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CHROMATOGRAPHIC FINGERPRINTING OF COAL EXTRACTS

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SUMMARY

Seven Hungarian coal samples of different ranks were examined by solvent extraction, liquid chromatographic (LC) separation of the extracts and analysis of the aliphatic and aromatic hydrocarbon LC fractions by high-resolution gas chromatography. The LC fraction distribution is characteristic of the coal. The gas chromatograms of the two hydrocarbon LC fractions show strong similarities for related samples and can serve as "fingerprints" of the coals. For the *n*-alkanes, parameters such as "carbon preference index" can be calculated. For other aliphatic and aromatic hydrocarbons, respectively, the retention and "PAH indices" are presented.

INTRODUCTION

The oil crisis has focused interest on other sources of energy, particularly on the most abundant fossil fuel, coal. Coal research had been dormant for a long period, and up-to-date analytical methods have only recently been applied to coal¹.

Gas chromatography (GC), especially high-resolution glass capillary GC, is a powerful tool in the study of complex mixtures such as those of biological origin. However, the range of GC is obviously restricted to volatile substances, while the bulk of coal is essentially non-volatile. As a consequence, GC has mainly been applied to "coal liquids". Bertsch *et al.*² analyzed a liquified coal sample, while Schultz *et al.*³ separated the aliphatic and polynuclear aromatic compounds of a "solvent refined coal". The rôle of GC in the analysis of coal products (together with the possibilities of high-performance liquid chromatography) has been reviewed⁴.

Another well-known "coal liquid" is tar. Instrumental methods (including GC) used in its analysis have been reviewed by Bartle⁵; an extensive study on the application of high-resolution glass capillary columns in analysis of coal tar aromatics was made by Borwitzky and Schomburg⁶.

It has become clear that even coal contains many small molecules accessible to GC and related methods. These substances can be removed from coal by extraction⁷ or by vacuum distillation⁸.

A class of extractable compounds which has earned special interest is the hydrocarbons (both aliphatic and aromatic). The results for aliphatic hydrocarbons have recently been reviewed⁹. These substances are present in coal at very low con-

centrations (0.1–0.3%)⁹, however, paraffinic and other saturated hydrocarbons, being chemically inert, are among the few compounds thought to be the last remnants of the living organisms from which coal originates. This “geochemical fossil”¹⁰ character of many hydrocarbon structures makes worthwhile their identification in coal as well as other geo-organic materials.

In this work a series of Hungarian coals was examined. The hydrocarbons were extracted, the extracts fractionated by liquid chromatography (LC) and the hydrocarbon fractions were analyzed by high-resolution GC.

EXPERIMENTAL

The procedure is summarized in Fig. 1.

Extraction

Coal samples were dried to constant weight at 105°C for about 5–6 h, then pulverized in a ball-mill in an argon atmosphere until the average particle size decreased to about 50 μm . A 25-g amount of each coal sample was extracted in a Soxhlet extractor with 160 cm³ benzene–ethanol (3:1). After extraction the solvent was evaporated under vacuum at room temperature and the extraction yield was determined.

All the solvents used in extraction and in column chromatography were carefully distilled before use and their purity was checked by GC.

Preseparation, column chromatography

Coal extracts, being very complex mixtures which are hardly volatile, require a preseparation step before GC analysis. This step provides a partial clean-up of the sample in order to protect the GC column from deterioration, and also yields more information about the mixture, without the application of any other instrumental analytical method.

A LC preseparation of saturated and aromatic hydrocarbons comprises part of

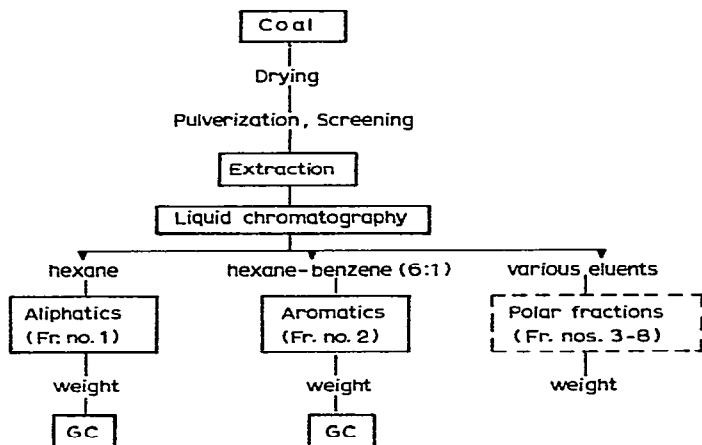


Fig. 1. Analytical scheme. For eluents used with polar fractions, see text.

TABLE I
LC SEPARATION SCHEME

<i>Fraction No.</i>	<i>Eluent (50 cm³)</i>	<i>Compound types eluted¹¹</i>
1	Hexane	Saturated hydrocarbons
2	Hexane-benzene (85:15)	Aromatic hydrocarbons
3	Chloroform	Polar aromatics, non-basic heterocyclics
4	Chloroform-diethyl ether (90:10)	Monophenols
5	Diethyl ether-ethanol (97:3)	Basic nitrogen heterocyclics
6	Methanol	Highly functional molecules
7	Chloroform-ethanol (97:3)	Polyphenols
8	Pyridine-ethanol (97:3) (100 cm ³)	Molecules with high O and N content

the more or less routine analysis of coal and petroleum (see ref. 10, p. 337). Instead, we applied a more rigorous LC pre-separation, as suggested by Farcasiu¹¹. The separation was performed on a silica gel column (30 × 1 cm I.D.), containing about 7.5 g of Kieselgel 60 (E. Merck, Darmstadt, G.F.R.). The sample was loaded in the following way: 100 mg of each extract were dissolved in benzene-ethanol (3:1), the thoroughly mixed with 500 mg of inert solid support (Chromosorb W) and the solvent was evaporated. The dry mixture was poured over the silica gel. In this way the disturbance of the polar extracting solvent could be avoided, the inert support acting as a "concentrating zone". For elution of the fractions, 50-cm³ volumes of different solvents were used (Table I) with a flow-rate of about 1 cm³/min.

In a model experiment with an aliphatic and an aromatic hydrocarbon, it was found that the former was eluted in the first 20 cm³ hexane, while even 100 cm³ hexane did not elute the latter.

The collected fractions were evaporated to dryness under vacuum at room temperature, and weighed. Fractions 1 and 2 were redissolved in high purity *n*-dodecane¹², and were injected into the gas chromatograph.

Gas chromatography

The gas chromatograph was a Perkin-Elmer Model F 22 instrument, with a

TABLE II
GAS CHROMATOGRAPHY PARAMETERS

Column	glass capillary (20 m × 0.23 mm), methylsilicone gum OV-1, phase ratio 600
Temperature	25°C at injection, up to 110°C after the hold-up time, to 330°C at 6°C/min, then isothermal
Injector	
Temperature	300°C
Material	glass insert (5 mm I.D.) packed with 3 cm of 1% OV-1 on Chromosorb W
Sample injection	ca. 1 μl with solvent flush
Splitting ratio	1:15
Carrier gas (hydrogen)	flow-rate 35 cm/sec
Flame ionization detector	
Temperature	240°C
Attenuation	8 × 10 ⁻¹¹ A f.s.d.

TABLE III
PETROGRAPHIC AND REFLECTANCE DATA OF COAL SAMPLES

No.	Origin	Type	Reflectance of vitrinite (%)	Petrography (%)				Natural coke	Inorganic matter
				Huminite	Liptinite	Inertinite			
I	Gyöngyösvisonta*	Lignite	0.35	60	2	2	—	36	
II	Torony**	Lignite	0.30	55	1	2	—	42	
III	Dorog***	Brown coal	0.50	84	7	2	—	7	
IV	Tatabánya K/I***	Brown coal	0.42	80	15	2	—	3	
V	Tatabánya K/II***	Brown coal	0.46	77	16	2	—	5	
VI	Komló †	Hard coal	0.95	67	3	8	2	16	
VII	Pécs †	Hard coal	1.23	73	1	5	2	19	

* North Hungary.

** West Hungary.

*** Trans-Danubian Coal Basin.

† Mecsek Coal Basin.

splitter injector and flame ionization detector. The separations were carried out on a glass capillary column (20 m \times 0.23 mm), coated with OV-1 stationary phase. The column was made as suggested by Borwitzky and Schomburg⁶. The GC conditions are summarized in Table II. The glass injector was filled with a small amount of GC column packing (1% OV-1 on silanized Chromosorb W, 60–80 mesh) in order to break the aerosol formed during injection. The discrimination for high-boiling compounds can thus be avoided. The injector configuration and other parameters are chosen (see Table II) as a result of an optimization experiment, reported elsewhere¹².

RESULTS AND DISCUSSION

Coal samples

The coals, together with simplified petrographic analysis results and data from vitrinite reflectance used as a rank parameter, are listed in Table III. The samples were representative of the whole range of ranks of Hungarian coals.

Extraction period

Exhaustive Soxhlet extraction of coals can be a lengthy operation; as long as 250 h were needed to obtain the maximum yield of aliphatic hydrocarbons from coal

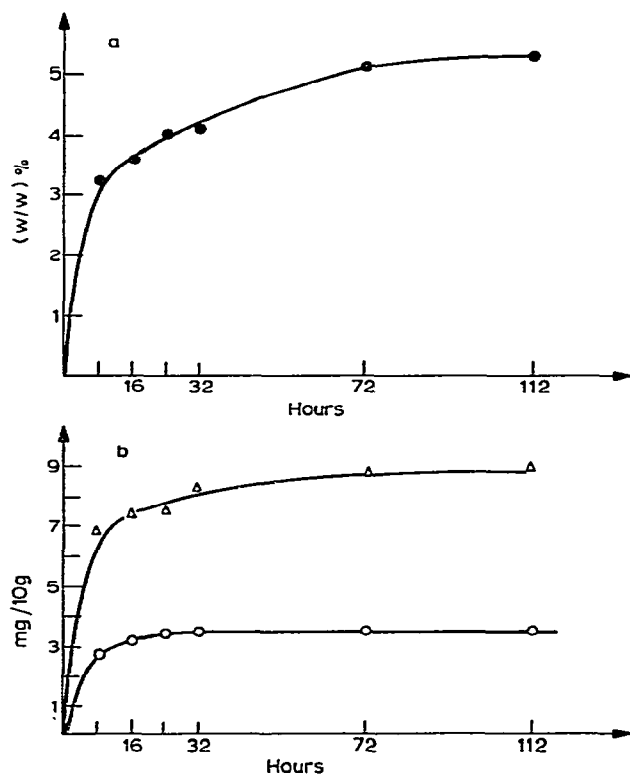


Fig. 2. Extraction yield of the Torony lignite as a function of extraction time. a, Total extraction yield; b, yields of fractions 1 (Δ , aliphatic hydrocarbons) and 2 (O, aromatic hydrocarbons).

with benzene-ethanol (7:3) as solvent¹³. The result of an experiment with Torony lignite to determine the optimal extraction time is presented in Fig. 2. The total amount extracted and also of LC fractions 1 and 2 as a function of extraction time are also shown*. As can be seen, even the longest period (112 h) was not sufficient to achieve maximum yield, but all the extractable aromatic and almost all the aliphatic hydrocarbons were obtained after about 30 h. Therefore all subsequent extractions were terminated after 40 h. It can be concluded that extraction of hydrocarbon molecules which are only weakly bonded to the macromolecular network of coal is easier and faster than that of the higher-molecular-weight and more polar compounds which are more strongly bonded¹⁴.

LC fractionation

The LC fractions of the different coal extracts are given in Table IV and in Fig. 3. The reproducibility of the distribution of the fractions, and of single extract weights is about 20%.

TABLE IV

LC FRACTIONATION OF COAL EXTRACTS

Origin of samples as in Table III. The results refer to dry but not ash-free coal.

No.	Total extraction yield (wt. %)	Weight (mg/10 g coal) of fraction no.							
		1	2	3	4	5	6	7	8
I	3.2	6.0	4.8	17	86	53	90	55	—
II	4.0	8.4	4.4	25	96	59	76	17	8.0
III	4.0	11	15	22	89	58	83	19	48
IV	6.0	16	18	29	140	60	134	35	41
V	7.2	26	33	65	180	87	140	36	12
VI	0.9	9.0	10.2	9.1	17	5.4	5.5	4.9	2.3
VII	0.6	5.3	8.5	8.7	16	4.5	7.4	3.1	0.8

The separation scheme given in Table I has the advantage that it can be directly correlated to the conventional fractionation of coal and petroleum extracts. According to Farcasiu¹¹, mixed fractions 1 and 2 correspond to "oils" (hexane soluble) and mixed fractions 3-6 correspond to "asphaltenes" (insoluble in hexane but soluble in benzene). The columns in Fig. 3 are "hatched" accordingly.

All efforts to obtain gas chromatograms from fractions 3-8 were unsuccessful (as in ref. 11), most probably because of the content of high-molecular-weight compounds. No attempt has been made until now either to volatilize these compounds by derivatization or pyrolysis, or to investigate them using other (*e.g.*, spectroscopic) methods. The following conclusions on the weight distribution pattern can be drawn:

(i) The amount of the oil fractions (1 and 2) from lignites is small compared to the yields of asphaltene and higher fractions.

(ii) The opposite is true for the hard coals, which yield extracts containing over 20% hydrocarbons, compared to 3% hydrocarbons in the lignite extracts.

* The weight percentages refer to dry but mineral-containing (not ash-free) coal.

- (iii) The brown coals have a much higher extraction yield than any other coal types, but intermediate hydrocarbon contents (about 6% of the extract).
- (iv) The higher fractions are almost absent from the hard coal extracts.
- (v) In all extracts the most abundant fractions are 4 and (except for hard coals) 6. This reflects the high phenol content in coal extractables.

Gas chromatography

Fractions 1 and 2 contain volatile compounds, accessible to GC.

Aliphatic compounds. Fraction 1 is a mixture of aliphatic compounds; it contains *n*-alkanes, branched chain and cyclic saturated hydrocarbons. It has been suggested (see ref. 10, p. 337) that *n*-alkanes may be separated from the other two classes by formation of urea adducts, or with 5-Å molecular sieves. However, this step was omitted in this work because the high separation power of the glass capillary column made possible the detection of numerous branched and cyclic compounds between the *n*-alkane peaks. The identification of the latter through standards and their regularly spaced elution pattern on the temperature programmed chromatograms facilitated estimation of the retention indices of other peaks. It was also possible to evaluate some characteristic coal parameters based on *n*-alkanes (see below).

Gas chromatograms of aliphatic fractions of lignite, brown coal and hard coal extracts are given in Figs. 4, 5 and 6, respectively. On each chromatogram an approximate scale of retention indices* is also given; the retention indices of the most abundant peaks are listed in Table V.

The first point to be noted is the striking similarity of the chromatograms within each group. This is even more remarkable, since the geographical distance between the two lignite mines is rather large, and all coal samples came from different mines.

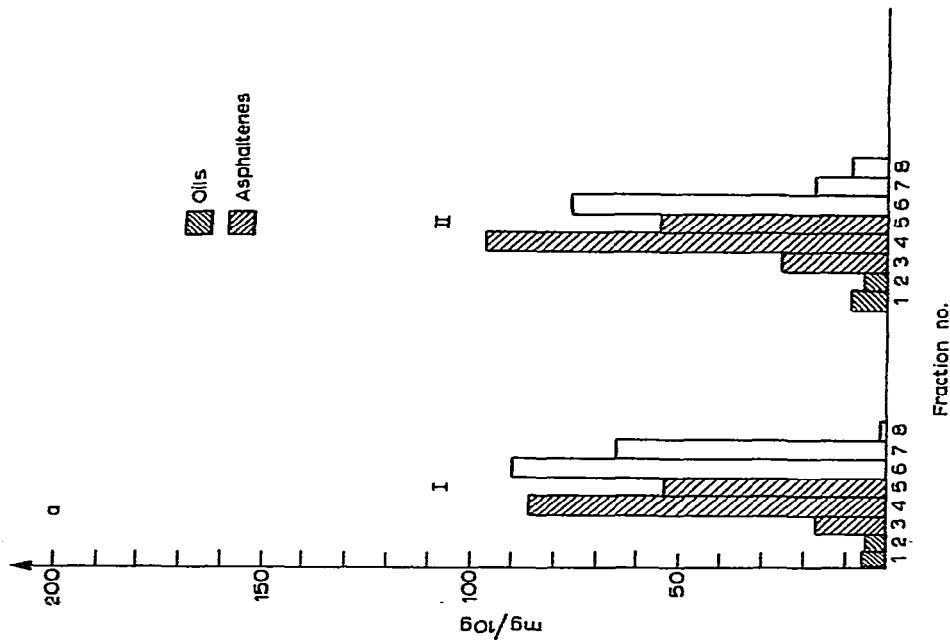
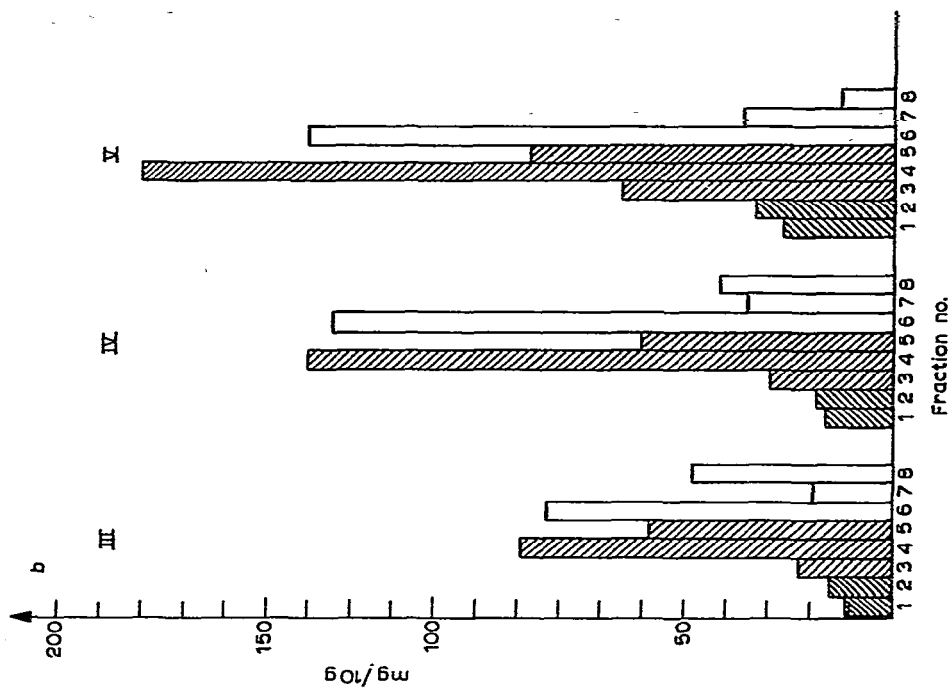
The *lignite* aliphatic fractions mainly (*ca.* 90%) comprise two compounds (peaks A and B) with retention indices of 1960 and 1980. They were identified in a single GC-mass spectrometric (MS) measurement as $C_{20}H_{34}$ and $C_{20}H_{36}$, respectively. Since the well-known acyclic saturated diterpanes pristane and phytane also appear with retention indices 1712 and 1815, A and B cannot be due to unsaturated branched diterpanes, since the retention indices would be smaller than that of the corresponding saturated compounds. The most possible structures, therefore, are saturated and unsaturated tricyclic diterpenoids. Such compounds are known geochemical fossils both in sediments and coals (see ref. 10, pp. 113 and 222). Besides peaks A and B and a few minor peaks in the retention index region of 3000, the *lignite* aliphatics contain only *n*-alkanes.

The chromatograms of the *brown coals* are dominated by a large number of

* The Kováts' retention index system defined under isothermal conditions cannot be applied for linear temperature programming. Instead, retention indices are calculated here using the approximately linear relationship

$$I = 100 \cdot \frac{TX - TC_n}{TC_{n+1} - TC_n} + 100n \quad (1)$$

where TX and TC are the retention times of the substance investigated and the *n*-alkanes, respectively, and *n* and *n* + 1 are the carbon numbers of the *n*-alkanes used as references.



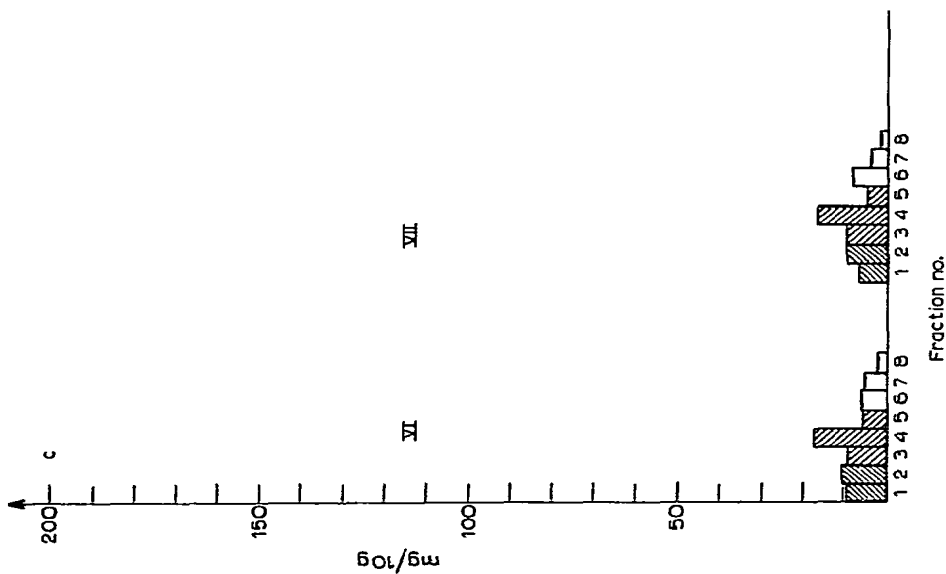


Fig. 3. LC fraction distribution of the coal extracts. Fractions are numbered as in Table I, coals as in Table III. a, Lignites; b, brown coals; c, hard coals.

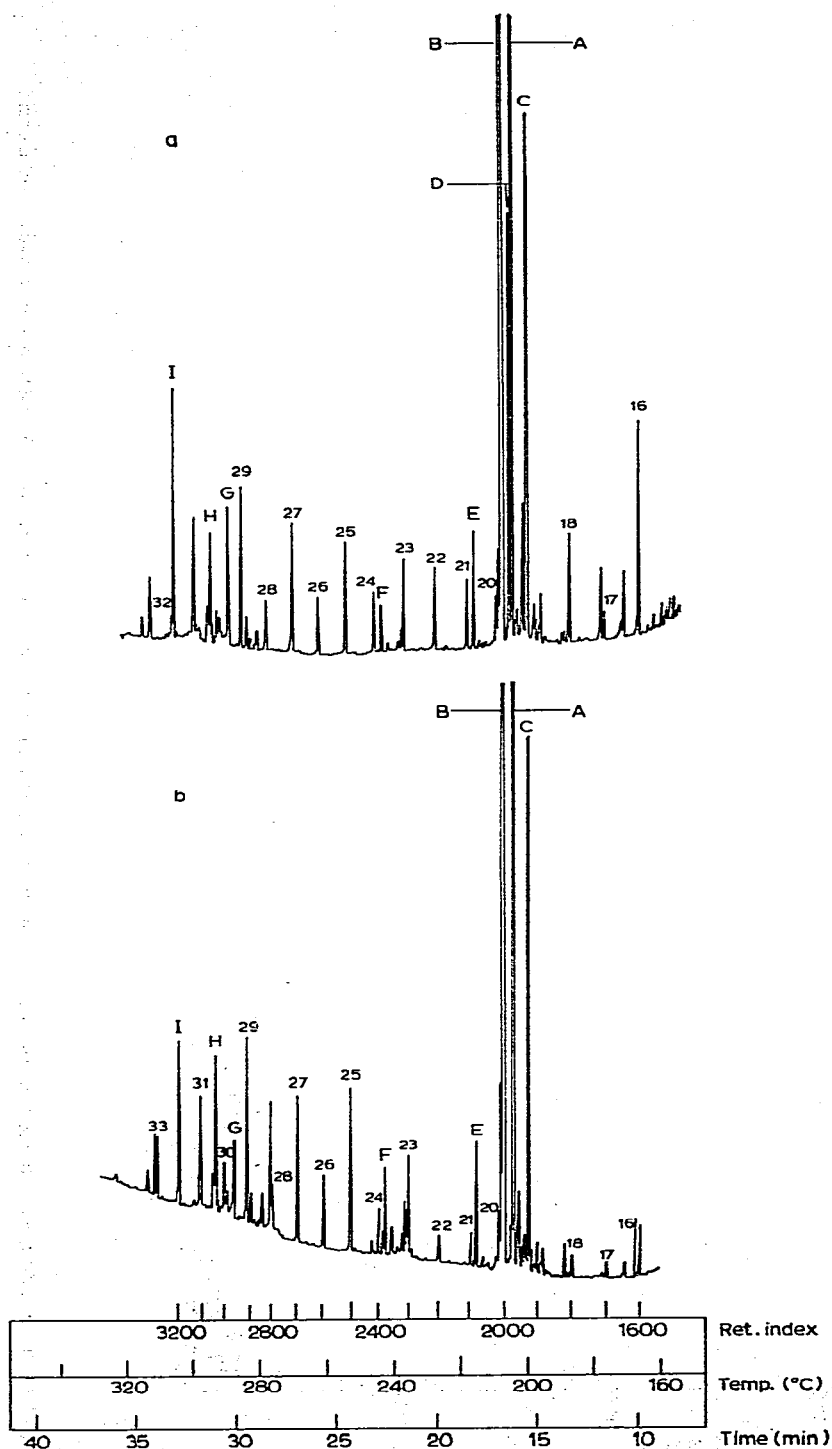


Fig. 4. Gas chromatograms of aliphatic hydrocarbons in lignites. The carbon numbers of the *n*-alkanes are indicated. For peaks marked with letters, the retention indices are listed in Table V. GC conditions are given in Table II. Origins: a, Gyöngyösvisonta; b, Torony.

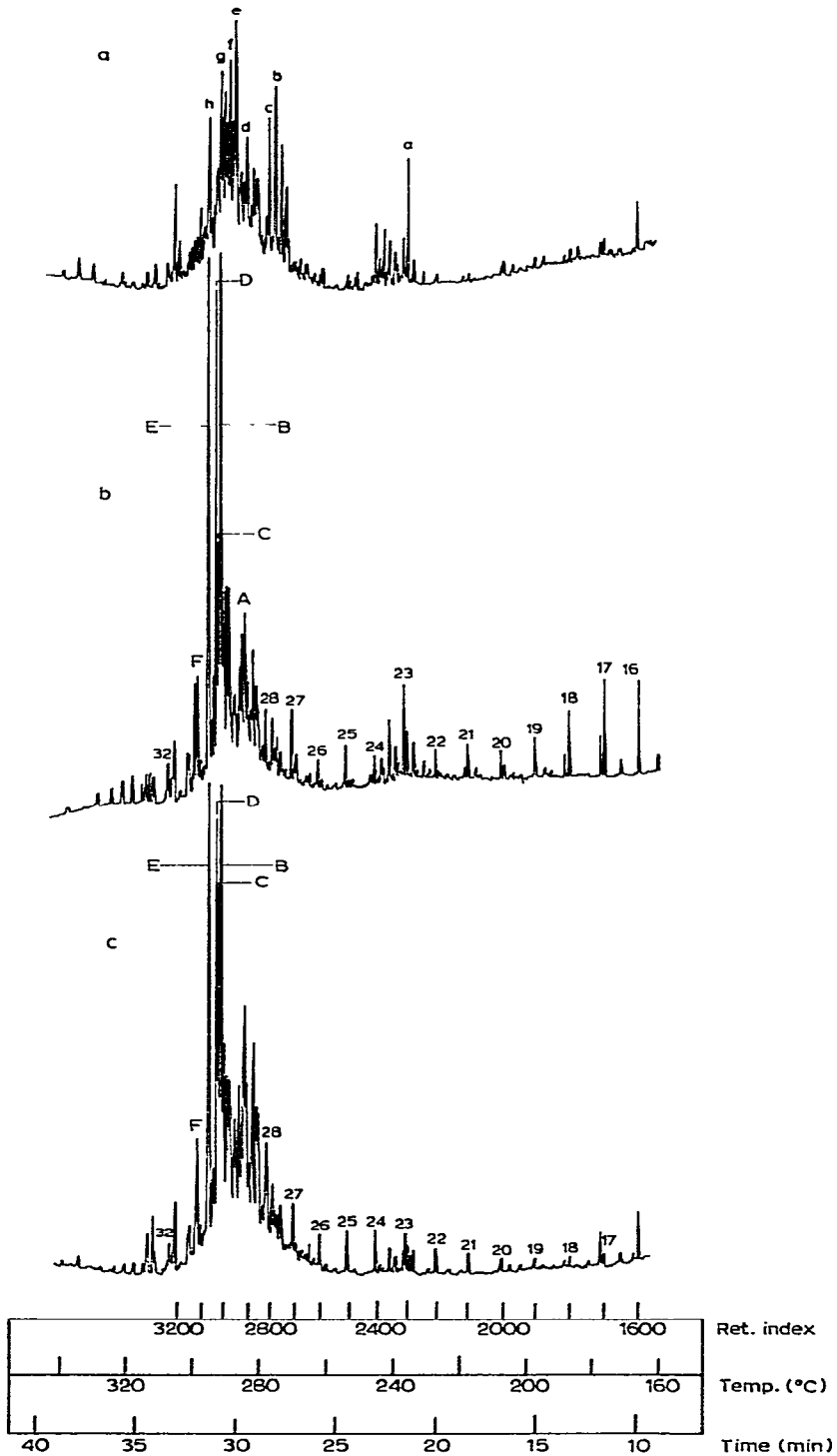


Fig. 5. Gas chromatograms of aliphatic hydrocarbons in brown coals. Details as in Fig. 4. Origins: a, Dorog; b, Tatabánya K/I; c, Tatabánya K/II.

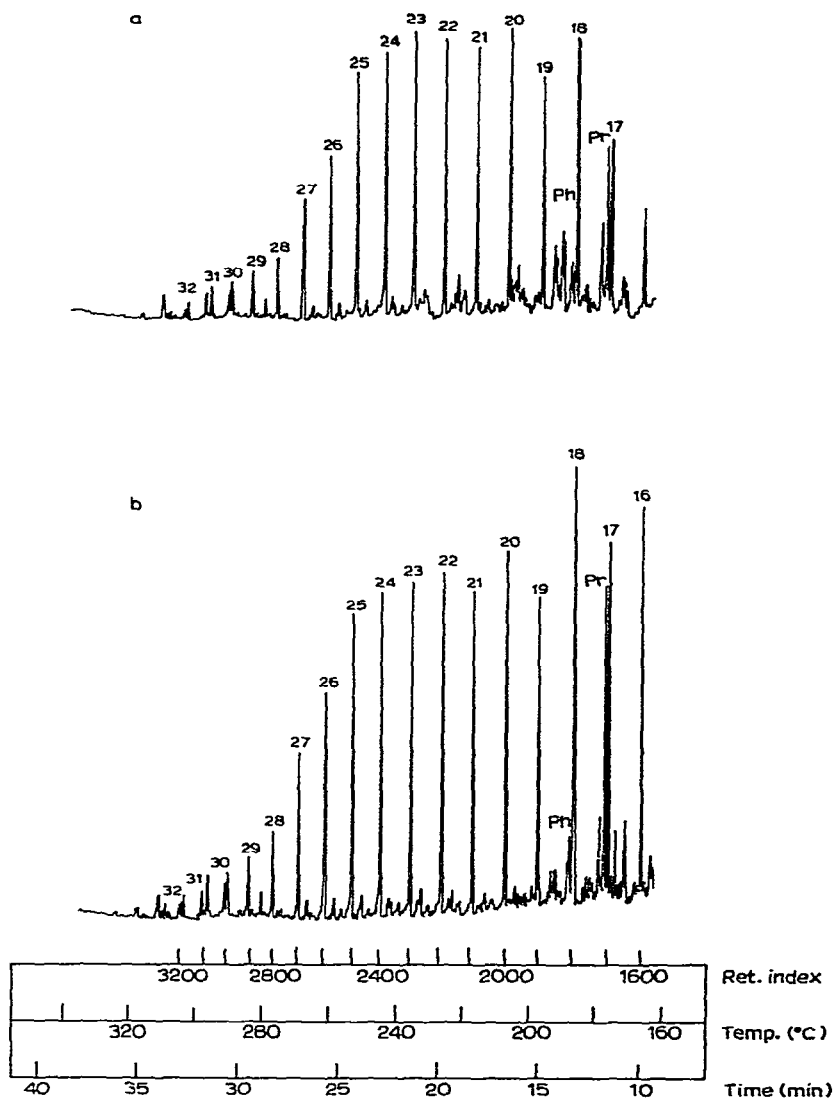


Fig. 6. Gas chromatograms of aliphatic hydrocarbons in hard coals. Details as in Fig. 4. Pr = Pristane; Ph = phytane. Origins: a, Komló; b, Pécs.

peaks in the retention index range 2800–3200. Retention indices of a few large peaks are listed in Table V. Considering their retention index range and aliphatic (non-polar) character, these peaks should belong to other groups of geochemical fossils: tetracyclic steranes and pentacyclic triterpanes¹⁰. Unfortunately, individual compounds cannot be identified at the moment; no coincidence can be found among the retention indices in Table V and the data of Allan *et al.*¹⁵ for triterpenoids of the hopane series in different coals.

The *hard coal* aliphatic fractions contain mainly *n*-alkanes. There are also traces of other homologous series appearing as small peaks between the equidistant *n*-

TABLE V

RETENTION INDICES OF THE MOST ABUNDANT COMPONENTS OF THE ALIPHATIC FRACTIONS

The values were calculated from temperature programmed gas chromatograms using eqn. 1. Pr = Pristane; Ph = phytane.

Coals	Peak	Retention index	
Lignites	A	1960	
	B	1980	
	C	1920	
	D	1967	
	E	2084	
	F	2381	
	G	2958	
	H	3030	
	I	3191	
Hard coals	Pr	1712	
	Ph	1815	
Brown coals Tatabánya K/I and K/II	A	2897	
	B	3009	
	C	3018	
	D	3026	
	E	3062	
	F	3096	
	Dorog	a	2296
		b	2778
c		2805	
d		2889	
e		2930	
f		2955	
	g	2989	
	h	3039	

alkanes. They are most probably iso-, anteiso- and other branched chain but acyclic hydrocarbons. The peaks characteristic of the lignites and the brown coals are completely absent here.

n-Alkane distribution in different coals. It is well known^{9,10} that *n*-alkanes in sediments, petroleum and coal are characteristically distributed according to carbon number. Most striking is the difference between the amounts of odd and even numbered alkanes. This difference is best expressed by the so-called "carbon preference index" (CPI) as defined by Maxwell *et al.*¹⁶:

$$\text{CPI} = \frac{1}{2} \left(\frac{\sum \text{concn. } C_{17}-C_{31}}{\sum \text{concn. } C_{16}-C_{30}} + \frac{\sum \text{concn. } C_{17}-C_{31}}{\sum \text{concn. } C_{18}-C_{32}} \right) \quad (2)$$

From the chromatograms in Figs. 4-6 and using peak heights as quantities proportional to concentration (within the range of the temperature program), CPI values for the seven coals were calculated and are listed in Table VI. Since CPI values

TABLE VI
CARBON PREFERENCE INDEX (CPI) OF COALS

Origin of samples as in Table III.

No.	CPI
I	1.31
II	3.54
III	0.98
IV	1.66
V	1.27
VI	0.99
VII	0.94

are thought to be related with coal rank^{7,17}, the data in Table VI are plotted vs. $R\%$ (vitrinite reflection) of the coals in Fig. 7. As it can be seen, the relationship found is non-linear.

The distribution of n -alkanes within the homologous series is also reported to vary characteristically with coal rank¹⁸: the maximum of the distribution curve was around carbon number 29–30 for low rank peat or lignite, and shifted toward lower carbon numbers with increasing rank, down to 20 for hard coals. This feature is clearly visible also in Figs. 4–6: the C_{29} peak is the maximum for lignite chromatograms, while the two hard coal chromatograms show broad plateaus around C_{20} – C_{22} .

Aromatic fractions. For characterization of aromatic peaks, a retention system based on naphthalene, phenanthrene, chrysene and picene as reference "homologous series" was used, as suggested by Lee *et al.*¹⁹. The reference polynuclear aromatic hydrocarbons (PAHs) have "PAH index" values of 200, 300, 400 and 500, respectively, where the PAH index is 100 times the number of condensed aromatic rings in the molecule. Interpolation of values for other aromatic substances should be made with an equation similar to 1, when linear temperature programming is used.

First the system was tested by determining the PAH index of a number of standard compounds (see also ref. 19). The values, calculated at different programming

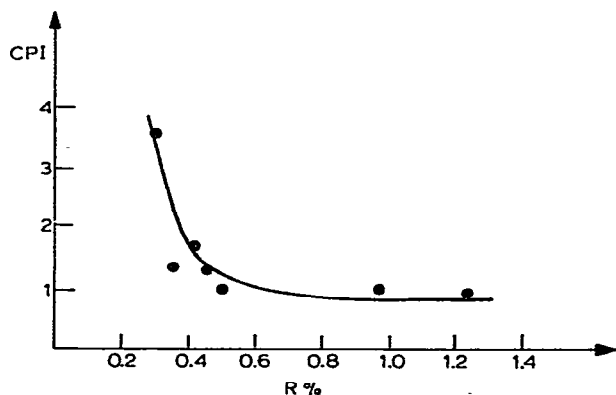


Fig. 7. Carbon preference index (CPI) as a function of vitrinite reflectance ($R\%$) of coals.

TABLE VII
PAH INDEX VALUES OF STANDARD COMPOUNDS

Compound	PAH index			Ref. 19, 2 and 4°C/min
	2°C/min	4°C/min	6°C/min	
Anthracene	301.5	301.8	302.6	301.7
Fluoranthene	344.2	344.6	345.0	344.0
Pyrene	350.9	351.5	352.2	351.2
Benz[a]anthracene	398.8	398.8	399.1	398.5
Benzo[k]fluoranthene	442.9	442.5	443.6	442.5
Benzo[a]pyrene	453.6	452.8	454.1	453.4
Perylene	456.7	456.2	457.2	456.2
Average difference from ref. 19	-0.16	-0.10	-0.90	
Standard deviation	0.28	0.35	0.17	

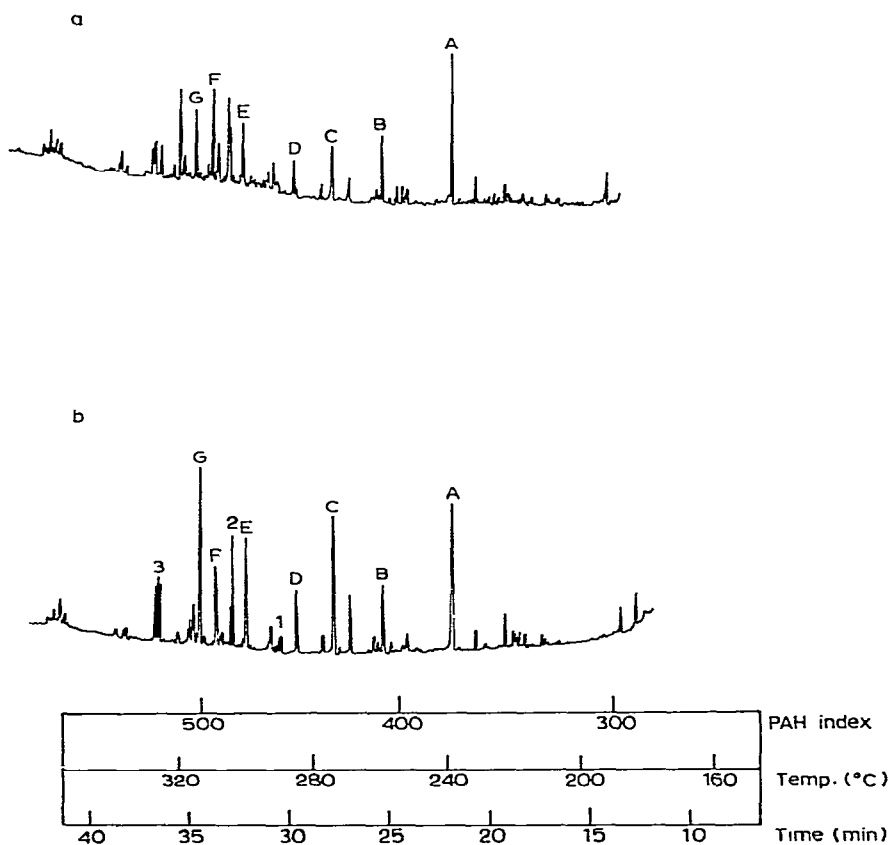


Fig. 8. Gas chromatograms of aromatic hydrocarbons in lignites. PAH indices are listed in Table VIII. Origins: a, Gyöngyösvisonta; b, Torony.

TABLE VIII
PAH INDICES OF THE MOST ABUNDANT COMPOUNDS OF THE AROMATIC FRACTIONS

Coals	Peak	PAH index at programming rate of			
		4°C/min	6°C/min	Difference	
Lignites	A	371.2	370.8	+0.4	
	B	404.5	403.7	+0.6	
	C	430.5	429.8	+0.7	
	D	454.0	451.1	+3.9	
	1	456.7	457.8	-1.1	
	E	480.7	477.9	+2.8	
	2	484.0	484.3	-0.3	
	F	493.2	492.8	+0.5	
	G	504.7*	502.0*	+2.7	
	3	521.3*	523.1*	-1.8	
Hard coals	A	—	300	—	
	B	319.8	320.0	-0.2	
	C	320.5	320.7	-0.2	
	D	323.0	323.3	-0.3	
	E	323.8	324.1	-0.3	
	F	342.2	341.8	+0.4	
	G	343.7	343.7	0	
	H	360.5	359.9	+0.6	
	I	367.2	366.6	+0.6	
	J	370.2	369.6	+0.6	
Brown coals	Common	A	390.5	390.0	+0.5
		B	395.4	395.3	+0.1
		C	506.9*	506.8*	+0.1
		D	537.0*	536.1*	+0.9
		E	545.6*	545.1*	+0.5
		F	552.2*	551.6*	+0.6
	Tatabánya K/I	d	—	465.0	—
		e	—	468.9	—
		f	—	475.9	—
		g	—	481.1	—
	Tatabánya K/II	i	—	488.3	—
		e	—	468.9	—
		g	—	481.1	—
		j	—	492.0	—
		m	—	520.3*	—

* Extrapolated value.

rates, are in Table VII. The reproducibility of the data is good; not generally larger than 0.1 index unit.

Indices at the same programming rate as in ref. 19 differ only slightly from the published data, in spite of the small difference (5% phenyl groups in SE-52 used by Lee *et al.*¹⁹, vs. our pure methylsiloxane, OV-1) between the two stationary phases. The average difference is even smaller. However, on changing the programming rate

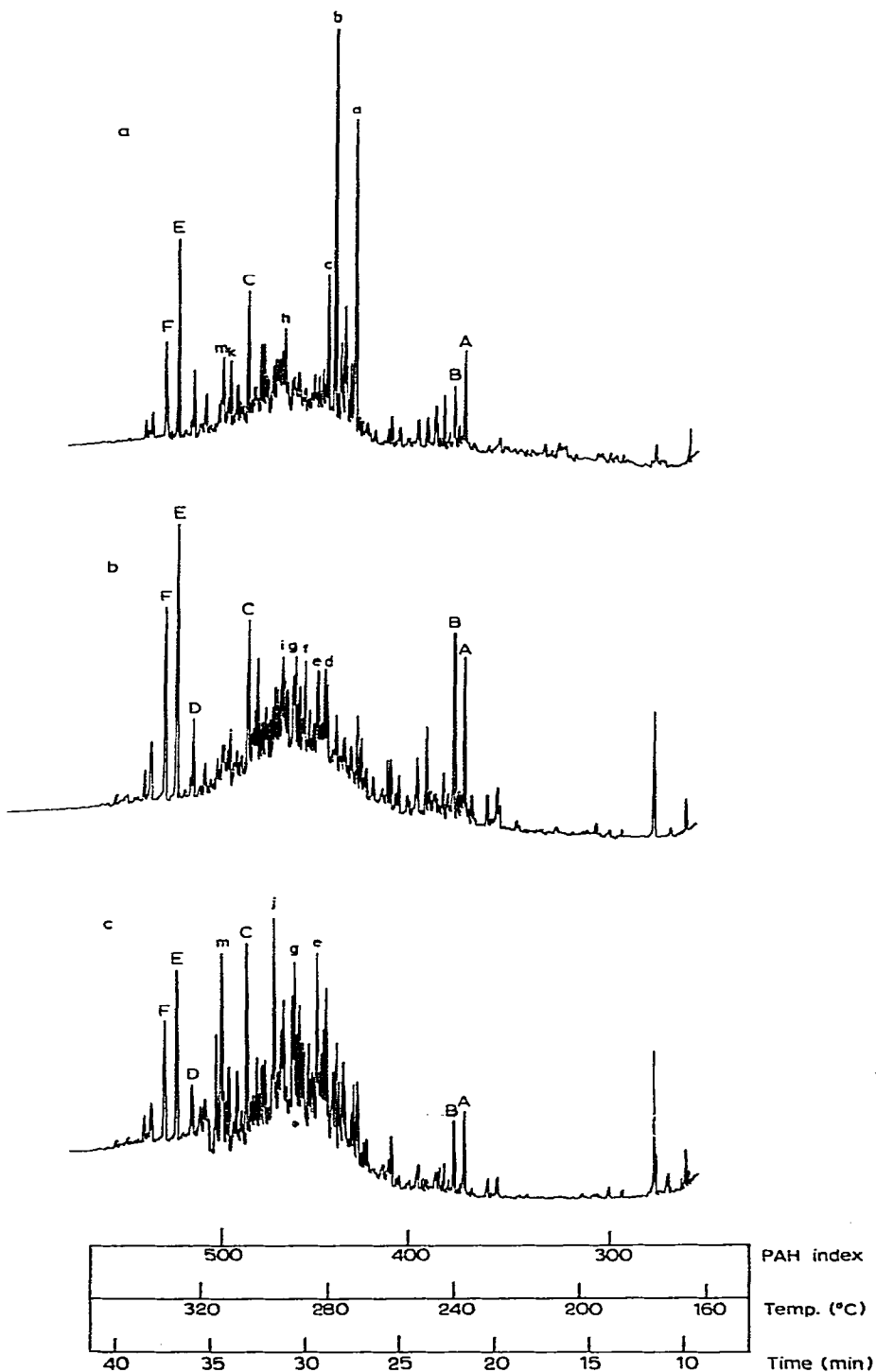


Fig. 9. Gas chromatograms of aromatic hydrocarbons in brown coals. PAH indices are listed in Table VIII. Origins: a, Dorog; b, Tatabánya K/I; c, Tatabánya K/II.

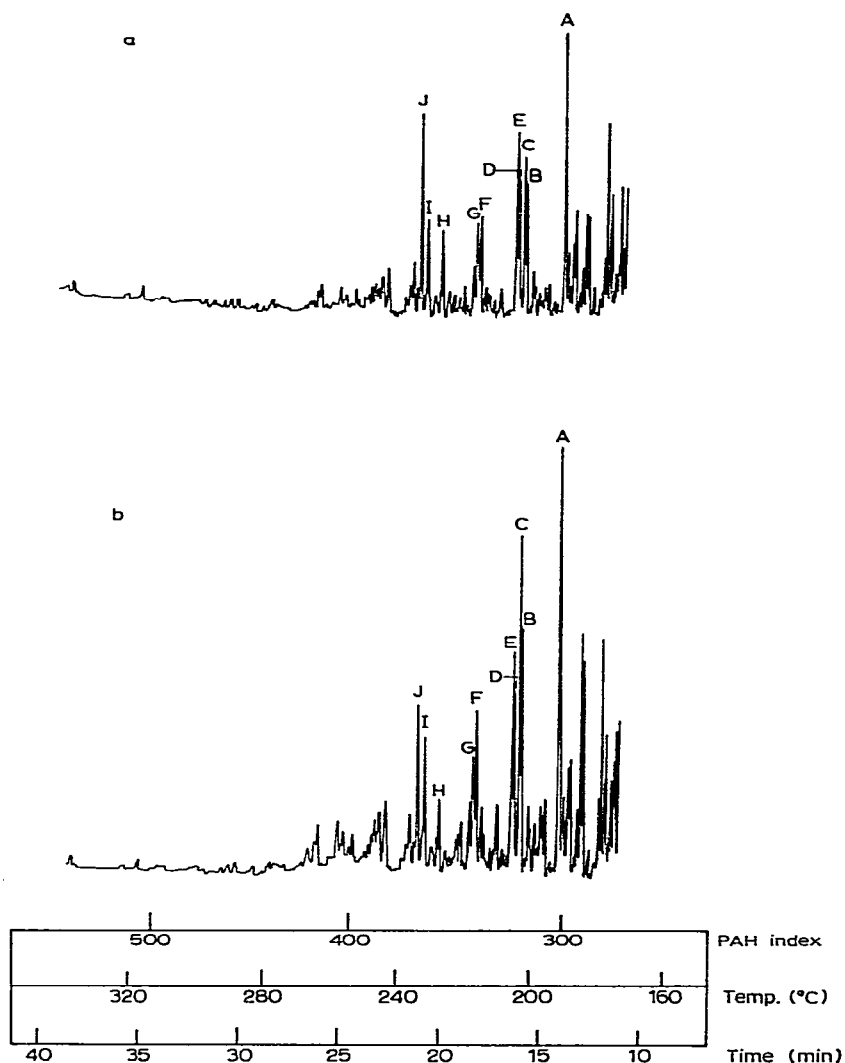


Fig. 10. Gas chromatograms of aromatic hydrocarbons in hard coals. PAH indices are listed in Table VIII. Origins: a, Komló; b, Pécs.

from $4^{\circ}\text{C}/\text{min}$ to $6^{\circ}\text{C}/\text{min}$, the average difference increases to 0.9 PAH index units, and the deviation from this is surprisingly low for the individual compounds. Therefore, not only the index values themselves, but also their dependence on program rate can provide useful data for identification.

In Figs. 8, 9 and 10 are given the chromatograms of aromatic fractions of coal extracts. The "fingerprint"-like similarities of and differences between the coal types are again visible and are the same as for the aliphatic chromatograms.

The PAH indices of a few major peaks were calculated at two different programming rates, $4^{\circ}\text{C}/\text{min}$ and $6^{\circ}\text{C}/\text{min}$; the data are presented in Table VIII. Beside the major peaks, a few small ones appeared on the chromatogram of one of the

lignites (numbered in Fig. 8), which deviate in behaviour considerably from other peaks: when changing the programming rate from 4°C/min to 6°C/min, their PAH index increased instead of the decrease shown by most of the peaks. The change is therefore in the same direction, and is approximately of the same magnitude, as that of the difference numbers in Table VII, that is for the PAH parent compounds (ring systems without side chains).

It can be concluded, therefore, that the compounds in aromatic extracts are not parent PAHs, but probably ring structures in various stages of aromatization. Such structures are known to exist in coals, and the polyaromatic rings are thought to originate from polycyclic saturated terpenoids⁹.

There are characteristic differences among the coals. The *brown coal* aromatic fractions contain a large number of peaks in the same retention range as the aliphatic compounds were eluted, again suggesting that this group of compounds is closely related to the aliphatic triterpanes. The *hard coal* aromatics comprise lower-molecular-weight compounds, having retentions corresponding to three rings. This is consistent with the fact that no pentacycles were found in the aliphatic fraction which would have been a source of higher-molecular-weight aromatics. The *lignites* contain a relatively small number of individual compounds distributed over the whole retention range. They are also probably hydroaromatic compounds.

CONCLUSIONS

(i) The extracts of different coals can be separated into various fractions by LC, and the weight distribution of these fractions differs according to the type and rank of coal.

(ii) The GC analysis of the more or less volatile aliphatic and aromatic fractions resulted in chromatograms which are useful in the fingerprint characterization of the coals. There are striking similarities between the gas chromatograms of related coals.

(iii) Groups of peaks at retention indices of 2000 and 3000 in the aliphatic gas chromatograms can be attributed to geochemical fossils of cyclic di- and triterpanes, respectively.

(iv) The *n*-alkanes in the chromatograms can be used to calculate certain parameters (CPI) related to coal rank.

(v) The PAH indices of the aromatic peaks and their dependence on the programming rate may be used to reveal their hydroaromatic character.

The work reported here can be extended in several ways. Further LC separation of the aromatics according to ring number will make the gas chromatograms simpler and help identification. The application of various spectroscopic techniques (MS, infrared and nuclear magnetic resonance spectroscopy) will facilitate the identification of unknown components in the extracts which can be correlated with other geochemical results for coals.

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