Journal of the Serbian Chemical Society
JSCS@tmf.bg.ac.rs • www.shd.org.rs/JSCS
J. Serb. Chem. Soc. *82* (6) S277–S300 (2017)
Supplementary material

SUPPLEMENTARY MATERIAL TO

Characterisation of lignite lithotypes from the "Kovin" deposit (Serbia) – Implications from petrographic, biomarker and isotopic analysis

DANICA MITROVIĆ[1], NATAŠA ĐOKOVIĆ[1], DRAGANA ŽIVOTIĆ[2], ACHIM BECHTEL[3], OLGA CVETKOVIĆ[4] and KSENIJA STOJANOVIĆ[5]*

[1]University of Belgrade, Innovation Center of the Faculty of Chemistry, Studentski trg 12–16, 11000 Belgrade, Serbia, [2]University of Belgrade, Faculty of Mining and Geology, Đušina 7, 11000 Belgrade, Serbia, [3]Montanuniversität Leoben, Department of Applied Geosciences and Geophysics, Peter-Tunner-Str. 5, A-8700 Leoben, Austria, [4]University of Belgrade, Institute of Chemistry, Technology and Metallurgy, Department of Chemistry, Njegoševa 12, 11000 Belgrade, Serbia and [5]University of Belgrade, Faculty of Chemistry, Studentski trg 12–16, 11000 Belgrade, Serbia

J. Serb. Chem. Soc. *82* (6) (2017) 739–754

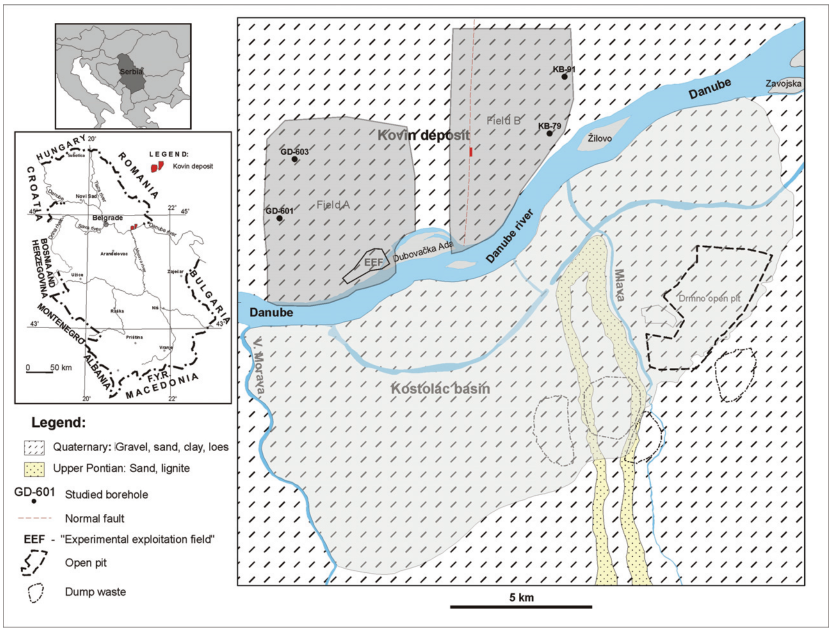

Fig. S-1. Simplified geological map of the Kovin deposit with sample locations.

* Corresponding author. E-mail: ksenija@chem.bg.ac.rs

SAMPLING LOCATIONS AND SAMPLE PREPARATION

Samples of four lignite lithotypes: matrix coal (MC), xylite-rich coal (XC), mixture of matrix and mineral-rich coal (MMiC) and mixture of matrix and xylite-rich coal (MXC) were taken from four boreholes, GD-601 and GD-603 (the "A" field), and KB-79 and KB-91 (the "B" field), representing different parts of all three coal seams (I, II and III), hosted in the Kovin deposit (Fig. S-1; Table S-I). The sampling interval was determined on the basis of lithological changes. The macroscopic description of the lignite lithotypes followed the nomenclature adopted by ICCP[1] (Table S-I).

TABLE S-I. The list of studied samples

Field	Borehole ID	Coal Seam	Sample ID	Depth interval m	Lithotype
B	KB-79	II	2/79	35.35-36.00	Matrix coal (MC)
		II	3/79	36.80-37.60	Mixture of matrix and xylite-rich coal (MXC)
		II	4/79	38.00-38.20	Xylite-rich coal (XC)
		II	5/79	38.50-39.00	Mixture of matrix and xylite-rich coal (MXC)
		II	6/79	39.00-39.10	Mixture of matrix and mineral-rich coal (MMiC)
		II	8/79	40.15-40.65	Mixture of matrix and xylite-rich coal (MXC)
		III	11/79	67.90-69.30	Mixture of matrix and mineral-rich coal (MMiC)
		III	14/79	114.10-114.25	Xylite-rich coal (XC)
		III	16/79	114.75-114.85	Xylite-rich coal (XC)
		III	17/79	115.00-115.30	Mixture of matrix and mineral-rich coal (MMiC)
		III	18/79	115.30-115.45	Mixture of matrix and xylite-rich coal (MXC)
		III	19/79	115.45-116.00	Mixture of matrix and mineral-rich coal (MMiC)
		III	20/79	116.05-116.30	Mixture of matrix and mineral-rich coal (MMiC)
	KB-91	I	26/91	22.50-24.25	Matrix coal (MC)
		I	27/91	24.60-25.00	Xylite-rich coal (XC)
		I	28/91	25.50-25.75	Matrix coal (MC)
		I	29/91	25.75-26.35	Xylite-rich coal (XC)
		I	30/91	26.35-27.65	Matrix coal (MC)
		I	31/91	27.65-28.15	Mixture of matrix and mineral-rich coal (MMiC)
		II	33/91	45.00-45.60	Mixture of matrix and xylite-rich coal (MXC)
		II	34/91	45.60-46.05	Xylite-rich coal (XC)
		II	36/91	47.05-48.35	Mixture of matrix and mineral-rich coal (MMiC)
		II	38/91	49.30-49.50	Xylite-rich coal (XC)
		II	39/91	50.60-50.90	Mixture of matrix and mineral-rich coal (MMiC)
		II	40/91	51.60-52.85	Matrix coal (MC)
A	GD-601	I (Ia)	42/601	42.65-43.10	Xylite-rich coal (XC)
		I (Ia)	43/601	43.10-43.50	Matrix coal (MC)

TABLE S-I. Continued

Field	Borehole ID	Coal Seam	Sample ID	Depth interval m	Lithotype
A	GD-601	I (Ib)	45/601	75.50-76.00	Mixture of matrix and xylite-rich coal (MXC)
		I (Ib)	46/601	76.00-76.40	Matrix coal (MC)
		II	48/601	96.40-97.00	Mixture of matrix and mineral-rich coal (MMiC)
		II	49/601	97.00-97.50	Matrix coal (MC)
	GD-603	I (Ia)	50/603	39.00-39.55	Xylite-rich coal (XC)
		I (Ib)	51/603	65.15-65.35	Matrix coal (MC)
		I (Ib)	52/603	65.60-65.70	Xylite-rich coal (XC)
		I (Ib)	53/603	65.70-66.65	Mixture of matrix and xylite-rich coal (MXC)
A	GD-603	II	54/603	88.00-88.12	Xylite-rich coal (XC)
		II	55/603	88.40-88.60	Mixture of matrix and xylite-rich coal (MXC)
		II	56/603	88.60-88.80	Mixture of matrix and mineral-rich coal (MMiC)

The area of the Kovin deposit consists of Palaeozoic schist, Tertiary, and Quaternary sediments. The basement of the Kovin deposit is formed of Devonian low grade schist overlain by Neogene sediments. Neogene of the Kovin deposit consists of the following units: Sarmatian (Middle Miocene), Pannonian (Late Miocene), Pontian (Late Miocene), Lower Pliocene and Quaternary. Three lignite seams: oldest III seam, middle II, and the youngest I seam, having maximal thickness of 48.7, 7.6 and 15.2 m, are respectively hosted in Pontian series. The detailed geological description of the Kovin deposit is given in the previous article.[2]

For the maceral analyses, the lignite samples were crushed to a maximum particle size of 1 mm, mounted in epoxy resin and polished. The maceral analysis was performed on a Leitz DMLP microscope in monochromatic and UV light illumination on 500 points. The maceral description follows the terminology developed by the ICCP for huminite,[3] liptinite[4] and inertinite[5] nomenclature. Elemental analysis, determination of ash content and calorific value measurements were performed according to procedures which were explained in detail in the previous papers.[6-8]

Extractable OM (bitumen) was obtained from pulverized lignites (<150 μm) in a Dionex ASE 200 accelerated solvent extractor using dichloromethane (DCM) for approximately one hour at 75°C. Copper was added in order to remove elemental sulphur during the extraction process. The asphaltenes were precipitated with *n*-hexane-DCM solution (80:1) and the remainder (maltenes) was separated into saturated, aromatic and NSO (polar fraction, which contains nitrogen, sulphur, and oxygen compounds) fractions using medium pressure liquid chromatography (MPLC) with a Köhnen–Willsch instrument.[9]

Vials of the aliphatic and aromatic fractions of the Kovin lignite samples after MPLC separation were weighted.

TABLE S-II. The maceral composition of lignite lithotypes based on mineral matter-free, vol. %; values of parameters for individual samples are given in Table S-III of the Supplementary material; *SD* – standard deviation

Com-ponent	Matrix coal (MC)				Xylite-rich coal (XC)				Mixture of matrix and mineral-rich coal (MMiC)				Mixture of matrix and xylite-rich coal (MXC)			
Maceral	Mean	Max.	Min.	*SD*	Mean	Max.	Min.	*SD*	Mean	Max.	Min.	*SD*	Mean	Max.	Min.	*SD*
T[a]	11.6	23	4.0	6.6	21.3	52.7	12.0	11.4	7.5	19.1	2.6	4.8	12.9	24.0	5.3	6.4
U[b]	26.6	45.6	14.3	8.5	40.0	47.9	17.2	8.7	21.3	32.2	9.0	7.0	24.9	37.2	6.6	10.1
A[c]	2.5	4.0	0.2	1.3	1.9	4.2	0.2	1.5	6.0	12.5	1.3	3.3	6.7	16.6	1.3	6.2
D[d]	40.5	52.1	17.8	9.6	19.5	24.9	10.2	4.6	42.6	58.4	32.6	8.8	36.1	47.5	30.6	5.4
G[e]	4.3	7.2	1.9	1.8	4.7	7.7	1.5	2.3	5.1	8.6	3.3	2.0	3.5	5.4	1.3	1.2
Ch[f]	3.4	6.9	1.6	1.7	3.5	7.2	1.4	1.7	3.1	6.0	1.6	1.4	3.6	6.8	1.3	2.1
HUM[g]	88.8	94.3	81.4	4.5	91.0	95.0	84.2	3.2	85.6	93.5	74.5	6.1	87.8	95.0	81.2	4.4
Sp[h]	1.2	1.8	0.2	0.6	1.1	1.9	0.5	0.4	1.1	1.7	0.6	0.4	1.4	2.2	0.5	0.7
Cu[i]	0.4	0.8	0.0	0.3	0.3	1.0	0.0	0.3	0.3	1.0	0.0	0.3	0.3	0.4	0.0	0.1
R[j]	0.4	1.2	0.2	0.3	0.6	2.0	0.2	0.5	0.6	1.1	0.0	0.3	0.6	1.6	0.0	0.5
Su[k]	0.4	1.0	0.0	0.3	0.4	1.0	0.0	0.3	0.1	0.7	0.0	0.2	0.4	1.0	0.2	0.3
Al[l]	0.2	0.7	0.0	0.3	0.0	0.0	0.0	0.0	0.1	0.3	0.0	0.1	0.2	0.7	0.0	0.3
Ld[m]	1.8	3.2	0.4	0.9	1.4	2.2	0.3	0.6	1.7	2.9	0.6	0.7	2.6	3.9	1.6	1.0
LIP[n]	4.4	6.8	2.0	1.3	3.8	5.9	2.6	0.9	4.0	7.3	1.1	1.6	5.4	7.4	3.0	1.7
F[o]	1.5	2.7	0.2	0.9	1.4	4.2	0.2	1.4	2.3	9.4	0.2	2.6	1.2	2.8	0.2	1.1
Sf[p]	0.6	2.5	0.2	0.7	0.8	3.9	0.2	1.1	1.1	3.0	0.0	0.9	0.6	1.2	0.0	0.4
Ma[q]	0.4	1.2	0.0	0.4	0.2	0.5	0.0	0.2	0.4	1.2	0.0	0.3	0.5	1.6	0.0	0.5
Fg[r]	0.8	1.6	0.2	0.5	0.6	1.7	0.2	0.4	0.6	1.4	0.2	0.4	0.8	1.8	0.2	0.5
Id[s]	3.5	10.6	0.6	3.1	2.2	4.4	0.7	1.4	6.1	13.3	1.4	4.0	3.6	8.8	0.8	2.6
IN[t]	6.7	14.8	2.2	4.1	5.2	13.2	2.0	3.5	10.5	24.4	2.6	6.7	6.7	14.6	2.0	4.0
MM[u]	9.7	16.8	4.3	4.1	7.6	11.4	3.3	2.8	17.5	29.7	11.4	5.6	15.1	23.9	8.6	5.1

[a]T – textinite; [b]U – ulminite; [c]A – attrinite; [d]D – densinite; [e]G – gelinite; [f]Ch – corpohuminite; [g]HUM – total huminite; [h]Sp – sporinite; [i]Cu – cutinite; [j]R – resinite; [k]Su – suberinite; [l]Al – alginite; [m]Ld – liptodetrinite; [n]LIP – total liptinite; [o]F – fusinite; [p]Sf – semifusinite; [q]Ma – macrinite; [r]Fg – funginite; [s]Id – inertodetrinite; [t]IN – total inertinite; [u]MM – total mineral matter

TABLE S-III. The maceral composition based on mineral matter-free, vol. %

Lithotype	Sample ID	T[a]	U[b]	A[c]	D[d]	G[e]	Ch[f]	HUM[g]	Sp[h]	Cu[i]	R[j]	Su[k]
MC	2/79	23.0	14.2	4.0	40.2	5.4	2.0	88.8	1.8	0.2	0.2	0.2
MXC	3/79	24.0	6.6	16.6	31.4	2.8	2.2	83.6	1.8	0.3	0.0	0.3
XC	4/79	52.7	17.2	4.2	10.2	3.4	2.3	90.0	1.5	0.0	0.2	0.0
MXC	5/79	17.4	12.9	15.8	33.6	3.2	5.3	88.2	2.2	0.4	0.4	1.0
MMiC	6/79	19.1	17.2	8.9	34.8	3.6	6.0	89.6	1.6	0.2	0.2	0.2
MXC	8/79	15.2	28.4	7.0	34.4	3.2	6.8	95.0	0.6	0.0	0.4	0.2
MMiC	11/79	9.5	9.0	12.5	53.5	3.3	2.8	90.6	0.9	0.0	0.3	0.0
XC	14/79	18.0	37.2	2.6	22.4	4.6	7.2	92.0	0.7	0.0	0.5	0.4
XC	16/79	12.0	40.9	0.6	18.0	7.7	5.0	84.2	1.1	0.0	0.2	1.0
MMiC	17/79	2.6	17.2	8.4	40.6	4.2	1.6	74.6	0.6	0.0	0.0	0.0
MXC	18/79	11.2	25.8	6.8	30.6	5.4	1.4	81.2	1.8	0.4	0.2	0.2
MMiC	19/79	5.8	23.8	4.2	35.0	8.6	1.6	79.0	1.2	0.6	0.6	0.0
MMiC	20/79	4.0	16.8	5.2	50.8	4.4	2.3	83.5	1.0	0.0	0.8	0.3

TABLE S-III. Continued

Lithotype	Sample ID	T[a]	U[b]	A[c]	D[d]	G[e]	Ch[f]	HUM[g]	Sp[h]	Cu[i]	R[j]	Su[k]
MC	26/91	16.6	19.8	3.0	40.0	6.0	6.9	92.3	0.7	0.2	0.4	0.4
XC	27/91	18.4	38.0	2.2	24.9	6.2	2.0	91.7	0.8	1.0	0.4	0.4
MC	28/91	8.8	25.4	3.6	41.4	2.4	2.6	84.2	1.8	0.4	1.2	0.0
XC	29/91	23.8	36.1	3.9	18.2	2.9	4.6	89.5	1.2	0.2	0.8	0.8
MC	30/91	4.0	25.1	2.4	39.8	7.2	3.1	81.6	1.1	0.8	0.2	0.6
MMiC	31/91	3.0	17.3	7.7	58.4	3.4	2.3	92.1	1.0	0.6	0.8	0.0
MXC	33/91	6.3	29.1	2.2	39.6	4.0	5.9	87.1	0.5	0.2	1.3	0.2
XC	34/91	14.6	47.4	1.6	23.6	2.2	4.4	93.8	0.7	0.2	0.2	0.4
MMiC	36/91	8.0	29.4	3.6	32.6	8.4	4.2	86.2	1.0	0.2	0.3	0.0
XC	38/91	24.2	47.8	1.7	14.1	3.0	2.8	93.6	0.7	0.2	1.2	0.5
MMiC	39/91	7.2	22.9	1.3	41.9	6.1	2.3	81.7	1.3	0.5	0.7	0.0
MC	40/91	8.2	28.8	3.0	46.0	4.6	3.0	93.6	0.6	0.4	0.2	0.4
XC	42/601	22.0	39.1	3.2	23.7	5.6	1.4	95.0	1.0	0.6	0.5	0.2
MC	43/601	8.4	25.1	2.2	52.1	4.0	2.6	94.4	1.6	0.0	0.2	0.2
MXC	45/601	7.9	27.3	2.2	47.5	4.6	2.5	92.0	0.7	0.2	0.7	0.2
MC	46/601	5.4	27.5	0.8	47.6	1.9	1.6	84.8	1.8	0.8	0.2	0.2
MMiC	48/601	10.4	26.8	4.7	42.8	4.9	3.9	93.5	0.8	0.2	1.1	0.2
MC	49/601	9.8	28.2	3.7	39.5	4.1	5.6	90.9	0.2	0.2	0.4	1.0
XC	50/603	13.2	44.7	0.4	16.8	7.4	4.3	86.8	1.2	0.2	0.4	0.4
MC	51/603	20.0	45.6	0.2	17.8	2.6	3.4	89.6	1.4	0.4	0.6	0.2
XC	52/603	13.0	47.4	0.2	22.6	7.5	1.9	92.6	1.9	0.2	0.2	0.2
MXC	53/603	5.3	37.2	2.1	34.5	3.8	3.5	86.4	1.7	0.2	0.2	0.7
XC	54/603	22.7	44.3	0.2	20.2	1.5	3.0	91.9	1.2	0.2	2.0	0.2
MXC	55/603	15.8	32.0	1.3	37.6	1.3	1.4	89.4	1.7	0.2	1.6	0.2
MMiC	56/603	5.8	32.2	3.3	36.1	3.8	4.2	85.4	1.7	1.0	1.0	0.7

TABLE S-III. Continuation

Lithotype	Sample ID	Al[l]	Ld[m]	LIP[n]	F[o]	Sf[p]	Ma[q]	Fg[r]	Id[s]	IN[t]	MM[u]
MC	2/79	0.7	2.7	5.8	2.0	0.4	0.0	1.6	1.4	5.4	8.0
MXC	3/79	0.7	3.9	7.0	2.8	1.2	0.3	0.4	4.7	9.4	23.9
XC	4/79	0.0	1.9	3.6	3.0	0.4	0.2	0.2	2.6	6.4	9.9
MXC	5/79	0.0	3.4	7.4	0.5	0.4	0.0	1.8	1.7	4.4	8.6
MMiC	6/79	0.2	2.4	4.8	0.6	0.3	0.2	1.0	3.5	5.6	13.0
MXC	8/79	0.0	1.8	3.0	0.4	0.0	0.0	0.8	0.8	2.0	9.4
MMiC	11/79	0.3	1.4	2.9	1.3	0.7	0.4	0.9	3.2	6.5	29.7
XC	14/79	0.0	1.8	3.4	1.2	0.4	0.5	0.8	1.7	4.6	8.8
XC	16/79	0.0	0.3	2.6	4.2	3.9	0.2	0.4	4.5	13.2	3.3
MMiC	17/79	0.0	0.6	1.2	9.4	1.2	0.2	0.2	13.2	24.2	11.4
MXC	18/79	0.0	1.6	4.2	2.8	0.8	1.6	0.6	8.8	14.6	14.4
MMiC	19/79	0.3	2.2	4.9	2.8	1.8	1.2	0.8	9.5	16.1	13.5
MMiC	20/79	0.0	0.7	2.8	2.0	3.0	0.4	0.3	8.0	13.7	20.4
MC	26/91	0.0	0.4	2.1	1.0	0.4	0.4	1.2	2.6	5.6	16.8
XC	27/91	0.0	1.4	4.0	0.8	0.2	0.2	0.2	2.9	4.3	4.2
MC	28/91	0.2	3.2	6.8	2.2	0.2	0.2	1.0	5.4	9.0	5.5
XC	29/91	0.0	2.0	5.0	1.0	0.4	0.4	0.5	3.2	5.5	8.8

TABLE S-III. Continued

Lithotype	Sample ID	Al[l]	Ld[m]	LIP[n]	F[o]	Sf[p]	Ma[q]	Fg[r]	Id[s]	IN[t]	MM[u]
MC	30/91	0.0	1.0	3.7	2.4	0.5	1.2	0.2	10.4	14.7	15.0
MMiC	31/91	0.0	1.6	4.0	1.4	0.0	0.3	0.6	1.6	3.9	22.9
MXC	33/91	0.2	2.5	4.9	1.8	0.2	0.2	0.8	5.0	8.0	14.8
XC	34/91	0.0	1.7	3.2	0.2	0.4	0.0	1.7	0.7	3.0	8.1
MMiC	36/91	0.0	1.7	3.2	2.6	0.8	0.2	0.6	6.4	10.6	13.9
XC	38/91	0.0	1.4	4.0	0.7	0.3	0.0	0.7	0.7	2.4	11.4
MMiC	39/91	0.0	1.8	4.3	1.0	1.5	0.0	1.4	10.1	14.0	15.9
MC	40/91	0.0	2.4	4.0	0.2	0.2	0.2	1.2	0.6	2.4	9.3
XC	42/601	0.0	0.7	3.0	0.5	0.2	0.0	0.2	1.1	2.0	11.2
MC	43/601	0.0	1.5	3.5	0.2	0.4	0.0	0.2	1.3	2.1	7.4
MXC	45/601	0.5	1.7	4.0	0.2	0.7	0.2	0.9	2.0	4.0	12.4
MC	46/601	0.6	1.0	4.6	2.7	2.5	0.6	0.6	4.2	10.6	11.5
MMiC	48/601	0.2	1.4	3.9	0.2	0.5	0.2	0.2	1.5	2.6	15.0
MC	49/601	0.4	2.1	4.3	1.0	0.4	0.4	0.8	2.2	4.8	9.9
XC	50/603	0.0	1.4	3.6	3.2	1.0	0.4	0.6	4.4	9.6	4.6
MC	51/603	0.0	2.2	4.8	2.0	0.4	0.2	0.4	2.6	5.6	4.3
XC	52/603	0.0	0.9	3.4	0.2	0.8	0.4	0.8	1.8	4.0	5.5
MXC	53/603	0.2	3.9	6.9	0.9	0.2	0.9	1.2	3.5	6.7	19.3
XC	54/603	0.0	2.2	5.8	0.2	0.2	0.0	0.9	1.0	2.3	7.8
MXC	55/603	0.0	2.3	6.0	0.5	1.1	0.5	0.2	2.3	4.6	17.8
MMiC	56/603	0.0	2.9	7.3	1.7	0.7	0.4	0.4	4.1	7.3	19.2

[a]T – Textinite; [b]U – ulminite; [c]A – attrinite; [d]D – densinite; [e]G – gelinite; [f]Ch – corpohuminite; [g]HUM – total huminite; [h]Sp – sporinite; [i]Cu – cutinite; [j]R – resinite; [k]Su – suberinite; [l]Al – alginite; [m]Ld – liptodetrinite; [n]LIP – total liptinite; [o]F – fusinite; [p]Sf – semifusinite; [q]Ma – macrinite; [r]Fg – funginite; [s]Id – inertodetrinite; [t]IN – total inertinite; [u]MM – total mineral matter

TABLE S-IV. Petrographic indices and bulk organic geochemical parameters of lignite lithotypes; values of parameters for individual samples are given in Table S-V of the Supplementary material

Parameter	Matrix coal (MC)				Xylite-rich coal (XC)				Mixture of matrix and mineral-rich coal (MMiC)				Mixture of matrix and xylite-rich coal (MXC)			
	Mean	Max.	Min.	*SD*	Mean	Max.	Min.	*SD*	Mean	Max.	Min.	*SD*	Mean	Max.	Min.	*SD*
ΣG[a] / vol. %	52.61	58.25	43.85	4.58	48.15	56.28	24.03	8.72	50.98	56.37	44.43	4.28	48.04	57.17	30.44	9.30
GI[b]	4.22	6.60	1.86	1.74	2.80	4.76	0.48	1.15	3.41	5.72	1.77	1.29	3.56	6.45	0.84	2.14
TPI[c]	1.20	3.90	0.67	1.02	3.24	5.15	2.17	0.98	0.76	1.21	0.34	0.30	1.01	1.26	0.73	0.23
VI[d]	1.02	3.10	0.63	0.78	2.74	4.22	1.91	0.75	0.64	0.97	0.31	0.24	0.88	1.22	0.65	0.21
GWI[e]	1.52	2.07	0.43	0.48	0.57	0.74	0.35	0.11	2.07	3.11	1.27	0.69	1.33	1.79	1.06	0.28
TOC[f] / %	40.77	57.97	29.58	10.21	51.66	57.01	40.44	4.67	25.54	48.90	8.04	12.37	35.41	45.79	17.14	10.96
S[g] / %	1.78	3.33	0.82	0.86	1.72	2.87	0.80	0.53	1.53	4.40	0.21	1.33	1.66	3.34	0.78	0.76
Q_g[h] / MJ kg^{-1}	24.30	28.30	22.80	1.70	25.80	27.80	24.20	0.90	20.80	25.80	15.70	3.30	23.10	25.10	18.90	2.10
Q_d[i] / MJ kg^{-1}	23.30	27.20	21.70	1.70	24.80	26.70	23.20	0.90	19.80	24.80	14.30	3.30	22.10	23.90	17.80	2.10
Ash, %	33.45	50.85	16.86	11.36	17.68	31.36	8.66	6.07	55.42	78.20	25.51	14.98	40.06	59.84	25.70	13.75
Bitumen mg (g *TOC*)$^{-1}$	59.99	105.33	36.89	21.13	49.27	64.38	22.65	12.72	64.65	131.69	34.78	32.04	61.18	87.97	36.78	17.17
Saturated HC[j], %	2.54	8.58	0.65	2.54	2.31	10.57	0.97	2.78	1.91	5.24	0.60	1.31	2.01	3.21	1.25	0.73
Aromatic HC, %	2.99	4.48	1.75	0.95	2.40	4.38	1.09	0.81	2.42	3.89	0.70	1.00	2.58	4.74	1.19	1.06
Asp[k]+ NSO[l], %	94.47	97.07	86.94	3.18	95.30	97.83	85.05	3.49	95.67	97.62	91.96	1.85	95.42	97.32	94.01	1.29

[a]ΣG = Gelinite + Corpohuminite + 0.67 (Ulminite + Densinite), (mineral matter-free basis); [b]*GI* – Gelification Index = (Ulminite + Corpohuminite + Densinite + Macrinite)/(Textinite + Attrinite + Fusinite + Inertodetrinite); [c]*TPI* – Tissue Preservation Index = (Textinite + Ulminite + Corpohuminite + Fusinite)/(Attrinite + Densinite + Macrinite); [d]*VI* – Vegetation Index = (Telohuminite + Fusinite + Semifusinite + Cutinite + Sporinite + Suberinite + Resinite)/(Detrohuminite + Inertodetrinite + Alginite + Liptodetrinite + Other liptinites); [e]*GWI* – Groundwater Index = (Gelohuminite + Densinite + Mineral Matter)/(Telohuminite + Attrinite); [f]*TOC* – Total organic carbon content, dry basis; [g]*S* – Total sulphur content, dry basis; [h]Q_g – Gross calorific value; [i]Q_d – Net calorific value; [j]HC – Hydrocarbons; [k]*Asp* – Asphaltenes; [l]*NSO* – Polar fraction, which contains nitrogen, sulphur and oxygen compounds

TABLE S-V. Petrographic indices and bulk organic geochemical parameters

Lithotype	Sample ID	ΣG[a] /vol. %	*GI*[b]	*TPI*[c]	*VI*[d]	*GWI*[e]	*TOC*[f] / %	*S*[g] /%
MC	2/79	43.85	1.86	0.93	0.86	1.35	56.06	1.88
MXC	3/79	30.44	0.84	0.74	0.65	1.28	24.23	1.67
XC	4/79	24.03	0.48	5.15	3.97	0.35	52.90	2.87
MXC	5/79	39.69	1.46	0.73	0.65	1.10	44.67	0.78
MMiC	6/79	44.43	1.81	0.98	0.79	1.27	20.21	0.51
MXC	8/79	52.12	2.97	1.23	1.03	1.06	45.79	3.34
MMiC	11/79	47.96	2.48	0.34	0.31	2.88	8.31	0.21
XC	14/79	51.73	2.86	2.49	2.05	0.74	51.64	1.53
XC	16/79	52.11	3.01	3.30	2.71	0.64	57.01	1.33
MMiC	17/79	44.47	1.77	0.63	0.49	2.05	27.16	0.82
MXC	18/79	44.58	2.01	1.06	0.90	1.18	43.97	1.45
MMiC	19/79	49.60	2.76	0.84	0.71	1.74	48.90	1.70
MMiC	20/79	51.94	3.66	0.45	0.43	3.00	27.52	2.13
MC	26/91	52.96	2.89	1.02	0.86	1.77	37.36	1.80
XC	27/91	50.31	2.68	2.17	1.91	0.64	50.80	1.98
MC	28/91	49.82	3.48	0.86	0.74	1.37	29.97	1.73
XC	29/91	43.82	1.86	2.91	2.36	0.54	49.29	1.41
MC	30/91	53.67	3.60	0.80	0.65	2.07	29.58	3.33
MMiC	31/91	56.37	5.72	0.36	0.35	3.11	26.10	4.40
MXC	33/91	55.86	4.89	1.03	0.80	1.71	39.65	1.46
XC	34/91	54.14	4.41	2.64	2.32	0.60	48.67	1.65
MMiC	36/91	54.10	3.22	1.21	0.95	1.44	26.22	1.35
XC	38/91	47.38	2.37	4.78	4.22	0.42	51.58	0.80
MMiC	39/91	51.74	3.42	0.77	0.64	2.11	39.27	1.00
MC	40/91	57.69	6.50	0.82	0.75	1.57	33.71	0.92
XC	42/601	49.16	2.40	2.34	2.23	0.65	40.44	2.28
MC	43/601	58.25	6.60	0.67	0.63	1.85	39.93	2.85
MXC	45/601	57.17	6.30	0.76	0.70	1.79	40.72	1.86
MC	46/601	53.77	5.90	0.76	0.76	1.86	41.38	1.69
MMiC	48/601	55.49	4.39	0.87	0.79	1.59	23.70	2.94
MC	49/601	55.02	4.41	1.02	0.86	1.42	41.01	0.97
XC	50/603	52.91	3.12	3.72	2.80	0.57	53.16	1.67
MC	51/603	48.49	2.70	3.90	3.10	0.43	57.97	0.82
XC	52/603	56.28	4.76	2.69	2.51	0.62	56.69	1.68
MXC	53/603	55.17	6.45	1.25	1.05	1.37	27.12	1.63
XC	54/603	47.72	2.80	3.44	3.01	0.48	56.06	1.67
MXC	55/603	49.30	3.59	1.26	1.22	1.18	17.14	1.07
MMiC	56/603	53.73	4.86	1.10	0.97	1.53	8.04	0.22

TABLE S-V. Continued

Lithotype	Sample ID	Q_g[h] MJ kg^{-1}	Q_d[i] MJ kg^{-1}	Ash %	Bitumen mg (g *TOC*)$^{-1}$	Saturated hydrocarbons, %	Aromatic hydrocarbons, %	Asphaltenes+ *NSO*[j] compounds, %
MC	2/79	25.9	24.8	19.00	65.99	1.04	3.39	95.56
MXC	3/79	18.9	17.8	59.84	87.97	1.94	2.26	95.81
XC	4/79	26.1	25.1	20.63	59.63	2.11	3.01	94.88
MXC	5/79	24.8	23.7	28.02	62.07	1.25	4.74	94.01
MMiC	6/79	17.9	17.0	63.83	44.25	0.91	2.13	96.96
MXC	8/79	25.1	23.9	25.70	36.78	3.21	2.75	94.04
MMiC	11/79	15.7	14.3	78.20	39.66	2.05	3.22	94.74
XC	14/79	26.3	25.3	12.62	52.62	1.08	2.16	96.76
XC	16/79	25.6	24.6	8.66	22.65	1.45	2.54	96.01
MMiC	17/79	23.5	22.5	56.29	39.40	1.75	0.70	97.54
MXC	18/79	24.2	23.3	27.62	51.75	1.49	1.19	97.32
MMiC	19/79	25.8	24.8	25.51	81.28	1.94	3.23	94.84
MMiC	20/79	21.3	20.3	58.27	34.78	2.27	1.70	96.02
MC	26/91	23.3	22.1	42.91	72.18	4.27	3.73	92.00
XC	27/91	25.1	24.1	17.90	48.64	2.50	2.19	95.31
MC	28/91	23.0	21.7	50.85	64.37	1.13	3.38	95.49
XC	29/91	25.3	24.2	20.08	54.20	0.97	2.27	96.75
MC	30/91	22.8	22.1	40.76	38.13	1.24	3.72	95.04
MMiC	31/91	21.0	20.1	52.56	60.52	1.30	3.26	95.44
MXC	33/91	24.3	23.3	35.95	75.09	1.28	1.92	96.81
XC	34/91	25.9	24.8	21.74	54.29	1.57	1.89	96.54
MMiC	36/91	21.2	19.9	56.11	131.69	0.60	1.79	97.62
XC	38/91	25.5	24.4	16.38	46.25	1.09	1.09	97.83

TABLE S-V. Continued

Lithotype	Sample ID	Q_g[h] MJ kg^{-1}	Q_d[i] MJ kg^{-1}	Ash %	Bitumen mg (g *TOC*)$^{-1}$	Saturated hydrocarbons, %	Aromatic hydrocarbons, %	Asphaltenes+ *NSO*[j] compounds, %
MMiC	39/91	24.4	23.3	37.05	73.43	2.10	3.89	94.01
MC	40/91	23.9	22.6	37.92	58.30	0.65	2.28	97.07
XC	42/601	24.2	23.2	31.36	57.62	10.57	4.38	85.05
MC	43/601	24.3	23.3	34.23	43.43	8.58	4.48	86.94
MXC	45/601	23.8	22.7	35.43	47.30	2.24	3.19	94.57
MC	46/601	23.4	22.5	24.40	55.28	1.75	1.75	96.49
MMiC	48/601	20.2	19.1	57.75	100.17	0.91	1.52	97.56
MC	49/601	24.2	23.1	34.11	105.33	2.93	2.05	95.01
XC	50/603	26.0	24.9	18.69	52.94	1.18	2.35	96.47
MC	51/603	28.3	27.2	16.86	36.89	1.24	2.17	96.59
XC	52/603	26.4	25.5	12.58	28.77	1.42	1.98	96.60
MXC	53/603	22.3	21.1	52.90	75.55	1.75	2.05	96.20
XC	54/603	27.8	26.7	13.85	64.38	1.42	2.49	96.09
MXC	55/603	21.7	20.9	54.98	52.94	2.92	2.50	94.58
MMiC	56/603	16.9	16.3	68.60	41.36	5.24	2.80	91.96

[a]ΣG = Gelinite + Corpohuminite + 0.67 (Ulminite + Densinite), (mineral matter-free basis); [b]*GI* – Gelification Index = (Ulminite + Corpohuminite + Densinite + Macrinite)/(Textinite + Attrinite + Fusinite + Inertodetrinite); [c]*TPI* – Tissue Preservation Index = (Textinite + Ulminite + Corpohuminite + Fusinite)/(Attrinite + Densinite + Macrinite); [d]*VI* – Vegetation Index = (Telohuminite + Fusinite + Semifusinite + Cutinite + Sporinite + Suberinite + Resinite)/(Detrohuminite + Inertodetrinite + Alginite + Liptodetrinite + Other liptinites); [e]*GWI* – Groundwater Index = (Gelohuminite + Densinite + Mineral Matter)/(Telohuminite + Attrinite); [f]*TOC* – Total organic carbon content, dry basis; [g]*S* – Total sulphur content, dry basis; [h]Q_g – Gross calorific value; [i]Q_d – Net calorific value; [j]*NSO* – Polar fraction, which contains nitrogen, sulphur and oxygen compounds

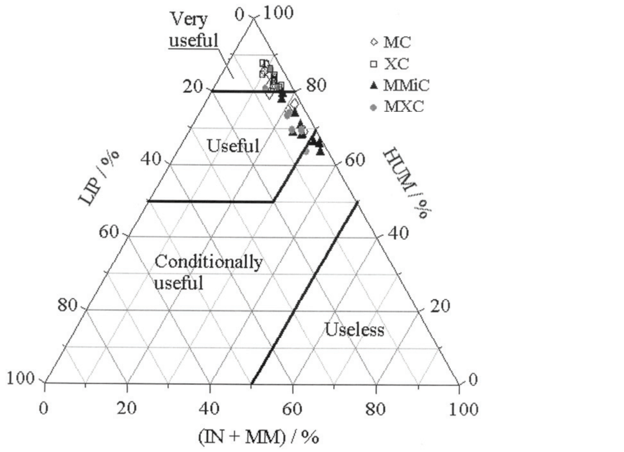

Fig. S-2. Evaluation of usefulness of investigated lithotypes in fluidized bed gasification based on petrographic composition. For the abbreviations of parameters, see the legend of Tables S-II and S-III.

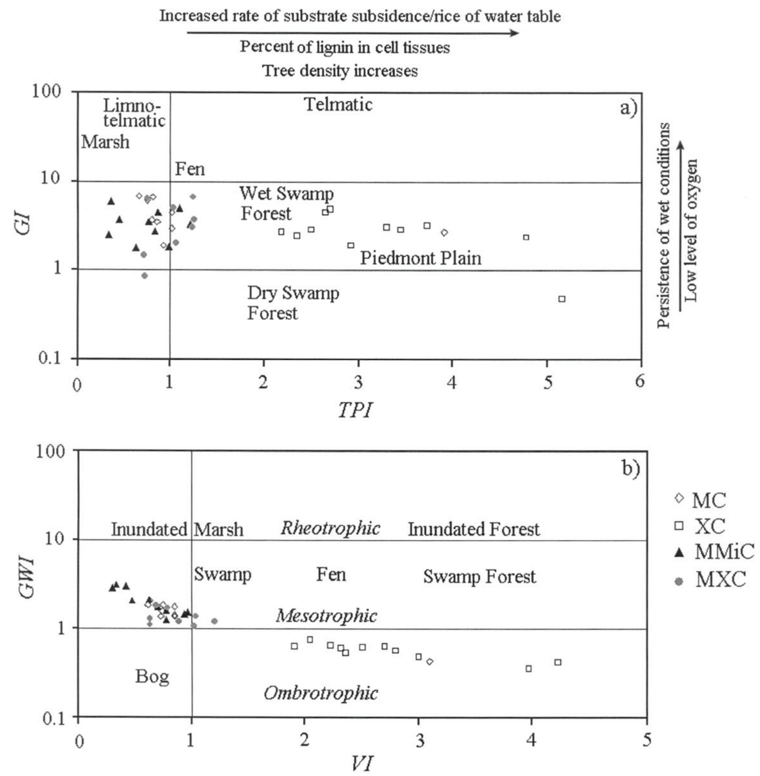

Fig. S-3. GI vs. TPI (a) and GWI vs. VI (b) plots. For the abbreviations of parameters, see the legend of Tables S-IV and S-V.

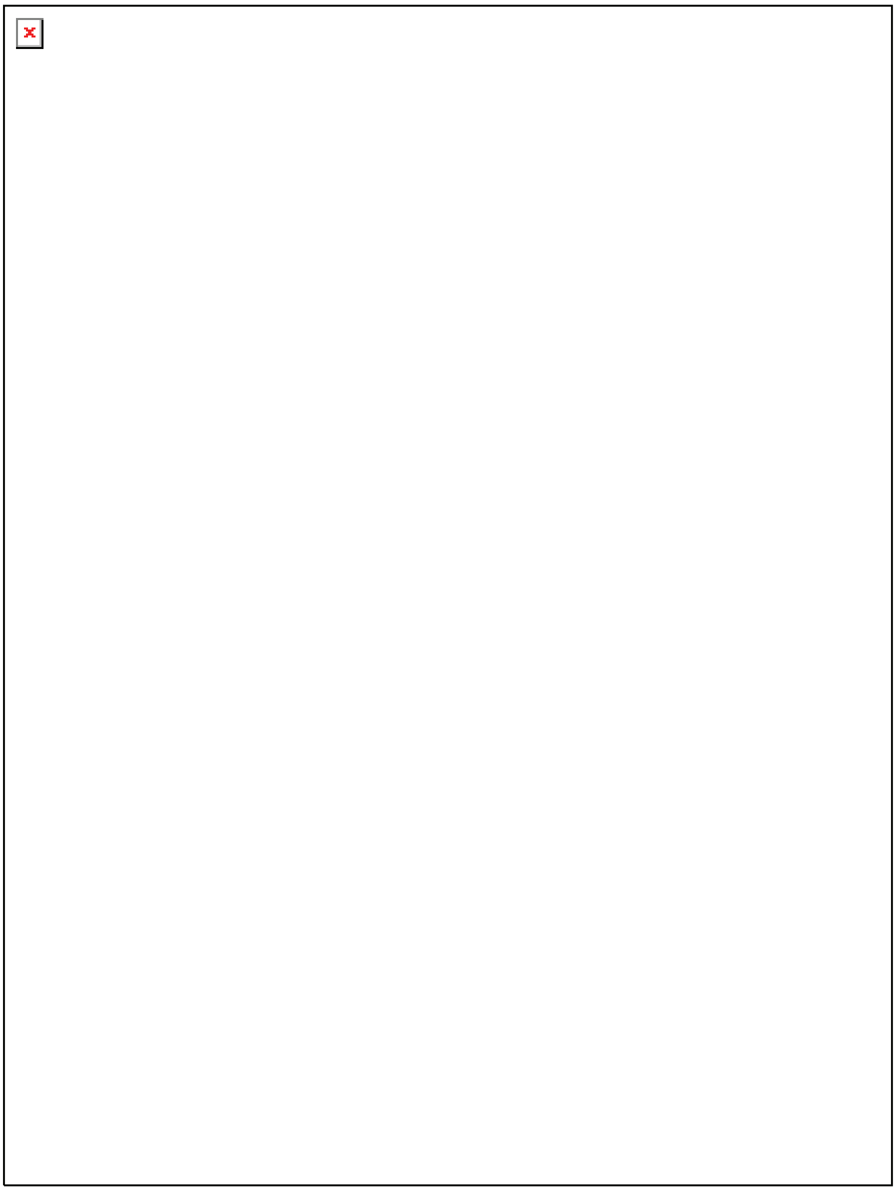

Fig. S-4. Total ion current (*TIC*) of saturated fraction typical for investigated lithotypes. Peak assignments: *n*-alkanes are labelled according to their carbon number; Pr – pristane; Ph – phytane; ΔPr – pristene; D1, D2 – isopimaradienes; D3 – norpimarane; D4 – beyerane; D5 – isophyllocladene; D6 – fichtelite; D7 – pimarane; D8 – 16*α*(H)-phyllocladane; D9 – 16*α*(H)-kaurane; D10 – dehydroabietane isomer; D11 – dehydroabietane; T1 – des-A-olean-13(18)-ene; T2 – des-A-olean-12-ene; Std – standard; T3 – des-A-lupane; T4 – des-A-urs-13(18)-ene; *ββ*, *βα* and *αβ* designate configurations at C-17 and C-21 in hopanes; (R) designates configuration at C-22 in hopanes.

Fig. S-5. *TIC* (Total Ion Current) of aromatic fraction typical for investigated lithotypes. Peak assignments:_1 – dihydro-ar-curcumene; 2 – cuparene; 3 – calamenene; 4 – eudalene; 5 – cadina-1(10),6,8-triene; 6 – methyldibenzofuran; 7 – 5,6,7,8-tetrahydrocadalene; 8 – cadalene; 9 – isocadalene; 10 – phenanthrene; 11 – 19-norabieta-8,11,13-triene; 12 – 19-norabieta-6,8,11,13-tetraene; 13 – 16,17-bisnordehydroabietane; 14, 15 – hibaenes;

Fig. S-5. (Continued) 16 – 18-norabieta-6,8,11,13-tetraene; 17 – 18-norabieta-8,11,13--triene; 18 – 16α(H)-phyllocladane; 19 – fluoranthene; 20 – dehydroabietane isomer; 21 – dehydroabietane; 22 – pyrene; 23 – 1,2,3,4-tetrahydroretene; 24 – 2-methyl, 1-(4'--methylpentyl), 6-*i*-propyl-naphthalene; 25 – simonellite; 26 – totarane; 27 – semper-virane; 28 – Retene; 29 – 4-methyl, 4,5-dihydropyrene; 30 – des-A-olean-diene; Std – standard; 31 – 2-methylretene; 32 – 3,4,7,12a-tetramethyl-1,2,3,4,4a,11,12,12a-octa-hydrochrysene; 33 – 3,3,7,12a-tetramethyl-1,2,3,4,4a,11,12,12a-octahydrochrysene; 34 – pentamethyldodecahydrochrysene; 35,36 – methylchrysenes; 37 – 3,4,7-trimethyl--1,2,3,4-tetrahydrochrysene; 38 – 3,3,7-trimethyl-1,2,3,4-tetrahydrochrysene; 39 – perylene; 40 – pentanorlupa-1,3,5(10)-triene; 41 – C_{27}Hop-17(21)-ene; 42 – D-ring monoaromatic hopane; 43 – 24,25-dinorursa-1,3,5(10),12-tetraene; 44 – 24,25-dinorlupa--1,3,5(10)-triene; 45 – Norlanosta(eupha)hexaene; 46 – C,D-ring diaromatic hopane; 47 – 1,2,4a,9-tetramethyl-1,2,3,4,4a, 5,6,14b-octahydropicene; 48 – 2,2,4a,9-tetramethyl--1,2,3,4,4a,5,6,14b-octahydropicene; 49 – 4-methyl, 24-ethyl, 19-norcholesta-1,3,5(10)--triene; 50 – B,C,D-ring triaromatic hopane; 51 – A,B,C,D-ring tetraaromatic hopane (7-methyl, 3'-ethyl, 1,2-cyclopentanochrysene); 52 – 1,2,9-trimethyl-1,2,3,4-tetrahyd-ropicene; 53 – 2,2,9-trimethyl-1,2,3,4-tetrahydropicene; 54 – C_{31} benzohopane cyclised at C-16.

TABLE S-VI. Contents of biomarkers, μg (g *TOC*)$^{-1}$ and values of biomarker ratios

Lithotype	Sample ID	*Di*[a]	*Tri*[b]	*n*-Alkanes	Hopanoids	Steroids
MC	2/79	1139.31	84.63	590.43	259.21	25.84
MXC	3/79	1108.06	318.22	1483.32	322.86	13.82
XC	4/79	1626.55	131.93	300.02	499.94	18.87
MXC	5/79	2934.05	203.75	275.28	228.14	20.05
MMiC	6/79	613.16	130.70	373.30	176.00	33.36
MXC	8/79	390.34	155.99	598.21	312.20	35.09
MMiC	11/79	741.27	118.40	578.86	128.63	17.27
XC	14/79	981.63	55.91	111.70	243.18	54.84
XC	16/79	321.58	49.55	178.48	111.41	10.54
MMiC	17/79	235.91	40.32	195.62	53.71	3.45
MXC	18/79	667.59	30.43	296.06	162.14	20.43
MMiC	19/79	1030.30	15.60	507.78	263.41	15.13
MMiC	20/79	691.39	111.94	292.94	220.98	27.81
MC	26/91	3463.61	84.66	567.22	417.51	45.51
XC	27/91	1544.68	77.73	179.78	135.10	23.63
MC	30/91	1152.86	206.61	149.17	213.27	25.20
MMiC	36/91	1973.07	187.79	255.32	143.52	15.22
XC	38/91	361.40	92.68	251.35	93.81	14.46
MMiC	39/91	1228.42	277.47	493.94	355.86	28.80
MC	40/91	439.23	196.65	529.10	152.65	27.95
MXC	45/601	1297.23	63.75	248.43	148.95	25.00
MC	46/601	401.86	90.64	639.55	187.27	9.21
MMiC	48/601	1154.87	133.22	104.93	59.10	17.27
MC	49/601	2603.85	59.40	708.22	239.95	22.39
MC	51/603	343.12	64.56	239.35	139.64	10.04
XC	52/603	286.72	65.96	263.16	156.83	33.57
MXC	53/603	1176.59	149.07	458.98	288.81	21.11

TABLE S-VI. Continued

Lithotype	Sample ID	*Di*[a]	*Tri*[b]	*n*-Alkanes	Hopanoids	Steroids
XC	54/603	1986.93	52.67	62.40	93.62	12.36
MXC	55/603	1842.38	124.73	388.71	117.31	8.78
MMiC	56/603	1278.70	130.57	1076.70	301.19	8.56
Lithotype	**Sample ID**	**Proportion of *Di***	**Diterpenoids/ *n*-Alkanes**	***Di*/(*Di*+*Tri*)**	**Aromatic *Di***	**Perylene**
MC	2/79	0.54	1.93	0.931	215.68	7.36
MXC	3/79	0.34	0.75	0.777	182.78	23.16
XC	4/79	0.63	5.42	0.925	481.57	18.16
MXC	5/79	0.80	10.66	0.935	408.89	21.42
MMiC	6/79	0.46	1.64	0.824	192.67	14.50
MXC	8/79	0.26	0.65	0.714	157.46	3.60
MMiC	11/79	0.47	1.28	0.862	139.40	9.44
XC	14/79	0.68	8.79	0.946	148.89	7.03
XC	16/79	0.48	1.80	0.866	43.90	1.94
MMiC	17/79	0.45	1.21	0.854	97.99	3.65
MXC	18/79	0.57	2.25	0.956	135.81	7.40
MMiC	19/79	0.56	2.03	0.985	117.19	0.57
MMiC	20/79	0.51	2.36	0.861	384.65	19.87
MC	26/91	0.76	6.11	0.976	213.45	2.36
XC	27/91	0.79	8.59	0.952	165.34	4.26
MC	30/91	0.66	7.73	0.848	383.88	15.68
MMiC	36/91	0.77	7.73	0.913	280.98	24.99
XC	38/91	0.44	1.44	0.796	48.69	4.41
MMiC	39/91	0.52	2.49	0.816	122.27	20.92
MC	40/91	0.33	0.83	0.691	97.65	16.64
MXC	45/601	0.73	5.22	0.953	173.16	8.19
MC	46/601	0.30	0.63	0.816	56.51	3.69
MMiC	48/601	0.79	11.01	0.897	366.77	N.D.[c]
MC	49/601	0.72	3.68	0.978	100.47	8.49
MC	51/603	0.43	1.43	0.842	71.38	5.26
XC	52/603	0.36	1.09	0.813	35.67	2.06
MXC	53/603	0.56	2.56	0.888	147.25	15.51
XC	54/603	0.90	31.84	0.974	377.30	7.12
MXC	55/603	0.74	4.74	0.937	139.48	11.63
MMiC	56/603	0.46	1.19	0.907	135.59	20.04

[a]*Di* – diterpenoids; [b]*Tri* – non-hopanoid triterpenoids; [c]N.D. – not determined. Note: biomarkers in the samples 28/91, 29/91, 31/91, 33/91, 34/91, 42/601, 43/601 and 50/603 have not been analysed

TABLE S-VII. The $\delta^{13}C$ values of individual diterpenoids and non-hopanoid triterpenoids of selected samples; A – 24,25-dinorlupa-1,3,5(10)-triene; B – 2,2,4a,9-tetramethyl--1,2,3,4,4a,5,6,14b-octahydropicene; N.D. – not determined

Litho-type	Sample ID	Beyer-ane	Pima-rane	16α(H)-Phyllo-cladane	Dehydro-abietane	Simon-ellite	Retene	A	B
MC	2/79	-25.3	-25.9	-26.9	-25.5	-25.9	-27.6	-28.1	N.D.[a]
MXC	3/79	N.D.	N.D.		-26.4	-26.8	-28.3	-28.9	-30.7
XC	4/79	-25.3	-25.9	-26.3	-26.4	-26.9	N.D.	-29.3	N.D.
MXC	5/79	N.D.	N.D.	N.D.	-27.0	-27.4	N.D.	N.D.	N.D.
MMiC	6/79	N.D.	N.D.	N.D.	-26.8	-26.7	N.D.	N.D.	N.D.
MXC	8/79	-26.0	-25.4	-26.9	N.D.	N.D.	N.D.	N.D.	N.D.
MMiC	11/79	-26.9	-27.4	-27.3	-25.2	-25.2	N.D.	-29.3	-30.5
XC	16/79	-27.3	-27.0	-26.7	-26.6	-27.3	-28.1	-28.2	-30.0
MXC	18/79	N.D.	N.D.	N.D.	-27.0	-27.5	N.D.	N.D.	N.D.
XC	27/91	-25.8	-26.4	-26.4	-27.4	-28.2	N.D.	-30.3	N.D.
MC	30/91	-25.1	-25.9	-26.0	-27.2	-28.1	-29.3	N.D.	-30.3
MXC	33/91	-26.0	-26.1	-26.1	-25.8	-26.2	N.D.	-29.6	N.D.
XC	34/91	-25.8	-26.1	-26.6	-26.8	-26.8	-28.1	-29.2	-29.6
XC	38/91	-26.3	-27.5	-27.8	-26.4	-26.6	-29.6	-29.0	-30.0
MC	40/91	-25.5	-26.2	-26.9	-26.7	-26.9	-27.9	-29.2	-29.8
MXC	45/601	-25.7	-26.5	-26.8	-27.0	-26.5	-28.9	-27.4	-27.8
MC	46/601	-26.1	-25.7	-26.4	-27.1	-27.3	N.D.	-28.6	-29.1
MMiC	48/601	-25.6	-25.6	-27.1	-27.2	-28.4	-28.5	-27.9	-27.9
MC	49/601	-27.0	-27.0	-27.4	-27.1	-27.7	N.D.	-27.6	-28.5
XC	50/603	-26.1	-27.1	-26.3	-27.5	-27.8	N.D.	-28.6	-28.7
MC	51/603	-25.6	-26.0	-26.9	-26.7	-25.9	-28.0	N.D.	-28.5
XC	52/603	N.D.	N.D.	N.D.	-27.2	-26.7	-30.7	-28.6	-29.9
MXC	53/603	N.D.	N.D.	N.D.	-26.2	-26.4	N.D.	-29.7	-29.8
XC	54/603	-26.9	-26.74	-27.3	-27.0	-28.1	-27.4	-28.1	-28.6
MMiC	56/603	-25.8	-26.64	-26.7	-25.5	-25.8	-28.2	N.D.	N.D.

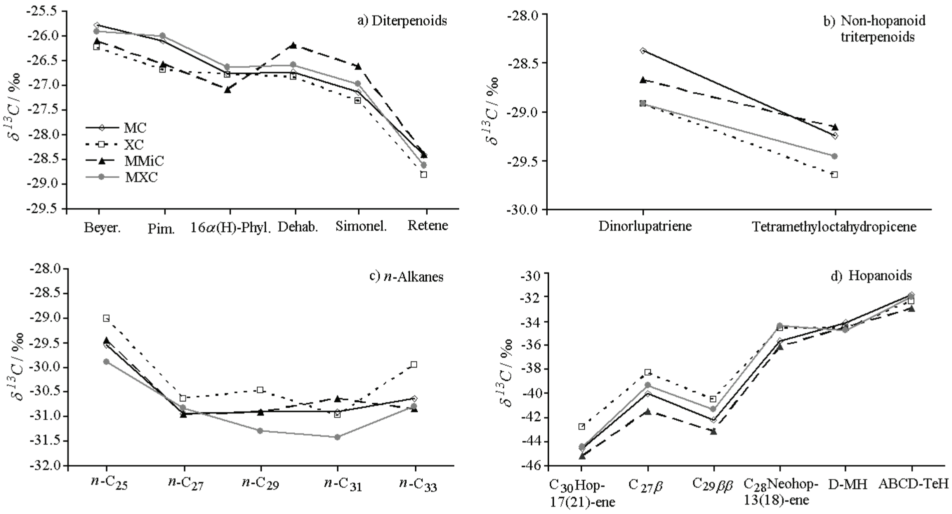

Fig. S-6. Average carbon isotopic compositions of individual biomarkers for investigated lithotypes. Beyer. – beyerane; Pim. – pimarane; 16*α*(H)-Phyl. – 16*α*(H)-phyllocladane; Dehab. – dehydroabietane; Simonel. – simonellite; Dinorlupatriene – 24,25-dinorlupa-1,3,5(10)-triene; tetramethyloctahydropicene – 2,2,4a,9-tetramethyl-1,2,3,4,4a,5,6,14b-octahydropicene; *β* designates configuration at C-17 in C_{27} hopane; *ββ* designate configurations at C-17 and C-21 in C_{29} hopane; D-MH – D-ring monoaromatic hopane; ABCD-TeH – A,B,C,D-ring tetraaromatic hopane.

TABLE S-VIII. Parameters calculated from distributions and abundances of *n*-alkanes and sterenes, and contents of main individual hopanoids, μg (g *TOC*)[-1] of lignite lithotypes; values of parameters for individual samples are given in Table S-IX of the Supplementary material

Parameter	Matrix coal (MC)				Xylite-rich coal (XC)				Mixture of matrix and mineral-rich coal (MMiC)				Mixture of matrix and xylite-rich coal (MXC)			
	Mean	Max.	Min.	*SD*	Mean	Max.	Min.	*SD*	Mean	Max.	Min.	*SD*	Mean	Max.	Min.	*SD*
CPI[a]	3.82	6.95	1.23	2.26	3.24	5.72	1.24	1.53	3.33	6.89	2.39	1.39	3.66	4.88	2.59	0.81
Proportion of C_{15}-C_{20} *n*-alkanes	0.11	0.20	0.08	0.04	0.09	0.18	0.03	0.05	0.14	0.20	0.07	0.05	0.12	0.31	0.04	0.09
Proportion of C_{21}-C_{25} *n*-alkanes	0.22	0.26	0.16	0.04	0.26	0.35	0.18	0.05	0.31	0.51	0.20	0.09	0.24	0.35	0.16	0.06
Proportion of C_{26}-C_{35} *n*-alkanes	0.67	0.76	0.57	0.06	0.65	0.73	0.56	0.06	0.55	0.70	0.36	0.09	0.65	0.80	0.46	0.10
C_{30} Hop-17(21)-ene	76.05	129.99	17.20	43.80	39.29	72.31	15.71	22.28	37.94	81.34	0.00	30.60	67.36	112.92	21.10	33.05
C_{27} 17β(H)-Hopane	18.20	45.38	7.98	13.64	7.87	13.73	3.96	3.73	23.60	107.53	2.36	33.88	15.11	27.56	6.36	7.59
C_{29} 17β(H) 21β(H)--Hopane	11.31	27.89	4.83	8.26	4.58	8.25	1.97	2.25	8.59	24.49	0.00	7.61	8.72	15.47	4.52	3.71
C_{31} 17α(H) 21β(H) 22(R)-Hopane	13.63	43.79	0.00	16.91	34.40	172.00	2.46	62.18	15.49	47.94	0.79	14.43	11.36	41.01	1.47	13.45
C_{28} 28,30-Bisnor-neo--hop-13(18)-ene	14.10	30.55	3.48	10.10	12.82	27.33	1.24	9.69	11.76	38.34	0.00	11.65	10.02	19.40	2.84	5.71
C_{27} S[b] / %	1.61	3.35	0.85	0.84	1.75	5.67	0.59	1.43	3.09	8.58	0.58	2.94	2.14	2.99	0.69	0.82
C_{28} S[c] / %	6.89	10.05	4.03	1.89	7.24	11.20	2.08	3.04	7.66	11.04	4.01	2.14	7.09	12.50	2.76	3.09
C_{29} S[d] / %	91.50	94.54	86.60	2.60	91.01	97.33	83.13	3.99	89.25	95.41	80.73	4.54	90.77	94.60	84.74	3.18

[a]*CPI* – Carbon Preference Index determined for distribution of *n*-alkanes C_{23}-C_{33}, $CPI = 1/2\ [\Sigma odd(n\text{-}C_{23} - n\text{-}C_{33})/\Sigma even(n\text{-}C_{22} - n\text{-}C_{32}) + \Sigma odd(n\text{-}C_{23} - n\text{-}C_{33})/\Sigma even(n\text{-}C_{24} - n\text{-}C_{34})]$; [b]$C_{27}\ S = 100 \times C_{27}(\Delta^2 + \Delta^4 + \Delta^5)$-Sterenes/$\Sigma(C_{27}$-$C_{29})(\Delta^2 + \Delta^4 + \Delta^5)$-Sterenes; [c]$C_{28}\ S = 100 \times C_{28}(\Delta^2 + \Delta^4 + \Delta^5)$-Sterenes/$\Sigma(C_{27}$-$C_{29})(\Delta^2 + \Delta^4 + \Delta^5)$-Sterenes; [d]$C_{29}\ S = 100 \times C_{29}(\Delta^2 + \Delta^4 + \Delta^5)$-Sterenes/$\Sigma(C_{27}$-$C_{29})(\Delta^2 + \Delta^4 + \Delta^5)$-Sterenes

TABLE S-IX. Parameters calculated from distributions and abundances of *n*-alkanes and sterenes, and contents of main individual hopanoids, μg (g *TOC*)$^{-1}$

Litho-type	Sample ID	*CPI*[a]	Proportion of C_{15}–C_{20} *n*-alkanes	Proportion of C_{21}–C_{25} *n*-alkanes	Proportion of C_{26}–C_{35} *n*-alkanes	C_{30} Hop-17(21)-ene	C_{27} 17β(H)--Hopane
MC	2/79	5.47	0.08	0.16	0.76	87.09	9.95
MXC	3/79	4.88	0.04	0.35	0.62	102.17	27.56
XC	4/79	1.67	0.03	0.23	0.73	72.31	13.73
MXC	5/79	2.59	0.04	0.16	0.80	57.75	6.36
MMiC	6/79	2.44	0.10	0.20	0.70	68.37	9.81
MXC	8/79	4.05	0.07	0.24	0.69	112.92	21.39
MMiC	11/79	4.38	0.13	0.33	0.54	35.55	10.63
XC	14/79	3.51	0.12	0.23	0.65	66.89	8.43
XC	16/79	1.24	0.06	0.28	0.66	40.77	7.38
MMiC	17/79	2.78	0.20	0.32	0.47	9.01	6.39
MXC	18/79	2.97	0.11	0.25	0.64	48.38	11.50
MMiC	19/79	3.35	0.07	0.35	0.58	81.34	19.30
MMiC	20/79	3.25	0.09	0.32	0.59	22.68	7.06
MC	26/91	N.D.[e]	0.09	0.25	0.66	129.77	45.38
XC	27/91	5.72	0.12	0.18	0.70	21.81	5.00
MC	30/91	1.23	0.14	0.23	0.62	17.20	7.98
MMiC	36/91	2.39	0.13	0.51	0.36	29.33	2.36
XC	38/91	2.86	0.07	0.27	0.66	24.16	4.76
MMiC	39/91	6.89	0.19	0.20	0.61	78.48	107.53
MC	40/91	3.06	0.08	0.18	0.73	70.82	10.01
MXC	45/601	3.26	0.14	0.19	0.66	46.45	10.83
MC	46/601	6.95	0.08	0.26	0.66	66.28	25.61
MMiC	48/601	2.45	0.18	0.28	0.53	16.72	5.49
MC	49/601	5.73	0.20	0.22	0.57	129.99	19.34
MC	51/603	1.26	0.11	0.24	0.65	31.22	9.13
XC	52/603	3.71	0.07	0.35	0.58	33.40	11.80
MXC	53/603	3.37	0.11	0.23	0.66	82.76	18.60
XC	54/603	4.85	0.18	0.26	0.56	15.71	3.96
MXC	55/603	4.67	0.31	0.23	0.46	21.10	9.51
MMiC	56/603	2.87	0.20	0.25	0.54	0.00	43.84

Lithotype	Sample ID	C_{29} 17β(H)21β-(H)-Hopane	C_{31} 17α(H)21β(H) 22(R)-Hopane	C_{28} 28.30-Bisnorneo-hop-13(18)--ene	C_{27} S[b] %	C_{28} S[c] %	C_{29} S[d] %
MC	2/79	8.87	0.00	14.60	1.43	4.03	94.54
MXC	3/79	15.47	8.73	12.04	2.64	2.76	94.6
XC	4/79	8.25	172.00	6.15	5.67	11.20	83.13
MXC	5/79	4.52	10.40	2.84	2.76	12.50	84.74
MMiC	6/79	5.32	21.21	3.90	1.69	6.23	92.08
MXC	8/79	9.41	41.01	19.40	0.69	7.48	91.83
MMiC	11/79	8.18	7.33	11.45	8.24	11.04	80.73
XC	14/79	4.02	41.11	16.67	0.71	6.29	93.00
XC	16/79	3.02	2.85	23.08	0.59	2.08	97.33

TABLE S-IX. Continued

Lithotype	Sample ID	C_{29} 17β(H)21β-(H)-Hopane	C_{31} 17α(H)21β(H) 22(R)-Hopane	C_{28} 28.30-Bisnorneo-hop-13(18)--ene	C_{27} S[b] %	C_{28} S[c] %	C_{29} S[d] %
MMiC	17/79	0.00	10.22	0.00	1.53	8.34	90.13
MXC	18/79	8.25	4.53	10.45	1.84	9.66	88.5
MMiC	19/79	10.24	22.54	15.31	1.00	7.03	91.98
MMiC	20/79	4.84	6.87	6.78	0.69	9.55	89.76
MC	26/91	27.89	43.79	30.55	N.D.	N.D.	N.D.
XC	27/91	3.47	5.31	7.93	1.33	7.40	91.26
MC	30/91	4.83	4.26	3.48	3.35	10.05	86.60
MMiC	36/91	6.02	3.88	12.94	2.56	8.92	88.52
XC	38/91	4.31	5.41	7.34	1.43	9.99	88.58
MMiC	39/91	16.22	18.66	16.31	0.58	4.01	95.41
MC	40/91	6.57	7.52	24.58	0.85	6.52	92.63
MXC	45/601	6.40	1.47	6.38	1.45	4.85	93.70
MC	46/601	15.85	2.94	9.69	0.95	5.65	93.40
MMiC	48/601	1.96	0.79	0.81	3.39	6.63	89.98
MC	49/601	10.32	5.48	11.28	1.25	6.50	92.25
MC	51/603	4.83	31.38	4.55	1.63	7.91	90.46
XC	52/603	7.05	2.46	27.33	1.72	2.88	95.40
MXC	53/603	11.08	8.88	13.87	1.84	7.41	90.76
XC	54/603	1.97	11.65	1.24	1.61	10.64	87.75
MXC	55/603	5.94	4.49	5.19	2.99	7.57	89.44
MMiC	56/603	24.49	47.94	38.34	2.68	5.52	91.80

[a]*CPI* – carbon preference index determined for distribution of *n*-alkanes C_{23}–C_{33}, *CPI* = 1/2 [Σodd(*n*-C_{23} – – *n*-C_{33})/Σeven(*n*-C_{22} – *n*-C_{32}) + Σodd(*n*-C_{23} – *n*-C_{33})/Σeven(*n*-C_{24} – *n*-C_{34})]; [b]C_{27} S = 100C_{27}(Δ^2 + Δ^4 + Δ^5)-Sterenes/Σ(C_{27}-C_{29})(Δ^2 + Δ^4 + Δ^5)-Sterenes; [c]C_{28} S = 100C_{28}(Δ^2 + Δ^4 + Δ^5)-Sterenes/Σ(C_{27}-C_{29})(Δ^2 + Δ^4 + Δ^5)-Sterenes; [d]C_{29} S = 100C_{29}(Δ^2 + Δ^4 + Δ^5)-Sterenes/Σ(C_{27}-C_{29})(Δ^2 + Δ^4 + Δ^5)-Sterenes; [e]N.D. – not determined

TABLE S-X. The $\delta^{13}C$ values of individual *n*-alkanes and hopanoids of lignite lithotypes; values of parameters for individual samples are given in Table S-XI of the Supplementary material; N.D. – not determined

Compound	Matrix coal (MC)				Xylite-rich coal (XC)				Mixture of matrix and mineral--rich coal (MMiC)				Mixture of matrix and xylite-rich coal (MXC)			
	Mean	Max.	Min.	*SD*	Mean	Max.	Min.	*SD*	Mean	Max.	Min.	*SD*	Mean	Max.	Min.	*SD*
n-C_{25}	29.5	28.2	30.2	0.7	29.0	27.2	30.2	1.0	29.4	28.9	29.8	0.5	29.9	28.9	30.5	0.8
n-C_{27}	30.9	29.4	31.6	0.8	30.6	29.1	32.0	0.9	31.0	30.6	31.5	0.4	30.8	30.5	31.0	0.3
n-C_{29}	30.9	29.4	32.0	1.0	30.5	28.9	31.8	1.1	30.9	30.8	31.0	0.1	31.3	31.1	31.7	0.3
n-C_{31}	30.9	29.5	31.8	1.0	31.0	29.7	31.8	0.9	30.6	29.2	31.3	1.2	31.4	31.3	31.5	0.1
n-C_{33}	30.6	29.4	31.5	0.8	30.0	29.0	30.9	0.8	30.8	30.4	31.1	0.4	30.8	30.3	31.4	0.5
C_{30} Hop-17(21)-ene	44.5	41.6	46.5	1.7	42.8	39.0	51.4	4.8	45.2	44.5	45.8	0.9	44.4	41.7	46.1	2.4
C_{27} 17β(H)-Hopane	40.0	37.7	41.7	1.7	38.3	36.8	39.6	1.0	41.4	38.4	43.9	2.8	39.3	37.0	42.0	2.5
C_{29} 17β(H) 21β(H)-Hopane	42.2	38.4	46.0	2.7	40.5	38.0	45.1	2.7	43.1	41.4	44.0	1.4	41.3	38.3	45.2	3.5
C_{31} 17α(H)21β(H) 22(R)-Hopane	26.5	25.7	27.3	1.2	25.3	24.2	26.1	0.9	26.1	26.1	26.1	N.D.	27.5	27.5	27.5	N.D.
C_{28} 28,30-Bisnor-neohop-13(18)-ene	35.6	33.6	36.6	1.3	34.6	34.1	35.8	0.8	36.1	36.1	36.1	N.D.	34.4	33.8	35.3	0.8
D-ring mono-aromatic hopane	34.1	32.9	36.5	1.6	34.6	32.4	38.0	2.0	34.5	34.5	34.5	N.D.	34.8	32.7	37.5	1.7
ABCD-ring tetra-aromatic hopane	31.8	30.9	34.1	1.2	32.3	30.1	34.4	1.7	32.9	31.3	34.5	2.3	32.0	30.3	33.3	1.5

TABLE S-XI. The $\delta^{13}C$ values of individual *n*-alkanes and hopanoids of selected samples

Litho-type	Sample ID	*n*-C_{25}	*n*-C_{27}	*n*-C_{29}	*n*-C_{31}	*n*-C_{33}	C_{30} Hop-17(21)-ene
MC	2/79	-30.2	-31.5	-31.7	-31.8	-30.2	-44.9
MXC	3/79	N.D.[a]	N.D.	N.D.	N.D.	N.D.	N.D.
XC	4/79	-29.7	-31.4	-31.2	-31.7	-30.5	-39.0
MXC	5/79	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
MMiC	6/79	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
MXC	8/79	-30.2	-30.9	-31.1	-31.5	-31.3	-41.7
MMiC	11/79	-29.7	-30.6	-30.9	-29.2	-31.0	-45.8
XC	16/79	-27.2	-29.1	-28.9	-29.7	-29.0	-39.9
MXC	18/79	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
XC	27/91	-29.1	-30.7	-30.6	-31.4	-30.2	-39.1
MC	30/91	-29.7	-30.7	-30.0	-30.2	-29.4	-41.6
MXC	33/91	-30.5	-31.0	-31.7	N.D. [a]	-30.7	-46.1
XC	34/91	-30.2	-31.0	-30.9	-31.6	-29.5	-47.4
XC	38/91	-28.8	-30.1	-30.6	-30.8	-30.4	-40.3
MMiC	39/91	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
MC	40/91	-30.2	-31.6	-32.0	N.D.	-31.4	-46.5
MXC	45/601	-28.9	-30.5	-31.1	-31.3	-30.3	-45.5
MC	46/601	-28.2	-29.4	-29.4	-29.5	-30.6	-45.5
MMiC	48/601	-29.8	-31.5	-31.0	-31.3	-30.4	-44.5
MC	49/601	-29.3	-31.5	-31.6	-31.7	-30.6	-44.7
XC	50/603	-29.0	-30.2	-29.2	-29.7	-29.0	-42.4
MC	51/603	-29.7	-30.9	-30.8	-31.3	-31.5	-44.0
XC	52/603	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
MXC	53/603	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
XC	54/603	N.D.	-31.9	-31.8	-31.8	-30.9	-51.3
MMiC	56/603	-28.9	-30.8	-30.8	-31.3	-31.1	N.D.
Litho-type	Sample ID	C_{27} 17β(H)-Hopane	C_{29} 17β(H)21β(H)-Hopane	C_{31} 17α(H)21β(H)22(R)-Hopane	C_{28} 28,30-Bisnor-neohop-13(18)-ene	D-ring monoaromatic hopane	ABCD-ring tetraaromatic hopane
MC	2/79	-41.3	-44.3	N.D.[a]	-35.0	N.D.	-34.1
MXC	3/79	N.D.	N.D.	N.D.	N.D.	-34.4	N.D.
XC	4/79	-36.8	-38.0	-25.9	N.D.	-32.3	N.D.
MXC	5/79	N.D.	N.D.	N.D.	N.D.	-37.5	N.D.
MMiC	6/79	N.D.	N.D.	N.D.	N.D.	-32.5	N.D.
MXC	8/79	-37.0	-38.3	-27.5	-34.0	N.D.	N.D.
MMiC	11/79	-43.9	-44.0	N.D.	-36.1	N.D.	-31.3
XC	16/79	-38.4	-39.0	N.D.	-34.3	-36.0	-33.3
MXC	18/79	N.D.	N.D.	N.D.	N.D.	-34.9	-33.3
XC	27/91	N.D.	N.D.	N.D.	N.D.	-33.3	-31.3
MC	30/91	-38.7	-40.7	-25.7	-36.3	-33.2	N.D.
MXC	33/91	-42.0	-45.2	N.D.	-35.3	-33.4	N.D.
XC	34/91	-38.4	-45.1	N.D.	-34.1	-35.0	-31.1
XC	38/91	-38.2	-39.8	-26.1	-34.1	-33.1	-30.1
MMiC	39/91	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.

TABLE S-XI. Continued

Litho-type	Sample ID	C_{27} 17β(H)-Hopane	C_{29} 17β(H)21β(H)-Hopane	C_{31} 17α(H)21β(H)22(R)-Hopane	C_{28} 28,30-Bisnor-neohop-13(18)-ene	D-ring monoaro-matic hopane	ABCD-ring tetraaro-matic hopane
MC	40/91	-41.3	-46.0	N.D.	-36.5	N.D.	-32.0
MXC	45/601	-39.0	-40.5	N.D.	-33.8	-32.7	-30.3
MC	46/601	-37.7	-38.4	N.D.	-33.6	-32.9	-30.9
MMiC	48/601	-42.0	-43.8	N.D.	N.D.	N.D.	N.D.
MC	49/601	-41.7	-42.6	N.D.	-36.6	-33.7	-31.0
XC	50/603	-39.6	-40.4	-25.2	-35.8	-32.8	N.D.
MC	51/603	-38.9	-40.8	-27.3	N.D.	-36.5	-31.3
XC	52/603	N.D.	N.D.	N.D.	N.D.	-38.0	-32.7
MXC	53/603	N.D.	N.D.	N.D.	N.D.	-35.8	-32.3
XC	54/603	N.D.	N.D.	-24.2	N.D.	-35.9	-34.4
MMiC	56/603	-38.4	-41.4	-26.1	N.D.	N.D.	-34.5

[a]N.D. – not determined

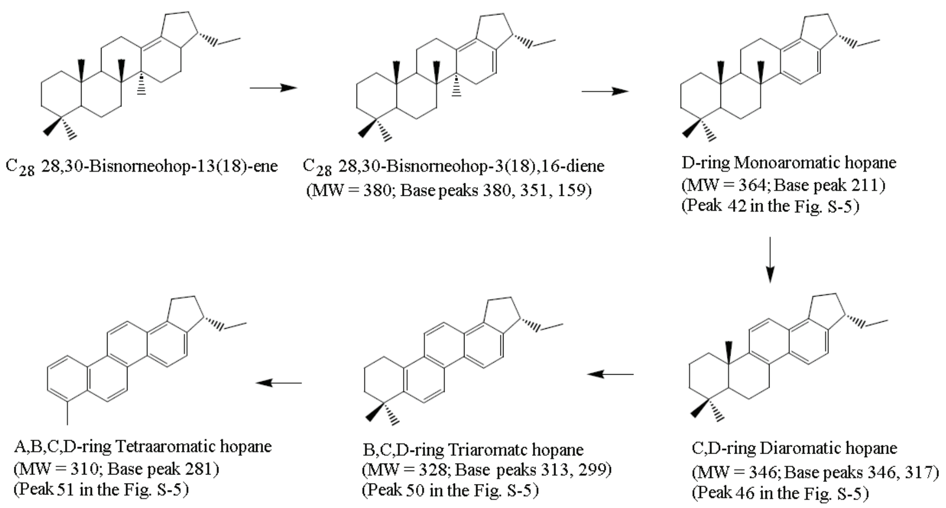

Fig. S-7. Diagenetic scheme showing the formation of series of orphan aromatic hopanoids bearing an ethyl group at C-21 from the C_{28} 28,30-bisnorneohop-13(18)-ene.

REFERENCES

1. http://www.iccop.org/documents/1993-iccp-international-handbook-of-coal-petrography-3rd-suppl-to-2nd-ed-pdf.pdf (last accessed November 21, 2016)
2. D. Mitrović, N. Đoković, D. Životić, A. Bechtel, A, Šajnović, K. Stojanović, *Int. J. Coal Geol.* **168** (2016) 80
3. I. Sykorovà, W. Pickel, K. Christanis, M. Wolf, G.H. Taylor, D. Flores, *Int. J. Coal Geol.* **62** (2005) 85

4. G.H. Taylor, M. Teichmüller, A. Davis, C.F.K. Diessel, R. Littke, P. Robert, *Organic Petrology*, Gebrüder Borntraeger, Berlin, 1998
5. International Committee for Coal Petrology (ICCP), *Fuel* **80** (2001) 459
6. K. Stojanović, D. Životić, A. Šajnović, O. Cvetković, H.P. Nytoft, G. Scheeder, *J. Serb. Chem. Soc.* **77** (2012) 1109
7. D. Životić, K. Stojanović, I. Gržetić, B. Jovančićević, O. Cvetković, A. Šajnović, V. Simić, R. Stojaković, G. Scheeder, *Int. J. Coal Geol.* **111** (2013) 5
8. N. Đoković, D. Mitrović, D. Životić, D. Španić, T. Troskot-Čorbić, O. Cvetković, K. Stojanović, *J. Serb. Chem. Soc.* **80** (2015) 575
9. M. Radke, H. Willsch, D.H. Welte, *Anal. Chem.* **52** (1980) 406.