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Polynuclear Aromatic Hydrocarbons of Tobacco Smoke: Isolation and Identification*

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INTRODUCTION

Fractionations of cigarette smoke condensate (CSC) for bioassay have resulted in the isolation of a neutral subfraction possessing high biological activity (1–4). Subfraction F-20 (Fig. 1) has been shown to contain the polynuclear aromatic hydrocarbons (PAH) known to occur in CSC (5, 6). Accordingly, the biological activity of this fraction has been ascribed to the PAH. Therefore, it became important to isolate and identify the PAH in this fraction. More recently, fraction F-20 was further fractionated for bioassay and the PAH successfully concentrated by preparative gel filtration (GF) chromatography (7). The success of the GF procedure stimulated the identification efforts, since, until now, interfering substances have deterred a complete analysis of the PAH in F-20 and similar neutral fractions.

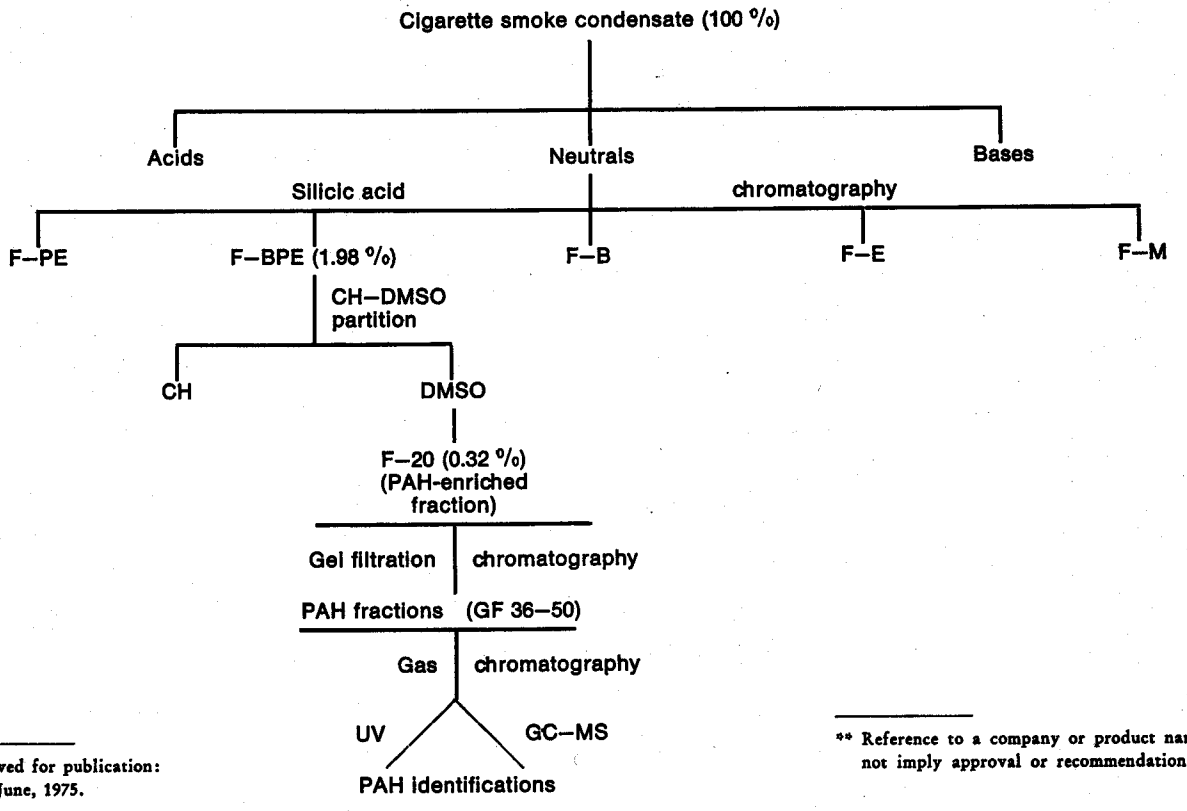
Utilizing our experience with gel filtration chromatography of PAH-containing CSC fractions (8, 9), we successfully separated the PAH of F-20 into relatively pure subfractions. Virtually all of the volatile constituents of the subfractions were identified by a combination of gas chromatographic, ultraviolet, and mass spectrometric methods. The methods of identification are detailed and the PAH are tabulated and discussed.

EXPERIMENTAL

Materials

All solvents used were Mallinckrodt** "nanograde" or Burdick and Jackson "distilled-in-glass" grade. Dimethylsulfoxide (DMSO) was Mallinckrodt analytical reagent

Figure 1. Abbreviated CSC fractionation and PAH isolation scheme.



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** Reference to a company or product name does not imply approval or recommendation by the USDA.

grade. CSC was prepared from commercial, non-filter cigarettes at the Roswell Park Memorial Institute and shipped to us under conditions previously described (10). The PAH standards were obtained from various commercial sources and used as received. Samples of the six isomeric methylchrysenes were kindly supplied by Dr. D. *Hoffmann*, American Health Foundation, Health Research Laboratory, Valhalla, New York.

Fractionation of CSC

The PAH-containing F-20 (Fig. 1) was obtained as described before (2). Acid-base extractions of 1 kg of CSC yielded a neutral fraction, which was chromatographed on a silicic acid column. Elution with petroleum ether (PE) followed by 25% benzene (B) in PE yielded fraction F-BPE. Partition of F-BPE between cyclohexane (CH) and DMSO yielded F-20.

Gel Filtration Chromatography

The gel filtration (GF) system consisted of four 1.25 cm × 109 cm Chromatronix LC columns, connected in series and packed with Bio-Beads SX-12 (a neutral, porous, styrene-divinylbenzene copolymer, M. exclusion 400, Bio-Rad Laboratories) in benzene. Total length of the wet gel bed was 400 cm (approximately 200 g of dry beads). Samples were placed on the gel column with a 1.0 ml injection loop. The eluting solvent was benzene, pumped by a Chromatronix CMP-3 pump at a rate of 120 ml/h; 8 ml fractions were collected. The effluent from the column was monitored at 280 nm with an Isco Model UA-5 absorbance monitor equipped with a micro-flowcell. The GF system was tested with known PAH and gave reproducible elution volumes for standard PAH, as found before (8). The total sample of F-20 (3.5 g) was chromatographed in lots of 0.5 g. Material eluted in GF fractions 24–50. Fractions with the same number were combined for subsequent gas chromatography (GC). Figure 2 contains the 280 nm UV trace of the elution of 2 mg of F-20 from the gel columns.

Analytical GC

GF fractions 40 through 45 were subjected to GC on a Hewlett-Packard Model 5750 gas chromatograph, equipped with 10′ × 1/8″ and 15′ × 1/8″ stainless steel (SS) columns, packed with 3% Dexsil 300 GC on 100/120 mesh Chromosorb W-AW (temperature program, 90–325° C at 2°/min; 48 ml/min He; injection temperature, 290° C; flame detector, 350° C). An Autolab System IV Integrator was used to determine peak areas of the GC volatiles. GF fractions 40 and 45 were analyzed on the 15′ column and GF fractions 41–44 were analyzed on the 10′ column.

Preparative GC

A Hewlett-Packard Model 5750 gas chromatograph equipped with a thermal conductivity (TC) detector was used for the preparative GC of GF fractions 40, 41, 43, and 45. The PAH were collected, as indicated below, at the exit port of the TC detector.

Preparative GC of GF Fraction 40

The compounds in GF fraction 40 were batch collected in six subfractions (into dry ice-cooled vials) from a 15′ × 1/8″ SS column, packed with 5% Dexsil on 100/120 mesh Chromosorb W-AW, at the same temperature conditions as above. Subfractions were collected according to the following relative retention time (RRT) intervals: GF 40-1, 0.113-0.308 RRT; GF 40-2, 0.324-0.476 RRT; GF 40-3, 0.520-0.610 RRT; GF 40-4, 0.629-0.821 RRT; GF 40-5, 0.842-1.107 RRT; and GF 40-6, 1.124 RRT and above. GF 40-1 was rechromatographed on the 15′ column and the PAH were collected by bubbling the GC effluent into vials containing 95% EtOH. GC program conditions were: 70° C for 10 min, followed by a 2°/min program, until all compounds had eluted. A total of 21 collection cuts were taken. GF 40-2 was chromatographed at 120° C, and 28 collection cuts were trapped in U-shaped capillary tubes, cooled with dry ice. The PAH in GF 40-3, GF 40-4 and GF 40-5 were collected from the Dexsil column isothermally at 150° C (22 collection cuts), at 175° C (28 collection cuts), and at 175° C (43 collection cuts), respectively. GF 40-6 was separated into 53 collection cuts using the following temperature program: 240° C for 20 min, followed by an increase of 1°/min to 275° C.

Preparative GC of Fraction 41

GF fraction 41 was first batch collected into 5 subfractions (GF 41-1, 0.165-0.350 RRT; GF 41-2, 0.360-0.503 RRT; GF 41-3, 0.520-0.754 RRT; GF 41-4, 0.760-0.877 RRT; and GF 41-5, 0.896-1.359 RRT) from a 10′ × 3/16″ SS 5% Dexsil column (100/120 mesh Chromosorb W-AW, 100-325° C at 2°/min, 35 ml/min He, injection temperature 290° C, thermal conductivity detector at 350° C). This column (75-125° C at 2°/min) was used to separate the PAH in GF 41-1 into 16 cuts, which were collected in vials containing 95% EtOH. GF 41-2 was subjected to preparative GC on the 10′ column (120° C; 35 ml/min He) and the PAH were trapped in dry ice-cooled capillary tubes (22 collection cuts). The PAH in GF 41-3, GF 41-4, and GF 41-5 were collected in capillary tubes at room temperature under the following conditions: 150° C, 35 ml/min He (28 collection cuts); 170° C, 20 ml/min He (18 collection cuts); and 170-325° C at 2°/min, 35 ml/min He (53 collection cuts), respectively.

Preparative GC of GF Fractions 43 and 45

GF fraction 43 was subjected to preparative GC on a 10′ × 1/8″ SS 5% Dexsil column (100-325° C at 2°/min, 20 ml/min He) and 105 cuts were collected in glass capillary tubes. GF fraction 45 was also separated on this column (150-340° C programming at 2°/min, 20 ml/min He) and the PAH were collected in 44 cuts.

Ultraviolet Spectral Data

The glass capillary tubes containing the PAH from the above preparative GC runs were rinsed individually into 0.4 ml cuvettes with 95% ethanol. UV spectra were obtained with a Beckman Acta C III spectrophotometer.

GC-Mass Spectral Data

A Varian 1400 GC instrument was interfaced with a DuPont 21-492 mass spectrometer. The gas chromatograph was equipped with a 10' × 1/8" SS column packed with 5% Dexsil 300 GC on 100/120 Chromosorb W-AW (injection temperature, 290° C; FID, 350° C; and 20 ml/min He). GF subfractions 40-1, -2, -3, -4, -5, and -6 were chromatographed isothermally at 100, 120, 165, 185, 240 and 285° C, respectively. GF fractions 41, 43, and 45 were chromatographed using a temperature program of 2°/min from 100° C to 325° C.

Mass spectral (MS) analyses were performed as follows. The GC effluent was split 1:1, one half going to the FID of the gas chromatograph and the other half to the source area of the mass spectrometer. A jet separator, at 300° C, stripped helium from the effluent before mass spectral analysis. Mass spectra of effluent GC peaks were obtained under the following conditions: a scan rate of 100 s/mass-decade, a minimal resolution of 1000, and 70 eV electron bombardment. Mass spectra were taken as often as possible during the elution time of a GC peak to determine mass integrity. The spectra were recorded by a high-speed recording oscillograph or an AEI DS-30 computerized data system. Mass spectral data were analyzed by both manual and computer aided techniques.

RESULTS

The characteristics of the GF step are presented in Fig. 2; the bar graph represents the weight percent of F-20 in each GF fraction. The smoke PAH, like the PAH standards, began to elute in GF fraction 36. Analytical GC data, such as relative retention times and percent composition of GC volatiles were calculated for GF fractions 40 through 45, inclusive. Chromatograms of GF fractions 40, 41, 43, and 45 are presented in Fig. 3, 4, 5, and 6. Peaks having the same RRT have been given the same number in all tables, chromatograms, and figures. This allows the comparison of the individual peak changes in increasing GF fractions. At least 115 peaks are discernable on the chromatograms. GF fractions 40 and 41 contain many early eluting components not found in GF fractions 43 and 45. Comparison of the chromatograms of GF fractions 40 to 45 shows that [1] many peaks decrease and disappear, [2] others, first increase then decrease, and [3] others mainly increase. This phenomenon will be shown later to be a characteristic of the GF step and actually aided in the identification of minor PAH components and isomeric PAH. Standard PAH were co-chromatographed with the GF fractions to determine GC retention time correlation.

Preparative GC was performed on GF fractions 40, 41, 43, and 45. Whenever possible, samples were collected while on the upslope, top, and downslope of the GC peaks to give at least three cuts for each peak. The object of taking multiple cuts of a single peak was to give selective enrichment of components for identification by UV spectroscopy. Analytical GC indicated that GF fractions 42 and 44 contained material also found in the adjacent GF fractions. Therefore, preparative GC separations and analyses on these fractions were not deemed necessary.

The results of the identification and quantitation of the components in the GF fractions are given in Table 1. Peak numbers refer to GC peaks in Figures 3 to 6. Peaks are tabulated in order of their RRT, with peak #70 (pyrene) equalling 1.000. The percent composition of the GF fraction, based on total GC volatiles and assuming unitary detector response, is also given. The tabulated values for percent composition of the GC peak components in each gel fraction depended on its percentage of total GC volatiles. The percentage

Figure 2. Gel filtration chromatography [A: percent weight distribution of F-20 gel fractions; B: 280 nm absorbance curve for the elution of F-20 (100 = 1.28 absorbance units); C: elution curves for standard PAH (1 — 3,6-dimethylphenanthrene; 2 — phenanthrene; 3 — pyrene; 4 — benzo(a)pyrene)].

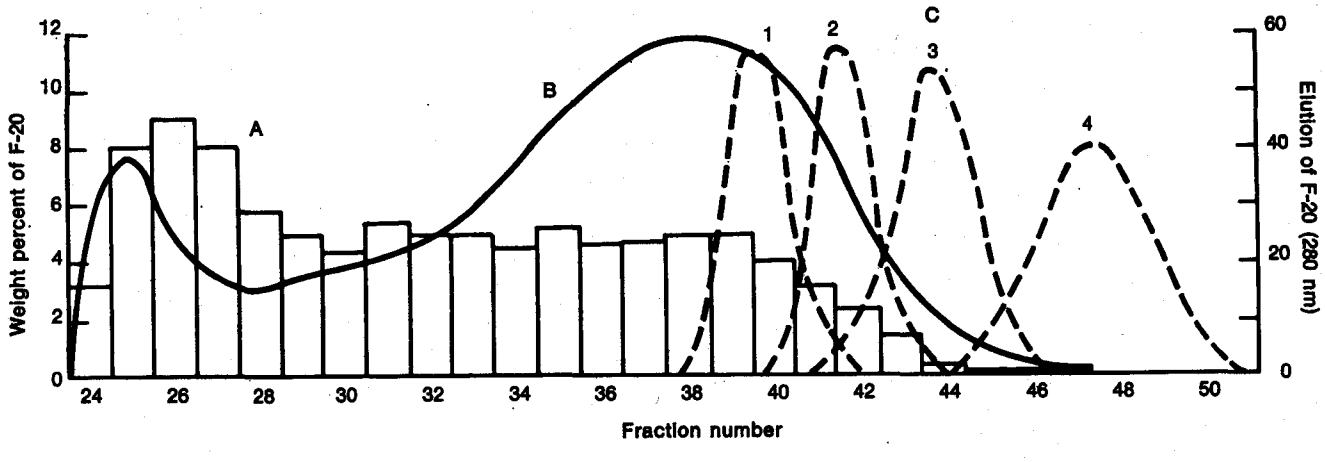


Figure 3. Gas chromatogram of gel filtration fraction 40.

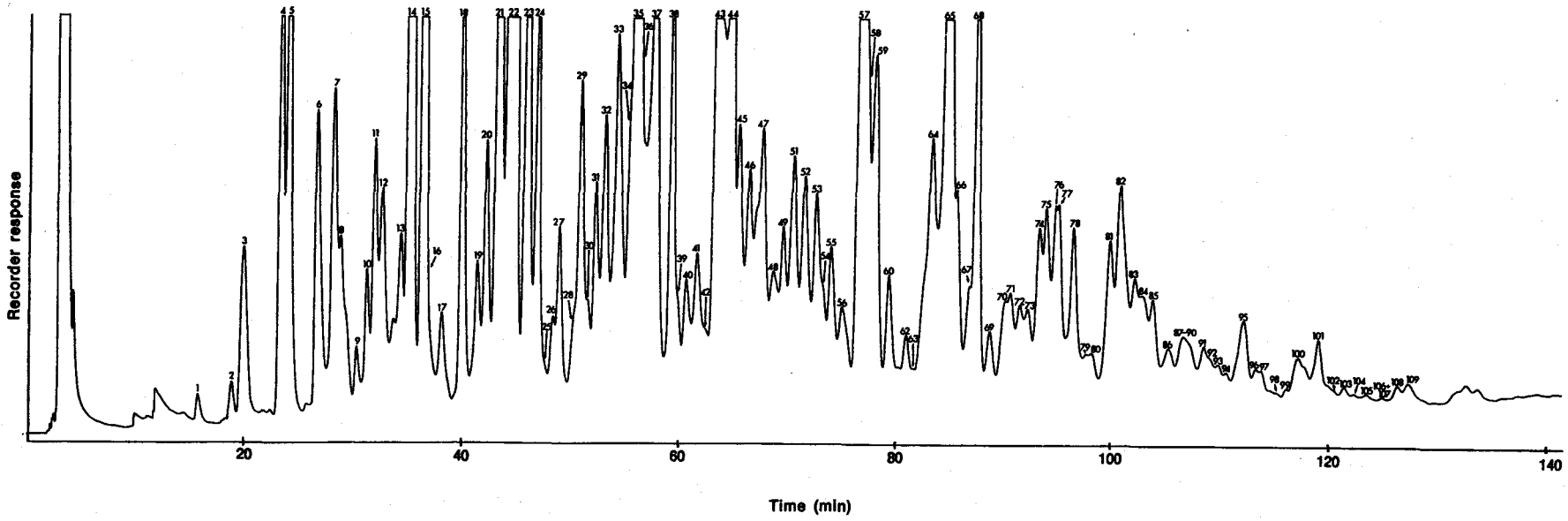
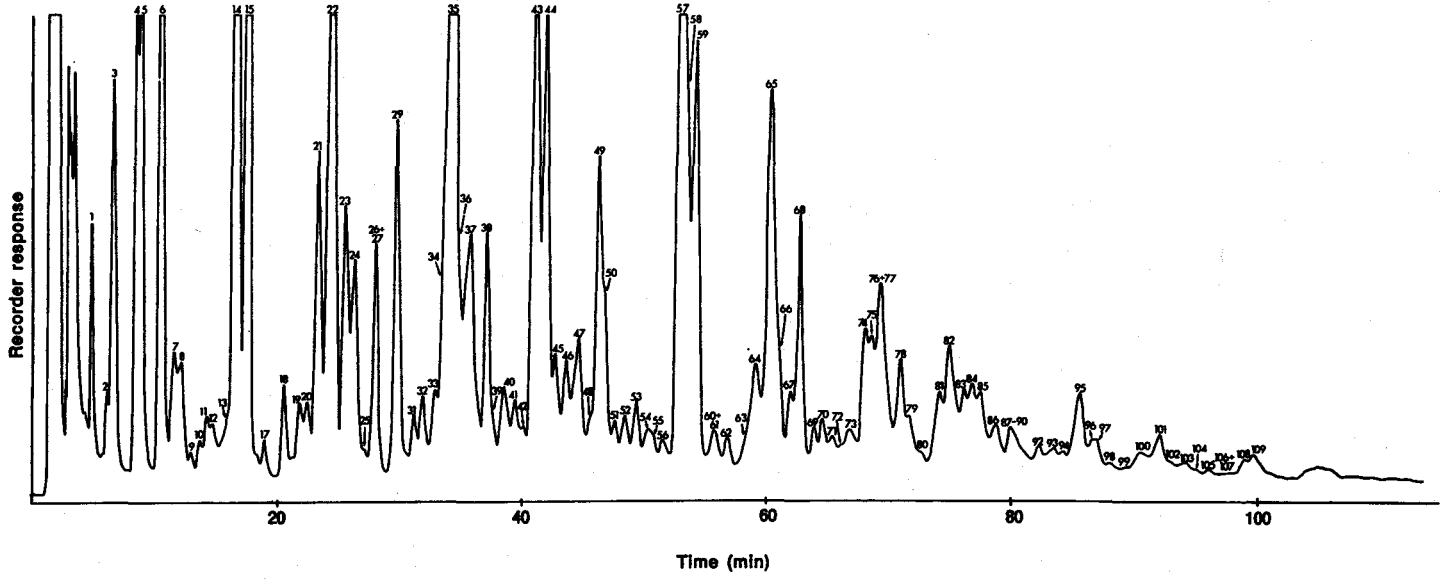


Figure 4. Gas chromatogram of gel filtration fraction 41.



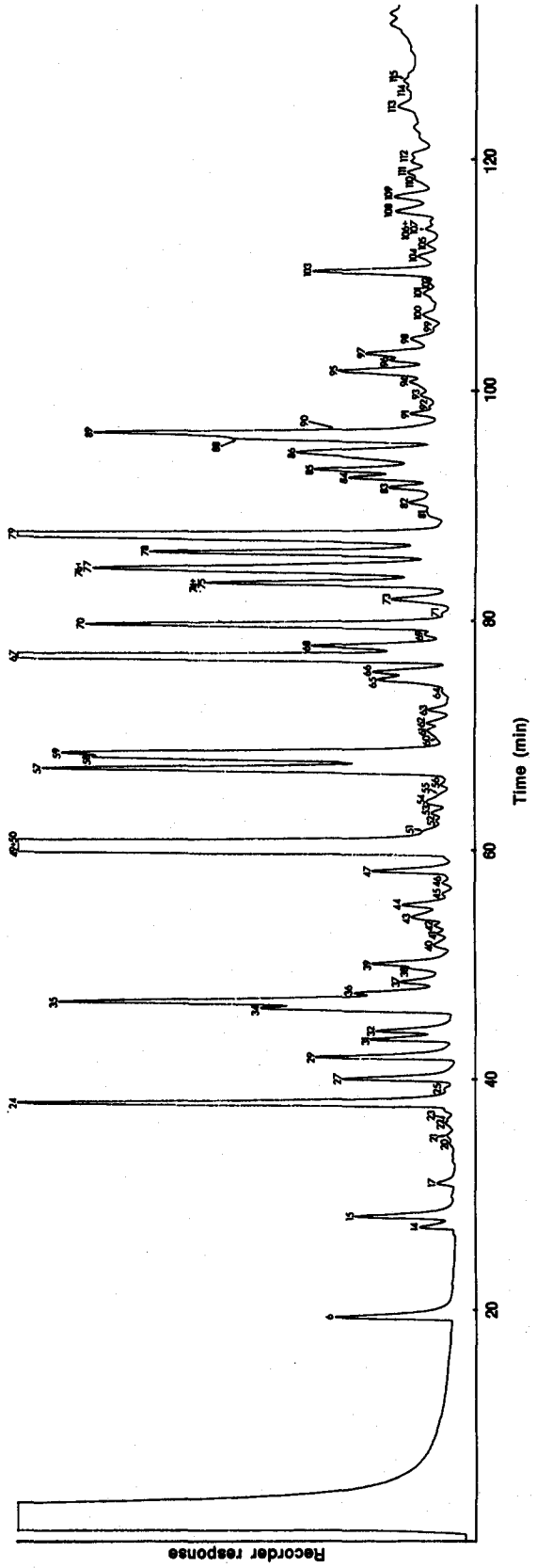


Figure 5. Gas chromatogram of gel filtration fraction 43.

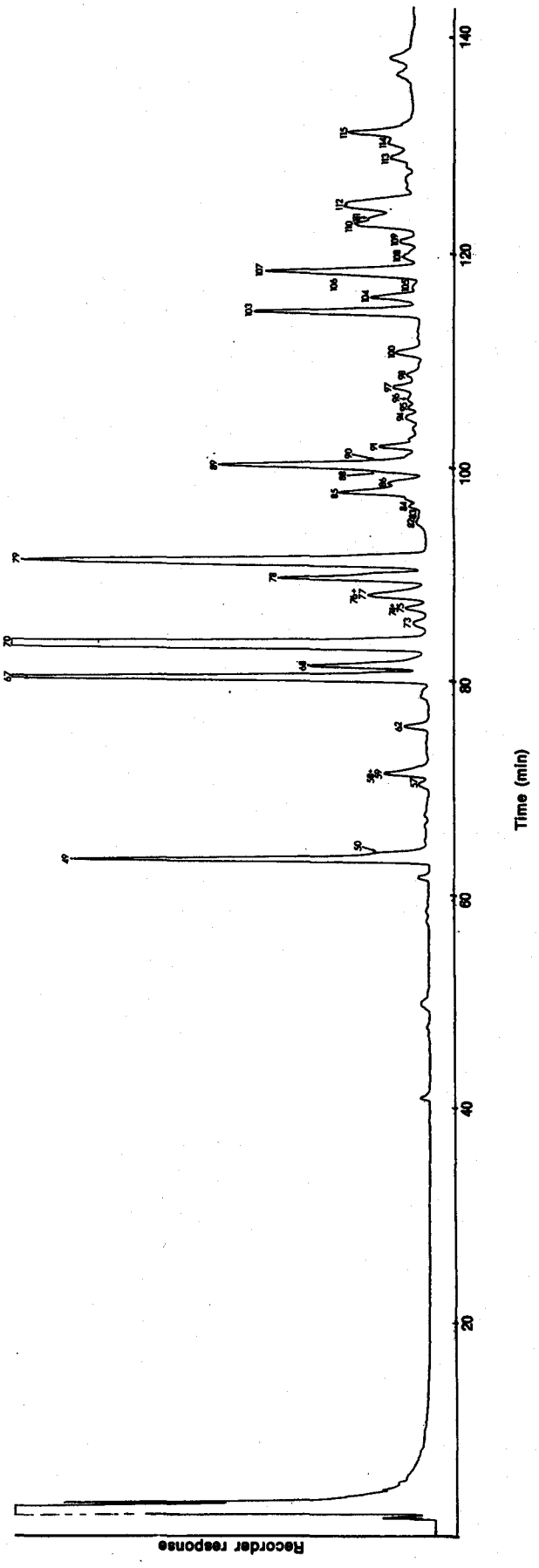


Figure 6. Gas chromatogram of gel filtration fraction 45.

values are strongly representative of increasing or decreasing concentrations of the components in successive gel fractions. Where possible, the major component of a peak is indicated. Frequently, the major component of the same peak changes, in progressing from GF fractions 40 to 45.
The criteria for identification of components are also indicated in Table 1. When GC retention times and/or literature UV data were unavailable, the data in Table 2 were the basis for identification.

DISCUSSION

Although numerous analytical methods for the PAH of tobacco smoke have been proposed (11-14), these techniques have utilized relatively crude CSC samples that contained many other compounds in addition to the PAH. By applying analytical GF chromatography to a PAH-enriched fraction (F-20), we obtained a highly refined PAH-isolate (GF fractions 36 to 50), which represented only 0.01% of the starting CSC. This GF method was an extension of preparative GF chromatography used to separate F-20 into subfractions for bioassay tests (7). The key to the successful identifications of the PAH was the analysis of each refined GF fraction. The only other compounds, in addition to the PAH that were detected in the GF fractions, were several oxygen-PAH analogues, such as benzo(b)-furan, naphthofurans, dibenzofuran, and their methylated derivatives. However, this was not unexpected as their properties are very similar to those of PAH. The Bio-Beads SX-12 gels separated PAH from other materials by an adsorption type mechanism, whereby the PAH were retained due to their aromatic character. Another separation factor involved early elution of methylated PAH before the parent PAH compound. Thus, increasing the number of methyl groups on a PAH decreases its elution volume. On the other hand, increasing the number of aromatic rings in a PAH increases its elution volume. These two gel properties have been discussed in detail (9). Fig. 2 shows that the order of elution of the standards was 3,6-dimethylphenanthrene, phenanthrene, pyrene, and benzo(a)-pyrene.
The partial separations of PAH by methyl substitution and ring number are also well illustrated by the data for the PAH of CSC. These two factors significantly aided in the identification of the PAH. That is, the methylated small ring PAH were found in the early GF fractions. Subsequent fractions contained the parent compounds and the methylated derivatives of higher ring PAH, while still later fractions contained predominantly the parent PAH. Thus, GF fractions 40 and 41 were rich in trimethyl- and dimethyl-derivatives of naphthalene, fluorene, phenanthrene, anthracene, fluoranthene, pyrene, and chrysene. GF fractions 40 and 41 were also rich in methyl-derivatives of naphthalene, fluorene, phenanthrene, and anthracene. GF fraction 43 contained large amounts of the methyl-derivatives of phenanthrene, fluoranthene, pyrene, 1,2-benzanthracene, chrysene, benzofluoranthene, benzo(a)pyrene, and benzo-(e)pyrene. The parent PAH — phenanthrene, anthracene, benzofluorenes, fluoranthene, pyrene, 1,2-benzanthracene, chrysene, benzofluoranthenes, acenaphthylene, and benz(f)indene — were concentrated in GF fraction 43. GF fraction 45 contained mainly the parent PAH — phenanthrene, anthracene, fluoranthene, pyrene, benzo(g,h,i)fluoranthene, chrysene, benzofluoranthene, benzo(a)pyrene, and benzo(e)pyrene. It also contained methyl-derivatives of fluoranthene, pyrene, benzo(a)-pyrene, and benzo(e)pyrene.
As mentioned before, the percent composition of gel fractions given in Table 1 only indicates trends, since the percentages for each peak depended upon the amount and type of GC volatiles. To quantitate individual PAH, calculations must be based on the combined data of all the gel fractions which contain the particular PAH. Such calculations have been performed in conjunction with a rapid analytical method for PAH of cigarette smoke (15).
The components of the GF fractions were identified by a combination of GC, UV, and GC-MS methods. These criteria together with the separation of PAH by GF, according to structure, have made many of the identifications more definitive. In only four cases was identification based on MS data alone. The lack of suitable PAH standards, particularly methyl- and dimethyl-derivatives, presented some problems in the unambiguous identification of the PAH. In some cases, additional criteria, such as NMR, spectrophotofluorometry, and high-speed liquid chromatography, will be needed to determine the position of methyls on the ring systems. Work will be continued in these areas. Obviously, previous identifications of PAH based on only one criterion (i.e., UV, MS data, or GC retention time) must be used cautiously.
Currently, work is continuing on the identification of the PAH constituents in GF fractions higher than 45. The material in these fractions constitutes only a small percentage of the total PAH, but should contain the higher ring PAH systems, from benzo(a)pyrenes and dibenzopyrenes to coronene and above. Due to the biological activity ascribed to some of the higher molecular weight PAH, this portion of the PAH spectrum should prove to be as interesting and as important as the lower molecular weight PAH.

SUMMARY

A neutral fraction of cigarette smoke condensate, which had shown biological activity and was known to contain polynuclear aromatic hydrocarbons (PAH), was fractionated by analytical gel filtration chromatography. These gel fractions were subjected to gas chromatographic separation and their components were identified by relative GC retention times, UV spectra, and mass spectral data. More than 300 PAH, ranging from indene to the dimethylbenzopyrenes, were characterized. This

method of isolation has yielded fractions which were more amenable to definitive identifications. The criteria used for identification are tabulated for all the identified PAH compounds.

ZUSAMMENFASSUNG

Eine neutrale Fraktion des Kondensates von Cigarettenrauch, bei der biologische Aktivität und ein Gehalt an polycyclischen aromatischen Kohlenwasserstoffen (PAH) beobachtet worden waren, wurde mittels analytischer Gel-Chromatographie fraktioniert. Nach gaschromatographischer Trennung dieser Gel-Fraktionen wurden deren Bestandteile auf Grund relativer GC-Retentionszeiten, UV-Spektren und massenspektrometrischen Werten identifiziert. Mehr als 300 polycyclische aromatische Kohlenwasserstoffe — vom Inden bis zum Dimethylbenzpyren — wurden nachgewiesen. Das Trennungsverfahren ergab Fraktionen, die für endgültige Identifizierungen geeigneter waren. Die zum Nachweis benutzten Kriterien werden für alle identifizierten Kohlenwasserstoffverbindungen tabellarisch aufgeführt.

RESUME

On a fractionné par chromatographie analytique à perméation de gel, une fraction neutre de condensat de fumée de cigarette, dont on a démontré une activité biologique et dont on sait qu'elle contient des hydrocarbures polynucléaires aromatiques (PAH). Ces fractions de «gel» sont soumises à une séparation par chromatographie en phase gazeuse, et on a identifié les composants par leurs temps de rétention relatifs, leurs spectres UV, et leurs données en spectrographie de masse. On a ainsi démontré la présence de plus de 300 PAH, variant de l'indène aux diméthylbenzopyrènes. Cette méthode d'isolation produit un groupe de fractions qu'il est plus aisé d'identifier avec certitude. Les critères employés pour l'identification de tous lesdits composés PAH sont présentés sous forme de tableau.

REFERENCES

1. Swain, A. P., J. E. Cooper, R. L. Stedman, and F. G. Bock: Beitr. Tabakforsch. 5 (1969) 109.
2. Bock, F. G., A. P. Swain, and R. L. Stedman: J. Natl. Cancer Inst. 44 (1970) 1305.
3. Bock, F. G., A. P. Swain, and R. L. Stedman: J. Natl. Cancer Inst. 49 (1972) 477.
4. Swain, A. P., F. G. Bock, J. E. Cooper, W. J. Chamberlain, E. D. Strange, L. Lakritz, and R. L. Stedman: Beitr. Tabakforsch. 7 (1973) 1.
5. Stedman, R. L., R. L. Miller, L. Lakritz, and W. J. Chamberlain: Chem. and Ind. 1968, 394.
6. Miller, R. L., W. J. Chamberlain, and R. L. Stedman: Tob. Sci. 13 (1969) 21.
7. Chamberlain, W. J., D. B. Walters, M. E. Snook, O. T. Chortyk, and F. J. Akin: Beitr. Tabakforsch. 8 (1975) 133.
8. Snook, M. E., W. J. Chamberlain, R. F. Severson, and O. T. Chortyk: Anal. Chem. 47 (1975) 1155.
9. Snook, M. E.: Anal. Chim. Acta. 81 (1976) 423.
10. Swain, A. P., J. E. Cooper, and R. L. Stedman: Cancer Res. 29 (1969) 579.
11. Carugno, N., and S. Rossi: Anal. Chem. 39 (1967) 103.
12. Davis, H. J.: Talanta 16 (1969) 621.
13. Rathkamp, G., and D. Hoffmann: Information Bulletin CORESTA 1972-Special, p. 16.
14. Hoffmann, D., G. Rathkamp, K. D. Brunnemann, and E. L. Wynder: Science of the Total Environment 2 (1973) 157.
15. Severson, R. F., M. E. Snook, O. T. Chortyk, and R. F. Arrendale: Beitr. Tabakforsch. 8 (1976) 273.
16. UV atlas of organic compounds; Plenum Press, New York, 1966.
17. Entwistle, I. D., and R. A. W. Johnstone: J. Chem. Soc. (C) 1968, 1818.
18. Stubbs, H. W. D., and S. H. Tucker: J. Chem. Soc. 1954, 227.
19. Clar, E.: Aromatische Kohlenwasserstoffe, polycyclische Systeme; Springer-Verlag, Berlin - Göttingen - Heidelberg, 1952.

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Tables 1 and 2 are shown on pages 257 to 272.

Table 1. Composition of gel filtration fractions 40 to 45.

Peak No.	Compound	Relative retention time[a]	Gel fraction 40	41	42	43	44	45	Criteria of identification GC-RT[c]	UV[d]	MS[e]
			Percent composition[b]								
1	Indene	0.113	0.06	1.27	0.04	<0.01	–	–	+	+	+
2	Methylbenzo(b)furan	0.156	0.11	0.53	0.02	<0.01	–	–		+	+
3	Methylbenzo(b)furan	0.165	0.66	2.52	0.15	<0.01	–	–		+	+
4	1-Methylindene	0.198	1.09	1.58	0.10	<0.01	–	–	+		+
	3-Methylindene		M[f]	M						+(16)	+
5	Methylindene	0.206	1.86	2.31	0.12	<0.01	–	–		+	+
6	Naphthalene	0.238	1.08	3.55	6.94	1.13	<0.01	–	+	+	+
	Dimethylbenzo(b)furan		M	M						+	+
7	Dimethylbenzo(b)furans	0.256	1.78	0.89	0.07	<0.01	–	–		+	+
8	Dimethylindene	0.259		0.76[g]		<0.01	–	–		+	+
9	Dimethylbenzo(b)furans	0.285	0.19	0.20	<0.01	–	–	–		+	+
	Dimethylindene		M	M						+	+
10	Dimethylindene	0.292	0.37	0.24	<0.01	–	–	–		+	+
11	Dimethylindene	0.300	0.78	0.36	<0.01	–	–	–		+	+
12	Dimethylindene	0.308	0.97	0.55	<0.01	–	–	–		+	+
13	Dimethylindene	0.327	0.76		0.05	<0.01	–	–		+	+
14	2-Methylnaphthalene	0.335	5.79	6.99	2.00	0.28	<0.01	–	+	+	+
15	1-Methylnaphthalene	0.350	4.64	6.46	3.87	0.98	<0.01	–	+	+	+
16	Trimethylindene							–		+	+
17	Trimethylindenes	0.372	0.41	0.43	<0.01	–	–	–		+	+
18	Biphenyl	0.396	1.29	0.54	<0.01	–	–	–	+	+	+
	Trimethylindenes		M	M						+	+
	Trimethylbenzo(b)furan									+	+
19	Trimethylindene	0.412	0.57	0.56	0.16	0.02	<0.01	–		+	+
	Trimethylbenzo(b)furan									+	+
20	2-Ethylnaphthalene	0.422	0.88	0.47	0.16	0.04	<0.01	–	+	+	+
	1-Ethylnaphthalene								+	+	+

Table 1. Composition of gel filtration fractions 40 to 45 (contd.).

Peak No.	Compound	Relative retention time[a]	Gel fraction 40	41	42	43	44	45	Criteria of identification GC-RT[c]	UV[d]	MS[e]
			Percent composition[b]								
21		0.434	2.96	1.56	0.30	0.07	<0.01	–			
	2,6-Dimethylnaphthalene		M	M					+	+	+
	2,7-Dimethylnaphthalene								+	+(16)	+
	1-Vinylnaphthalene								+	+	+
22		0.450	7.67	4.21	0.63	0.09	<0.01	–			
	1,3-Dimethylnaphtalene								+	+	+
	1,6-Dimethylnaphthalene								+	+	+
	2-Vinylnaphthalene								+	+	+
23		0.467	2.16	1.40	3.72	0.12	<0.01	–			
	2,3-Dimethylnaphthalene								+	+	+
	1,4-Dimethylnaphthalene								+	+	+
	1,5-Dimethylnaphthalene								+	+	+
24		0.476	1.33	1.46		3.52	1.25	0.17			
	1,7-Dimethylnaphthalene		M	M						+(17)	+
	Acenaphthylene					M		M	+	+	+
25		0.489	0.15[h]	0.10	0.11	0.07	<0.01	–			
	3-Methylbiphenyl								+	+	+
26		0.497	0.26[h]		<0.01	–	–	–			
	4-Methylbiphenyl								+	+	+
27		0.503	0.64	1.32	1.55	0.90	0.13	<0.01			
	1,8-Dimethylnaphthalene								+	+	+
	Acenaphthene								+	+	+
	Trimethylnaphthalene										+
28		0.526	1.32	1.89	2.09	1.14	0.21	<0.01			
	Trimethylnaphthalenes									+	+
29											
	Dibenzofuran		M	M		M			+	+	+
30		0.537	0.31		<0.01	–	–	–			
	Trimethylnaphthalene									+	+
31		0.545	0.74	0.38	0.66	0.63	0.26	0.07			
	Trimethylnaphthalene		M							+	+
	Unknown					M		M		+	+
32		0.555	1.06	0.52	0.53	0.72	0.35	0.09			
	Trimethylnaphthalene		M	M						+	+
	Naphtho(2,1-b)furan					M		M		+(18)	+
33		0.568	1.80[h]	0.55[h]	<0.01	–	–	–			
	Trimethylnaphthalene									+	+
34		0.581	0.86[h]	[h]		1.51[h]	1.76	<0.01			
	Trimethylnaphthalene		M							+	+
	1-Methylacenaphthylene					M				+(19)	+
35		0.588	5.40	8.50	10.13	3.76		0.33			
	Fluorene		M	M		M			+	+	+
	Methylacenaphthylene									+	+
	Trimethylnaphthalene									+	+
36		0.596				0.84		<0.01			
	9-Methylfluorene								+	+	+
	Trimethylnaphthalene									+	+
	Methylacenaphthylenes					M				+	+

Table 1 (contd.)

Peak No.	Compound	Relative retention time[a]	Gel fraction 40	41	42	43	44	45	Criteria of identification GC-RT[c]	UV[d]	MS[e]
			Percent composition[b]								
37		0.612	2.69	2.34	1.48	0.61	<0.01	–			
	Methylacenaphthene		M	M						+	+
	Trimethylnaphthalene										+
	Unknown					M				+	+
38		0.629	1.68	1.38	1.00	0.36	<0.01	–			
	Methyldibenzofuran		M							+	+
	Unknown					M				+	+
39		0.636				0.80	0.20	<0.01			
	Benz(f)indene									+(18)	+
40		0.647	0.58	0.75	0.40	0.29	<0.01	–			
	Methyl-unknown of RRT 0.545		M	M						+	+
	Dimethylacenaphthene									+	+
41		0.660	0.92	0.57	0.16	0.14	<0.01	–			
	Dimethylacenaphthene		M							+	+
	Methyl-unknown of RRT 0.545					M				+	+
42		0.671	[h]	0.23[h]	0.23	0.16[h]	<0.01	–			
	Dimethylacenaphthene									+	+
43		0.682	5.10	3.11	1.00	0.56	0.09	0.10			
	2-Methylfluorene		M	M					+	+	+
	3-Methylfluorene								+(13)		+
	Dimethylacenaphthylene									+	+
	Methyl-unknown of RRT 0.545					M				+	+
44		0.694	3.92	2.44	0.90	0.53	0.16	0.09			
	1-Methylfluorene		M	M					+	+	+
	4-Methylfluorene		M	M					+(13)	+(16)	+
	Dimethylacenaphthylene					M				+	+
	Methyldibenzofuran									+	+
45		0.704	1.03	0.76	0.14	0.14	<0.01	–			
	Dimethylacenaphthene		M	M						+	+
	Dimethylacenaphthylenes			M						+	+
	Dimethyldibenzofuran									+	+
46		0.716	0.91	0.69	0.02	0.12	<0.01	–			
	Dimethylacenaphthene									+	+
	Dimethyldibenzofuran									+	+
	Methylbenz(f)indene		M							+	+
47		0.731	1.69	1.21	0.44	0.70[g]	0.51	0.23			
	Dimethylacenaphthene									+	+
	Dimethyldibenzofuran									+	+
	Methylbenz(f)indene									+	+
	Tetramethylnaphthalene									+	+
48		0.745	0.41		<0.01	–	–	–			
	Trimethylacenaphthene									+	+
	Trimethylacenaphthylene									+	+
	Methylbenz(f)indene									+	+
	Dimethyl-unknown of RRT 0.545									+	+
49		0.754	0.76	2.60	17.26	20.32	20.87	6.75			
	Phenanthrene		M	M		M		M	+	+	+
	Trimethylacenaphthene									+	+
50		0.760				9.13					
	Anthracene								+	+	+
51		0.769	1.11	0.43			<0.01	–			
	Dimethylfluorenes		M	M						+	+
	Trimethylacenaphthene									+	+

Table 1. Composition of gel filtration fractions 40 to 45 (contd.).

Peak No.	Compound	Relative retention time[a]	Gel fraction 40	41	42	43	44	45	Criteria of identification GC-RT[c]	UV[d]	MS[e]
			Percent composition[b]								
52		0.780	1.04	0.48	0.01	0.03	0.03	<0.01			
	Dimethylfluorene		M	M						+	+
	Trimethylacenaphthene									+	+
	Dimethyl-unknown of RRT 0.545									+	+
53		0.794	0.90[h]	0.54[h]	0.10	0.08[g]	<0.01	0.14			
	Dimethylfluorene		M	M						+	+
	Trimethylacenaphthylene									+	+
54		0.804	0.26[h]	0.62	0.17	0.17	0.12	0.14			
	Trimethylacenaphthylene									+	+
	Dimethylfluorene									+	+
55		0.810	0.66[h]	[h]		[g]					
	Dimethylfluorene									+	+
	Trimethylacenaphthylene									+	+
56		0.821	0.58[h]	0.35[h]	0.06	0.01[g]	<0.01	–			
	Dimethylbenz(f)indene									+	+
	Trimethylacenaphthylene									+	+
57		0.843	3.70	5.45	5.98	3.67	1.05	0.26			
	2-Methylphenanthrene		M	M		M		M	+	+	+
	3-Methylphenanthrene		M	M		M		M	+	+	+
	Dimethylfluorene									+	+
	Trimethylacenaphthylene									+	+
58		0.849	1.49	2.45	6.15	2.66	3.14	1.09			
	2-Methylanthracene								+	+	+
59		0.859				3.29					
	9-Methylphenanthrene									+(18)	+
	1-Methylphenanthrene								+	+	+
	1-Methylanthracene									+(18)	+
60		0.877	0.66	0.59	0.12	0.23	0.06	<0.01			
	9-Methylanthracene					M			+	+	+
	4-Methylphenanthrene		M	M						+(18)	+
61		0.881	<0.01	[h]	0.03	[h]	<0.01	–			
	Dimethylphenanthrene									+	+
	Tetramethylacenaphthene									+	+
	Tetramethylacenaphthylene									+	+
62		0.897	0.03[h]	0.36[h]	0.05	0.06	0.11	0.44			
	Dimethylphenanthrene					M				+	+
	Tetramethylacenaphthene		M							+	+
	Tetramethylacenaphthylene		M							+	+
63		0.905	<0.01		<0.01	0.02	<0.01	–			
	Dimethylphenanthrene									+	+
	Dimethylanthracene					M				+	+
64		0.924	1.87[h]	1.24	0.10	0.03	<0.01	–			
	Dimethylphenanthrenes			M						+	+
	Dimethylanthracene									+	+
	Tetramethylacenaphthylene									+	+
65		0.941	3.13	3.43	2.22	0.70	0.34	0.21			
	Dimethylphenanthrenes									+	+
	Dimethylanthracene									+	+
66		0.951	0.62			0.62	0.35	<0.01			
	Dimethylphenanthrene		M							+	+
	Dimethylenephenanthrene									+	+

Table 1 (contd.)

Peak No.	Compound	Relative retention time[a]	Gel fraction						Criteria of identification		
			40	41	42	43	44	45			
			Percent composition[b]						GC-RT[c]	UV[d]	MS[e]
67		0.964	0.42	0.50	3.23	7.20	9.76	9.06			
	Fluoranthene					M		M	+	+	+
	Dimethylphenanthrene		M							+	+
	Dimethylanthracene									+	+
68		0.973	1.48	1.43	0.91	1.28	1.77	2.52			
	Dimethylphenanthrene		M	M						+	+
	Trimethylphenanthrene										+
	Unknown					M		M		+	+
69		0.993	0.31	0.32	0.12	0.16	<0.01	–			
	Dimethylphenanthrene									+	+
	Trimethylphenanthrene									+	+
70		1.000	[h]	0.46[h]	1.07	2.86	7.06	21.45			
	Pyrene					M		M	+	+	+
	Dimethylphenanthrene									+	+
	Trimethylphenanthrene									+	+
	Cyclopentenophenanthrene									+	+
71		1.013	0.60	0.32		0.03	<0.01	–			
	Trimethylphenanthrene									+	+
	Dimethylphenanthrene									+	+
	Cyclopentenophenanthrene									+	+
72		1.023	0.42[h]		<0.01	–	–	–			
	Trimethylphenanthrene		M							+	+
	Trimethylanthracene									+	+
	Cycopentenophenanthrene									+	+
73		1.032	0.34	0.72	0.42	0.45[g]	0.48	0.45[g]			
	Trimethylphenanthrene									+	+
74		1.044	0.60[h]	0.86	2.11	1.95	1.22	0.51			
	Trimethylphenanthrene									+	+
	8-Methylfluoranthene			M		M		M		+(20)	+
75		1.051	0.63[h]	0.62							
	Trimethylphenanthrene									+	+
	1,2-Benzofluorene			M					+	+	+
76		1.060	0.54[h]	1.65	4.26	4.59	3.14	1.66			
	1-Methylfluoranthene		M			M		M		+(20)	+
	2-Methylfluoranthene		M							+(20)	+
	Trimethylphenanthrene									+	+
77		1.067	0.53								
	2,3-Benzofluorene			M		M		M	+	+	+
	3,4-Benzofluorene			M		M		M	+	+	+
	Trimethylphenanthrene		M							+	+
78		1.080	0.85	0.88	1.61	2.62	3.17	2.93			
	Trimethylphenanthrene		M							+	+
	Cyclopentenophenanthrene			M						+	+
	Methylcyclopentenophenanthrene									+	+
	2-Methylpyrene			M		M		M	+	+	+
79		1.095	0.13	0.54	3.10	6.35	9.32	10.56			
	Dimethylfluoranthene									+	+
	Trimethylphenanthrene									+	+
	Cyclopentenophenanthrene		M							+	+
	Methylcyclopentenophenanthrene									+	+
	1-Methylpyrene					M		M	+	+	+
	4-Methylpyrene					M		M	+	+	+

Table 1. Composition of gel filtration fractions 40 to 45 (contd.).

Peak No.	Compound	Relative retention time[a]	Gel fraction 40	41	42	43	44	45	Criteria of identification GC-RT[c]	UV[d]	MS[e]
			Percent composition[b]								
80		1.107	0.20	0.20	<0.01	–	–	–			
	Dimethylfluoranthene									+	+
	Cyclopentenophenanthrene									+	+
	Methylcyclopentenophenanthrene									+	+
81		1.124	0.70	0.76	0.35	0.08	0.14	<0.01			
	Dimethylfluoranthene			M						+	+
	Methyl-1,2-benzofluorene									+	+
	Methylcyclopentenophenanthrene									+	+
82		1.133	1.18	1.14	0.66	0.13	0.40	0.35			
	Dimethylfluoranthenes									+	+
	Methyl-1,2-benzofluorene									+	+
	Methyl-2,3-benzofluorene									+	+
	Methyl-3,4-benzofluorene									+	+
83		1.150	0.42[h]	0.54[h]	0.59	0.27	0.59	0.35			
	Dimethylfluoranthene		M							+	+
	Dimethylpyrene			M		M				+	+
	Methyl-1,2-benzofluorene									+	+
	Methyl-3,4-benzofluorene									+	+
84		1.160	0.53[h]	0.69	0.77	0.62	0.85	0.12			
	Dimethylpyrene			M		M				+	+
	Dimethylfluoranthenes									+	+
	Methylbenzofluorene		M							+	+
85		1.167	0.44[h]	0.67[h]	1.06	0.96	0.97	2.55			
	Dimethylpyrenes		M	M		M				+	+
	Dimethylfluoranthene									+	+
	Methylbenzofluorene									+	+
	Benzo(g,h,i)fluoranthene							M	+	+	+
86		1.186	0.32[h]	0.56	1.48	1.87	1.63	0.85			
	Dimethylpyrenes		M	M		M		M		+	+
	Methylbenzofluorene									+	+
	Trimethylfluoranthene									+	+
87		1.207	0.58	0.87	2.35	3.85	5.76	5.62			
	Methylbenzofluorene									+	+
88											
	1,2-Benzanthracene			M		M			+	+	+
89											
	Chrysene			M		M		M	+	+	+
90											
	Triphenylene					M		M	+	+	+
	Trimethylfluoranthene									+	+
	Trimethylpyrene		M							+	+
91		1.230	0.18	<0.01	0.12	0.02	0.87	1.32			
	Trimethylpyrene		M							+	+
	Trimethylfluoranthene									+	+
	Dimethylbenzofluorene									+	+
	3,4-Dimethylenepyrene							M		+	+
92		1.236	0.10	0.39			<0.01	–			
	Trimethylpyrene									+	+
	Trimethylfluoranthene									+	+
93		1.246	0.13	0.35	0.33	0.02	0.33	0.40			
	Trimethylpyrenes									+	+

Table 1 (contd.)

Peak No.	Compound	Relative retention time[a]	Gel fraction 40	41	42	43	44	45	Criteria of identification GC-RT[c]	UV[d]	MS[e]
			Percent composition[b]								
94		1.255	0.10	0.18		0.16	0.58	0.64			
	Trimethylpyrenes		M	M		M				+	+
	Methyl-1,2-benzanthracene									+	+
	Methylbenzo(g,h,i)fluoranthene									+	+
95		1.276	0.46	0.77	1.28	0.84	0.94	0.40			
	2-Methylchrysene		M	M		M			+	+	+
	3-Methylchrysene								+	+	+
	Methyl-1,2-benzanthracene									+	+
	Methyltriphenylene									+	+
	Methylbenzo(g,h,i)fluoranthene							M		+	+
	Trimethylpyrene									+	+
96		1.288	0.10	0.18	0.92	0.25	1.36	0.49			
	4-Methylchrysene		M	M		M			+	+	+
	Trimethylpyrene									+	+
	Tetramethylpyrene									+	+
	Methyl-1,2-benzanthracenes									+	+
97		1.294	0.08			0.52		0.93			
	1-Methylchrysene								+	+	+
	6-Methylchrysene								+	+	+
	Methyl-1,2-benzanthracene									+	+
	Trimethylpyrene									+	+
	Tetramethylpyrene									+	+
	Methyltriphenylene									+	+
98		1.310	0.02	0.01	0.27	0.07	0.80	0.61			
	Dimethylchrysene									+	+
	Tetramethylpyrene									+	+
	Trimethylpyrene									+	+
	3,4-Trimethylenepyrene			M		M		M		+(21)	+
99		1.322	0.04			0.03	<0.01	–			
	Dimethylchrysene		M							+	+
	Dimethyl-1,2-benzanthracene									+	+
	Tetramethylpyrene									+	+
100		1.336	0.25	0.17	0.07	0.02	0.56	0.64			
	Dimethylchrysenes		M	M		M		M		+	+
	Dimethyl-1,2-benzanthracenes									+	+
	Dimethyltriphenylene									+	+
	Tetramethylpyrene									+	+
101		1.359	0.19	0.27	0.14	0.02	0.41	0.20			
	Dimethylchrysenes		M	M						+	+
	Dimethyl-1,2-benzanthracene									+	+
	Dimethyltriphenylene									+	+
102		1.371	0.17	0.08	0.04	0.03	<0.01	–			
	Dimethylchrysene		M	M						+	+
	Dimethyl-1,2-benzanthracene									+	+
	Dimethyltriphenylene									+	+
	Trimethylchrysene									+	+
	Trimethyl-1,2-benzanthracene									+	+
	Trimethyltriphenylene									+	+
103		1.384	0.02	0.01	0.30	0.71	2.24	3.31			
	Benzo(b)fluoranthene					M		M	+	+	+
	Benzo(j)fluoranthene					M		M		+(21)	+
	Benzo(k)fluoranthene					M		M		+(21)	+
	Dimethylchrysene		M							+	+
	Trimethylchrysene		M							+	+

Table 1. Composition of gel filtration fractions 40 to 45 (contd.).

Peak No.	Compound	Relative retention time[a]	Gel fraction 40	41	42	43	44	45	Criteria of identification GC-RT[c]	UV[d]	MS[e]
			Percent composition[b]								
104		1.401	<0.01[h]	0.01	0.50	0.02	0.71	1.08			
	Benzo(a)fluoranthene					M		M		+(21)	+
	Trimethylchrysene		M	M						+	+
105		1.413	<0.01[h]	0.01	0.05	0.01	0.38	0.17			
	Trimethylchrysene		M							+	+
	Trimethyl-1,2-benzanthracene									+	+
	Trimethyltriphenylene									+	+
106		1.429	<0.01[h]	0.01	0.01	0.01	0.88	3.67			
	Benzo(e)pyrene							M	+	+	+
107											
	Benzo(a)pyrene							M	+	+	+
	Trimethylchrysene		M							+	+
	Trimethyltriphenylene									+	+
108		1.449	0.04	0.07	0.27	0.13	0.97	0.57			
	Methylbenzo(b)fluoranthene									+	+
	Methylbenzo(j)fluoranthene									+	+
	Methylbenzo(k)fluoranthene									+	+
	Perylene							M	+	+	+
	Trimethylchrysene		M							+	+
109		1.464	0.07	0.13	0.24	0.12	1.00	0.53			
	Methylbenzo(b)fluoranthene									+	+
	Methylbenzo(j)fluoranthene									+	+
	Methylbenzo(k)fluoranthene									+	+
110		1.484	–	–	–	<0.01	0.95	2.78			
	Methylbenzo(e)pyrene									+	+
111		1.492	–	–	<0.01	0.03	0.97	1.95			
	Methylbenzo(a)pyrene									+	+
112		1.508	–	–	<0.01	0.03	1.83	1.09			
	Methylbenzo(e)pyrenes									+	+
	Methylbenzo(a)pyrenes							M		+	+
113		1.561	–	–	<0.01	0.42	1.80	1.04[h]			
	Dimethylbenzo(a)pyrenes									+	+
	Dimethylbenzo(e)pyrene									+	+
114		1.575	–	–	<0.01	0.04	0.63	1.03			
	Dimethylbenzo(a)pyrenes									+	+
	Dimethylbenzo(e)pyrene									+	+
115		1.587	–	–	<0.01		0.93	2.14[h]			
	σ-Phenylenepyrene								+	+	+

a: Relative to pyrene; a factor of 80.5 converts RRT to minutes from point of injection.
b: Based on total GC volatiles in gel fraction, assuming unitary detector response; represents total percent composition of all components listed for GC peak(s) up to next listed percentage.
c: GC retention time identical to standard.
d: UV spectra identical to standard, identical to literature, or analogous to parent compound.
e: Molecular ion and fragmentation pattern correlation.
f: Major component, greater than 40 % of composition, subsequently denoted by "M".
g: Major component unidentified.
h: Contains other unidentified material.
M: Major component, greater than 40% of composition.

Table 2. PAH identification data[a].

Relative retention time	Compound	λ_{max} (nm)	Mass (m/e)
0.156	methylbenzo(b)furan	243, 270, 280	132
0.165	methylbenzo(b)furan	245, 275, 282	132
0.206	methylindene	253, 295	130, 115
0.238	dimethylbenzo(b)furan	248, 275, 282	146, 131
0.256	dimethylbenzo(b)furan (2 isomers)	248, 271, 282 248, 275, 288	146, 131
0.259	dimethylindene	253, 279	144
0.285	dimethylbenzo(b)furan (2 isomers)	245, 278, 288 247, 282	146, 131
	dimethylindene	253	144
0.292	dimethylindene	252, 283, 293	144, 129
0.300	dimethylindene	255	144, 129
0.308	dimethylindene	255 (broad)	144, 129
0.327	dimethylindene	255 (broad)	144, 129
0.350	trimethylindene	255	158, 142, 141
0.372	trimethylindenes (2 isomers)	223, 252, 256	158, 142, 141
0.396	trimethylindenes	223, 252 (broad) (located on upslope and downslope)	158, 142, 141
	trimethylbenzo(b)furan	280, 288, 302	160, 145
0.412	trimethylindene	223, 254	158, 142, 141
	trimethylbenzo(b)furan	broad 260-280, 288, 294, 301	160, 145
0.526 upslope	trimethylnaphthalenes (2 isomers)	227, 279, 285, 300, 306, 311 320	170, 155
downslope	(1 isomer)	226	170, 155
0.537	trimethylnaphthalene	228, 273, 280, 285, 296, 318, 325	170, 155
0.545	trimethylnaphthalene	229, 264, 284, 295	170, 155
	unknown (possibly a naphthofuran)	238, 244	168
0.555	trimethylnaphthalene	229, 278, 285, 295, 323	170, 155
0.568	trimethylnaphthalene	229, 270, 277, 294, 300, 318, 325	170, 155
0.581	trimethylnaphthalene	228, 263, 272, 283, 294, 318, 329	170, 155
	unidentified	232, 240, 294, 308, 318, 332	168

Table 2. PAH identification data[a] (contd.).

Relative retention time	Compound	λ_{max} (nm)	Mass (m/e)
0.588	methylacenaphthylene	233, 315, 325, 343	166, 165
	trimethylnaphthalene	226, 324	170, 155
0.596	methylacenaphthylene (2 isomers)	231, 233, 300, 309, 315, 323 330, 344	166
	trimethylnaphthalene	228, 308, 314, 323	170, 155
0.612	methylacenaphthene	228, 280, 290, 308, 317, 323	168, 167, 166
	unknown (possibly benz(e)indene)	229, 245, 254, broad 280, 320	166, 165
0.629	methyldibenzofuran	210, 219, 242, 250, 286, 296, 307	182, 181
	unknown (possibly methylbenz(e)indene)	236, 244, 254, 276, 287, 300	180
0.647	methyl-unknown of RRT 0.545 (possibly a methylnaphthofuran)	230, 238, 246, broad 270-285	182, 167
	dimethylacenaphthene	308, 314, 321, 330	182, 167, 152
0.660	methyl-unknown of RRT 0.545 (possibly a methylnaphthofuran)	240, 246, 247	182
	dimethylacenaphthene	231, 211, 319, 326	182, 181, 180
0.671	dimethylacenaphthene	232, 240, 325	182, 181, 180
0.682	dimethylacenaphthylene	235, 321, 326, 336	180
	methyl-unknown of RRT 0.545 (possibly a methylnaphthofuran)	210, 239, 243	182
0.694	dimethylacenaphthylene	233, broad 322, 334	180
	methyldibenzofuran	248, 256	182
0.704	dimethylacenaphthylenes (2 isomers)	232, 235, broad 328, 345	180, 165
	dimethylacenaphthene	230, 326	182
	dimethyldibenzofuran	248, 257	196
0.716	dimethylacenaphthene	232, broad 328	182, 167
	methylbenz(f)indene	278, 288, 300	180, 165
	dimethyldibenzofuran	245, 255	196, 181
0.731	methylbenz(f)indene	broad 238-245, 277, 287, 300	180, 165
	dimethyldibenzofuran	248, 258	196, 181
	dimethylacenaphthene	233, broad 325	182, 167
	tetramethylnaphthalene	231, 257, 261, 275, 280, 285	184
0.745	trimethylacenaphthene	232, 325	196, 181
	trimethylacenaphthylene	232, 325	194
	methylbenz(f)indene	278, 288, 300	180, 165
	dimethyl-unknown of RRT 0.545 (possibly a dimethylnaphthofuran)	248, 257	196, 181

Table 2 (contd.)

Relative retention time	Compound	λ_{max} (nm)	Mass (m/e)
0.754	trimethylacenaphthene	234, broad 324	196, 181
0.769	dimethylfluorenes (2 isomers)	266, 294, 299, 306	194, 179
	trimethylacenaphthene	231, 328	196
0.780	dimethylfluorene	268, 289, 301	194, 179
	dimethyl-unknown of RRT 0.545 (possibly a dimethylnaphthofuran)	246, broad 280	196
	trimethylacenaphthene	236, 326	196
0.794	dimethylfluorene	209, 258, 264, 276, 306	194, 179
	trimethylacenaphthylene	234, 325, 345	194
	unidentified	258, 292	196, 181
0.804	trimethylacenaphthylene	232, 300, 312, 328	194, 179
	dimethylfluorene	204, 305	194, 179
	unidentified		196
0.810	dimethylfluorene	208, 261, 300	194, 179
	trimethylacenaphthylene	232, 325	194
	unidentified	237, 251, 262, 284, 292, 300, 311	198, 196 ,192
0.821	trimethylacenaphthylene	234, broad 320-340	194, 179
	dimethylbenz(f)indene	279, 288, 300	196, 181
	unidentified	236, 251, 289	208, 198
0.843 (front shoulder)	dimethylfluorene	203, 259, 289, 292, 302	194, 179
(front shoulder)	trimethylacenaphthylene	235, 330	194, 179
0.881	dimethylphenanthrene	252, 275, 283, 295	206, 191
	tetramethylacenaphthene	238, broad 310-340	208
	unidentified	246	204
0.897	dimethylphenanthrene	252, 304, 310, 318	206
	tetramethylacenaphthene	232	210
	tetramethylacenaphthylene	238	208
	unidentified	275, 288	212, 192
0.905	dimethylphenanthrene	275, 288	212, 192
	dimethylanthracene		
0.924	dimethylphenanthrenes (3 isomers)	252, 275, 283, 293 253, 277, 284, 296 252, 275, 285, 296	206, 191
	dimethylanthracene	255, 262, 370, 381	206, 191
	tetramethylacenaphthylene	242, 328	208, 193

Table 2. PAH identification data[a] (contd.).

Relative retention time	Compound	λ_{max} (nm)	Mass (m/e)
0.941	dimethylphenanthrene (3 isomers)	255, 277, 286, 287, 299 253, 278, 285, 297 254, 278, 287, 300	206, 191
	dimethylanthracene	255, 341, 350, 359, 380	206, 191
0.951	dimethylphenanthrene	252, 277, 288, 296	206, 191
	dimethylenephenanthrene	256, 275, 286, 301	204
0.964	dimethylphenanthrene	255, 274, 280, 291, 304	206, 191
	dimethylanthracene	255, 340, 357, 378	206, 191
0.973	dimethylphenanthrene	257, 278, 287, 300	206, 191
	unknown (possibly acephenanthrylene and/or aceanthrylene)	261, 286, 298, 328, 347, 365	202
0.993	dimethylphenanthrene	257, 276, 283, 295, 315, 322, 329, 337	206, 191
	trimethylphenanthrene	(same as above)	220, 205
1.000	dimethylphenanthrene	254, 277, 289, 300	206, 191
	trimethylphenanthrene	(same as above)	220, 205
	unidentified	245, 313, 321, 330, 336	218
1.013	dimethylphenanthrene	253, 255, 257, 270, 280, 288, 300, 315, 320	206, 191
	trimethylphenanthrene	(same as above)	220, 205
	cyclopentenophenanthrene[b]	(same as above)	218
1.023	cyclopentenophenanthrene	255, 280, 286, 301, 335, 350	218
	trimethylphenanthrene	254, 279, 291, 303	220, 205
	trimethylanthracene	350, 360, 381	220, 205
	unidentified	240, 256, 272, 303, 318, 333	
1.032	trimethylphenanthrene	253, 283, 292, 303	220, 205
1.044	trimethylphenanthrene (2 isomers)	253, 257, 300	220, 205
	unidentified		218
1.051	trimethylphenanthrene	254, 255, 256, 282	220, 205
	unidentified	327, 342, 359	218
1.060	trimethylphenanthrene	254	220, 205
	unidentified	323, 338	218
1.067	trimethylphenanthrene	259, 282, 293, 305	220, 205

Table 2 (contd.)

Relative retention time	Compound	λ_{max} (nm)	Mass (m/e)
1.080	trimethylphenanthrene	258, 278, 288, 300, 335, 351	220, 205
	cyclopentenophenanthrene	(same as above)	218
	methylcyclopentenophenanthrene	(same as above)	232
1.095	dimethylfluoranthene	238, 275, 286	230
	cyclopentenophenanthrene	253, 258, 261, 300	218
	methylcyclopentenophenanthrene	(same as above)	234
	trimethylphenanthrene	(same as above)	220, 205
1.107	dimethylfluoranthene	236, 277, 282, 288, 323, 342, 359	230, 215
	methylcyclopentenophenanthrene	254, 300	232, 217
	cyclopentenophenanthrene	(same as above)	218
1.124	dimethylfluoranthene	237, 279, 284, 290, 342, 360	230, 215
	methyl-1,2-benzofluorene	262	230, 215
	methylcyclopentenophenanthrene	254, 300	232, 217
1.133	dimethylfluoranthene (2 isomers)	238, 276, 288, 364 240, 280, 291, 362	230, 215
1.150	dimethylpyrene	247, 277, 310, 323, 337	230, 215
	dimethylfluoranthene	240, 272, 290, 364	230, 215
	methyl-1,2-benzofluorene	254, 260, 263	230, 215
	methyl-3,4-benzofluorene	311, 322, 337	230, 215
	unidentified	301	246, 232
1.160	dimethylpyrene	245, 266, 277, 307, 323, 339	230, 215
	dimethylfluoranthene (2 isomers)	242, 282, 361 247, 290	230, 215
	methylbenzofluorene	254, 262	230, 215
	unidentified		246, 232
1.167	dimethylpyrene (2 isomers)	243, 266, 277, 307, 309, 323 324, 338, 342	230, 215
	dimethylfluoranthene	288	230, 215
	methylbenzofluorenes	254, 262	230, 215
	unknown (possibly a methylcyclopentenophenanthrene)		232, 217
	unknown (possibly a dimethyl-cyclopentenophenanthrene)		246
1.186	dimethylpyrene (2 isomers)	243, 266, 277, 323, 327, 338 343	230, 215
	methylbenzofluorene	255, 263	230, 215
	trimethylfluoranthene	245, 288, 292	244
	unknown (possibly a methylcyclopentenophenanthrene)		232, 217

Table 2. PAH identification data[a] (contd.).

Relative retention time	Compound	λ_{max} (nm)	Mass (m/e)
1.207	methylbenzofluorene	255, 265	230, 215
	trimethylfluoranthene	290, 363	244
	trimethylpyrene (2 isomers)	245, 276, 326, 338, 341	244, 229
1.230	trimethylpyrene	243, 277, 312, 324, 339	244
	trimethylfluoranthene	290, 293	244, 299
	dimethylbenzofluorene	254, 265	244, 229
	3,4-dimethylenepyrene	242, 254, 265, 275, 313, 327, 343	228
1.236	trimethylpyrene	243, 266, 277, 313, 324, 339	244, 229
	trimethylfluoranthene	246, 289	244
1.246	trimethylpyrenes (2 isomers)	245, 255, 265, 279, 324, 340 245, 257, 267, 280, 326, 345	244, 229
1.255	trimethylpyrene (2 isomers)	245, 257, 267, 279, 313, 328 340, 344	244, 229
	methyl-1,2-benzanthracene	290	242
	methylbenzo(g, h, i)fluoranthene	234, 290	240
1.276	trimethylpyrene	244, 278, 329, 346	244, 229
	methyl-1,2-benzanthracene	277, 288	242
	methylbenzo(g, h, i)fluoranthene	233	240
	methyltriphenylene	249, 259	242
1.288	trimethylpyrene	245, 326, 345	244, 229
	tetramethylpyrene	(same as above)	258, 243
	methyl-1,2-benzanthracene (2 isomers)	270, 289, 293	242
1.294	trimethylpyrene	245, 279, 330, 345	244, 229
	tetramethylpyrene	(same as above)	258, 243
	methyl-1,2-benzanthracene	279, 290	242, 227
	methyltriphenylene	249, 259	242
1.310	trimethylpyrene	244, 279, 327, 343	244, 229
	tetramethylpyrene	(same as above)	258, 243
	dimethylchrysene	257, 268	256, 239
1.322	dimethylchrysene	259, 269, 320	256, 241
	dimethyl-1,2-benzanthracene	279, 289	256, 241
	tetramethylpyrene	279, 330, 344	258, 243

Table 2 (contd.)

Relative retention time	Compound	λ_{max} (nm)	Mass (m/e)
1.366	dimethylchrysene (2 isomers by GC)	259, 269, 319	256, 241
	dimethyl-1,2-benzanthracene (2 isomers by GC)	279, 289	256, 241
	dimethyltriphenylene	249, 260	256, 241
	tetramethylpyrene	249, 279, 330, 344	258, 243
1.359	dimethylchrysene (2 isomers by GC)	250, 260, 310, 324	256, 241
	dimethyl-1,2-benzanthracene	270, 280	256, 241
	dimethyltriphenylene	249, 259	256, 241
1.371	dimethylchrysene	259, 270, 313, 328	256
	trimethylchrysene	(same as above)	270
	di- and/or trimethyl-1,2-benzanthracene	280, 288	256, 270
	di- and/or trimethyltriphenylene	248, 259	256, 270
1.384	dimethylchrysene	261, 270, 325	256
	trimethylchrysene	(same as above)	270
1.401	trimethylchrysene	261, 270	270
	unidentified		268
1.413	trimethylchrysene	261, 271	270
	trimethyl-1,2-benzanthracene	280, 292	270
	trimethyltriphenylene	261	270
	unidentified		268
1.429	trimethylchrysene	261, 272	270
	trimethyltriphenylene	252, 261	270
	unidentified	224	268
1.449	trimethylchrysene	262, 272	270
	methylbenzo(b)fluoranthene	254, 276, 292, 302	266
	methylbenzo(j)fluoranthene	223, 242, 319, 332, 345, 364, 382	266
	methylbenzo(k)fluoranthene	240, 402	266
	methylbenzo(a)fluoranthene	256, 363	266
1.464	methylbenzo(b)fluoranthene	255, 290, 301	266
	methylbenzo(j)fluoranthene	242, 308, 317, 332, 384	266
	methylbenzo(k)fluoranthene	240, 308, 402	266
1.489	methylbenzo(e)pyrene	204, 215, 223, 237, 257, 266, 278, 289, 317, 331	266
1.492	methylbenzo(a)pyrene	255, 267, 285, 297, 348, 366, 386	266

Table 2. PAH identification data[a] (contd.).

Relative retention time	Compound	λ_{max} (nm)	Mass (m/e)
1.508	methylbenzo(a)pyrene (2 isomers)	254, 265, 285, 296, 348, 366 broad 380–387	266
	methylbenzo(e)pyrene (2 isomers)	204, 279, 290, 318, 331 280, 290, 320, 336	266
1.561	dimethylbenzo(a)pyrene (2 isomers)	257, 266, 367, 386 257, 267, 368, 388	280, 265
	dimethylbenzo(e)pyrene	204, 224, 280, 292, 319, 333	280, 265
1.575	dimethylbenzo(a)pyrene (2 isomers)	296, 365, 367, 389	280, 265
	dimethylbenzo(e)pyrene	204, 224, 281, 291, 332, 337	280, 265
	unidentified	257	276

a: This table presents only data for compounds whose GC retention time and/or literature UV data are lacking.
b: One of several possible isomeric phenanthrenes with m/e 218.