

## Interpretation of Serbian surface sediments' maturation parameters based on factor analysis

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**Abstract:** The factor analysis, used in this work for the interpretation of maturation parameters observed in an exploration study of a group of surface sediments of diverse age originating from different localities in Serbia, resulted in two significant factors. Factor 1 involved parameters related mainly to maturation changes within the aliphatic chains of the organic matter and factor 2 involved parameters based mainly on changes in the terpane and sterane rings. A statistically significant inversely proportional linear dependence between factors 1 and 2 was observed with older, in contrast to younger sediments, suggesting that the reactions of the aliphatic chains in the older sediments did not occur simultaneously with the reactions in the rings and, also, that the older surface sediments examined in this study may be characterized by a degree of thermal maturity corresponding to changes in the biomarker sterane and terpane rings, while the younger sediments by intensive changes in the aliphatic chains.

**Keywords:** factor analysis, maturation parameters, biological markers, surface sediments.

### INTRODUCTION

In organic geochemical studies of the petroleum source potential of sedimentary deposits, in addition to the proportion and type of the kerogen, organic matter maturity represents one of the most important evaluation characteristics. Maturation parameters are mainly based on chemical transformations of different classes of organic compounds in the bitumen fraction of the sediment such as *n*-alkanes, isoprenoid aliphatic alkanes, polycyclic alkanes of the sterane and terpane type, mono- and triaromatic steroids *etc.*<sup>1–4</sup> Due to the fact that the maturation transformations of sedimentary organic matter are influenced by several different factors, such as heat, pressure and catalytic effect of minerals, a correlation between the geological age of a sediment and its organic matter maturity does not necessarily

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exist.<sup>5,6</sup> Moreover, since the equilibria of the maturation reactions are attained at different stages of the diagenetic-catagenetic sequence, individual maturation parameters, logically, are of limited specificity and informativeness.<sup>5</sup> Some maturation parameters have also been shown to substantially depend on the origin of the organic matter.<sup>5,7,8</sup> Therefore, a reliable estimation of the thermal maturity of sediments requires the determination of a number of different maturation parameters.

On the other hand, in exploration studies of vast geological basins, involving the investigation of sediments of different age, origin and history, determination of a large number of maturation parameters may bring interpretational ambiguity. Consequently, this study was aimed at checking the potentials of a statistical method, *i.e.*, factor analysis, for interpreting, or solving possible uncertainties in interpreting the maturation parameters observed in organic geochemical explorations. More specifically, factor analysis was used in this work for the first time for the interpretation of maturation parameters observed in an exploration study of a group of surface sediments of diverse age (Devonian, Lower Carboniferous, Upper Cretaceous and Neogene-Middle Miocene) originating from different localities in Serbia. The ultimate goal was to help in establishing a hierarchy of maturation parameters in this particular case, *i.e.*, to possibly classify maturation parameters according to their role in defining maturity of the examined sediments. For this purpose, the factor analysis observations are compared here with the accumulated organic geochemical experience concerning the sequence of individual maturation reactions and the significance of the corresponding maturation parameters.

#### EXPERIMENTAL

##### *Samples*

Thirteen samples of Serbian surface sedimentary rocks were investigated in this study. A list of the samples involving data on lithology, stratigraphy and geotectonics is presented in Table I.

TABLE I. The investigated sedimentary rocks

No.	Locality	Lithological composition	Age	Geotectonic unit
1	Lipe	Oil shale	M <sub>2</sub>	GMN
2	Kraljevo–Guča	Marly limestone	M <sub>2</sub>	ČKN
3	Kraljevo–Guča	Calcareous sandstone	K <sub>2</sub> <sup>3</sup>	ZVZ
4	Kraljevo–Guča	Fine-grain sandstone	K <sub>2</sub> <sup>3</sup>	ZVZ
5	Guča	Fine-grain sandstone	K <sub>2</sub> <sup>3</sup>	ZVZ
6	Lučani	Marly limestone	K <sub>2</sub> <sup>3</sup>	ZVZ
7	Rajićeva Gora	Aleurolite	K <sub>2</sub> <sup>3</sup>	IVZ
8	Gornja Kravarica	Quartzose-sericitous shale	C <sub>1</sub>	ZVZ
9	Brodarevo	Fine-grain sandstone	C <sub>1</sub>	LP
10	Brodarevo	Aleurolitic limestone	C <sub>1</sub>	LP
11	Jabuka	Fine-grain sandstone	C <sub>1</sub>	LP

TABLE I. Continued

No.	Locality	Lithological composition	Age	Geotectonic unit
12	Prijepolje	Aleurolite	C <sub>1</sub>	LP
13	Stublica–Vrnjačka Banja	Metaclay	D	CVZ

M<sub>2</sub> – Middle Miocene; K<sub>2</sub><sup>3</sup> – Upper Cretaceous (Cenomanian); C<sub>1</sub> – Lower Carboniferous; D – Devonian; GMN – Gornji Milanovac Neogene; ČKN – Čačak-Kraljevo Neogene; ZVZ – West Vardar zone; IVZ – East Vardar zone; CVZ – Central Vardar zone; LP – River Lim Paleozoic

The present spatial distribution of Paleozoic and Mesozoic formations in Serbia resulted from complex tectonic events in the Pre- and Post-Maastrichtian period (Upper Cretaceous). Consequently, it is not known which sediments, regardless of their age, were exposed to higher or lower temperatures. Geotectonic units in the investigated area, characterized by different geological evolution during Paleozoic and Mesozoic, and hence, by different sedimentation locations, are found today to be in direct contact. Tertiary complexes, deposited on a base of tectogenetic origin after intensive tectonic events, are composed of diverse sedimentary and magmatic products.<sup>9</sup>

The essential difference between the investigated sedimentary samples lies in their stratigraphy, *i.e.*, in their age (Table I). Samples 1 and 2 are the youngest, originating from Middle Miocene (around 20 million years). Samples 3-7 originate from Cretaceous (~65 million years). Samples 8-13 are the oldest, originating from Lower Pre-Tertiary, *i.e.*, Paleozoic (Carboniferous and Devonian, ~300, and ~400 million years, respectively).<sup>10</sup>

Pre-Tertiary samples (Paleozoic and Mesozoic) were taken from localities close to deep faults which represent boundaries between geotectonic units. In earlier exploration of these localities, the amount of bitumen in the samples closest to the faults was found to be the highest. With increasing distance, a trend of decreasing bitumen content, or, generally, of lower petroleum-gas source potential, was observed.<sup>9</sup>

#### Analytical methods

The samples were powdered (<0.063 mm) and Soxhlet extracted for 36 h with a dichloro-methane-methanol azeotrope. The individual fractions of saturated hydrocarbons were isolated from the bitumen by column chromatography. Silica gel and aluminium oxide were used as adsorbents and petroleum ether as the eluent.

The alkane fractions were analyzed by a Hewlett Packard 5890, Series II, gas chromatograph, with a HP-5MS capillary column, using helium as the carrier gas (1 cm<sup>3</sup>/min). The gas chromatograph was coupled with a mass selective Hewlett Packard 5972 MSD (70 eV) detector. The Single Ion Monitoring (SIM) method was used for the identification of the individual components.

*n*-Alkanes and isoprenoid aliphatic alkanes pristane (Pr) and phytane (Phyt) were identified on the basis of *m/z* 71, and polycyclic alkanes of terpane and sterane types on the basis of *m/z* 191 and *m/z* 217 fragmentograms. The retention times of the individual peaks were compared with literature data.<sup>3</sup>

#### Factor analysis

Factor analysis as a statistical method has been known since the nineteenfifties.<sup>11,12</sup> However, its more intensive application in nonmathematical fields began only recently, due to the development of SPSS 10.0 and S-PLUS type computer programs, which led to results by very simple mathematical operations.<sup>13-15</sup> Factor analysis represents an analytical process of transforming statistical data (as measurements) into linear combinations of variables. It is a statistical method used for combining a larger number of data into a considerably smaller number of *factors*. Factors represent groups of initial mutually linearly dependent parameters and contain the same amount of information as their constituent parameters. The values of the coefficients preceding the parameters included in a factor define the significance of a particular parameter for the characterization of the analyzed samples.<sup>15,16</sup> Variables belonging to a given factor are in high correlation with other variables within that factor, and in low correlation with those belonging to other factors. The analytical

process is done statistically, first by determining the strongest factor, then removing that factor (statistically) from the data matrix and looking for the next strongest factor. After each step a new factor is removed and the next strongest interrelationship determined.<sup>13,14</sup>

The feasibility of the factor analysis in a particular case is determined on the basis of the results of the Kaiser-Meyer-Olkin Measure of Sample Adequacy (KMO) and the Bartlett's Test (significance, *sig*). The KMO value has to be  $> 0.50$ , and the *sig* value  $< 0.05$ .<sup>13,14</sup>

The factor analysis produces a large number of factors. However, only those complying with the Kaiser's and Cattell's rules<sup>13,14</sup> are considered to be significant. For the sake of enhancing the coefficients of parameters of high significance within the defined factors, and thus of facilitating the interpretation of geological and geochemical data, the so-called varimax rotation is used.<sup>17</sup> Thus, the factor analysis results in a matrix of factor loadings. Since variables correlate differently with each other, each variable will correlate differently with the identified factor. Variables will also, generally, show some correlation with other factors.<sup>13,14,17</sup>

## RESULTS AND DISCUSSION

### *Maturation parameters*

CPI (Carbon Preference Index) and Phyt/*n*-C<sub>18</sub> (phytane/C<sub>18</sub> *n*-alkane ratio) were calculated on the basis of the distribution of *n*-alkanes and isoprenoid aliphatic

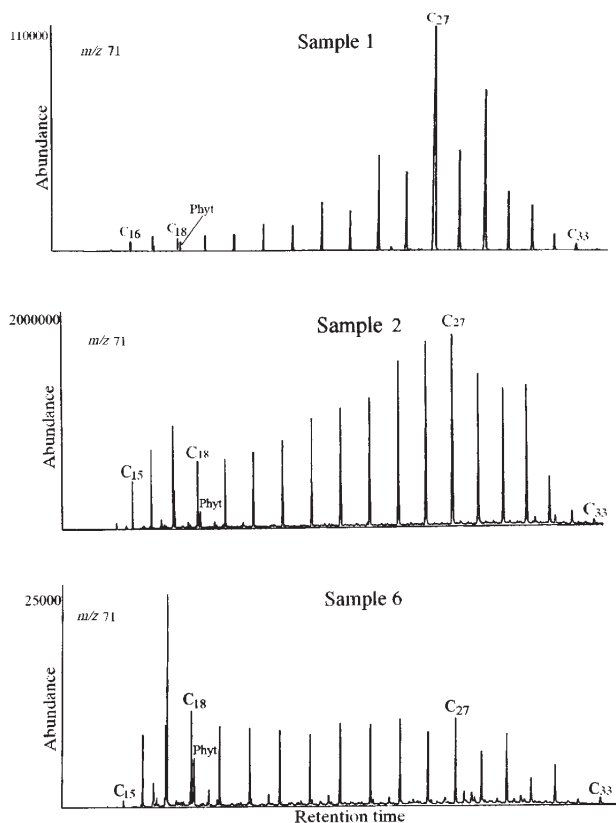


Fig. 1.  $m/z$  71 fragmentograms typical of the investigated alkane fractions.

TABLE II. Maturation parameters calculated on the basis of the *n*-alkane, phytane, triterpane and sterane distributions

Sample	<i>n</i> -Alkanes and phytane		Triterpanes			Steranes		
	CPI	Phyt/ <i>n</i> -C18	Ts/Ts+Tm	22S/22S+22R	M/H	$\beta\beta/\beta\beta+\alpha\alpha$	20S/20S+20R	Dia/Dia+Ster
1	1.80	0.77	0.07	0.17	0.32	0.21	0.04	0.03
2	1.06	0.23	0.21	0.61	0.14	0.31	0.39	0.41
3	0.72	0.23	0.11	0.59	0.25	0.45	0.42	0.44
4	1.02	0.45	0.06	0.60	0.37	0.31	0.41	0.37
5	1.17	0.62	0.28	0.61	0.20	0.44	0.45	0.38
6	1.17	0.48	0.10	0.61	0.42	0.29	0.38	0.31
7	0.92	0.87	0.46	0.59	0.09	0.55	0.48	0.44
8	0.88	0.84	0.49	0.59	0.08	0.54	0.49	0.35
9	0.91	0.96	0.47	0.62	0.07	0.55	0.48	0.33
10	0.93	1.09	0.45	0.60	0.09	0.55	0.47	0.40
11	0.83	0.65	0.45	0.58	0.08	0.55	0.48	0.41
12	1.12	0.67	0.46	0.60	0.08	0.53	0.46	0.43
13	0.96	1.29	0.44	0.61	0.08	0.54	0.44	0.39

CPI – Carbon Preference Index; Phyt – Phytane; Ts – C<sub>27</sub>-18 $\alpha$ (H)-22,29,30-trisnorhopane; Tm – C<sub>27</sub>-17 $\alpha$ (H)-22,29,30-trisnorhopane; 22S – C<sub>31</sub>-17 $\alpha$ (H),21 $\beta$ (H),22S-hopane; 22R – C<sub>31</sub>-17 $\alpha$ (H),21 $\beta$ (H),22R-hopane; H – C<sub>30</sub>-17 $\alpha$ (H),21 $\beta$ (H)-hopane; M – C<sub>30</sub>-17 $\beta$ (H),21 $\alpha$ (H)-moretane;  $\beta\beta$ -C<sub>29</sub>-14 $\beta$ (H),17 $\beta$ (H),20R-sterane;  $\alpha\alpha$  – C<sub>29</sub>-14 $\alpha$ (H),17 $\alpha$ (H),20R-sterane; 20S – C<sub>29</sub>-14 $\alpha$ (H),17 $\alpha$ (H),20S-sterane; 20R – C<sub>29</sub>-14 $\alpha$ (H),17 $\alpha$ (H),20R-sterane; Dia – C<sub>27</sub>-13 $\beta$ (H),17 $\alpha$ (H),20S-diasterane and Ster – C<sub>27</sub>-14 $\alpha$ (H),17 $\alpha$ (H),20R-sterane

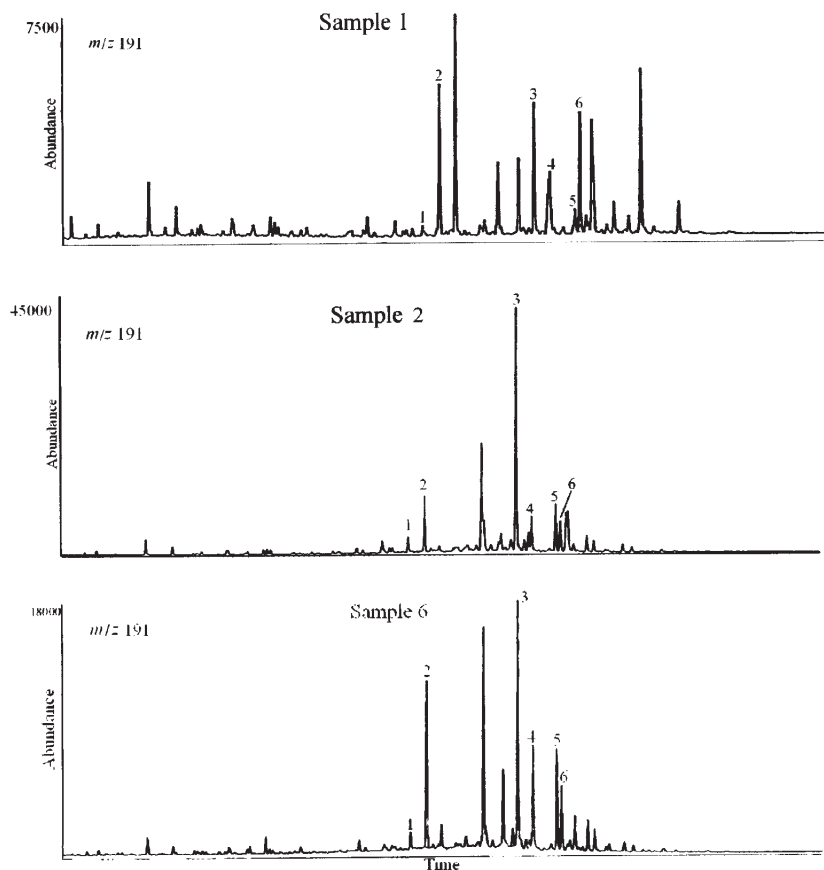


Fig. 2.  $m/z$  191 fragmentograms typical of terpanes observed in the investigated alkane fractions. 1 –  $C_{27}$ -18 $\alpha$ (H)-22,29,30-trisnorhopane (Ts); 2 –  $C_{27}$ -17 $\alpha$ (H)-22,29,30-trisnorhopane (Tm); 3 –  $C_{30}$ -17 $\alpha$ (H),21 $\beta$ (H)-hopane; 4 –  $C_{30}$ -17 $\beta$ (H),21 $\alpha$ (H)-moretane; 5 –  $C_{31}$ -17 $\alpha$ (H),21 $\beta$ (H),22*S*-hopane and 6 –  $C_{31}$ -17 $\alpha$ (H),21 $\beta$ (H),22*R*-hopane (Detailed identification of the corresponding peaks was discussed in previous papers<sup>3,5</sup>).

alkanes. Characteristic examples of  $m/z$  71 fragmentograms, demonstrating qualitative and quantitative differences between the various samples, are shown in Fig. 1. It is well known that during maturation the concentrations of odd and even  $n$ -alkane homologues become equalized, the CPI value approaches unity.<sup>5,6</sup> Simultaneously, the amount of  $n$ - $C_{18}$  increases relative to phytane, resulting in a decrease in the Phyt/ $n$ - $C_{18}$  ratio.<sup>5,6</sup> The values of these two parameters, calculated for the 13 examined samples of Serbian surface sediments, are shown in Table II.

The following maturation parameters were calculated based on the distribution of polycyclic alkanes of the triterpane type: the ratio between the more stable  $C_{27}$ -18 $\alpha$ (H)-22,29,30-trisnorhopane and its less stable precursor  $C_{27}$ -17 $\alpha$ (H)-22,29,30-trisnorhopane (parameter Ts/Ts+Tm); furthermore, the ratio between the thermody-

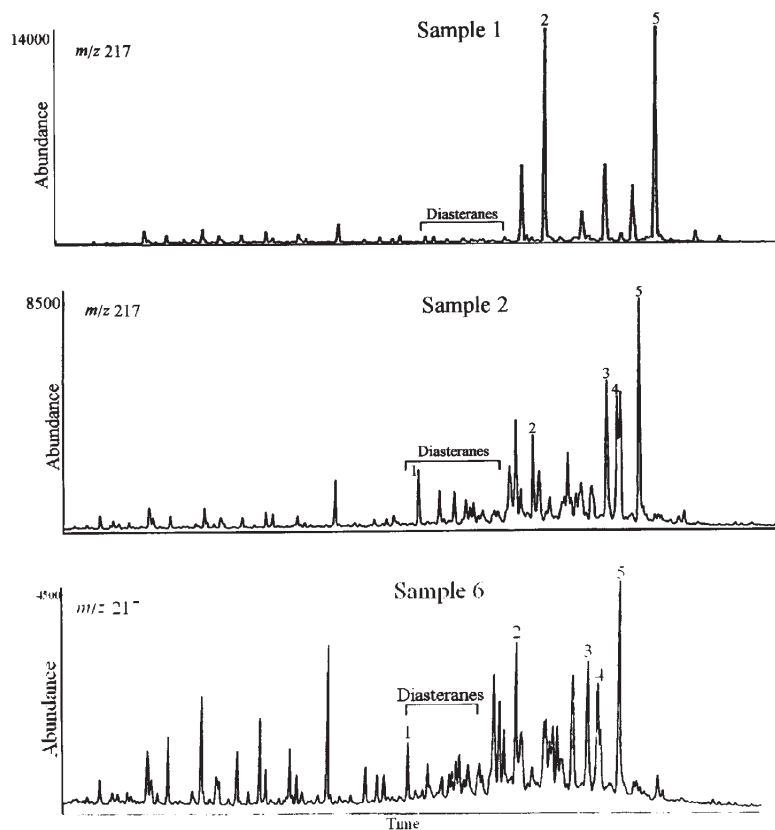


Fig. 3.  $m/z$  217 fragmentograms typical of steranes observed in the investigated alkane fractions. 1 –  $C_{27}$ -13 $\beta$ (H),17 $\alpha$ (H),20*S*-diasterane; 2 –  $C_{27}$ -14 $\alpha$ (H),17 $\alpha$ (H),20*R*-sterane; 3 –  $C_{29}$ -14 $\alpha$ (H),17 $\alpha$ (H)-sterane; 4 –  $C_{29}$ -14 $\beta$ (H),17 $\beta$ (H),20*R*-sterane; 5 –  $C_{29}$ -14 $\alpha$ (H),17 $\alpha$ (H),20*R*-sterane. (Detailed identification of the corresponding peaks was discussed in previous papers<sup>3,5</sup>).

namically more stable  $C_{31}$ -17 $\alpha$ (H),21 $\beta$ (H),22*S*-hopane and the corresponding less stable isomer  $C_{31}$ -17 $\alpha$ (H),21 $\beta$ (H),22*R*-hopane (parameter 22*S*/22*S*+22*R*); finally, the ratio between  $C_{30}$ -17 $\beta$ (H),21 $\alpha$ (H)-moretane and the thermodynamically more stable  $C_{30}$ -17 $\alpha$ (H),21 $\beta$ (H)-hopane (M/H). Other parameters were calculated on the basis of the distribution of polycyclic alkanes of the sterane type, *i.e.*, the ratio of the thermodynamically more stable  $C_{29}$ -14 $\beta$ (H),17 $\beta$ (H),20*R*-sterane and its less stable precursor  $C_{29}$ -14 $\alpha$ (H),17 $\alpha$ (H),20*R*-sterane (parameter  $\beta\beta/\beta\beta+\alpha\alpha$ ); the ratio between the more stable  $C_{29}$ -14 $\alpha$ (H),17 $\alpha$ (H),20*S*- and the less stable  $C_{29}$ -14 $\alpha$ (H),17 $\alpha$ (H),20*R*-sterane (parameter 20*S*/20*S*+20*R*); the ratio of the typical geoisomer, diasterane  $C_{27}$ -13 $\beta$ (H),17 $\alpha$ (H),20*S* and the less stable sterane  $C_{27}$ -14 $\alpha$ (H),17 $\alpha$ (H),20*R* (parameter Dia/Dia+Ster).

The characteristic  $m/z$  191 (triterpanes) and  $m/z$  217 (steranes) fragmento-

TABLE III. Correlation matrix

	CPI	Phyt/n-C <sub>18</sub>	Ts/Ts+Tm	22S/22S+22R	M/H	$\beta\beta/\beta\beta+\alpha\alpha$	20S/20S+20R	Dia/Dia+Ster
CPI	1.000	0.002	-0.459	-0.835	0.470	-0.702	-0.888	-0.867
Phyt/n-C <sub>18</sub>	0.002	1.000	0.672	-0.050	-0.533	0.556	0.133	-0.109
Ts/Ts+Tm	-0.459	0.672	1.000	0.397	-0.925	0.910	0.637	0.431
22S/22S+22R	-0.835	-0.050	0.397	1.000	-0.334	0.549	0.938	0.904
M/H	0.470	-0.533	-0.925	-0.334	1.000	-0.848	-0.556	-0.455
$\beta\beta/\beta\beta+\alpha\alpha$	-0.702	0.556	0.910	0.549	-0.848	1.000	0.778	0.626
20S/20S+20R	-0.888	0.133	0.637	0.938	-0.556	0.778	1.000	0.901
Dia/Dia+Ster	-0.867	-0.109	0.431	0.904	-0.455	0.626	0.901	1.000

Determinant =  $5.283 \times 10^{-7}$ 

TABLE IV. KMO and Bartlett's Test sig

Kaiser-Mayer-Olkin Measure of Sampling Adequacy.	0.678
Bartlett's Test (sig)	0.000



grams, selected as examples demonstrating the qualitative and quantitative differences between the examined samples, are shown in Figs. 2 and 3, respectively. The calculated values of terpane and sterane maturation parameters for the 13 investigated samples are shown in Table II.

#### Factor analysis

The eight maturation parameters calculated for the thirteen investigated Serbian surface sedimentary samples (Table II) were submitted to factor analysis (computer program SPSS 10.0). Table III shows the resulting positively defined correlation matrix (determinant =  $5.283 \times 10^{-7}$ ), and Table IV the values of KMO and *sig.* The results presented in these tables evidently justified the application of the selected model of factor analysis in this particular case study.<sup>11,12</sup>

The factor analysis was expected to define the significance of individual maturation parameters calculated on the basis of the distribution of biological markers of the *n*-alkane, isoprenoid aliphatic alkane, triterpane and sterane type (Figs. 1–3, Table II).

The factors observed for the calculated maturation parameters, together with the corresponding variance values representing the percentage of samples which may be characterized only on the basis of parameters involved in the factor under consideration, or the percentage of the variance in the total data are shown in Table Va. The corresponding cumulative values („cumulative”) are also shown in Table Va.

TABLE V. The observed factors together with the corresponding “variance” and “cumulative” percents before (a) and after (b) varimax rotation

Factor	Before varimax rotation (a)			After varimax rotation (b)		
	Total	Variance/%	Cumulative/%	Total	Variance/%	Cumulative/%
1	<b>5.25</b>	<b>65.49</b>	<b>65.49</b>	<b>4.09</b>	<b>51.19</b>	<b>51.19</b>
2	<b>2.00</b>	<b>25.02</b>	<b>90.51</b>	<b>3.15</b>	<b>39.32</b>	<b>90.51</b>
3	0.38	4.73	95.24			
4	0.19	2.43	97.67			
5	$9.15 \times 10^{-2}$	1.14	98.81			
6	$7.34 \times 10^{-2}$	0.92	99.73			
7	$1.54 \times 10^{-2}$	0.19	99.92			
8	$6.65 \times 10^{-3}$	0.08	100.00			

The significant factors, determined on the basis of Kaiser’s rule<sup>13,14</sup> (total > 1, bold in Table Va), and Cattell’s rule<sup>13</sup> (“scree plot” shown in Fig. 4), were exposed to varimax rotation. The corresponding “variance” and “cumulative” values observed after rotation are shown in Table Vb.

Table VI shows the loadings values of the individual parameters in factors 1 and 2 which had already been defined as significant according to Kaiser’s and

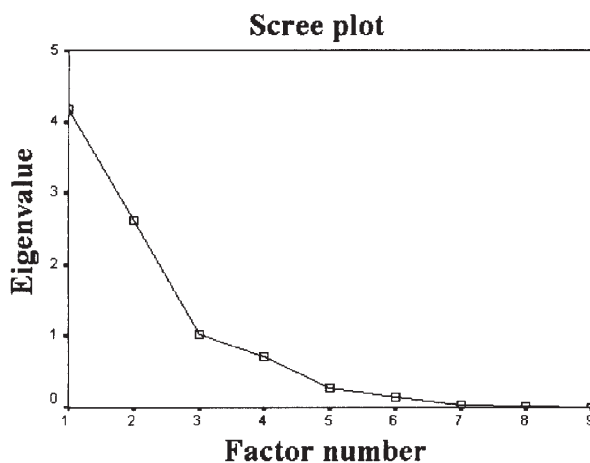


Fig. 4. "Scree plot" for the Cattell's rule.

Cattell's rules before (Table Va) and after (Table Vb) varimax rotation. Based on the up-to-date statistical investigations, the results of factor analysis after varimax rotation were shown to be more suitable for application. Therefore, only the results from Table VIb are interpreted in this paper.

TABLE VI. Loadings observed for individual parameters in factors 1 and 2 before (a) and after (b) varimax rotation

Parameters	Factor (a)		Factor (b)	
	1	2	1	2
CPI	<b>-0.857</b>	0.382	<b>-0.916</b>	-0.203
Phyt/ <i>n</i> -C <sub>18</sub>	0.347	<b>0.830</b>	-0.214	<b>0.874</b>
Ts/Ts+Tm	<b>0.819</b>	0.535	0.340	<b>0.917</b>
22 <i>S</i> /22 <i>S</i> +22 <i>R</i>	<b>0.810</b>	-0.500	<b>0.949</b>	7.960×10 <sup>-2</sup>
M/H	<b>-0.780</b>	-0.485	-0.339	<b>-0.854</b>
ββ/ββ+αα	0.422	0.309	0.558	<b>0.796</b>
20 <i>S</i> /20 <i>S</i> +20 <i>R</i>	<b>0.943</b>	-0.273	<b>0.921</b>	0.341
Dia/Dia+Ster	<b>0.843</b>	-0.474	<b>0.959</b>	0.120

According to factor analysis principles, only parameters whose loadings are higher than |0.6| are valuable for defining a factor. Table VIb shows that parameters CPI, 22*S*/22*S*+22*R*, 20*S*/20*S*+20*R* and Dia/Dia+Ster, represented by boldfaced figures in the factor 1 column, are characterized by loadings higher than |0.6|. This particular observation suggests the following maturation processes were dominant in the bitumens of the investigated sediments: equalization of the concentrations of the odd and even carbon number *n*-alkanes, stereochemical changes at C<sub>22</sub> in C<sub>31</sub> pentacyclic terpanes and C<sub>20</sub> in C<sub>29</sub> regular steranes, as well as transformation of steranes into diasteranes.

On the other hand, in the factor 2 column, involving less dominant processes, the parameters Phyt/ $n$ -C<sub>18</sub>, Ts/Ts+Tm, M/H and  $\beta\beta/\beta\beta+\alpha\alpha$  had loadings significantly higher than  $|0.6|$  (Table VI b). The ratios Ts/Ts+Tm, M/H and  $\beta\beta/\beta\beta+\alpha\alpha$  are based on epimerization reactions occurring in the rings of polycyclic alkanes of the terpane and sterane type. Considering the fact that the Phyt/ $n$ -C<sub>18</sub> parameter was classified as a group 2 factor, it may be presumed that increasing  $n$ -alkane and decreasing isoprenoid concentrations in the bitumen of the investigated sediments were processes taking place parallel with isomerization reactions in the C<sub>31</sub> terpane and C<sub>29</sub> sterane rings.

It was of interest to consider the interdependence of factors 1 and 2 observed for the investigated samples (Fig. 5). A statistically very significant inversely proportional linear dependence was observed with the older sediments, in contrast to the younger sediments which did not show a statistically significant correlation between factors 1 and 2. This observation suggests that the reactions of the aliphatic chain in the older sediments did not occur simultaneously with reactions in the rings. That is to say, transformations in the aliphatic chains were dominant, they occurred first, until an equilibrium was approached or attained. Following these reactions, epimerization reactions in ring structures became dominant.

Based on the positive correlation of factors 1 and 2 (Fig. 5), it may be concluded that the older surface sediments examined in this paper are characterized by a maturity corresponding to changes in the sterane and terpane biomarker rings. On the other hand, the lack of a linear dependence between factors 1 and 2 with the younger sediments indicates their degree of thermal maturity to be characterized by intensive changes in the aliphatic chains, while isomerization reactions in the terpane and sterane rings have not yet begun.

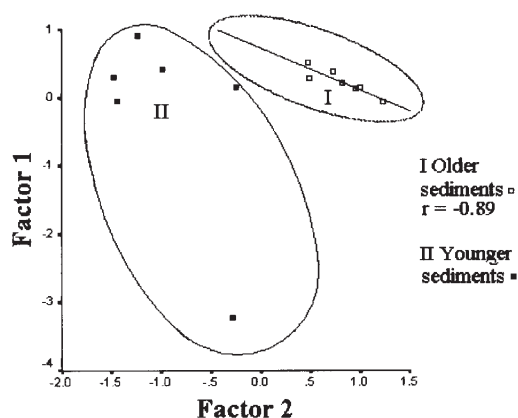


Fig. 5. Correlation between factors 1 and 2 observed for the investigated surface sediments.

Conclusions based on the factor analysis are in quite good agreement with known organic geochemical reasoning.<sup>2,3,5,6</sup> The sole apparent discrepancy was observed with parameters Dia/Dia+Ster and Ts/Ts+Tm. Namely, the factor analy-

sis classified these two parameters into two different factors, while according to up-to-date organic geochemical experience, sterane  $\rightarrow$  diasterane and Tm  $\rightarrow$  Ts transformations take place under similar conditions, involving the catalytic effect of silicates.<sup>6</sup> However, the discrepancy observed with the examined surface sediments suggests that the sterane  $\rightarrow$  diasterane and the Tm  $\rightarrow$  Ts transformations must not necessarily have occurred simultaneously, presumably as a result of the possible different catalytic effects of the mineral constituents in the examined samples, or the different behavior during the catagenetic evolution of the individual isomers figuring in the corresponding parameters.<sup>18</sup> Such a presumption should be verified by further investigations.

The results of the performed factor analysis confirmed that the geological age does not necessarily correlate with the maturity of the sedimentary organic matter. Thus, based on the factor analysis, sample no. 7 (Rajićeva Gora), the only one from the group of five Upper Cretaceous samples (Table I), was classified into the factor 1 column (Table VI), together with the older Lower Carboniferous and Devonian sediments. This observation, which nevertheless demonstrated the advantageous feasibilities of the factor analysis, was not surprising, since sample no. 7 belongs to a different geotectonic unit compared to the other four examined Upper Cretaceous sediments, and is also of a different lithological (aleurolitic) composition. Namely, aleurolite was shown to have a substantial catalytic effect on maturation transformations of biomarkers.

#### CONCLUSIONS

The factor analysis of eight maturation parameters observed in an explorative study of thirteen samples of diverse age originating from different localities in Serbia, resulted in two significant factors.

Factor 1 involved CPI (*n*-alkanes), 22S/22S+22R (pentacyclic terpanes), 20S/20S+20R (steranes) and Dia/Dia+Ster (diasterane-sterane) parameters. Hence, the following maturation processes are suggested to have been dominant in the bitumens of the corresponding sediments: equalization of the concentrations of odd and even carbon number *n*-alkanes, stereochemical changes at C<sub>22</sub> in C<sub>31</sub> pentacyclic terpanes and C<sub>20</sub> in C<sub>29</sub> regular steranes, as well as transformation of steranes into diasteranes.

Factor 2 involved Phyt/*n*-C<sub>18</sub> (isoprenoid-*n*-alkane), Ts/Ts+Tm (pentacyclic terpanes), M/H (pentacyclic terpanes) and  $\beta\beta/\beta\beta+\alpha\alpha$  (steranes) parameters, suggesting that the increase in the concentrations of *n*-alkanes and the decrease in the concentrations of isoprenoids in the bitumen of corresponding sediments took place simultaneously with isomerization reactions in C<sub>31</sub> terpane and C<sub>29</sub> sterane rings.

A statistically very significant linear inverse proportionality between factors 1 and 2 was observed with the older sediments, including just one of the Upper Cretaceous samples, in contrast to the younger sediments, suggesting that reactions of

the aliphatic chains in older sediments were dominant and did not occur simultaneously with reactions in the rings. Hence, it can be concluded that the degree of thermal maturity in the older sediments is characterized by changes in the biomarker sterane and terpane rings, and of the younger sediments by intense changes in the aliphatic chains, in contrast to isomerization reactions in the terpane and sterane rings which have not yet begun.

The conclusions based on factor analysis were in agreement with known organic geochemical reasoning. The sole apparent discrepancy was observed with the parameters Dia/Dia+Ster and Ts/Ts+Tm, suggesting that in the examined surface sediments the corresponding transformations must not necessarily have occurred simultaneously, presumably as a result of possible different catalytic effects of mineral constituents in the examined samples, or different behavior during the catagenetic evolution of the individual isomers figuring in the corresponding parameters.

In conclusion, it has been shown that factor analysis may be of great help in establishing the hierarchy of maturation parameters in exploration studies of vast geological basins.

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#### ИЗВОД

#### ПРИМЕНА ФАКТОРСКЕ АНАЛИЗЕ У ИНТЕРПРЕТАЦИЈИ МАТУРАЦИОНИХ ПАРАМЕТАРА ПОВРШИНСКИХ СЕДИМЕНАТА СРБИЈЕ

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Београд

У овом раду факторска анализа је примењена за интерпретацију осам матурационих параметара израчунатих у оквиру експлорационог истраживања тринаест узорка површинских седимената различите старости, узетих са различитих локалитета у Србији. Анализом су утврђена два значајна фактора. Фактор 1 је обухватио параметре засноване претежно на матурационим променама алифатичних низова, а фактор 2 параметре засноване углавном на променама у терпанским и стеранским прстеновима. Статистички значајна, обрнуто пропорционална, линеарна зависност између фактора 1 и 2 утврђена је код старијих, за разлику од млађих седимената. На основу тога претпостављено је да се код старих седимената реакције у алифатичном низу и прстену нису одигравале истовремено, и такође, да се старији седименти испитивани у овом раду могу окарактерисати степеном термичке зрелости који одговара променама у биомаркерским стеранским и терпанским прстеновима, а млађи интензивним променама у алифатичним низовима.

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