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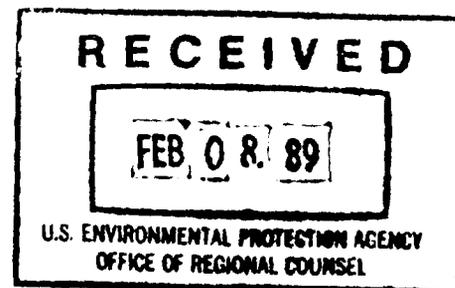
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Polychlorinated Biphenyl (PCB) Movement and Transformation
in Acushnet Estuary Sediments

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ABSTRACT



The polychlorinated biphenyls (PCBs) in the sediments of the Acushnet River estuary (New Bedford, MA) vary widely in both level and composition. Detailed examination of these PCBs by capillary gas chromatography and mass spectrometry (GC and GC/MS) now shows the following: (a) The original releases consisted of Aroclors 1254 and 1242, probably laid down on the sediments in that order, both rather unevenly. (b) Since the original deposition, these PCBs have undergone partial extraction into the estuarine waters (at a rapidly declining rate), considerable vertical diffusion within the sediments, and partial dechlorination at subsurface levels. However, they have undergone little or no aerobic microbial biodegradation or horizontal transport between sediment sites. (c) The dechlorinating agent(s) present, presumably anaerobic bacteria, apparently became established in the north end of the estuary by the late 1950's and have subsequently spread south about 6 Km (to the hurricane barrier) with at least one minor mutation. (d) The two closely related dechlorination processes (designated H and

H') carried out by these agents are distinct from those thus far observed at other PCB spill sites. They are attacking most of the more heavily chlorinated PCB congeners with half-times ranging between about 7 and 50 years, with the pharmacologically active species being among those most rapidly dechlorinated. Thus, the current fate of the PCBs in the Acushnet estuary sediments is dechlorination, detoxication, slow extraction into the tidal waters, and dissipation into the Atlantic.

INTRODUCTION

The commercial PCB products (e.g., Aroclors) that were so widely released into the environment in past decades possessed one unique feature of chemical composition: These products were complex mixtures of chlorinated biphenyl isomers and homologs (generically referred to as "congeners") that were originally present in fixed relative proportions. The chemical complexity arose because there are many different patterns (theoretically, 209) in which 1 to 10 chlorine atoms can become attached to a biphenyl nucleus. The invariance of original composition occurred because a single manufacturing process, iron-catalysed chlorination of biphenyl to a fixed weight gain, was used by all manufacturers during the entire period of PCB production (1).

Because of this chemical peculiarity - complex but fixed composition - the commercial PCBs, unlike other environmental contaminants, can preserve a record of their origin, transformation history, and environmental movement. This happens because the various product grades (classified mainly by weight gain during the original chlorination) each possessed a characteristic distribution of PCB con-

generators, and because each individual type of transformation process, whether physical, chemical, or biological, attacks the various PCB congeners according to its own selectivity rules, and hence may generate a distinctive new type of congener distribution pattern. Thus, given an environmental PCB sample, a determination of its congener distribution pattern, (e.g., by gas chromatography, or GC) may provide information on the original Aroclor released, the nature of the environmental agents that have altered it, and sometimes also, its route through the environment.

Since the availability of high resolution capillary GC techniques, substantial progress has been made in both the empirical and chemical characterization of the changes effected by individual transformation processes. Thus, the congener selectivity patterns for the oxidative biodegradation of PCBs by 25 strains of aerobic bacteria isolated from PCB spill sites have been reported (3). Most or all of these bacteria are believed to effect biodegradation via dioxygenase attack (4). None of the selectivity patterns observed corresponded to that

displayed in warm blooded animals, such as humans (5, 6), where the active enzymes are believed to be monooxygenases of the cytochrome P450 type (7, 8, 9). The changes in Aroclor peak distribution pattern resulting from partial vaporization, extraction into water, or adsorption on soils have also been reported (10). Briefly, all of these phase-transfer processes increase the relative concentrations of individual PCB congeners in the less condensed phase in approximate proportion to their volatilities (as indicated by elution rates on a GC column) without the structure-dependent selectivities exhibited by the biodegradation processes (3-6).

When the GC patterns of PCBs from heavily contaminated aquatic sediments were examined to see which of the above sorts of alteration patterns might be present, there were observed instead unusual congener distribution patterns, unlike any that had been previously reported (11, 12, 13). Patterns that were seen often enough to be sure of their individuality were given letter designations in approximate order of their discovery (11, 13). Further investigation showed that most of these novel patterns, e.g., Patterns B, B', C, and E of the upper Hudson sediments, and Patterns F and G of Silver Lake (Pittsfield, MA) resulted from the occurrence of reductive dechlorination in the sediments, probably mediated by anaerobic bacteria (11, 13). Since these discoveries we have been endeavoring to collect either sediment samples or gas chromatograms from other PCB spill sites, in order to determine the range and extent of this phenomenon.

In this regard, the sediments of the New Bedford area presented particular interest since they, unlike the others under investigation, had been deposited in salt water, and since there had already been enough survey work around the site (14) to

define the geographical distribution of the PCBs (15). Accordingly, we requested copies of some of the original analytical chromatograms and received several from Paul Serabian of the Massachusetts Department of Environmental Quality Engineering, some reprints of published articles showing GC patterns for New Bedford biota and sediments from John Farrington of the Woods Hole Oceanographic Inst. (16, 17, 18) and an extensive collection of chromatograms (19), originally run by Versar, Inc. on samples collected for EPA .

Examination of these chromatograms indicated that at least two PCB-alteration processes had occurred. The first had effected a partial loss of the lower congener peaks (i.e., those arising from dichlorobiphenyls and di-ortho trichlorobiphenyls) in most sediments, but particularly those of the outer harbor. The second had produced a sharp decline in the higher congener peaks (mainly those of penta- and hexachlorobiphenyls), particularly in the inner harbor and upper estuary. The latter alteration suggested possible dechlorination, but the resolution of the analytical GC's did not permit rigorous characterization of either alteration process, and none of the original sediment samples were available. Therefore, we undertook the collection and detailed examination of a new set of samples.

The area selected for study consisted of the upper estuary of the Acushnet River. This is a shallow body of salt water (depth at mean low tide generally 0.2-1.0 m) and surrounding tidal mudflats that is about 2.3 Km long, located between the entrance of the Acushnet (a small stream) at $41^{\circ}40'37''$ N and the narrow passage under the Coggeshall St. bridge at $41^{\circ}39'22''$ N. This area is thus about 2

Km above (north of) the dock area of New Bedford inner harbor, and about 3.7 Km above the hurricane barrier that forms the boundary between the inner and outer harbors, the latter being alternatively described as either the lower estuary, or an arm of Buzzard's Bay (Figure 1).

Previous sampling studies (14, 15) reported high (>5,000 ppm) PCB levels in parts of the upper estuary, particularly at "shallow" (4-8 cm) depths, albeit in a very "patchy" distribution. The highest PCB levels occurred near the capacitor manufacturing plant located near the northern end of the estuary. This plant is believed (14, 19) to have begun using Aroclor 1254 in substantial quantities in the 1950's, to have switched over most usage to Aroclor 1242 in 1962-65, to have switched again to Aroclor 1016 during 1970-72, and to have used this latter Aroclor until 1978, when all manufacturing use of PCB was banned by law. There is also a report indicating minor usage of Aroclor 1262 in the New Bedford area (14). The 23 different analytical laboratories who have performed PCB analyses on Acushnet estuary air, sediments, water, and biota have reported their findings in terms of Aroclors 1221, 1232, 1016, 1242, 1248, 1254, and 1260 (15).

Thus, it was apparent that our study would have to be concerned with the original Aroclor composition of the PCBs found in the sediment samples, as well as with their transformation.

EXPERIMENTAL

Sample Collection - Samples were collected from the tidal flats near the low tide

line by GHR Analytical Inc. of Lakeville, MA in June, 1986 from 17 sites along the west side of the estuary and six along the east. At each site the surface layers were removed and the two sets of samples taken: Set A at 5-7.5 cm depth and Set B at 15-17.5 cm. At least one sample of each set was retained by GHR for determination of total oil and grease content (reported in Table 3 below) and another was sent to us.

In selecting samples for detailed PCB analysis we first rejected two of the 17 west side samples that appeared to consist mainly of coarse gravel or cultural artifacts. The six of the remaining 15 west side sample pairs that permitted the most even spacing of sample sites, along with all six east side sample pairs, were then analysed.

Analytical Procedures. - The 24 selected sediment samples were air-dried, sieved to remove gravel, extracted in a Soxhlet overnight with 1:1 hexane:acetone, evaporated, and the concentrates extracted with concentrated sulfuric acid, mercury, and florisil. All concentrates were then examined by packed column GC (Hewlett Packard 5880 gas chromatograph; 6'x0.25" glass column packed with 1.5% SP2250 and 1.9% SP2401 on Supelcoport) to monitor the success of the cleanup and determine the appropriate loading for capillary GC. Capillary GC was performed with a Varian 4600 gas chromatograph equipped with an autosampler, splitter/-injector option 1070, a nickel electron capture detector, a Vista 402 data system, and a fused silica capillary column (J&W Scientific, 30m x 0.25 mm I.D., coated with an 0.25u bonded liquid phase of Durabond 1 (DB-1, a cross-linked polydimethylsiloxane). This was operated with an He flow of 30 cm/sec, and a temperature program as follows: 40°C for 2 min; 40° to 80° at 10°/min.; 80° to

225° at 6°/min.; 225° for 10 min. All data obtained was stored on discs so as to permit plotting of the chromatograms on the various scales needed to reveal particular features of interest.

The mass spectra of the effluent from a DB-1 capillary column (30 m x 0.25 mm I.D.; Du Durabond 1) were determined by positive ion electron impact using a ZAB VG Analytical organic mass spectrometer. Full mass scans of the mass range 50-500 were completed at 2 second intervals, giving approximately 900 low resolution mass spectra per chromatogram when the column was taken through the temperature range 70°-290°C at 8°/min, or about 1600 mass spectra when taken through the range 150°-290°C at 2°/min. The former GC temperature program was found to permit better detection of weak peaks, the latter greater peak resolution. The mass spectra were used solely to identify the GC peaks of the environmental specimens as indeed arising from PCBs, and to resolve coeluting congeners having different chlorine numbers, since ion fragmentation patterns do not serve to distinguish between PCB isomers (22).

The response factors (weight PCB per unit area of GC peak) for the electron capture detector (ECD) used were generated for all sizeable DB-1 capillary peaks exhibited by Aroclors 1221 through 1262 by the procedure of Webb and McCall (26); that is, by coulometric determination of weight chlorine per unit area of peak (using a Hall electrolytic conductivity detector from Tracor, Inc.) combined with mass spectrometric determination of homolog ratios and hence weight chlorine per weight PCB in the individual peaks. Response factors for the weaker peaks (which could not be reliably measured with the Hall detector) were estimated from published values (21).

PCB Peak Identification - The chromatograms of the Aroclor standards and sediment extracts observed in this and previous studies with our DB-1 capillary system have revealed distinguishable peaks at 118 different relative retention times, which we have designated Peaks 1-118. Of these 22 have been further resolved by mass spectrometry, making a total of 140 chromatographically distinguishable congeners or sets of coeluting isomers.

The prior literature reports PCB congener assignments for the GC peaks given by several Aroclors on columns coated with polydimethylsiloxane (e.g., OV-1, SE-30, SF-96), as determined from relative retention times that were mostly calculated from retention indices (23, 24); and also assignments for Aroclor 1260 peaks on coatings of SE-54 (6), based on measured relative retention times for all 209 congeners on that coating (21). Because of some disparities among the earlier assignments, we determined the positions of 70 individual congeners with respect to the Aroclor GC patterns on DB-1 by spiking Aroclor standards with specimens of the commercially available synthetic congeners and then chromatographing. This showed that within isomer sets (distinguishable by GC-MS) the elution sequences on DB-1 closely paralleled those on SE-54, as might be expected from their chemical similarity (pure polydimethylsiloxane vs. copolymer with 5% diphenylsiloxane). Accordingly, we were able to make assignments for the generally minor DB-1 peaks not adequately identified by our own spiking experiments or the prior literature (23, 24) by use of the observed patterns of relative retention on SE-54 (21). This indicated that 180 congeners had retention times close enough to those of the 118 resolvable GC peaks to require consideration as possible components thereof (Appendix A). In 22 cases, however, the mass spectra permitted resolution of non-

isomeric coeluting congeners. In several cases consideration of the relative proportions of the individual chlorophenyl groups in the particular sample being examined indicated that certain of the coeluting isomers would be present at levels too low to merit reporting as significant peak components. Finally, in one case, that of DB-1 Peak 17, the two coeluting congeners, 2,2',3- and 2,4',6-trichlorobiphenyl, were found to be adequately resolved on the packed column GCs, which contained a slightly more polar coating.

In hopes of improved comprehensibility, individual PCB congeners will be designated by a terminology paralleling that commonly used in verbal communication; that is by numbers indicating the substitution pattern on each ring separately, separated by a dash. Thus, 2,2',3,4',5,5',6-heptachlorobiphenyl will be called 2356-245 CB or simply 2356-245.

Calculation of Original Aroclor Ratios and Solubilization Losses. - In order to calculate x , the original ratio of Aroclor 1242 to Aroclor 1242 + 1254, and y , the fractional weight loss attributable to evaporative type processes such as true solution, from raw data on the weight fractions of the various PCB congener peaks in the sediment samples and the Aroclor standards, we used an "indicator peak" procedure. This presumes that we can identify in the sample chromatograms at least two peaks, A and B, which, after correction if appropriate, can be considered to be unaffected by the chemical transformation(s) underway. If we define the following parameters:

- a fraction Peak A in sample
- a_1 fraction Peak A in Aroclor 1242 standard
- a_2 fraction Peak A in Aroclor 1254 standard
- b fraction Peak B in sample
- b_1 fraction Peak B in Aroclor 1242 standard
- b_2 fraction Peak B in Aroclor 1254 standard
- c_1 relative effect of evaporative loss on A, i.e., $\Delta a / a \Delta y$
- c_2 relative effect of evaporative loss on B, i.e., $\Delta b / b \Delta y$
- c relative effect of evaporative loss on A/B ratio

then simple material balances indicate that:

$$(1) \quad a = [(1-c_1y)/(1-y)] [a_1x+a_2(1-x)]$$

$$(2) \quad b = [(1-c_2y)/(1-y)] [b_1x+b_2(1-x)]$$

$$(3) \quad \frac{a}{b} = \frac{(1-cy) [(a_1-a_2)x+a_2]}{[(b_1-b_2)x+b_2]}$$

Examination of the chromatograms (described below) indicated that congeners 26-34 and 236-34 were probably not being significantly formed or destroyed by the transformation processes at work in the sediments examined, and hence that Peaks 39 (originally mainly 26-34 CB, with a little 236-4 and 234-2) and 61 (originally mainly 236-34 CB, with a trace of 34-34) could be used as indicators for Aroclors 1242 and 1254 respectively. The only correction applied was that the 234-2 in Peak 39 was presumed to be originally present at the 10% level, but to then decline in proportion to any observed decline in Peak 50 (23-34 plus a little 234-4). For these peaks we were able to evaluate the constants in equations 1-3 from

Aroclor 1242 and 1254 standards, and from a sample of Aroclor 1242 that had been evaporated to 34% weight loss in the laboratory as follows: a_1 , 0.03160; a_2 , 0.00789; b_1 , 0.00743; b_2 , 0.0895; c_1 , 0.43; c_2 , 0.1; c , 0.382.

Using these values, equations 1-3 were solved for x and y by a process of successive approximations. Examination of the sensitivity of the solutions to variations in the observed parameters a and b indicated no particular magnification of errors in the case of the x values (mainly because the intensity ratios a_1/a_2 and b_2/b_1 are quite large for both peaks). For the y values, however, where $1/(1-y)$ is roughly proportional to $(a+b)$, errors in a or b could be magnified. As a check for such errors, we roughly estimated y from the loss in the very strong pair of Aroclor 1242 peaks, Nos. 23 and 24, given by 25-4 and 24-4 CB, and made note of the cases where the calculation via eq. 1-3 had given a questionable result.

RESULTS

Aroclor and Alteration Pattern Identification. - The raw data collected during this investigation consisted of SP2250/SP2401 (packed column) and DB-1 (capillary) gas chromatograms, and peak quantitations by weight and mole fractions on the 118 resolvable DB-1 peaks for each of the 24 sediment samples and the Aroclor standards. It also included GC-MS ion chromatograms measured with two different temperature programs (to optimize either sensitivity or resolution) for the standards and for representative samples. All of the DB-1 chromatograms and data print-outs, along with keys to the peak number assignments and congener identifications, are attached as Appendix A.

Visual inspection of the DB-1 chromatograms revealed a variety of patterns. Some GC patterns (e.g., 9A) resembled that of Aroclor 1242; some (e.g., 18A) were quite similar to Aroclor 1254; most, however, resembled Aroclor 1242-1254 mixtures that had been subjected to either or both of two types of pattern alteration.

The first of these types of alteration consisted of a general, non-selective loss of peaks with short retention times, very similar to that seen when Aroclor 1242 samples were simply allowed to evaporate in the laboratory (Fig. 2 below). There was no hint of the patterns of selective PCB congener removal (i.e., rapid loss of 2-3 and 2-4 CB; slower of 25-2 and 24-2; very slow for 26-2, 26-3, and 26-4 CB) that have been repeatedly observed for aerobic microbial biodegradation by either pure cultures (3,4) or sewage sludge (10). This observation is consistent with those we have made at other sites, where PCB pattern alterations resembling those effected by aerobic microbial degradation were often seen in river water, ground water, and soil samples, but only rarely in aquatic sediments.

The second type of alteration consisted of parallel declines in the major peaks 25, 26, 46, 47, 48, 50, 53, 58, 59, 63, 69, 74, 82, 89, 95, 102, and 106, and in many weaker ones as well, along with the increases in peaks 7, 12, 13, 21, 22, 31, 32, 33, 40, 43, 44, 49, 54, 55, 62, and 88. This pattern of alteration was thus somewhat intermediate between, but clearly distinct from, those previously designated as Pattern B (11, 13) and Pattern F (13), which were seen in many sediment samples of the upper Hudson River (NY) and Silver Lake (Pittsfield, MA), respectively. Accordingly we concluded that it represented a new type of

alteration, and designated it Pattern H. Subsequent reexamination of the chromatograms revealed an occasional slightly different pattern, characterized by greater relative declines in Peaks 26, 27, 37, 38, and 45 than with Pattern H; this was designated Pattern H'. Figure 2 shows representative examples of well-developed Patterns H and H' (from sediments 19B and 12B, respectively), along with reference chromatograms of Aroclors 1016, 1242, 1254, and 1242 after 34% evaporative weight loss.

Attention was then given to the possibilities that the original PCB discharge may have contained Aroclors 1016, 1248, or 1262 rather than just 1242 and 1254.

Fig. 2 shows that in Aroclor 1242 there is a prominent Peak 50 (mainly 23-34 CB) that is much weaker in Aroclor 1254 and only 1.5% as strong in Aroclor 1016. Thus, in undechlorinated 1242 specimens (such as those of the outer harbor) loss of Peak 50 (relative to indicator Peak 39) can provide a sensitive measure of admixed Aroclor 1016. To extend this method to lightly dechlorinated samples, we found that in the deeper, and hence presumably older (pre-1016), sediments undergoing dechlorination by System H, the disappearance rates for the trichlorobiphenyl component of Peak 25 (mainly 34-2 CB) and for Peak 50 were about equal. Accordingly, we could subtract any percentage loss in Peak 25 trichlorobiphenyls from that in Peak 50, to get an approximate measure of the portion of the Peak 50

In the case of Aroclor 1248, which gives a chromatogram virtually identical to that of 1242 after ca. 50% evaporation, chromatographic proof of presence or absence in admixture with extractively devolatilized Aroclor 1242 would be very difficult. However, the site contamination history (14, 19) indicates no known releases of Aroclor 1248, which was never used in electrical devices (1). Accordingly, we conclude that the "Aroclor 1248" reportings by previous analysts (15) all represent devolatilized Aroclor 1242 rather than actual 1248.

Regarding Aroclor 1262, careful inspection of the sediment chromatograms showed that the major octachlorobiphenyl peaks (Peaks 109, 110, 112, and 115) were always slightly stronger than in our Aroclor 1254 standard, i.e., with a total weight percent (of Aroclor 1254 content) about 0.3% rather than 0.15%. The excess octachlorobiphenyls were accompanied by only modest proportions of nonachlorobiphenyls (Peaks 113, 114, and 117) indicating the additional Aroclors, if any, to be Aroclor 1260 or 1262 rather than 1268. Since Aroclor 1262 contains 14% by weight of the measured octachlorobiphenyls, the observed increase in octachlorobiphenyls could have been produced by 1% contamination of the 1254 with 1262. Alternatively, it may simply be that the average Aroclor 1254 produced during the period of discharge contained 0.15% more octachlorobiphenyl than did our analytical reference standard.

Characterization of Alteration Processes H and H⁺. - The alterations in PCB congener distribution effected by Process H are probably most easily seen in the GC-MS ion chromatograms run under conditions that maximized resolution, even though such tracings lacked a few of the weaker peaks, including those of the

mono- and octachlorobiphenyls, which were present only at very low levels. Fig. 3 shows the di- through heptachlorobiphenyl ion chromatograms for sample 19A, for which the quantitatively more reliable capillary GC is shown in Fig. 2.

Beginning with the dichlorobiphenyl panels of Fig. 3, it is evident that there has occurred in the sediments a marked increase in Peaks 7, 12, and 13 (2-3, 3-3, and 3-4 CB) relative to the originally prominent Peaks 5, 8, and 14 (2-2, 2-4, and 4-4 CB). There is also a possibility that the latter peaks may all be increased slightly relative to Peak 6 (24- and 25-CB), which is probably the least likely of the group to be either increased or decreased by dechlorination.

The trichlorobiphenyl tracings of Fig. 3 and Fig. 2 show little or no change in the relative levels of Peaks 10, 14, 15, 16, 23, 24, and the component of Peak 17 that elutes earlier on the packed column GC; the congeners responsible for these peaks are 26-2, 25-2, 24-2, 26-3, 25-4, 24-4, and 26-4, respectively. Very prominent increases are shown for the peaks for 25-3 and 24-3 CB, and small increases for 35-2, 34-3, and possibly 35-3 (Peak 27). Marked decreases were seen for Peaks 25, 26, and 38, given mainly by 34-2, 23-4, and 34-4 CB, respectively.

Among the tetrachlorobiphenyls, the unaffected congeners appeared to be 26-25, 26-24, 236-2, and 236-34. Large increases were seen in 25-25, 25-24, and 24-24, with lesser absolute, though still proportionately important, increases in 24-35, 235-3, and 245-3. The peaks exhibiting 50% decline include those for 245-2, 23-23, 245-4, 25-34, 24-34, 234-3, 23-34 (+234-4), and 34-34. Congeners 23-25 and 23-24 CB showed sizeable losses in sediments derived primarily from Aroclor 1242, small losses in most of those with higher Aroclor 1254 content, and an actual gain at one

such site (samples 21A, 21B).

Among the pentachlorobiphenyls, there appeared to be little or no net change in ^{the} peaks for 236-26, 236-25, 236-23 + 235-25, 235-23, and 235-34 CB, although there may have been a slight increase in 236-25. Unequivocal increases occurred in 246-25, 246-24, 236-24, 245-24, and in Peak 55 (246-34 + 2356-3). All of the other pentachlorobiphenyls declined, with the largest losses being in 245-25, 234-25, 234-24, 234-23, 245-34, and 234-34 CB.

With the hexachlorobiphenyls, there appeared to be little change in 236-236, 235-236, 245-236, 2356-23, or 235-245. The only clear gains were in the minor components 245-246 and 2356-24. All of the other hexachlorobiphenyl peaks declined, with the largest absolute losses being in 234-236, 245-245, 2345-25, 234-245, 234-234, and 2345-34.

Among the heptachlorobiphenyls, there was probably no change in Peak 78 (2356-236 CB); but a clear 30-40% increase in Peak 88 (2345-246 + 2356-245), and clear decreases in all the other congeners. The octachlorobiphenyls were not reliably detected by GC-MS, but were on amplified versions of the DB-1 capillary chromatograms. Because of the uncertainties regarding the octachlorobiphenyl levels in the original discharges, it was not possible to establish their alterability by System H; however, the clear increase in heptachlorobiphenyl Peak 88 suggests that some dechlorination of octachlorobiphenyls had occurred.

Figures 2 and 3 thus show that alteration Pattern H arises from marked decreases in the levels of most of the higher (more heavily chlorinated) PCB

congeners, and corresponding increases in some of the lower congeners, as was seen also for the previously discovered PCB dechlorination systems (11, 13). In order to identify the simplest set of dechlorination process steps that would account for this pattern of change we sorted out the congeners responsible for the observed changes according to the types of individual chlorophenyl (CP) groups present (Table 1). We thus identified as not dechlorinatable by System H groups 2-, 3-, 4-, 2,4-, 2,5-, 2,6-, 3,5-, 2,3,6-, 2,4,6-, and 2,3,5,6-CP on the grounds that there was no clear evidence of decline in any PCB congeners containing only these CP groups. The remaining types of CP groups, namely, 2,3-, 3,4-, 2,3,4-, 2,3,5-, 2,4,5-, 3,4,5-, 2,3,4,5-, 2,3,4,6-, and 2,3,4,5,6-CP, were all identified as potentially reactive to System H on the grounds that one or more PCB congeners containing these CP groups attached to one of the unreactive CP's did show a decline. We did observe, however, that when 2,3-, 3,4-, 2,3,5-, and possibly 2,4,5-CP groups were attached to a CP having two ortho chlorines, as in 2,6-, 2,3,6-, 2,4,6-, or 2,3,5,6-CP, there was no longer any reactivity. This phenomenon is reminiscent of the reactivity pattern exhibited by upper Hudson dechlorination Systems B, B', C, and E, where congeners 236-34 and 2356-34 CB showed reduced reactivities (11, 13), although not as markedly so as towards System H. The effect was not universal, however. PCB congeners containing 2,3,4- or 2,3,4,5-CP groups attached to unreactive di-ortho substituted CP's were still attacked by the System H.

The mass balance analyses that were useful in establishing that the compositional changes seen in the upper Hudson (11) and Waukegan Harbor (25) sediments proceeded solely by loss of chlorine atoms located meta or para (rather than ortho) to the other ring could not be strictly applied because of the elutriative losses; however, there was no obvious indication of reduced ortho chlorine content in the

dechlorinated products, nor any evidence of the marked decline in tri- and tetra-ortho CB's that was exhibited by the ortho-reactive System F (13). Accordingly, it was tentatively concluded that System H, like the upper Hudson and Waukegan Harbor System, is a meta/para-selective dechlorination system. This conclusion, plus consideration of the relative mole fractions of CP groups lost and gained, permitted identification of the source of the small gain in PCB congeners containing 2-CP groups as 2,3-CP group dechlorination; of the large gain in congeners containing 3-CP's as 3,4-CP loss; of the occasionally increased 2,3-CP as 2,3,4- (also conceivably 2,3,5-) loss; of the sizeable 2,4-CP gain as 2,3,4- (plus conceivably 2,4,5-) loss; of the large 2,5-CP gain as 2,4,5- (plus the smaller 2,3,5-) loss; of the occasionally increased 2,3,5-CP as 2,3,4,5-CP loss; and of the small but unequivocal gains in congeners containing 3,5- or 2,4,6-CP groups as 3,4,5- or 2,3,4,6-CP dechlorinations, respectively. The extent to which this set of conclusions is supported by the various observations of PCB congener level change is set forth in Table 1. This Table shows that a simple stepwise matching between congener loss and congener gain is frequently precluded by the fact that the congener that is the product of one dechlorination step may still be the substrate for another; however, there are still enough unequivocal observations to define a self-consistent pattern.

In order to estimate relative dechlorination rates for the various chlorophenyl groups, we first determined the numbers of half-losses (calculated as $-\log_2$ of the fraction of the original congener level still present) for various penta-, hexa-, and heptachlorobiphenyls (which are primarily derived from Aroclor 1254) in sediments showing well-advanced Aroclor 1254 dechlorination. We then did the same for the

reactive tri- and tetrachlorobiphenyls (which are primarily derived from Aroclor 1242) in sediments where Aroclor 1242 dechlorination was prominent. We then presumed, on the basis of the mean values shown in Table 3 below, that in sediments where the dechlorinations of Aroclor 1254 and 1242 were equally advanced the reductions in Peaks 50 (mainly 23-34 CB) and 58 (234-25 CB) would be about equal. This permitted the estimates of the relative reactivities for all of the major PCB congeners shown in Table 2.

This Table shows that PCB congener reactivity towards dechlorination System H is determined not only by the arrangement of chlorine atoms on the presumably reactive CP group, but also by their arrangement on the other, presumably unreactive, CP group, where ortho (2 and/or 6) substituents appear particularly important in reducing reactivity. Table 2 also shows that the minor dechlorination system, H', differs from H in exhibiting higher reactivities for 2,3-, 2,3,5-, and 2,3,6-CP groups, relative to the rest of the pattern. The conversion of these observed relative reactivities to absolute rates, (i.e., dechlorination half-times) will be addressed in the Discussion.

Compositional Variations in Upper Estuary Sediments. - The resistance to dechlorination of 26-34 and 236-34 CB, congeners which give rise to prominent peaks in Aroclors 1242 and 1254, respectively, meant that these peaks could be used to estimate the original Aroclor 1242-1254 ratios by the "indicator peak" method described in the experimental section. Likewise, the identification of Peaks 50 and 58 (prominent in Aroclors 1242 and 1254, respectively) as containing only easily dechlorinated congeners (i.e., 23-34 plus a little 234-4 CB and 234-25 CB, respectively) meant that the declines in these peaks could be used as indicators of

the dechlorination states of the two Aroclors. The resulting compositional data are presented, along with information on site locations and total levels for oils and PCBs, in Table 3. This table lists the site numbers for samples taken along either the west or east side of the estuary in either the first or second column, respectively, and in the same order as the north-to-south sequence of sites; thus the arrangement of the site numbers within the first two columns also constitutes a rough map of the relative positions of the sites.

From Table 3, the following findings were noted. First, the usual range of estuarine bottom textures (mud, sand, gravel, and marsh bed in various proportions) was represented. No measurements of oxygen levels were made, but it was noted that the sediments after drying generally graded in color from the black of FeS to the brown of Fe_2O_3 upon moving from north to south over the range studied. The odor of H_2S was apparent in the samples denoted "soft black mud," indicating that they, at least, were anoxic. Unfortunately, however, there were no obvious correlations between either PCB level or alteration state and sediment textures.

The large excess of hydrocarbon oils (some of which do give weak responses on the electron capture detector used for the GC analyses) and other minor contaminants meant that the measurements of relative PCB peak heights were unreliable for samples containing only low levels of PCBs; accordingly the compositional indices calculated for such samples, if reported at all, are flagged with an approximation sign.

Third, there was a general tendency for the A and B (shallow and deep)

specimens at each site to be similar in color, texture, and odor; in levels of both oils and PCBs; in the calculated 1242:1254 ratios, extractive losses, and dechlorination indices; in the dechlorination pattern; and also in the patterns of minor, non-PCB peaks on the chromatogram. These similarities occurred despite much wider variations between sites in all of these parameters, and hence suggest that both the oils and the Aroclors had been undergoing vertical diffusion within the sediments at most sites.

The Metcalf & Eddy (15) summary of previous sampling data also noted wide site-to-site variations in PCB level in the upper estuary. In addition, however, this compilation suggested that PCB levels there were highest at "shallow" (4-8 cm) depths, corresponding to our depth "A", somewhat lower at the "surface" (0-4 cm), and one to two orders of magnitude lower in the "deep" (>8 cm) layers, which would correspond to our depth "B". This latter generalization is in clear discord with the data shown in Table 3. For all sites examined, the average total PCB levels at depths A and B were 1187 and 839 ppm, respectively, indicating a mean B-depth (15-17.5 cm) PCB level only 29% lower than at depth "A" (5-7.5 cm).

Fifth, there was a general tendency for the total PCB levels, and particularly that of the Aroclor 1254 components, to decline from north to south, in accord with the previous report (15), indicating an upstream source for the Aroclors.

Sixth, despite the diffusive blurring of the stratification, it was still possible to see three compositional differences between the PCBs at depths A and B: (a) at every site where the PCB levels were high enough for reliable peak area measurements, the Aroclor 1242:1254 ratio was similar to or larger in the upper

("A") sample than in sample B, suggesting that the Aroclor 1242 deposition came generally later than that of Aroclor 1254. (b) Again at every site with PCB peaks strong enough for reliable comparison, the extent of dechlorination, whether of the Aroclor 1242-derived Peak 50 (23-34 CB), or of the 1254-derived Peak 58 (234-25 CB) was equal to or greater in the "B" (lower) sample than in "A", indicating that the dechlorination was occurring preferentially in the lower layers, as in the upper Hudson sediments (11). (c) At both "A" and "B" depths, the dechlorination was more advanced in the Aroclor 1254-derived peak in the more northerly (upriver) sites, and more advanced in the Aroclor 1242-derived peak in the more southerly sites, indicating that seeding with the dechlorinating agent occurred before the time of Aroclor 1242 deposition at the former sites, and after that time in the latter.

PCB Compositional Changes in Other New Bedford Area Specimens. - Prior to collecting the upper estuary samples for DB-1 capillary GC analysis, a careful study of the Versar (19) and Woods Hole (16-18) chromatograms was made to identify features indicative of compositional change.

The sediment samples analysed by Versar included 72 grab samples collected by GCA/Technology Division for EPA throughout the New Bedford area and surrounding waterways in August 1982 and 72 upper estuary core sections similarly collected in January 1983, as well as sediments taken from sewage lines and sewer overflow areas. The analyses were done by conventional packed column GC on a polydimethylsiloxane column. We observed the chromatograms of the Aroclor standards, which accompanied those of the sediments, to be very similar in general

appearance to those reported by Webb and McCall (26). Accordingly, we used the Webb and McCall peak designations (which describe retention times relative to DDE=100 for peaks obtained on an isothermal (195°C) SE-30 packed column) for denoting the Versar GC peaks seen. Such packed column peaks rarely represent individual PCB congeners; instead they correspond to unresolved aggregates of the peaks seen on polydimethylsiloxane-coated capillary columns, such as DB-1. The correspondence between the packed column and DB-1 peak numbers is given in Figure 4 (Appendix A).

The Versar chromatograms of the various sediments showed all of the low resolution peaks seen in the Aroclor 1242 and 1254 standards, but with often sizeable differences in relative peak heights, and occasionally slight differences in the apparent relative retention time (RRT). In virtually all cases the peaks with RRT 21, 28, 32, and 40 were clearly depressed relative to the very strong peak at RRT 37 (which corresponds to Peaks 21-24 on Fig. 1). In the tetrachlorobiphenyl region there was usually enhancement of the peak at RRT 47, and depression of those at RRT 54 and 78. In the penta- to hexachlorobiphenyl region, some GC patterns showed the peaks at RRT 84, 125, 146, and 174 at the same relative peak heights as in the Aroclor standards, whereas others showed a marked "high end drop-off," meaning that the observed pattern of relative peak height became $84 > 125 > 146 > 174$. (The pentachlorobiphenyl peaks at RRT 96 and 104 were not observable on the Versar GC's because DDE, RRT=100, had been added to all samples as an internal standard). This was a sufficiently unambiguous feature of the packed column chromatograms to permit the GC's of sediments that contained >1 ppm PCB to be scored for "high and drop-off." This scoring was done before we had the key indicating the relationship between the separate sets of identification

numbers used by the sampler and the analyst.

When the key became available, a striking geographic correlation emerged: all of the samples collected in the estuary north of the hurricane barrier showed the "high end drop-off" feature in their chromatograms, whereas this feature was not detectable in the samples from any of the other marine collection sites: e.g., those in the lower estuary, south of the hurricane barrier, those in Clark's Cove, or in the surrounding areas of Buzzard's Bay. The only other sediment chromatograms exhibiting the "high end drop-off" feature were those of a small group of otherwise 1254-like specimens that were collected in a short section of the East Rodney French Blvd. (ERFB) sewer line near David St. The effluent from this line ultimately discharges into the outer harbor.

Correlation of the packed column and capillary chromatograms showed that the packed column peaks at RRT 84, 125, 146, and 174 must be produced mainly by the congeners responsible for DB-1 Peaks 51-54, 69, 74-75, and 82 respectively, indicating that a sample that had undergone dechlorination by System H or H' would indeed exhibit the observed "high end drop-off" in the packed column GC. However, because of the lower resolution of the packed column chromatograms we cannot exclude the possibility that the dechlorination system operating in the middle estuary (e.g., inner harbor) or in the ERFB sewer line may have been of a subtype different from H or H'.

Brownawell and Farrington (18) have published SE-30 capillary gas chromatograms for two sections (3-5 and 35-45 cm) taken from a single outer harbor core collected in September, 1983. Reference to the Figure 1 standards indicated that

these two PCB samples resembled a simple mixture of Aroclor 1254 with evaporated 1242 and virtually pure Aroclor 1254, respectively. The accompanying plots (18) of peak height data for intermediate core sections showed a nearly smooth decline with depth for the Aroclor 1242:1254 ratio. Our measurements on the published chromatograms indicated that for the upper sediment sample the peak corresponding to DB-I peak 50 had a height of $103 \pm 5\%$ of that in the Aroclor 1242 standard, both measured relative to peak 39, indicating that no detectable Aroclor 1242 dechlorination or admixture with Aroclor 1016 had occurred. However, the Peak 58 heights were depressed 37% and 8% relative to the Aroclor 1254 standard in the upper and lower sediments respectively, indicating some deposition of dechlorinated 1254 (possibly from the ERFB sewer line) in the upper sample. The 3-5 cm sediment GC also showed small losses in congeners 105 and 138, corresponding to DB-I peaks 74 and 82 (234-34 and 234-245 CB), and a small gain in peak 54 (245-24 CB), consistent with, but not unambiguously demonstrative of, Pattern H. None of these small changes would have been large enough to produce an observable "high end drop-off" in the packed column GC.

Water samples collected from just south of the hurricane barrier in September, 1982, were reported to contain approximately half their PCBs in true solution and half as suspended particulates (16). This report shows a pair of DB-5 capillary gas chromatograms for dissolved and suspended PCB fractions of a water sample collected at ebb tide. We noted that the GC of the dissolved fraction resembled that of a partially dechlorinated Aroclor 1242 with marked enhancement of dichlorobiphenyl peaks 5 and 7 and/or 8, (2-2 and 2-3 and/or 2-4 CB), while that of the suspended particulates looked more like the sort of lightly dechlorinated

1242-rich Aroclor 1242-1254 mixture seen in some of our least altered "A" level sediments from the upper estuary (e.g., 2A) except for the absence of all dichlorobiphenyl peaks. Relative peak height measurements indicated the losses in the Aroclor 1242-derived Peak 50 to be 44 and 20%, and those in the Aroclor 1254-derived Peak 58 to be 42 and 41% in the dissolved and suspended fractions, respectively. The losses for both these peaks averaged 67% (1.6 half-clearance) in the upper estuary sediments (Table 3). Thus, the levels of Aroclor 1242 and 1254 dechlorination in the water at the north end of the outer harbor at ebb tide were intermediate between those of the upper estuary sediments and those of the outer harbor.

The Woods Hole group also reported chromatograms of mussels (Mytilus edulis), green crab (Neopanope taxons) and lobster (Homarus americanus) from about the same location (17). The mussel PCBs resembled an Aroclor 1242 + 1254 mixture, but with those peaks that are most sensitive to System H dechlorination (e.g., DB-I peaks 25, 26, 50, 58, 59, and 74, corresponding to 34-2, 23-4, 23-34, 234-25, 234-24, 234-23, and 234-34 CB) largely removed. These same peaks were also largely removed from the chromatograms of the lobster and crab, along with those of all PCB congeners lacking in 4,4'-substitution. Thus, the GC pattern of the residual PCBs in the lobster showed strong peaks for 245-34, 245-245, and 245-234, and medium ones for 24-4, 24-24, 245-4, 24-34, and 245-24 CB. In the crab, there was much additional loss of congeners other than 245-245 CB; 245-34 was down by a half, and 245-4, 24-34, 245-24, and 245-234 still more so. These PCB congener-persistence patterns are quite similar to those seen in the human (5,6) and indicate that the two crustaceans, unlike the mussel, possess active eukaryotic

P450 cytochrome systems (7,8) for metabolizing lipophilic xenobiotics. The chromatograms of flounders (Lephopsetta maculata and Pseudopleuronectes americanus) from the same area were not published, but were stated to be intermediate in appearance between those of the mussels and lobsters (17), implying the presence of a P450 cytochrome system, but at lower levels. Because of the biodegradative activities thus exhibited by the crabs, lobsters, and flounder, we cannot be certain whether the sharply reduced levels of System H-sensitive congeners, such as 23-34, 234-25, 234-24, 234-23, and 234-34, that were seen in their tissues resulted from reductive dechlorination in the sediments or oxidative metabolism in the animal; however, their reduced levels in the mussels are clearly relatable to dechlorination.

DISCUSSION

This investigation resulted in the accumulation of a body of very detailed compositional information (in the form of quantitated capillary gas chromatograms) on the PCBs in upper Acushnet estuary sediments, and also provided more limited compositional information on those of other sediment, biota, and water samples from the New Bedford area. The PCB congener distributions observed in individual samples permitted deductions as to the original Aroclor compositions of the PCB releases, and the transformation processes that subsequently occurred. Comparison between the Aroclor compositions and transformation states of the PCBs in different samples permit deductions as to PCB diffusion and translocation, and the timing of the observed dechlorination processes. In this section we shall discuss these findings and deductions, and examine their implications as to the future progress of natural decontamination and detoxication processes in the Acushnet.

Vertical Movement of Estuarine Sediment PCBs. - Previous investigations of PCBs in freshwater sediments, e.g., those of Lake Superior (27), Lake Michigan (28), and the Upper Hudson (11) have shown good preservation of stratification, indicating very little vertical mobility for the PCBs. In sharp contrast, our 12 pairs of samples showed no large compositional differences between the 5-7.5 cm and 15-17.5 cm levels for any of the 7 parameters listed in Table 3, strongly suggesting diffusive blurring of stratification. Also suggestive of vertical diffusion are the various reports (15, 16, 18) indicating PCB levels in the sediment surface layers to be equal or nearly equal to those in the subsurface, despite the cessation of significant PCE releases (14), the continuation of active sedimentation (29), and losses of PCBs to the water column (16).

There are two possible mechanisms by which vertical diffusion might occur. First, Brownawell and Farrington (18) have shown that the pore water in these sediments contains detergent-like agents that solubilize the PCBs. This would permit the movement of the otherwise highly water-insoluble PCBs from particle to particle in the sediments. Alternatively, it could be that bioturbation processes are much more important in the tidal flats of the Acushnet estuary than in freshwater sediments. Whatever the cause, this vertical diffusivity of the PCBs has some significant consequences. One is that observations of substantial levels of PCBs even below 40 cm at some sites (15, 18) may not mean that that much sedimentation has actually occurred over the past 20-30 years. Another is that whether or not further sedimentation does occur, all of the PCBs now in the sediments may be able to reach those anaerobic layers where dechlorination is proceeding. A third is that they may also be able to reach the surface, and then

elute out into the water.

Flution of PCBs from Sediments into Water. - There are two well established mechanisms by which PCBs could be transferred into the aqueous phase. One is by true, evaporative-type, molecular solution in the water. Evidence for the occurrence of this process in the Acushnet is presented by the non-selective loss of the more volatile and water-soluble congeners from the PCBs now in the sediments (Figure 1), and the corresponding enrichment of these congeners in the PCBs found in filtered water (16). Since this process results in a compositional change we could calculate its extent (Table 3). For the upper estuary subsurface PCBs as a whole, the average loss due to this mechanism of solubilization was 18% (Table 3). The second possible mechanism of transfer to the water column consists of facilitated solubilization by either organic solubilizing agents or suspended particles. This type of process does not result in significant change in PCB composition (18). Brownawell and Farrington's analyses of the state of the PCBs in the estuarine waters indicated both of these processes to be of about the same importance (16), whereas the Batelle data (43), as averaged by ASA (44), indicated a ratio of 1:1.61. These two ratios indicate the total losses of PCBs from the sediments to the water column to be 31% and 36%, respectively.

In order to estimate the absolute magnitude of this loss, we assumed (a) the near equivalency of PCB concentration values expressed as g/g (dry weight) to those expressed as g/cm³ (wet sediments) on the basis of the reported (16) water content of outer harbor sediments; (b) that the mean level of PCB in the top 20 cm. of the sediments of the northern half of the upper estuary was 1000 ppm (Table 3; also consistent with ref. 15); (c) that the corresponding level in the southern half

was 100 ppm (15); and that the total area of the sediments in the upper estuary was about $9 \times 10^5 \text{ m}^2$ (from ref. 44). Multiplication then indicated the total current weight of PCB in the upper 20 cm. of the upper estuary sediments to be about 10^5 Kg., showing the total losses to the water column to have been about 50,000 Kg.

ASA (44) has estimated the current flux of PCBs from the sediments to the water by a two-dimensional vertically averaged finite element pollutant transport model as 189 Kg/yr. Three calculations using a simple one-dimensional model gave fluxes averaging 99 Kg/yr. Even the larger, and presumably more reliable, value represents a current annual flux of only 1/265 the total estimated losses. The inescapable conclusion is that during and shortly after the period of active discharges the rate of PCB extraction into the water column must have been between 10- and 100-fold greater than at present, and that the elution rate has been dropping sharply since that time.

Horizontal Movement of Estuarine Sediment PCBs. - There are two obvious mechanisms by which PCBs might move from one patch of sediment to another. One would be by scouring and redeposition of sediment particles carrying bound PCBs. The other would be dissolution into and readsorption from the water column. A priori, both mechanisms would appear eminently plausible: there is an abundance of heavily contaminated sediments present (14, 15), and there must have been very substantial levels in the estuarine waters in the recent past. The available evidence, however, indicates that neither translocation process has been occurring to a significant extent in the Acushnet. This evidence is of two types. First, both we (Table 3) and others (15) have observed an extraordinarily spotty distribution of both Aroclor 1242 and 1254 in the upper estuary sediments, with

many instances of 1000-fold concentration differences between nearby sites. Second, there are virtually none of the dechlorinated PCBs, which are ubiquitous in the sediments located north of the hurricane barrier, in those located south of it. Neither observation would be possible if there had been any significant horizontal transport between sediment banks, by whatever mechanism.

This current immobility of the PCBs now present in Acushnet estuary sediments raises the question of how the PCBs could have become so broadly distributed over the estuary in the first place.

We suggest that the PCBs, which are heavy, water-insoluble oils (1) were originally released to the estuary in the form of suspended droplets, and that these droplets moved various distances before sinking into the sediments. This would result in a rather spotty deposition on the sediments, the deposition pattern for each release being determined by the location of the discharge point and the state of the tide. Once adsorbed onto the sediment particles, however, little further horizontal movement between sediment sites could occur except by scouring and redeposition, which require higher water flow rates than normally occur in the estuary (44).

Where horizontal movement is occurring, of course, is in those PCBs that have become dissolved or suspended in the tidal waters. It would appear from the considerations outlined in the previous section that about 35% of the PCBs originally released into the upper estuary have already traveled this route through the waters of the lower estuary and Buzzard's Bay to the Atlantic, where their ultimate fate will be photolysis by sunlight (30) and oxidative biodegradation by various aerobic life forms (3, 4, 7). However, the Versar (19) and Brownawell (18)

chromatograms both indicate that these partially dechlorinated PCBs are not being reabsorbed from the water column by outer harbor sediments.

The inability of PCBs to move from one sediment bank to another, by whatever mechanism, along with the observed differences in composition, means that there must have been separate sources for the PCBs found in the sediments of the upper estuary, Clarks Cove, and the outer harbor. However, the composition of the PCBs in the water of the latter site indicates that they must have been derived partly from the sediments of the upper and middle estuary, and partly from local, outer harbor sediments.

Characteristics of Dechlorination Systems H and H^o. - The results show that the upper and middle Acushnet Estuary PCBs are undergoing dechlorination by at least two closely related dechlorination systems, herein designated H and H^o, which can be characterized in detail as to their relative reactivities toward the various individual PCB congeners present in the Aroclor mixtures released (Figs. 2,3; Tables 1,2).

In Table 4 we summarize the derived information on chlorophenyl group reactivities for System H, and show comparable summaries for two other dechlorination systems: System B, which is one of four meta/para PCB-dechlorinating systems (B, B', C, and E) found in upper Hudson River sediments (11, 13) and System F, which is one of two ortho/meta/para PCB dechlorinating systems (F and G) found in the sediments of Silver Lake (Pittsfield, MA) (13). Also included in Table 4 is a list of the reported electrochemical reduction potentials of the various chlorophenyl groups (31), not because of any evidence that the environmental dechlorinations proceed by simple electron transfer reactions, but simply because

these reduction potentials represent the only currently available indicators of the intrinsic chemical reactivities of the various chlorophenyl groupings toward reductive processes.

Table 4 shows that the susceptibility of chlorophenyl groups to attack by System H (indicated by "R" rather than "-" in Column H of the Table) does correlate to a fair extent with this index of reactivity, and also with the reactivity pattern shown by System F. Moreover, the pattern of chlorophenyl groups that appear in the dechlorinated product is also similar to that of System F. From this we may conclude that the intrinsic chemical reactivity, or reduction potential, of the agent responsible for System H must be quite similar to that responsible for F, and roughly equivalent to that of an Hg-Pt electrode set at -1.94 volts (relative to a standard calomel electrode in dimethyl sulfoxide). The equivalent potential for System H' may be slightly more negative, judging from the greater reactivity towards the borderline groups 2,3- and 2,3,6-CP.

However, the relative reactivities of the various PCB congeners towards Systems H and H' are clearly influenced by structural, or steric, effects as well as intrinsic susceptibilities to reduction. There would appear to be three sorts of steric effects involved: First, hindrance at the ortho (2 or 6) position by the opposite ring, regardless of chlorination pattern. As a result, we have a meta/para-selective dechlorination, like those of the upper Hudson river (11, 13), rather than the ortho/meta/para dechlorinations of Silver Lake Systems F and G (13). Second, hindrance by additional ortho substitution on the reacting ring. Thus, groups 2-,2,3,6-CP and 2,3,5,6- are progressively less reactive than 2,3-CP; and 2,3,4,6- and 2,3,4,5,6-CP are less reactive than 2,3,4-CP. This effect may be

particularly significant when the ortho chlorine is located opposite the meta chlorine that is to be removed; thus, the reactivity of 3,4-CP is undepressed in 2,3,4-CP, but significantly so in 2,4,5-CP, and the same relative positioning (3 vs. 6, or 5 vs. 2) is also present in 2,3,6- and 2,3,5,6-CP. The third steric effect, shown by the vertical progressions in Table 4, is a general reduction in reactivity produced by substituents on the opposite ring, particularly when in ortho (2 or 6) positions.

The first and third of these steric effects are also exhibited by System B (and the other upper Hudson systems as well), but the second is unique to H and H'. It would appear that removal of a chlorine from position 3 by System H is inhibited by the presence of a chlorine in position 6, whereas for Systems B, B', or C the inhibition is greater if the blocking chlorine is in position 5 (13). At any event, System H is more reactive than B to 2,3,4-, 2,3,5-, 2,3,4,5-, and possibly also 2,3,4,6-CP groups, but less reactive to 2,4,5-, 2,3,6-, 2,3-, 2,4-, and 2,5-CPs. As a result of this reactivity pattern, an Aroclor that has undergone dechlorination by this system will develop the characteristic pattern of GC peak gains and losses that we have termed Pattern H (Figure 1): prominent declines in the peaks of almost all congeners containing 3,4-, 2,3,4-, 2,3,4,5-, or 3,4,5-CP groups, and corresponding increases in those containing 3-, 2,4-, 2,5-, or 3,5-CPs.

Toxicological Implications of System H Dechlorination. - In the U.S., the PCBs were widely used in the manufacture of electrical devices for nearly fifty years (1930-1978) without generating any findings of significant health effects (32-35). Concern over PCB toxicity arose in the 1970's after reports of widespread human

poisoning in Japan caused by ingestion of rice oil ("yusho") that had been contaminated by PCBs (36). Eventually, further analyses of the rice oil identified polychlorinated dibenzofurans as the toxic contaminants, and the indictment of PCBs was withdrawn (37, 38). Meanwhile, however, studies with heavily dosed animals showed that a variety of toxic responses could be elicited, particularly by the more heavily chlorinated Aroclors, including hepatocellular carcinoma in rats (by Aroclor 1260) (39). Further studies with individual congeners then showed that only a very small subset of the 209 possible chlorinated biphenyls were active in producing observable toxic effects. These congeners were all found to be species having chlorines in both of the para (4 and 4') positions, in at least two of the four meta (3,3',5,5') positions, and in no more than one ortho (2 or 6) position. More specifically, a typical toxic response, thymic involution in rats, was elicited by 34-34, 345-4, 345-34, 345-345, 2345-4, 234-34, 2345-34, and 234-345 CB, but not by 34-4, 345-24, 245-34, 245-345, 2345-345, or any di-ortho substituted PCB (8). Three of the toxic congeners, namely 345-4, 345-34, and 345-345, have not been found in the commercial Aroclors; however, the other five are present at detectable levels (Appendix A). Thus, although occupational exposures of types permitting Aroclor (mixed PCB congener) uptakes up to several grams per year (5, 34) have not been sufficient to produce medically observable effects (32-35), the specific congeners of concern for their ability to produce toxic effects at still higher dosages are 34-34, 234-34, 234-345, 2345-4 and 2345-34.

Of secondary toxicological concern is the ability of a somewhat larger group of PCB congeners to induce the microsomal enzyme aromatic hydrocarbon hydroxylase (AHH), which has been more specifically identified in the rat as cytochrome P450c (8). This activity does not appear to be a component of the toxic response,

but is frequently induced by the same pharmaceutical agents, and hence is often considered a warning sign. The Aroclor constituents that induce this response are the toxic congeners just listed, and also 34-4, 245-34, 345-24, 234-234, 234-245, 245-345, 2345-24, 2346-34, and 2345-234 CB (8).

Upon comparing these two lists of pharmacologically active PCB congeners with the lists of congeners attacked by Systems H and H' (Table 1), and their relative susceptibilities to attack (Tables 2, 4) a notable correlation emerges: All of the congeners that are of primary toxicological concern, as producing demonstrable toxicity in rats, are among the group that is most rapidly attacked by System H and H'. All those congeners that are of secondary toxicological concern, as being cytochrome P450c inducers, are either also among this group or among those that are only slightly less rapidly attacked. Thus, an Aroclor mixture being transformed by System H or H' will undergo loss of pharmacologically active congeners (detoxication) much faster than the overall rate of dechlorination.

An exact estimate of the extent of detoxication is somewhat complicated by the fact that the two congeners of greatest concern, 34-34 and 234-34 CB, both coelute with other, non-isomeric congeners on DB-1 capillary columns, so that the less reliable GC-MS data (e.g., Fig. 3) rather than the GC-ECD measurements (e.g., Figure 2) must be used for their quantitation. These data, along with the reactivity patterns of Tables 2 and 4, do show, however, that the toxic congeners are being removed at least as rapidly as the Peaks 50 and 58 that we have routinely used as indicators of dechlorination status. On this basis, Table 3 shows detoxication of at least 90% (3.3 half-clearances) in sediments 17B, 19B, and 22B) or at least 67% (1.6

half-clearances) averaged over all of the upper estuary sediment samples collected. The similar levels of toxic congener loss that occur in the mussels, crabs, and lobsters collected south of the hurricane barrier in the outer harbor are somewhat easier to observe, since the DB-5 gas chromatograms that were reported (17) provide greater separation of the 234-34 CB peak (IUPAC 105) from nearby congeners than does the DB-1 column that we used.

Microbial Ecology of System H. - As pointed out earlier (11, 13) there are no known environmental chemical agents having the negative reduction potentials or other activities needed to reductively dechlorinate aromatic chlorine compounds such as the PCBs, and no simple chemical agents of any type that show the steric selectivities exhibited by dechlorination systems B, B', C, E, H, and H'. Accordingly, these dechlorinating agents must be enzymes, presumably each associated with a specific strain of anaerobic bacteria. No PCB-dechlorinating bacteria have yet been isolated, nor is early success in such an endeavor likely, in view of the experimental difficulties normally attendant upon work with environmental anaerobes. However, it has been demonstrated through use of microbial inhibitors that the analogous dechlorinations of chlorobenzoic acids and chlorophenyls are microbially mediated (40, 41), and the same approach has recently been found to show that PCB dechlorination by upper Hudson sediments is also dependent upon microbial action (42). Thus, there appears no reason to doubt that agents H and H' are microbial.

The dechlorinase enzymes H and H' are clearly much more closely related to each other than to those of the other dechlorination systems found to date. This suggests the possibility that agents H and H' may be mutant varieties of the same microbial species.

The ecological relationships between environmental xenobiotics and environmental bacteria cover a range of patterns. At one extreme is the situation where the xenobiotic chemical is non-beneficially cometabolized by a variety of common endogenous microbes, with no resulting alteration in population distribution. The oxidative biodegradation of PCBs by aerobic bacteria (3,4) apparently fits this pattern: Many strains of bacteria having the ability to cometabolize PCBs have been discovered, but none can grow on PCB as a sole carbon source, and no population enhancements of the PCB-degrading aerobes in PCB-contaminated areas have been noted.

At the other extreme is the situation where the xenobiotic selectively favors the growth of a rare organism. This is normally manifested by a long induction period during which seeding, adaptation, and clonal expansion occur, followed by the appearance of a homogeneous population of xenobiotic-dependent organisms. PCB dechlorination in aquatic sediments appears to follow this latter pattern; we have thus far examined several hundred gas chromatograms (albeit of widely varying quality) from five different PCB spill sites where dechlorination is occurring, and found at least nine different dechlorination patterns, implying at least nine different strains of PCB-dechlorinating microbes. However, where multiple patterns have appeared at the same site, they generally appeared to be closely related (e.g., H and H⁺ in the Acushnet; B, B' and C in the upper Hudson; and F and G in Silver Lake); thus, the original seeding in each case could have involved only a single organism that then underwent mutation. At all spill sites, most individual sediment specimens have shown only a single pattern, implying a patchy distribution of the dechlorinating organisms in the sediments, each patch

presumably representing a single clone. PCB-containing sediments that were not undergoing dechlorination as of the time of observation were seen downriver of the actively dechlorinating patches in both the upper Hudson (12) and the Acushnet. All of these observations suggest localized population blooms of otherwise very rare environmental bacteria.

It is a stoichiometric necessity that if some chemical species is being reduced, as the PCBs are when dechlorinated, some other species must be oxidized. Thus, the anaerobic bacteria that effect dechlorination must be using the PCBs as oxidizing agents (e.g., terminal electron acceptors) in their metabolic processes. We have shown earlier that this is strongly allowed on thermodynamic grounds; in fact, the free energy gain in oxidizing glucose (for example) to carbon dioxide and water using PCBs as the oxidants is calculated to be about three times that available from sulfate (13). Thus, the rare anaerobic bacterial strain that happens to possess enzyme systems that can effect PCB dechlorination should be at a selective advantage, and would be expected to proliferate. What is notable about the Acushnet dechlorinating strains H and H' is that they were evidently able to compete with the endogeneous sulfate-utilizing anaerobes even in estuarine sediments, where the sulfate level was found to be almost as high as in seawater (18).

Dechlorination Initiation and Rates. - As we saw above, it would appear that the upper and middle Acushnet estuary sediments have received between 100 and 200 metric tons of PCBs. Several minor routes of PCB entry into the estuary have been noted (14); however, the large quantities present are virtually inexplicable unless they be presumed to have occurred predominantly in connection with

ongoing manufacturing operations. This indicates the possible period for significant Aroclor 1254 release as between 1945 and 1965, and that for Aroclor 1242 as between 1962 and 1972. We have thus far been unable to detect any Aroclor 1016 (in manufacturing use 1970-78) in the sediments. Presumably, the growing concerns over environmental accumulation that led to the switchover to Aroclor 1016 beginning in 1970 also led to a curtailing of practices leading to releases.

In order to estimate the absolute rates of System H dechlorination from this chronology, we shall make two presumptions. The first is that the dechlorination process, once past the induction period, proceeded according to first order kinetics. This conventional presumption is not yet demonstrated for System H; however, for the analogous System B of the upper Hudson we have seen one core where the expected linear relationship between half-clearance number and depth was maintained over 30 cm. The second is that the intrinsic reactivities of the Aroclor 1242-associated Peak 50 (mainly 23-34 CB) and the Aroclor 1254-associated Peak 58 (234-25 CB) are about the same. This is the same presumption as that previously used in deriving a single scale for Table 2, and is based upon the identity of the mean numbers of half-clearances of these two peaks, when averaged over all sites listed in Table 3.

The first presumption means that we may take all of the "numbers of half-clearances" listed on the last three columns of Table 3 as equivalent to the numbers of half-times that the dechlorination has been proceeding. Thus, in the most advanced sediments of the northern end of the upper estuary, e.g., 17B, 19B, and 22B, we conclude that Peak 58 (and also those of the other Aroclor 1254-associated 234-XY CBs) has undergone about 3.5 half-times of clearance. The

second presumption tells us that in these more northerly sediments there was an approximately one half-time time lapse between the time of initiation of the Aroclor 1254 dechlorination and the mean arrival time of Aroclor 1242 in the subsurface zone where dechlorination was occurring (last column, Table 3). If we conservatively estimate the mean time of deposition of the Aroclor 1242 as roughly 1966, and the sample was collected in 1986, this means that the 2.5 half-times of dechlorination that elapsed after the arrival of the 1242 in the dechlorination zone took 20 years. If there was no transit time between deposition and arrival, or perhaps 15 years if there was a 5-year delay during which downward diffusion and/or burial occurred, indicating respective values of 8 and 6 years for the half-time. Consideration of the observed variances and uncertainties in the values used in this calculation indicates that the $t-1/2$ for Peak 58 (234-25 CB) removal in actively dechlorinating sediments should be estimated as 7 ± 3 years.

This number is equivalent to giving the period of active dechlorination of the sediments used for determining the relative rate data of Table 2 as 25 ± 10 years. Thus, the actual dechlorination $t-1/2$ for any of the individual congeners listed in Table 3 can be determined by dividing 25 ± 10 by the number of half-clearances given in the Table.

All such $t-1/2$ values refer, of course, to sediment strata where dechlorination is actively progressing. However, it is very likely that there may be a thin layer at the surface that is too aerobic for anaerobic bacterial growth. For the PCBs in this zone to dechlorinate, they must diffuse down into the active layers. Table 3 indicates that relative to the presumably fully active lower ("B") layer, the extent of dechlorination was 20-25% lower in the upper ("A") layer, or about 10-15% lower for the average of the two, which is probably representative of the

average for the sediment column as a whole. Thus, while the clearance $t-1/2$ for species like 234-25 CB in the active layers of the sediments can be stated as 7 ± 3 years it probably should be stated as 8 ± 3 years for the whole of the PCBs present.

We can now use the differences in the relative extents of dechlorination of the Aroclor 1254-derived peaks (last column, Table 3) to sketch out a chronology of events. First, there were sizeable releases of Aroclor₁₂₅₄ on various occasions within the period 1945 to 1965. Next, organism H appeared in PCB-adapted form, probably near the north end of the estuary. It was probably established in several locations, e.g., our sampling sites 17, 19, and 22, by the late 1950's; in the remainder of the northern half of the upper estuary (with the probable exception of site 18) by the time of the switchover to Aroclor 1242 (1962-65), and in most sites in the southern half of the upper estuary during the mid-1960's. During the period of spread, either a second seeding or mutation occurred, giving organism H'. This became established in one small area near sites 9 and 12, which are within 100m of each other. Also during this period a limited seeding of the Aroclor 1254 deposits in the ERFB sewer line occurred, possibly via sewage overflow connections that permit reverse flow into the sewer system during periods of high water levels (14). Sizeable releases of Aroclor 1242 to the upper estuary presumably then occurred on various occasions within the period 1962-1971, along with continued colonization of subsurface sediment layers by anaerobe H. In the absence of capillary GC data we cannot say when H reached the inner harbor; only that as of the time of the GCA sampling (1982-83) dechlorination was well along at all sites north of the hurricane barrier, but not to the south.

Future Course of Acushnet Sediment Dechlorination. - Presuming that all sedi-

ments north of the hurricane barrier are now seeded with the agent responsible for System H (or H') dechlorination, and that this dechlorination will continue to proceed in the future as it has over the past 25 years, we may project its future course. Our projection must, however, take into account the facts that the commercial Aroclors that were released into the estuary were complex mixtures of PCB congeners having quite different dechlorination rates, and also posing quite different levels of environmental concern. Of greatest concern must be those congeners that actually produce toxic effects or unusual enzyme inductions in animals; notably, those containing only 3,4-, 2,3,4-, 3,4,5-, and 2,3,4,5-CP groups attached to each other. Fortunately, it happens that these are also the groups most rapidly attacked by System H (Table 2). Judging overall detoxication (probably conservatively) by the disappearance rate of Peak 58 (234-25 CB), about 67% of these congeners have already been lost from the upper estuary (1.6 half-lives; Table 3). Overall average reduction to the 90% level (3.2 half-lives) will accordingly require 1.6 additional half-times, or 13±5 years. Further declines in the levels of toxic congeners in the upper estuary sediments will probably not have much further effect on those in outer harbor fish and shellfish, since these organisms will be exposed to water-borne PCBs originating in undechlorinated outer harbor sediments as well as those of the upper estuary.

Of secondary concern will be those PCB congeners which, while not particularly toxic, do show considerable persistence in crustaceans, birds, mammals, and man. This is because it is these persistent congeners that determine the total levels of PCBs actually measured in the blood or tissues of these species, and thus serve as a basis for regulatory actions. The most persistent PCB congeners in all these groups of species (which share the ability to biodegrade most PCB congeners

by microsomal oxidases of the cytochrome P450 type) are those having a 2,4,5- or 2,3,4,5-CP group attached to any other 4-substituted CP, e.g., 4-, 2,4-, 3,4-, 2,3,4-, 2,4,5-, etc. (5,6). System H does attack all of these congeners, but sometimes only slowly, notably in the case of 245-245 CB, for which the $t-1/2$ may be estimated only roughly from the available data (Table 2) as about 35 years. We estimate that to achieve 90% overall reduction in the level of P450-resistant congeners in the sediments will require 2 half-losses of 245-245 CB, which equates to roughly 70 years, starting in 1965, or 50 years from the present. Again, further dechlorination beyond the 90% level may not be helpful, since the lobsters are exposed to water containing PCBs from undechlorinating sources as well. This calculation applies, of course, to the proportion of P450-resistant congeners in the PCBs of the upper and middle estuary sediments. The actual quantity of such congeners reaching the outer harbor lobsters will be additionally determined by future elution rates from the sediments.

Of tertiary concern will be those many PCB congeners that are neither more toxic nor more persistent (in higher animals) than the petroleum hydrocarbons that are present along with them but which are regulated as PCBs nevertheless. These congeners include those Aroclor constituents that are not attacked by System H in the first place (e.g., 25-4, 24-4, 26-34, 236-34 CB, etc.) or else are products of System H dechlorination (e.g., 2-3, 25-3, 24-3, 25-25, 25-24, 24-24 CB, etc.) These congeners will still contribute to the measured PCB levels in mussels and some fish (i.e., those lacking cytochrome P450 activity for degrading PCBs), but not significantly to those of lobsters, crabs, or warm blooded animals. Their total levels in upper estuary sediments will decline only as elution occurs. However, their levels in the surface layers of the sediments, and hence

also their elution rates, concentrations in the upper estuary waters, and concentrations in lower estuary mussels should all continue to decline in response to elutriative depletion of the surface layers and continued sedimentation (29).

The foregoing projections assumed no change in the ongoing dechlorination system or its area of occupancy. Actually, of course, there are several alternative scenarios that should be considered. The most notable are (a) that System H may spread south into the outer harbor, (b) that System H may mutate to give a new strain with a broader range of PCB congener competence (like H'), (c) that the sediments may become seeded with some unrelated organism having the ability to utilize the congeners left unattacked by System H, a development that will become increasingly likely in the future as both the supply of H-dechlorinatable congeners and the population of System H organisms decline, and (d) that it may be decided to deliberately seed the sediments with an organism having a broader range of PCB congener competence, such as upper Hudson Systems C or E, or Silver Lake Systems F or G, or whatever other PCB-dechlorinating bacteria may be capable of survival in the Acushnet. The objectives of such seeding would be to accelerate the loss of P450-resistant congeners (which are attacked more rapidly by most other dechlorinating systems than by Systems H and H') and/or to carry the dechlorination all the way down to the mono- and dichlorobiphenyls, which would be more readily eluted from the sediments and also more readily biodegraded by aerobic microorganisms in the water.

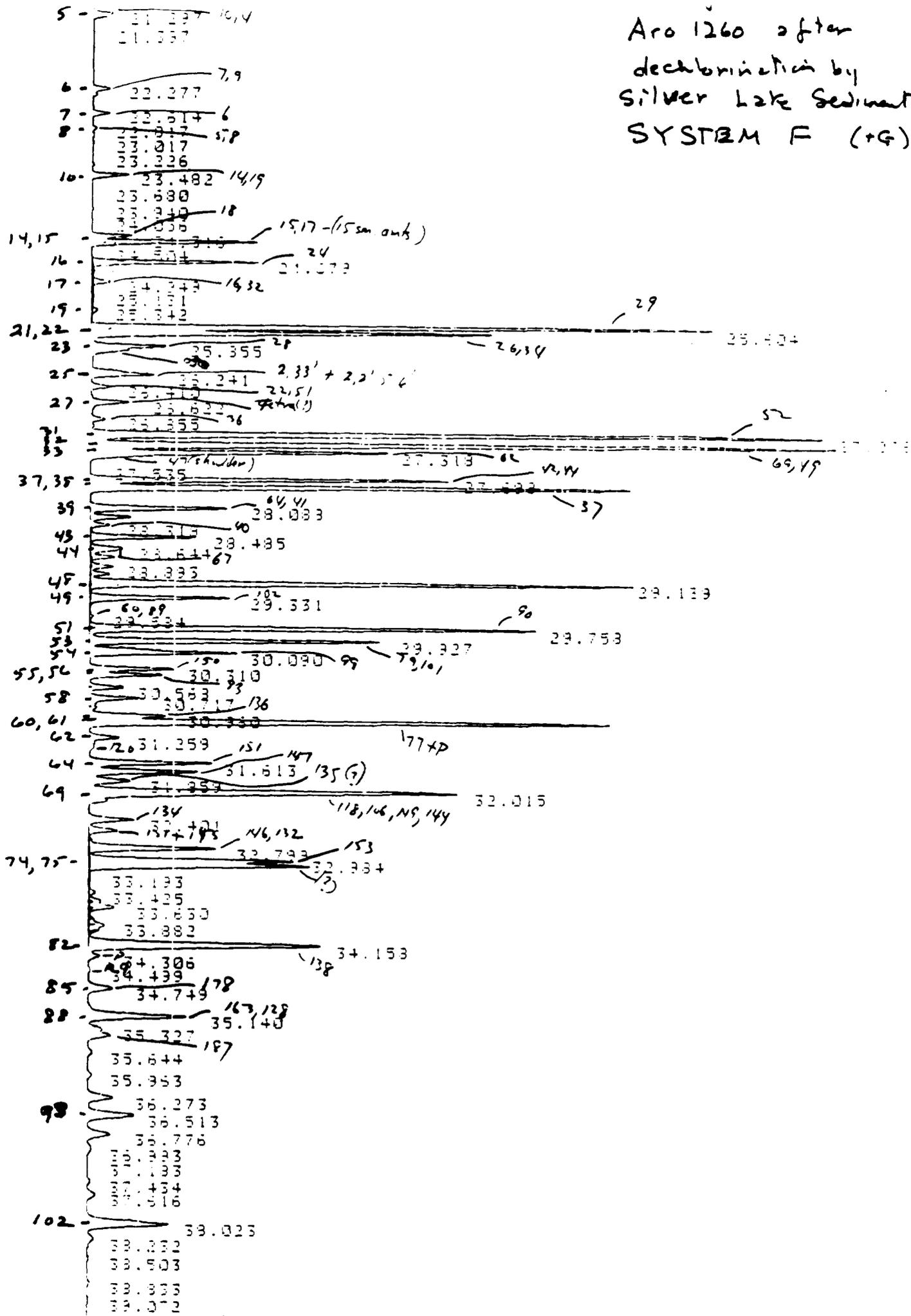
In summary, for upper and middle estuary sediments, for upper, middle, and lower estuary waters, and for lower estuary (outer harbor) biota, a projection of

current trends indicates a fairly rapid decline in the levels of those PCB congeners that are toxic in warm-blooded animals; a slower decline in those that are persistent but not toxic; and a still slower decline in the total PCB levels. However, there are conceivable developments that could speed up the natural processes by which detoxication and decontamination have been occurring.

Finally, we must add a cautionary note. The above projections are based upon observations of PCB transport and transformation processes that may be specific to the Acushnet estuary. Accordingly, they should not be used to predict the course of events at other PCB spill sites, unless the comparability of such processes has been established.

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Aro 1260 after
dechlorination by
Silver Lake Sediment
SYSTEM F (+G)



N.B.
2A

2A

5	20.097	
	20.417	
	20.829	
6	21.208	
7	21.532	
10	22.214	
11	22.600	
12	23.000	
14, 17	23.350	
18	23.700	
19	23.947	
21, 22	24.200	
23, 24	24.374	
	24.536	
31, 32	25.050	
37, 38	25.500	
39	25.771	
42	27.140	
46, 47, 48	27.700	
49	28.197	
53	28.676	
58	29.243	
61	29.825	29.540
69	30.100	30.345
74, 75	30.640	31.100
	31.329	
82	31.767	32.024
	32.315	
89	32.503	32.953
	33.100	
95	34.072	
	34.390	
102	34.701	
	35.006	
	35.375	
	35.690	
106	35.974	
	36.344	
109	37.141	
110	37.483	
	38.195	
	39.700	Int. Std.
	39.174	
	39.452	
115	40.778	
	41.802	
	42.000	
117	44.226	

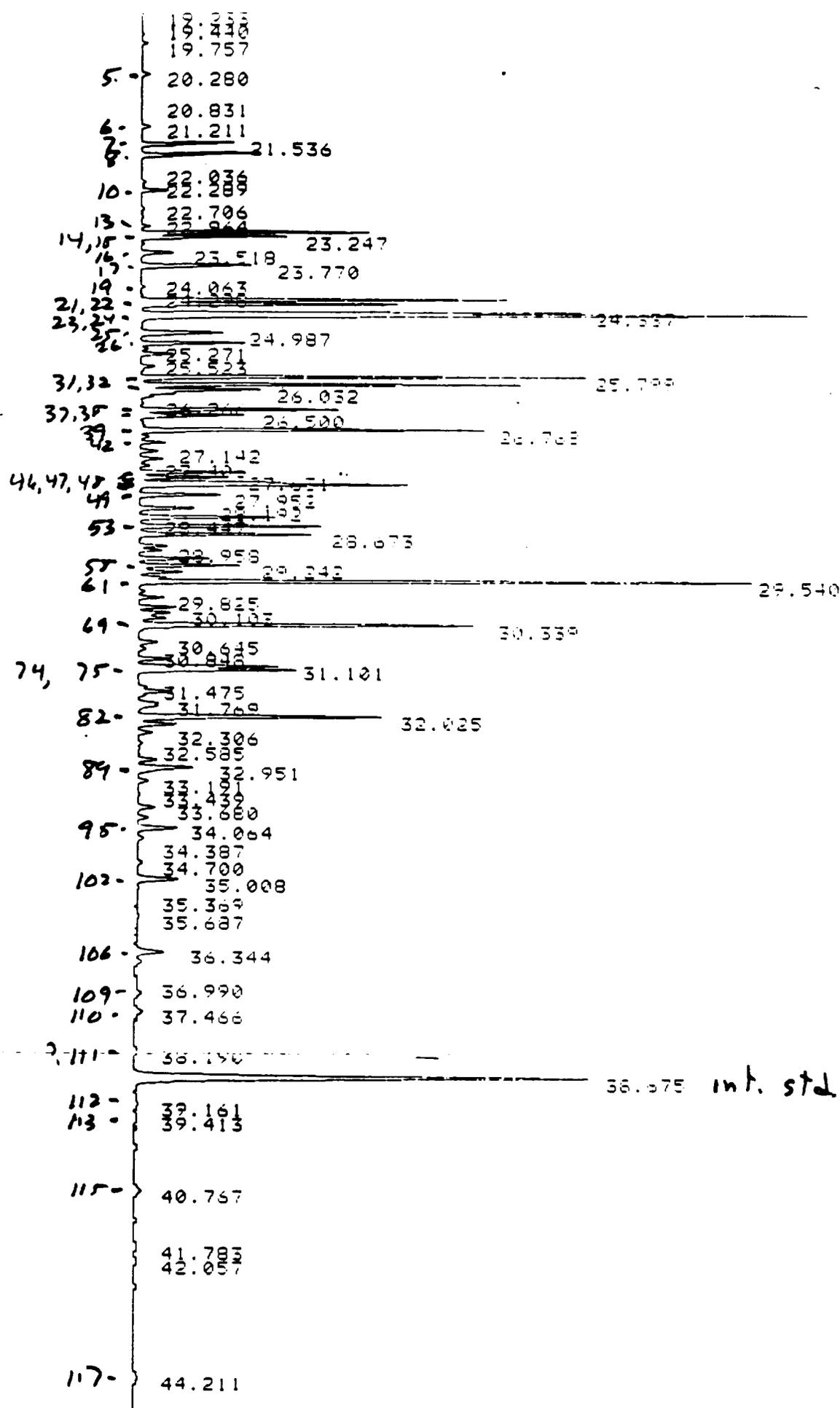
N.B. 2A

PLANK	RLT. TIME	T-CL:O-CL	IUPACH	RTT	CONDENSERS	WEIGHT %	MOLE %
1	40.64	0:0	000	.0997	BIPHENTYL	0.0000	0.0000
2	46.67	1:1	001	.1944	2	0.6904	0.9766
3	50.00	1:0	002	.1937	3	1.9107	2.0512
4	50.62	1:0	003	.1975	4	0.7360	1.0903
5	52.35	2:2	004 010	.2293	22' 1 26'	0.7350	0.9207
6	54.75	2:1	007 009	.2566	24' 1 25'	0.3599	0.4479
7	55.50	2:1	006	.2709	25'	1.4994	1.0874
8	56.1	2:1	005 000	.2785	23' 1 24'	2.3260	2.9343
9	57.46	2:0	010	.2973	35	0.0427	0.0530
10	57.75	2:3	019	.3095	22'6	0.4094	0.5352
11	58.06	3:2	030	.3165	246	0.0000	0.0043
12	59.15	2:0	011	.3230	33'	0.0000	0.0000
13	59.46	2:0	012 013	.3297	34' 1 34'	0.2401	0.3030
14	59.82	4:2 2:0	010 015	.3387	22'9 1 94'	5.6120	6.3937
15	60.02	3:2	017	.3390	22'0	2.0413	3.1071
16	60.72	3:2	024 027	.3500	236 1 23'6	0.4965	0.8029
17	61.34	4:2	016 032	.3625	22'9 1 20'6	2.6799	2.9306
18	62.12	3:1	033	.3770	235	0.0195	0.0213
19	62.32	3:1 4:0	034 050	.3800	2'35 1 22'66'	0.0713	0.0750
20	62.74	3:1	029	.3820	245	0.0512	0.0560
21	63	3:1	026	.3911	23'9	2.5990	2.0426
22	63.10	3:1	025	.3937	23'0	2.0063	2.1940
23	63.62	3:1	031	.4024	24'9	0.0770	0.5519
24	63.75	3:1 4:3	020 050	.4031	244' 1 22'06'	6.5779	7.1741
25	64.49	3:1 4:3	021 033	.4170	233' 1 230' 1 22'56'	3.0649	3.0272
26	65.01	3:1 4:3	022 051	.4267	234' 1 22'06'	1.9249	2.0000
27	65.5	4:3	045	.4334	22'36	0.6955	0.6787
28	65.89	3:1	036	.4379	33'5	0.0000	0.0000
29	66.07	4:3	046	.4450	22'36'	0.4779	0.4609
30	66.45	3:1	039	.4480	34'5	0.0000	0.0000
31	66.61	4:2	052 073	.4554	22'55' 1 23'5'6	5.4206	5.2273
32	66.90	4:2	049	.4610	22'45	3.5003	3.3755
33	67.21	4:2	047	.4639	22'44'	1.2975	1.2512
34	67.36	4:2	040 075	.4651	22'45 1 244'6	0.9367	0.9033
35	67.6	4:2	065 062	.4665	23'46 1 23'56	0.0000	0.0000
36	67.83	3:0	035	.4758	33'4	0.1040	0.1138
37	68.16	3:0 4:2	104 044	.4832	22'46'6' 1 22'35'	3.4610	3.3345
38	68.42	3:0 4:2	037 042	.4870	344' 1 22'34' 1 234'6	2.7200	2.6440
39	69.15	4:2	064 071	.4990	23'34 1 234'6 1 23'4'6	2.7125	2.6157
40	69.25	4:1	060	.5040	23'45' 7	0.0000	0.0000
41	69.4	3:0	096	.5057	22'36'6'	0.1600	0.1432
42	69.69	4:2	040	.5104	22'33'	0.7657	0.7304
43	70.1	5:3 4:1	103 057	.5155	22'45'6' 1 233'5	0.2210	0.2002
44	70.46	5:3 4:1	100 067	.5212	22'44'6' 1 23'4'5	0.4274	0.3849
45	70.77	4:1	058 063	.5267	233'5' 1 234'5	0.2470	0.2390
46	71.11	4:1 5:3	074 094	.5340	244'5 1 22'35'6	1.0343	1.2916
47	71.37	4:1	070 061	.5407	23'4'5 1 2'34'5 1 240'9	2.1640	2.0910
48	71.6	4:1 5:3	066 095	.5447	23'44' 1 22'35'6 1 22'30'6	2.5110	2.1770
49	72.1	5:3 4:1	091 090	.5549	22'30'6 1 22'3'06 1 230'9	0.0063	0.0030
50	72.8	4:1	056 060	.5676	233'4' 1 2344'	1.0051	1.7400
51	73.2	6:4 5:3	155 084	.5666	22'44'66' 1 22'33'61 22'35'5'	1.5000	1.3624
52	73.4	5:3	089	.5779	22'30'6'	0.0337	0.0291
53	73.6	5:2	101 090	.5814	22'30'5' 1 22'45'5'	2.6440	2.2017
54	74	5:2	099	.5800	22'44'5	1.6070	1.3671
55	74.6	6:4 5:2	150 112	.5969	22'30'66' 1 233'56 1 23'44'6	0.1265	0.1092
56	74.83	5:2	083 109	.6029	22'33'5 1 233'46	0.0000	0.0000
57	75.1	6:4 5:2	152 097	.6062	22'35'66' 1 22'34'5 1 22'3'45	0.0464	0.0241
58	75.5	5:2	087 111	.6175	22'34'5' 1 233'55' 1 2444'6	1.0760	0.9203
59	75.8	5:2	085 116	.6224	22'344' 1 234567	0.4970	0.4207
60	76.1	6:4	136	.6257	22'33'66'	0.3067	0.2393
61	76.3	4:0 5:2	077 110	.6295	33'44' 1 233'4'6	4.0402	3.4055
62	76.7	6:3	154	.6349	22'44'56'	0.0374	0.0291
63	77	5:2	082	.6453	22'33'4	0.3629	0.3131
64	77.4	6:3	151	.6499	22'35'5'6	0.3901	0.3106
65	77.7	6:3 5:1	135 124	.6563	22'33'56' 1 2'444'5	0.4359	0.3501
66	77.9	6:3	144	.6584	22'34'5'6	0.2652	0.2069
67	78.01	5:1 6:3	107 108	.6628	233'4'5 1 233'45' 1 22'30'56	0.0000	0.0000
68	78.3	5:1	123	.6650	2'344'5	4.1024	3.6002
69	78.41	6:3 5:1	149 110	.6672	22'30'5'6 1 23'44'5 1 233'45	0.0000	0.0000
70	78.7	6:3	139 140	.6707	22'344'6 1 22'344'6'	0.0034	0.0026
71	79.1	6:3 5:1	134 143	.6796	22'33'56' 1 22'3456' 1 2344'5	0.2046	0.2421
72	79.4	5:1 6:3	122 131	.6871	2'33'45' 1 22'33'46' 1 22'33'55'	0.1030	0.0859
73	79.9	6:2	146 161	.6955	22'34'55' 1 233'45'6	0.3620	0.2831
74	80.5	6:3 5:1	132 105	.7035	22'33'46' 1 233'44'	1.0375	0.8055
75	80.52	6:2	153	.7036	22'44'55'	0.0000	0.0000
76	81.2	6:2	160	.7060	23'44'5'6	0.0676	0.0527
77	81.5	6:2	141	.7204	22'3453'	0.2597	0.2026
78	81.7	7:4	179	.7205	22'33'566'	0.0000	0.0000
79	82	6:2	130	.7204	22'33'45'	0.2593	0.2023
80	82.2	6:2	137	.7329	22'344'5	0.0000	0.0000
81	82.35	7:4	176	.7305	22'33'466'	0.0000	0.0000
82	82.7	6:2	130 163	.7403	22'344'5' 1 233'4'56 1 +2	2.2023	1.7007
83	83	6:2	150	.7429	233'44'6	0.3490	0.2725
84	84.4	6:2	129	.7501	22'33'45	0.2206	0.1703
85	85.9	7:3	170	.7537	22'33'55'6	0.0577	0.0411
86	86.25	6:2	166	.7572	2344'56	0.0000	0.0000
87	86.4	7:3	173	.7611	22'33'45'6	0.0106	0.0100
88	86.7	7:3	107 102	.7653	22'34'55'6 1 22'444'56'	0.1630	0.1167
89	89.1	6:2	120	.7761	22'33'44'	0.5177	0.4039
90	89.4	7:3	103	.7720	22'344'5'6	0.0000	0.0000
91	89.76	6:1	167	.7814	23'44'55'	0.0000	0.0000
92	86.8	7:3	105	.7800	22'3453'6	0.0196	0.0140
93	87	7:3	174 101	.7965	22'33'56' 1 22'344'56	0.1520	0.1006
94	87.4	7:3	177	.8031	22'33'4'56	0.1172	0.0837
95	88	7:3 6:1	171 156	.8109	22'33'44'6 1 233'44'5	0.4227	0.3206
96	88.44	6:4	202	.8009	22'33'55'66'	0.0000	0.0000
97	88.5	6:1	157	.8104	233'44'5'	0.0552	0.0415
98	88.8	7:3	173	.8152	22'33'456	0.0004	0.0031
99	89.2	6:4	200 204	.8197	22'33'45'66' 1 22'344'566'	0.0051	0.0034
100	89.6	7:2	172 192	.8270	27'33'55' 1 233'445'6	0.0666	0.0475
101	90.2	6:4	197	.8293	22'33'44'66'	0.0000	0.0000
102	90.4	7:2	100	.8362	22'344'55'	0.3143	0.2259
103	91	7:2	193	.8397	233'44'5'6	0.0013	0.0009
104	91.44	7:2	191	.8447	233'44'5'6	0.0000	0.0000
105	92.15	6:4	199	.8494	22'33'4566'	0.0000	0.0000
106	93.8	7:2	170	.8740	22'33'44'5	0.2071	0.1475
107	94.3	7:2	190	.8740	233'44'56	0.0537	0.0300
108	95.4	6:3	196	.8845	22'33'455'6	0.0017	0.0011
109	95.9	6:3	201	.8875	22'33'4'55'6	0.0327	0.0245
110	96.0	6:3	194 203	.8935	22'33'44'5'6 1 22'444'55'6	0.0515	0.0357
111	96.6	7:1	189	.9102	213'44'55'	0.0063	0.0059
112	101.1	6:3	195	.9321	22'33'44'56	0.0252	0.0165
113	101.8	9:4	208	.9320	22'33'455'66'	0.0060	0.0037
114	103.29	9:4	207	.9421	22'33'44'566'	0.0000	0.0000
115	103.3	6:2	194	.9620	22'33'44'55'	0.0394	0.0250
116	106.4	6:2	205	.9670	233'44'55'6	0.0000	0.0000
117	114.2	9:3	206	1.010	22'33'44'55'6	0.0570	0.0346
118	126.35	10:4	209	1.050	22'33'44'55'66'	0.0000	0.0000

CONCENTRATION = 2.751815
TOTAL RICHMONDES = 0.0090

AVERAGE MOLECULAR WEIGHT = 201.50772
NUMBER OF CALIBRATED PEAKS FOUND = 118

N.B.
2 B



2 B

N.B 2B

PCARR	RET. TIME	T-CL:D-CL	IUPAC#	RTT	CONCENTERS	WEIGHT %	MOLE %
1	40.57	0:0	000	.0997	BIPHENYL	0.0000	0.0000
2	46.72	1:1	001	.1544		0.0000	0.0000
3	50.29	1:0	002	.1937		0.0000	0.0000
4	50.94	1:0	003	.1975		0.2190	0.0000
5	52.27	2:2	004 010	.2295	22' 1 26'	2.3357	2.8644
6	54.7	2:1	007 009	.2566	24' 1 25'	0.7154	0.8773
7	55.53	2:1	006	.2709	23'	4.6591	5.7139
8	56.02	2:1	005 008	.2705	23' 1 24'	4.9803	6.1127
9	57.09	2:0	019	.2973	35'	0.0000	0.0000
10	57.67	3:3	019	.3045	22'6'	0.9000	0.9371
11	58.55	3:2	030	.3165	24'	0.0353	0.0375
12	59.21	2:0	011	.3250	33'	0.0000	0.0000
13	59.4	2:0	012 013	.3297	34' 1 30'	0.4000	0.5946
14	59.74	3:2 2:0	010 015	.3307	22'5' 1 00'	10.6696	11.0103
15	59.95	3:2	017	.3390	22'0'	5.5513	5.8905
16	60.64	3:2	024 027	.3500	23' 1 23'6'	1.0236	1.0877
17	61.29	3:2	016 032	.3625	22'3' 1 24'6'	2.5019	2.6504
18	62.04	3:1	023	.3770	235'	0.0097	0.0103
19	62.43	3:1 4:0	034 054	.3800	2'35' 1 22'66'	0.0000	0.0000
20	62.66	3:1	029	.3820	245'	0.0229	0.0243
21	62.92	3:1	026	.3911	23'5'	3.9378	4.1041
22	63.22	3:1	025	.3937	23'4'	0.0000	0.0000
23	63.54	3:1	031	.4024	24'5'	7.6590	8.1300
24	63.77	3:1 4:3	020 050	.4031	244' 1 22'46'	0.0000	0.0000
25	64.04	3:1 4:3	021 033	.4170	233' 1 234' 1 22'56'	1.5530	1.6903
26	64.93	3:1 4:3	022 051	.4270	234' 1 22'46'	0.0077	0.0933
27	65.42	4:3	043	.4334	22'36'	0.9407	0.8849
28	65.79	3:1	036	.4379	33'5'	0.0164	0.0174
29	65.99	4:3	046	.4450	22'36'	0.6757	0.6331
30	66.54	3:1	039	.4488	34'5'	0.5417	0.0760
31	66.66	4:2	052 073	.4554	22'55' 1 23'5'6'	0.0000	0.0000
32	66.92	4:2	049	.4610	22'45'	5.2815	4.9488
33	67.16	4:2	047	.4639	22'44'	2.2498	2.1041
34	67.41	4:2	048 075	.4651	22'45' 1 244'6'	0.1369	0.1470
35	67.6	4:2	065 062	.4665	234' 1 2356'	0.0000	0.0000
36	67.75	3:0	035	.4730	33'4'	0.1540	0.1645
37	68.09	3:4 4:2	104 044	.4832	22'466' 1 22'35'	5.0200	2.8265
38	68.47	3:0 4:2	037 042	.4870	344' 1 22'30' 1 233'6'	0.0000	0.0000
39	69.04	4:2	064 071	.4990	23'34' 1 234'6' 1 23'0'6'	3.6099	3.3825
40	69.45	4:1	048	.5044	23'05' 7'	0.0000	0.0000
41	69.42	3:4	096	.5057	22'366'	0.0000	0.0000
42	69.58	4:2	040	.5102	22'33'	0.3751	0.3515
43	70.02	3:3 4:1	103 057	.5155	22'45'6' 1 233'5'	0.1360	0.1209
44	70.54	3:3 4:1	100 067	.5212	22'44'6' 1 23'4'5'	0.6115	0.5351
45	70.7	4:1	050 063	.5267	233'5' 1 234'5'	0.1302	0.1220
46	71.03	4:1 5:3	074 094	.5340	244'5' 1 22'356'	1.5204	1.3373
47	71.48	4:1	070 061	.5407	25'4'5' 1 2'345' 1 24057	0.0000	0.0000
48	71.52	4:1 5:3	066 095	.5447	23'00' 1 22'356' 1 22'55'6'	3.0009	2.6022
49	72.09	3:3 4:1	091 098	.5549	22'34'6' 1 22'3'46' 1 233'4'	0.9351	0.7925
50	72.74	4:1	056 060	.5676	233'4' 1 2346'	0.9305	0.8719
51	73.18	6:4 5:3	155 084	.5666	22'44'66' 1 22'33'61 1 22'355'	1.0031	0.8362
52	73.59	5:3	049	.5779	22'346'	1.7727	1.4664
53	73.71	5:2	101 090	.5814	22'34'5' 1 22'495'	0.0000	0.0000
54	73.94	5:2	099	.5880	22'44'5'	1.3081	1.1636
55	74.49	6:4 5:2	150 112	.5949	22'34'66' 1 233'56' 1 23'00'6'	0.1360	0.1140
56	74.88	5:2	085 109	.6029	22'33'5' 1 233'46'	0.0000	0.0074
57	75.11	6:4 5:2	152 097	.6044	22'3366' 1 22'345' 1 22'3'05'	0.3405	0.3506
58	75.42	5:2	087 111	.6175	22'343' 1 233'55' 1 2344'6'	0.4292	0.3598
59	75.76	5:2	085 116	.6224	22'344' 1 234567	0.3114	0.2610
60	76.2	4:4	116	.6257	22'33'66'	5.2630	3.9906
61	76.32	4:0 5:2	077 110	.6295	33'00' 1 233'0'6'	0.0000	0.0000
62	76.64	6:3	154	.6349	22'44'56'	0.0494	0.0375
63	76.95	5:2	082	.6403	22'33'4'	0.1506	0.1329
64	77.41	6:3	151	.6499	22'335'6'	0.2033	0.2140
65	77.7	6:3 5:1	135 124	.6563	22'33'56' 1 2'344'5'	0.3034	0.2360
66	77.93	6:3	144	.6584	22'345'6'	0.1020	0.1303
67	78.01	5:1 6:3	107 108	.6628	233'4'5' 1 233'43' 1 22'34'56'	0.0000	0.0000
68	78.29	5:1	125	.6650	22'344'5'	3.0764	2.5974
69	78.41	6:3 5:1	149 118	.6672	22'34'5'6' 1 23'44'5' 1 233'45'	0.0000	0.0000
70	78.55	6:3	134 140	.6707	22'344'6' 1 22'344'6'	0.0000	0.0000
71	79.07	6:3 5:1	134 143	.6796	22'33'56' 1 22'3456' 1 2344'5'	0.1929	0.1583
72	79.55	5:1 6:3	122 131	.6871	2'33'43' 1 22'33'46' 1 22'34'56'	0.0000	0.0000
73	79.87	6:2	146 161	.6955	22'34'55' 1 233'45'6'	0.2347	0.1779
74	80.23	6:3 5:1	132 105	.7035	22'33'46' 1 233'44'	0.4431	0.3674
75	80.52	6:2	153	.7036	22'44'55'	0.0000	0.0000
76	81.19	6:2	164	.7060	23'44'5'6'	0.0440	0.0333
77	81.57	6:2	141	.7203	22'3455'	0.0271	0.0205
78	81.7	7:4	179	.7203	22'33'566'	0.0000	0.0000
79	81.94	6:2	130	.7208	22'33'45'	0.1654	0.1254
80	82.2	6:2	137	.7329	22'344'5'	0.0000	0.0000
81	82.35	7:4	176	.7305	22'33'466'	0.0000	0.0000
82	82.61	6:2	130 163	.7403	22'344'5' 1 233'4'56' 1 2	1.1715	0.8001
83	82.97	6:2	150	.7429	233'44'6'	0.2391	0.1013
84	83.36	6:2	129	.7501	22'33'45'	0.1422	0.1070
85	83.85	7:3	178	.7537	22'33'55'6'	0.0206	0.0190
86	84.23	6:2	166	.7572	2344'56'	0.0000	0.0000
87	84.4	7:3	175	.7611	22'33'45'6'	0.0000	0.0000
88	84.62	7:3	187 182	.7653	22'34'55'6' 1 22'344'56'	0.1570	0.1087
89	85.03	6:2	128	.7761	22'33'44'	0.3078	0.2349
90	85.4	7:3	185	.7720	22'344'5'6'	0.0000	0.0000
91	85.68	6:1	167	.7814	23'44'55'	0.1901	0.1441
92	86.25	7:3	185	.7840	22'3455'6'	0.0154	0.0135
93	86.9	7:3	174 101	.7963	22'33'456' 1 22'344'56'	0.1307	0.0907
94	87.46	7:3	177	.8031	22'33'4'56'	0.0955	0.0663
95	87.88	7:3 6:3	171 156	.8105	22'33'44'6' 1 233'44'5'	0.2636	0.1957
96	88.34	6:4	202	.8009	22'33'55'66'	0.0317	0.0202
97	88.55	6:1	157	.8108	233'44'5'	0.0000	0.0000
98	88.91	7:3	175	.8152	22'33'456'	0.0000	0.0000
99	89.48	6:4	200 204	.8197	22'33'45'66' 1 22'344'566'	0.0497	0.0316
100	89.68	7:2	172 192	.8270	22'33'455' 1 233'455'6'	0.0000	0.0000
101	90.1	7:2	197	.8293	22'33'44'66'	0.2963	0.1804
102	90.7	7:2	180	.8362	22'344'55'	0.0135	0.0094
103	90.91	7:2	193	.8397	233'4'55'6'	0.0000	0.0000
104	91.44	7:2	191	.8447	233'44'5'6'	0.0000	0.0000
105	91.84	6:4	199	.8494	22'33'4566'	0.0137	0.0007
106	92.17	7:2	170	.8740	22'33'44'5'	0.1679	0.1162
107	92.44	7:2	190	.8740	233'44'56'	0.0000	0.0000
108	92.7	6:3	190	.8845	22'33'455'6'	0.0345	0.0219
109	92.99	6:3	201	.8873	22'33'4'55'6'	0.0000	0.0000
110	93.05	6:3	196 203	.8933	22'33'44'5'6' 1 22'344'55'6'	0.0000	0.0000
111	93.72	7:1	189	.9142	233'44'55'	0.0000	0.0000
112	100.9	6:3	195	.9321	22'33'44'56'	0.0134	0.0097
113	101.87	9:4	208	.9320	22'33'455'66'	0.0000	0.0000
114	103.29	9:4	207	.9423	22'33'44'566'	0.0000	0.0000
115	103.1	8:2	194	.9620	22'33'44'53'	0.0404	0.0308
116	106.77	8:2	205	.9670	233'44'53'6'	0.0000	0.0000
117	114.34	9:3	206	1.010	22'33'44'55'6'	0.0000	0.0000
118	126.33	10:4	209	1.050	22'33'44'55'66'	0.0000	0.0000

CONCENTRATION = 2.56605
TOTAL MICROMOLEL = 0.0094

AVERAGE MOLECULAR WEIGHT = 273.6050
NUMBER OF CALIBRATION PLANS FOUND = 110

N. B.
5A

19.229
19.595
20.074

21.198
21.522

22.206
22.691

23.337
23.755
24.045

24.966
24.966

25.780
25.017

26.482
26.755

27.130
27.617

28.179
28.000

29.229
29.521

30.330
30.632

31.237
31.642

32.142
32.489

32.794
33.174
33.426
33.600

34.054
34.370

34.681
34.984
35.348
35.671

36.321

36.965

37.456

38.173

38.557 int. STD.

39.142
39.389

40.737

41.757
42.037

44.180

5A

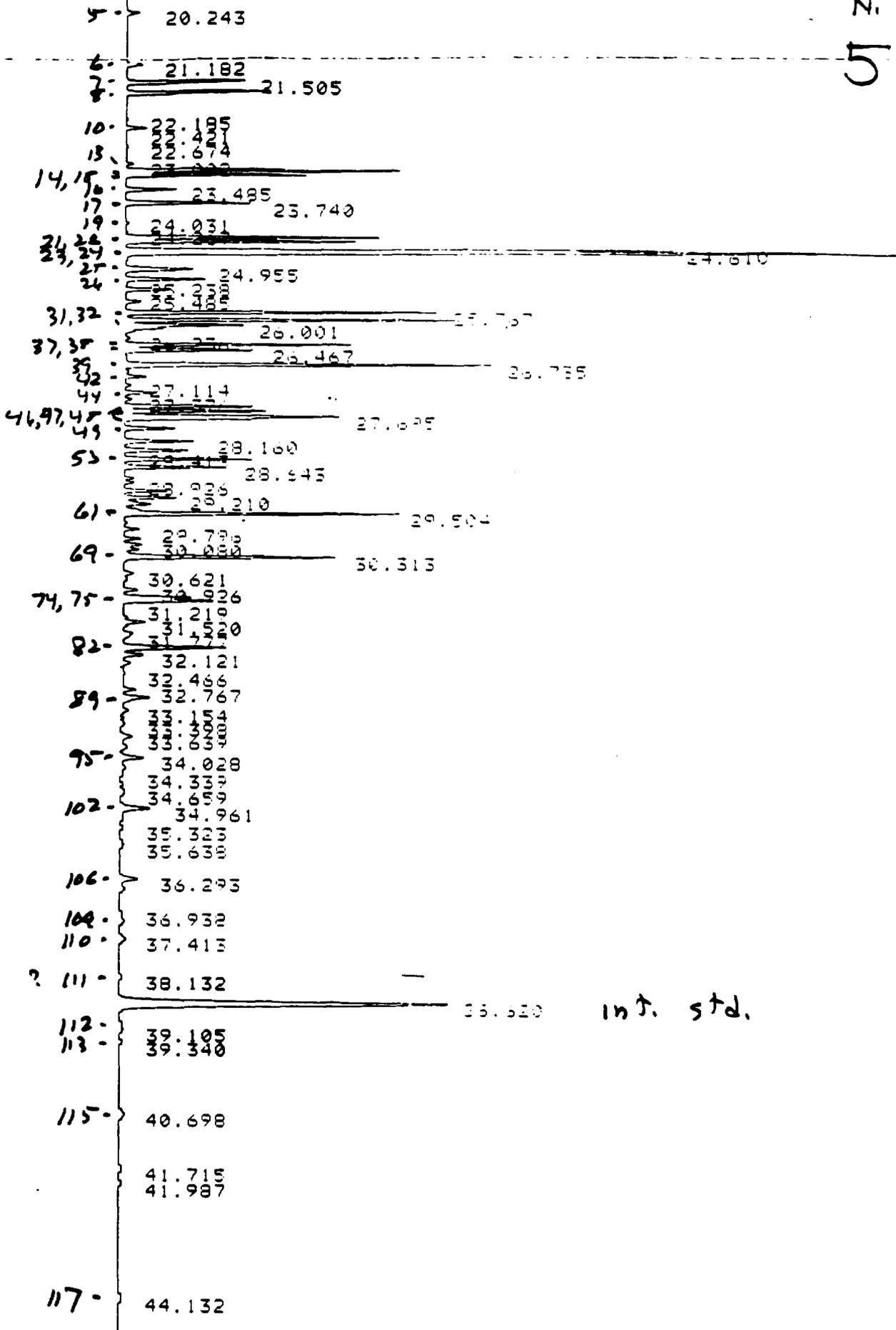
NB 5A

PEAK#	RET. TIME	T-LL:O-CL	IUPACC	RTT	CONDENSERS	WEIGHT %	MOLE %
1	40.64	0:0	000	.0997	BIPHENYL	0.0000	0.0000
2	46.72	1:1	001	.1544	2	0.0000	0.0000
3	50.29	1:0	002	.1937	3	0.0000	0.0000
4	50.62	1:0	003	.1975	4	0.3761	0.0695
5	52.55	4:2	004 010	.2245	22' 1 26	1.4077	1.7972
6	54.76	2:1	007 009	.2566	24' 1 25	0.3285	0.4194
7	55.61	2:1	006	.2709	23'	2.1489	2.7435
8	56.1	2:1	005 000	.2785	23' 1 20'	2.6878	3.4315
9	57.47	2:0	014	.2973	35	0.0417	0.0333
10	57.75	3:3	019	.3045	22'6	0.6800	0.7619
11	58.63	3:2	030	.3165	246	0.0517	0.0371
12	59.22	2:0	011	.3230	33'	0.0000	0.0000
13	59.96	2:0	012 013	.3297	34' 1 30'	0.2461	0.3141
14	59.02	3:2 2:0	010 015	.3307	22'5' 1 44'	6.2240	7.1730
15	60.07	3:2	017	.3398	22'6	5.5465	5.9230
16	60.7	3:2	024 027	.3500	236' 1 23'6	0.6433	0.7337
17	61.37	3:2	016 052	.3625	22'3' 1 24'6	1.9651	2.1737
18	62.1	5:1	023	.3770	235	0.0005	0.0004
19	62.43	5:1 4:4	034 054	.3800	2'35' 1 22'66'	0.0000	0.0000
20	62.72	5:1	029	.3820	245	0.0201	0.0222
21	62.98	5:1	026	.3911	25'5	2.4144	2.6706
22	63.18	5:1	025	.3957	23'0	2.1623	2.3910
23	63.6	5:1	031	.4024	24'5	4.6367	5.1289
24	64.73	5:1 4:5	020 050	.4031	244' 1 22'46	0.1435	0.1837
25	64.5	5:1 4:5	021 053	.4170	233' 1 234' 1 22'56'	1.7975	1.7956
26	64.39	5:1 4:5	022 051	.4267	234' 1 22'46'	1.0030	1.0530
27	65.48	4:3	045	.4354	22'36	0.8232	0.8030
28	65.87	5:1	036	.4379	35'5	0.0140	0.0159
29	66.08	4:3	046	.4450	22'36'	0.6079	0.5930
30	66.45	5:1	039	.4480	34'5	0.0000	0.0000
31	66.6	4:2	052 073	.4554	22'55' 1 23'5'6	5.3435	5.2123
32	66.98	4:2	049	.4618	22'45	4.2329	4.1209
33	67.27	4:2	047	.4639	22'44'	1.9163	1.8693
34	67.47	4:2	040 075	.4651	22'45' 1 240'6	1.0034	0.9788
35	67.6	4:2	045 062	.4865	2346' 1 2356	0.0000	0.0000
36	67.84	5:0	035	.4750	35'0	0.1470	0.1626
37	68.15	5:4 4:2	104 044	.4832	22'466' 1 22'35'	2.7938	2.7221
38	68.45	5:0 4:2	037 042	.4870	344' 1 22'38' 1 233'6	2.7572	2.7119
39	69.13	4:2	064 071	.4998	23'30' 1 250'6 1 23'4'6	3.1721	3.0942
40	69.25	4:1	048	.5040	23'45' 7	0.0000	0.0000
41	69.39	5:4	096	.5057	22'366'	0.3446	0.3087
42	69.67	4:2	040	.5102	22'53'	0.4715	0.4399
43	70.09	5:3 4:1	103 057	.5155	22'45'6' 1 235'5	0.1544	0.1474
44	70.45	5:3 4:1	100 067	.5212	22'40'6' 1 23'4'5	0.4647	0.4232
45	70.78	4:1	090 063	.5267	235'5' 1 234'5	0.1585	0.1544
46	71.12	4:1 3:5	074 094	.5340	244'5' 1 22'336'	1.6219	1.4773
47	71.35	4:1	070 061	.5407	23'4'5' 1 2'345' 1 24457	2.3999	2.3418
48	71.59	4:1 3:5	066 095	.5447	23'40' 1 22'336' 1 22'38'6	3.2661	2.6819
49	72.18	5:3 4:1	091 096	.5549	22'34'6' 1 22'3'46' 1 234'4	0.9294	0.8195
50	72.85	4:1	056 060	.5676	233'4' 1 2300'	1.3903	1.3440
51	73.24	6:4 5:3	155 084	.5666	22'40'66' 1 22'33'61 22'355'	1.1491	0.9972
52	73.48	5:3	089	.5779	22'366'	0.0000	0.0000
53	73.68	5:2	101 090	.5814	22'34'3' 1 22'455'	2.3740	2.0734
54	74.07	5:2	099	.5880	22'40'5	1.7292	1.5090
55	74.58	6:4 5:2	150 112	.5969	22'30'66' 1 233'56' 1 23'40'6	0.1605	0.1400
56	74.79	5:2	083 109	.6029	22'33'5' 1 233'46	0.2690	0.2394
57	75.2	6:4 5:2	152 097	.6062	22'3566' 1 22'340' 1 22'3'45	0.7608	0.6672
58	75.52	5:2	087 111	.6175	22'340' 1 233'55' 1 2340'6	0.4719	0.3864
59	75.83	5:2	085 116	.6224	22'340' 1 234567	0.1157	0.1027
60	76.13	6:4	136	.6257	22'33'66'	0.0000	0.0000
61	76.49	4:0 5:2	077 110	.6295	35'44' 1 233'4'6	3.2224	2.8122
62	76.75	6:3	154	.6349	22'40'56'	0.0541	0.0487
63	77.01	5:2	082	.6453	22'33'8	0.2630	0.2299
64	77.48	6:3	151	.6499	22'35'6	0.3307	0.2673
65	77.74	6:3 5:1	135 124	.6563	22'33'56' 1 2'344'5	0.3760	0.3055
66	77.9	6:3	144	.6584	22'34'6	0.0000	0.0000
67	78	5:1 6:3	107 100	.6628	233'4'5' 1 233'45' 1 22'30'56	0.3144	0.2659
68	78.25	5:1	123	.6658	2'344'5	0.0000	0.0000
69	78.38	6:3 5:1	149 118	.6672	22'30'5'6' 1 23'40'5' 1 233'45	3.3778	2.7437
70	78.59	6:3	139 140	.6707	22'340'6' 1 22'340'6'	0.0000	0.0000
71	79.16	6:3 5:1	144 143	.6794	22'35'56' 1 22'3406' 1 2344'5	0.2359	0.2015
72	79.47	5:1 6:3	122 151	.6871	2'33'40'1 22'33'46'1 22'35'55'	0.0927	0.0774
73	79.96	4:2	146 161	.6955	22'34'55' 1 233'45'6	0.3007	0.2436
74	80.32	6:3 5:1	132 105	.7035	22'33'46' 1 233'44'	0.7080	0.6112
75	80.68	6:2	173	.7034	22'40'55'	2.7641	2.1815
76	81.31	6:2	140	.7064	23'40'3'6	0.1810	0.1435
77	81.44	6:2	143	.7203	22'3405'	0.2115	0.1649
78	81.67	7:4	179	.7205	22'33'566'	0.0925	0.0647
79	82.06	6:2	130	.7284	22'33'45'	0.2064	0.1629
80	82.19	6:2	137	.7329	22'340'5	0.2112	0.1666
81	82.35	7:4	174	.7305	22'33'466'	0.0000	0.0000
82	82.73	6:2	140 163	.7404	22'340'5' 1 233'4'56' 1 2	1.6174	1.2765
83	83.06	6:2	150	.7429	233'40'6	0.2940	0.2327
84	83.45	6:2	129	.7501	22'33'45	0.1825	0.1400
85	83.94	7:3	170	.7537	22'33'55'6	0.0410	0.0301
86	84.10	6:2	166	.7572	2340'56	0.0111	0.0067
87	84.46	7:3	175	.7611	22'33'45'6	0.0122	0.0080
88	84.78	7:3	187 182	.7659	22'30'55'6 1 22'344'56'	0.1956	0.1409
89	85.11	6:2	120	.7761	22'33'44'	0.4307	0.3399
90	85.4	7:3	183	.7790	22'340'5'6	0.0000	0.0000
91	85.7	6:1	167	.7814	23'44'56'	0.2390	0.1847
92	86.57	7:3	185	.7840	22'40'55'6	0.0227	0.0164
93	86.99	7:4	174 181	.7900	22'43'456' 1 22'444'56	0.1593	0.1150
94	87.40	7:3	177	.8031	22'33'4'56	0.1164	0.0842
95	88	7:3 6:1	171 156	.8103	22'33'40'6' 1 233'44'5	0.3504	0.2750
96	88.47	8:4	202	.8009	22'33'35'66'	0.0457	0.0363
97	88.55	6:1	157	.8104	233'44'5'	0.0000	0.0000
98	88.91	7:3	174	.8134	22'33'456	0.0000	0.0000
99	89.36	8:4	208 200	.8197	22'33'45'66' 1 22'444'566'	0.0000	0.0000
100	89.6	7:2	172 192	.8270	22'33'455' 1 233'455'6	0.0797	0.0574
101	90.2	8:4	197	.8293	22'33'40'66'	0.0000	0.0000
102	90.4	7:2	180	.8362	22'340'56'	0.3436	0.2476
103	90.91	7:2	193	.8397	233'4'55'6	0.0000	0.0000
104	91.3	7:2	191	.8447	233'44'5'6	0.0047	0.0034
105	92.1	8:4	199	.8494	22'33'4566'	0.0261	0.0173
106	92.6	7:2	170	.8740	22'33'40'5	0.2180	0.1335
107	93.3	7:2	190	.8740	233'40'56	0.0544	0.0400
108	93.63	8:3	190	.8849	22'33'455'6	0.0000	0.0000
109	93.9	8:3	201	.8875	22'33'4'55'6	0.0567	0.0376
110	96.7	8:3	194 203	.8935	22'33'40'5'6 1 22'444'55'6	0.0721	0.0470
111	98.72	7:1	189	.9142	233'44'55'	0.0000	0.0000
112	101.1	8:3	195	.9321	22'33'40'56	0.0192	0.0127
113	101.87	9:4	200	.9320	22'33'455'66'	0.0000	0.0000
114	103.29	9:4	207	.9423	22'33'40'566'	0.0000	0.0000
115	105.2	8:2	194	.9620	22'33'40'55'	0.0426	0.0415
116	106.77	8:2	205	.9670	233'44'55'6	0.0000	0.0000
117	114.1	9:3	204	1.010	22'33'40'55'6	0.0344	0.0211
118	126.35	10:4	209	1.090	22'33'40'55'66'	0.0000	0.0000

CONCENTRATION = 1.633279
 TOTAL MICROMOLES = 0.0050
 AVERAGE MOLECULAR WEIGHT = 204.83194
 NUMBER OF CALIBRATED PLANS FOUND = 118

N. B.
5B

100.017
100.000
99.983
99.966
99.949



38.520 int. std.

5B

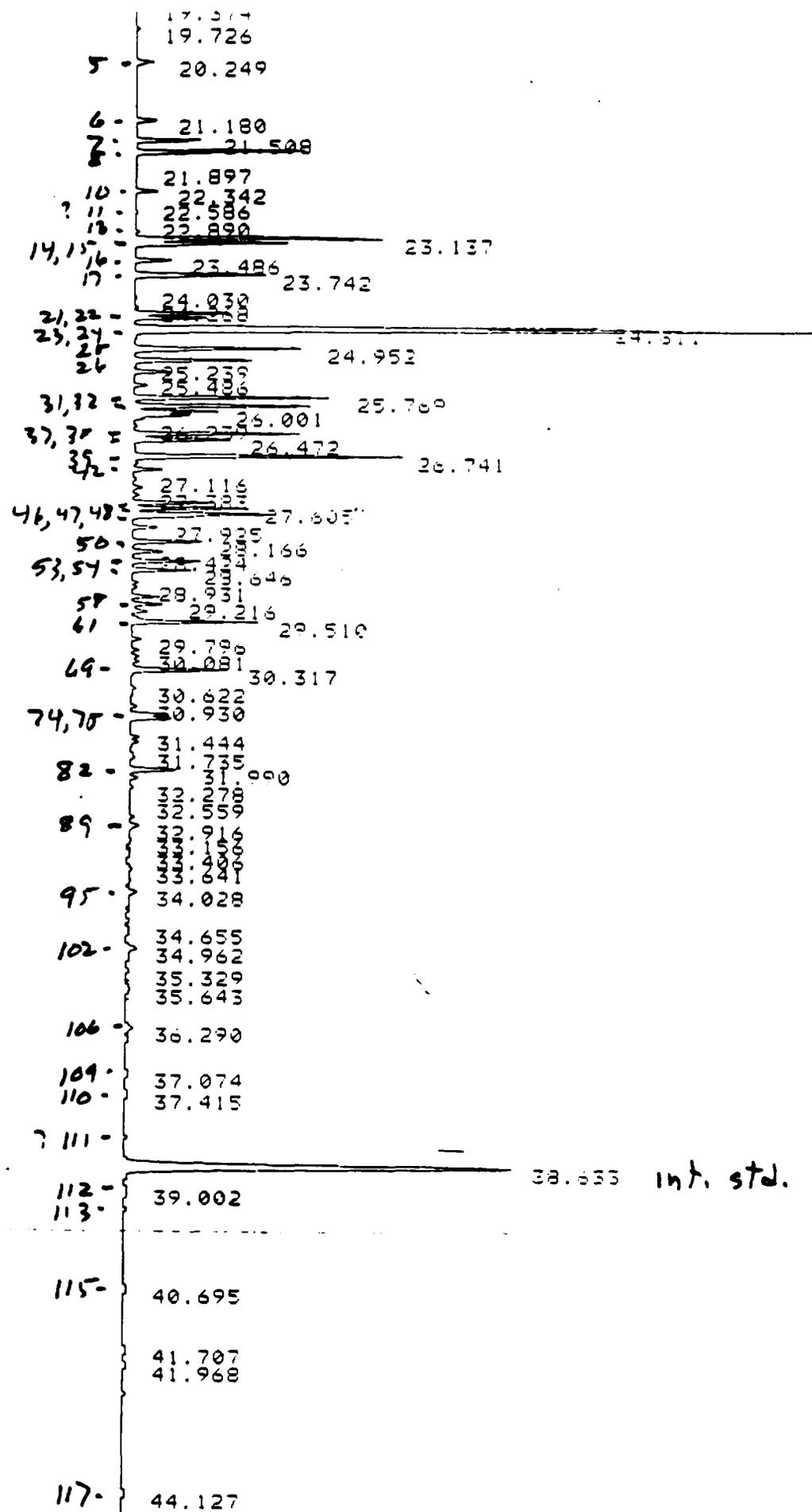
NB 5 B

PEAK#	HLT. TIME	T-CL:O-CL	IUMACH	RTT	CONGENERS	WEIGHT %	ROLE %
1	40.61	0:0	000	.0997	BIPHENYL	0.0000	0.0000
2	46.72	1:1	001	.1344	2	0.0000	0.0000
3	50.29	1:0	002	.1937	3	0.0000	0.0000
4	50.59	1:0	003	.1975	4	0.1859	0.2703
5	52.33	2:2	004 010	.2245	22' 1 26	1.9829	2.4390
6	54.76	2:1	007 009	.2566	24' 1 25	2.6073	0.7473
7	55.59	2:1	006	.2709	23'	3.9594	4.0668
8	56.00	2:1	005 008	.2785	23' 1 24'	4.2313	3.2063
9	57.49	2:0	014	.2973	55	0.0000	0.0000
10	57.73	3:3	019	.3045	22' 6	0.7647	0.8152
11	58.59	3:2	030	.3165	246	0.0300	0.0320
12	59.21	2:0	011	.3238	33'	0.0000	0.0000
13	59.47	2:0	012 013	.3297	34' 1 30'	0.4116	0.3064
14	59.8	3:2 2:0	018 015	.3387	22' 5' 1 40'	9.9500	10.0594
15	60.01	3:2	017	.3396	22' 4	4.7126	3.0241
16	60.71	3:2	024 027	.3500	236' 1 23' 6	0.0678	0.9264
17	61.35	3:2	016 032	.3625	22' 3' 1 24' 6	2.1248	2.2643
18	62.1	3:1	023	.3770	235	0.0002	0.0007
19	62.31	3:1 4:4	034 054	.3800	2' 35' 1 22' 66'	0.0721	0.0739
20	62.72	3:1	029	.3820	245	0.0194	0.0207
21	62.98	3:1	026	.3921	23' 5	3.3430	3.5638
22	63.16	3:1	025	.3937	23' 4	3.3280	3.5487
23	63.6	3:1	031	.4024	24' 5	6.5021	6.9316
24	63.73	3:1 4:3	028 050	.4031	244' 1 22' 46	0.5169	9.0551
25	64.31	3:1 4:3	021 033	.4170	233' 1 234' 1 22' 56'	1.3184	1.2694
26	65	3:1 4:3	022 051	.4267	234' 1 22' 46'	0.7537	0.7626
27	65.49	3:1	045	.4334	22' 34	0.0034	0.7571
28	65.85	3:1	036	.4379	33' 5	0.0139	0.0148
29	66.06	4:3	046	.4450	22' 34'	0.5736	0.5392
30	66.45	3:1	039	.4488	34' 5	0.0000	0.0000
31	66.6	4:2	052 073	.4554	22' 55' 1 23' 5' 6	5.6045	3.2687
32	66.99	4:2	049	.4610	22' 45	4.0838	4.2151
33	67.23	4:2	047	.4639	22' 44	1.9100	1.7956
34	67.33	4:2	048 075	.4651	22' 45' 1 244' 6	0.5642	0.5304
35	67.6	4:2	063 062	.4865	2346' 1 2356	0.0000	0.0000
36	67.82	3:0	035	.4738	33' 4	0.1314	0.1401
37	68.16	3:4 4:2	104 044	.4832	22' 466' 1 22' 35'	2.5639	2.4075
38	68.42	3:0 4:2	037 042	.4870	344' 1 22' 34' 1 233' 6	2.5607	2.4274
39	67.11	4:2	064 071	.4490	23' 34' 1 234' 6 1 23' 4' 6	3.0647	2.0811
40	69.25	4:1	060	.4040	25' 45' 7	0.0000	0.0000
41	69.42	3:4	096	.5057	22' 366'	0.0000	0.0000
42	69.66	4:2	040	.5102	22' 33'	0.3184	0.2994
43	70.1	3:3 4:1	053 057	.5155	22' 45' 6' 1 233' 5	0.1158	0.1063
44	70.44	3:3 4:1	100 067	.5212	22' 44' 4' 1 23' 4' 5	0.3192	0.4557
45	70.77	4:1	058 063	.5267	233' 5' 1 234' 5	0.1109	0.1039
46	71.11	4:1 3:4	074 094	.5340	244' 5' 1 22' 356'	1.2973	1.1390
47	71.34	4:1	070 061	.5407	23' 4' 5' 1 2' 345' 1 23457	1.6984	1.5968
48	71.6	4:1 3:4	066 095	.5447	25' 44' 1 22' 356' 1 22' 35' 6	2.6224	2.2164
49	72.17	3:3 4:1	091 098	.5549	22' 34' 6' 1 22' 3' 46' 1 233' 4	0.7938	0.6744
50	72.81	4:1	056 060	.5676	253' 4' 1 2344'	0.7899	0.7426
51	73.25	4:4 3:4	155 044	.5666	22' 44' 66' 1 22' 33' 61 22' 355'	0.0516	0.7122
52	73.43	3:3	089	.5779	22' 346'	0.0033	0.0045
53	73.67	3:2	101 090	.5814	22' 34' 5' 1 22' 455'	1.5999	1.3406
54	74.05	3:2	099	.5880	22' 44' 5	1.1784	0.9911
55	74.57	6:4 3:2	150 112	.5969	22' 34' 66' 1 233' 36' 1 23' 44' 6	0.1159	0.0971
56	74.70	3:2	083 109	.6029	22' 33' 5' 1 233' 46	0.1864	0.1569
57	75.14	6:4 3:2	152 097	.6064	22' 3566' 1 22' 346' 1 22' 3' 46	0.4589	0.3830
58	75.3	3:2	067 111	.6175	22' 345' 1 233' 35' 1 2444' 6	0.3644	0.3063
59	75.44	3:2	085 114	.6224	22' 344' 1 234567	0.2644	0.2223
60	76.13	6:4	136	.6257	22' 33' 66'	0.0000	0.0000
61	76.28	4:0 3:2	077 110	.6295	33' 44' 1 233' 4' 6	2.2718	1.9106
62	76.72	6:3	134	.6347	22' 44' 36'	0.0419	0.0319
63	77.03	3:2	082	.6453	22' 33' 4	0.1364	0.1132
64	77.49	6:3	151	.6499	22' 335' 6	0.2405	0.1830
65	77.78	6:3 3:1	135 124	.6563	22' 33' 56' 1 2' 344' 5	0.2576	0.2017
66	77.7	6:3	144	.6584	22' 345' 6	0.0000	0.0000
67	78.01	3:1 6:4	147 148	.6628	233' 4' 5' 1 233' 45' 1 22' 34' 36	0.2126	0.1733
68	78.25	3:1	123	.6658	2' 344' 5	0.0000	0.0000
69	78.37	6:3 3:1	149 118	.6672	22' 34' 5' 6' 1 23' 44' 5' 1 233' 45	2.3795	1.0632
70	78.55	6:3	139 140	.6707	22' 344' 6' 1 22' 344' 6'	0.0000	0.0000
71	79.13	6:3 3:1	134 143	.6796	22' 33' 56' 1 22' 3456' 1 2344' 5	0.1638	0.1349
72	79.53	3:1 6:4	122 141	.6871	2' 33' 45' 1 22' 33' 46' 1 22' 34' 36	0.0000	0.0000
73	79.45	6:2	146 161	.6955	22' 34' 55' 1 233' 45' 6	0.1993	0.1516
74	80.31	6:3 3:1	137 145	.7035	22' 33' 46' 1 233' 44'	0.3761	0.3130
75	80.47	6:2	153	.7036	22' 44' 35'	1.9314	1.0690
76	81.27	6:2	148	.7068	23' 44' 3' 6	0.0373	0.0204
77	81.48	6:2	141	.7203	22' 3455'	0.1421	0.1081
78	81.64	7:4	179	.7205	22' 33' 366'	0.0784	0.0469
79	82.02	6:2	138	.7284	22' 33' 45'	0.1404	0.1068
80	82.15	6:2	137	.7329	22' 344' 5	0.1329	0.1011
81	82.35	7:4	176	.7305	22' 33' 466'	0.0000	0.0000
82	82.64	6:2	134 163	.7403	22' 344' 5' 1 233' 4' 36' 1 42	0.9945	0.7363
83	83.04	6:2	158	.7429	233' 44' 6	0.2039	0.1544
84	83.44	6:2	129	.7501	22' 33' 45	0.1207	0.0918
85	83.93	7:3	170	.7537	22' 33' 33' 4	3.8243	3.0169
86	84.14	6:2	146	.7572	2344' 56	0.0864	0.0649
87	84.4	7:3	175	.7611	22' 33' 45' 6	0.0000	0.0000
88	84.71	7:3	187 182	.7654	22' 34' 55' 6' 1 22' 344' 36'	0.1333	0.0926
89	85.1	6:2	124	.7761	22' 33' 44'	0.2630	0.2001
90	85.4	7:3	183	.7720	22' 344' 3' 6	0.0000	0.0000
91	85.72	6:11	167	.7814	23' 44' 55'	0.1614	0.1227
92	86.34	7:3	185	.7848	22' 3455' 6	0.0163	0.0113
93	86.49	7:3	174 181	.7963	22' 33' 456' 1 22' 344' 36	0.1109	0.0772
94	87.43	7:3	177	.8031	22' 33' 4' 36	0.0811	0.0563
95	87.97	7:3 6:11	171 156	.8105	22' 33' 44' 6' 1 233' 44' 5	0.2255	0.1667
96	88.44	8:4	202	.8089	22' 33' 35' 66'	0.0269	0.0172
97	88.55	6:11	157	.8184	233' 44' 3'	0.0000	0.0000
98	88.91	7:3	173	.8152	22' 33' 456	0.0000	0.0000
99	89.36	8:4	240 244	.8197	22' 33' 45' 66' 1 22' 344' 366'	0.0000	0.0000
100	89.57	7:2	172 192	.8276	22' 33' 455' 1 233' 455' 6	0.0454	0.0317
101	90.2	8:4	197	.8293	22' 33' 44' 66'	0.0000	0.0000
102	90.4	7:2	180	.8362	22' 344' 33'	0.2456	0.1703
103	90.79	7:2	193	.8397	233' 4' 55' 6	0.0679	0.0053
104	91.44	7:2	191	.8447	233' 44' 3' 6	0.0000	0.0000
105	92.13	8:4	199	.8494	22' 33' 466'	0.0116	0.0074
106	93.4	7:2	178	.8748	22' 33' 44' 3'	0.1425	0.0990
107	94.44	7:2	190	.8748	233' 44' 36	0.0000	0.0000
108	95.8	8:3	198	.8805	22' 33' 455' 6	0.0293	0.0107
109	95.99	8:3	201	.8875	22' 33' 4' 55' 6	0.0000	0.0000
110	96.85	8:3	194 203	.8935	22' 33' 44' 5' 6' 1 22' 344' 55' 6	0.0000	0.0000
111	98.72	7:1	189	.9142	233' 44' 35'	0.0000	0.0000
112	101	8:3	195	.9321	22' 33' 44' 36	0.0000	0.0000
113	103.07	9:4	208	.9320	22' 33' 455' 66'	0.0133	0.0085
114	103.24	9:4	207	.9423	22' 33' 44' 366'	0.0000	0.0000
115	105.2	8:2	194	.9628	22' 33' 44' 36'	0.0000	0.0000
116	104.77	8:2	205	.9678	233' 44' 36'	0.0411	0.0263
117	114.24	9:3	204	1.010	22' 33' 44' 35' 6	0.0000	0.0000
118	126.55	10:4	209	1.058	22' 33' 44' 35' 66'	0.0000	0.0000

CONCENTRATION = 3.023534
TOTAL MICROMOLES = 0.0110

... ..

N. B.
9A



9A

PEAK#	RET. TIME	I-CLD-CL	IUPACH	RT	COMBENERS	WEIGHT %	MOLE %
1	40.61	0:0	000	.0997	BIPHENYL	0.0000	0.0000
2	46.72	1:1	001	.1599		0.0000	0.0000
3	50.00	1:0	002	.1937		1.3630	1.9190
4	50.62	1:0	003	.1975		0.6300	0.8670
5	52.33	2:2	004 010	.2295	22' 1 26'	3.7890	4.4166
6	54.73	2:1	007 009	.2566	24' 1 25'	1.0615	1.2640
7	55.59	2:1	006	.2709	23'	2.6335	3.1360
8	56.1	2:1	005 008	.2785	23' 1 24'	6.3036	7.5064
9	57.4	2:0	014	.2973	35	0.0761	0.0906
10	57.73	2:1	013	.3045	22' 6'	1.1825	1.1375
11	58.61	2:2	030	.3165	246	0.0396	0.0480
12	59.16	2:0	011	.3250	33'	0.1032	0.1229
13	59.47	2:0	012 013	.3297	34' 1 34'	0.2691	0.3205
14	59.8	3:2 2:0	010 015	.3307	22' 5' 1 44'	10.6706	11.4687
15	60.01	2:2	017	.3390	22' 0'	3.4099	3.9815
16	60.71	2:2	024 027	.3500	236' 1 23' 6'	0.0620	0.0693
17	61.30	3:2	016 032	.3625	22' 3' 1 24' 6'	3.1937	3.2970
18	62.1	3:1	023	.3770	255	0.0093	0.0096
19	62.51	3:1 0:0	034 034	.3800	2' 55' 1 22' 66'	0.0712	0.0707
20	62.72	3:1	029	.3820	245	0.0731	0.0755
21	62.98	3:1	026	.3911	23' 5'	1.6321	1.6902
22	63.19	3:1	025	.3957	23' 0'	1.4760	1.5228
23	63.6	3:1	031	.4024	24' 5'	7.1224	7.3663
24	63.73	3:1 0:0	028 030	.4031	244' 1 22' 46'	0.0730	0.0730
25	64.31	3:1 0:0	021 033	.4170	233' 1 234' 1 22' 56'	3.4115	3.1790
26	65	3:1 0:0	022 031	.4267	234' 1 22' 46'	1.0864	1.3772
27	65.49	4:3	045	.4374	22' 36'	0.9759	0.0861
28	65.68	3:1	036	.4379	33' 5'	0.0472	0.0487
29	66.09	4:3	046	.4450	22' 36'	0.6307	0.5759
30	66.45	3:1	039	.4488	34' 5'	0.0008	0.0000
31	66.6	4:2	052 073	.4554	22' 55' 1 23' 5' 6'	4.6361	4.2100
32	66.97	4:2	049	.4610	22' 45'	3.6524	3.3230
33	67.23	4:2	047	.4639	22' 44'	1.6140	1.4684
34	67.35	4:2	048 075	.4651	22' 45' 1 240' 6'	1.3541	1.2320
35	67.51	4:2	065 062	.4665	2346' 1 2356'	0.0838	0.0763
36	67.82	3:0	035	.4738	33' 4'	0.1484	0.1531
37	68.16	3:0 4:2	104 044	.4832	22' 466' 1 22' 35'	2.3752	2.3402
38	68.44	3:0 4:2	037 042	.4870	344' 1 22' 36' 1 233' 6'	2.5047	2.2978
39	69.14	4:2	064 071	.4990	23' 34' 1 230' 6' 1 23' 4' 6'	2.9902	2.7206
40	69.25	4:1	064	.5040	23' 45' 7'	0.0000	0.0000
41	69.4	3:0	046	.5057	22' 366'	0.1031	0.1490
42	69.68	4:2	040	.5102	22' 33'	0.5225	0.4754
43	70.1	3:3 4:1	103 057	.5155	22' 45' 6' 1 233' 5'	0.0923	0.0820
44	70.46	3:3 4:1	100 067	.5212	22' 44' 6' 1 231' 4' 5'	0.2508	0.2192
45	70.79	4:1	058 063	.5267	233' 5' 1 234' 5'	0.1176	0.1072
46	71.13	4:1 5:3	074 094	.5340	244' 5' 1 22' 356'	1.0203	0.8737
47	71.36	4:1	070 061	.5407	23' 4' 5' 1 2' 345' 1 24457'	1.6800	1.5892
48	71.6	4:1 5:3	066 095	.5447	23' 44' 1 22' 356' 1 22' 35' 6'	2.5534	2.0903
49	72.19	3:3 4:1	091 098	.5549	22' 34' 6' 1 22' 3' 46' 1 234' 4'	0.5012	0.4122
50	72.81	4:1	056 060	.5674	233' 4' 1 2344'	0.9936	0.9035
51	73.25	6:4 5:3	155 084	.5666	22' 44' 66' 1 22' 33' 6' 1 22' 355'	0.3428	0.4394
52	73.49	3:3	089	.5779	22' 346'	0.0000	0.0000
53	73.67	3:2	101 090	.5814	22' 34' 5' 1 22' 455'	1.1046	0.8991
54	74.05	3:2	099	.5840	22' 44' 5'	0.8522	0.6934
55	74.6	6:4 5:2	150 112	.5969	22' 34' 66' 1 233' 56' 1 23' 44' 6'	0.0003	0.0004
56	74.8	3:2	084 109	.6029	22' 33' 5' 1 233' 46'	0.1264	0.1029
57	75.22	6:4 5:2	152 097	.6062	22' 3566' 1 22' 345' 1 22' 3' 45'	0.3667	0.2968
58	75.53	3:2	087 111	.6175	22' 345' 1 233' 55' 1 2344' 6'	0.2074	0.2339
59	75.80	3:2	085 116	.6224	22' 344' 1 234467'	0.1900	0.1344
60	76.13	6:4	136	.6257	22' 33' 66'	0.0000	0.0000
61	76.28	4:0 5:2	077 110	.6295	35' 44' 1 233' 4' 6'	1.2809	1.0426
62	76.72	6:3	154	.6349	22' 44' 56'	0.0296	0.0218
63	77.03	3:2	082	.6453	22' 33' 4'	0.1192	0.0970
64	77.49	6:3	151	.6499	22' 335' 6'	0.1296	0.0954
65	77.70	6:3 5:1	135 124	.6563	22' 33' 56' 1 2' 344' 5'	0.1455	0.1102
66	77.9	6:3	144	.6584	22' 345' 6'	0.0000	0.0000
67	77.99	3:1 6:3	107 108	.6628	233' 4' 5' 1 233' 45' 1 22' 34' 56'	0.1419	0.1119
68	78.25	3:1	123	.6650	2' 344' 5'	0.0000	0.0000
69	78.37	6:3 5:1	149 118	.6672	22' 34' 5' 6' 1 23' 44' 5' 1 233' 45'	1.0057	1.0652
70	78.55	6:3	139 140	.6707	22' 344' 6' 1 22' 344' 6'	0.0000	0.0000
71	79.10	6:3 5:1	134 143	.6796	22' 33' 56' 1 22' 3456' 1 2344' 5'	0.0925	0.0737
72	79.41	5:1 6:3	122 131	.6871	2' 33' 45' 1 22' 33' 46' 1 22' 33' 55' 6'	0.0390	0.0304
73	79.75	6:2	146 161	.6955	22' 34' 53' 1 233' 45' 6'	0.1236	0.0911
74	80.3	6:3 5:1	132 105	.7035	22' 33' 46' 1 233' 44'	0.2509	0.2085
75	80.32	6:2	133	.7036	22' 44' 53'	0.0000	0.0000
76	81.3	6:2	144	.7068	23' 44' 5' 6'	0.0004	0.0021
77	81.5	6:2	141	.7203	22' 3455'	0.0604	0.0504
78	81.8	7:4	179	.7205	22' 33' 566'	0.0145	0.0097
79	82	6:2	130	.7284	22' 33' 45'	0.0673	0.0495
80	82.2	6:2	137	.7329	22' 344' 5'	0.0000	0.0000
81	82.34	7:4	176	.7305	22' 33' 466'	0.0000	0.0000
82	82.7	6:2	134 163	.7403	22' 344' 5' 1 233' 4' 56' 1 42'	0.3495	0.4445
83	83	6:2	150	.7429	233' 44' 6'	0.1075	0.0791
84	84.4	6:2	129	.7501	22' 33' 45'	0.0633	0.0466
85	84.9	7:3	170	.7537	22' 32' 55' 6'	0.0229	0.0134
86	84.25	6:2	146	.7572	2344' 56'	0.0000	0.0000
87	84.4	7:3	175	.7611	22' 33' 45' 6'	0.0000	0.0000
88	84.7	7:3	187 182	.7654	22' 34' 55' 6' 1 22' 344' 56'	0.0634	0.0424
89	85.1	6:2	128	.7761	22' 33' 44'	0.1365	0.1085
90	85.4	7:3	183	.7728	22' 344' 5' 6'	0.0000	0.0000
91	85.7	6:1	167	.7814	23' 44' 55'	0.0951	0.0700
92	86.8	7:3	185	.7848	22' 3455' 6'	0.0042	0.0042
93	86.9	7:3	174 101	.7965	22' 33' 56' 1 22' 344' 56'	0.0436	0.0309
94	87.4	7:3	177	.8031	22' 33' 4' 56'	0.0359	0.0242
95	87.9	7:3 6:1	171 154	.8105	22' 33' 44' 6' 1 233' 44' 5'	0.1275	0.0911
96	88.4	6:4	202	.8089	22' 33' 55' 66'	0.0174	0.0107
97	88.55	6:1	157	.8184	233' 44' 5'	0.0000	0.0000
98	88.91	7:3	173	.8152	22' 33' 456'	0.0000	0.0000
99	89.3	8:4	208 204	.8197	22' 33' 45' 66' 1 22' 344' 566'	0.0293	0.0101
100	89.68	7:2	172 172	.8278	22' 33' 455' 1 233' 455' 6'	0.0000	0.0000
101	90.2	8:4	197	.8293	22' 33' 44' 66'	0.0000	0.0000
102	90.4	7:2	180	.8362	22' 344' 55'	0.1063	0.0714
103	90.91	7:2	193	.8397	233' 44' 55' 6'	0.0000	0.0000
104	91.3	7:2	191	.8447	233' 44' 5' 6'	0.0017	0.0011
105	92.1	8:4	199	.8494	22' 33' 4566'	0.0219	0.0134
106	93.8	7:2	178	.8748	22' 33' 44' 5'	0.0640	0.0434
107	94.3	7:2	190	.8748	233' 44' 56'	0.0206	0.0139
108	95.8	8:3	194	.8845	22' 33' 455' 6'	0.0047	0.0029
109	96	8:3	201	.8875	22' 33' 455' 6'	0.0000	0.0000
110	96.7	8:3	196 203	.8935	22' 33' 44' 55' 6' 1 22' 344' 55' 6'	0.0245	0.0151
111	98.6	7:1	189	.9142	233' 44' 55'	0.0033	0.0023
112	100.7	8:3	195	.9321	22' 33' 44' 56'	0.0000	0.0000
113	101.87	9:4	200	.9320	22' 33' 455' 66'	0.0000	0.0000
114	103.29	9:4	207	.9423	22' 33' 44' 566'	0.0000	0.0000
115	105.2	8:2	194	.9620	22' 33' 44' 55'	0.0171	0.0106
116	106.77	8:2	205	.9678	233' 44' 55' 6'	0.0000	0.0000
117	110.1	9:3	206	1.010	22' 33' 44' 55' 66'	0.0313	0.0179
118	126.45	10:4	209	1.050	22' 33' 44' 55' 66'	0.0000	0.0000

CONCENTRATION = 2.060414
TOTAL MICROMOLES = 0.0070
AVERAGE MOLECULAR WEIGHT = 265.46769

N.B.
9B

1000.924
1000.211
1000.411
1000.732

5 - 20.252

6 - 21.190

7 - 21.512

10 - 22.192

11 - 22.410

12 - 22.604

11, 13

14 - 23.489

23.746

19 - 24.036

21, 22

23, 24

25 - 24.960

25.512

31, 32

37, 38 - 26.005

26.775

39

40 - 26.478

26.741

44

46, 47

48 - 27.007

49

54

61

69

30.315

74, 75

82

89 - 31.742

31.001

91

102

106

36.298

109

110

37.087

37.427

? 111

38.146

int. STD.

112

113

39.107

39.346

115

40.709

41.715

41.980

117

44.136

9B

N.B 9B

PLAKR	HLI. TIME	T-CL:O-CL	IUPACH	RTT	CONDENSER	WEIGHT %	MOLE %
1	40.63	0:0	000	.0997	MIPHENYL	0.0000	0.0000
2	46.72	1:1	001	.1544	2	0.0000	0.0000
3	50.29	1:0	002	.1937	3	0.0000	0.0000
4	50.61	1:0	003	.1975	4	0.1944?	0.2767
5	52.34	2:2	004 010	.2205	22' 1 26	2.3912	3.1193
6	54.70	2:1	007 009	.2564	24' 1 25	0.6003	0.8109
7	55.6	2:1	006	.2709	23'	4.0734	4.9835
8	56.09	2:1	005 000	.2785	23' 1 20'	4.0020	5.7006
9	57.33	2:0	014	.2973	35	0.0141	0.0169
10	57.75	3:3	019	.3045	22'6	0.9355	0.9757
11	58.6	3:2	030	.3165	246	0.0314	0.0327
12	59.17	2:0	011	.3230	33'	0.0956	0.1151
13	59.40	2:0	012 013	.3297	34' 1 30'	0.3662	0.6016
14	59.61	3:2 2:0	010 015	.3367	22'5' 1 40'	10.2050	11.1757
15	60.42	3:2	017	.3398	22'4	5.3103	5.5468
16	60.69	3:2	024 027	.3500	236' 1 23'6	0.7505	0.7820
17	61.37	3:2	016 032	.3625	22'3' 1 20'6	2.4292	2.5335
18	62.12	3:1	023	.3770	235	0.0066	0.0089
19	62.32	3:1 4:0	034 034	.3800	2'35' 1 22'66'	0.1036	0.1039
20	62.74	3:1	029	.3820	245	0.0271	0.0282
21	62.99	3:1	026	.3911	23'5	4.7563	4.9627
22	63.10	3:1	025	.3937	23'4	0.6046	0.8027
23	63.62	3:1	031	.4024	24'5	7.3051	7.6190
24	63.72	3:1 4:3	028 030	.4031	244' 1 22'06	0.7206	0.9794
25	64.49	3:1 4:3	021 033	.4170	235' 1 234' 1 22'56'	1.6250	1.5315
26	65.01	3:1 4:3	022 031	.4267	234' 1 22'06'	0.6460	0.6799
27	65.40	4:3	045	.4334	22'36	0.7909	0.7274
28	65.84	3:1	036	.4379	33'5	0.0000	0.0000
29	66.07	4:3	046	.4450	22'36'	0.5365	0.6935
30	66.45	3:1	039	.4480	34'5	0.0000	0.0000
31	66.61	4:2	052 073	.4554	22'55' 1 23'5'6	6.0960	5.6006
32	66.90	4:2	049	.4610	22'45	4.5941	4.2354
33	67.21	4:2	047	.4639	22'44'	1.8976	1.7453
34	67.36	4:2	040 075	.4651	22'45' 1 244'6	0.7947	0.7309
35	67.6	4:2	063 062	.4865	23'6' 1 2356	0.0000	0.0000
36	67.83	3:0	035	.4730	33'4	0.0002	0.0006
37	68.14	3:0 4:2	104 044	.4852	22'466' 1 22'55'	2.0577	1.8963
38	68.43	3:0 4:2	037 042	.4870	344' 1 22'34' 1 234'6	1.7047	1.6551
39	69.12	4:2	064 071	.4990	23'34' 1 234'6 1 23'0'6	3.2115	2.9550
40	69.25	4:1	060	.5000	23'45' 7	0.0000	0.0000
41	69.30	5:4	096	.5057	22'366'	0.3489	0.2871
42	69.67	4:2	040	.5102	22'33'	0.2320	0.2137
43	70.08	5:3 4:1	104 057	.5155	22'45'6' 1 233'5	0.0997	0.0896
44	70.44	5:3 4:1	100 067	.5212	22'44'6' 1 23'4'5	0.2022	0.2424
45	70.78	4:1	050 063	.5267	233'5' 1 234'5	0.0770	0.0780
46	71.11	4:1 5:3	074 094	.5300	244'5' 1 22'356'	1.3660	1.1752
47	71.35	4:1	070 061	.5407	23'4'5' 1 2'345' 1 23457	1.0000	1.0000
48	71.61	4:1 5:3	066 093	.5447	23'44' 1 22'356' 1 22'35'6	1.7325	1.4326
49	72.17	5:3 4:1	091 090	.5549	22'34'6' 1 22'3'46' 1 233'4	0.7050	0.5067
50	72.8	4:1	056 060	.5676	233'4' 1 2344'	0.6194	0.5657
51	73.24	6:4 5:3	155 084	.5666	22'44'66' 1 22'33'61 22'335'	0.6991	0.5720
52	73.49	5:3	089	.5779	22'346'	0.0000	0.0000
53	73.65	5:2	101 090	.5814	22'34'5' 1 22'455'	0.9279	0.7625
54	74.06	5:2	099	.5800	22'44'5	1.0320	0.8492
55	74.50	6:4 5:2	150 112	.5969	22'34'66' 1 233'56' 1 23'00'6	0.1146	0.1146
56	74.79	5:2	083 104	.6029	22'31'5' 1 233'46	0.1249	0.1249
57	75.17	6:4 5:2	152 097	.6062	22'3566' 1 22'345' 1 22'3'45	0.3575	0.3525
58	75.34	5:2	087 111	.6175	22'345' 1 233'55' 1 2344'6	0.2350	0.1941
59	75.82	5:2	085 116	.6224	22'344' 1 234567	0.1759	0.1447
60	76.13	6:4	156	.6257	22'33'66'	0.0000	0.0000
61	76.29	6:0 5:2	077 110	.6290	33'44' 1 233'4'6	1.0993	1.5620
62	76.73	6:3	154	.6349	22'44'56'	0.0329	0.0245
63	77.01	5:2	082	.6453	22'33'4	0.0909	0.0814
64	77.5	6:5	151	.6499	22'55'6	0.1429	0.1043
65	77.76	6:3 5:1	135 124	.6568	22'32'96' 1 2'344'5	0.1405	0.1130
66	77.9	6:3	144	.6564	22'345'6	0.0000	0.0000
67	77.99	5:1 6:3	107 104	.6620	233'4'5' 1 233'45' 1 22'34'56	0.1263	0.1007
68	78.25	5:1	125	.6650	2'344'5	0.0000	0.0000
69	78.56	6:3 5:1	149 110	.6672	22'34'5'6' 1 23'44'5' 1 233'45	1.3905	1.0652
70	78.56	6:3	139 140	.6707	22'344'6' 1 22'344'6'	0.0134	0.0100
71	79.10	6:3 5:1	134 143	.6796	22'33'56' 1 22'3456' 1 2344'5	0.0996	0.0762
72	79.44	5:1 6:3	122 141	.6871	2'33'451 22'33'461 22'33'55'	0.0361	0.0205
73	79.96	6:2	146 161	.6955	22'34'55' 1 233'45'6	0.1302	0.0949
74	80.32	6:3 5:1	132 105	.7033	22'33'46' 1 233'44'	0.0294	0.1067
75	80.45	6:2	153	.7036	22'44'55'	1.1247	0.8369
76	81.20	6:2	160	.7060	23'44'5'6	0.0725	0.0540
77	81.40	6:2	141	.7203	22'3455'	0.0590	0.0439
78	81.67	7:4	179	.7205	22'32'466'	0.0402	0.0273
79	82.40	6:2	150	.7204	22'33'45'	0.0667	0.0494
80	82.10	6:2	137	.7329	22'344'5	0.0455	0.0634
81	82.30	7:4	176	.7305	22'33'466'	0.0000	0.0000
82	82.73	6:2	150 163	.7403	22'344'5' 1 233'4'56' 1 43	0.5310	0.3951
83	83.00	6:2	150	.7429	233'44'6	0.1120	0.0839
84	83.42	6:2	129	.7501	22'33'45	0.0541	0.0402
85	83.90	7:3	170	.7537	22'33'50'6	0.0127	0.0066
86	84.10	6:2	166	.7572	2344'56	0.0022	0.0017
87	84.4	7:3	175	.7611	22'33'45'6	0.0000	0.0000
88	84.72	7:3	187 102	.7633	22'34'55'6 1 22'344'56'	0.0770	0.0523
89	85.1	6:2	120	.7761	22'33'44'	0.1363	0.1014
90	85.4	7:3	183	.7720	22'344'5'6	0.0000	0.0000
91	85.73	6:1	167	.7814	23'44'50'	0.0000	0.0455
92	86.44	7:3	185	.7840	22'3453'6	0.0000	0.0000
93	86.97	7:3	174 103	.7945	22'33'456' 1 22'344'56	0.0401	0.0327
94	87.46	7:3	177	.8031	22'33'4'56	0.0349	0.0251
95	87.90	7:3 6:1	171 156	.8105	22'33'44'6 1 233'44'5	0.1140	0.0630
96	88.47	6:4	202	.8047	22'33'55'66'	0.0161	0.0100
97	88.53	6:1	157	.8104	233'44'5'	0.0000	0.0000
98	88.91	7:3	173	.8132	22'33'456	0.0000	0.0000
99	89.34	6:4	200 204	.8197	22'33'45'66' 1 22'344'566'	0.0000	0.0000
100	89.50	7:2	172 192	.8270	22'33'455' 1 233'453'6	0.0257	0.0174
101	90.2	6:4	197	.8292	22'33'44'66'	0.0000	0.0000
102	90.41	7:2	180	.8362	22'344'53'	0.1132	0.0702
103	90.91	7:2	193	.8397	233'4'55'6	0.0000	0.0000
104	91.44	7:2	191	.8447	233'44'5'6	0.0000	0.0000
105	92.14	6:4	199	.8494	22'33'4566'	0.0102	0.0063
106	92.8	7:2	178	.8740	22'33'44'5	0.0649	0.0460
107	94.3	7:2	190	.8740	233'44'56	0.0164	0.0111
108	95.0	6:3	190	.8845	22'33'453'6	0.0131	0.0002
109	95.99	6:3	201	.8875	22'33'4'55'6	0.0000	0.0000
110	96.7	6:3	196 203	.8935	22'33'44'5'6 1 22'344'55'6	0.0227	0.0142
111	98.72	7:1	109	.9142	233'44'53'	0.0000	0.0000

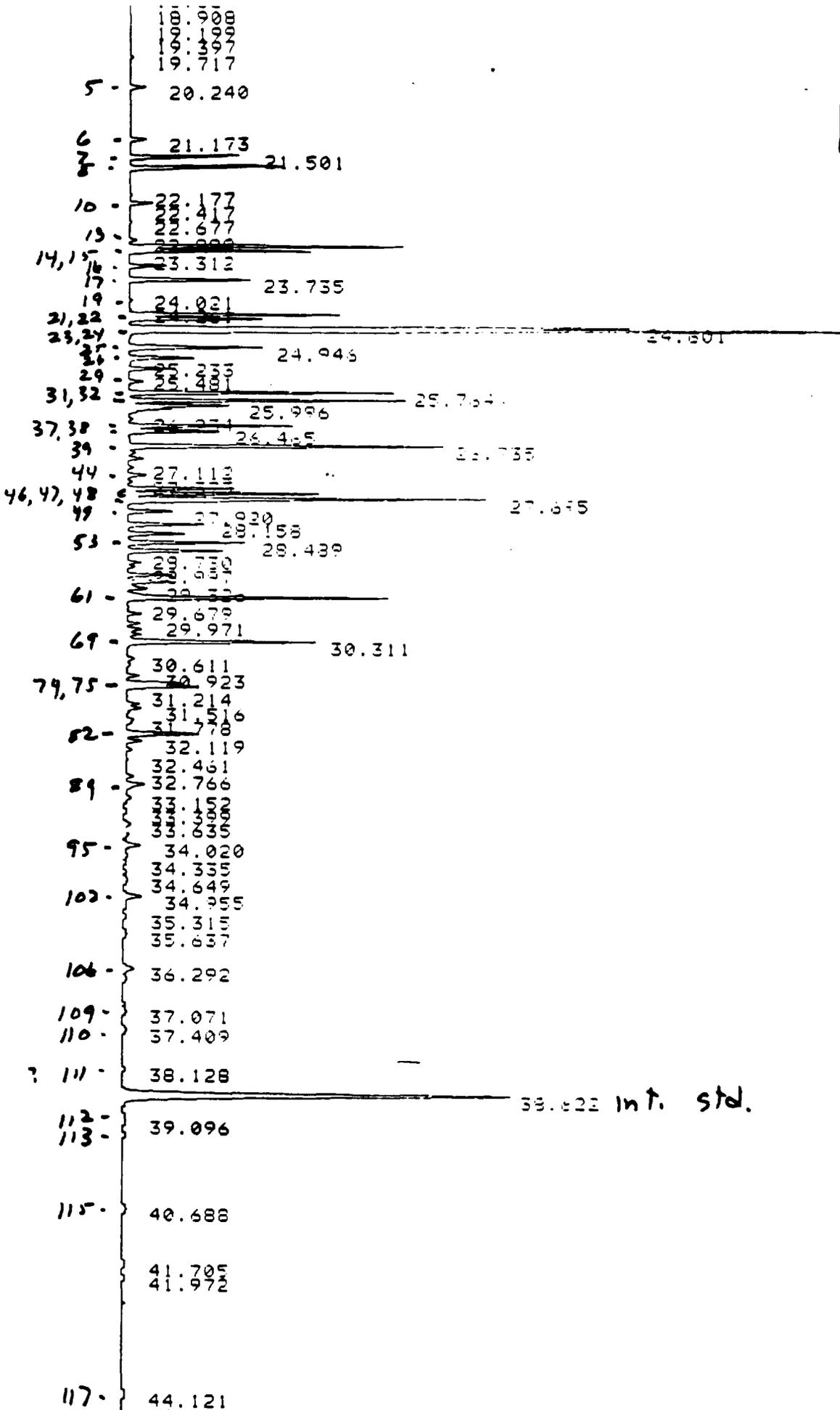
CONCENTRATION = 2.7760%

TOTAL MICROMOLES = 0.0103

AVERAGE MOLECULAR WEIGHT = 260.36478

NUMBER OF CALIBRATED PEAKS FOUND = 111

N. B.
12A



12A

38.622 int. std.

N.B. 12 A

PEAK #	RET. TIME	T-CL:O-CL	IUPAC#	RT	CONSERNS	WEIGHT %	ROLE %
1	40.62	0:0	000	.0997	BIPHENYL	0.0000	0.0000
2	46.82	1:1	001	.1500		0.2693	0.3892
3	50.29	1:0	002	.1957		0.0000	0.0000
4	50.61	1:0	003	.1975		0.1817	0.2626
5	52.34	2:2	004 010	.2200	22' 1 26'	2.6600	3.2560
6	54.75	2:1	007 009	.2566	20' 1 25'	0.6210	0.7600
7	55.50	2:1	006	.2709	23'	3.5000	4.2000
8	56.09	2:1	005 008	.2709	23' 1 24'	5.0601	6.1051
9	57.49	2:0	014	.2973	35'	0.0000	0.0000
10	57.70	0:3	019	.3093	22'6	0.0900	0.0929
11	58.63	0:2	030	.3163	206	0.0293	0.0311
12	59.21	2:0	011	.3230	33'	0.0000	0.0000
13	59.46	2:0	012 013	.3297	30' 1 30'	0.4400	0.5400
14	59.79	3:2 2:0	010 015	.3307	22'5' 1 40'	9.5300	10.5200
15	60.03	0:2	017	.3390	22'6	0.9710	5.2600
16	60.7	0:2	020 027	.3508	236' 1 23'6	0.7300	0.7021
17	61.37	3:2	016 032	.3625	22'5' 1 24'6	2.2150	2.3457
18	62.1	3:1	023	.3770	235	0.0000	0.0005
19	62.43	3:1 0:0	024 029	.3800	2' 35' 1 22'06'	0.0000	0.0000
20	62.72	3:1	029	.3820	245	0.0190	0.0201
21	62.98	3:1	026	.3911	23'5	3.0359	3.2151
22	63.18	3:1	025	.3957	23'6	2.3000	2.4362
23	63.62	3:1	031	.4024	24'5	7.1307	7.5516
24	63.73	3:1 0:3	020 050	.4031	240' 1 22'06'	0.3519	0.0212
25	64.5	3:1 0:3	021 033	.4170	233' 1 23' 1 22'56'	2.3016	2.2014
26	64.99	3:1 0:3	022 051	.4267	230' 1 22'06'	0.6420	0.6453
27	65.51	0:3	043	.4330	22' 36'	0.7393	0.6905
28	65.80	3:1	036	.4379	33'5	0.0000	0.0000
29	66.08	0:3	046	.4450	22' 36'	0.5321	0.4960
30	66.45	3:1	034	.4480	34'5	0.0000	0.0000
31	66.62	4:2	052 073	.4554	22' 55' 1 23'5'6	5.1017	4.7645
32	66.99	4:2	049	.4610	22' 45'	0.0730	3.0030
33	67.22	4:2	047	.4639	22' 44'	1.6746	1.5619
34	67.43	4:2	048 075	.4651	22' 45' 1 24'6	0.7199	0.6723
35	67.6	4:2	065 062	.4663	230' 1 2356	0.0000	0.0000
36	67.84	3:0	035	.4730	33'4	0.1205	0.1360
37	68.10	5:4 0:2	104 044	.4832	22' 46' 1 22' 35'	2.0620	1.9235
38	68.43	5:0 4:2	037 042	.4870	340' 1 22' 30' 1 236'6	2.0319	1.9134
39	69.15	4:2	060 071	.4990	23' 34' 1 230'6 1 23'0'6	2.7000	2.5967
40	69.25	4:1	060	.5040	23' 45' 7	0.0000	0.0000
41	69.39	5:4	096	.5057	22' 366'	0.2236	0.1060
42	69.68	4:2	040	.5102	22' 33'	0.2407	0.2200
43	70.12	5:3 4:1	103 057	.5155	22' 45'6' 1 233'5	0.0990	0.0911
44	70.45	5:3 4:1	100 067	.5212	22' 44'6' 1 23'0'5	0.3505	0.3127
45	70.79	4:1	050 063	.5267	233'5' 1 234'5	0.0760	0.0720
46	71.15	4:1 5:0	074 094	.5340	240'5' 1 22' 356'	1.1323	1.0049
47	71.36	4:1	070 061	.5407	23' 4'5' 1 2' 40'5' 1 23457	2.3600	2.2047
48	71.62	4:1 5:3	066 095	.5447	23' 44' 1 22' 356' 1 22' 35'6	0.5069	3.7042
49	72.19	5:3 4:1	091 090	.5549	22' 34'6' 1 22' 3'06' 1 233'0	0.7391	0.6239
50	72.81	4:1	056 060	.5676	233' 4' 1 2300'	0.0409	0.7053
51	73.25	6:4 5:0	155 084	.5666	22' 40'66' 1 22' 34'0' 1 22' 355'	0.7607	0.6320
52	73.49	5:3	049	.5779	22' 346'	0.0000	0.0000
53	73.66	5:2	101 090	.5814	22' 30'5' 1 22' 435'	1.3414	1.2070
54	74.05	5:2	099	.5800	22' 44'5	1.2273	1.0254
55	74.49	6:4 5:2	150 112	.5969	22' 30'66' 1 233'56' 1 23' 40'6	0.1349	0.1124
56	74.8	5:2	083 109	.6024	22' 33'5' 1 233'06	0.1499	0.1219
57	75.21	6:4 5:2	152 097	.6042	22' 3566' 1 22' 340' 1 22' 3'03	0.4611	0.3031
58	75.32	5:2	087 111	.6175	22' 345' 1 233'55' 1 2300'6	0.3290	0.2715
59	75.83	5:2	085 116	.6224	22' 344' 1 230567	0.2114	0.1766
60	76.13	6:4	136	.6257	22' 33'66'	0.0000	0.0000
61	76.3	4:0 5:2	077 110	.6293	33' 40' 1 233'0'6	2.2467	1.0771
62	76.74	6:3	154	.6349	22' 40'56'	0.0410	0.0310
63	77.02	5:2	082	.6453	22' 33'0	0.1200	0.1069
64	77.52	6:3	151	.6499	22' 355'6	0.1743	0.1482
65	77.75	6:3 5:1	135 120	.6563	22' 33'56' 1 2' 300'5	0.2003	0.1620
66	77.9	6:3	144	.6584	22' 305'6	0.0000	0.0000
67	78.01	5:1 6:0	107 100	.6626	233' 4'5' 1 230'40' 1 22' 30'56	0.1491	0.1491
68	78.25	5:1	123	.6656	2' 300'5	0.0000	0.0000
69	78.37	6:3 5:1	149 114	.6672	22' 30'5'6' 1 23' 40'5' 1 233'05	2.1902	1.7037
70	78.55	6:3	139 140	.6707	22' 300'6' 1 22' 300'6'	0.0000	0.0000
71	79.17	6:3 5:1	134 103	.6796	22' 33'56' 1 22' 3056' 1 2300'5	0.1264	0.1034
72	79.46	5:1 6:0	124 131	.6871	22' 33'05' 1 22' 33'46' 1 22' 30'55'	0.0906	0.0405
73	79.47	6:2	146 161	.6955	22' 30'55' 1 233'05'6	0.1607	0.1214
74	80.34	6:3 5:1	132 105	.7035	22' 33'46' 1 233'00'	0.3663	0.2532
75	80.49	6:2	153	.7036	22' 40'53'	1.6060	1.2135
76	81.29	6:2	160	.7068	23' 40'5'6	0.0939	0.0709
77	81.5	6:2	141	.7203	22' 3455'	0.0939	0.0710
78	81.7	7:4	179	.7205	22' 33'566'	0.0000	0.0000
79	82.04	6:2	130	.7200	22' 33'05'	0.1039	0.0705
80	82.17	6:2	137	.7129	22' 340'5	0.0949	0.0717
81	82.35	7:4	176	.7305	22' 33'466'	0.0000	0.0000
82	82.74	6:2	138 163	.7403	22' 340'5' 1 233'0'56' 1 02	0.7312	0.5525
83	83.05	6:2	150	.7429	233' 40'6	0.1519	0.1148
84	83.47	6:2	129	.7501	22' 33'05	0.0042	0.0636
85	84	7:3	174	.7537	22' 35'55'6	0.0000	0.0000
86	84.17	6:2	166	.7572	2300' 36	0.0042	0.0032
87	84.6	7:3	175	.7611	22' 33'05'6	0.0000	0.0000
88	84.73	7:3	187 182	.7653	22' 30'55'6' 1 22' 300'56'	0.0091	0.0615
89	85.1	6:2	128	.7761	22' 33'00'	0.1029	0.1302
90	85.4	7:3	184	.7720	22' 340'5'6	0.0000	0.0000
91	85.74	6:1	167	.7814	23' 40'53'	0.1303	0.0904
92	86.36	7:3	185	.7840	22' 3455'6	0.0053	0.0037
93	86.99	7:3	174 181	.7965	22' 33'056' 1 22' 300'56	0.0555	0.0304
94	87.05	7:3	177	.8031	22' 33'0'56	0.0014	0.0204
95	87.99	7:3 6:1	171 156	.8105	22' 33'00'6' 1 230'00'5	0.1624	0.1193
96	88.46	8:4	202	.8009	22' 33'50'66'	0.0207	0.0131
97	88.55	6:1	157	.8184	233' 40'5'	0.0000	0.0000
98	88.91	7:3	173	.8152	22' 33'056	0.0000	0.0000
99	89.36	8:4	200 200	.8197	22' 33'05'66' 1 22' 300'566'	0.0000	0.0000
100	89.6	7:2	172 192	.8270	22' 33'05'6' 1 233'05'6	0.0306	0.0213
101	90.2	8:4	197	.8293	22' 33'00'66'	0.0000	0.0000
102	90.4	7:2	180	.8362	22' 340'30'	0.1413	0.0975
103	90.79	7:2	193	.8397	233' 4'55'6	0.0031	0.0021
104	91.44	7:2	191	.8447	233' 40'5'6	0.0000	0.0000
105	92.16	8:4	199	.8494	22' 33'4566'	0.0114	0.0072
106	92.87	7:2	170	.8740	22' 33'00'5	0.0073	0.0602
107	94.31	7:2	190	.8740	233' 40'36	0.0255	0.0176
108	95.63	8:3	198	.8845	22' 33'05'6	0.0000	0.0000
109	95.86	8:3	201	.8875	22' 33'0'55'6	0.0190	0.0126
110	96.74	8:3	196 203	.8935	22' 33'00'5'6' 1 22' 300'55'6	0.0259	0.0144
111	98.72	7:1	189	.9142	233' 40'35'	0.0000	0.0000
112	101.23	8:3	195	.9321	22' 33'00'56	0.0000	0.0000
113	101.87	9:4	200	.9320	22' 33'055'66'	0.0000	0.0000
114	103.29	9:4	207	.9423	22' 33'00'566'	0.0000	0.0000
115	105.2	8:2	194	.9620	22' 33'00'50'	0.0140	0.0094
116	106.77	8:2	205	.9670	233' 40'30'6	0.0000	0.0000
117	114.24	9:3	206	1.010	22' 33'00'55'6	0.0000	0.0000
118	126.35	10:4	209	1.050	22' 33'00'55'66'	0.0000	0.0000

CONCENTRATION = 2.860115
 TOTAL MICROMOLES = 0.0105
 AVERAGE MOLECULAR WEIGHT = 272.69987
 NUMBER OF CALIBRATED PEAKS FOUND = 118

N. B.
12B

100.7
100.2
100.0
19.7

5 - 20.245
20.469

6 - 21.182
21.507

10 - 22.010
22.010
22.010
22.010
22.010
22.010
22.010
22.010

14, 15 -

16 - 23.322
23.322
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21, 22 - 24.137
24.653

25, 26 - 24.964
24.964
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24.964
24.964
24.964
24.964
24.964

31, 32 - 25.771

37, 38 - 25.001

39 - 26.467
26.751

44 - 26.953
27.261

46, 47, 48 - 27.734

54 - 28.159
28.493

61 - 29.735
29.895

69 - 29.684
29.979
30.310

74, 75 - 30.614
30.920

82 - 31.237
31.521
31.771

89 - 32.117
32.459
32.764

95 - 33.154
33.592
33.833

102 - 34.020
34.338
34.652
34.958

106 - 35.323
35.643

109 - 36.293

110 - 36.941
37.407

? 111 - 38.134
38.618 int. std.

112 - 39.097
39.354

115 - 40.692

41.717
41.987

117 - 44.122

12B

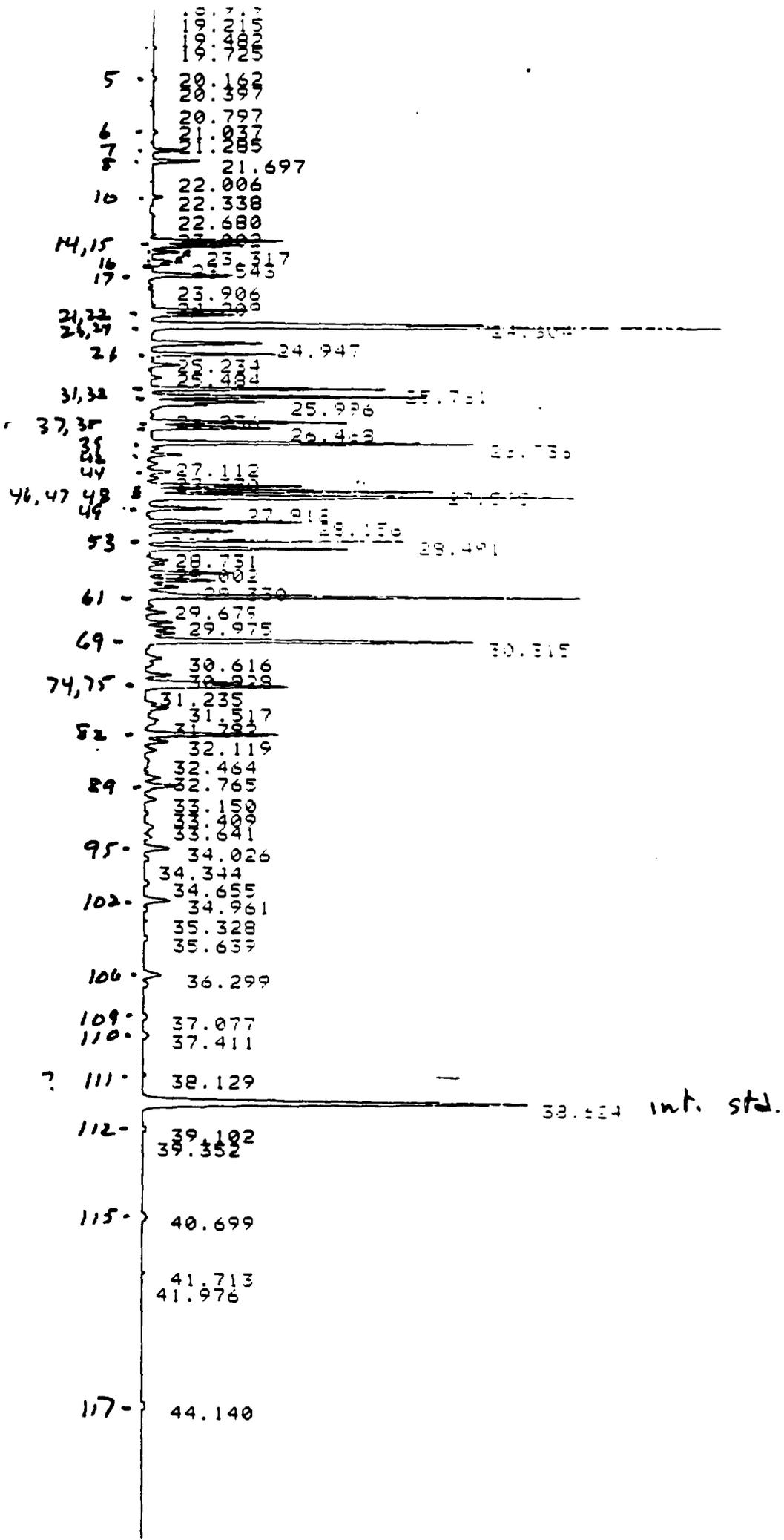
NB 12B

PEAK#	RET. TIME	T-CL:O-CL	IUPAC#	RTT	CONDENSERS	WEIGHT %	ROLE %
1	40.64	0:0	000	.0997	BIPHENYL	0.0000	0.0000
2	46.72	1:1	001	.1504		0.0000	0.0000
3	50.29	1:0	002	.1937		0.0000	0.0000
4	50.63	1:0	003	.1979		0.3939	0.3939
5	52.37	2:2	004 010	.2245	22' 1 26	1.0555	1.3504
6	54.8	2:1	007 009	.2566	24 1 25	0.2566	0.3253
7	55.63	2:1	006	.2709	25'	2.0045	2.6432
8	56.12	2:1	005 000	.2785	25 1 24'	2.4006	3.0401
9	57.39	2:0	014	.2973	35	0.1816	0.2303
10	57.8	3:3	019	.3045	22'6	1.2089	1.3194
11	58.68	3:2	030	.3165	246	0.0497	0.0546
12	59.2	2:0	011	.3238	33'	0.7136	0.9049
13	59.51	2:0	012 013	.3297	34 1 34'	0.4305	0.5459
14	59.85	2:2 2:0	010 015	.3387	22'5 1 44'	6.6036	7.6496
15	60.06	2:2	017	.3398	22'4	3.2340	3.6496
16	60.76	2:2	024 027	.3508	236 1 23'6	0.6450	0.7307
17	61.4	3:2	016 032	.3625	22'3 1 24'6	2.0538	2.2564
18	62.15	3:1	023	.3770	235	0.0058	0.0064
19	62.34	3:1 4:4	034 054	.3800	2'35 1 22'66'	0.0767	0.0810
20	62.78	3:1	029	.3820	245	0.0000	0.0000
21	63.03	3:1	026	.3911	23'5	5.2287	5.7350
22	63.22	3:1	025	.3937	23'4	3.2740	3.5979
23	63.66	3:1	031	.4024	24'5	5.1563	5.6650
24	63.78	3:1 4:3	028 030	.4031	244' 1 22'46	5.2790	5.7843
25	64.59	3:1 4:3	021 063	.4170	253' 1 254' 1 22'56'	1.6006	1.6677
26	65.03	3:1 4:3	022 031	.4267	234' 1 22'46'	0.5978	0.6234
27	65.50	4:3	045	.4534	22'36	0.4099	0.3972
28	65.84	3:1	036	.4579	33'5	0.0000	0.0000
29	66.11	4:3	046	.4650	22'36'	0.3964	0.3840
30	66.45	3:1	039	.4680	34'5	0.0000	0.0000
31	66.60	4:2	052 073	.4554	22'55' 1 23'5'6	10.0901	9.7759
32	67.02	4:2	049	.4610	22'45	7.9677	7.7196
33	67.20	4:2	047	.4634	22'44'	2.0265	2.7305
34	67.41	4:2	048 075	.4651	22'45 1 244'6	0.0000	0.0000
35	67.56	4:2	065 062	.4665	2346 1 2356	0.0009	0.0822
36	67.87	3:0	035	.4738	33'4	0.0777	0.0854
37	68.21	5:4 4:2	104 044	.4832	22'466' 1 22'35'	1.0910	1.0550
38	68.47	3:0 4:2	037 042	.4870	344' 1 22'34' 1 233'6	0.9734	0.9518
39	69.14	4:2	064 071	.4990	23'34 1 234'6 1 23'4'6	3.1172	3.0201
40	69.25	4:1	060	.5040	23'45' 7	0.0000	0.0000
41	69.45	5:4	096	.5057	22'366'	0.5278	0.4575
42	69.74	4:2	040	.5102	22'33'	0.1194	0.1157
43	70.15	5:3 4:1	105 057	.5155	22'45'6 1 233'5	0.2562	0.2425
44	70.54	5:3 4:1	100 067	.5212	22'44'6 1 23'4'5	0.4274	0.3867
45	70.83	4:1	058 063	.5267	233'5' 1 234'5	0.0308	0.0330
46	71.16	4:1 5:3	074 094	.5340	244'5 1 22'356'	0.4782	0.4326
47	71.42	4:1	070 061	.5407	23'4'5 : 2'345 1 24457	1.3089	1.2601
48	71.65	4:1 5:3	066 095	.5447	23'44' 1 22'356 1 22'35'6	2.3450	2.0430
49	72.22	5:3 4:1	091 098	.5549	22'34'6 1 22'3'46 1 234'4	1.5482	1.3550
50	72.84	4:1	056 060	.5676	253'4' 1 2344'	0.4672	0.4526
51	73.31	6:4 5:3	155 044	.5666	22'44'64' 1 22'33'61 22'359'	0.9749	0.8437
52	73.49	5:3	089	.5774	22'346'	0.0000	0.0000
53	73.73	5:2	101 090	.5814	22'34'5 1 22'433'	1.7053	1.6781
54	74.09	5:2	099	.5880	22'44'5	1.7791	1.5420
55	74.63	6:4 5:2	150 112	.5969	22'34'64' 1 233'56 1 23'44'6	0.9350	0.8444
56	74.84	5:2	083 109	.6029	22'33'5 1 233'46	0.1210	0.1056
57	75.25	6:4 5:2	152 097	.6062	22'3566' 1 22'345 1 22'3'45	0.4382	0.3734
58	75.59	5:2	087 111	.6175	22'345' 1 233'55' 1 2344'6	0.3030	0.2633
59	75.87	5:2	085 116	.6224	22'344' 1 230567	0.1704	0.1478
60	76.13	6:4	136	.6257	22'33'64'	0.4599	0.3605
61	76.37	4:0 5:2	077 110	.6295	33'44' 1 233'4'6	3.3939	2.9434
62	76.81	6:3	154	.6349	22'44'54'	0.1749	0.1571
63	77.09	5:2	082	.6454	22'33'4	0.0956	0.0828
64	77.56	6:3	151	.6499	22'355'6	0.2794	0.2190
65	77.82	6:3 5:1	155 124	.6563	22'33'56' 1 2'444'5	0.2868	0.2514
66	77.9	6:3	144	.6584	22'345'6	0.0000	0.0000
67	78.07	5:1 6:3	107 108	.6620	233'4'5 1 233'45' 1 22'34'56	0.2530	0.2132
68	78.25	5:1	123	.6658	2'344'5	0.0000	0.0000
69	78.44	6:3 5:1	149 110	.6672	22'34'5'6 1 23'44'5 1 233'45	3.0944	3.1426
70	78.55	6:3	139 140	.6707	22'344'6 1 22'344'6'	0.0000	0.0000
71	79.21	6:3 5:1	154 143	.6794	22'33'56' 1 22'3456' 1 2344'5	0.1529	0.1290
72	79.52	5:1 6:3	122 131	.6871	2'33'45 1 22'33'46 1 22'56'53'	0.0604	0.0578
73	80.02	6:2	146 161	.6955	22'34'55' 1 233'45'6	0.2475	0.1940
74	80.4	6:3 5:1	132 105	.7035	22'33'46' 1 233'44'	0.2036	0.2432
75	80.56	6:2	155	.7056	22'44'55'	3.3127	2.5968
76	81.36	6:2	168	.7068	23'44'5'6	0.0739	0.0579
77	81.57	6:2	141	.7203	22'3455'	0.0994	0.0779
78	81.75	7:4	179	.7204	22'33'366'	0.0954	0.0663
79	82.11	6:2	130	.7204	22'33'45'	0.1298	0.1018
80	82.22	6:2	137	.7329	22'344'5	0.1451	0.1130
81	82.55	7:4	176	.7300	22'33'466'	0.0000	0.0000
82	82.79	6:2	158 163	.7404	22'344'5' 1 233'4'56 1 42	1.0059	0.7885
83	83.1	6:2	158	.7429	233'44'6	0.2049	0.1606
84	84.51	6:2	129	.7501	22'33'45	0.0979	0.0767
85	84	7:3	170	.7537	22'33'55'6	0.0468	0.0329
86	84.24	6:2	164	.7572	2344'56	0.0092	0.0072
87	84.82	7:3	175	.7611	22'33'45'6	0.0083	0.0068
88	84.78	7:3	187 182	.7654	22'34'55'6 1 22'344'56'	0.2101	0.1532
89	85.17	6:2	128	.7761	22'33'44'	0.2354	0.1846
90	85.4	7:3	183	.7784	22'344'5'6	0.0000	0.0000
91	85.79	6:1	167	.7814	23'44'55'	0.2948	0.2342
92	86.04	7:3	185	.7848	22'3455'6	0.0000	0.0000
93	87.08	7:3	174 181	.7965	22'33'456' 1 22'344'56	0.0787	0.0568
94	87.5	7:3	177	.8031	22'33'4'56	0.0576	0.0413
95	88	7:3 6:1	171 156	.8105	22'33'44'6 1 233'44'5	0.2198	0.1649
96	88.44	8:0	202	.8060	22'33'38'64'	0.0000	0.0000
97	88.5	8:1	137	.8100	233'44'5'	0.0308	0.0239
98	88.91	7:3	173	.8154	233'44'56	0.0000	0.0000
99	89.56	8:4	200 204	.8197	22'33'45'64' 1 22'344'564'	0.0000	0.0000
100	89.6	7:2	172 192	.8270	22'33'455' 1 233'455'6	0.0473	0.0339
101	89.8	8:4	197	.8294	22'33'44'64'	0.0000	0.0000
102	89.4	7:2	180	.8362	22'344'55'	0.2100	0.1539
103	90.8	7:2	193	.8387	233'44'55'6	0.0181	0.0073
104	91.5	7:2	191	.8447	233'44'5'6	0.0043	0.0031
105	92.2	8:4	194	.8490	22'33'4564'	0.0179	0.0110
106	94.9	7:2	170	.8748	22'33'44'75	0.1374	0.0903
107	94.3	7:2	198	.8748	233'44'56	0.0482	0.0345
108	95.63	8:3	190	.8843	22'33'455'6	0.0000	0.0000
109	95.3	8:3	201	.8874	22'33'44'55'6	0.0472	0.0311
110	96.7	8:3	194 203	.8938	22'33'44'5'6 1 22'344'55'6	0.0710	0.0472
111	98.6	7:1	189	.9142	233'44'55'	0.0053	0.0040
112	101.1	8:3	199	.9321	22'33'44'56	0.0169	0.0111
113	101.87	9:4	200	.9380	22'33'455'64'	0.0000	0.0000
114	102.29	9:4	207	.9423	22'33'44'564'	0.0000	0.0000
115	105.2	8:2	194	.9620	22'33'44'55'	0.0560	0.0374
116	106.77	8:2	203	.9670	233'44'55'6	0.0000	0.0000
117	110.1	9:3	206	1.010	22'33'44'55'6	0.0900	0.0551
118	120.55	10:4	209	1.0500	22'33'44'55'64'	0.0000	0.0000

meth. 20 -
shown from
of 2-nd 4
mono's -
priority not
deducted by
GC/DC

- only guthy
6-5 CB -
single cell -
in right column

N. B.
14A



14A

N.B. 14A

PEARL	RET. TIME	T-CL:O-CL	IUPACO	RTT	CONDENSERS	WEIGHT %	MOLC %
1	40.64	0:0	000	.0997	BIPHENYL	0.0000	0.0000
2	46.65	1:1	001	.1544	2	0.3422	0.5217
3	50.37	1:0	002	.1937	3	1.9982	3.0461
4	50.63	1:0	003	.1975	4	0.3079	0.4694
5	52.37	2:2	004 010	.2249	22' 1 26'	0.7101	0.9259
6	54.77	2:1	007 009	.2566	24' 1 25'	0.1913	0.2470
7	55.63	2:1	006	.2709	23'	0.9632	1.2443
8	56.12	2:1	005 008	.2785	23' 1 24'	1.6132	2.0000
9	57.39	2:0	014	.2973	35'	0.0112	0.0144
10	57.70	2:0	019	.3045	22' 6'	0.4500	0.5316
11	58.06	2:2	030	.3165	24'	0.0124	0.0139
12	59.2	2:0	011	.3238	33'	0.3027	0.3902
13	59.51	2:0	012 013	.3297	34' 1 34'	0.1793	0.2312
14	59.82	2:2 2:0	018 015	.3387	22' 5' 1 44'	5.1973	6.4083
15	60.05	2:2	017	.3398	22' 6'	2.7471	3.0607
16	60.75	2:2	024 027	.3508	23' 1 23' 6'	0.4799	0.5311
17	61.4	3:2	016 052	.3625	22' 3' 1 24' 6'	1.7761	1.9081
18	62.15	3:1	023	.3770	23'	0.0340	0.0579
19	62.53	3:1 4:0	034 036	.3800	2' 35' 1 22' 66'	0.0373	0.0400
20	62.77	3:1	029	.3820	24'	0.0482	0.0539
21	63.01	3:1	026	.3911	23' 5'	1.5931	1.7796
22	63.21	3:1	025	.3937	23' 6'	1.5064	1.6020
23	63.65	3:1	031	.4024	24' 5'	0.3751	0.4074
24	63.78	3:1 4:3	028 030	.4031	24' 1 22' 46'	6.4592	7.4190
25	64.33	3:1 4:3	021 033	.4178	23' 1 23' 1 22' 56'	2.1404	2.1596
26	65.05	3:1 4:3	022 031	.4267	23' 1 22' 46'	1.1944	1.2664
27	65.54	4:3	045	.4334	22' 36'	0.6263	0.6170
28	65.91	3:1	036	.4379	33' 5'	0.0115	0.0129
29	66.11	4:3	046	.4450	22' 36'	0.4749	0.4678
30	66.45	3:1	039	.4488	34' 5'	0.0000	0.0000
31	66.66	4:2	052 073	.4534	22' 55' 1 23' 5' 6'	4.8062	4.7346
32	67.02	4:2	049	.4610	22' 45'	4.2517	4.1886
33	67.25	4:2	047	.4639	22' 44'	1.9793	1.9498
34	67.38	4:2	040 075	.4631	22' 45' 1 24' 6'	1.0056	0.9906
35	67.54	4:2	045 062	.4665	23' 46' 1 23' 56'	0.0019	0.0007
36	67.87	3:0	035	.4738	33' 6'	0.1368	0.1519
37	68.18	3:4 4:2	104 044	.4832	22' 46' 6' 1 22' 33'	2.6331	2.6105
38	68.47	3:0 4:2	057 042	.4870	34' 4' 1 22' 34' 1 23' 6'	2.7540	2.7356
39	69.17	4:2	044 071	.4990	25' 34' 1 23' 6' 1 23' 4' 6'	2.9125	2.8691
40	69.25	4:1	064	.5048	23' 45' 7'	0.0000	0.0000
41	69.43	3:4	096	.5037	22' 36' 6'	0.3157	0.2783
42	69.71	4:2	040	.5102	22' 33'	0.5073	0.4990
43	70.15	3:3 4:1	103 057	.5155	22' 45' 6' 1 23' 5'	0.1635	0.1574
44	70.51	3:3 4:1	100 067	.5212	22' 44' 6' 1 23' 4' 5'	0.4470	0.4112
45	70.8	4:1	058 063	.5267	23' 5' 1 23' 4' 5'	0.1829	0.1802
46	71.16	4:1 5:3	074 094	.5340	24' 4' 5' 1 22' 35' 6'	1.6010	1.5463
47	71.39	4:1	070 061	.5407	23' 4' 5' 1 2' 34' 5' 1 24' 57'	3.6159	3.5620
48	71.65	4:1 5:3	066 095	.5447	23' 44' 1 22' 35' 6' 1 22' 35' 6'	6.1019	5.4084
49	72.22	3:3 4:1	091 098	.5549	22' 54' 6' 1 22' 3' 4' 6' 1 23' 4' 6'	1.1648	1.1367
50	72.44	4:1	056 060	.5674	23' 4' 1 23' 44'	1.9073	1.8789
51	73.28	4:4 5:3	155 084	.5666	22' 44' 66' 1 22' 33' 6' 1 22' 35' 6'	1.2197	1.0609
52	73.49	3:3	089	.5779	22' 34' 6'	0.0000	0.0000
53	73.72	3:2	101 098	.5814	22' 34' 5' 1 22' 45' 6'	3.2158	2.8386
54	74.04	3:2	099	.5880	22' 44' 5'	2.5584	2.2549
55	74.66	6:4 5:2	158 112	.5969	22' 34' 66' 1 23' 56' 1 28' 44' 6'	0.2537	0.2236
56	74.84	3:2	083 109	.6029	22' 33' 5' 1 23' 4' 6'	0.2700	0.2430
57	75.25	6:4 5:2	152 097	.6062	22' 33' 66' 1 22' 34' 6' 1 22' 3' 4' 6'	0.9667	0.7946
58	75.56	5:2	087 111	.6175	22' 34' 5' 1 23' 55' 1 23' 4' 6'	0.5313	0.4680
59	75.9	3:2	085 116	.6224	22' 34' 4' 1 23' 46' 7'	0.2985	0.2586
60	76.14	4:4	136	.6257	22' 33' 66'	0.0000	0.0000
61	76.34	4:0 5:2	077 110	.6295	33' 44' 1 23' 4' 6'	3.6996	3.2684
62	76.70	6:3	154	.6349	22' 44' 56'	0.0738	0.0580
63	77.09	5:2	082	.6433	22' 33' 4'	0.1868	0.1646
64	77.55	6:3	151	.6499	22' 35' 6'	0.3349	0.2649
65	77.81	6:3 5:1	135 124	.6563	22' 33' 56' 1 2' 34' 4' 5'	0.3713	0.3046
66	77.9	6:3	144	.6580	22' 34' 5' 6'	0.0000	0.0000
67	78.07	3:1 6:3	107 108	.6628	23' 4' 5' 1 23' 45' 1 22' 34' 56'	0.3640	0.3280
68	78.25	5:1	173	.6650	2' 34' 4' 5'	0.0000	0.0000
69	78.43	6:3 5:1	149 118	.6672	22' 34' 5' 6' 1 23' 44' 5' 1 23' 45'	4.3668	3.5338
70	78.55	6:3	139 140	.6707	22' 34' 4' 6' 1 22' 34' 4' 6'	0.0000	0.0000
71	79.21	6:3 5:1	134 143	.6796	22' 33' 56' 1 22' 34' 56' 1 23' 44' 5'	0.2284	0.1971
72	79.5	3:1 6:3	122 131	.6871	2' 33' 45' 1 22' 33' 46' 1 22' 33' 55' 6'	0.0943	0.0797
73	80.01	6:2	146 161	.6955	22' 34' 55' 1 23' 45' 6'	0.3464	0.2761
74	80.30	6:3 5:1	132 105	.7035	22' 33' 46' 1 23' 44' 6'	0.4995	0.4355
75	80.53	6:2	153	.7036	22' 44' 55'	3.2250	2.5711
76	81.43	6:2	160	.7060	23' 44' 5' 6'	0.0729	0.0581
77	81.54	6:2	141	.7204	22' 34' 55'	0.1470	0.1172
78	81.72	7:4	179	.7205	22' 33' 56' 6'	0.0742	0.0540
79	82.11	6:2	130	.7284	22' 33' 49'	0.1635	0.1319
80	82.44	6:2	137	.7329	22' 34' 4' 5'	0.1566	0.1240
81	82.55	7:4	176	.7385	22' 33' 46' 6'	0.0000	0.0000
82	82.76	6:2	138 163	.7483	22' 34' 4' 5' 1 23' 4' 56' 1 2'	1.3445	1.0716
83	83.12	6:2	158	.7429	23' 44' 6'	0.2442	0.1946
84	83.51	6:2	129	.7501	22' 33' 45'	0.1499	0.1195
85	84	7:3	178	.7537	22' 33' 53' 6'	0.0302	0.0220
86	84.2	6:2	164	.7572	23' 44' 56'	0.0009	0.0071
87	84.5	7:3	175	.7611	22' 33' 49' 6'	0.0040	0.0035
88	84.7	7:3	187 182	.7653	22' 34' 35' 6' 1 22' 34' 4' 56'	0.1626	0.1183
89	85.1	6:2	126	.7761	22' 33' 44'	0.2903	0.2310
90	85.4	7:3	183	.7720	22' 34' 4' 5' 6'	0.0000	0.0000
91	85.7	6:1	167	.7814	23' 44' 55'	0.2942	0.2361
92	86.44	7:3	185	.7840	22' 34' 38' 6'	0.0000	0.0000
93	87	7:3	174 181	.7965	22' 33' 45' 6' 1 22' 34' 4' 56'	0.1209	0.0802
94	87.5	7:3	177	.8031	22' 33' 4' 56'	0.0047	0.0410
95	88	7:3 6:1	171 156	.8105	22' 33' 44' 6' 1 23' 44' 5'	0.2996	0.2322
96	88.44	8:4	202	.8089	22' 33' 53' 66'	0.0000	0.0000
97	88.5	6:1	157	.8104	23' 44' 5'	0.0247	0.0197
98	88.91	7:3	173	.8152	22' 33' 45' 6'	0.0000	0.0000
99	89.36	8:4	200 204	.8197	22' 33' 45' 66' 1 22' 34' 4' 56' 6'	0.0000	0.0000
100	89.6	7:2	172 192	.8270	22' 33' 45' 5' 1 23' 45' 5' 6'	0.0523	0.0380
101	90.2	8:4	197	.8294	22' 33' 44' 66'	0.0000	0.0000
102	90.4	7:2	188	.8362	22' 34' 4' 55'	0.2413	0.1756
103	90.8	7:2	193	.8397	23' 4' 55' 6'	0.0079	0.0057
104	91.4	7:2	191	.8447	23' 44' 3' 6'	0.0037	0.0027
105	92.2	8:4	199	.8494	22' 33' 45' 66'	0.0148	0.0097
106	93.9	7:2	170	.8740	22' 33' 44' 5'	0.1588	0.1158
107	94.3	7:2	190	.8748	23' 44' 56'	0.0476	0.0346
108	95.63	8:3	198	.8845	22' 33' 45' 5' 6'	0.0000	0.0000
109	95.9	8:3	201	.8875	22' 33' 4' 55' 6'	0.0303	0.0236
110	96.8	8:3	196 203	.8935	22' 33' 44' 5' 6' 1 22' 34' 4' 55' 6'	0.0470	0.0320
111	98.72	7:1	189	.9142	23' 44' 55'	0.0000	0.0000
112	101.23	8:3	195	.9321	22' 33' 44' 56'	0.0000	0.0000
113	101.87	9:4	208	.9328	22' 33' 45' 55' 66'	0.0000	0.0000
114	103.29	9:4	207	.9423	22' 33' 44' 56' 6'	0.0000	0.0000
115	105.3	8:2	194	.9620	22' 33' 44' 55'	0.0376	0.0252
116	106.77	8:2	205	.9670	23' 44' 55' 6'	0.0000	0.0000
117	119.24	9:3	206	1.010	22' 33' 44' 55' 6'	0.0000	0.0000
118	126.85	10:4	209	1.050	22' 33' 44' 55' 66'	0.0000	0.0000

CONCENTRATION = 2.640816
TOTAL RICHMOLES = 0.0092
AVAILABLE MOLECULAR WEIGHT = 287.65237

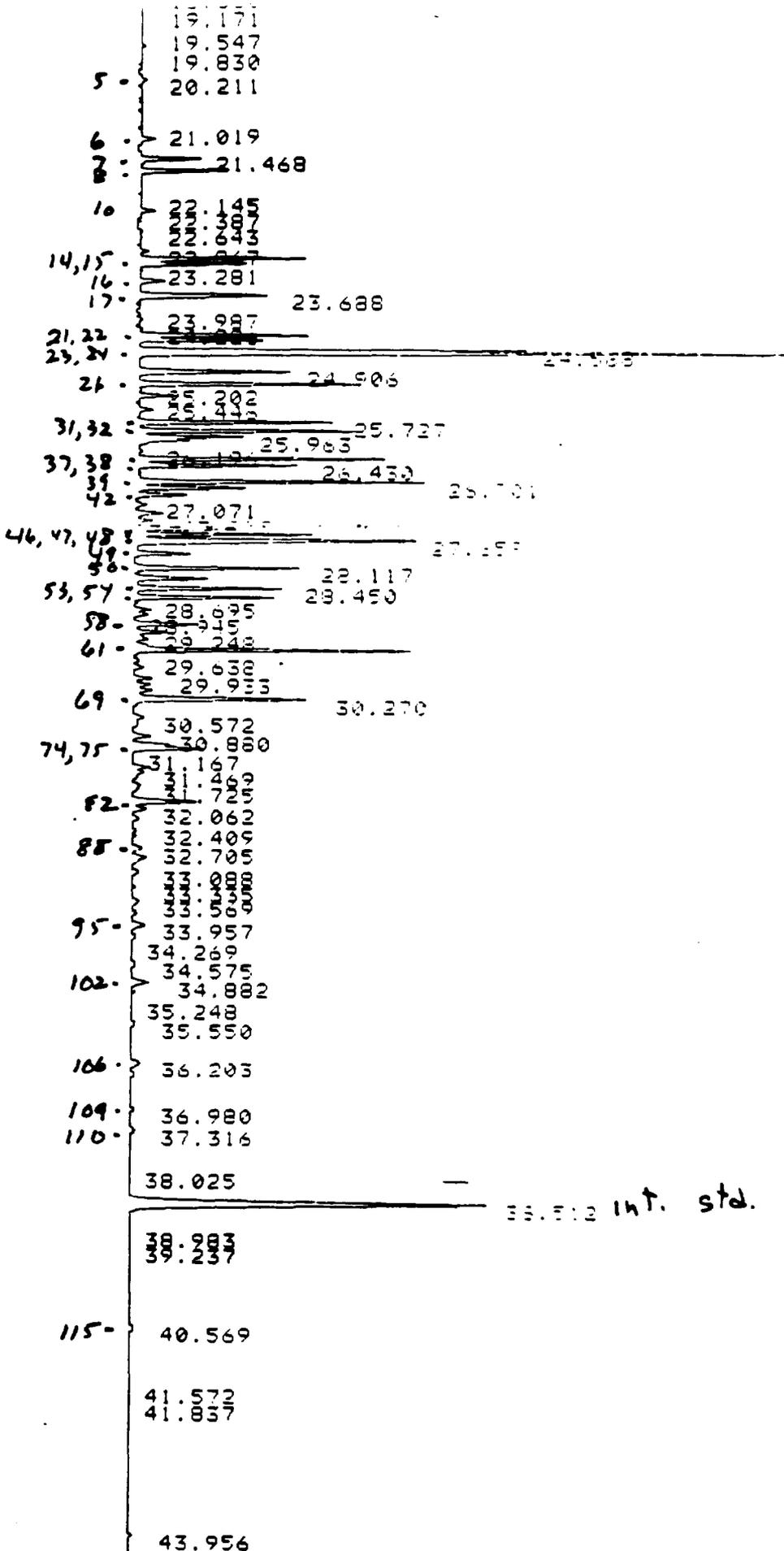
N.B. 14B

PEAK#	RET. TIME	T-CLIO-CL	IUPACH	RRT	CONDENSERS	WEIGHT %	ROLE #
1	49.64	010	000	.0997	BIPHENYL	0.0000	0.0000
2	46.64	111	001	.1300		0.0000	0.0000
3	50.12	110	002	.1937		0.0000	0.0000
4	50.66	110	003	.1875		0.0000	0.0000
5	52.14	212	004 010	.2245	22' 1 26	0.0007	0.0021
6	54.73	211	007 009	.2566	24' 1 25	0.0629	0.0633
7	55.61	211	006	.2709	23'	0.0000	0.0000
8	56.82	211	005 008	.2789	23' 1 24'	0.3956	0.4000
9	57.37	210	014	.2973	35	0.3223	0.3356
10	57.78	212	019	.3045	22'6	0.0700	0.0630
11	58.77	212	030	.3163	246	0.1700	0.1570
12	59.21	210	011	.3236	35'	0.0000	0.0000
13	59.52	210	012 013	.3297	34' 1 34'	0.0000	0.0000
14	59.78	312 2:0	018 015	.3387	22'5' 1 40'	0.0000	0.0000
15	60.06	312	017	.3390	22'4	0.7382	0.6500
16	60.47	312	024 027	.3500	236' 1 23'6	0.7725	0.6969
17	61.36	312	016 032	.3625	22'3' 1 24'6	0.0000	0.0000
18	62.16	311	023	.3770	235	9.2142	0.3180
19	62.43	311 4:4	034 034	.3800	2'35' 1 22'64'	0.0000	0.0000
20	62.78	311	029	.3820	245	0.0000	0.0000
21	63.04	311	026	.3911	23'5	0.5286	0.4769
22	63.22	311	025	.3937	23'4	2.1046	1.0908
23	63.66	311	031	.4024	24'5	1.2299	1.1044
24	63.76	311 4:3	028 030	.4031	240' 1 22'46	1.2214	1.0900
25	64.37	311 4:3	021 033	.4170	233' 1 234' 1 22'56'	0.9327	0.7600
26	64.83	311 4:3	022 031	.4267	236' 1 22'46'	0.1576	0.1351
27	65.55	413	043	.4334	22'36	0.1769	0.1408
28	65.84	311	036	.4379	33'5	0.0000	0.0000
29	66.07	413	046	.4450	22'36'	0.9450	0.7837
30	66.45	311	039	.4488	34'5	0.0000	0.0000
31	66.66	412	052 073	.4554	22'55' 1 23'5'6	1.2528	0.9968
32	67.03	412	049	.4610	22'45	1.0753	0.8553
33	67.26	412	047	.4639	22'44'	0.4567	0.3633
34	67.49	412	048 075	.4651	22'45' 1 244'6	0.2005	0.1627
35	67.52	412	063 062	.4663	2346' 1 2356	0.0717	0.0571
36	67.87	310	035	.4738	33'4	0.0000	0.0000
37	68.19	5:0 4:2	104 044	.4832	22'466' 1 22'35'	0.5389	0.4216
38	68.40	310 4:2	037 042	.4870	340' 1 22'30' 1 233'6	0.6506	0.5219
39	69.18	412	064 071	.4990	23'34' 1 234'6' 1 23'4'6'	0.5489	0.4367
40	69.25	411	060	.5040	23'45' 7	0.0000	0.0000
41	69.41	3:0	096	.5037	22'366'	0.1659	0.1181
42	69.72	4:2	040	.5102	22'33'	0.1176	0.0936
43	70.34	5:3 4:1	103 057	.5155	22'45'6' 1 233'5	0.0000	0.0000
44	70.49	5:3 4:1	100 067	.5212	22'44'6' 1 23'4'5	0.0000	0.0000
45	70.83	4:1	050 063	.5267	233'5' 1 234'5	0.0481	0.0319
46	71.17	4:1 3:3	074 094	.5300	244'5' 1 22'356'	0.3260	0.2528
47	71.4	4:1	070 061	.5407	23'4'5' 1 2'345' 1 23437	0.5982	0.4759
48	71.64	4:1 3:3	066 095	.5447	23'44' 1 22'356' 1 22'39'6	0.9031	0.7446
49	72.26	5:3 4:1	091 098	.5549	22'34'6' 1 22'3'46' 1 234'4	0.2511	0.1662
50	72.88	4:1	036 060	.5676	233'4' 1 2344'	0.4198	0.3336
51	73.3	6:4 5:4	155 084	.5666	22'44'66' 1 22'33'61 1 22'395'	0.2727	0.2000
52	73.49	5:3	089	.5779	22'346'	0.0000	0.0000
53	73.71	5:2	101 090	.5814	22'34'5' 1 22'455'	0.5411	0.4051
54	74.12	5:2	099	.5880	22'44'5	0.3710	0.2800
55	74.67	6:4 5:2	150 112	.5969	22'34'66' 1 233'56' 1 23'44'6	0.0290	0.226
56	74.85	5:2	083 109	.6029	22'33'5' 1 233'46	0.0329	0.231
57	75.26	6:4 5:2	152 097	.6062	22'3566' 1 22'345' 1 22'3'43	0.1506	0.1066
58	75.57	5:2	087 111	.6173	22'345' 1 233'55' 1 2344'6	0.1304	0.0983
59	75.86	5:2	085 116	.6224	22'344' 1 234567	0.1111	0.0791
60	76.13	6:4	136	.6257	22'33'66'	0.0000	0.0000
61	76.25	4:0 5:2	077 110	.6295	33'44' 1 233'4'6	0.6131	0.463
62	76.79	6:3	134	.6349	22'44'56'	0.0000	0.0000
63	77.08	5:2	082	.6453	22'33'4	0.0473	0.0336
64	77.57	6:3	131	.6499	22'355'6	0.0595	0.043
65	77.78	6:3 5:1	135 124	.6563	22'33'56' 1 2'344'5	0.0000	0.0000
66	77.9	6:3	144	.6584	22'345'6	0.0000	0.0000
67	78.09	5:1 6:4	107 108	.6628	233'4'5' 1 233'45' 1 22'34'56	0.0631	0.0435
68	78.25	5:1	123	.6650	2'344'5	0.0000	0.0000
69	78.45	6:3 5:1	149 118	.6672	22'34'5'6' 1 23'44'5' 1 233'45	0.6635	0.4977
70	78.55	6:3	139 148	.6707	22'344'6' 1 22'344'6'	0.0000	0.0000
71	79.23	6:3 5:1	134 143	.6796	22'33'56' 1 22'3456' 1 2344'5	0.0201	0.0196
72	79.53	5:1 6:3	122 131	.6871	2'33'45' 1 22'33'46' 1 22'33'55'	0.0000	0.0000
73	80.03	6:2	146 161	.6955	22'34'55' 1 233'45'6	0.0433	0.0379
74	80.3	6:3 5:1	132 105	.7033	22'33'46' 1 233'44'	0.1321	0.0930
75	80.5	6:2	153	.7034	22'44'55'	0.5343	0.3939
76	81.3	6:2	160	.7068	23'44'5'6	0.0613	0.0423
77	81.5	6:2	141	.7203	22'3455'	0.0510	0.0285
78	81.7	7:4	179	.7205	22'33'566'	0.0000	0.0000
79	82.09	6:2	130	.7204	22'33'45'	0.0000	0.0000
80	82.2	6:2	137	.7329	22'344'5	0.0000	0.0000
81	82.35	7:4	176	.7305	22'33'466'	0.0000	0.0000
82	82.7	6:2	130 163	.7483	22'344'5' 1 233'4'56' 1 +2	0.2500	0.1661
83	83.1	6:2	130	.7429	233'44'6	0.0345	0.0222
84	83.49	6:2	129	.7501	22'33'45	0.0000	0.0000
85	84	7:3	170	.7537	22'33'55'6	0.0000	0.0000
86	84.28	6:2	166	.7572	2344'56	0.0000	0.0000
87	84.4	7:3	173	.7611	22'33'45'6	0.0000	0.0000
88	84.7	7:3	187 182	.7653	22'34'55'6 1 22'344'56'	0.0301	0.0244
89	85.1	6:2	128	.7761	22'33'44'	0.0515	0.0322
90	85.4	7:3	183	.7720	22'344'5'6	0.0000	0.0000
91	85.78	6:1	167	.7814	23'44'55'	0.0000	0.0000
92	86.44	7:3	185	.7848	22'3455'6	0.0000	0.0000
93	87.83	7:3	174 181	.7963	22'33'456' 1 22'344'86	0.0000	0.0000
94	87.97	7:3	177	.8031	22'33'4'56	0.0000	0.0000
95	88	7:3 6:1	171 156	.8105	22'33'44'6' 1 233'44'5	0.0523	0.0272
96	88.44	8:4	202	.8007	22'33'55'66'	0.0000	0.0000
97	88.55	6:1	157	.8184	233'44'5'	0.0000	0.0000
98	88.91	7:3	173	.8152	22'33'456	0.0000	0.0000
99	89.36	8:4	200 204	.8197	22'33'45'66' 1 22'344'566'	0.0000	0.0000
100	89.68	7:2	172 192	.8278	22'33'455' 1 233'455'6	0.0000	0.0000
101	90.2	8:4	197	.8293	22'33'44'66'	0.0000	0.0000
102	90.49	7:2	188	.8362	22'344'55'	0.0000	0.0000
103	90.91	7:2	193	.8397	233'4'55'6	0.0000	0.0000
104	91.44	7:2	191	.8447	233'44'5'6	0.0000	0.0000
105	92.13	8:4	199	.8494	22'33'4566'	0.0000	0.0000
106	92.8	7:2	178	.8748	22'33'44'5	0.0139	0.0042
107	94.44	7:2	198	.8748	233'44'56	0.0000	0.0000
108	95.63	8:3	198	.8843	22'33'455'6	0.0000	0.0000
109	95.99	8:3	201	.8873	22'33'4'55'6	0.0000	0.0000
110	96.85	8:3	196 203	.8935	22'33'44'5'6 1 22'444'55'6	0.0000	0.0000
110	98.72	7:1	189	.9142	233'44'55'	0.0000	0.0000

CONCENTRATION = 4.782611
 TOTAL MICROMOLS = 0.0202

AVERAGE MOLECULAR WEIGHT = 242.31413
 NUMBER OF CALIBRATED PEAKS FOUND = 111

N. B
17A



17A

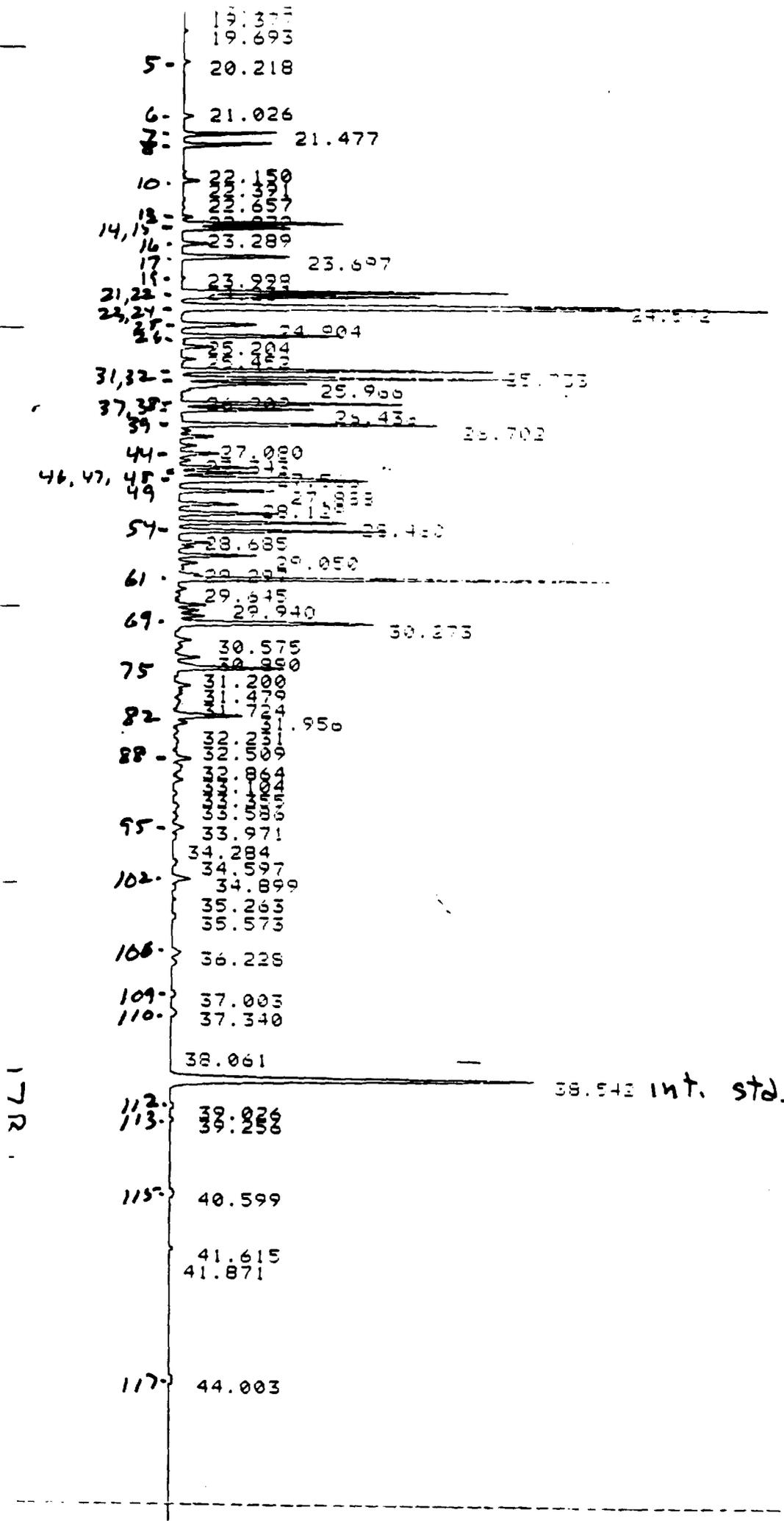
N.B. 17A

PEAK#	RET. TIME	F-CL:O-CL	IUPAC#	RTT	CONGENERS	WEIGHT %	ROLE %
1	40.62	0:0	800	.8997	81PHENYL	0.0000	0.0000
2	46.63	1:1	801	.1344	2	0.3909	0.3764
3	50.08	1:0	802	.1937	3	1.1410	1.6028
4	50.59	1:0	803	.1975	4	0.1759	0.2593
5	52.36	2:2	804 810	.2205	22' 1 26	1.1720	1.4615
6	54.77	2:1	807 809	.2546	24' 1 25	0.6290	0.7845
7	55.6	2:1	806	.2709	23'	2.3446	2.9241
8	56.12	2:1	805 808	.2785	23' 1 24'	3.1907	3.9889
9	57.46	2:0	814	.2974	35	0.0637	0.0794
10	57.77	3:3	819	.3049	22'6	0.0442	0.6982
11	58.66	4:2	820	.3165	246	0.0370	0.0409
12	59.82	4:0	811	.3230	33'	0.2593	0.3234
13	59.49	2:0	812 813	.3297	34' 1 30'	0.5122	0.6387
14	59.82	4:2 2:0	818 819	.3347	22'9' 1 44'	6.4245	7.2512
15	60.83	4:2	817	.3398	22'4	3.6265	3.9163
16	60.73	5:2	824 827	.3508	256' 1 23'6	0.6289	0.6799
17	61.35	5:2	816 832	.3625	22'3' 1 24'6	3.0737	3.3210
18	62.13	5:1	823	.3770	255	0.0078	0.0084
19	62.34	5:1 4:0	834 854	.3800	2'35' 1 22'66'	0.1023	0.1062
20	62.75	5:1	829	.3820	245	0.0551	0.0595
21	63.01	5:1	826	.3911	25'5	2.7915	2.9729
22	64.14	5:1	825	.3937	25'4	2.2605	2.4422
23	63.65	5:1	831	.4024	24'5	5.3088	5.7351
24	64.76	5:1 4:5	830 850	.4031	244' 1 22'46	7.4260	8.4331
25	64.51	5:1 4:5	821 833	.4170	253' 1 234' 1 22'56'	2.8967	2.7877
26	65.03	5:1 4:5	822 851	.4267	254' 1 22'46'	2.1039	2.2396
27	65.52	4:3	845	.4334	22'36	0.0463	0.0463
28	65.91	5:1	836	.4379	33'5	0.0263	0.0284
29	66.49	4:3	846	.4454	22'36'	0.6281	0.5985
30	66.5	5:1	839	.4488	34'5	0.0336	0.0363
31	66.64	4:2	852 873	.4554	22'55' 1 23'5'6	4.4960	4.2838
32	67.03	4:2	849	.4610	22'45	3.9415	3.7855
33	67.26	4:2	847	.4639	22'44'	1.8447	1.7576
34	67.39	4:2	848 875	.4651	22'45' 1 240'6	0.9782	0.9321
35	67.52	4:2	865 862	.4865	2346' 1 2356	0.0463	0.0432
36	67.86	5:0	835	.4738	33'4	0.1594	0.1679
37	68.19	5:4 4:2	104 844	.4832	22'466' 1 22'35'	3.3955	3.2515
38	68.45	5:0 4:2	837 842	.4870	344' 1 22'34' 1 234'6	3.1116	2.9894
39	68.95	4:2	864 871	.4990	25'34' 1 230'6 1 23'4'6	0.0274	0.0264
40	69.25	4:1	868	.5040	23'45' 7	0.0000	0.0000
41	69.41	5:1	896	.5057	22'346'	2.8853	2.4594
42	69.72	4:2	840	.5102	22'33'	0.8048	0.7687
43	70.11	5:3 4:1	103 857	.5155	22'45'6' 1 233'9	0.1803	0.1679
44	70.48	5:3 4:1	100 867	.5212	22'44'6' 1 233'4'5	0.5822	0.5242
45	70.81	4:1	858 863	.5267	233'5'	0.2594	0.2434
46	71.15	4:1 5:3	874 894	.5348	244'5' 1 22'556'	1.4639	1.3024
47	71.48	4:1	870 841	.5407	23'45' 1 2'305' 1 24497	2.1958	2.0893
48	71.64	4:1 5:3	866 895	.5447	23'44' 1 22'556' 1 22'35'6	4.3872	3.7583
49	72.21	5:3 4:1	891 898	.5549	22'34'6' 1 22'3'46' 1 234'4	0.9399	0.8994
50	72.86	4:1	856 864	.5674	233'4' 1 2344'	1.9367	1.8472
51	73.27	6:4 5:3	155 884	.5666	22'44'46' 1 22'35'6' 1 22'355'	1.0000	0.9272
52	73.49	5:3	889	.5779	22'346'	0.0000	0.0000
53	73.72	5:2	101 890	.5814	22'34'5' 1 22'495'	2.0330	1.7500
54	74.08	5:2	899	.5880	22'44'5	1.7382	1.4748
55	74.69	5:4 5:2	150 112	.5949	22'34'44' 1 234'56' 1 26'44'6	0.1806	0.1589
56	74.83	5:2	883 889	.6029	22'33'5' 1 233'46	0.2783	0.2546
57	75.2	5:4 5:2	152 897	.6042	22'5566' 1 22'349' 1 22'3'45	0.7369	0.6246
58	75.3	5:2	887 111	.6175	22'345' 1 233'55' 1 2344'6	0.2434	0.2273
59	75.8	5:2	885 116	.6224	22'344' 1 234567	0.1222	0.1041
60	76.13	4:4	136	.6257	22'33'66'	0.0000	0.0000
61	76.3	4:0 5:2	877 110	.6295	33'44' 1 233'4'6	2.4760	2.1105
62	76.7	4:3	154	.6344	22'44'56'	0.0599	0.0459
63	77	5:2	882	.6433	22'33'4	0.0460	0.0733
64	77.5	4:3	151	.6499	22'55'6	0.2401	0.1913
65	77.8	4:3 5:1	135 124	.6562	22'33'56' 1 2'344'5	0.2310	0.1833
66	77.9	4:3	144	.6584	22'345'6	0.0000	0.0000
67	78	5:1 6:3	107 108	.6628	233'4'5' 1 233'45' 1 22'34'56	0.2925	0.2416
68	78.25	5:1	123	.6658	2'344'5	0.0000	0.0000
69	78.4	4:3 5:1	149 118	.6672	22'34'5'6' 1 23'44'5' 1 233'45	2.3465	1.8621
70	78.55	4:3	139 140	.6707	22'344'6' 1 22'344'6'	0.0000	0.0000
71	79.2	4:3 5:1	134 143	.6796	22'33'56' 1 22'3496' 1 2344'5	0.1671	0.1393
72	79.4	5:1 6:3	122 131	.6871	2'33'45' 1 22'33'46' 1 22'33'55'	0.6620	0.0587
73	80	4:2	146 161	.6935	22'34'55' 1 233'45'6	0.2403	0.1852
74	80.3	4:3 5:1	132 185	.7035	22'33'46' 1 233'44'	0.2081	0.1687
75	80.5	4:2	153	.7036	22'44'55'	1.8745	1.4451
76	81.3	4:2	168	.7068	23'44'5'6	0.1237	0.0953
77	81.5	4:2	141	.7203	22'3455'	0.0731	0.0579
78	81.7	7:4	179	.7205	22'33'566'	0.0666	0.0468
79	82	4:2	138	.7284	22'33'45'	0.0925	0.0713
80	82.2	4:2	137	.7329	22'344'5	0.0000	0.0000
81	82.35	7:4	176	.7385	22'33'466'	0.0000	0.0000
82	82.7	4:2	138 163	.7408	22'344'5' 1 233'4'56' 1 2	0.7104	0.5477
83	83	4:2	158	.7429	233'44'6	0.1474	0.1133
84	83.4	4:2	129	.7501	22'33'45	0.0774	0.0597
85	83.9	7:3	178	.7537	22'33'55'6	0.0260	0.0189
86	84.25	4:2	164	.7572	2344'56	0.0000	0.0000
87	84.4	7:3	175	.7611	22'33'45'6	0.0000	0.0000
88	84.7	7:3	187 182	.7654	22'34'55'6' 1 22'344'56'	0.1161	0.0817
89	85.1	4:2	128	.7761	22'33'44'	0.1524	0.1175
90	85.4	7:3	143	.7728	22'344'5'6	0.0000	0.0000
91	85.7	6:1	167	.7814	23'44'55'	0.1460	0.1129
92	86.0	7:3	183	.7848	22'3455'6	0.0104	0.0073
93	86.4	7:3	174 181	.7965	22'33'456' 1 22'444'56	0.0300	0.0415
94	87.4	7:3	177	.8031	22'33'4'56	0.0367	0.0259
95	87.9	7:3 6:1	171 136	.8105	22'33'44'6' 1 233'44'5	0.1515	0.1136
96	88.4	4:0	202	.8089	22'33'55'66'	0.0182	0.0118
97	88.7	6:1	157	.8184	233'44'5'	0.0035	0.0027
98	88.91	7:3	173	.8134	22'33'456	0.0000	0.0000
99	89.2	4:0	208 204	.8197	22'33'45'66' 1 22'444'566'	0.0000	0.0000
100	89.68	7:2	172 192	.8276	22'33'455' 1 233'455'6	0.0000	0.0000
101	90.3	4:0	197	.8293	22'33'44'66'	0.1401	0.0987
102	90.49	7:2	188	.8362	22'344'55'	0.0000	0.0000
103	90.91	7:2	193	.8397	233'4'55'6	0.0000	0.0000
104	91.3	7:2	191	.8447	233'44'5'6	0.0029	0.0020
105	92	4:0	199	.8494	22'33'4566'	0.0184	0.0119
106	93.8	7:2	178	.8748	22'33'44'5	0.0005	0.0566
107	94.3	7:2	198	.8748	233'44'56	0.0296	0.0209
108	95.8	8:3	196	.8845	22'33'455'6	0.0178	0.0113
109	96.2	8:3	201	.8875	22'33'4'55'6	0.0000	0.0000
110	96.6	8:3	194 203	.8935	22'33'44'5'6' 1 22'344'55'6	0.0364	0.0234
111	98.3	7:1	189	.9142	233'44'55'	0.0042	0.0030
112	101.7	8:3	195	.9321	22'33'44'56	0.0050	0.0033
113	101.7	9:4	208	.9328	22'33'455'66'	0.0010	0.0011
114	103.4	9:4	207	.9424	22'33'44'566'	0.0016	0.0018
115	103.1	8:2	194	.9420	22'33'44'55'	0.0266	0.0172
116	106.1	8:2	205	.96'4	233'44'55'6	0.0000	0.0000
117	113.8	9:3	206	1.018	22'33'44'55'6	0.0472	0.0263
118	126.35	10:4	209	1.058	22'33'44'55'66'	0.0000	0.0000

CONCENTRATION = 2.746371
 TOTAL NICHROMULES = 0.0099
 AVERAGE MOLECULAR WEIGHT = 278.21794
 NUMBER OF CALIBRATED PEAKS FOUND = 118

N. B.

17B



17R

N.B. 17B

PLA#	RET. TIME	T-CL:O-CL	LUPAC#	RTT	CONCENTR	WEIGHT %	MOLE %
1	40.62	0:0	000	.0997	BIPHENYL	0.0000	0.0000
2	46.72	1:1	001	.1900	2	0.0000	0.0000
3	50.29	1:0	002	.1937	3	0.0000	0.0000
4	50.59	1:0	003	.1975	4	0.1609	0.2300
5	52.33	2:2	004 010	.2245	22' 1 26	1.1239	1.4133
6	54.74	2:1	007 009	.2266	24' 1 23	0.4234	0.5300
7	55.59	2:1	006	.2709	23'	3.1207	3.9273
8	56.09	2:1	005 008	.2705	23' 1 20'	2.9266	3.6734
9	57.44	2:0	014	.2973	35	0.0816	0.1024
10	57.77	2:1	019	.3045	22'6	0.7039	0.7655
11	58.02	2:2	030	.3163	24	0.0000	0.0000
12	59.04	2:0	021	.3230	53'	0.3164	0.3971
13	59.48	2:0	012 013	.3297	34' 1 30'	0.5436	0.6423
14	59.82	2:2 2:0	010 015	.3307	22'5' 1 00'	6.1000	7.0117
15	60	2:2	017	.3390	22'4	3.4074	3.7057
16	60.72	3:2	024 027	.3508	23' 1 23'6	0.5623	0.6115
17	61.35	3:2	016 032	.3625	22'3' 1 24'6	2.4853	2.7030
18	62.12	3:1	023	.3770	235	0.0071	0.0077
19	62.43	3:1 4:4	034 036	.3800	2'05' 1 22'66'	0.0000	0.0000
20	62.72	3:1	029	.3820	245	0.0056	0.0061
21	62.98	3:1	026	.3911	23'5	4.6749	5.0864
22	63.10	3:1	025	.3937	24'4	3.9424	4.2676
23	63.6	3:1	031	.4024	24'5	6.0700	6.6111
24	63.73	3:1 4:3	028 030	.4031	244' 1 22'46	6.0032	7.4660
25	64.48	3:1 4:3	021 033	.4170	233' 1 234' 1 22'56'	1.7056	1.6753
26	65	3:1 4:3	022 031	.4267	234' 1 22'46'	1.6090	1.7026
27	65.32	4:3	043	.4334	22'36	0.6757	0.6481
28	65.84	3:1	036	.4379	31'5	0.0000	0.0000
29	66.09	4:3	044	.4450	22'36'	0.3094	0.4003
30	66.45	3:1	039	.4480	34'5	0.0000	0.0000
31	66.63	4:2	052 073	.4554	22'55' 1 23'5'6	6.2090	6.0315
32	66.97	4:2	049	.4614	22'45	5.1212	4.9116
33	67.23	4:2	047	.4639	22'44'	2.2035	2.1133
34	67.36	4:2	040 075	.4651	22'45' 1 244'6	0.5360	0.5332
35	67.51	4:2	065 062	.4865	23'4' 1 2356	0.0856	0.0821
36	67.85	3:0	035	.4738	33'4	0.0663	0.0721
37	68.16	5:1 4:2	104 044	.4832	22'66' 1 22'35'	3.0201	2.9000
38	68.44	3:0 4:2	037 042	.4870	344' 1 22'34' 1 233'6	2.5001	2.5028
39	69.14	4:2	064 071	.4990	23'34' 1 234'6 1 23'4'6	2.4017	2.3034
40	69.25	4:1	060	.5044	25'45' 7	0.0000	0.0000
41	69.42	5:1	096	.5057	22'366'	0.3465	0.2973
42	69.69	4:2	048	.5102	22'33'	0.5302	0.5003
43	70.1	5:3 4:1	103 057	.5135	22'45'6 1 233'5	0.3064	0.2871
44	70.49	5:3 4:1	100 067	.5212	22'44'6 1 23'4'5	0.8325	0.7456
45	70.8	4:1	050 063	.5267	233'5' 1 234'5	0.1859	0.1703
46	71.11	4:1 5:3	074 074	.5340	244'5' 1 22'356'	0.7070	0.7056
47	71.37	4:1	070 061	.5407	23'4'5' 1 2'345' 1 25457	0.9331	0.8949
48	71.66	4:1 5:3	066 075	.5447	23'44' 1 22'356' 1 22'35'6	1.3137	1.1343
49	72.2	5:3 4:1	091 094	.5549	22'34'6' 1 22'3'46' 1 234'4	1.4901	1.2907
50	72.42	6:1	056 060	.5676	233'4' 1 2344'	0.7052	0.7531
51	73.24	6:1 5:3	155 084	.5666	22'44'66' 1 22'33'61 1 22'355'	1.4601	1.2450
52	73.49	5:3	089	.5779	22'346'	0.0000	0.0000
53	73.69	5:3	101 090	.5814	22'34' 5' 1 22'435'	2.2093	1.7642
54	74.61	5:2	099	.5880	22'44'5'	2.5669	2.2024
55	74.82	6:1 5:2	150 112	.5967	22'34'66' 1 233'56' 1 24'44'6	0.3100	0.3132
56	75.21	6:1 5:2	083 109	.6029	22'33'5' 1 233'46	0.3100	0.2639
57	75.24	6:1 5:2	152 097	.6062	22'3566' 1 22'340' 1 22'3'45	0.0502	0.7254
58	75.54	5:2	087 111	.6173	22'345' 1 233'55' 1 244'6	0.1627	0.1394
59	75.72	5:2	085 116	.6224	22'344' 1 234567	0.0494	0.0424
60	76.11	6:1	136	.6257	22'33'66'	0.3641	0.2023
61	76.37	4:0 5:2	077 110	.6295	33'44' 1 233'4'6	3.4709	2.7040
62	76.76	6:1	154	.6349	22'44'96'	0.1225	0.0950
63	77.04	5:2	084	.6433	22'33'4'	0.0252	0.0216
64	77.31	6:1	151	.6499	22'355'6	0.3973	0.3003
65	77.77	6:1 5:1	135 124	.6563	22'33'56' 1 2'344'5	0.2002	0.2302
66	77.9	6:1	144	.6584	22'345'6	0.0000	0.0000
67	78.03	5:1 6:3	107 104	.6620	233'4'5' 1 233'45' 1 22'34'56	0.3605	0.3164
68	78.25	5:1	123	.6650	2'344'5	0.0000	0.0000
69	78.39	6:1 5:1	149 118	.6672	22'34'5'6' 1 23'44'5' 1 233'45	2.7690	2.2123
70	78.55	6:1	139 140	.6707	22'34'6' 1 22'344'6'	0.0000	0.0000
71	79.17	6:1 5:1	134 143	.6746	22'33'56' 1 22'3'56' 1 2344'5	0.1065	0.1564
72	79.44	5:1 6:3	122 131	.6871	2'33'45' 1 22'33'46' 1 22'33'59'	0.0607	0.0563
73	80	6:2	146 161	.6955	22'34'55' 1 233'45'6	0.3492	0.2709
74	80.45	6:1 5:1	132 105	.7033	22'33'46' 1 233'44'	0.0000	0.0000
75	80.52	6:2	153	.7036	22'44'55'	3.1224	2.4229
76	81.24	6:2	160	.7066	21'44'0'6	0.1170	0.0914
77	81.5	6:2	143	.7101	22'3456'	0.0325	0.0252
78	81.71	7:1	174	.7105	22'33'566'	0.0907	0.0784
79	82.04	6:2	130	.7204	22'33'45'	0.0920	0.0714
80	82.2	6:2	157	.7329	22'340'3	0.0000	0.0000
81	82.45	7:1	174	.7305	22'33'466'	0.0000	0.0000
82	82.74	6:2	150 163	.7403	22'340'3' 1 233'4'56' 1 2	0.7395	0.5730
83	83.05	6:2	150	.7429	233'44'6	0.1345	0.1044
84	83.44	6:2	129	.7501	22'33'45	0.0336	0.0261
85	83.94	7:1	170	.7537	22'33'55'6	0.0305	0.0273
86	84.23	6:2	166	.7572	2344'56	0.0000	0.0000
87	84.8	7:1	175	.7611	22'33'45'6	0.0000	0.0000
88	84.76	7:1	187 182	.7653	22'34'55'6' 1 22'344'56'	0.1943	0.1374
89	85.1	6:2	120	.7761	22'33'44'	0.0445	0.0454
90	85.4	7:1	183	.7720	22'340'3'6	0.0000	0.0000
91	85.72	6:2	167	.7814	23'44'55'	0.1021	0.1413
92	86.44	7:1	189	.7844	22'3456'6	0.0000	0.0000
93	86.97	7:1	174 181	.7905	22'33'456' 1 22'344'56	0.0445	0.0316
94	87.46	7:1	177	.8031	22'33'4'56	0.0505	0.0217
95	87.98	7:1 6:1	171 156	.8105	22'33'44'6' 1 233'44'5	0.1104	0.0833
96	88.44	6:1	202	.8004	22'33'55'66'	0.0133	0.0007
97	88.55	6:1	157	.8104	133'44'5'	0.0000	0.0000
98	88.91	7:1	173	.8132	22'33'456	0.0000	0.0000
99	89.46	6:1	200 204	.8197	22'33'45'66' 1 22'344'566'	0.0000	0.0000
100	89.50	7:2	172 192	.8270	22'33'455' 1 233'455'6	0.0364	0.0254
101	90.4	6:1	197	.8293	22'33'44'66'	0.1444	0.0941
102	90.7	7:2	180	.8362	22'344'55'	0.0139	0.0000
103	90.91	7:2	175	.8397	23'44'55'6	0.0000	0.0000
104	91.44	7:2	181	.8447	23'44'5'6	0.0000	0.0000
105	92.15	6:1	199	.8494	22'33'4566'	0.0000	0.0000
106	92.9	7:2	170	.8740	22'33'44'5	0.0736	0.0521
107	94.2	7:2	190	.8740	233'44'56	0.0339	0.0240
108	95.0	6:3	201	.8875	22'33'455'6	0.0235	0.0153
109	95.99	6:3	201	.8875	22'33'455'6	0.0000	0.0000
110	96.6	6:3	196 203	.8933	22'33'44'5'6' 1 22'344'55'6	0.0000	0.0000
111	98.72	7:1	189	.9142	23'44'55'	0.0000	0.0000
112	101.23	6:1	191	.9321	22'33'44'56	0.0000	0.0000
113	101.87	6:1	200	.9324	22'33'455'66'	0.0000	0.0000
114	103.29	6:1	207	.9423	22'33'44'566'	0.0000	0.0000
115	105.1	6:2	194	.9620	22'33'44'55'	0.0337	0.0220
116	106.77	6:2	209	.9678	233'44'55'6	0.0000	0.0000
117	114.24	9:3	206	1.010	22'33'44'55'6	0.0000	0.0000
118	126.35	10:4	209	1.050	22'33'44'55'66'	0.0000	0.0000

mass spec. shows traces of all three mono's - but probably not being detected by GC/SC

N.B.

18A

18A

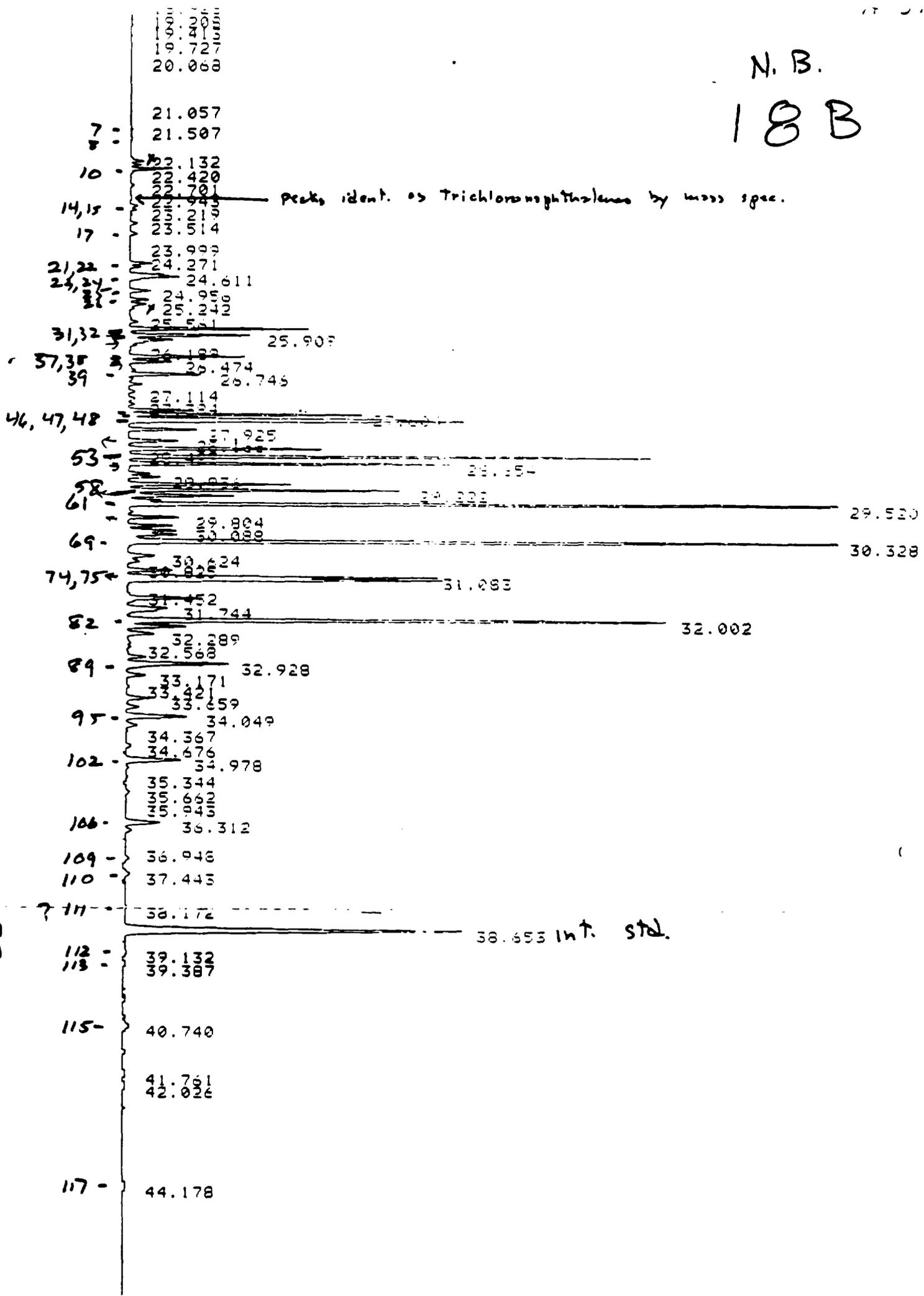
	17.711	
	19.716	
	20.059	
	21.157	
8 -	21.494	
	22.001	
	22.249	
	22.000	
14, 15 -	22.000	
	22.000	
17 -	23.400	
	23.719	
21, 22 -	24.000	
23, 24 -	24.300	
	24.000	
	24.940	
	25.111	
31, 32 -	25.901	
37, 38 -	26.100	
39	26.466	
	26.755	
	27.102	
46, 47, 48 -	27.500	
	27.915	
53 -	28.410	
	28.555	
58 -	29.021	
61	29.215	
	29.704	
69 -	30.000	
	30.316	
74, 75 -	30.620	
	31.072	
	31.447	
82 -	31.738	
	32.275	
89 -	32.500	
	32.910	
	33.159	
	33.400	
95 -	33.842	
	34.029	
	34.350	
102 -	34.653	
	34.970	
	35.331	
	35.651	
106 -	36.296	
109 -	36.951	
110 -	37.422	
111 -	38.137	
	38.625 int. std.	
112 -	39.109	
113 -	39.352	
115 -	40.710	
	41.719	
	42.008	
117 -	44.129	

N.B 18A

PCARR	RLI. TIME	T-CL:O-CL	IMPACH	RRY	CONDENSERS	WEIGHT S	MOLE S
1	40.59	0:0	000	.0997	IMPMENTL	0.0000	0.0000
2	46.57	1:1	001	.1304	2	0.2006	0.3206
3	50.19	1:0	002	.1937	3	0.5132	0.7553
4	50.61	1:0	003	.1975	4	0.8119	1.3302
5	52.13	2:2	004 010	.2245	22' 1 26'	0.0000	0.0000
6	54.69	2:1	007 009	.2566	20' 1 25'	0.0021	0.0503
7	55.57	2:1	006	.2789	23'	0.0215	0.0290
8	56.07	2:1	005 000	.2705	23' 1 20'	0.1013	0.1400
9	57.31	2:0	010	.2973	33'	0.7059	0.9701
10	57.79	0:3	019	.3003	22' 6'	1.6833	2.0105
11	58.63	0:2	030	.3163	24'	0.0720	0.0074
12	59.27	2:0	011	.3230	33'	0.6632	0.9217
13	59.52	2:0	012 013	.3297	30' 1 20'	0.0000	0.0000
14	59.79	3:2 2:0	018 015	.3307	22' 5' 1 00'	0.3001	0.6254
15	60	3:2	017	.3390	22' 6'	0.2019	0.3304
16	60.75	3:2	024 027	.3500	23' 1 23' 6'	0.3630	0.4350
17	61.32	3:2	016 032	.3625	22' 3' 1 20' 6'	0.2001	0.3363
18	62.3	3:1	023	.3770	23'	0.0120	0.0144
19	62.48	3:1 4:0	030 034	.3800	2' 35' 1 22' 66'	0.0394	0.0454
20	62.72	3:1	029	.3820	24'	0.0094	0.0113
21	62.97	3:1	026	.3911	23' 5'	0.2772	0.3326
22	63.15	3:1	025	.3937	23' 4'	0.1576	0.1892
23	63.59	3:1	031	.4024	20' 5'	0.5966	0.7163
24	63.72	3:1 4:3	028 030	.4031	24' 1' 1 22' 06'	0.0090	1.0604
25	64.47	3:1 4:3	021 033	.4170	23' 1' 1 23' 1 22' 56'	0.3509	0.6060
26	64.99	3:1 4:3	022 031	.4267	23' 1' 1 22' 06'	0.2522	0.2074
27	65.48	4:3	045	.4334	22' 36'	0.1104	0.1254
28	65.84	3:1	036	.4379	33' 5'	0.0000	0.0000
29	66.00	4:3	046	.4450	22' 36'	0.1310	0.1395
30	66.45	3:1	039	.4480	34' 5'	0.0000	0.0000
31	66.6	4:2	052 073	.4554	22' 55' 1 23' 5' 6'	4.3300	4.5927
32	66.90	4:2	049	.4610	22' 45'	2.1307	2.2034
33	67.22	4:2	047	.4639	22' 44'	0.7903	0.8454
34	67.55	4:2	048 075	.4651	22' 45' 1 24' 6'	0.3079	0.3260
35	67.73	4:2	065 062	.4863	23' 06' 1 23' 56'	0.0420	0.0445
36	67.87	5:0	035	.4730	33' 4'	0.0000	0.0000
37	68.15	5:0 4:2	104 044	.4832	22' 44' 1 22' 35'	2.0226	2.1309
38	68.43	3:0 4:2	037 042	.4870	34' 1' 1 22' 30' 1 23' 6'	1.0000	1.0769
39	69.13	4:2	064 071	.4990	23' 34' 1 23' 6' 1 23' 6' 6'	0.9200	0.9749
40	69.25	4:1	060	.5040	23' 43' 7'	0.0000	0.0000
41	69.42	5:0	096	.5037	22' 346'	0.0971	0.0920
42	69.67	4:2	040	.5104	22' 33'	0.2471	0.2592
43	70.09	5:3 4:1	103 057	.5153	22' 45' 6' 1 233' 9'	0.1903	0.2050
44	70.48	5:3 4:1	100 067	.5212	22' 44' 6' 1 23' 0' 5'	0.1612	0.1594
45	70.76	4:1	094 063	.5267	233' 5' 1 230' 5'	0.1231	0.1324
46	71.1	4:1 5:3	074 074	.5300	244' 5' 1 22' 356'	0.0070	0.0975
47	71.36	4:1	070 061	.5407	23' 4' 5' 1 2' 349' 1 24457'	1.3900	3.0055
48	71.62	4:1 5:3	066 075	.5447	23' 44' 1 22' 356' 1 22' 35' 6'	2.6439	2.5166
49	72.10	5:3 4:1	091 070	.5549	22' 30' 6' 1 22' 3' 46' 1 230' 4'	1.2191	1.1666
50	72.81	4:1	056 060	.5674	233' 4' 1 2344'	0.9276	0.9926
51	73.25	6:0 5:3	155 084	.5666	22' 44' 66' 1 22' 33' 6' 1 22' 350'	3.1404	2.9579
52	73.49	5:3	089	.5779	22' 346'	0.0000	0.0000
53	73.66	5:2	101 090	.5814	22' 30' 5' 1 22' 438'	0.2360	7.0012
54	74.07	5:2	099	.5800	22' 44' 5'	4.1290	3.9115
55	74.59	6:4 5:2	150 112	.5969	22' 30' 66' 1 233' 56' 1 23' 44' 6'	0.2500	0.2440
56	74.8	5:2	083 109	.6029	22' 33' 5' 1 233' 46'	0.6444	0.6402
57	75.21	6:4 5:2	152 097	.6062	22' 30' 66' 1 22' 340' 1 22' 3' 49'	2.0917	1.9701
58	75.5	5:2	087 111	.6175	22' 34' 5' 1 233' 55' 1 2344' 6'	2.7234	2.5794
59	75.8	5:2	085 116	.6224	22' 344'	1.1093	1.1264
60	76.13	6:4	136	.6257	22' 33' 66'	0.0000	0.0000
61	76.4	4:0 5:2	077 110	.6295	33' 44' 1 233' 4' 6'	0.9400	0.9070
62	76.7	6:3	154	.6349	22' 44' 36'	0.1145	0.0961
63	77	5:2	082	.6453	22' 33' 4'	0.6990	0.6620
64	77.5	6:3	151	.6499	22' 33' 5' 6'	0.7639	0.6543
65	77.7	6:3 5:1	137 124	.6564	22' 33' 36' 1 2' 344' 5'	0.9372	0.8264
66	77.9	6:3	144	.6584	22' 34' 5' 6'	0.0000	0.0000
67	78	5:1 6:3	107 100	.6620	233' 0' 5' 1 233' 45' 1 22' 34' 56'	0.0370	0.7602
68	78.3	5:1	123	.6650	2' 344' 5'	12.2911	11.6412
69	78.41	6:3 5:1	149 110	.6672	22' 30' 5' 6' 1 23' 44' 5' 1 233' 45'	0.0000	0.0000
70	78.7	6:3	139 140	.6707	22' 344' 6' 1 22' 344' 6'	0.0062	0.0053
71	79.2	6:3 5:1	134 143	.6746	22' 33' 36' 1 22' 3456' 1 2344' 5'	0.3700	0.3293
72	79.4	5:1 6:3	122 131	.6871	2' 33' 45' 1 22' 33' 46' 1 22' 33' 55'	0.2160	0.1963
73	79.9	6:2	146 161	.6953	22' 30' 55' 1 233' 45' 6'	0.7660	0.6397
74	80.3	6:3 5:1	132 105	.7033	22' 33' 46' 1 233' 44'	2.2104	2.0704
75	80.7	6:2	153	.7036	22' 44' 59'	0.0123	0.0106
76	81.4	6:2	160	.7060	23' 44' 5' 6'	0.0000	0.0000
77	81.5	6:2	141	.7204	22' 3455'	0.6479	0.5349
78	81.7	7:0	179	.7205	22' 33' 366'	0.0000	0.0000
79	82	6:2	130	.7244	22' 33' 45'	0.6563	0.5622
80	82.2	6:2	137	.7329	22' 344' 5'	0.6102	0.5227
81	82.55	7:0	176	.7305	22' 33' 466'	0.0000	0.0000
82	82.7	6:2	150 163	.7403	22' 344' 5' 1 233' 4' 36' 1 42'	6.4902	5.5663
83	83	6:2	150	.7429	233' 44' 6'	0.0310	0.7110
84	83.4	6:2	129	.7501	22' 33' 45'	0.3521	0.4729
85	83.9	7:3	170	.7537	22' 33' 55' 6'	0.0025	0.0645
86	84.25	6:2	166	.7574	2344' 56'	0.0000	0.0000
87	84.3	7:3	175	.7611	22' 33' 49' 6'	0.0342	0.0260
88	84.7	7:3	107 102	.7650	22' 30' 55' 6' 1 22' 344' 56'	0.2757	0.2156
89	85.1	6:2	120	.7761	22' 33' 44'	1.2071	1.0300
90	85.4	7:3	105	.7720	22' 344' 5' 6'	0.0000	0.0000
91	85.7	6:1	167	.7814	23' 44' 59'	0.3020	0.4904
92	86.3	7:3	105	.7840	22' 3455' 6'	0.0399	0.0313
93	87	7:3	174 101	.7940	22' 33' 456' 1 22' 344' 56'	0.2914	0.2205
94	87.5	7:3	177	.8031	22' 33' 4' 56'	0.2136	0.1690
95	87.9	7:3 6:1	171 156	.8105	22' 33' 44' 6' 1 233' 44' 5'	0.9060	0.7551
96	88.4	6:0	202	.8049	22' 33' 53' 66'	0.1175	0.0045
97	88.59	6:1	157	.8104	233' 44' 5'	0.0000	0.0000
98	88.91	7:3	173	.8132	22' 33' 456'	0.0000	0.0000
99	89.3	6:0	200 204	.8197	22' 33' 45' 66' 1 22' 344' 566'	0.0097	0.0034
100	89.6	7:2	172 192	.8270	22' 33' 455' 1 233' 455' 6'	0.1072	0.0030
101	90.2	6:0	197	.8293	22' 33' 44' 66'	0.0000	0.0000
102	90.4	7:2	100	.8362	22' 344' 59'	0.6200	0.4911
103	90.91	7:2	193	.8397	233' 0' 55' 6'	0.0000	0.0000
104	91.3	7:2	191	.8447	233' 44' 5' 6'	0.0132	0.0103
105	92.1	6:0	199	.8494	22' 33' 4566'	0.0395	0.0204
106	93.0	7:2	170	.8740	22' 33' 44' 5'	0.4055	0.3172
107	94.8	7:2	190	.8740	233' 44' 56'	0.1064	0.0032
108	95.4	6:3	190	.8845	22' 33' 455' 6'	0.0030	0.0022
109	95.99	6:3	201	.8870	22' 33' 45' 55' 6'	0.0000	0.0000
110	96.7	6:3	194 203	.8900	22' 33' 44' 5' 6' 1 22' 344' 55' 6'	0.0074	0.0030
111	98.6	7:1	109	.9142	233' 44' 59'	0.0174	0.0136
112	101.1	6:3	195	.9321	22' 33' 44' 56'	0.0463	0.0333
113	101.7	9:0	200	.9320	22' 33' 455' 66'	0.0056	0.0037
114	103.29	9:0	207	.9423	22' 33' 44' 366'	0.0000	0.0000
115	105.2	6:2	194	.9620	22' 33' 44' 59'	0.0019	0.0009
116	106.2	6:2	205	.9670	233' 44' 55' 6'	0.0023	0.0017
117	110.1	9:3	206	1.010	22' 33' 44' 55' 6'	0.0640	0.0430
118	126.35	10:0	209	1.030	22' 33' 44' 55' 66'	0.0000	0.0000

probability Cl₂ - in a patholens

N. B.
18B



18B

N.B 18B

PEAK#	RET. TIME	I-CLD-CL	IUMACH	RTT	CONDENSERS	WEIGHT %	MOLE %
1	40.64	0:0	000	.0997	BIPHENYL	0.0000	0.0000
2	46.72	1:1	001	.1544	2	0.0000	0.0000
3	50.21	1:0	002	.1937	3	1.6647	2.8195
4	50.62	1:0	003	.1978	4	0.5130	0.8680
5	52.46	2:2	004 010	.2243	22' 1 26'	0.0000	0.0000
6	54.71	2:1	007 009	.2566	24' 1 25'	0.0399	0.0572
7	55.59	2:1	006	.2709	23'	0.0007	0.0503
8	56.00	2:1	005 000	.2705	23' 1 24'	0.0908	0.1373
9	57.34	2:0	014	.2973	35	0.5308	0.7719
10	57.70	2:3	019	.3003	22'6	1.3036	1.8662
11	58.04	2:2	020	.3165	246	0.0069	0.0086
12	59.28	2:0	011	.3238	33'	0.5043	0.7224
13	59.41	2:0	012 013	.3297	34' 1 34'	0.0096	0.1204
14	59.8	3:2 2:0	010 015	.3307	22'5' 1 00'	0.4994	0.6406
15	60.03	3:2	017	.3390	22'4	0.2313	0.2874
16	60.70	3:2	024 027	.3500	236' 1 23'6	0.2293	0.2846
17	61.35	3:2	016 032	.3625	22'3' 1 20'6	0.2163	0.2604
18	62.1	3:1	023	.3770	235	0.0113	0.0141
19	62.31	3:1 4:4	034 054	.3800	2'35' 1 22'66'	0.0000	0.0000
20	62.78	3:1	029	.3820	245	0.0000	0.0000
21	62.90	3:1	026	.3911	23'5	0.3906	0.4947
22	63.19	3:1	025	.3937	23'4	0.2092	0.2596
23	63.63	3:1	031	.4024	24'5	0.5400	0.6402
24	63.73	3:1 4:3	028 050	.4031	244' 1 22'46	0.7541	0.9335
25	64.31	3:1 4:3	021 043	.4170	233' 1 230' 1 22'56'	0.4590	0.5146
26	65	3:1 4:3	022 051	.4267	234' 1 22'46'	0.2279	0.2603
27	65.49	4:3	045	.4334	22'36	0.1122	0.1220
28	65.84	3:1	036	.4379	33'5	0.0000	0.0000
29	66.06	4:3	046	.4450	22'36'	0.1437	0.1593
30	66.45	3:1	039	.4480	34'5	0.0000	0.0000
31	66.63	4:2	052 073	.4554	22'55' 1 23'5'6	4.1409	4.5410
32	66.97	4:2	049	.4610	22'45	2.3400	2.5700
33	67.23	4:2	047	.4639	22'44'	0.9249	1.0123
34	67.35	4:2	040 075	.4651	22'45' 1 244'6	0.3027	0.3313
35	67.51	4:2	065 062	.4665	2346' 1 2356'	0.0796	0.0871
36	67.87	3:0	035	.4730	33'4	0.0000	0.0000
37	68.16	5:4 4:2	104 044	.4832	22'466' 1 22'35'	1.7602	1.9331
38	68.44	3:0 4:2	037 042	.4870	344' 1 22'30' 1 233'6	0.9539	1.0550
39	69.14	4:2	064 071	.4990	23'50' 1 234'6' 1 23'4'6'	0.0777	0.0866
40	69.25	4:1	060	.5000	23'45' 7	0.0000	0.0000
41	69.4	5:0	074	.5057	22'366'	0.1447	0.1417
42	69.60	4:2	040	.5102	22'33'	0.2520	0.2540
43	70.1	5:3 4:1	103 057	.5155	22'45'6' 1 233'5	0.1691	0.1800
44	70.46	5:3 4:1	100 067	.5212	22'44'6' 1 23'4'5	0.2005	0.2049
45	70.79	4:1	050 063	.5267	233'5' 1 234'5	0.1106	0.1290
46	71.13	4:1 5:3	074 094	.5300	244'5' 1 22'356'	0.0101	0.0279
47	71.36	4:1	070 061	.5407	23'4'5' 1 2'345' 1 24457	3.2037	3.5066
48	71.73	4:1 5:3	066 075	.5447	23'44' 1 22'356' 1 22'35'6	4.2010	4.1340
49	72.19	5:3 4:1	071 070	.5549	22'30'6' 1 22'3'46' 1 233'4	1.1904	1.1056
50	72.81	4:1	056 060	.5676	233'4' 1 2344'	0.7977	0.0731
51	73.25	6:4 5:3	153 084	.5666	22'44'66' 1 22'33'61 1 22'355'	2.9595	2.0769
52	73.49	5:3	089	.5779	22'306'	0.0000	0.0000
53	73.69	5:2	101 098	.5814	22'30'5' 1 22'405'	7.7900	7.6353
54	74.00	5:2	099	.5800	22'44'5	4.1910	4.1044
55	74.6	6:4 5:2	150 112	.5969	22'30'66' 1 233'56' 1 23'44'6	0.2695	0.2639
56	74.8	5:2	083 109	.6029	22'33'5' 1 233'46	0.6406	0.6390
57	75.22	6:4 5:2	152 097	.6062	22'3566' 1 22'345' 1 22'3'45	1.9166	1.0663
58	75.55	5:2	087 111	.6175	22'345' 1 233'55' 1 2344'6	2.1102	2.0662
59	75.86	5:2	085 116	.6224	22'344' 1 234567	0.9903	0.9696
60	76.1	6:4	136	.6257	22'33'64'	0.6173	0.3467
61	76.3	4:0 5:2	077 110	.6295	33'44' 1 233'4'6	0.2012	0.1806
62	76.7	6:3	154	.6349	22'44'56'	0.0060	0.0769
63	77	5:2	082	.6453	22'33'4	0.3470	0.5354
64	77.5	6:3	151	.6499	22'355'6	0.7239	0.6411
65	77.7	6:3 5:1	135 124	.6563	22'33'56' 1 2'344'5	0.0514	0.7762
66	77.9	6:3	144	.6584	22'345'6	0.0000	0.0000
67	78	5:1 6:3	107 100	.6628	233'4'5' 1 233'45' 1 22'34'56	0.0064	0.7653
68	78.25	5:1	123	.6658	2'344'5	0.0000	0.0000
69	78.4	6:3 5:1	149 110	.6674	22'44'5'6' 1 23'44'5' 1 233'45	10.4394	9.5132
70	78.8	6:3	139 146	.6707	22'344'6' 1 22'344'6'	0.0039	0.0052
71	79.1	6:3 5:1	134 143	.6796	22'33'56' 1 22'3456' 1 2344'5	0.4994	0.4707
72	79.5	5:1 6:3	122 131	.6871	2'33'451 1 22'33'46122'33'55'	0.1905	0.1709
73	79.9	6:2	146 161	.6955	22'34'55' 1 233'45'6	0.7070	0.6260
74	80.3	6:3 5:1	132 105	.7035	22'33'46' 1 233'44'	1.0592	1.0009
75	80.5	6:2	153	.7036	22'44'55'	7.9606	7.0566
76	81.3	6:2	160	.7060	23'44'5'6	0.0104	0.0163
77	81.5	4:2	141	.7203	22'3455'	0.5450	0.5003
78	81.7	7:4	179	.7205	22'33'566'	0.0000	0.0000
79	82	6:2	130	.7204	22'33'45'	0.6044	0.5352
80	82.2	6:2	137	.7324	22'344'5	0.5210	0.4621
81	82.35	7:4	176	.7305	22'33'466'	0.0000	0.0000
82	82.7	6:2	130 163	.7403	22'344'5' 1 233'4'56' 1 2	5.9107	5.2343
83	83	6:2	156	.7429	233'44'6	0.7569	0.6703
84	83.4	6:2	129	.7501	22'33'45	0.4075	0.4317
85	83.9	7:3	170	.7547	22'33'55'6	0.0702	0.0632
86	84.25	6:2	166	.7572	2344'56	0.0000	0.0000
87	84.4	7:3	175	.7611	22'33'45'6	0.0000	0.0000
88	84.7	7:3	107 102	.7653	22'34'55'6' 1 22'444'56'	0.2613	0.2112
89	85.1	6:2	120	.7761	22'33'44'	1.1047	0.9703
90	85.4	7:3	103	.7720	22'344'5'6	0.0000	0.0000
91	85.7	6:1	167	.7814	23'44'55'	0.3709	0.5056
92	86.3	7:3	105	.7800	22'3455'6	0.0370	0.0307
93	87	7:3	174 181	.7965	22'33'456' 1 22'344'56	0.2762	0.2230
94	87.5	7:3	177	.8031	22'33'4'86	0.2043	0.1606
95	88	7:3 6:1	171 154	.8105	22'33'44'6' 1 233'44'5	0.0309	0.7222
96	88.44	8:4	202	.8009	22'33'55'66'	0.0000	0.0000
97	88.5	6:1	157	.8104	233'44'5'	0.1055	0.0934
98	88.8	7:3	173	.8152	22'33'456	0.0076	0.0061
99	89.3	8:4	200 204	.8197	22'33'45'66' 1 22'444'566'	0.0045	0.0033
100	89.4	7:2	172 192	.8278	22'33'455' 1 233'455'6	0.1161	0.0939
101	90.2	8:4	197	.8293	22'33'44'66'	0.0000	0.0000
102	90.4	7:2	100	.8362	22'344'55'	0.6205	0.5016
103	90.8	7:2	193	.8397	233'44'55'6	0.0262	0.0212
104	91.3	7:2	191	.8447	233'44'5'6	0.0167	0.0135
105	92.2	8:4	199	.8494	22'33'4566'	0.0535	0.0390
106	92.8	7:2	170	.8740	22'33'44'5	0.3990	0.3286
107	94.3	7:2	190	.8740	233'44'56	0.1045	0.0845
108	93.5	8:3	190	.8845	22'33'455'6	0.0064	0.0064
109	93.9	8:3	201	.8875	22'33'4'55'6	0.0710	0.0534
110	94.8	8:3	194 203	.8935	22'33'44'5'6' 1 22'444'55'6	0.0063	0.0642
111	98.6	7:1	109	.9142	233'44'55'	0.0165	0.0133
112	101.23	8:3	199	.9321	22'33'44'56	0.0000	0.0000
113	101.7	9:4	200	.9320	22'33'455'66'	0.0000	0.0000
114	103.6	9:4	207	.9423	22'33'44'566'	0.0000	0.0000
115	105.3	8:2	194	.9620	22'33'44'55'	0.0036	0.0622
116	106.77	8:2	208	.9670	233'44'55'6	0.0000	0.0000
117	114.2	9:3	206	1.010	22'33'44'55'6	0.0612	0.0421
118	120.35	10:4	209	1.050	22'33'44'55'66'	0.0000	0.0000

- R 0.5043 g -
 Ident. as
 -Trichloronaphth
 1cm by M.S.

N. B.

19A

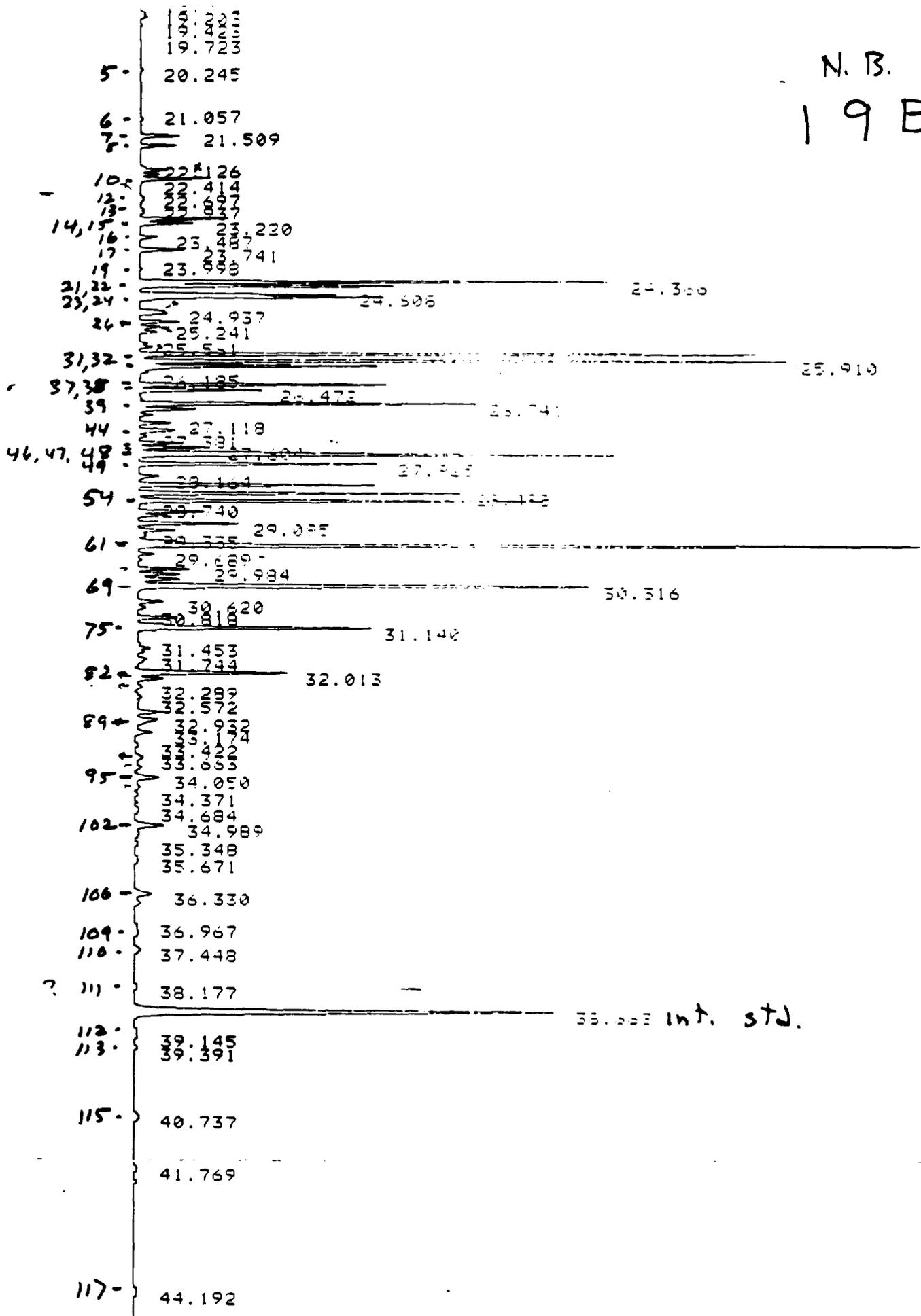
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113	39.153	
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115	40.743	
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117	44.177	

19A

PEAK#	RET. TIME	T-CLIO-CL	IUPAC#	RTT	CONGENERS	WEIGHT %	MOLE %
1	40.63	0:0	000	.0997	BIPHENYL	0.0000	0.0000
2	46.72	1:1	001	.1944	2	0.0000	0.0000
3	50.22	1:0	002	.1937	3	0.7903	1.4600
4	50.61	1:0	003	.1973	4	0.2933	0.4524
5	52.31	2:2	004 010	.2245	22' 1 26	0.4920	0.6375
6	54.75	2:1	007 009	.2564	24' 1 25	0.2182	0.2827
7	55.6	2:1	006	.2709	23'	1.0201	2.3600
8	56.09	2:1	005 008	.2785	23' 1 24'	1.3342	1.9906
9	57.33	2:0	014	.2973	35	0.2032	0.2634
10	57.77	0:0	019	.3093	22'6	0.9043	1.0152
11	58.03	3:2	030	.3163	244	0.0675	0.0750
12	59.4	2:0	011	.3234	33'	0.3170	0.2822
13	59.49	2:0	012 013	.3297	34' 1 34'	0.3704	0.4903
14	59.81	4:2 2:0	010 015	.3307	22'5' 1 44'	4.1291	4.0293
15	60.02	4:2	017	.3390	22'4	2.2247	2.4973
16	60.69	3:2	024 027	.3500	236' 1 23'6	0.4200	0.4713
17	61.34	3:2	016 032	.3625	22'3' 1 25'6	1.3073	1.4677
18	62.01	3:1	023	.3770	235	0.0261	0.0293
19	62.32	3:1 4:0	034 054	.3800	2'35' 1 22'64'	0.0572	0.0610
20	62.78	3:1	029	.3820	245	0.0000	0.0000
21	62.99	3:1	026	.3911	23'5	4.5707	5.1403
22	63.10	3:1	025	.3937	23'4	3.6941	4.1516
23	63.62	3:1	031	.4024	24'5	4.2764	4.8009
24	63.72	3:1 4:0	020 050	.4031	244' 1 22'46	4.9390	5.3309
25	64.47	3:1 4:0	021 033	.4170	253' 1 23' 1 22'56'	1.0062	1.0202
26	65.01	3:1 4:0	022 031	.4267	234' 1 22'46'	0.4032	0.4559
27	65.5	4:0	045	.4334	22'36	0.4845	0.4794
28	65.89	3:1	036	.4379	33'5	0.0110	0.0124
29	66.07	4:0	046	.4450	22'36'	0.3035	0.3797
30	66.45	3:1	039	.4480	34'5	0.0000	0.0000
31	66.61	4:2	052 073	.4554	22'55' 1 23'5'6	7.7312	7.6540
32	66.98	4:2	049	.4610	22'45	6.1607	6.0991
33	67.24	4:2	047	.4639	22'44'	2.4523	2.4270
34	67.34	4:2	048 075	.4651	22'45' 1 24'6	0.4356	0.4312
35	67.52	4:2	045 062	.4663	234' 1 2356	0.0004	0.0075
36	67.83	3:0	035	.4738	33'4	0.0609	0.0603
37	68.17	5:4 4:2	104 044	.4852	22'46' 1 22'35'	2.8204	2.7969
38	68.45	3:0 4:2	037 042	.4870	344' 1 22'36' 1 234'6	2.2997	2.2957
39	69.12	4:2	064 071	.4990	23'34' 1 234'6 1 23'4'6	2.5072	2.5614
40	69.25	4:1	048	.5040	23'45' 7	0.0000	0.0000
41	69.36	5:4	096	.5057	22'366'	1.3021	1.1532
42	69.69	4:2	040	.5102	22'33'	0.3033	0.3023
43	70.11	5:3 4:1	103 057	.5155	22'45'6' 1 233'5	0.3315	0.3399
44	70.47	5:3 4:1	100 067	.5212	22'44'6' 1 23'4'5	0.0410	0.7774
45	70.70	4:1	050 063	.5267	233'5' 1 234'5	0.1462	0.1440
46	71.11	4:1 5:3	074 094	.5340	244'5' 1 22'356'	0.7000	0.7210
47	71.35	4:1	070 061	.5407	23'4'5' 1 2'345' 1 24457	0.0649	0.0562
48	71.71	4:1 5:3	064 095	.5447	23'44' 1 24'356' 1 22'35'6	4.1871	3.7002
49	72.17	5:3 4:1	071 098	.5544	22'34'6' 1 22'3'46' 1 234'4	1.9100	1.7099
50	72.82	4:1	056 060	.5674	233'4' 1 2344'	0.3264	0.5211
51	73.24	6:0 5:3	155 084	.5666	22'44'66' 1 22'33'61 22'335'	1.0003	1.5037
52	73.49	5:3	089	.5779	22'346'	0.0000	0.0000
53	73.67	5:2	101 090	.5814	22'34'5' 1 22'455'	2.8999	2.5603
54	74.04	5:2	099	.5880	22'44'5	3.3200	2.9404
55	74.61	6:4 5:2	150 112	.5969	22'34'66' 1 233'56' 1 23'44'6	0.4654	0.4122
56	74.79	5:2	083 109	.6029	22'33'5' 1 233'46	0.3674	0.3254
57	75.2	6:0 5:2	152 097	.6062	22'3566' 1 22'346' 1 22'3'49	0.0730	0.7609
58	75.54	5:2	087 111	.6175	22'345' 1 234'53' 1 2344'6	0.0411	0.2135
59	75.82	5:2	085 116	.6224	22'344' 1 234567	0.0763	0.0674
60	76.08	6:4	136	.6257	22'33'66'	0.4435	0.3569
61	76.29	4:0 5:2	077 110	.6295	33'44' 1 233'4'6	4.3406	4.0215
62	76.75	6:3	154	.6344	22'44'56'	0.1499	0.1200
63	77.44	5:2	082	.6453	22'33'4	0.0433	0.0304
64	77.5	6:3	151	.6499	22'359'6	0.4662	0.3094
65	77.76	6:3 5:1	135 124	.6563	22'33'56' 1 2'344'5	0.3632	0.2995
66	77.9	6:3	144	.6584	22'345'6	0.0000	0.0000
67	78.02	5:1 6:3	107 104	.6628	233'4'5' 1 233'45' 1 22'34'56	0.4605	0.3962
68	78.25	5:1	123	.6650	2'344'5	0.0000	0.0000
69	78.30	6:3 5:1	149 114	.6672	22'34'5'6' 1 23'44'5' 1 233'45	3.9903	3.2970
70	78.55	6:3	139 140	.6707	22'344'6' 1 22'344'6'	0.0000	0.0000
71	79.16	6:3 5:1	134 103	.6796	22'33'56' 1 22'3456' 1 2344'5	0.2327	0.2016
72	79.47	5:1 6:3	122 131	.6871	2'33'45' 1 22'33'46' 1 22'33'58'	0.0022	0.0699
73	79.98	6:2	146 161	.6955	22'34'53' 1 233'45'6	0.4312	0.3454
74	80.35	6:3 5:1	132 105	.7039	22'33'66' 1 233'44'	0.0000	0.0000
75	80.5	6:2	154	.7036	22'44'55'	4.3900	3.5235
76	81.3	6:2	168	.7068	23'44'5'6	0.0140	0.0119
77	81.51	6:2	141	.7203	22'3455'	0.0531	0.0425
78	81.72	7:4	174	.7205	22'33'566'	0.1169	0.0033
79	82.05	6:2	130	.7284	22'33'45'	0.0946	0.0750
80	82.21	6:2	137	.7329	22'344'5	0.0731	0.0505
81	82.35	7:4	176	.7305	22'33'466'	0.0000	0.0000
82	82.75	6:2	134 163	.7403	22'344'5' 1 233'4'56' 1 42	1.0110	0.0105
83	83.06	6:2	130	.7429	233'4'6	0.1662	0.1332
84	83.40	6:2	129	.7501	22'33'45	0.0547	0.0439
85	83.97	7:3	170	.7537	22'33'55'6	0.0430	0.0329
86	84.8	6:2	166	.7572	2344'56	0.0102	0.0062
87	84.8	7:3	178	.7611	22'33'45'6	0.0000	0.0000
88	84.74	7:3	107 108	.7633	22'34'55'6' 1 22'344'56'	0.2256	0.1650
89	85.1	6:2	128	.7761	22'33'44'	0.1125	0.0944
90	86.4	7:3	165	.7720	22'344'5'6	0.0000	0.0000
91	86.7	6:1	147	.7814	23'44'55'	0.2451	0.1943
92	86.8	7:3	188	.7840	22'3455'6	0.0109	0.0000
93	86.9	7:3	174 181	.7965	22'33'56' 1 22'344'56	0.0444	0.0472
94	87.5	7:3	177	.8031	22'33'45'6	0.0440	0.0320
95	88	7:3 6:1	171 154	.8105	22'33'44'6' 1 234'44'5	0.1602	0.1247
96	88.44	8:4	202	.8009	22'33'55'66'	0.0000	0.0000
97	88.55	6:1	157	.8104	233'44'5'	0.0000	0.0000
98	88.91	7:3	173	.8152	22'33'56	0.0000	0.0000
99	89.46	8:4	200 204	.8197	22'33'45'66' 1 22'344'566'	0.0000	0.0000
100	89.6	7:2	172 192	.8278	22'33'45' 1 234'455'6	0.0334	0.0244
101	90.2	8:4	197	.8293	22'33'44'66'	0.0000	0.0000
102	90.4	7:2	160	.8368	22'344'56'	0.1040	0.1304
103	90.6	7:2	193	.8397	233'44'55'6	0.0106	0.0092
104	91.44	7:2	191	.8447	233'44'5'6	0.0000	0.0000
105	92.1	8:4	199	.8494	22'33'466'	0.0106	0.0075
106	93.9	7:2	170	.8740	22'33'44'5	0.1047	0.0766
107	94.3	7:2	190	.8740	233'44'56	0.0496	0.0354
108	95.63	8:3	190	.8845	22'33'455'6	0.0000	0.0000
109	95.9	8:3	201	.8875	22'33'455'6	0.0347	0.0247
110	96.8	8:3	196 203	.8935	22'33'44'5'6' 1 22'344'55'6	0.0592	0.0390
111	96.72	7:1	169	.9142	233'44'55'	0.0000	0.0000
112	101.1	8:3	195	.9321	22'33'44'56	0.0105	0.0071
113	101.87	9:4	208	.9320	22'33'455'66'	0.0000	0.0000
114	103.29	9:4	207	.9423	22'33'44'566'	0.0000	0.0000
115	105.3	8:2	194	.9620	22'33'44'55'	0.0044	0.0312
116	106.77	8:2	205	.9670	233'44'55'6	0.0000	0.0000
117	114.34	9:3	204	1.010	22'33'44'55'6	0.0000	0.0000
118	126.35	10:4	209	1.050	22'33'44'50'66'	0.0000	0.0000

CONCENTRATION = 3.004791
 INITIAL MICROGRAMS = 0.0104
 AVAILABLE MOLECULAR WEIGHT = 209.00233
 NUMBER OF CALIBRATED PEAKS FOUND = 118

N. B.
19B



Int. std.

OR

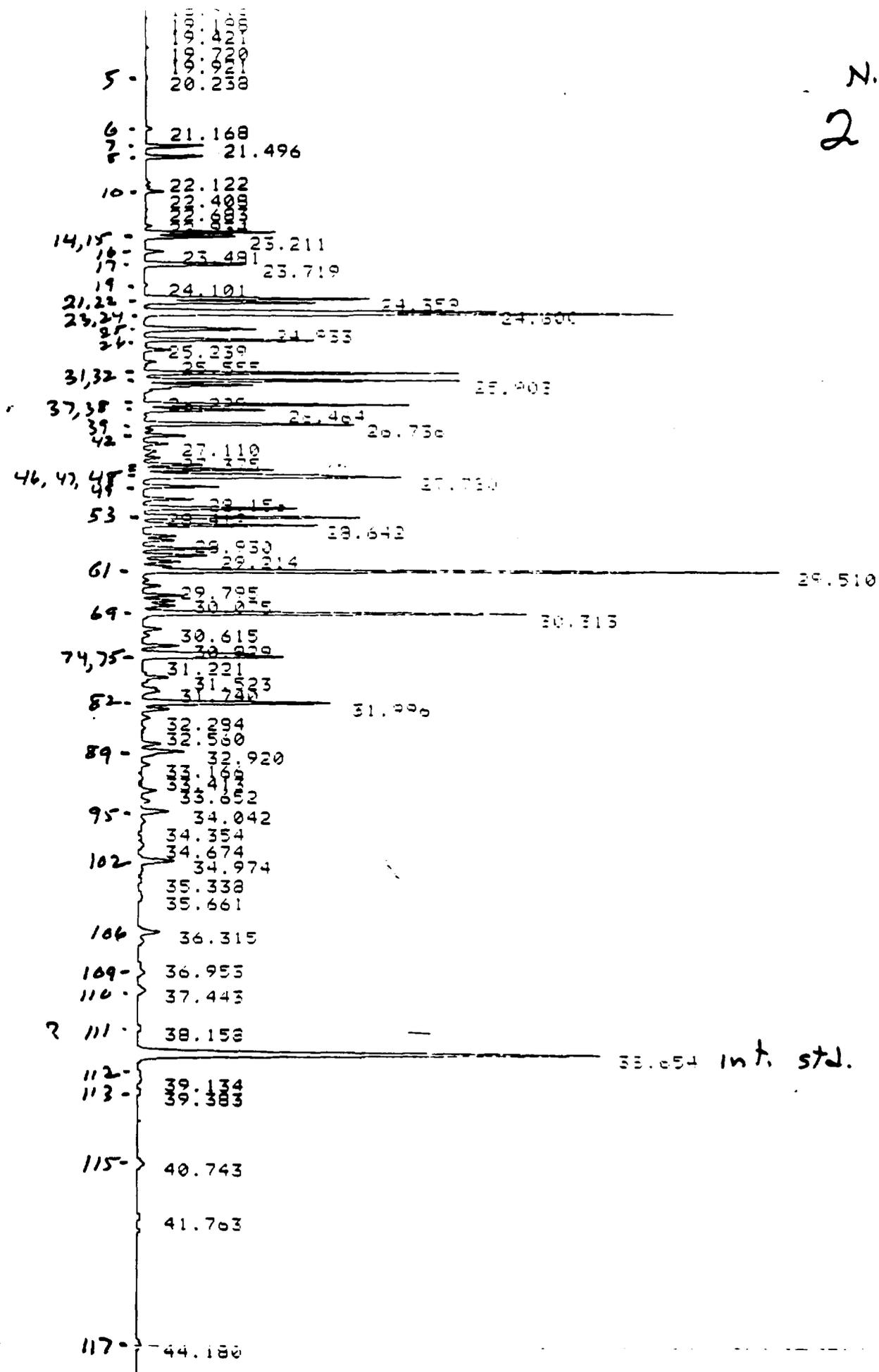
NR 19B

PEAK#	RET. TIME	T-CL:O-CL	IUPAC#	RRT	CONDENSERS	WEIGHT %	MOLE %
1	40.66	0:0	000	.0997	BIPHENYL	0.0000	0.0000
2	46.61	1:1	001	.1344	2	0.1210	0.1067
3	50.10	1:0	002	.1937	3	3.1799	4.9050
4	50.62	1:0	003	.1975	4	0.1633	0.2319
5	52.33	2:2	004 010	.2245	22' 1 20'	0.4354	0.5601
6	54.73	2:1	007 009	.2566	24 1 25'	0.1143	0.1491
7	55.59	2:1	006	.2709	23'	1.1277	1.4715
8	56.00	2:1	005 008	.2705	20 1 20'	0.0924	1.1643
9	57.50	2:0	014	.2973	35	0.4614	0.6021
10	57.78	0:0	019	.3045	22'6	2.2378	2.5523
11	58.02	0:0	020	.3163	246	0.0615	0.0699
12	59.00	0:0	011	.3238	33'	0.2400	0.3143
13	59.47	2:0	012 013	.3297	34 1 34'	0.2283	0.2979
14	59.8	3:2 2:0	010 015	.3307	22'5 1 40'	2.5374	2.9005
15	60.01	3:2	017	.3390	22'6	1.2360	1.8974
16	60.71	3:2	024 027	.3500	236 1 23'6	0.2707	0.3151
17	61.30	3:2	016 032	.3625	22'3 1 20'6	0.7011	0.7926
18	62.1	3:1	023	.3770	235	0.0072	0.0082
19	62.34	3:1 4:0	034 034	.3800	2'35 1 22'66'	0.0475	0.0516
20	62.78	3:1	029	.3820	245	0.0000	0.0000
21	62.90	3:1	026	.3911	23'5	5.3529	6.0510
22	63.19	3:1	025	.3937	23'4	3.3929	3.8350
23	63.6	3:1	031	.4024	24'5	2.0161	2.2793
24	63.73	3:1 4:3	020 030	.4031	244' 1 22'46	2.1320	2.4040
25	64.46	3:1 4:3	021 033	.4174	233' 1 234' 1 22'36'	0.2506	0.2640
26	65	3:1 4:3	022 031	.4267	230' 1 22'46'	0.3221	0.3456
27	65.49	4:3	045	.4334	22'36	0.2766	0.2778
28	65.73	3:1	036	.4379	13'5	0.0000	0.0000
29	66.09	4:3	046	.4450	22'36'	0.2704	0.2776
30	66.45	3:1	039	.4480	34'5	0.0000	0.0000
31	66.63	4:2	052 073	.4554	22'55' 1 23'5'6	9.0363	9.0066
32	66.97	4:2	049	.4610	22'45'	7.7913	7.7677
33	67.23	4:2	047	.4639	22'40'	2.9743	2.9653
34	67.41	4:2	048 075	.4651	22'45 1 244'6	0.0000	0.0000
35	67.51	4:2	065 062	.4663	2346 1 2356	0.0600	0.0606
36	67.87	3:0	035	.4730	13'4	0.0000	0.0000
37	68.16	5:4 4:2	104 044	.4832	22'466' 1 22'35'	2.4510	2.4407
38	68.44	3:0 4:2	037 042	.4870	344' 1 22'30' 1 233'6	1.6467	1.6554
39	69.11	4:2	064 071	.4990	23'34 1 234'6 1 23'4'6	2.2644	2.2575
40	69.25	4:1	040	.5040	23'45' 7	0.0000	0.0000
41	69.4	5:4	096	.5057	22'366'	1.2561	1.1203
42	69.60	4:2	040	.5102	22'33'	0.1420	0.1420
43	70.1	5:3 4:1	103 057	.5159	22'45'6 1 233'5	0.4127	0.4020
44	70.40	5:3 4:1	100 067	.5212	22'40'6 1 23'4'5	0.7052	0.6566
45	70.79	4:1	050 063	.5267	233'5' 1 244'5	0.0917	0.0910
46	71.73	4:1 5:3	074 094	.5300	244'5 1 22'396'	0.3639	0.3300
47	71.86	4:1	070 061	.5407	23'4'5 1 2'345 1 23457	0.7196	0.7177
48	71.73	4:1 5:3	066 095	.5447	23'40' 1 22'356 1 22'35'6	4.7901	4.2936
49	72.19	5:3 4:1	091 078	.5544	22'34'6 1 22'3'46 1 233'0	2.5002	2.3251
50	72.81	4:1	056 060	.5674	233'4' 1 2344'	0.2230	0.2223
51	73.25	6:1 5:3	155 084	.5666	22'44'66' 1 22'33'61 22'335'	2.3171	2.0552
52	74.49	5:3	089	.5779	22'366'	0.0000	0.0000
53	73.67	5:2	101 090	.5814	22'30'5 1 22'455'	3.2973	2.8962
54	74.45	5:2	099	.5880	22'40'5	3.6995	3.2996
55	74.6	6:1 5:2	130 112	.5969	22'30'66' 1 233'56 1 20'40'6	0.3967	0.5322
56	74.8	5:2	083 109	.6029	22'33'5 1 233'46	0.4198	0.3741
57	75.22	6:1 5:2	132 097	.6062	22'3566' 1 22'349 1 22'3'40	0.0000	0.7182
58	75.95	5:2	087 111	.6175	22'345' 1 233'55' 1 2344'6	0.2361	0.2016
59	75.04	5:2	085 116	.6224	22'340' 1 234567	0.0660	0.0560
60	76.1	6:1	134	.6254	22'33'56'	0.4907	0.4022
61	76.6	4:0 5:2	077 110	.6295	31'40' 1 233'4'6	5.3504	4.9370
62	76.74	6:1	134	.6349	22'40'56'	0.1650	0.1337
63	77	5:2	082	.6453	22'33'4	0.0200	0.0257
64	77.5	6:3	151	.6499	22'355'6	0.3329	0.4379
65	77.7	6:3 5:1	135 124	.6563	22'33'56' 1 2'344'5	0.4017	0.3336
66	77.9	6:3	144	.6584	22'305'6	0.0000	0.0000
67	78	5:1 6:3	107 100	.6628	233'4'5 1 233'45' 1 22'30'36	0.4923	0.4255
68	78.3	5:1	123	.6658	2'344'5	3.2360	4.6787
69	78.41	6:1 5:1	149 110	.6672	22'30'5'6 1 23'40'5 1 233'45	2.0000	0.0000
70	78.55	6:1	139 100	.6707	22'304'6 1 22'344'6'	0.0000	0.0000
71	79.1	6:3 5:1	134 103	.6796	22'33'56' 1 22'3456' 1 2344'5	0.2650	0.2314
72	79.4	5:1 6:3	122 131	.6871	2'33'45 1 22'35'40 1 22'33'55'	0.0909	0.0770
73	79.9	6:1	146 161	.6955	22'30'55' 1 233'45'6	0.4630	0.3741
74	80.35	6:3 5:1	132 105	.7035	22'33'45' 1 233'44'	0.0000	0.0000
75	80.5	6:2	153	.7068	22'40'35'	4.0656	3.9240
76	81.3	6:2	148	.7088	22'40'3'6	0.0211	0.0170
77	81.9	6:2	147	.7201	22'345'	0.0450	0.0400
78	81.7	7:1	179	.7209	22'33'566'	0.1100	0.0869
79	82	6:2	130	.7284	22'33'45'	0.1066	0.1007
80	82.4	6:2	137	.7329	22'304'5	0.0000	0.0000
81	82.35	7:1	176	.7385	22'33'466'	0.0000	0.0000
82	82.7	6:2	130 163	.7403	22'304'5' 1 233'4'56 1 42	1.1065	0.9367
83	83	6:2	150	.7429	233'40'6	0.2025	0.1640
84	83.4	6:2	129	.7501	22'33'45	0.0443	0.0319
85	83.9	7:1	170	.7537	22'33'35'6	0.0569	0.0429
86	84.2	6:2	166	.7572	1300'36'	0.0132	0.0104
87	84.4	7:1	175	.7611	22'33'45'6	0.0000	0.0000
88	84.7	7:1	187 102	.7653	22'34'55'6 1 22'344'56'	0.2311	0.1702
89	85.1	6:2	120	.7741	22'33'44'	0.1852	0.1490
90	85.4	7:1	183	.7720	22'304'5'6	0.0000	0.0000
91	85.7	6:1	167	.7810	22'40'35'	0.2096	0.2356
92	86.0	7:1	185	.7808	22'345'6	0.0096	0.0071
93	87	7:1	174 101	.7965	22'33'456' 1 22'344'56	0.0663	0.0491
94	87.5	7:1	177	.8031	22'33'4'56	0.0496	0.0366
95	88	7:1 6:1	171 154	.8100	22'33'40'6 1 233'40'5	0.2004	0.1639
96	88.4	8:1	202	.8009	22'33'35'66'	0.0256	0.0160
97	88.55	8:1	157	.8104	233'40'5	0.0000	0.0000
98	88.8	7:1	173	.8154	22'33'36	0.0019	0.0014
99	89.4	8:1	200 204	.8197	22'33'45'66' 1 22'344'566'	0.0029	0.0019
100	89.6	7:2	172 192	.8270	22'33'35'6 1 234'455'6	0.0370	0.0272
101	90.2	8:1	197	.8293	22'33'45'66'	0.0000	0.0000
102	90.4	7:2	186	.8347	22'304'35'66'	0.2036	0.1499
103	90.8	7:2	193	.8397	233'40'35'6	0.0167	0.0123
104	91.3	7:2	191	.8447	233'40'5'6	0.0066	0.0049
105	92.2	8:1	199	.8494	22'33'4566'	0.0156	0.0092
106	93.9	7:2	170	.8748	22'33'44'5	0.1214	0.0894
107	94.5	7:2	190	.8740	233'40'36	0.0439	0.0350
108	95.6	8:1	190	.8805	22'33'35'6	0.0037	0.0023
109	95.9	8:1	201	.8875	22'33'40'36	0.0356	0.0241
110	96.0	8:1	194 203	.8955	22'33'40'36 1 22'344'55'6	0.0406	0.0329
111	96.7	7:1	189	.9102	233'40'35'	0.0079	0.0050
112	101.2	8:1	195	.9321	22'33'45'86	0.0209	0.0142
113	101.7	9:1	206	.9321	22'33'45'66'	0.0017	0.0011
114	105.1	4:0	207	.9473	22'33'40'366'	0.0000	0.0000
115	105.3	8:2	194	.9620	22'33'40'35'	0.0410	0.0283
116	106.6	8:1	205	.9670	233'40'35'6	0.0000	0.0000
117	114.3	9:1	206	1.010	22'33'40'35'6	0.0146	0.0092
118	126.55	10:1	209	1.058	22'33'40'35'66'	0.0000	0.0000

CONCENTRATION = 3.327554
TOTAL MICROMOLES = 0.0114

AVERAGE MOLECULAR WEIGHT = 293.1197

N. B.
21A



21A

33.654 int. std.

NB. 21A

PEARL	RLT. TIME	T-CL:O-CL	IUPACO	RRT	CONDENSERS	WEIGHT %	MOLE %
1	40.59	0:0	000	.0997	BIPHENYL	0.0000	0.0000
2	44.72	1:1	001	.1904	2	0.0000	0.0000
3	50.06	1:0	002	.1937	3	2.1139	3.2103
4	50.63	1:0	003	.1979	4	0.1629	0.2473
5	52.31	2:2	004 010	.2249	22' 1 26	0.3799	0.4079
6	54.72	2:1	007 009	.2546	24' 1 25	0.2706	0.3579
7	55.57	2:1	006	.2709	23'	2.0034	2.5734
8	56.09	2:1	005 008	.2703	23' 1 24'	1.9016	2.4426
9	57.33	2:0	010	.2973	33	0.1632	0.2122
10	57.75	3:3	019	.3095	22'6	0.7690	0.8563
11	58.68	0:2	030	.3165	246	0.0307	0.0301
12	59.00	0:0	011	.3230	33'	0.3202	0.4113
13	59.46	2:0	012 015	.3307	34' 1 30'	0.3900	0.5110
14	59.79	4:2 2:0	010 015	.3387	22'5' 1 00'	4.0016	5.4132
15	60	3:2	017	.3390	22'0	2.5701	2.8692
16	60.72	3:2	024 027	.3508	236' 1 23'6	0.3905	0.4345
17	61.32	3:2	016 032	.3625	22'8' 1 24'6	2.3345	2.5901
18	62.3	3:1	023	.3770	235	0.0063	0.0060
19	62.43	4:1 0:0	034 036	.3800	2'35' 1 22'66'	0.0000	0.0000
20	62.72	3:1	029	.3820	245	0.0057	0.0063
21	64.97	3:1	046	.3911	23'5	5.5029	5.8903
22	65.10	3:1	025	.3937	23'0	2.0773	3.2021
23	65.54	3:1	031	.4024	24'5	4.6007	5.1201
24	66.72	3:1 4:3	020 030	.4031	244' 1 22'06	5.5045	6.1095
25	66.87	3:1 4:3	021 033	.4170	233' 1 230' 1 22'56'	2.1810	2.1320
26	66.99	3:1 4:3	022 051	.4267	234' 1 22'06'	1.5706	1.6390
27	65.48	0:3	045	.4334	22'36	0.5343	0.5244
28	65.80	3:1	036	.4370	15'5	0.0000	0.0000
29	66.00	0:3	046	.4450	22'36'	0.4090	0.4022
30	66.45	3:1	039	.4480	10'5	0.0000	0.0000
31	66.62	4:2	052 073	.4554	22'55' 1 23'5'6	6.3494	6.2313
32	66.94	4:2	049	.4610	22'45	4.7745	4.6057
33	67.22	4:2	047	.4639	22'44'	1.6430	1.6125
34	67.35	4:2	040 075	.4651	22'45' 1 240'6	0.3569	0.3503
35	67.6	4:2	065 062	.4665	23'06' 1 2356	0.0000	0.0000
36	67.81	3:0	035	.4730	33'0	0.0576	0.0641
37	68.15	3:0 4:2	104 044	.4832	22'466' 1 22'35'	3.4373	3.3697
38	68.43	3:0 4:2	037 042	.4870	344' 1 22'38' 1 230'6	2.3448	2.3203
39	69.13	4:2	064 071	.4990	23'30' 1 230'6 1 23'4'6	1.0760	1.0419
40	69.25	4:1	060	.5000	23'45' 7	0.0000	0.0000
41	69.42	3:0	096	.5057	22'366'	0.2672	0.2346
42	69.7	4:2	040	.5102	22'38'	0.6200	0.6093
43	70.09	3:3 4:1	103 057	.5155	22'45'6' 1 233'5	0.3996	0.3831
44	70.48	3:3 4:1	100 067	.5212	22'46'6' 1 23'4'5	0.3213	0.2945
45	70.79	4:1	050 063	.5267	233'0' 1 234'5	0.2327	0.2400
46	71.12	4:1 5:3	074 090	.5340	244'3' 1 22'356'	0.6570	0.6029
47	71.36	4:1	070 061	.5407	23'4'5' 1 2'345' 1 24457	1.5340	1.5062
48	71.62	4:1 5:3	066 095	.5447	23'44' 1 22'356' 1 22'35'6	1.4991	1.3220
49	72.10	3:3 4:1	091 090	.5509	22'34'6' 1 22'3'46' 1 233'0	1.0674	0.9469
50	72.81	4:1	056 060	.5676	233'0' 1 2300'	0.5510	0.5015
51	73.25	0:4 5:3	153 004	.5666	22'40'66' 1 22'33'61 22'355'	2.1450	1.8735
52	73.49	3:3	089	.5779	22'346'	0.0000	0.0000
53	73.69	3:2	101 090	.5814	22'34'5' 1 22'455'	3.0301	2.6603
54	74.07	3:2	099	.5880	22'44'5	2.1220	1.8630
55	74.59	6:4 5:2	150 112	.5969	22'34'66' 1 233'56' 1 23'00'6	0.3500	0.3073
56	74.82	3:2	083 109	.6029	22'33'5' 1 233'46	0.5621	0.4935
57	75.21	6:4 5:2	152 097	.6062	22'3566' 1 22'345' 1 22'3'45	0.7544	0.6307
58	75.55	3:2	087 111	.6175	22'345' 1 233'55' 1 2300'6	0.4939	0.4336
59	75.86	3:2	085 116	.6224	22'346' 1 234567	0.3070	0.2702
60	76.09	6:4	136	.6257	22'33'66'	0.4446	0.3530
61	76.3	4:0 5:2	077 110	.6295	33'44' 1 233'4'6	3.1776	4.5458
62	76.76	6:3	154	.6349	22'40'56'	0.0027	0.0636
63	77.05	3:2	082	.6436	22'33'0	0.1721	0.1511
64	77.51	6:3	151	.6499	22'355'6	0.5210	0.4144
65	77.77	6:3 5:1	133 124	.6563	22'33'56' 1 2'300'5	0.4278	0.3497
66	77.9	6:3	144	.6580	22'345'6	0.0000	0.0000
67	78.01	3:1 6:3	107 100	.6628	233'0'5' 1 233'05' 1 22'30'56	0.4909	0.4177
68	78.25	3:1	123	.6650	2'300'5	0.0000	0.0000
69	78.39	6:3 5:1	149 110	.6672	22'34'5'6' 1 23'00'5' 1 233'05	4.4029	3.5990
70	78.55	6:3	139 140	.6707	22'340'6' 1 22'300'6'	0.0000	0.0000
71	79.17	6:3 5:1	134 143	.6796	22'33'56' 1 22'3456' 1 2300'5	0.2600	0.2304
72	79.40	3:1 6:4	122 131	.6871	2'33'43' 22'33'46' 22'33'55'	0.0937	0.0769
73	79.97	6:2	146 161	.6955	22'34'55' 1 233'45'6	0.4712	0.3741
74	80.36	6:3 5:1	132 105	.7035	22'33'46' 1 233'44'	0.5404	0.4694
75	80.52	6:2	153	.7036	22'44'55'	3.3757	2.0393
76	81.37	6:2	168	.7060	23'44'5'6	0.0327	0.0260
77	81.52	6:2	141	.7203	22'3455'	0.1647	0.1304
78	81.68	7:4	179	.7205	22'33'566'	0.1121	0.0813
79	82.09	6:2	130	.7200	22'33'45'	0.1751	0.1390
80	82.22	6:2	137	.7329	22'340'5	0.3000	0.2302
81	82.35	7:4	176	.7305	22'33'466'	0.0000	0.0000
82	82.74	6:2	138 163	.7403	22'340'5' 1 233'4'56' 1 2	1.9577	1.5545
83	83.00	6:2	154	.7429	233'00'6	0.2647	0.2110
84	83.49	6:2	129	.7501	22'33'45	0.1359	0.1079
85	83.90	7:3	178	.7537	22'33'55'6	0.0603	0.0437
86	84.22	6:2	166	.7572	2344'56	0.0094	0.0075
87	84.5	7:3	175	.7611	22'33'45'6	0.0206	0.0149
88	84.76	7:3	107 102	.7653	22'34'55'6 1 22'344'56'	0.2304	0.1670
89	85.15	6:2	120	.7761	22'33'44'	0.4316	0.3427
90	85.4	7:3	103	.7720	22'340'5'6	0.0000	0.0000
91	85.77	6:3	167	.7810	23'44'55'	0.2212	0.1736
92	86.44	7:3	105	.7800	22'3455'6	0.0000	0.0000
93	87.01	7:3	174 101	.7965	22'33'456' 1 22'344'56	0.1611	0.1171
94	87.33	7:3	177	.8031	22'33'4'56	0.1320	0.0960
95	88.04	7:3 6:1	171 156	.8109	22'33'44'6' 1 233'44'5	0.3222	0.2407
96	88.44	8:4	202	.8089	22'33'55'66'	0.0000	0.0000
97	88.51	6:1	157	.8104	233'44'5'	0.0399	0.0205
98	88.91	7:3	173	.8152	22'33'456	0.0000	0.0000
99	89.36	0:4	200 204	.8197	22'33'45'66' 1 22'344'566'	0.0000	0.0000
100	89.67	7:2	172 192	.8278	22'33'455' 1 233'455'6	0.0553	0.0401
101	90.2	0:4	197	.8293	22'33'44'66'	0.0000	0.0000
102	90.43	7:2	100	.8362	22'344'55'	0.3256	0.2360
103	90.86	7:2	193	.8397	233'44'55'6	0.0111	0.0080
104	91.5	7:2	191	.8447	233'44'5'6	0.0053	0.0030
105	92.2	0:4	199	.8494	22'33'4566'	0.0119	0.0079
106	92.9	7:2	170	.8700	22'33'44'5	0.1937	0.1404
107	94.3	7:2	190	.8700	233'44'56	0.0372	0.0415
108	95.64	0:3	198	.8845	22'33'455'6	0.0000	0.0000
109	96.9	0:3	201	.8875	22'33'4'55'6	0.0633	0.0422
110	96.8	0:3	196 203	.8930	22'33'44'5'6 1 22'344'55'6	0.0700	0.0520
111	98.72	7:1	109	.9102	233'44'55'	0.0000	0.0000
112	101.1	0:3	195	.9321	22'33'44'56	0.0163	0.0100
113	101.87	9:0	200	.9320	22'33'455'66'	0.0000	0.0000
114	103.29	9:0	207	.9423	22'33'44'566'	0.0000	0.0000
115	105.3	0:2	194	.9620	22'33'44'55'	0.0607	0.0405
116	106.77	0:2	205	.9670	233'44'55'6	0.0000	0.0000
117	110.24	0:3	206	1.010	22'33'44'55'6	0.0000	0.0000
118	126.35	10:4	209	1.050	22'33'44'55'66'	0.0000	0.0000

CONCENTRATION = 2.38673
TOTAL RICHMONDES = 0.0000

AVERAGE MOLECULAR WEIGHT = 206.57000
NUMBER OF CALIBRATED PEARLS FOUND = 118

N.B.
21B

19.190
19.471
19.715
5. 20.235

6 21.170
7 21.499

10 22.123
22.599
23.000

14,15 - 23.211

17 - 24.017
24.719

21,22 - ~~24.027~~

25,24 - ~~24.027~~

26 25.230

31,32 - ~~25.901~~

37,38 - ~~26.466~~
26.737

42 27.111

46,47,48 - ~~27.733~~

53 - ~~28.152~~

61 - ~~28.800~~
29.082

69 - ~~29.631~~
29.976

74,75 - ~~30.615~~ 30.315

82 - ~~31.222~~
31.955

88 - ~~32.284~~ 31.950
32.564

94 - ~~33.100~~ 32.1
33.440

95 - ~~34.037~~
34.355

102 - ~~34.667~~
34.975

106 - 35.341
35.663

109 - 36.318

109 - 36.949

110 - 37.434

? 111 - 38.158

112 - 38.652 Int. std

113 - ~~39.131~~
39.370

115 - 40.731

41.742
42.022

117 - 44.176

21B

N.B 21B

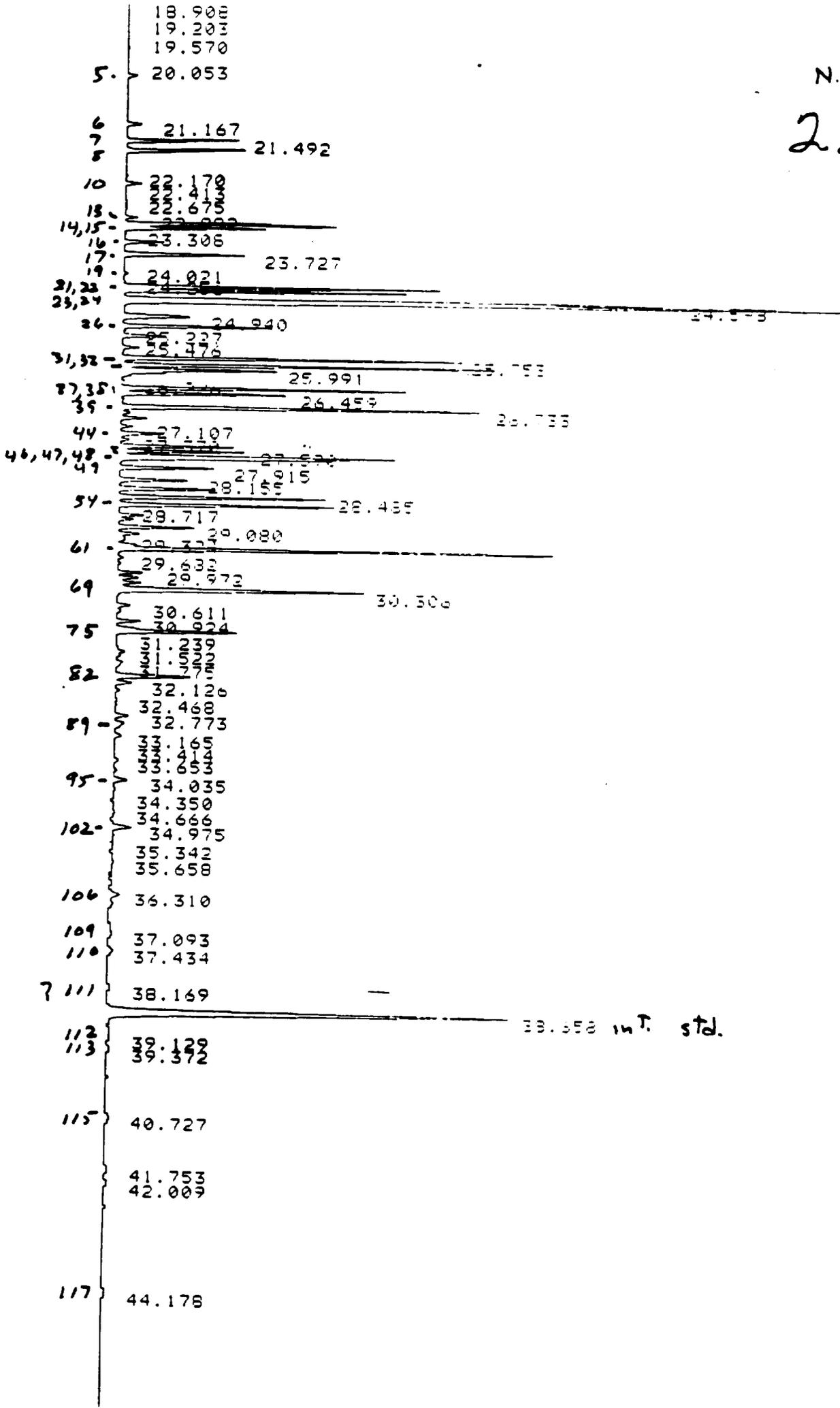
PEAK#	RET. TIME	T-CL:O-CL	IUPAC#	RTT	COMPOUNDS	WEIGHT %	ROLE #
1	40.39	0:0	000	.0997	BIPMENTL	0.0000	0.0000
2	46.72	1:1	001	.1504		0.0000	0.0000
3	50.29	1:0	002	.1937		0.0000	0.0000
4	50.63	1:0	003	.1975		0.0000	0.0000
5	52.31	2:2	004 010	.2245	22' 1 26	0.1945	0.2503
6	54.70	2:1	007 009	.2566	24' 1 23	0.0000	0.0000
7	59.97	2:1	006	.2709	23'	1.5007	2.1126
8	56.02	2:1	005 008	.2705	23' 1 24'	1.4111	1.0763
9	57.33	2:0	014	.2973	35	0.1971	0.2621
10	57.75	3:3	019	.3045	22'6	0.0162	0.0403
11	58.68	4:2	030	.3163	246	0.0209	0.0241
12	59.27	2:0	011	.3238	33'	0.1911	0.2341
13	59.46	2:0	012 013	.3297	34' 1 30'	0.3622	0.4817
14	59.79	3:2 2:0	010 015	.3307	22'5' 1 40'	3.9641	4.7601
15	60.02	3:2	017	.3398	22'6	2.0511	2.3630
16	60.7	3:2	024 027	.3508	236' 1 23'6	0.3317	0.3021
17	61.32	3:2	016 032	.3625	22' 3' 1 24'6	1.0473	2.1203
18	62.09	3:1	023	.3778	235	0.0315	0.0393
19	62.43	3:1 4:0	034 034	.3800	2' 35' 1 22'64'	0.0000	0.0000
20	62.72	3:1	029	.3820	245	0.0330	0.0390
21	62.97	3:1	026	.3911	23'5	3.3152	3.0195
22	63.18	3:1	025	.3937	23'6	2.0374	3.2690
23	63.39	3:1	031	.4024	24'5	3.6314	4.2067
24	63.72	3:1 4:3	020 050	.4031	244' 1 22'46	4.6492	5.3650
25	64.45	3:1 4:3	021 033	.4170	233' 1 234' 1 22'56'	1.6507	1.7260
26	64.99	3:1 4:0	022 051	.4267	234' 1 22'46'	1.2594	1.3771
27	65.48	4:3	045	.4334	22' 36	0.4504	0.4578
28	65.84	3:1	036	.4379	33'5	0.0000	0.0000
29	66.5	4:3	046	.4450	22' 36'	0.3620	0.3686
30	66.75	3:1	039	.4480	34'5	0.0000	0.0000
31	66.82	4:2	052 073	.4554	22' 55' 1 23'5'6	6.4591	6.5623
32	66.90	4:2	049	.4610	22' 45	4.0940	4.9722
33	67.22	4:2	047	.4639	22' 44'	2.0740	2.1071
34	67.5	4:2	048 075	.4651	22' 45' 1 244'6	0.1630	0.1644
35	67.6	4:2	045 062	.4665	234' 1 2356	0.0000	0.0000
36	67.81	3:0	035	.4730	33'6	0.0343	0.0396
37	68.17	3:4 4:2	104 044	.4832	22' 46' 1 22' 39'	3.2011	3.2404
38	68.45	3:0 4:2	037 042	.4870	344' 1 22' 34' 1 234'6	2.0967	2.1479
39	69.13	4:0	064 071	.4990	23' 34' 1 234'6 1 23'4'6	1.4931	1.7202
40	69.25	4:1	068	.5040	23' 45' 7	0.0000	0.0000
41	69.42	3:4	094	.5057	22' 366'	0.2292	0.2003
42	69.67	4:2	040	.5102	22' 33'	0.5274	0.5359
43	70.11	3:2 4:1	103 057	.5155	22' 45'6' 1 233'5	0.4120	0.4097
44	70.45	3:3 4:1	100 067	.5212	22' 44'6' 1 23'4'5	0.4120	0.3912
45	70.79	4:1	050 063	.5267	233' 5' 1 234'5	0.2245	0.2201
46	71.12	4:1 3:3	074 094	.5340	244' 5' 1 22' 306'	0.6709	0.6368
47	71.36	4:1	070 061	.5407	23' 4' 5' 1 2' 345' 1 24457	1.0821	1.5058
48	71.72	4:1 3:3	066 093	.5447	23' 44' 1 22' 356' 1 22' 35'6	4.9961	4.1963
49	72.18	3:3 4:1	091 090	.5549	22' 34'6' 1 22' 3'46' 1 244'6	1.3914	1.2770
50	72.81	4:1	056 060	.5676	233' 4' 1 2344'	0.4767	0.4403
51	73.25	4:4 3:3	155 084	.5666	22' 44'66' 1 22' 33'61 22' 385'	2.3532	2.1278
52	73.49	3:3	089	.5779	22' 346'	0.0000	0.0000
53	73.66	3:2	101 090	.5814	22' 34'5' 1 22' 455'	3.0502	3.5067
54	74.07	3:2	099	.5884	22' 44'5	2.0465	2.5072
55	74.39	4:4 3:2	150 112	.5969	22' 34'66' 1 233'56' 1 23'44'6	0.3948	0.3905
56	74.8	3:2	083 109	.6029	22' 33'5' 1 233'46	0.5030	0.5317
57	75.21	4:4 3:2	152 097	.6062	22' 3566' 1 22' 340' 1 22' 3'48	1.0948	0.6628
58	75.55	3:2	087 111	.6175	22' 305' 1 233'53' 1 2344'6	0.5773	0.5247
59	75.86	3:2	085 116	.6224	22' 306' 1 234967	0.3494	0.3139
60	76.09	4:4	136	.6257	22' 33'66'	0.0000	0.0132
61	76.5	4:0 3:2	077 110	.6295	33' 44' 1 233'4'6	5.0006	5.3449
62	76.76	3:3	154	.6349	22' 40'36'	0.0906	0.0811
63	77.05	3:2	082	.6434	22' 33'4	0.1711	0.1558
64	77.51	3:3	151	.6499	22' 355'6	0.5942	0.4804
65	77.77	4:3 3:1	135 124	.6563	22' 33'56' 1 2' 344'5	0.3105	0.4320
66	77.9	3:3	144	.6584	22' 349'6	0.0000	0.0000
67	78.43	3:1 4:3	107 100	.6628	233' 4' 5' 1 233' 45' 1 22' 34' 56	0.5656	0.4902
68	78.25	3:1	123	.6650	2' 344'5	0.0000	0.0000
69	78.49	4:3 3:1	149 114	.6672	22' 34' 5'6' 1 23' 44'5' 1 233' 45	5.3392	4.5101
70	78.58	4:3	149 140	.6707	22' 344'6' 1 22' 344'6'	0.0000	0.0000
71	79.17	4:3 3:1	134 103	.6796	22' 33'56' 1 22' 3456' 1 2344'5	0.3153	0.2006
72	79.51	3:1 4:3	122 131	.6871	2' 33' 45' 22' 33' 46' 22' 33' 55'6	0.1110	0.0975
73	80	4:2	146 161	.6950	22' 34' 55' 1 233' 45'6	0.4415	0.4451
74	80.36	4:3 3:1	132 105	.7039	22' 33' 44' 1 233' 44'	0.5672	0.3100
75	80.52	4:2	153	.7036	22' 44' 55'	0.3799	3.6166
76	81.40	4:2	148	.7040	23' 44' 5'6	0.0139	0.0113
77	81.52	4:2	141	.7203	22' 3433'	0.1966	0.1616
78	81.73	7:4	179	.7205	22' 33' 366'	0.1137	0.0853
79	82.07	4:2	130	.7284	22' 33' 45'	0.2312	0.1900
80	82.22	4:2	137	.7329	22' 304'5	0.2778	0.2204
81	82.35	7:4	176	.7309	22' 33' 466'	0.0000	0.0000
82	82.77	4:2	138 163	.7403	22' 304'5' 1 233' 4' 56' 1 2	2.1740	1.7671
83	85.06	4:2	156	.7429	233' 44'6	0.3202	0.2698
84	85.49	4:2	129	.7501	22' 33' 45	0.1622	0.1333
85	85.98	7:3	170	.7537	22' 33' 55'6	0.0463	0.0349
86	86.22	4:2	166	.7578	2344' 36	0.0067	0.0055
87	86.5	7:3	175	.7611	22' 33' 45'6	0.0061	0.0046
88	86.76	7:3	187 182	.7633	22' 34' 55'6' 1 22' 344' 56'	0.2303	0.1700
89	89.12	4:2	180	.7741	22' 33' 44'	0.4501	0.3766
90	89.4	7:3	183	.7720	22' 344' 5'6	0.0000	0.0000
91	89.77	4:1	167	.7814	23' 44' 35'	0.2704	0.2290
92	86.91	7:3	185	.7840	22' 3433'6	0.0201	0.0151
93	87.04	7:3	174 181	.7845	22' 33' 46' 1 22' 344' 56	0.1640	0.1234
94	87.5	7:3	177	.7831	22' 33' 4' 56	0.1364	0.1026
95	88.02	7:3 4:1	171 156	.7895	22' 33' 44'6' 1 233' 44'5	0.3605	0.3072
96	88.44	8:0	202	.7889	22' 33' 35'66'	0.0000	0.0000
97	88.55	4:1	157	.7894	233' 44' 5'	0.0000	0.0000
98	88.91	7:3	173	.7832	22' 33' 456	0.0000	0.0000
99	89.36	8:0	208 204	.7897	22' 33' 45'66' 1 22' 444' 566'	0.0000	0.0000
100	89.65	7:2	172 192	.7874	22' 33' 35' 1 233' 455'6	0.0623	0.0468
101	90.2	8:0	197	.8243	22' 33' 44' 66'	0.0000	0.0000
102	90.49	7:2	188	.8344	22' 344' 35'	0.3530	0.2644
103	90.84	7:2	193	.8397	233' 44' 35'6	0.0133	0.0100
104	91.21	7:2	191	.8447	233' 44' 3'6	0.0047	0.0036
105	92.21	8:0	199	.8494	22' 33' 4566'	0.0162	0.0112
106	94.7	7:2	170	.8740	22' 33' 44' 5	0.2179	0.1635
107	94.5	7:2	198	.8740	233' 44' 36	0.0620	0.0471
108	95.63	8:3	198	.8843	22' 33' 45'6	0.0000	0.0000
109	95.7	8:3	201	.8875	22' 33' 4' 35'6	0.0635	0.0430
110	96.0	8:3	194 203	.8935	22' 33' 44' 5'6' 1 22' 344' 55'6	0.0700	0.0330
111	96.72	8:1	195	.9140	233' 44' 35'	0.0000	0.0000
112	101.25	9:1	195	.9321	22' 33' 44' 56	0.0000	0.0000
113	101.07	9:4	200	.9320	22' 33' 45' 66'	0.0000	0.0000
114	103.29	9:4	207	.9423	22' 33' 44' 366'	0.0000	0.0000
115	103.37	8:2	194	.9420	22' 33' 44' 35'	0.0000	0.0000
116	106.77	8:2	203	.9670	233' 44' 35'6	0.0000	0.0000
117	114.2	9:3	206	1.0110	22' 33' 44' 38'6	0.0099	0.0044
118	126.35	10:4	209	1.0500	22' 33' 44' 55' 66'	0.0000	0.0000

CONCENTRATION = 2.705922
TOTAL MICROMOLES = 0.0091

AVERAGE MOLECULAR WEIGHT = 296.66582
NUMBER OF CALIBRATED PEAKS FOUND = 118

N. B.

22A



33.658 int. std.

22A

NB 22 A

PEARL	MLT. TIME	T-CLIO-CL	IUPACR	ART	CONDENSERS	WEIGHT %	ROLE %
1	40.6	0:0	000	.0997	01PHEMTL	0.0000	0.0000
2	46.62	1:1	001	.1544	2	0.2681	0.3905
3	50.19	1:0	002	.1937	3	0.0000	0.0000
4	50.58	1:0	003	.1975	4	0.1700	0.2635
5	52.29	2:2	004 010	.2245	22' 1 26	1.0074	2.3022
6	54.72	2:1	007 009	.2566	24 1 25	0.6250	0.7799
7	55.50	2:1	006	.2709	23'	3.6033	4.4927
8	56.07	2:1	005 008	.2705	23 1 20'	3.7617	4.6876
9	57.31	2:0	014	.2973	35	0.0910	0.0646
10	57.75	0:8	019	.3045	22'6	0.6729	0.7265
11	58.01	0:2	030	.3165	206	0.0240	0.0260
12	59.02	2:0	011	.3238	33'	0.5278	0.6573
13	59.46	2:0	012 013	.3297	30 1 30'	0.6450	0.8048
14	59.79	3:2 2:0	018 015	.3387	22'5 1 04'	7.7882	8.7507
15	60	0:2	017	.3398	22'0	4.0730	4.3975
16	60.7	0:2	024 027	.3508	236 1 23'6	0.7550	0.8161
17	61.35	0:2	016 032	.3625	22'3 1 20'6	2.2532	2.4349
18	62.1	3:1	023	.3770	235	0.0079	0.0085
19	62.43	3:1 4:4	030 054	.3800	2'35 1 22'66'	0.0000	0.0000
20	62.72	3:1	029	.3820	245	0.0312	0.0336
21	62.98	3:1	026	.3911	23'5	4.2047	4.5828
22	63.16	3:1	025	.3937	23'4	3.9792	4.2962
23	63.4	3:1	031	.4024	20'5	6.7102	7.2491
24	63.77	3:1 4:3	028 050	.4031	200' 1 22'06	0.0000	0.0000
25	64.48	3:1 4:3	021 033	.4170	233' 1 230 1 22'56'	1.5510	1.5125
26	64.99	3:1 4:3	022 051	.4267	230' 1 22'06'	1.2069	1.3167
27	65.49	4:3	049	.4334	22'36	0.0371	0.7978
28	65.72	3:1	036	.4379	33'5	0.0268	0.0289
29	66.05	4:3	046	.4450	22'36'	0.6678	0.6350
30	66.45	3:1	039	.4488	34'5	0.0000	0.0000
31	66.6	4:2	052 073	.4554	22'55' 1 23'5'6	6.5243	6.2118
32	66.96	4:2	049	.4618	22'45	5.4083	5.1493
33	67.19	4:2	047	.4639	22'44'	2.4557	2.3381
34	67.35	4:2	048 075	.4651	22'45 1 240'6	0.6650	0.6530
35	67.6	4:2	065 042	.4865	23'6 1 2356	0.0000	0.0000
36	67.81	3:0	035	.4758	33'4	0.1264	0.1365
37	68.15	5:0 4:2	109 044	.4832	22'46' 1 22'35'	3.3986	3.2320
38	68.41	3:0 4:2	037 042	.4870	344' 1 22'30' 1 233'6	2.7855	2.6741
39	69.13	4:2	064 071	.4990	23'34 1 230'6 1 23'0'6 +	3.1665	3.0339
40	69.25	4:1	068	.5040	23'45' 7	0.0000	0.0000
41	69.34	5:0	096	.5057	22'366'	0.3026	0.2577
42	69.68	4:2	040	.5102	22'33'	0.3756	0.3578
43	70.09	5:3 4:1	103 057	.5155	22'45'6 1 233'5	0.1034	0.1706
44	70.45	5:3 4:1	100 067	.5212	22'44'6 1 23'0'5	0.0122	0.7221
45	70.76	4:1	090 063	.5267	233'5' 1 230'5	0.1017	0.1349
46	71.1	4:1 5:6	074 094	.5340	200'5 1 22'356'	1.2172	1.0822
47	71.33	4:1	070 061	.5407	23'4'5 1 2'005 1 24457	1.3195	1.4467
48	71.62	4:1 5:3	048 095	.5447	23'44' 1 22'356 1 22'38'6	2.4662	2.4662
49	72.19	5:3 4:1	091 090	.5544	22'34'6 1 22'3'06 1 233'0	1.3346	1.1485
50	72.81	4:1	056 060	.5676	233'0' 1 2300'	0.7778	0.7405
51	73.25	6:4 5:3	155 084	.5666	22'44'66' 1 22'33'61 22'355'	1.2612	1.0853
52	73.49	5:3	089	.5779	22'346'	0.0000	0.0000
53	73.66	5:2	101 090	.5814	22'34'5 1 22'455'	2.3772	2.1932
54	74.05	5:2	099	.5880	22'40'5	2.5649	2.1846
55	74.59	6:4 5:2	150 112	.5969	22'34'66' 1 233'56 1 22'44'6	0.2648	0.2253
56	74.8	5:2	083 109	.6029	22'33'5 1 233'06	0.2696	0.2262
57	75.21	6:4 5:2	152 097	.6062	22'3566' 1 22'345 1 22'3'05	0.7782	0.6524
58	75.52	5:2	087 111	.6175	22'345' 1 233'55' 1 2340'6	0.1613	0.1374
59	75.83	5:2	085 116	.6225	22'340' 1 230467	0.0580	0.0443
60	76.09	6:4	136	.6257	22'33'66'	0.3019	0.2326
61	76.3	4:0 5:2	077 110	.6295	33'00' 1 233'0'6	3.2463	2.7651
62	76.77	6:3	134	.6344	22'40'56'	0.0756	0.0503
63	77.02	5:2	082	.6453	22'33'0	0.0200	0.0230
64	77.52	6:3	151	.6499	22'355'6	0.3312	0.2552
65	77.75	6:3 5:1	135 124	.6563	22'33'56' 1 2'344'5	0.2904	0.2303
66	77.9	6:3	144	.6584	22'30'6	0.0000	0.0000
67	78.03	5:1 6:3	107 109	.6628	233'0'5 1 233'05' 1 22'30'56	0.3393	0.2801
68	78.25	5:1	123	.6658	2'300'5	0.0000	0.0000
69	78.47	6:3 5:1	149 118	.6672	22'30'5'6 1 23'40'5 1 233'05	3.0904	2.4587
70	78.55	6:3	139 140	.6707	22'300'6 1 22'300'6	0.0000	0.0000
71	79.17	6:3 5:1	134 143	.6796	22'33'56' 1 22'3056' 1 2300'5	0.1665	0.1555
72	79.46	5:1 6:3	122 131	.6871	2'33'451 22'33'06122'33'55'	0.0644	0.0542
73	79.9	6:2	146 161	.6955	22'30'55' 1 233'45'6	0.3019	0.2325
74	80.4	6:3 5:1	132 105	.7035	22'33'06' 1 233'00'	0.7141	0.6017
75	80.7	6:2	153	.7036	22'40'55'	0.0062	0.0063
76	81.2	6:2	160	.7068	25'00'5'6	0.0128	0.0099
77	81.5	6:2	141	.7204	22'3055'	0.0603	0.0464
78	81.7	7:4	179	.7205	22'33'566'	0.0000	0.0000
79	82	6:2	140	.7284	22'33'05'	0.1023	0.0780
80	82.2	6:2	137	.7329	22'340'5	0.0541	0.0417
81	82.35	7:4	176	.7385	22'43'666'	0.0000	0.0000
82	82.7	6:2	138 163	.7483	22'304'5' 1 233'0'56 1 +2	0.7371	0.5678
83	83	6:2	158	.7429	233'00'6	0.1670	0.1293
84	83.4	6:2	129	.7501	22'33'05	0.0500	0.0447
85	83.9	7:3	178	.7537	22'33'55'6	0.0390	0.0274
86	84.25	6:2	166	.7572	2300'56	0.0000	0.0000
87	84.5	7:3	175	.7611	22'33'05'6	0.0113	0.0080
88	84.7	7:3	187 182	.7653	22'34'55'6 1 22'340'56'	0.1518	0.1068
89	85.1	6:2	120	.7761	22'33'00'	0.1367	0.1053
90	85.4	7:3	184	.7724	22'300'5'6	0.0000	0.0000
91	85.7	6:1	167	.7814	23'00'55'	0.2159	0.1663
92	86.4	7:3	185	.7808	22'3455'6	0.0105	0.0074
93	87	7:3	174 181	.7963	22'33'056' 1 22'340'56	0.0972	0.0404
94	87.5	7:3	177	.8031	22'33'0'06	0.0407	0.0287
95	88	7:3 6:1	171 156	.8105	22'33'00'6 1 224'00'5	0.1590	0.1197
96	88.4	8:4	202	.8089	22'33'55'66'	0.0203	0.0131
97	88.55	6:1	157	.8104	233'00'5	0.0000	0.0000
98	88.8	7:3	173	.8152	22'33'056	0.0021	0.0013
99	89.3	8:4	200 204	.8197	22'33'05'66' 1 22'300'566'	0.0062	0.0040
100	89.68	7:2	172 192	.8278	22'33'055' 1 233'055'6	0.0000	0.0000
101	90.2	8:4	197	.8293	22'33'00'66'	0.0000	0.0000
102	90.4	7:2	188	.8362	22'340'55'	0.1699	0.1193
103	90.8	7:2	193	.8397	233'00'55'6	0.0107	0.0075
104	91.4	7:2	191	.8447	233'00'5'6	0.0004	0.0021
105	92.2	8:4	199	.8494	22'33'0566'	0.0168	0.0109
106	93.9	7:2	170	.8748	22'33'04'5	0.0901	0.0662
107	94.3	7:2	190	.8748	233'00'56	0.0332	0.0247
108	95.63	8:3	194	.8845	22'33'055'6	0.0000	0.0000
109	95.9	8:3	201	.9073	22'33'0'35'6	0.0340	0.0216
110	96.8	8:3	196 203	.8935	22'33'00'5'6 1 22'300'55'6	0.0417	0.0269
111	98.7	7:1	184	.9142	233'00'55'	0.0050	0.0040
112	101.2	8:3	195	.9321	22'33'00'56	0.0076	0.0049
113	101.4	9:4	204	.9328	22'33'055'66'	0.0017	0.0022
114	103.2	9:4	207	.9423	22'33'00'566'	0.0000	0.0000
115	105.3	8:2	194	.9628	22'33'04'35'	0.0333	0.0218
116	106.77	8:2	205	.9678	233'00'55'6	0.0000	0.0000
117	110.2	9:3	206	1.018	22'33'04'55'6	0.0408	0.0287
118	126.85	10:4	209	1.058	22'33'04'55'66'	0.0000	0.0000

CONCENTRATION = 2.302769
TOTAL MICROMOLEX = 0.8104

AVERAGE MOLECULAR WEIGHT = 270.81408
NUMBER OF CALIBRATED PEARLS FOUND = 118

N. B.
22B

5
100.951
100.100
19.562
19.842
20.222

6
21.160
21.484

10
22.102
22.397
23.874

14, 15
23.464 23.192
17
23.716

21, 22
24.006
24.931

31, 32
25.219
25.511
25.838

37, 38
26.215
26.451
26.716

44
27.095

46, 47, 48
27.000
27.141

54
28.705
29.067

61
29.069
29.960
30.269

75
30.602
30.913
31.229
31.510

82
31.993

88
32.264
32.549
32.909
33.246
33.541

95
34.021

102
34.511
34.962

35.322
35.650

106
36.296

109
37.078
110
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39.365

115
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41.747

117
44.158

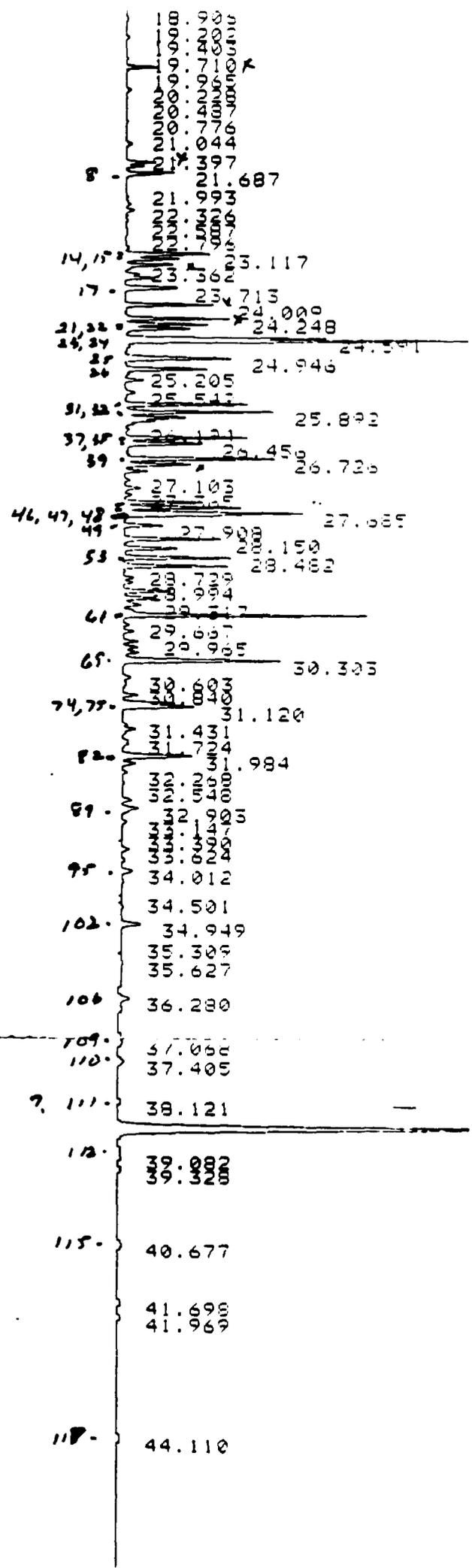
22B

N.B 22B

PLANN	HLT. TIME	I-CL:O-CL	IUPAC9	RRY	CONDENSERS	WEIGHT B	ROLE B
1	40.62	0:0	000	.0997	BIPHENYL	0.0000	0.0000
2	46.6	1:1	001	.1304	2	0.2132	0.3107
3	50.19	1:0	002	.1937	3	2.0010	4.1069
4	50.58	1:0	003	.1979	4	0.2670	0.4301
5	52.32	2:2	004 010	.2245	22' 1 26	1.0549	1.3334
6	54.75	2:1	007 009	.2564	24' 1 25	0.3133	0.3960
7	55.50	2:1	006	.2709	23'	2.1700	2.7427
8	56.07	2:1	005 008	.2785	23' 1 24'	2.5527	3.2263
9	57.52	2:0	014	.2973	35	0.1251	0.1501
10	57.75	3:3	019	.3045	22'6	1.1039	1.2960
11	58.01	4:2	030	.3165	246	0.0159	0.0170
12	59.20	2:0	011	.3230	33'	0.2120	0.2602
13	59.44	2:0	012 013	.3297	34' 1 30'	0.4350	0.5509
14	59.8	3:2 2:0	010 015	.3307	22'5' 1 44'	5.2932	6.0306
15	60.01	3:2	017	.3390	22'4	2.9679	3.2497
16	60.7	3:2	024 027	.3500	236' 1 23'6	0.9146	0.9635
17	61.35	3:2	016 032	.3625	22'3' 1 20'6	1.7649	1.9320
18	62.1	3:1	025	.3770	235	0.0127	0.0139
19	62.31	3:1 4:0	034 034	.3800	2'35' 1 22'66'	0.0697	0.0734
20	62.72	3:1	029	.3820	245	0.0301	0.0329
21	62.98	3:1	026	.3911	23'5	2.7051	3.0500
22	63.16	3:1	025	.3937	23'4	2.3245	2.9455
23	63.6	3:1	031	.4024	24'5	0.6411	0.6624
24	63.73	3:1 4:3	020 050	.4031	244' 1 22'46	6.1712	6.7000
25	64.51	3:1 4:3	021 033	.4170	233' 1 234' 1 22'56'	1.5501	1.5332
26	65	3:1 4:3	022 051	.4267	234' 1 22'46'	1.0720	1.1151
27	65.49	4:3	045	.4334	22'36	0.6093	0.3036
28	65.84	3:1	036	.4379	33'5	0.0000	0.0000
29	66.09	4:3	046	.4450	22'36'	0.5023	0.4451
30	66.45	3:1	039	.4480	34'5	0.0000	0.0000
31	66.61	4:2	052 073	.4554	22'55' 1 23'5'6	5.3690	5.1657
32	66.97	4:2	049	.4610	22'45	4.5000	4.3461
33	67.2	4:2	047	.4639	22'44'	2.2649	2.1916
34	67.36	4:2	048 075	.4651	22'45 1 244'6	0.5021	0.5622
35	67.6	4:2	065 062	.4865	2346' 1 2356	0.0000	0.0000
36	67.82	3:0	035	.4730	33'4	0.1102	0.1207
37	68.13	5:0 4:2	104 044	.4832	22'466' 1 22'35'	2.5414	2.4514
38	68.44	3:0 4:2	037 042	.4870	344' 1 22'30' 1 230'6	2.2070	2.1494
39	69.12	4:2	064 071	.4990	23'34' 1 234'6 1 23'4'6	2.2490	3.1726
40	69.25	4:1	068	.5040	23'45' 7	0.0000	0.0000
41	69.4	5:0	096	.5057	22'366'	0.2207	0.1974
42	69.66	4:2	040	.5102	22'33'	0.2036	0.2739
43	70.1	5:3 4:1	103 057	.5155	22'45'6 1 234'5	0.2213	0.2000
44	70.46	5:3 4:1	100 067	.5212	22'44'6 1 23'4'5	0.9160	0.8260
45	70.77	4:1	050 063	.5267	23'5' 1 234'5	0.1100	0.1101
46	71.11	4:1 5:0	074 094	.5340	244'5 1 22'306'	1.8217	0.9213
47	71.34	4:1	070 061	.5407	23'4'5 1 2'345 1 24457	1.6774	1.6199
48	71.63	4:1 5:0	064 095	.5447	23'44' 1 22'356 1 22'45'6	3.0157	2.1803
49	72.17	5:3 4:1	091 098	.5544	22'34'6 1 22'3'46 1 231'4	1.6302	1.4039
50	72.82	4:1	056 060	.5676	233'4' 1 2344'	0.6607	0.6601
51	73.23	6:4 5:3	155 084	.5664	22'44'66' 1 22'33'6 1 22'355'	1.4797	1.2712
52	73.49	5:3	089	.5779	22'346'	0.0000	0.0000
53	73.67	5:2	101 090	.5814	22'34'5 1 22'455'	3.6442	3.1404
54	74.06	5:2	099	.5880	22'44'5	3.8796	3.3514
55	74.61	6:4 5:2	150 112	.5969	22'34'66' 1 233'56 1 23'44'6	0.3906	0.3404
56	74.79	5:2	084 109	.6029	22'33'5 1 233'46	0.2030	0.2400
57	75.2	6:4 5:2	152 097	.6062	22'3566' 1 22'345 1 22'3'45	0.9949	0.8847
58	75.54	5:2	087 111	.6175	22'345' 1 233'55' 1 2344'6	0.1477	0.1276
59	75.85	5:2	085 116	.6224	22'344' 1 234567	0.0233	0.0201
60	76.11	6:4	136	.6257	22'33'66'	0.4003	0.3191
61	76.3	4:0 5:2	077 110	.6295	33'44' 1 233'4'6	3.9700	3.4371
62	76.7	6:3	154	.6349	22'44'66'	0.1250	0.1013
63	77	5:2	082	.6453	22'33'4	0.0113	0.0097
64	77.5	6:3	151	.6494	22'325'6	0.4357	0.3405
65	77.7	6:3 5:1	135 124	.6563	22'33'56' 1 2'344'5	0.3574	0.2873
66	77.9	6:3	144	.6584	22'345'6	0.0000	0.0000
67	78	5:1 6:3	107 100	.6620	233'4'5 1 233'45' 1 22'34'56	0.4350	0.3632
68	78.3	5:1	123	.6658	2'344'5	4.7672	4.1105
69	78.41	6:3 5:1	149 118	.6672	22'34'5'6 1 23'44'5 1 233'45	0.0000	0.0000
70	78.55	6:3	139 140	.6707	22'34'56' 1 22'344'6	0.0000	0.0000
71	79.1	6:3 5:1	134 143	.6796	22'33'56' 1 22'3456' 1 2344'5	0.2201	0.1862
72	79.4	5:1 6:3	122 131	.6871	2'33'45' 1 22'33'46 1 22'33'58'	0.0001	0.0044
73	79.4	6:2	146 161	.6955	22'34'55' 1 233'45'6	0.4000	0.3163
74	80.55	6:3 5:1	152 105	.7035	22'33'46' 1 233'44'	0.0000	0.0000
75	80.5	6:2	153	.7036	23'44'55'	3.9966	3.1243
76	81.3	6:2	148	.7060	23'44'5'6	0.0160	0.0129
77	81.5	6:2	141	.7203	22'3458'	0.0000	0.0000
78	81.7	7:0	179	.7205	22'33'564'	0.1139	0.0816
79	82	6:2	138	.7204	22'33'45'	0.1152	0.0904
80	82.2	6:2	137	.7329	22'344'5	0.0000	0.0000
81	82.3	7:0	176	.7305	22'33'464'	0.0033	0.0023
82	82.7	6:2	130 163	.7403	22'344'5' 1 233'4'56 1 2	0.7672	0.5993
83	83	6:2	150	.7429	233'44'6	0.1546	0.1200
84	84.4	6:2	129	.7501	22'33'45	0.0000	0.0000
85	84.9	7:3	178	.7537	22'33'55'6	0.0501	0.0350
86	84.2	6:2	164	.7572	2344'56	0.0116	0.0091
87	84.4	7:3	175	.7611	22'33'45'6	0.0016	0.0000
88	84.7	7:3	167 182	.7653	22'34'55'6 1 22'344'56'	0.2146	0.1530
89	85.1	6:2	126	.7761	22'33'44'	0.0532	0.0416
90	85.6	7:3	183	.7720	22'344'5'6	0.0647	0.0461
91	85.7	6:1	167	.7814	23'44'55'	0.2606	0.2036
92	86.4	7:3	185	.7800	22'3458'6	0.0127	0.0091
93	87	7:3	174 181	.7965	22'33'456' 1 22'444'56	0.0000	0.0000
94	87.5	7:3	177	.8031	22'33'4'56	0.0273	0.0275
95	88.1	7:3 6:1	171 156	.8109	22'33'44'6 1 233'44'5	0.0000	0.0000
96	88.44	8:4	202	.8009	22'33'55'66'	0.0000	0.0000
97	88.5	6:1	157	.8184	233'44'5'	0.0159	0.0124
98	88.91	7:3	173	.8152	22'33'456	0.0000	0.0000
99	89.3	6:4	200 204	.8197	22'33'45'66' 1 22'444'566'	0.0056	0.0053
100	89.6	7:2	172 192	.8274	22'33'458' 1 233'455'6	0.0353	0.0252
101	90.2	6:4	197	.8293	22'33'44'66'	0.0000	0.0000
102	90.4	7:2	180	.8362	22'344'58'	0.1750	0.1254
103	90.91	7:2	193	.8397	233'4'58'6	0.0000	0.0000
104	91.4	7:2	191	.8447	233'44'5'6	0.0050	0.0042
105	92.2	6:4	199	.8494	22'33'4566'	0.0148	0.0100
106	94.9	7:2	170	.8740	22'33'44'5	0.7709	0.5564
107	94.4	7:2	190	.8740	233'44'56	0.0000	0.0200
108	95.63	8:3	198	.8845	22'33'455'6	0.0000	0.0000
109	95.9	8:3	201	.8875	22'33'4'55'6	0.0350	0.0235
110	96.8	8:3	196 203	.8935	22'33'44'5'6 1 22'444'55'6	0.0577	0.0379
111	98.7	7:1	149	.9142	233'44'55'	0.0004	0.0003
112	101.2	8:3	195	.9321	22'33'44'56	0.0123	0.0081
113	101.9	9:0	208	.9320	22'33'455'66'	0.0015	0.0009
114	103.29	9:0	207	.9423	22'33'44'566'	0.0000	0.0000
115	103.3	8:2	194	.9420	22'33'44'58'	0.0452	0.0297
116	104.0	8:2	203	.9670	233'44'58'6	0.0000	0.0000
117	114.2	9:3	204	1.810	22'33'44'58'6	0.0729	0.0403
118	124.35	10:0	209	1.850	22'33'44'55'66'	0.0000	0.0000

CONCENTRATION = 3.027572
 TOTAL MICROMOLES = 0.0107
 AVERAGE MOLECULAR WEIGHT = 201.98793

N. B.
24 A



38.604 int. std.

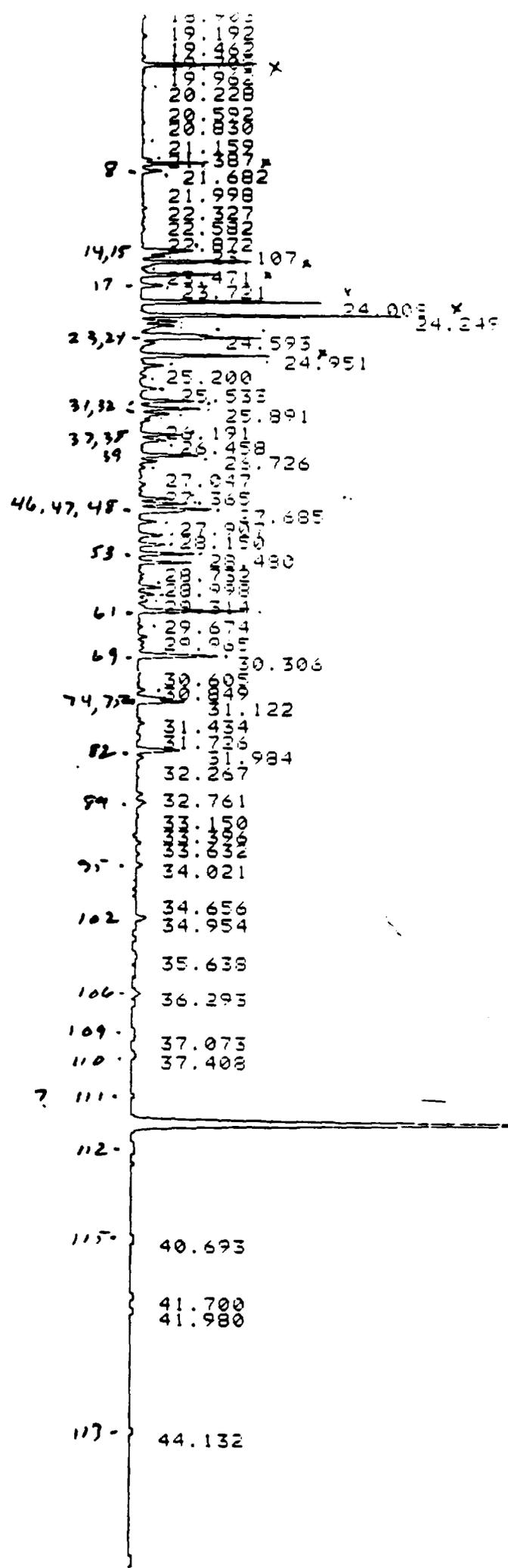
24 A

NB. 24A

PEAR#	MLI. TIME	I-CL:O-CL	IUMACH	RRT	CONGENERS	WEIGHT %	ROLE %
1	40.8	0:0	000	.0997	BIMENTYL	0.0000	0.0000
2	40.62	1:1	001	.1944		13.3520	18.7600
3	50.46	1:0	002	.1937		10.3625	13.6770
4	50.61	1:0	003	.1975		0.2903	0.3913
5	52.32	2:2	004 010	.2245	22' : 26'	1.1125	1.2440
6	54.75	2:1	007 009	.2564	24 : 25	0.3273	0.3732
7	55.6	2:1	006	.2789	23'	1.2557	1.4310
8	56.09	2:1	005 00A	.2709	21' : 24'	1.0770	1.2546
9	57.30	2:0	014	.2974	35	0.0315	0.0360
10	57.75	2:3	019	.3045	22' 6	0.4064	0.4015
11	58.74	2:2	030	.3163	24	0.0751	0.0732
12	59.21	2:0	011	.3230	31'	0.0000	0.0000
13	59.49	2:0	012 013	.3297	34' : 30'	0.2347	0.2499
14	59.8	3:2 2:0	016 015	.3387	22' 5 : 44'	4.7663	4.9051
15	60.03	3:2	017	.3390	22' 0	1.9054	1.9614
16	60.73	3:2	024 027	.3500	236 : 23' 6	0.3244	0.3205
17	61.35	3:2	016 032	.3625	22' 3 : 24' 6	1.4966	1.4704
18	62.1	3:1	023	.3770	235	2.0106	1.9941
19	62.31	3:1 4:3	034 034	.3800	2' 35 : 22' 66'	0.0492	0.0460
20	62.72	3:1	029	.3820	245	1.7507	1.7374
21	62.90	3:1	026	.3911	23' 5	1.5021	1.4839
22	63.19	3:1	025	.3937	23' 4	1.4024	1.4644
23	63.6	3:1	031	.4024	24' 5	3.0373	3.0005
24	63.73	3:1 4:3	028 030	.4031	244' : 22' 46	4.4639	4.3900
25	64.55	3:1 4:3	021 033	.4170	233' : 234' : 22' 36'	2.4927	2.2241
26	65	3:1 4:3	022 031	.4267	234' : 22' 46'	1.0633	0.9970
27	65.49	4:3	045	.4334	22' 36	0.4026	0.4204
28	65.84	3:1	036	.4379	33' 5	0.0000	0.0000
29	66.09	4:3	044	.4450	22' 36'	0.6127	0.5338
30	66.45	3:1	039	.4480	34' 5	0.0000	0.0000
31	66.63	4:2	052 073	.4554	22' 55' : 23' 5' 6	3.2542	2.8349
32	66.99	4:2	049	.4610	22' 45	2.0620	2.4933
33	67.23	4:2	047	.4639	22' 44'	1.3375	1.1652
34	67.30	4:2	048 075	.4651	22' 45 : 244' 6	0.5995	0.5222
35	67.51	4:2	045 062	.4865	2346 : 2356	0.1159	0.1009
36	67.77	3:0	055	.4738	33' 0	0.1967	0.1943
37	68.16	3:4 4:2	104 044	.4832	22' 46' 6 : 22' 35'	2.0145	1.7529
38	68.40	3:0 4:2	037 042	.4870	344' : 22' 34' : 233' 6	2.0330	1.7050
39	68.93	4:2	044 071	.4990	23' 34 : 234' 6 : 23' 4' 6	0.0420	0.0373
40	69.25	4:1	040	.5040	23' 45' 7	0.0000	0.0000
41	69.4	3:4	046	.5057	22' 36' 6'	2.2401	1.7450
42	69.71	4:2	040	.5102	22' 33'	0.4361	0.3799
43	70.13	3:5 4:1	103 057	.5155	22' 45' 6 : 233' 5	0.1542	0.1312
44	70.46	3:5 4:1	100 047	.5212	22' 44' 6 : 23' 4' 5	0.3990	0.3253
45	70.8	4:1	054 063	.5267	233' 5' : 234' 5	0.1629	0.1419
46	71.13	4:1 3:3	074 094	.5340	244' 5 : 22' 35' 6	1.0003	0.8700
47	71.37	4:1	070 061	.5407	23' 4' 5 : 2' 34' 5 : 244' 57	1.9277	1.6794
48	71.63	4:1 3:3	046 095	.5447	23' 44' : 22' 35' 6 : 22' 35' 6	3.4967	2.7340
49	72.2	3:3 4:1	091 048	.5549	22' 34' 6 : 22' 3' 46 : 244' 0	0.7368	0.5955
50	72.82	4:1	056 060	.5676	233' 4' : 2344'	1.4310	1.2470
51	73.26	4:4 3:3	154 084	.5664	22' 44' 66' : 22' 33' 6 : 22' 35' 6	0.9290	0.7206
52	73.44	3:3	089	.5779	22' 34' 6	0.0000	0.0000
53	73.7	3:2	101 090	.5814	22' 34' 5 : 22' 45' 6	1.0007	1.4720
54	74.09	3:2	099	.5880	22' 44' 5	1.3774	1.2293
55	74.6	4:4 3:2	150 112	.5969	22' 34' 66' : 233' 36 : 23' 44' 6	0.1629	0.1270
56	74.81	3:2	083 109	.6029	22' 33' 5 : 233' 46	0.2214	0.1725
57	75.22	4:4 3:2	152 097	.6062	22' 35' 66' : 22' 34' 9 : 22' 3' 45	0.6420	0.4976
58	75.34	3:2	087 111	.6175	22' 34' 5 : 233' 55' : 2344' 6	0.3251	0.2534
59	75.80	3:2	085 114	.6224	22' 34' 4 : 234567	0.2462	0.1919
60	76.1	4:4	136	.6257	22' 33' 66'	0.2005	0.1470
61	76.31	4:0 3:2	077 110	.6295	33' 44' : 233' 4' 6	2.3193	1.0075
62	76.75	4:5	154	.6349	22' 44' 56'	0.1064	0.0790
63	77.06	3:2	082	.6453	22' 33' 4	0.1221	0.0952
64	77.5	4:5	151	.6499	22' 35' 6	0.2731	0.1925
65	77.7	4:3 3:1	135 124	.6563	22' 33' 56' : 2' 344' 5	0.2495	0.1811
66	77.9	4:3	144	.6584	22' 34' 6	0.0000	0.0000
67	78	3:1 4:3	107 108	.6620	233' 4' 5 : 233' 45' : 22' 34' 56	0.2067	0.2165
68	78.25	3:1	123	.6650	2' 344' 5	0.0000	0.0000
69	78.4	4:3 3:1	149 110	.6674	22' 34' 5' 6 : 23' 44' 5 : 233' 45	2.5241	1.6315
70	78.55	4:3	139 140	.6707	22' 344' 6 : 22' 344' 6	0.0000	0.0000
71	79.1	4:3 3:1	134 143	.6796	22' 33' 56' : 22' 3456' : 2344' 5	0.1514	0.1155
72	79.4	3:1 4:3	172 131	.6871	22' 33' 45 : 22' 33' 44 : 22' 34' 55' 6	0.0566	0.0423
73	79.9	4:2	146 141	.6955	22' 34' 55' : 233' 45' 6	0.2294	0.1617
74	80.3	4:3 3:1	132 105	.7035	22' 33' 46' : 233' 44'	0.3425	0.2641
75	80.5	4:2	153	.7036	22' 44' 55'	2.2203	1.5706
76	81.3	4:2	140	.7040	23' 44' 5' 6	0.0437	0.0300
77	81.5	4:2	141	.7204	22' 3455'	0.1060	0.0707
78	81.7	7:4	179	.7205	22' 33' 56' 6	0.0049	0.0546
79	82	4:2	140	.7204	22' 33' 45'	0.0994	0.0702
80	82.2	4:2	137	.7329	22' 344' 5	0.1437	0.1013
81	82.35	7:4	176	.7383	22' 33' 46' 6	0.0000	0.0000
82	82.7	4:2	130 163	.7403	22' 344' 5' : 233' 4' 56 : 4' 2	0.9401	0.6626
83	83	4:2	144	.7429	233' 44' 6	0.1733	0.1221
84	83.4	4:2	129	.7501	22' 33' 45	0.0041	0.0593
85	83.9	7:3	174	.7537	22' 33' 55' 6	0.0253	0.0163
86	84.25	4:2	144	.7572	2344' 56	0.0000	0.0000
87	84.4	7:3	175	.7611	22' 33' 55' 6	0.0000	0.0000
88	84.7	7:3	187 182	.7633	22' 34' 55' 6 : 22' 344' 56'	0.1533	0.0907
89	85.1	4:2	128	.7761	22' 33' 44'	0.2257	0.1591
90	85.4	7:3	183	.7770	22' 344' 5' 6	0.0000	0.0000
91	85.7	4:1	147	.7814	23' 44' 55'	0.1533	0.1001
92	86.04	7:3	189	.7840	22' 3455' 6	0.0000	0.0000
93	87	7:4	174 181	.7945	22' 33' 456' : 22' 344' 56	0.0993	0.0640
94	87.4	7:3	177	.8031	22' 33' 4' 56	0.0743	0.0479
95	88	7:3 6:1	171 156	.8109	22' 33' 44' 6 : 234' 44' 5	0.1052	0.1269
96	88.4	4:4	202	.8409	22' 33' 55' 66'	0.0255	0.0191
97	88.55	4:1	157	.8104	233' 44' 5'	0.0000	0.0000
98	89.91	7:3	174	.8152	22' 33' 456	0.0000	0.0000
99	89.36	4:4	200 204	.8197	22' 33' 45' 66' : 22' 344' 566'	0.0000	0.0000
100	89.6	7:2	172 192	.8270	22' 33' 45' 6 : 233' 45' 6	0.0411	0.0264
101	90.2	4:4	197	.8293	22' 33' 44' 66'	0.0000	0.0000
102	90.4	7:2	140	.8364	22' 344' 55'	0.2721	0.1429
103	90.8	7:2	193	.8397	233' 4' 55' 6	0.0862	0.0440
104	91.44	7:2	191	.8447	233' 44' 5' 6	0.0000	0.0000
105	92.1	4:4	199	.8494	22' 33' 4566'	0.0257	0.0152
106	93.0	7:2	170	.8740	22' 33' 44' 5	1.1229	0.0793
107	94.3	7:2	190	.8740	233' 44' 56	0.0347	0.0223
108	95.63	4:3	190	.8849	22' 33' 455' 6	0.0000	0.0000
109	95.9	4:3	201	.8875	22' 33' 4' 55' 6	0.0429	0.0254
110	96.7	4:3	194 203	.8935	22' 33' 44' 5' 6 : 22' 444' 55' 6	0.0545	0.0322
111	98.72	7:1	189	.9102	233' 44' 55'	0.0000	0.0000
112	101.23	4:3	195	.9321	22' 33' 44' 56	0.0000	0.0000
113	101.87	9:4	208	.9320	22' 33' 455' 66'	0.0000	0.0000
114	103.29	4:4	207	.9473	22' 33' 44' 566'	0.0000	0.0000
115	105.2	4:2	194	.9628	22' 33' 44' 55'	0.0371	0.0220
116	106.77	4:2	205	.9678	233' 44' 55' 6	0.0000	0.0000
117	114.24	4:3	206	1.010	22' 33' 44' 55' 6	0.0000	0.0000
118	126.35	10:4	209	1.050	22' 33' 44' 55' 66'	0.0000	0.0000

CONCENTRATION = 1.94321
 TOTAL MICROLITERS = 0.0076
 APPROXIMATE MOLECULAR WEIGHT = 340.47000

N. B.
24 B



24 B

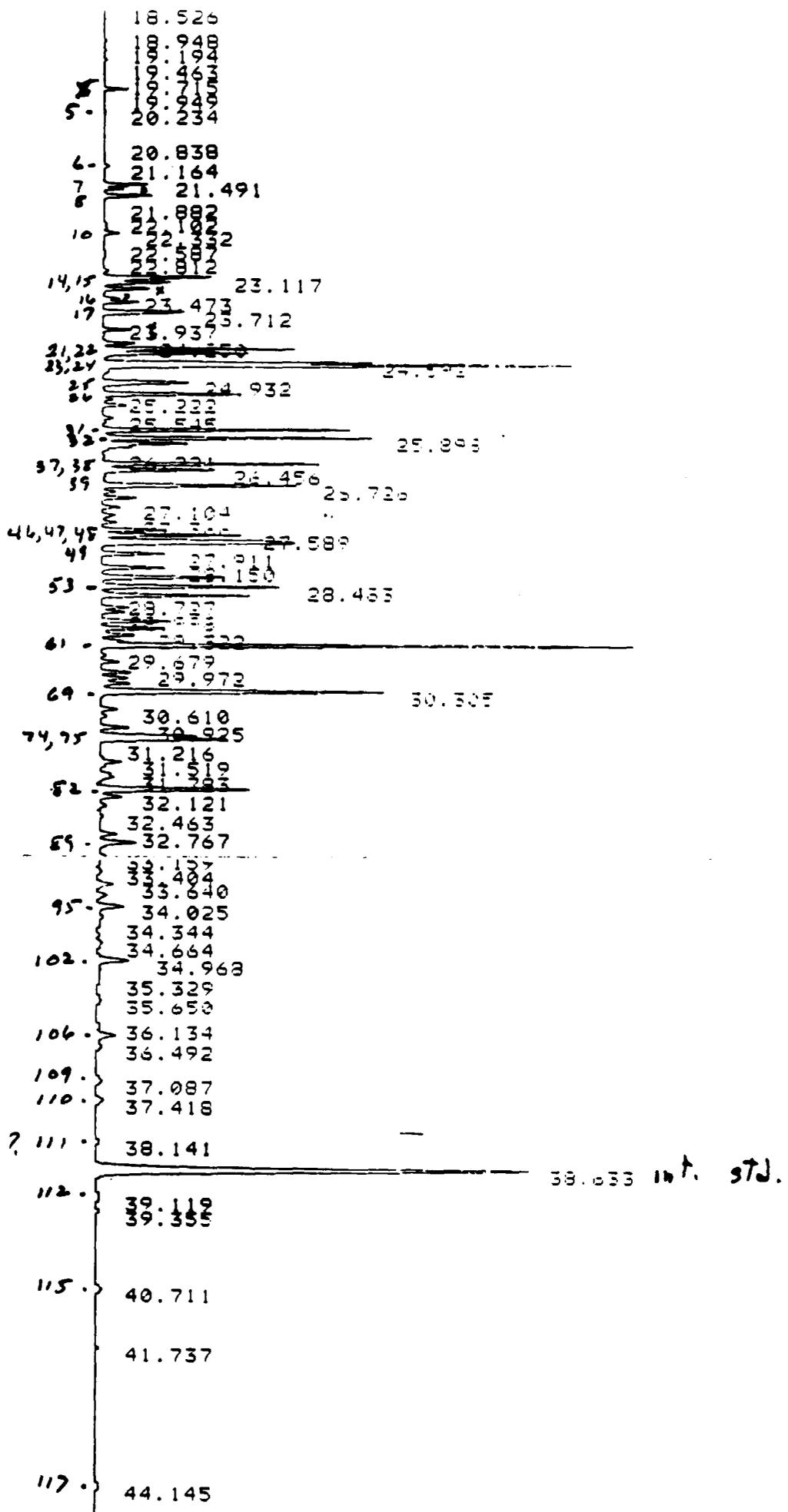
N.B 24B

PEAK#	RET. TIME	T-CL:O-CL	IUPAC#	RTT	CONDENSERS	WEIGHT %	MOLE %
1	40.77	0:0	000	.0997	BIPHENYL	0.0000	0.0000
2	46.6	1:1	001	.1500		0.0000	0.0000
3	50.32	1:0	002	.1937		0.0000	0.0000
4	50.50	1:0	003	.1975		0.0000	0.0000
5	52.52	2:2	004 010	.2245	22' 1 26	0.0000	0.0000
6	54.70	2:1	007 009	.2566	20' 1 23	0.0000	0.0000
7	55.50	2:1	006	.2709	23'	0.0000	0.0000
8	56.1	2:1	005 006	.2785	23' 1 20'	0.0000	0.0000
9	57.07	2:0	014	.2973	35	0.0000	0.0000
10	57.75	3:3	019	.3005	22'6	0.0000	0.0000
11	58.74	3:2	030	.3165	206	0.0000	0.0000
12	59.21	2:0	011	.3250	33'	0.0000	0.0000
13	59.66	2:0	012 013	.3297	34' 1 30'	0.0000	0.0000
14	59.77	4:2 2:0	010 015	.3307	22'5' 1 00'	0.0000	0.0000
15	60.01	4:2	017	.3398	22'4	0.0000	0.0000
16	60.7	3:2	024 027	.3500	236' 1 23'6	0.0000	0.0000
17	61.38	4:2	016 032	.3625	22'5' 1 20'6	0.0000	0.0000
18	62.1	3:1	023	.3770	235	0.0000	0.0000
19	62.33	3:1 4:4	034 034	.3800	2'35' 1 22'66'	0.0000	0.0000
20	62.72	3:1	029	.3820	245	0.0000	0.0000
21	62.98	3:1	026	.3911	23'5	0.0000	0.0000
22	63.19	3:1	025	.3957	23'4	0.0000	0.0000
23	63.63	3:1	031	.4024	24'5	0.0000	0.0000
24	63.73	3:1 4:3	028 030	.4051	244' 1 22'06	0.0000	0.0000
25	64.56	3:1 4:3	021 033	.4170	233' 1 230' 1 22'56'	0.0000	0.0000
26	65	3:1 4:3	022 031	.4267	230' 1 22'06'	0.0000	0.0000
27	65.49	4:3	045	.4354	22'36	0.0000	0.0000
28	65.84	3:1	036	.4379	33'5	0.0000	0.0000
29	66.06	4:3	046	.4450	22'36'	0.0000	0.0000
30	66.43	3:1	039	.4488	34'5	0.0000	0.0000
31	66.63	4:2	052 073	.4554	22'55' 1 23'5'6	0.0000	0.0000
32	66.99	4:2	049	.4618	22'45	0.0000	0.0000
33	67.23	4:2	047	.4639	22'44'	0.0000	0.0000
34	67.38	4:2	048 075	.4651	22'45' 1 200'6	0.0000	0.0000
35	67.51	4:2	065 062	.4663	2306' 1 2356	0.0000	0.0000
36	67.77	3:0	039	.4758	33'4	0.0000	0.0000
37	68.19	5:4 4:2	104 044	.4832	22'466' 1 22'33'	0.0000	0.0000
38	68.44	3:0 4:2	037 042	.4870	344' 1 22'30' 1 230'6	0.0000	0.0000
39	69.14	4:2	064 071	.4990	23'30' 1 234'6 1 23'4'6	0.0000	0.0000
40	69.25	4:1	060	.5040	23'45' 7	0.0000	0.0000
41	69.4	3:4	096	.5057	22'366'	0.0000	0.0000
42	69.65	4:2	040	.5102	22'33'	0.0000	0.0000
43	70.1	5:3 4:1	103 057	.5155	22'45'6 1 233'5	0.0000	0.0000
44	70.49	5:3 4:1	100 067	.5212	22'44'6 1 23'4'5	0.0000	0.0000
45	70.8	4:1	058 063	.5267	233'5' 1 234'9	0.0000	0.0000
46	71.14	4:1 5:3	074 094	.5300	244'5' 1 22'356'	0.0000	0.0000
47	71.37	4:1	070 061	.5307	23'4'5' 1 2'308' 1 24457	0.0000	0.0000
48	71.63	4:1 5:3	066 095	.5347	23'44' 1 22'356' 1 22'55'6	0.0000	0.0000
49	72.2	5:3 4:1	091 090	.5394	22'30'6 1 22'3'46 1 234'6	0.0000	0.0000
50	72.84	4:1	056 060	.5676	233'4' 1 2344'	0.0000	0.0000
51	73.26	6:4 5:3	155 084	.5666	22'44'66' 1 22'30'61 22'350'	0.0000	0.0000
52	73.49	5:3	089	.5779	22'346'	0.0000	0.0000
53	73.67	5:2	101 090	.5814	22'34'5' 1 22'455'	0.0000	0.0000
54	74.09	5:2	099	.5880	22'44'5	0.0000	0.0000
55	74.6	6:4 5:2	159 112	.5969	22'34'66' 1 233'56 1 23'00'6	0.0000	0.0000
56	74.8	5:2	084 109	.6029	22'32'5' 1 233'46	0.0000	0.0000
57	75.2	6:4 5:2	152 097	.6062	22'3566' 1 22'340' 1 22'3'40	0.0000	0.0000
58	75.5	5:2	087 111	.6175	22'345' 1 233'55' 1 2344'6	0.0000	0.0000
59	75.8	5:2	085 116	.6224	22'344' 1 234067	0.0000	0.0000
60	76.1	6:4	134	.6257	22'33'66'	0.0000	0.0000
61	76.3	4:0 5:2	077 110	.6295	33'44' 1 233'4'6	0.0000	0.0000
62	76.7	6:3	154	.6349	22'44'96'	0.0000	0.0000
63	77	5:2	082	.6433	22'38'4	0.0000	0.0000
64	77.5	6:3	151	.6499	22'355'6	0.0000	0.0000
65	77.7	6:3 5:1	135 124	.6563	22'33'96' 1 2'344'5	0.0000	0.0000
66	77.9	6:3	144	.6584	22'345'6	0.0000	0.0000
67	78	5:1 6:4	107 100	.6628	233'4'5' 1 233'45' 1 22'34'56	0.0000	0.0000
68	78.25	5:1	123	.6658	2'344'5	0.0000	0.0000
69	78.4	6:3 5:1	149 110	.6672	22'34'5'6 1 23'44'5 1 233'45	0.0000	0.0000
70	78.55	6:3	139 140	.6707	22'344'6 1 22'344'6	0.0000	0.0000
71	79.1	6:3 5:1	134 143	.6796	22'33'96' 1 22'3456' 1 2344'5	0.0000	0.0000
72	79.4	5:1 6:4	122 131	.6871	2'33'451 22'33'46122'33'55'	0.0000	0.0000
73	79.9	6:2	146 161	.6955	22'34'55' 1 233'45'6	0.0000	0.0000
74	80.3	6:3 5:1	132 105	.7035	22'33'46' 1 233'44'	0.0000	0.0000
75	80.5	6:2	153	.7036	22'44'55'	0.0000	0.0000
76	81.3	6:2	160	.7064	23'44'5'6	0.0000	0.0000
77	81.5	6:2	141	.7203	22'3455'	0.0000	0.0000
78	81.7	7:4	179	.7205	22'33'566'	0.0000	0.0000
79	82	6:2	130	.7284	22'33'45'	0.0000	0.0000
80	82.2	6:2	137	.7329	22'344'5	0.0000	0.0000
81	82.35	7:4	176	.7380	22'33'466'	0.0000	0.0000
82	82.7	6:2	130 163	.7404	22'344'5' 1 233'4'56 1 0 2	0.0000	0.0000
83	83.1	6:2	158	.7429	233'44'6	0.0000	0.0000
84	83.4	6:2	129	.7501	22'33'45	0.0000	0.0000
85	83.9	7:3	178	.7537	22'33'55'6	0.0000	0.0000
86	84.25	6:2	164	.7572	2344'96	0.0000	0.0000
87	84.4	7:3	175	.7611	22'33'45'6	0.0000	0.0000
88	84.7	7:3	187 182	.7654	22'34'55'6 1 22'344'56'	0.0000	0.0000
89	85.1	6:2	120	.7761	22'33'44'	0.0000	0.0000
90	85.4	7:3	183	.7720	22'344'5'6	0.0000	0.0000
91	85.7	6:1	167	.7814	23'44'55'	0.0000	0.0000
92	86.4	7:3	185	.7848	22'3455'6	0.0000	0.0000
93	87	7:3	174 181	.7965	22'33'456' 1 22'344'56	0.0000	0.0000
94	87.5	7:3	177	.8031	22'33'456	0.0000	0.0000
95	88	7:3 6:1	171 154	.8105	22'32'44'6 1 233'44'5	0.0000	0.0000
96	88.44	6:4	202	.8195	22'32'55'66'	0.0000	0.0000
97	88.5	6:1	157	.8184	233'44'5'	0.0000	0.0000
98	88.91	7:3	173	.8152	22'33'456	0.0000	0.0000
99	89.36	6:4	200 204	.8197	22'33'45'66' 1 22'444'566'	0.0000	0.0000
100	89.6	7:2	172 192	.8278	22'33'455' 1 233'455'6	0.0000	0.0000
101	90.2	6:4	197	.8293	22'33'44'66'	0.0000	0.0000
102	90.4	7:2	188	.8362	22'344'55'	0.0000	0.0000
103	90.8	7:2	193	.8397	233'44'55'6	0.0000	0.0000
104	91.44	7:2	191	.8447	233'44'5'6	0.0000	0.0000
105	92.2	6:4	199	.8494	22'33'4566'	0.0000	0.0000
106	92.9	7:2	178	.8748	22'33'44'5	0.0000	0.0000
107	94.44	7:2	190	.8746	233'44'56	0.0000	0.0000
108	95.63	6:3	190	.8845	22'33'455'6	0.0000	0.0000
109	95.9	6:3	201	.8875	22'33'44'55'6	0.0000	0.0000
110	96.7	6:3	194 203	.8925	22'33'44'5'6 1 22'344'55'6	0.0000	0.0000
111	98.72	7:1	189	.9132	233'44'55'	0.0000	0.0000
112	101.23	6:3	195	.9321	22'33'44'56	0.0000	0.0000
113	101.67	9:4	208	.9320	22'33'455'66'	0.0000	0.0000
114	103.29	9:4	207	.9425	22'33'44'566'	0.0000	0.0000
115	105.2	6:2	194	.9620	22'33'44'55'	0.0000	0.0000
116	106.77	6:2	205	.9678	233'44'55'6	0.0000	0.0000
117	110.24	9:3	206	1.010	22'33'44'55'6	0.0000	0.0000
118	126.35	10:4	209	1.050	22'33'44'55'66'	0.0000	0.0000

CONCENTRATION = 1.671311
 TOTAL MOLECULES = 0.0074
 AVERAGE MOLECULAR WEIGHT = 226.69184
 NUMBER OF CALIBRATED PEAKS FOUND = 118

N.B.
26A

V/A



N.B. 26A

PLANK	RET. TIME	T-CL:O-CL	IUPAC#	RTT	CONDENSERS	WEIGHT %	MOL% %
1	40.81	0:0	000	.0997	BIPHENYL	0.0000	0.0000
2	46.62	1:1	001	.1504	2	9.1040	13.2503
3	50.34	1:0	002	.1937	3	2.0061	0.2509
4	50.4	1:0	003	.1975	4	0.1441	0.2081
5	52.34	2:2	004 010	.2243	22' 1 26'	0.3362	0.4105
6	54.74	2:1	007 009	.2566	24' 1 25'	0.1909	0.2326
7	55.6	2:1	006	.2709	23'	1.6242	1.9033
8	56.09	2:1	005 000	.2703	23' 1 24'	1.6101	1.9790
9	57.33	2:0	014	.2973	35	0.1253	0.1530
10	57.77	2:2	019	.3049	22'6	0.6033	0.6403
11	58.03	2:2	030	.3165	246	0.0135	0.0164
12	59.21	2:0	011	.3230	33'	0.0000	0.0000
13	59.48	2:0	012 013	.3297	34' 1 34'	0.2646	0.3200
14	59.79	3:2 2:0	010 015	.3307	22'5' 1 40'	5.0034	5.6024
15	60.02	3:2	017	.3390	22'4	2.1214	2.2443
16	60.72	3:2	024 027	.3500	236' 1 23'6	0.3200	0.3470
17	61.32	3:2	016 032	.3625	22'5' 1 24'6	1.0092	1.1906
18	62.12	3:1	023	.3778	255	0.0154	0.0182
19	62.43	3:1 4:4	034 054	.3800	2'35' 1 22'66'	0.0000	0.0000
20	62.72	3:1	029	.3820	245	0.0370	0.0492
21	62.97	3:1	026	.3911	23'5	2.7203	2.8843
22	63.16	3:1	025	.3937	23'4	2.4564	2.5990
23	64.6	3:1	031	.4024	24'5	3.0075	4.0200
24	63.72	3:1 4:5	020 050	.4031	244' 1 22'46	5.1767	5.4410
25	64.5	3:1 4:5	021 033	.4170	233' 1 23' 1 22'56'	1.0790	1.1962
26	65.02	3:1 4:5	022 051	.4267	234' 1 22'46'	1.3610	1.3674
27	65.31	4:3	045	.4334	22'36	0.4910	0.4500
28	65.80	3:1	036	.4379	33'5	0.0000	0.0000
29	66.00	4:3	044	.4450	22'36'	0.3147	0.4002
30	66.45	3:1	039	.4480	34'5	0.0000	0.0000
31	66.62	4:2	052 073	.4554	22'55' 1 23'5'6	5.2700	4.9247
32	66.99	4:2	049	.4610	22'45	4.1827	3.9021
33	67.22	4:2	047	.4639	22'44'	1.5275	1.4250
34	67.27	4:2	040 075	.4651	22'45' 1 244'6	0.4059	0.4333
35	67.6	4:2	065 062	.4845	2546' 1 2356'	0.0000	0.0000
36	67.84	3:0	035	.4730	33'0	0.0849	0.0900
37	68.15	5:4 4:2	104 044	.4832	22'46'6' 1 22'35'	2.9014	2.7036
38	68.44	5:0 4:2	037 042	.4878	344' 1 22'30' 1 234'6	2.2956	2.1594
39	69.13	4:2	064 071	.4990	23'34' 1 234'6' 1 23'4'6	1.0451	1.1213
40	69.25	4:1	064	.5044	23'45' 7	0.0000	0.0000
41	69.47	5:4	076	.5057	22'366'	0.3749	0.3145
42	69.7	4:2	040	.5104	22'33'	0.3500	0.3213
43	70.12	5:3 4:1	103 057	.5155	22'45'6' 1 233'9	0.3378	0.3079
44	70.46	5:3 4:1	100 067	.5212	22'44'6' 1 233'4'5	0.3219	0.2804
45	70.79	4:1	050 063	.5267	233'5' 1 234'5	0.2236	0.2006
46	71.13	4:1 5:3	074 094	.5307	244'5' 1 22'396'	0.7763	0.6762
47	71.46	4:1	070 061	.5347	23'4'5' 1 2'345'	1.6803	1.5751
48	71.62	4:1 5:3	066 095	.5347	23'44' 1 22'356' 1 22'35'6	1.7102	1.4413
49	72.19	5:3 4:1	091 098	.5349	22'34'6' 1 22'3'46' 1 233'4	0.9705	0.8252
50	72.44	4:1	056 060	.5676	233'4' 1 2344'	0.0163	0.0615
51	74.25	6:4 5:3	155 084	.5666	22'44'66' 1 22'33'61' 22'355'	1.7431	1.4404
52	73.49	5:3	089	.5779	22'346'	0.0000	0.0000
53	73.89	5:2	101 090	.5814	22'34'5' 1 22'455'	2.6727	2.2307
54	74.00	5:2	099	.5880	22'44'5	1.9507	1.6201
55	74.6	6:4 5:2	150 112	.5969	22'34'66' 1 233'56' 1 23'44'6	0.2960	0.2470
56	74.8	5:2	083 109	.6029	22'33'5' 1 233'46	0.4620	0.3062
57	75.22	6:4 5:2	152 097	.6062	22'3566' 1 22'345' 1 22'3'48	0.7247	0.6014
58	75.55	5:2	087 111	.6175	22'345' 1 233'59' 1 2344'6	0.4774	0.3904
59	75.84	5:2	085 116	.6224	22'344' 1 234567	0.3096	0.2504
60	76.12	6:4	136	.6257	22'33'66'	0.3021	0.2091
61	76.33	4:0 5:2	077 110	.6295	33'44' 1 233'4'6	4.2425	3.5408
62	76.7	6:3	154	.6349	22'44'56'	0.0012	0.0614
63	77	5:2	082	.6453	22'33'4	0.1692	0.1412
64	77.5	6:3	151	.6499	22'335'6	0.4491	0.3390
65	77.8	6:3 5:1	153 124	.6544	22'33'96' 1 2'344'5	0.3020	0.2969
66	77.9	6:3	144	.6584	22'345'6	0.0000	0.0000
67	78	5:1 6:3	107 108	.6620	233'4'5' 1 233'45' 1 22'34'56	0.4345	0.3514
68	78.25	5:1	123	.6630	2'344'5	0.0000	0.0000
69	78.4	6:3 5:1	149 110	.6672	22'34'5'6' 1 23'44'5' 1 233'48	3.7356	2.9027
70	78.55	6:3	139 140	.6707	22'344'6' 1 22'344'6'	0.0000	0.0000
71	79.2	6:3 5:1	134 143	.6746	22'33'96' 1 22'3456' 1 2344'5	0.2330	0.1911
72	79.5	5:1 6:3	122 131	.6871	2'33'451' 22'33'461' 22'33'59'	0.0029	0.0044
73	80	6:2	146 161	.6955	22'34'55' 1 233'45'6	0.0093	0.3009
74	80.5	6:3 5:1	132 105	.7035	22'33'66' 1 233'44'	0.5132	0.4237
75	80.5	6:2	153	.7036	22'44'55'	3.0922	2.3346
76	81.3	6:2	160	.7044	25'44'5'6	0.0310	0.0234
77	81.5	6:2	141	.7203	22'3455'	0.1506	0.1137
78	81.7	7:4	174	.7205	22'33'566'	0.1141	0.0706
79	82	6:2	140	.7204	22'33'45'	0.1740	0.1319
80	82.2	6:2	137	.7329	22'344'5	0.2734	0.2064
81	82.35	7:4	176	.7303	22'33'666'	0.0000	0.0000
82	82.7	6:2	133 163	.7403	22'344'5' 1 233'4'56' 1 42	1.6362	1.2363
83	83.1	6:2	150	.7429	233'44'6	0.2450	0.1856
84	83.5	6:2	129	.7501	22'33'45	0.1203	0.0908
85	83.9	7:3	170	.7537	22'33'53'6	0.0533	0.0367
86	84.2	6:2	166	.7572	2344'56	0.0100	0.0075
87	84.5	7:3	175	.7611	22'33'45'6	0.0102	0.0126
88	84.7	7:3	107 102	.7634	22'34'53'6' 1 22'344'56'	0.2093	0.1443
89	85.1	6:2	120	.7741	22'33'44'	0.3432	0.2606
90	85.4	7:3	183	.7720	22'344'5'6	0.0000	0.0000
91	85.8	6:1	167	.7814	23'44'59'	0.2121	0.1601
92	86.4	7:3	185	.7840	22'3458'6	0.0191	0.0132
93	87	7:3	174 101	.7965	22'33'456' 1 22'344'56	0.1405	0.0970
94	87.57	7:3	171	.8031	22'33'4'56	0.0000	0.0000
95	88	7:3 4:1	171 156	.8170	22'33'44'6' 1 234'44'5	0.2960	0.2177
96	88.44	8:4	202	.8009	22'33'53'66'	0.0000	0.0000
97	88.5	6:1	157	.8104	233'44'5'	0.0341	0.0273
98	88.8	7:3	173	.8132	22'33'456	0.0025	0.0016
99	89.36	8:4	200 204	.8197	22'33'45'66' 1 22'344'566'	0.0000	0.0000
100	89.6	7:2	172 192	.8270	22'33'458' 1 233'455'6	0.0516	0.0356
101	90.2	8:4	197	.8298	22'33'44'66'	0.0000	0.0000
102	90.4	7:2	180	.8362	22'344'58'	0.2001	0.1704
103	90.8	7:2	193	.8397	233'4'55'6	0.0006	0.0059
104	91.44	7:2	191	.8447	233'44'3'6	0.0000	0.0000
105	92.2	8:4	199	.8490	22'33'4366'	0.0196	0.0124
106	93.9	7:2	170	.8740	22'33'44'5	0.1690	0.1170
107	94.4	7:2	190	.8740	233'44'56	0.0506	0.0349
108	95.63	8:3	190	.8845	22'33'455'6	0.0000	0.0000
109	95.9	8:3	201	.8875	22'33'4'55'6	0.0540	0.0355
110	96.4	8:3	196 203	.8935	22'33'44'5'6' 1 22'344'55'6	0.0690	0.0437
111	98.72	7:1	189	.9142	233'44'58'	0.0000	0.0000
112	101.23	8:3	195	.9321	22'33'44'56	0.0000	0.0000
113	101.07	9:4	200	.9320	22'33'455'66'	0.0000	0.0000
114	103.29	9:4	207	.9428	22'33'44'566'	0.0000	0.0000
115	103.3	8:2	194	.9620	22'33'44'55'	0.0394	0.0331
116	106.77	8:2	205	.9670	233'44'55'6	0.0000	0.0000
117	114.2	9:3	206	1.010	22'33'44'55'6	0.0644	0.0378
118	126.33	10:4	209	1.050	22'33'44'55'66'	0.0000	0.0000

CONCENTRATION = 2.321319
TOTAL MICROROLLS = 0.0005

AVERAGE MOLECULAR WEIGHT = 272.41290
NUMBER OF CALIBRATED PEAKS FOUND = 118

N.B. 26 B

PEAK#	RET. TIME	T-CL:D-CL	IUPAC#	RTT	COMBENERS	WEIGHT %	MOLE %
1	40.81	0:0	000	.0997	BIPHENYL	0.0000	0.0000
2	46.62	1:1	001	.1384	2	29.6481	37.7411
3	50.35	1:0	002	.1937	3	6.0336	8.7667
4	50.61	1:0	003	.1975	4	0.2196	0.2895
5	52.34	2:2	004 010	.2243	22' 1 26'	0.4210	0.4550
6	54.73	2:1	007 009	.2564	24' 1 29'	0.1146	0.1241
7	55.50	2:1	006	.2709	23'	0.7939	0.8595
8	56.1	2:1	005 000	.2785	23' 1 24'	1.1278	1.2201
9	57.07	2:0	010	.2974	35	0.1963	0.2147
10	57.70	2:3	019	.3045	22'6	0.3132	0.2934
11	58.74	2:0	030	.3165	246	0.0340	0.0319
12	59.20	2:0	011	.3230	33'	0.1533	0.1601
13	59.49	2:0	012 013	.3297	34' 1 34'	0.2576	0.2709
14	59.75	2:2 2:0	018 015	.3307	22'5' 1 44'	4.9073	4.8732
15	60.01	2:2	017	.3390	22'4	1.0300	0.9649
16	60.73	3:2	024 027	.3500	236' 1 23'6	0.1540	0.1445
17	61.30	3:2	016 032	.3625	22'3' 1 20'6	0.7305	0.6852
18	62.13	3:1	023	.3770	235	2.5102	2.3545
19	62.37	3:1 4:0	034 034	.3800	2'35' 1 22'66'	0.0612	0.0552
20	62.75	3:1	029	.3820	245	2.0411	2.6649
21	63.01	3:1	026	.3911	23'5	1.0190	0.9550
22	63.19	3:1	025	.3937	23'4	1.7049	1.5992
23	63.63	3:1	031	.4024	24'5	2.1175	1.9862
24	63.74	3:1 4:0	028 030	.4031	244' 1 22'46	2.6142	2.6326
25	64.54	3:1 4:0	021 033	.4170	233' 1 24' 1 22'36'	1.0799	0.9140
26	65.01	3:1 4:0	022 031	.4267	236' 1 22'46'	0.6349	0.5831
27	65.5	4:3	045	.4334	22'34	0.2764	0.2286
28	65.84	4:1	036	.4379	33'5	0.0000	0.0000
29	66.07	4:3	046	.4430	22'36'	0.7521	0.6221
30	66.45	4:1	039	.4480	34'5	0.0000	0.0000
31	66.64	4:2	052 073	.4534	22'55' 1 23'5'6	2.7489	2.2737
32	67	4:2	049	.4610	22'45	2.4144	1.9970
33	67.23	4:2	047	.4639	22'44'	1.1045	0.9136
34	67.36	4:2	048 075	.4651	22'43' 1 244'6	0.7992	0.3964
35	67.52	4:2	065 062	.4665	23'46' 1 2396	0.0817	0.0676
36	67.70	4:0	035	.4738	33'4	0.1737	0.1629
37	68.17	5:4 4:2	104 044	.4832	22'466' 1 22'35'	1.4292	1.1800
38	68.4	3:0 4:2	037 042	.4870	344' 1 22'30' 1 233'6	1.6020	1.3367
39	69.1	4:2	064 071	.4990	23'34' 1 234'6' 1 23'4'6	1.3605	1.1253
40	69.25	4:1	048	.5044	23'43' 7	0.0000	0.0000
41	69.4	5:4	096	.5057	22'366'	0.4751	0.3516
42	69.7	4:2	040	.5102	22'33'	0.2756	0.2279
43	70.1	5:3 4:1	103 057	.5135	22'43'6' 1 233'5	0.1774	0.1433
44	70.5	5:3 4:1	100 067	.5212	22'44'6' 1 23'4'5	0.2626	0.2020
45	70.8	4:1	050 063	.5267	233'5' 1 234'5	0.1112	0.0920
46	71.1	4:1 5:0	074 094	.5348	244'5' 1 22'396'	0.7800	0.6493
47	71.3	4:1	070 061	.5407	23'4'5' 1 2'34'5' 1 24497	1.5419	1.2754
48	71.6	4:1 5:3	066 095	.5447	23'44' 1 22'396' 1 22'39'6	2.0262	1.5060
49	72.4	5:3 4:1	091 090	.5549	22'34'6' 1 22'3'46' 1 233'4	0.7043	0.5266
50	72.8	4:1	056 060	.5676	233'4' 1 2344'	1.0782	0.8919
51	73.2	6:4 5:3	155 084	.5666	22'44'64' 1 22'33'6' 1 22'350'	0.0431	0.0204
52	73.6	5:3	089	.5779	22'306'	1.6932	1.2544
53	73.71	5:2	101 090	.5814	22'30'5' 1 22'493'	0.0000	0.0000
54	74.1	5:2	099	.5880	22'44'5	1.4223	1.0524
55	74.6	6:4 5:2	150 112	.5969	22'30'66' 1 233'36' 1 23'44'6	0.1504	0.1178
56	74.8	5:2	083 109	.6029	22'33'5' 1 233'46	0.1470	0.1470
57	75.2	6:4 5:2	152 097	.6062	22'3566' 1 22'340' 1 22'3'46	0.5662	0.4166
58	75.5	5:2	087 111	.6175	22'340' 1 233'55' 1 2344'6	0.4012	0.2969
59	75.8	5:2	085 116	.6224	22'344' 1 23467	0.2075	0.2127
60	76.1	6:4	136	.6257	22'33'66'	0.2110	0.1410
61	76.3	4:0 5:2	077 110	.6295	33'44' 1 233'4'6	2.2266	1.6476
62	76.7	6:3	154	.6349	22'44'36'	0.0497	0.0497
63	77	5:2	082	.6434	22'33'4	0.1401	0.1037
64	77.5	6:3	151	.6499	22'359'6	0.2493	0.1802
65	77.8	6:3 5:1	135 124	.6563	22'33'36' 1 2'444'5	0.2814	0.1732
66	77.9	6:3	144	.6584	22'345'6	0.0000	0.0000
67	78	5:1 6:4	107 100	.6628	233'4'5' 1 233'45' 1 22'44'36	0.2791	0.2001
68	78.25	5:1	123	.6650	2'344'5	0.0000	0.0000
69	78.4	6:3 5:1	149 110	.6672	22'30'3'6' 1 23'44'5' 1 233'45	2.3634	1.7660
70	78.55	6:3	139 140	.6707	22'344'6' 1 22'344'6'	0.0000	0.0000
71	79.2	6:3 5:1	134 143	.6796	22'33'36' 1 22'4436' 1 2344'5	0.1644	0.1220
72	79.4	5:1 6:3	122 131	.6871	2'33'45' 1 22'35'46' 1 22'33'59'	0.0293	0.0208
73	80	6:2	146 161	.6955	22'34'55' 1 233'45'6	0.2792	0.1849
74	80.3	6:3 5:1	132 105	.7033	22'33'46' 1 233'44'	0.4204	0.3070
75	80.5	6:2	153	.7036	22'44'55'	2.2200	1.8462
76	81.3	6:2	160	.7060	23'44'3'6	0.0242	0.0162
77	81.5	6:2	141	.7203	22'3455'	0.1290	0.0843
78	81.7	7:4	179	.7205	22'33'366'	0.0797	0.0487
79	82.1	6:2	130	.7280	22'33'49'	0.1132	0.0750
80	82.2	6:2	137	.7329	22'344'5	0.1024	0.1221
81	82.35	7:4	176	.7385	22'33'466'	0.0000	0.0000
82	82.7	6:2	130 163	.7404	22'344'3' 1 233'4'36' 1 2	1.0049	0.7261
83	83.1	6:2	150	.7429	23'44'6	0.1796	0.1202
84	83.4	6:2	129	.7501	22'33'45	0.0932	0.0637
85	83.9	7:3	170	.7537	22'33'39'6	0.0450	0.0200
86	84.2	6:2	164	.7572	2344'36	0.0107	0.0073
87	84.5	7:3	173	.7611	22'33'48'6	0.0166	0.0102
88	84.7	7:3	147 182	.7693	22'34'55'6' 1 22'344'36'	0.1720	0.1036
89	85.1	6:2	128	.7761	22'33'44'	0.2943	0.1715
90	85.5	7:3	183	.7720	22'344'3'6	0.0110	0.0072
91	85.7	6:1	167	.7814	23'44'39'	0.1047	0.1249
92	86.4	7:3	180	.7808	22'3458'6	0.0106	0.0114
93	87	7:3	174 181	.7963	22'32'456' 1 22'444'36	0.1164	0.0713
94	87.3	7:3	177	.8031	22'44'40'	0.0929	0.0579
95	88	7:3 6:1	171 154	.8105	22'33'44'6' 1 233'44'5	0.2349	0.1501
96	88.44	8:4	202	.8084	22'32'55'66'	0.0000	0.0000
97	88.5	6:1	157	.8104	23'44'3'	0.0330	0.0226
98	88.9	7:3	173	.8132	22'33'456	0.0004	0.0004
99	89.44	8:4	200 204	.8197	22'32'43'66' 1 22'344'366'	0.0000	0.0000
100	89.6	7:2	172 192	.8278	22'32'456' 1 233'495'6	0.0344	0.0344
101	90.2	8:4	197	.8293	22'33'40'66'	0.0000	0.0000
102	90.49	7:2	180	.8362	22'344'35'	0.0000	0.0000
103	90.8	7:2	193	.8397	233'40'38'6	0.0001	0.0049
104	91.3	7:2	191	.8447	233'40'3'6	0.0034	0.0021
105	92.2	8:4	199	.8490	22'33'4866'	0.0231	0.0130
106	92.9	7:2	170	.8740	22'33'44'5	0.1337	0.0617
107	94.4	7:2	190	.8740	23'44'36'	0.0429	0.0262
108	95.2	8:3	198	.8845	22'33'455'6	0.0000	0.0000
109	95.9	8:3	201	.8875	22'33'43'6	0.0324	0.0295
110	96.7	8:3	196 203	.8934	22'33'44'3'6' 1 22'344'35'6	0.0334	0.0314
111	98.6	7:1	184	.9142	23'44'35'	0.0004	0.0032
112	101.1	8:3	195	.9321	22'33'44'36	0.0345	0.0194
113	101.8	9:4	208	.9320	22'33'435'66'	0.0004	0.0020
114	103.2	9:4	207	.9423	22'33'44'366'	0.0010	0.0005
115	105.4	8:2	194	.9620	22'33'44'35'	0.0441	0.0240
116	106.5	8:2	205	.9678	233'44'38'6	0.0009	0.0005
117	110.2	9:3	206	1.0110	22'33'44'38'6	0.0333	0.0277
118	126.35	10:4	209	1.0550	22'33'44'38'66'	0.0000	0.0000

CONCENTRATION = 2.523900
 TOTAL RICHMONDS = 0.0104
 AVERAGE MOLECULAR WEIGHT = 241.32657
 NUMBER OF CALIBRATED PEAKS FOUND = 110

Table 3. PCB Levels, Distributions, and Alteration States in Subsurface Sediments of the Upper Acushnet River Estuary, New Bedford, MA

No., ^a side	Latitude (41°N)	Sample texture ^d	Total oils, ppm ^e	Total PCBs, ppm ^e	Orig. 1242: 1254	Soln., loss (%)	Dechlor'n Status ^f			
							Pat- tern	half- losses P50	half- losses P58	half- losses 58-5
- 19A	40'30"	sft mud	20,000	1,637	68:32	40	H	2.5	3.1	0.6
- 19B	40'30"	sft mud	28,400	1,126	57:43	40 ^g	H	3.2	3.5	0.3
- 18A	40'30"	snd	20,700	3,285	05:95	5	H?	~0.0	0.6	0.6
- 18B	40'30"	snd	7,040	739	06:94	6	H?	~0.1	0.8	0.7
- 21A	40'26"	gr, snd	11,100	3,775	47:53	4	H	1.9	2.2	0.3
- 21B	40'26"	gr, snd	1,400	417	40:60	5	H	2.0	2.2	0.2
17A -	40'21"	sft mud	46,300	3,292	80:20	9	H	0.8	2.3	1.5
17B -	40'21"	sft mud	40,300	3,724	70:30	12 ^h	H	1.9	3.2	1.3
- 22A	40'16"	snd	5,390	765	81:19	33 ^h	H	2.3	3.1	0.8
- 22B	40'16"	snd	8,110	1,444	64:32	14	H	1.9	3.5	1.6
14A -	40'16"	snd, mud	3,840	40.4	74:26	34	H	0.9	1.6	0.7
14B -	40'16"	snd, mud	3,390	0.9	~76:24	-	H?	~0.7	~0.8	-
12A -	40'14"	gr, snd	8,730	505	84:16	11	H'	2.1	1.6	-0.5
12B -	40'14"	gr, snd	6,070	526	82:18	51	H'	3.1	2.3	-0.8
- 24A	40'12"	gr, snd	<150	0.7	~70:30	-	H?	~0.6	~1.6	-
- 24B	40'12"	gr, snd	<150	0.3	~65:35	-	H?	~0.9	~1.6	-
9A -	40'11"	gr, mud	26,700	490	94:06	8	H'	1.9	1.0	-0.9
9B -	40'11"	gr, mud	22,900	1,135	91:09	30 ^h	H'	2.7	1.8	-0.9
5A -	40'01"	gr, snd	12,800	304	82:18	44 ^h	H	1.2	1.1	-0.1
5B -	40'01"	gr, snd	34,500	785	86:14	22	H	2.3	1.4	-0.9
2A -	39'55"	gr, snd	1,570	150	71:29	29	H	0.9	0.7	-0.2
2B -	39'55"	gr, snd	2,050	171	67:33	22	H	2.3	1.6	-0.7
- 26A	39'39"	fiber	<440	3.2	~54:46	-	H	~1.3	~1.9	-
- 26B	39'39"	fiber	<370	0.6	~64:36	-	H?	~0.5	~1.3	-
Average for all sites:			13,000	1,013	61:39	18	-	1.6	1.6	0.0

- a. Depth of "A: samples 5-7.5 cm; of "B" samples 15-17.5 cm.
- b. Sites located on west side of estuary, 70°55'06-09" W.
- c. Sites located on east side of estuary, 70°54'51-59" W.
- d. Key: sft, soft black mud, H₂S odor; snd, sand; gr, gravel; fiber, apparently spartina root mass (marsh bed).
- e. Parts per million of air-dried sediment weight.
- f. -Log₂ fractional retention of peak 50 (mainly 23-34 CB from Aroclor 1242) or of peak 58 (mainly 234-25 CB from Aroclor 1254), or differences between these numbers of half-losses.
- g. This calculated value probably an underestimate.
- h. This calculated value probably an overestimate.