.4)') VALUEA(X10)
          WRITE(6,'(3X,"DECA CONC. ON B =",F8.4)') VALUEB(X10)
          Else
          X10 = X10-1
          End if
        PCB11C=PCB1C+PCB2C+PCB3C+PCB4C+PCB5C+PCB6C+CPB7C+PCB8C+PCB9C
        PCB11D=PCB1D+PCB2D+PCB3D+PCB4D+PCB5D+PCB6D+PCB7D+PCB8D+PCB9D
        WRITE(6,'(2X,"TOTAL CONFIRMED PCBs ON A =",F8.4)') PCB11C
        WRITE(6,'(2X,"TOTAL CONFIRMED PCBs ON B =",F8.4)') PCB11D
 27       Format('0')
          Print 27
          X10 = X10+1
```

```
            If (X11.eq.0) then
            Write(6,'(1x,"No OCA s")')
            PRINT 650
            Go to 651
            End if
            Write(6,'(14X,"ANALYSIS OF OCA S")')
            Print 27
      Write(6,'(1x,"COMPOUND",20X,"CONC.       CONC.       RT.A    RT.B")')
        Write(6,'(30X,"ON A       ON B")')
           Do M= X10,X10+X11-1
          Write(6,814) CNAME(M)(5:29),VALUEA(M),VALC(M),C(M),CC(M)
814      FORMAT(1X,A25,2X,F8.5,2X,F8.5,3X,F5.2,2X,F5.2)
           End do
            PRINT 650
650         FORMAT('1')
 30     CALL LAS TELLCLOSE
651     STOP
        End
```

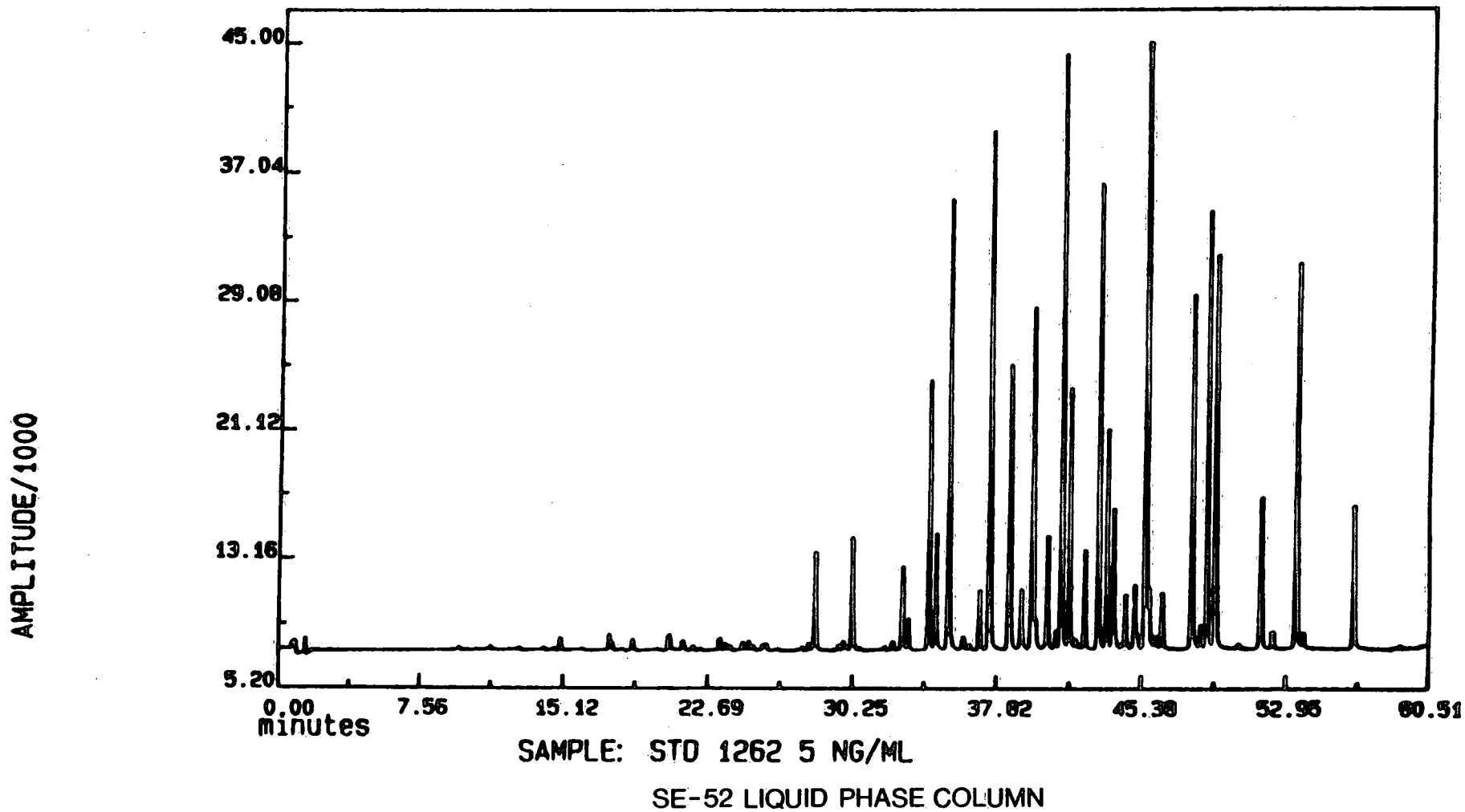
45.00
37.04
29.08
21.12
13.16
5.20
AMPLITUDE/1000
0.00
7.56
15.12
22.69
30.25
37.82
45.38
52.95
60.51
minutes
SAMPLE: STD 1262 5 NG/ML
SE-52 LIQUID PHASE COLUMN

Fig. 1

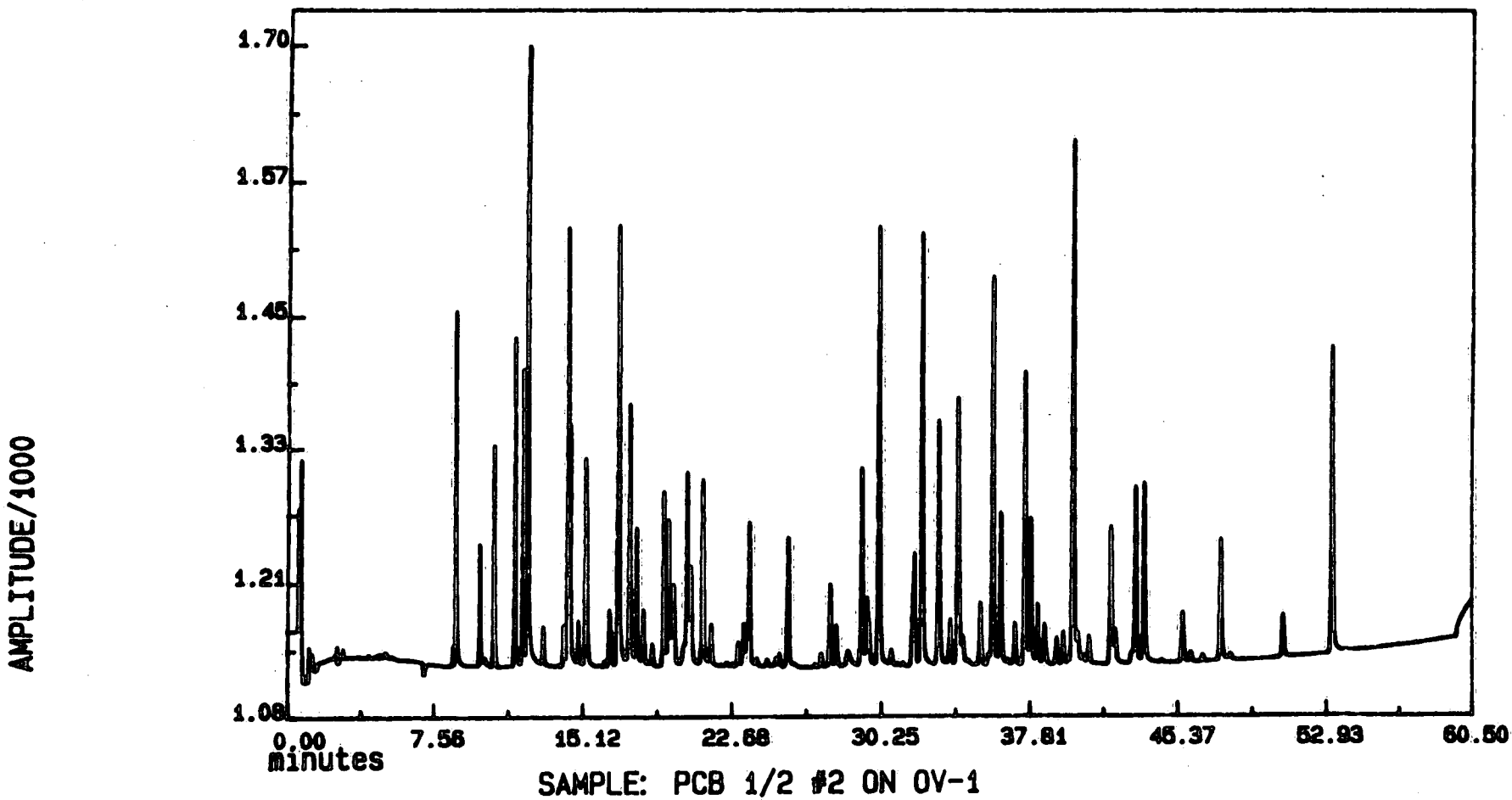
AMPLITUDE/1000
1.70
1.57
1.45
1.33
1.21
1.08
0.00
7.56
15.12
22.68
30.25
37.81
45.37
52.93
60.50
minutes
SAMPLE: PCB 1/2 #2 ON OV-1

Fig. 2

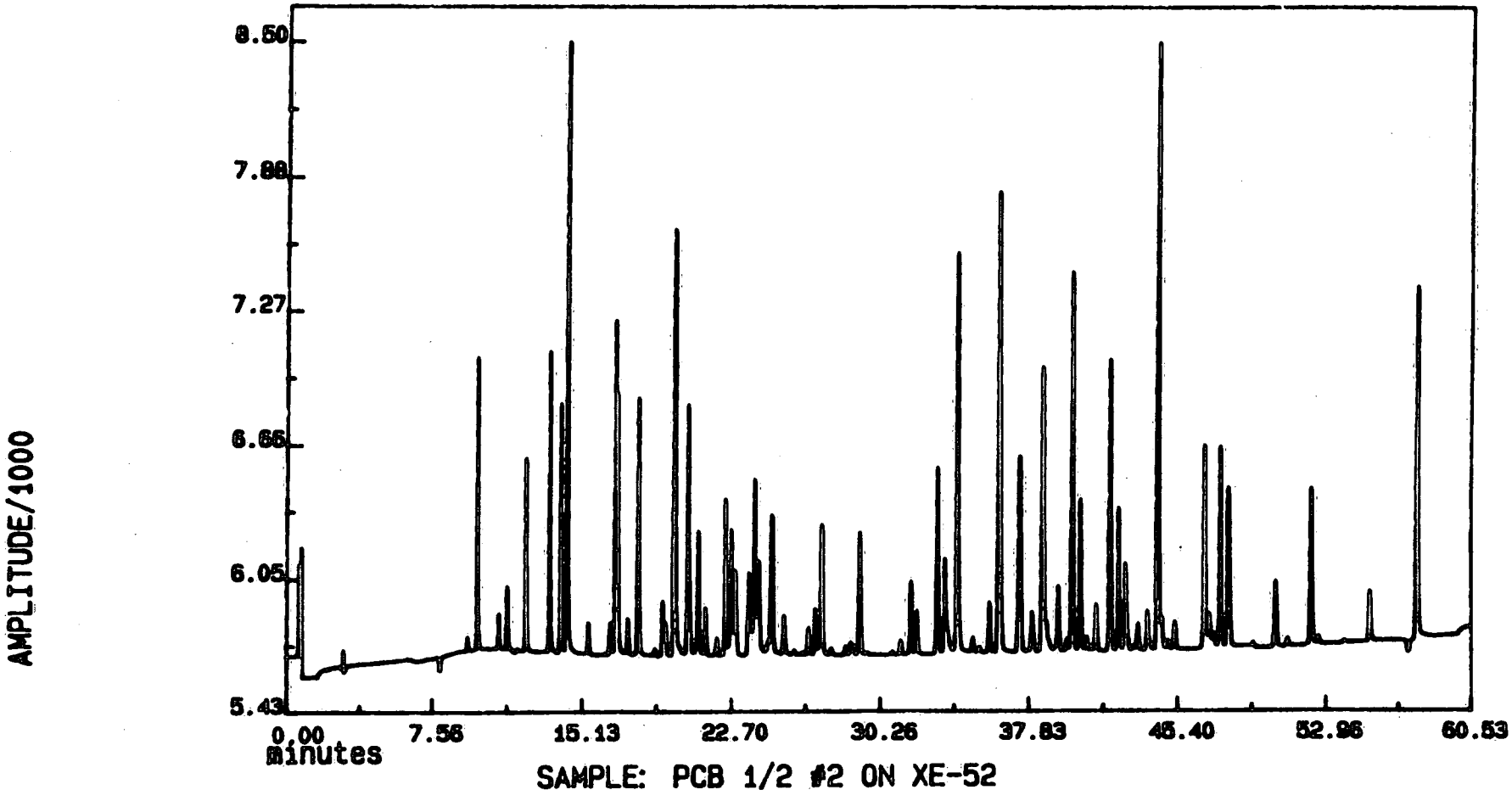
AMPLITUDE/1000
8.50
7.88
7.27
6.66
6.05
5.43
0.00
7.56
15.13
22.70
30.26
37.83
45.40
52.96
60.53
minutes
SAMPLE: PCB 1/2 #2 ON XE-52

Fig. 3

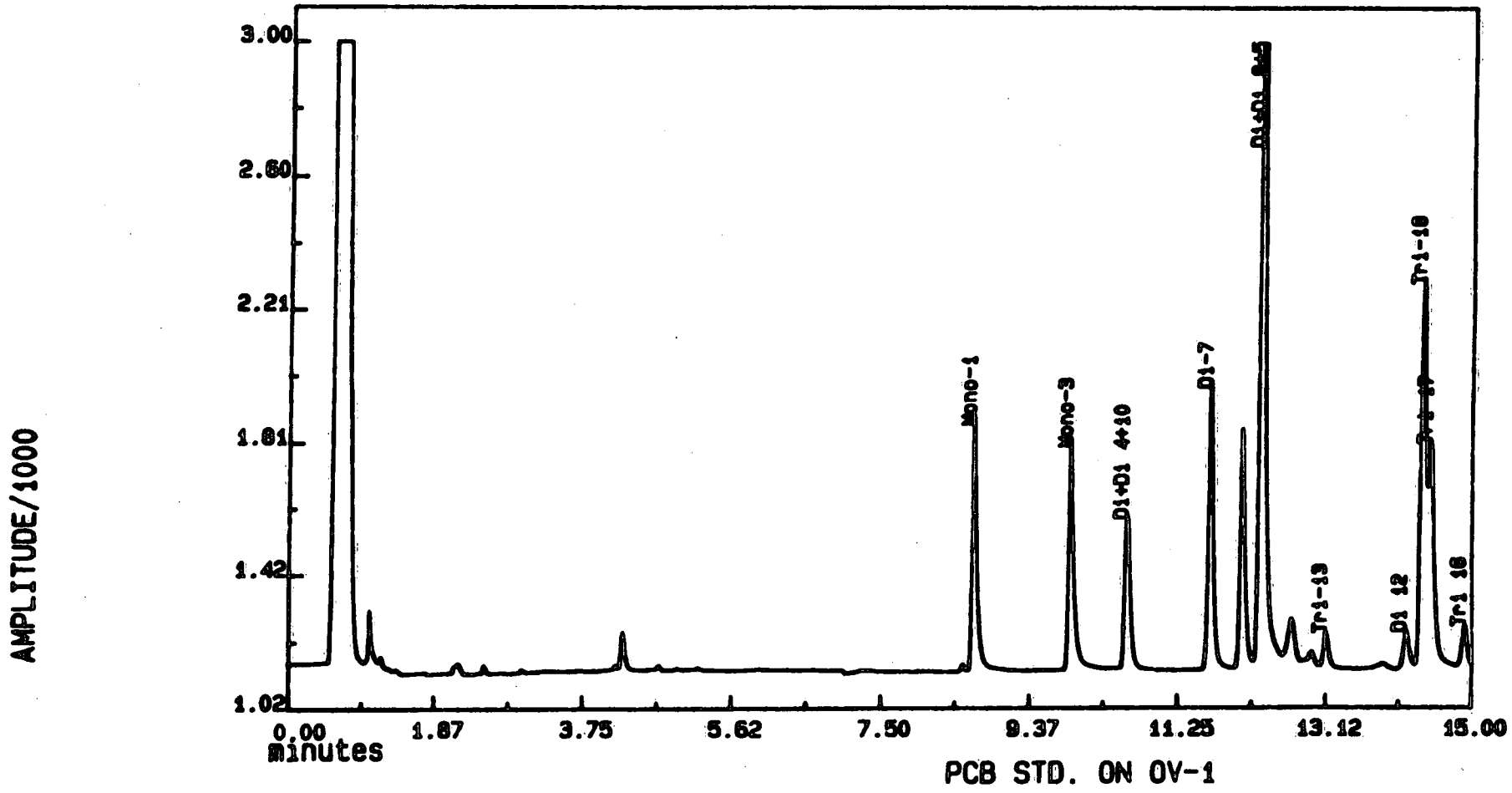
AMPLITUDE/1000
3.00
2.60
2.21
1.81
1.42
1.02
0.00
1.87
3.75
5.62
7.50
9.37
11.25
13.12
15.00
minutes
Mono-1
Mono-3
D1+D1 4+10
D1-7
Tr1-13
D1 12
Tr1 16
PCB STD. ON OV-1

Fig. 4(a)

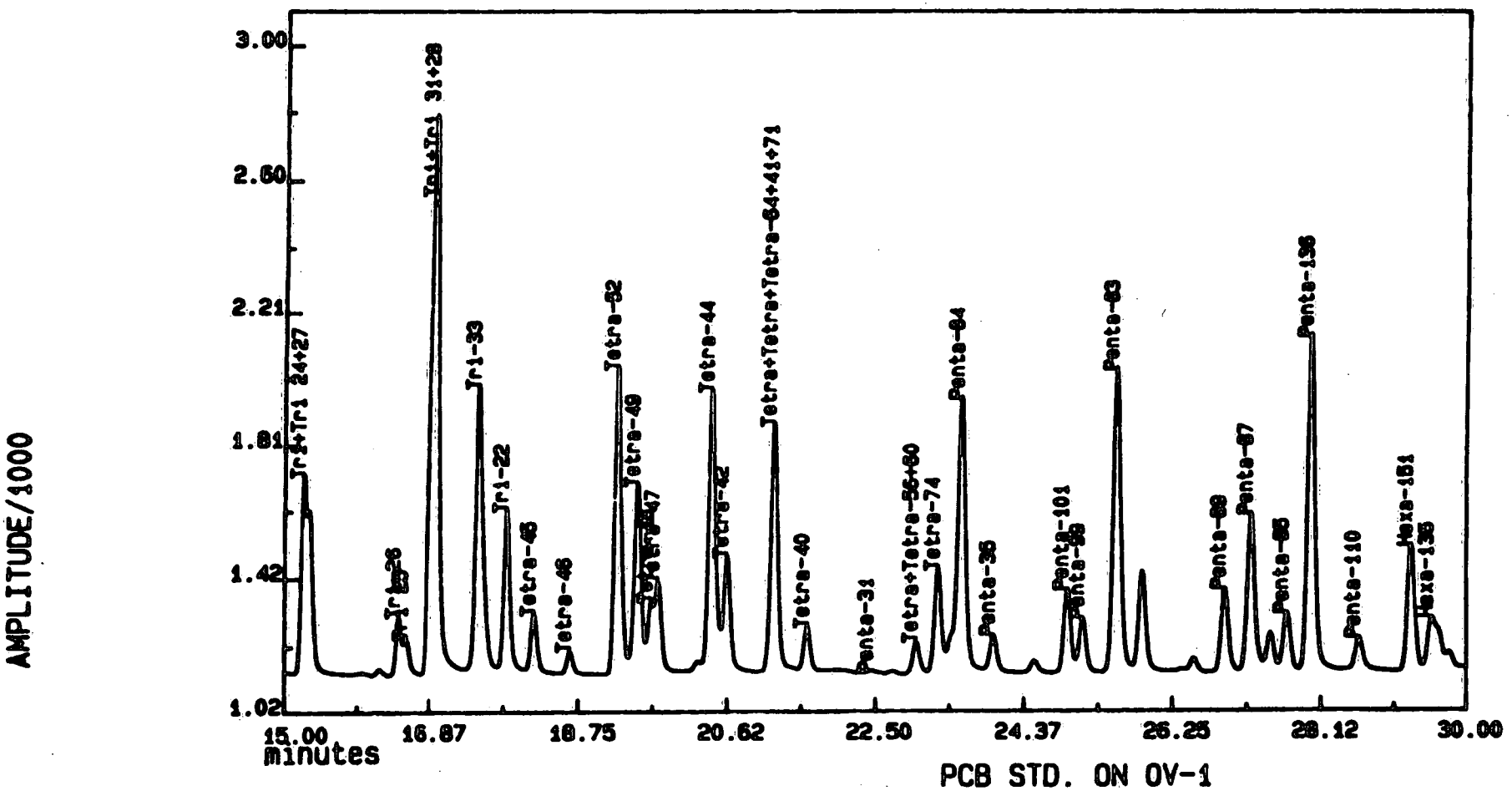
AMPLITUDE/1000
3.00
2.60
2.21
1.81
1.42
1.02
15.00
16.87
18.75
20.62
22.50
24.37
26.25
28.12
30.00
minutes
PCB STD. ON OV-1
Tri+Tri 24+27
Tri-33
Tri-22
Tetra-45
Tetra-46
Tetra-52
Tetra-49
Tetra-44
Tetra-42
Tetra+Tetra+Tetra-64+41+71
Tetra-40
Penta-31
Tetra+Tetra-56+60
Tetra-74
Penta-64
Penta-35
Penta-101
Penta-83
Penta-87
Penta-85
Penta-110
Penta-136
Hexa-151
Hexa-135

Fig. 4(b)

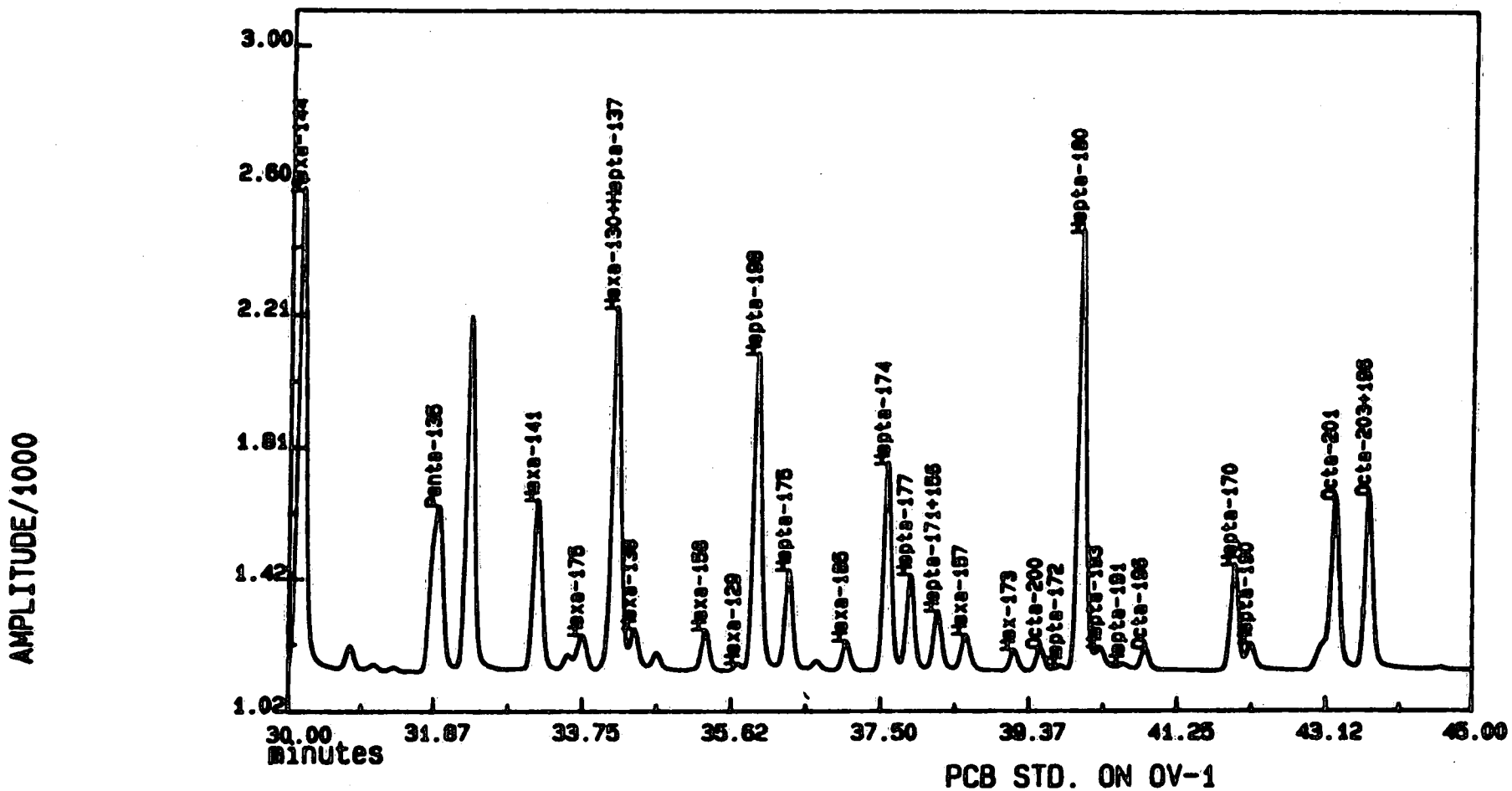
AMPLITUDE/1000
3.00
2.60
2.21
1.81
1.42
1.02
Hexa-134
Penta-135
Hexa-141
Hexa-176
Hexa-130+Hepta-137
Hexa-138
Hexa-158
Hexa-129
Hepta-178
Hepta-175
Hexa-165
Hepta-174
Hepta-177
Hepta-171+156
Hexa-167
Hex-173
Octa-200
Hepta-172
Hepta-180
Hepta-183
Hepta-191
Octa-196
Hepta-170
Hepta-190
Octa-201
Octa-203+196
30.00
31.87
33.75
35.62
37.50
39.37
41.25
43.12
45.00
Minutes
PCB STD. ON OV-1

Fig.4(c)

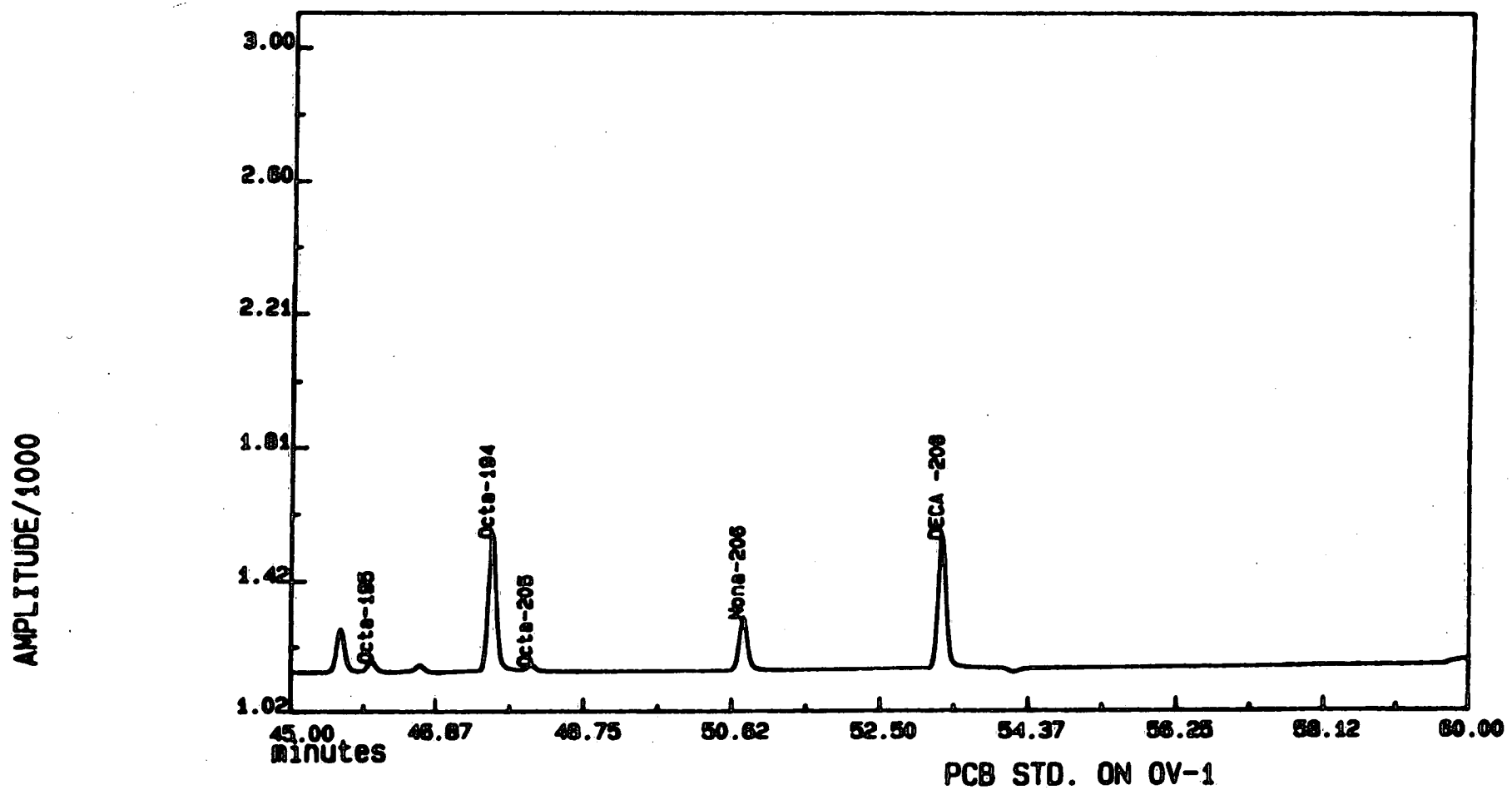
AMPLITUDE/1000
3.00
2.60
2.21
1.81
1.42
1.02
Octa-195
Octa-194
Octa-205
Nona-206
DECA -208
45.00
46.87
48.75
50.62
52.50
54.37
56.25
58.12
60.00
minutes
PCB STD. ON OV-1

Fig. 4 (d)

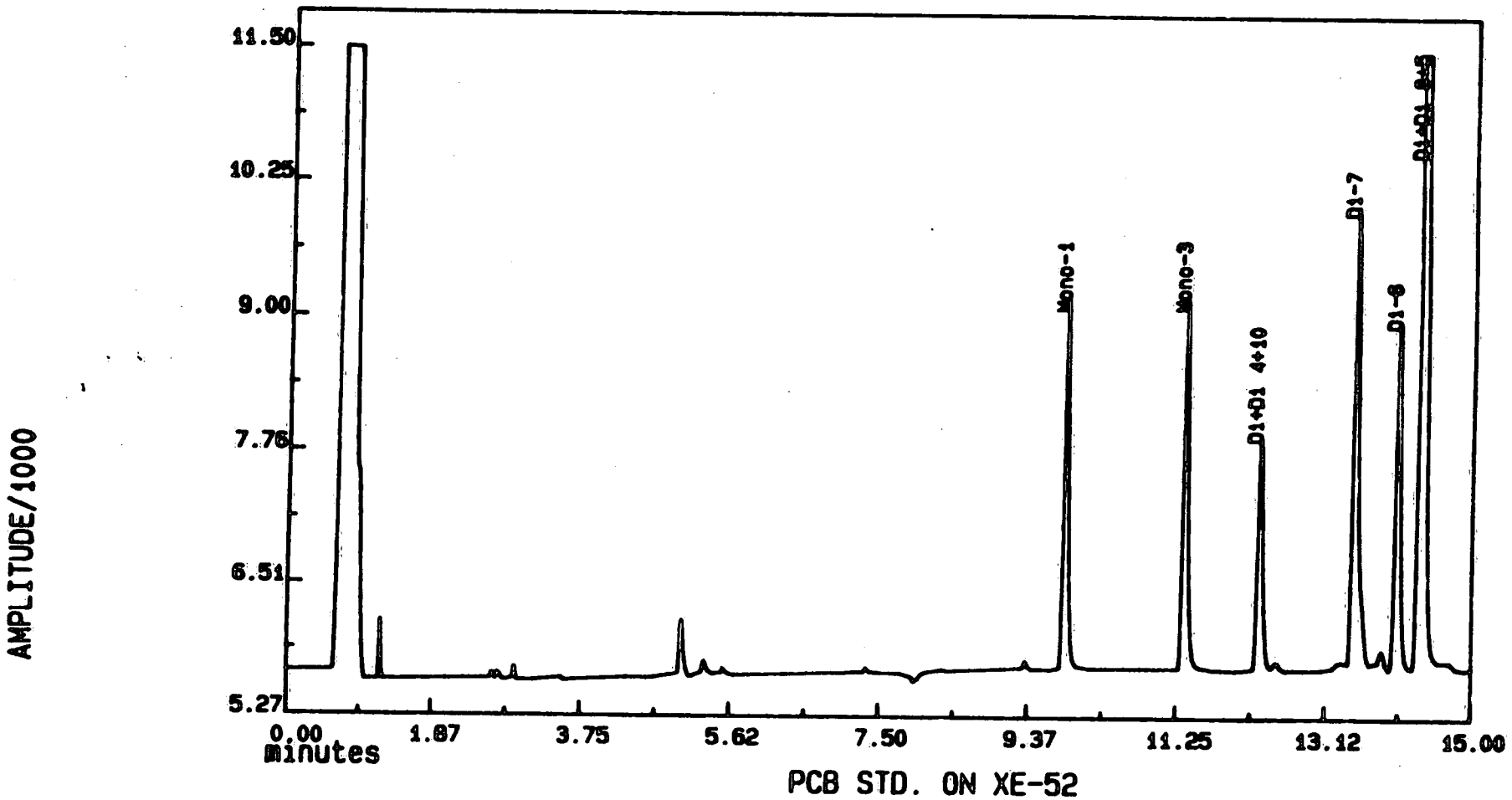
AMPLITUDE/1000
11.50
10.25
9.00
7.76
6.51
5.27
0.00
minutes
1.87
3.75
5.62
7.50
9.37
11.25
13.12
15.00
Mono-1
Mono-3
D1+D1 4+10
D1-7
D1-8
D1-10
PCB STD. ON XE-52

Fig. 5(a)

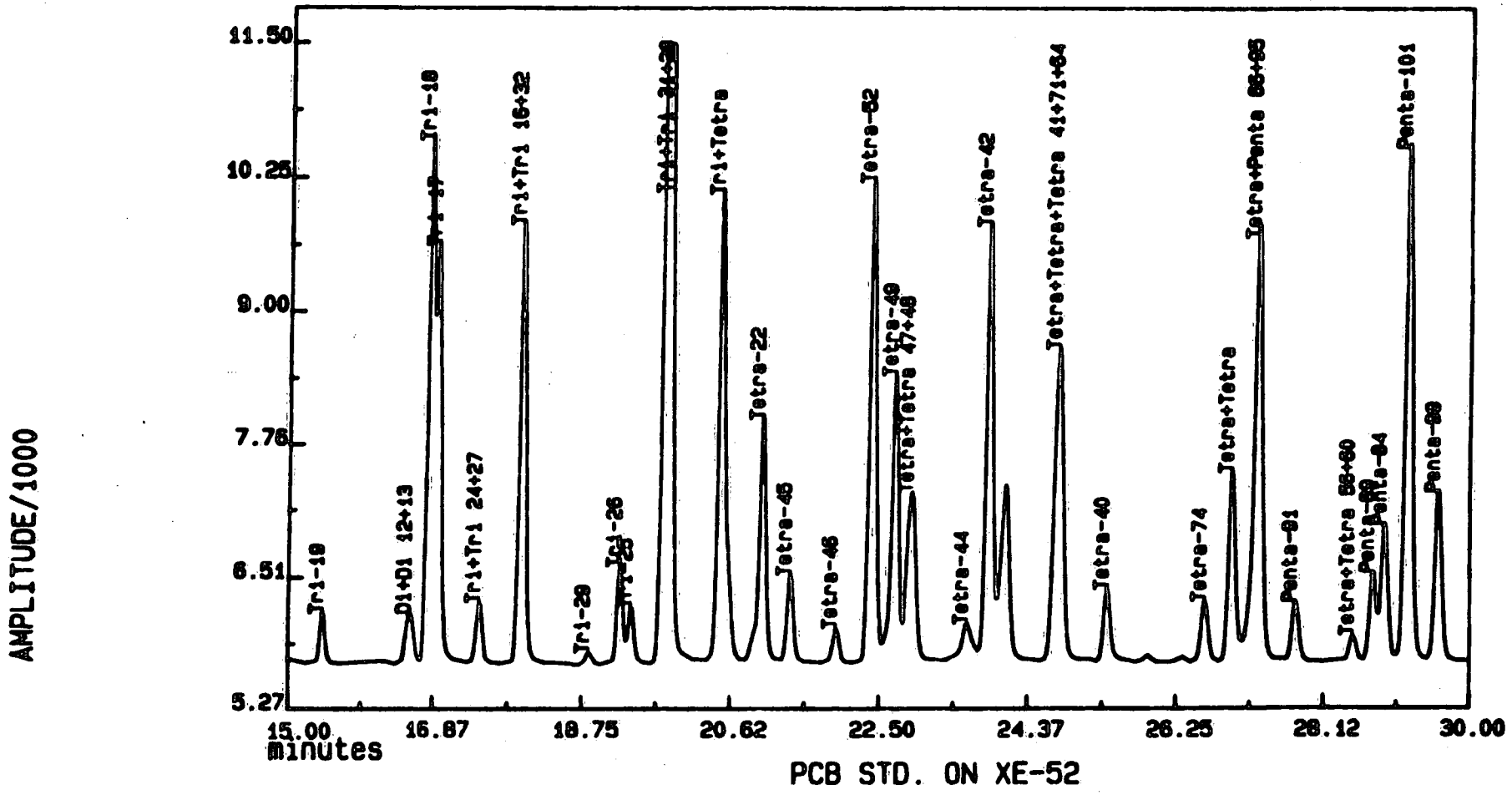
AMPLITUDE/1000
11.50
10.25
9.00
7.76
6.51
5.27
15.00
16.87
18.75
20.62
22.50
24.37
26.25
28.12
30.00
minutes
PCB STD. ON XE-52
Tri-18
Di+Di 12+13
Tri+Tri 24+27
Tri-29
Tri-26
Tri+Tetra
Tetra-22
Tetra-45
Tetra-46
Tetra-52
Tetra-49
Tetra 47+48
Tetra-44
Tetra-42
Tetra+Tetra 41+71+64
Tetra-40
Tetra-74
Tetra+Tetra
Tetra+Penta 86+85
Penta-91
Tetra+Tetra 58+60
Penta-84
Penta-101
Penta-99

Fig.5(b)

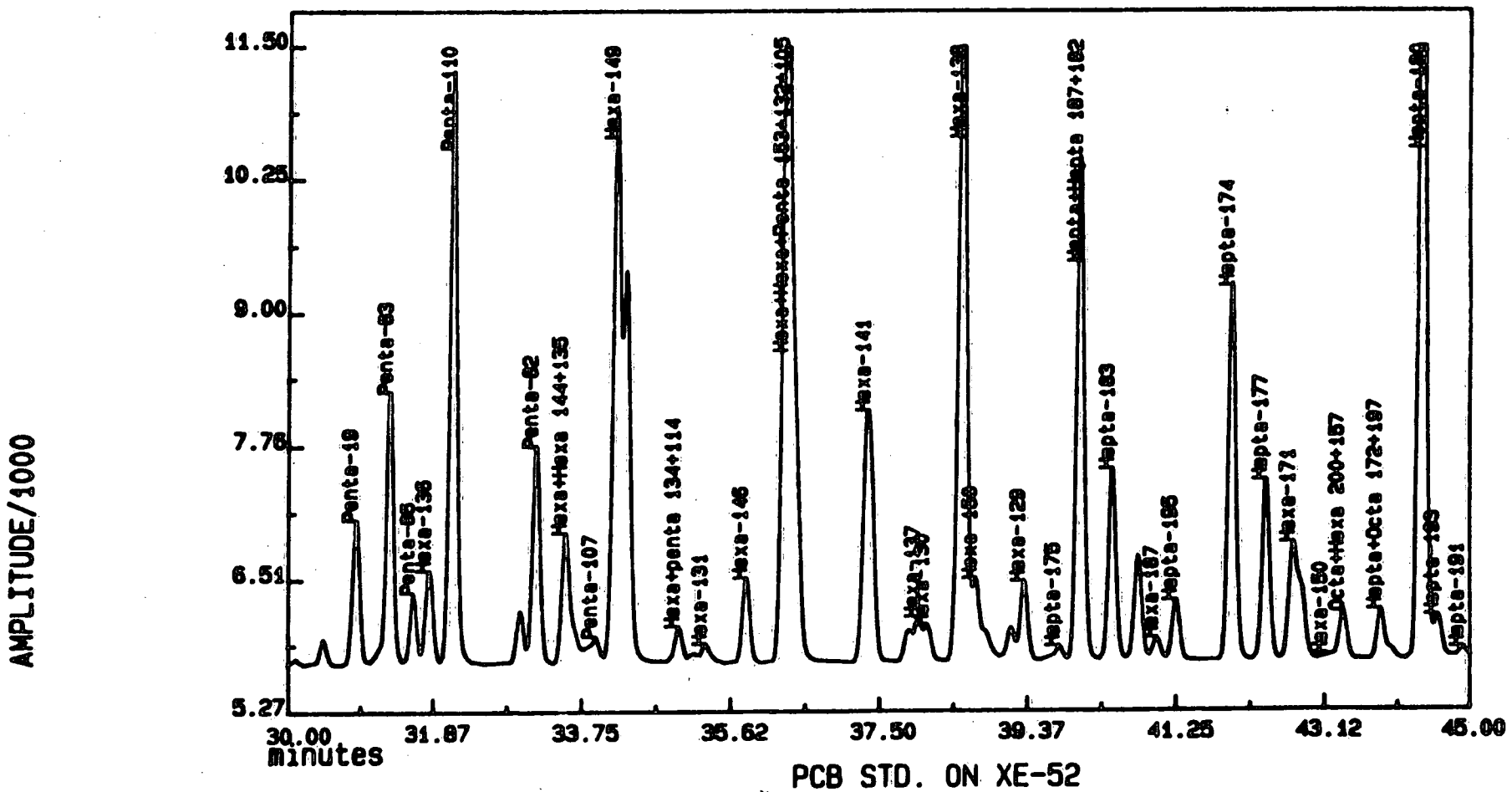
AMPLITUDE/1000
11.50
10.25
9.00
7.76
6.51
5.27
30.00
31.87
33.75
35.62
37.50
39.37
41.25
43.12
45.00
minutes
PCB STD. ON XE-52
Penta-110
Penta-82
Hexa-149
Hexa-141
Hepta-174
Hepta-177
Hepta-183
Hepta-187+182
Hepta-191

Fig. 5(c)

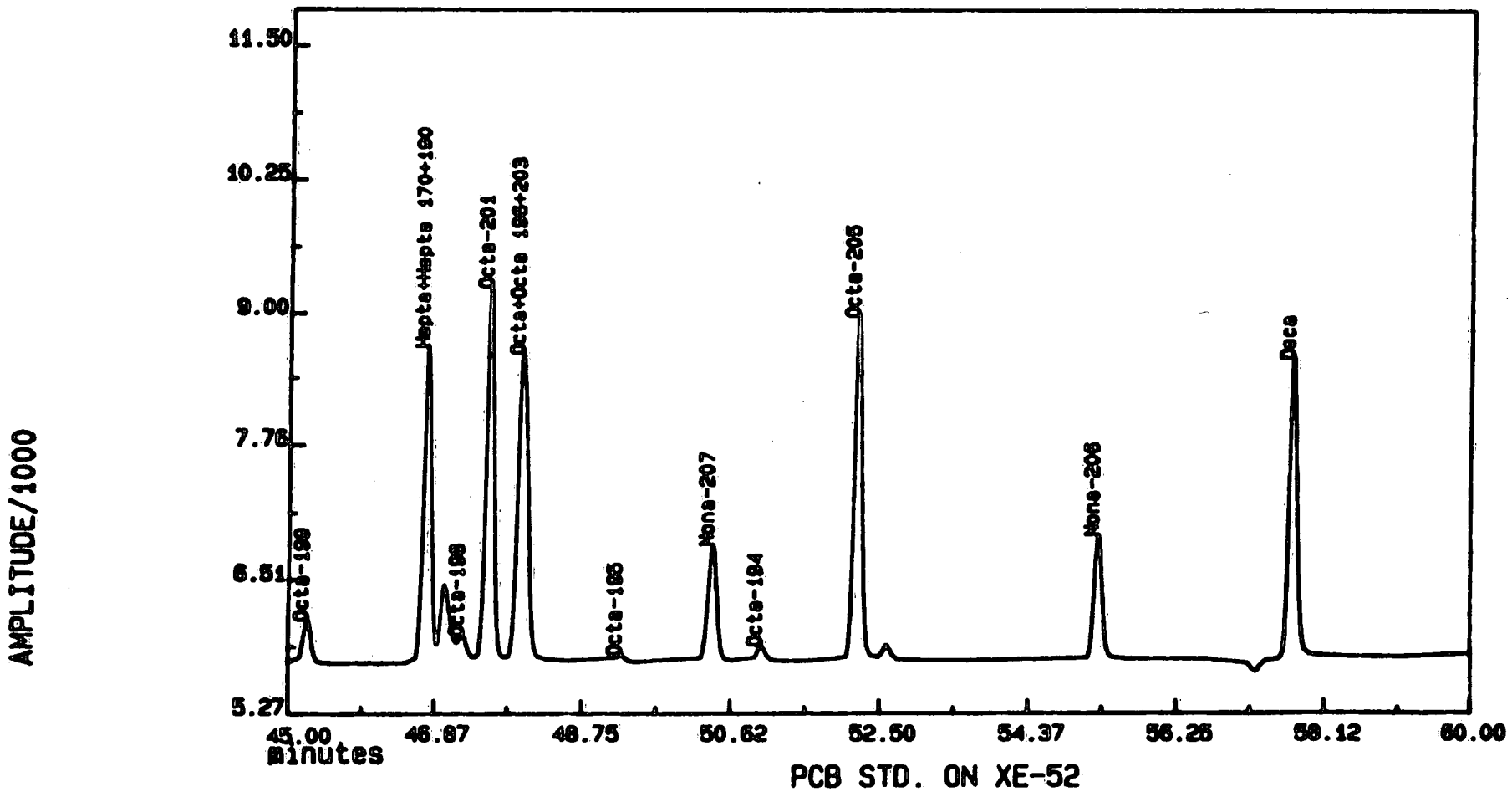
AMPLITUDE/1000
11.50
10.25
9.00
7.76
6.51
5.27
Hepta+Hepta 170+190
Octa-201
Octa+Octa 188+203
Octa-195
Nona-207
Octa-194
Octa-205
Nona-206
Deca
45.00
46.87
48.75
50.62
52.50
54.37
56.25
58.12
60.00
minutes
PCB STD. ON XE-52

Fig. 5 (d)

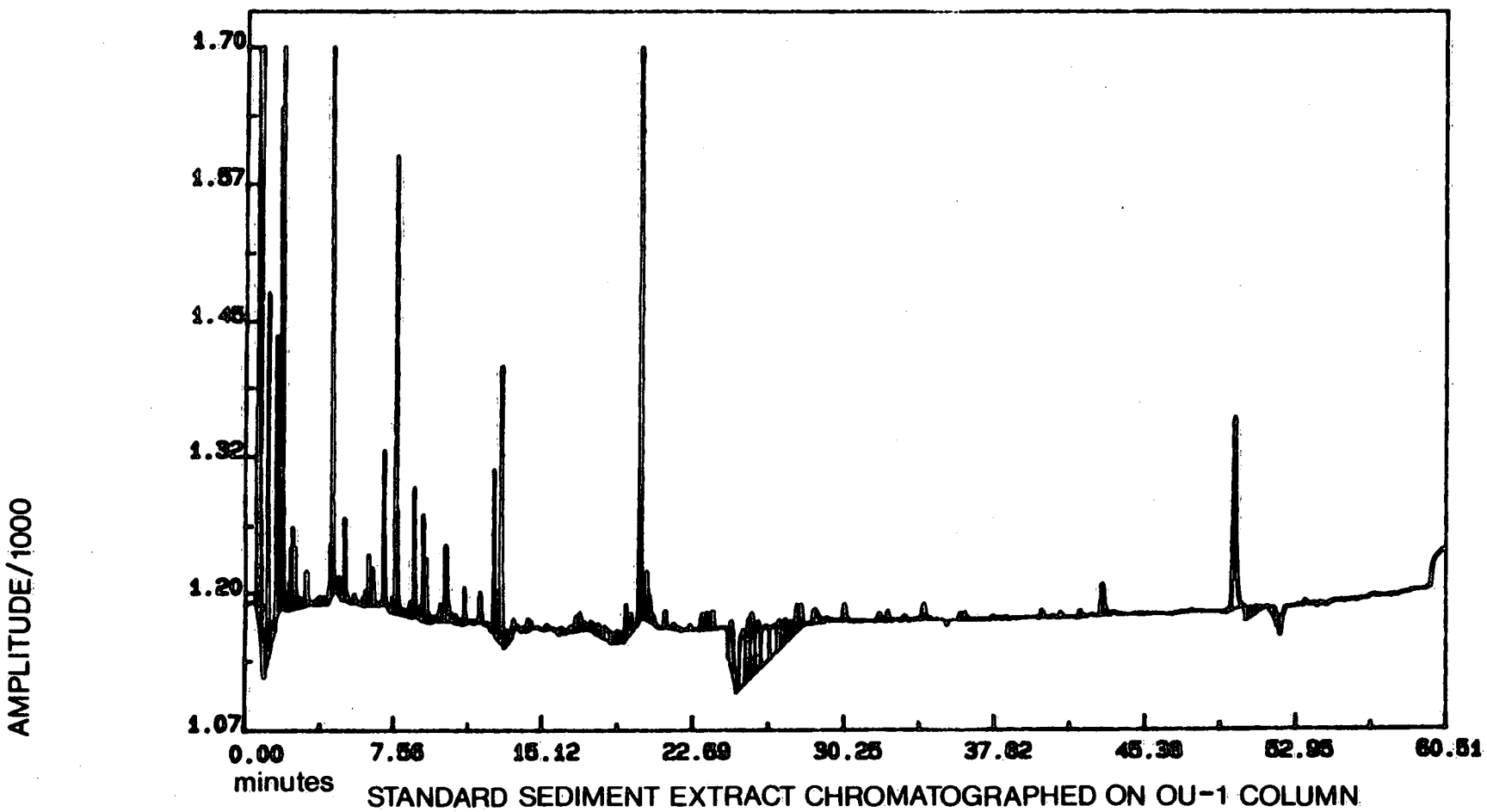
AMPLITUDE/1000
1.70
1.57
1.45
1.32
1.20
1.07
0.00
7.56
15.12
22.69
30.25
37.82
45.38
52.95
60.51
minutes
STANDARD SEDIMENT EXTRACT CHROMATOGRAPHED ON OU-1 COLUMN

Fig. 6

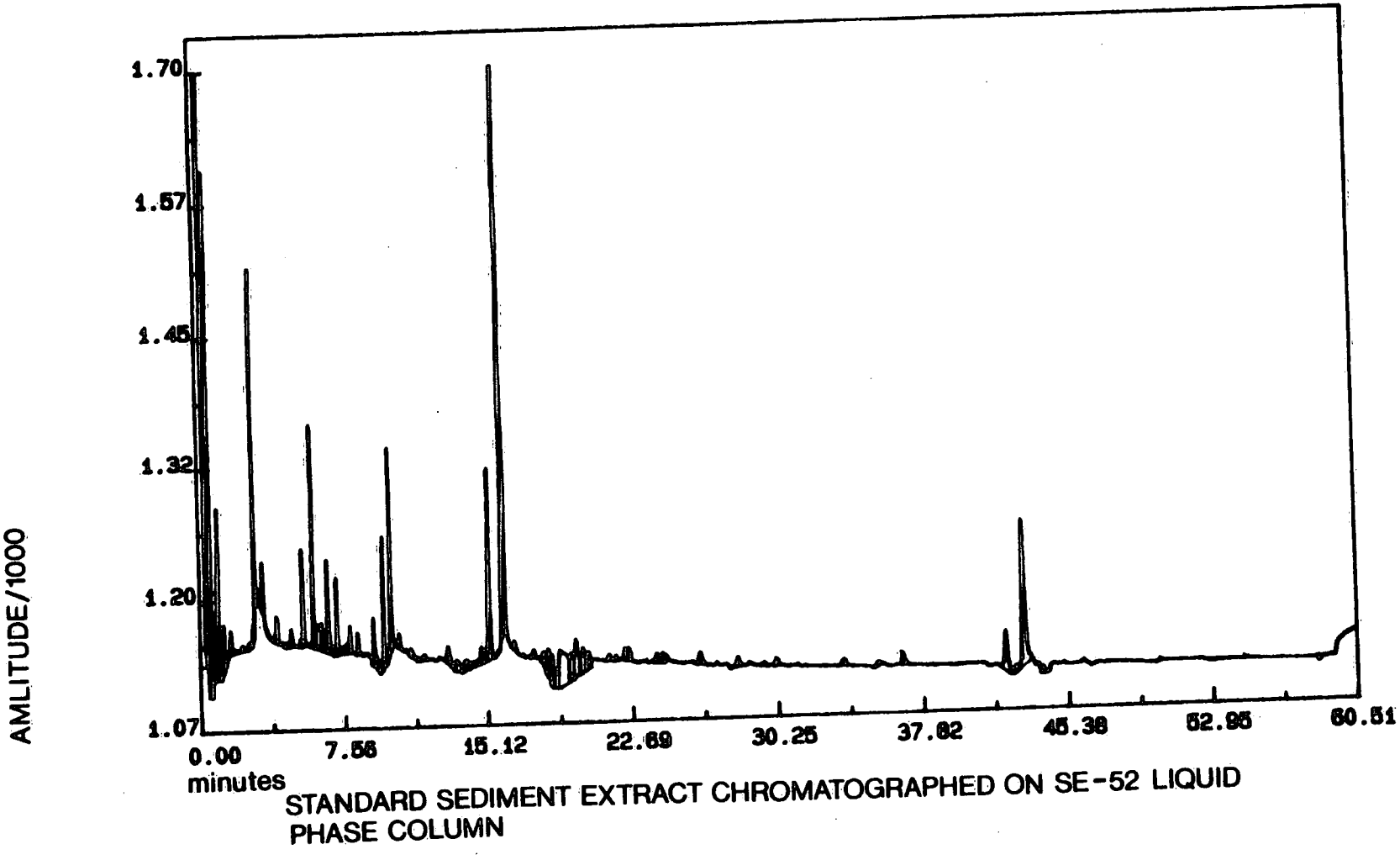
AMLITUDE/1000
1.70
1.57
1.45
1.32
1.20
1.07
0.00
7.56
15.12
22.69
30.25
37.82
45.38
52.95
60.51
minutes
STANDARD SEDIMENT EXTRACT CHROMATOGRAPHED ON SE-52 LIQUID PHASE COLUMN

Fig. 7

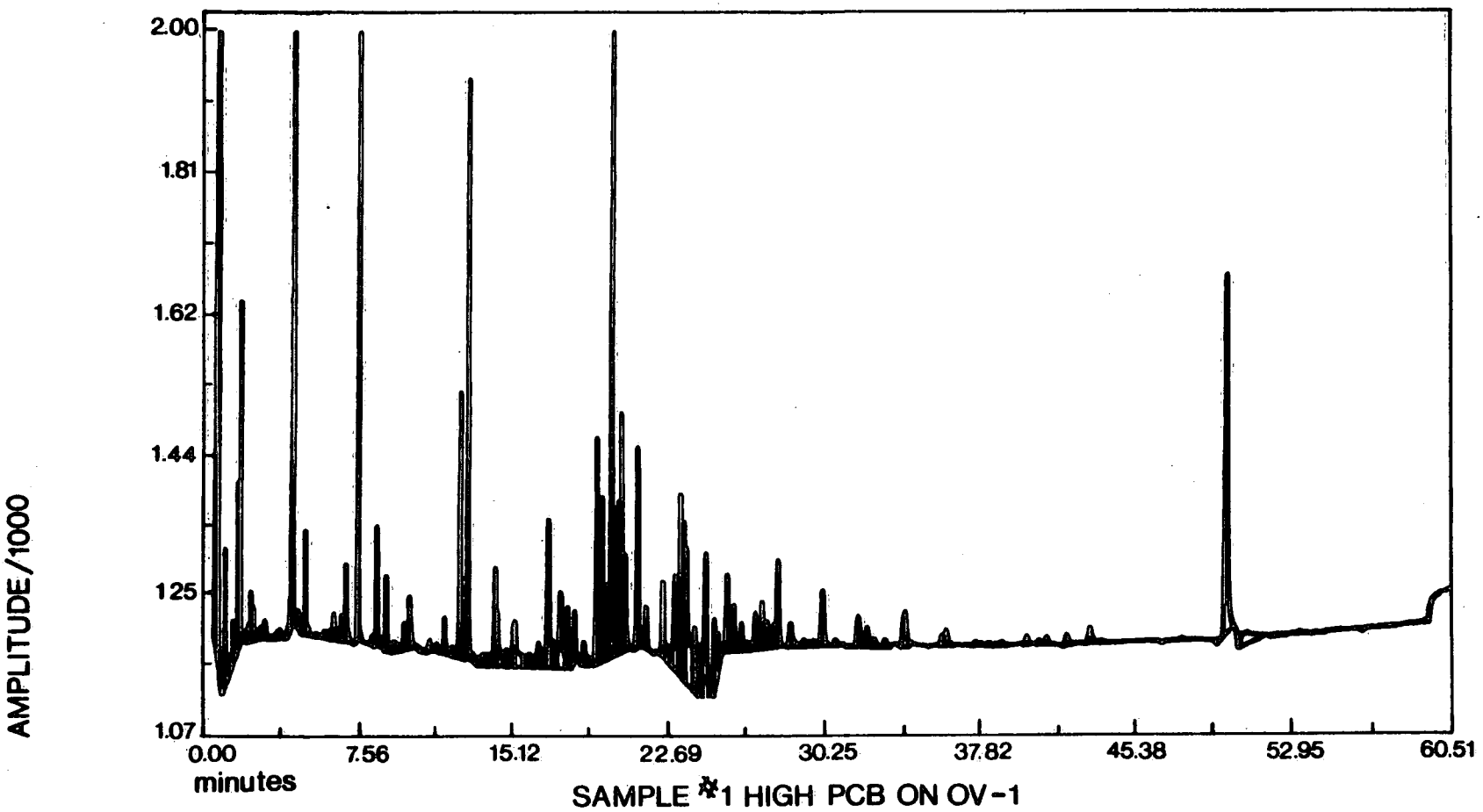
2.00
1.81
1.62
1.44
1.25
1.07
AMPLITUDE/1000
0.00
7.56
15.12
22.69
30.25
37.82
45.38
52.95
60.51
minutes
SAMPLE *1 HIGH PCB ON OV-1

Fig. 8