

29. BITUMINOLOGICAL STUDIES OF THE SAMPLES FROM SITE 379 AND LABORATORY SIMULATION OF DISPERSED ORGANIC MATTER TRANSFORMATION¹

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INTRODUCTION

The studies of bitumoids from the Black Sea sediments are of great interest because these sediments are regarded by most geologists as recent analogs of the oil-producing facies of the past. The analyses of 23 samples from the cores taken at Site 379 were made at the Laboratory of Oil and Gas Prospecting of the Sea Regions of the P. P. Shirshov Institute of Oceanology, the USSR Academy of Sciences. A list of the samples is given in Table 1. Five samples were analyzed in triplicate, two samples were stored in a special fluorine plastic capsule for further laboratory simulation of the oil and gas formation processes. Such simulation, though not giving a full reproduction of the complicated natural processes, makes it possible to evaluate the trend of a catagenic transformation of dispersed organic matter and to study the products generated during the experiment.

CHARACTERISTICS OF BITUMOID "A"

Experimental Methods and Procedure

Bitumoid "A" was extracted from the sediment by a consecutive extraction with chloroform (chloroform bitumoid "A" - A_{chl}) and alcohol-benzene (alcohol-benzene bitumoid "A" - A_{alb}).

The fractional composition of the bitumoids (6-15 mg) was determined by absorption chromatographic analyses on silica gel columns (AKS, acid washed, 100-200 mesh; dimensions 15 cm × 0.5 cm). Solvent was removed from the eluting fractions with a nitrogen stream.

Elution was carried out first with hexane for 30 minutes to give a hydrocarbon (HC) fraction, then with benzene to give a "benzene resin" fraction. Most of the condensed ring hydrocarbons were found in the benzene resin fraction. The benzene elution was continued until disappearance of color from the eluting solvent. An "acid resin" fraction remaining on the silica gel was desorbed with alcohol benzene (1:1) to give an "alcohol-benzene" resin fraction.

Infrared spectra were obtained on carbon tetrachloride (CCl_4) solutions in NaCl cuvettes using a scanning Hilger spectrometer in the range from 1800 to 900 cm^{-1} . Simultaneously the IR spectra were recorded on a punched tape and then treated on the digital computer.

TABLE 1
List of Samples Examined

No	Core	Section	Sediment Depth (m)
Hole 379			
1	1	CC	0-7.0
2	5 ^a	3	73.5-83.0
3	7	CC	121.0-130.5
4	8	CC	130.5-140.0
5	9	CC	149.5-159.0
Hole 379A			
6	21	1	187.5-197.0
7	25	4	225.5-235.0
8	27	4	244.5-254.0
9	29	4	263.5-273.0
10	31	6	282.5-292.0
11	34	3	311.0-320.5
12	34	CC	311.0-320.5
13	35 ^a	5	320.5-330.0
14	36	5	330.0-339.5
15	37	CC	339.5-349.0
16	43	3	387.0-396.5
17	47 ^a	0	425.0-434.5
18	51	0	463.0-472.5
19	54		491.5-501.0
20	57 ^a	CC	520.0-529.5
21	59	3	539.0-548.5
22	65	4	586.5-596.0
23	68 ^a	6	615.0-624.5

^a Triplicate samples chosen for simulating.

UV-spectra were obtained on a scanning "Specord" instrument, "Carl Zeiss," Jena, DDR using a quartz cuvette (2 ml; 1 cm thick). The scanning range was 5400 to 16,000 cm^{-1} .

Data on the composition of paraffin hydrocarbons in the paraffin-naphthene fractions were obtained by means of gas-liquid chromatography. The analyses were performed on a Pye gas chromatograph with the use of a 25 meter Apiezon L capillary column with temperature programming from 125° to 300°C.

Results and Preliminary Discussion

Organic matter content of the section is fairly constant and ranges from 0.40% to 1.43%, except for Sample 29 in which it is 3.79% (Table 2). Carbonate content of the sediments varies from 2.74% to 15.28%.

The physical properties of the bitumoid A_{chl} and A_{alb} extracts are different. The concentrate from the chloroform extract is light colored, solid, waxy; the solid residue from the alcohol-benzene extract is dark brown to black, resinous, solid. Both extracts are rich

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TABLE 2
Bituminological Characteristics of Organic Matter of Sediments

Sample	Depth, (m)	C _{org}	CO ₂	OM (percent) K = 1.76	% in OM		Σ Achl+ Aalb	A chl		Σ A in OM %	HC in %			
					Achl	Aalb		Aalb	βchl ^a		Achl	Aalb	OM	Sedi-ment
1	0-7	0.48	6.50	0.84	1.79	1.79	3.58	1.00	3.13	3.58	29.82	21.05	0.91	0.0076
5	73.5-83.0	0.50	3.13	0.88	2.27	0.01	2.28	0.50	2.00	2.38	10.00	2.00	0.06	0.0005
7	121.0-130.5	0.34	7.36	0.60	3.17	3.00	6.17	1.05	5.89	6.17	16.88	3.57	0.56	0.0034
8	130.5-140.5	0.47	8.45	0.83	—	3.25	—	—	—	—	—	4.76	—	—
9	149.5-159.0	0.59	2.74	1.04	—	6.70	—	—	—	—	—	0.96	—	—
20	187.5-197.0	0.52	7.50	0.92	3.59	3.37	6.96	1.06	6.35	6.96	12.82	4.54	0.61	0.0056
25	225.5-235.0	0.66	4.06	1.16	1.90	0.43	2.33	4.40	3.33	2.33	12.24	4.88	0.30	0.0035
27	244.5-254.0	0.62	5.12	1.09	3.26	1.01	4.27	2.73	4.84	4.27	17.50	4.76	0.63	0.0068
29	263.5-273.0	2.15	4.45	3.79	5.29	2.65	7.94	2.00	9.30	7.94	4.27	2.70	0.32	0.0121
31	282.5-292.0	0.46	4.32	0.81	—	—	—	—	—	—	—	—	—	—
34 (CC)	311.0-320.5	0.45	10.54	0.79	2.15	3.42	5.57	0.63	3.78	5.57	5.10	8.54	0.40	0.0031
34 (3)	311.0-320.5	0.50	10.70	0.88	1.25	0.91	2.16	1.38	2.20	2.16	16.13	4.44	0.24	0.0021
35	320.5-330.0	0.42	10.57	0.74	0.68	2.30	2.98	0.29	1.19	2.98	16.67	7.35	0.28	0.0021
36	330.0-339.5	0.37	8.68	0.65	2.31	1.85	4.16	1.25	4.05	4.16	23.33	2.14	0.58	0.0037
37	339.5-349.0	0.57	4.02	1.00	1.20	0.47	1.67	0.60	2.10	1.67	16.67	3.45	0.22	0.0022
43	387.0-396.5	0.23	7.42	0.40	0.50	2.50	3.00	0.20	0.87	3.00	—	6.82	—	—
47	425.0-434.5	0.44	9.29	0.77	1.56	1.95	3.51	0.80	2.73	3.51	26.19	5.0	0.51	0.0039
51	463.0-472.5	0.27	7.91	0.48	2.08	2.90	4.98	0.71	3.70	4.98	18.18	1.45	0.42	0.0020
54	491.5-501.0	0.35	10.65	0.62	1.13	2.58	3.71	0.44	2.00	3.71	5.55	1.18	0.09	0.0005
57	520.0-529.5	0.45	15.06	0.79	2.15	3.42	5.57	0.63	3.78	5.57	8.22	3.90	0.31	0.0024
59	539.0-548.5	0.44	11.56	0.77	2.21	0.78	2.99	2.83	3.86	2.99	3.70	2.20	0.10	0.0006
65	586.5-596.0	0.52	5.26	0.92	1.41	2.93	4.34	0.48	2.50	4.34	15.69	2.86	0.22	0.0020
68	615.0-624.5	0.81	15.28	1.43	2.80	1.82	4.62	1.54	4.94	4.62	6.94	4.81	0.28	0.0040

$${}^a\beta_{chl} = \frac{\text{Achl (sediment)} 100}{\text{C}_{org}}$$

in elemental sulfur, and the alcohol-benzene extract contains a large amount of mineral salts.

Bitumoid "A" accounts for 1.67% to 7.94% of the organic carbon, the highest quantity being found in the samples with average organic carbon values (Figure 1). No relationship is apparent between the concentration of bitumoid "A" and the depth of the sample. The concentration of the bitumoid and its fractional composition depend to a high degree on the initial type of organic matter and its earlier transformations. Table 2 shows that A_{chl} concentration is insignificant (from 0.5% to 5% of the organic matter) and bitumoid "A" is represented mainly by the alcohol-benzene extract of the "acid resin" components,

$$\frac{A_{chl}}{A_{alb}} < 1, \beta = \frac{A_{chl} (\text{sediment}) \times 100}{C_{org}} = 0.8 - 6.0,$$

except for Sample 29,

where $\beta_{chl} = 9.30$.

These data may be indicative, on one hand, of a low level transformation of organic matter, and, on the other hand, of organic matter that underwent a long oxidation in the water column.

The bitumoids A_{chl} and A_{alb} differ in fractional composition (Table 3). A_{chl} is composed mainly of resins material² (70%-96%) with an appreciable prevalence of acid alcohol-benzene resins over benzene resins ([benz.res.]/[alc/benz.res.] = 0.07-0.67). Asphaltenes are absent in the group composition of

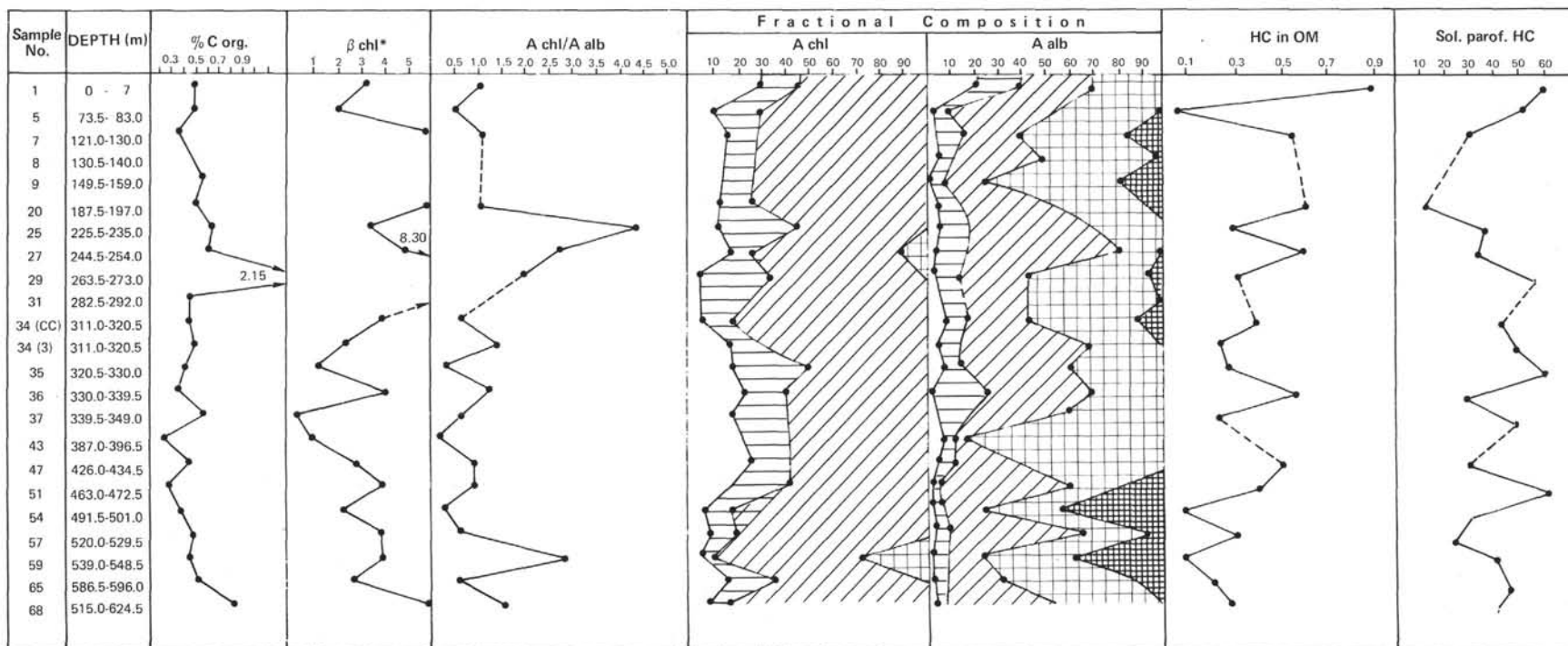
A_{chl}, except for Samples 27 and 59 (Figure 1). The latter samples were found to contain a rather high A_{chl}/A_{alb} ratio (about 3), a high concentration of alcohol-benzene resins in A_{chl} which is much in excess of benzene resins ([benz.res.]/[alc/benz.res.] = 0.12-0.08). However, Samples 27 and 59 differ sharply from each other in A_{alb} composition. In the first sample the A_{alb} composition is represented by resin components (resins/asphaltenes = 4.13), and in the second sample, by asphaltenes and a fraction insoluble in chloroform (resins/asphaltenes = 0.26).

Based on the IR spectrometric data, benzene and alcohol-benzene resins of these samples differ considerably in the relationships between separate structural fragments (Table 4). As shown in Table 4, benzene and alcohol-benzene resins of both samples are rich in oxygen-containing groups in the form of acids, ethers and ketones, associated mainly with aliphatic structures. However, a relatively high content of carbonyl is noted in Sample 59 as related to aromatic rings (absorption band—1670 cm⁻¹), and a high proportion of aromatic structures, especially in alcohol-benzene resins. According to the UV spectrometric data (Table 5), the aromatic structures of this sample are of a more condensed character than those of Sample 27 and are represented by anthracene and phenanthrene derivatives.

Benzene resins are the major source of the aromatic structures in Sample 27 represented mainly by benzene and naphthalene derivatives and to a lesser extent by anthracene and phenanthrene.

The above-mentioned similarity and differences in the composition of A_{chl} and A_{alb} of bitumoids and in the structure of benzene and alcohol-benzene resins of these samples may be attributed to either the similar

²Resins material = benzene resins + alc-benz resins where benzene resins and alcohol-benzene resins are materials eluted from the silica gel column with benzene and benzene-alcohol, respectively.



$$*\beta \text{ chl} = \frac{(\text{A chl/lq sediment}) \cdot 100}{\text{C org}}$$

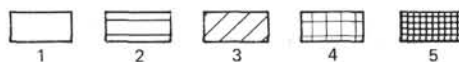


Figure 1. Distribution of C_{org} and bitumoid components in the samples from the section. (1) hexane fraction; (2) benzene resins; (3) alcohol-benzene resins; (4) asphaltenes; (5) chloroform insoluble fraction.

TABLE 3
Fractional Composition of Bitumoid "A"

Sample	Benzene Resins								Alcohol-Benzene Resins							
	Absorption (cm ⁻¹)															
	1740	1710	1670	1600	1470	1380	1115	1030	1740	1710	1670	1600	1470	1380	1115	1030
1	1.50	1.10	0.40	14.30	9.00	12.30	4.50	23.00	1.57	2.64	0.89	12.95	7.14	8.93	3.10	60.87
5	0.90	1.26	—	8.60	6.70	6.30	8.30	9.20	1.43	1.79	0.46	8.21	6.71	10.27	5.00	60.44
7	1.00	0.15	—	11.32	7.79	1.40	7.30	12.13	1.57	1.86	0.68	10.23	7.79	12.73	4.35	28.49
20	0.51	1.20	1.21	15.80	4.30	10.10	4.80	22.60	0.89	1.39	0.36	4.69	4.57	7.67	1.85	9.64
25	2.10	2.00	0.82	13.60	10.29	12.33	5.05	28.13	1.57	3.00	1.07	22.95	5.93	15.00	4.68	3.65
27	5.10	8.60	5.17	76.97	30.21	47.47	15.73	—	2.43	3.64	0.89	14.92	9.86	9.40	3.00	8.27
29	0.79	1.96	0.21	5.50	6.50	5.50	1.60	8.90	2.04	5.04	1.61	22.68	20.71	21.00	6.18	8.27
34 (CC)	1.07	0.46	0.25	0.65	3.60	6.60	0.87	1.98	2.50	2.86	0.46	3.16	7.71	16.40	5.68	10.40
34 (3)	0.43	0.36	0.25	4.70	2.76	2.90	1.05	7.07	1.68	2.53	—	—	7.93	—	—	6.69
35	2.40	3.30	1.75	4.29	15.14	24.07	15.73	43.24	2.07	2.64	0.79	17.70	7.29	16.47	2.83	42.69
36	4.40	2.60	1.39	33.77	17.86	4.47	13.55	59.80	—	—	2.84	36.06	10.29	19.07	7.00	46.73
37	0.53	0.50	0.64	16.07	5.28	12.33	5.45	31.25	1.94	2.75	0.79	16.19	9.64	14.40	—	35.75
47	2.90	3.40	1.46	44.87	14.29	20.13	4.63	47.98	3.29	1.96	0.71	17.77	8.79	6.73	4.18	27.73
51	1.90	1.30	0.36	14.39	4.57	6.47	2.38	12.40	2.23	4.04	0.71	11.08	7.71	10.47	2.93	7.69
54	1.40	1.30	1.61	21.50	8.00	18.20	12.20	32.50	1.50	2.14	0.79	12.31	7.86	11.40	4.50	—
57	2.76	5.01	1.25	56.62	18.93	28.30	7.00	6.00	1.00	1.36	0.29	3.58	4.07	5.67	1.28	5.04
59	8.20	16.10	8.61	29.09	71.64	61.40	10.13	8.76	11.43	23.57	4.46	51.04	58.57	53.33	20.25	—
65	2.70	3.57	1.68	35.52	13.00	19.80	10.50	44.40	0.18	3.00	0.14	—	9.21	—	8.03	36.53
68	1.25	1.60	1.68	20.91	8.43	—	6.00	22.40	0.75	1.18	0.36	6.36	3.57	5.20	0.88	4.91

TABLE 4
Molar Relationships of Functional Groups in Chromatographic Fractions of Bitumoid A_{chl}

Sample	A chl, %					Σ resins	A alb, %					Σ resins	Benz. z. A.-b. res.	Σ asph.+ unsol.	Σ asph. + unsol.	
	HC	Benz. resins	Alc.-benz. resins	Asphal.	Σ resins		Benz. res. A.-b. res.	HC	Benz. resins	Alc.-benz. resins	Asph.					Fraction unsol. in Chlorof.
1	29.82	15.79	54.39	—	70.18	0.29	21.05	19.30	31.58	21.05	7.02	50.88	0.61	27.07	1.88	
5	10.00	20.00	70.00	—	90.00	0.28	2.00	7.00	45.00	46.00	—	52.00	0.16	46.00	0.88	
7	16.88	11.69	71.43	—	83.12	0.16	3.57	13.10	21.12	47.62	14.29	34.22	0.62	61.91	0.55	
8	—	—	—	—	—	—	4.76	6.35	38.10	50.79	—	44.45	0.17	50.79	0.86	
9	—	—	—	—	—	—	0.96	5.74	17.18	48.80	17.22	22.92	0.33	66.02	0.35	
20	12.82	12.82	74.36	—	87.18	0.17	4.57	10.61	43.94	37.88	3.03	54.55	0.24	40.91	1.33	
25	12.24	30.61	57.15	—	87.76	0.54	4.88	14.63	53.66	26.83	—	68.29	0.27	26.83	2.55	
27	17.50	17.50	63.50	12.50	71.00	0.12	4.76	11.90	64.77	18.57	—	76.67	0.18	18.57	4.13	
29	4.27	29.89	65.84	—	95.73	0.45	2.70	10.81	28.38	52.03	6.08	39.19	0.38	58.11	0.67	
31	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	
34 (CC)	5.10	11.84	83.06	—	94.90	0.14	8.54	8.54	26.82	45.12	10.98	35.36	0.32	56.10	0.63	
34 (3)	16.13	12.90	70.97	—	83.87	0.18	4.44	8.88	55.57	31.11	—	64.45	0.16	31.11	2.07	
35	16.67	33.33	50.00	—	83.33	0.67	7.35	7.35	44.12	41.18	—	51.47	0.17	41.18	1.25	
36	23.33	16.67	60.00	—	76.67	0.28	2.14	25.12	42.38	30.36	—	67.50	0.59	30.36	2.22	
37	16.67	25.00	58.33	—	83.33	0.43	3.45	12.07	40.41	44.07	—	52.48	0.30	44.07	1.19	
43	—	—	—	—	—	—	6.22	4.55	2.27	86.36	—	6.82	—	86.36	—	
47	26.19	16.67	57.14	—	73.81	0.29	5.00	6.67	30.00	58.33	—	36.67	0.22	58.33	0.63	
51	18.18	22.73	59.09	—	81.82	0.38	1.45	1.45	57.97	21.74	17.39	59.42	0.03	39.13	1.52	
54	5.55	11.11	83.34	—	94.45	0.13	1.18	4.71	15.29	31.76	47.06	20.00	0.31	78.82	0.25	
57	8.22	10.96	80.82	—	91.78	0.14	3.90	4.68	57.04	34.38	—	61.72	0.08	34.38	1.80	
59	3.70	64.94	62.96	28.40	67.90	0.08	2.20	5.55	14.47	38.89	38.89	20.02	0.38	77.78	0.26	
65	15.69	23.53	60.78	—	84.31	0.39	2.86	4.76	22.85	58.10	11.43	27.61	0.21	69.53	0.40	
68	6.94	6.25	86.81	—	93.06	0.07	4.81	2.88	51.93	40.38	—	54.81	0.06	40.38	1.36	

conditions of organic matter transformation, or to the differences in organic matter's initial composition.

These samples differ considerably from one another in the content of the "hydrocarbon" fraction or hexanecluant (Sample 27; 29%, Sample 59; 6%). However, the composition of these samples, according to the gas-liquid chromatography and mass spectrometry, is very similar (Tables 6, 7).

The paraffin-naphthene fraction was found to contain solid high-molecular weight paraffins with the number of carbon atoms in a molecule from C₁₇ to C₃₅ with clear-cut maxima in the regions of C₂₇, C₂₉, and C₃₁, and with a noticeable predominance of the normal structure hydrocarbons (more than 95%) over iso-paraffins. The n-alkanes series is characterized by a predominance of n-alkanes with an odd number of carbon atoms in molecules; the odd/even ratio ranges from 1.08 to 2.35 (Table 6). All the samples were found to contain pristane and phytane; the ratio of pristane to phytane ranges from 0.30 to 0.93.

Paraffin hydrocarbons comprise from 25% to 59% in the paraffin-naphthene fraction (Table 7), i.e., amounts of paraffin hydrocarbons vary widely and, as seen from Figure 1, do not show any dependence on sediment depth. The surface sediments are characterized by the highest content of paraffin hydrocarbons (Sample 1, depth 0-7 m).

Among cyclic hydrocarbons, 1-6-ring structures with a predominance of mono-, bi-, and tricyclic ones were distinguished.

Such a composition of the "hydrocarbon" fraction is evidently determined by the facial and ecological peculiarities of the sedimentation and early diagenesis stages.

Interesting data were obtained for Sample 47 (depth 425-434 m). Despite the low level of the transformation of organic matter ($A_{chl}/A_{alb}=0.97$), the sum of "hydrocarbons" per bitumoid "A" is rather large (31%, 26% of them in A_{chl}). The composition of A_{chl} was found to lack asphaltenes, and A_{alb} contains no

TABLE 5
Relative Content of Aromatic Structures in Resins of Bitumoid "A" Based on UV-Spectroscopic Data (internal standard)

Sample	Benzene Resins					Alcohol-Benzene Resins				
	Sulfides	Thiophenes	Naphthalenes	Benzenes	Anthracenes	Sulfides	Thiophenes	Naphthalenes	Benzenes	Anthracenes
1	4.2	4.3	3.8	3.9	—					
5	3.6	2.9	—	2.1	—	3.3	4.4	3.8	2.7	3.8
7	13.3	—	14.8	11.1	—					
8						9.7	9.4	7.8	5.4	7.5
9						6.8	—	5.6	3.6	5.4
20	7.0	4.4	7.6	5.4	—					
25	3.6	2.6	—	—	2.0					
27	21.0	28.6	30.8	—	32.6					
29	1.0	1.0	1.0	—	1.0					
34 (CC)	4.1	5.7	—	2.9	8.0	5.3	6.7	5.9	4.4	6.2
34 (3)	3.1	4.1	4.2	—	4.0					
35	8.1	11.9	11.4	—	—	14.3	—	12.2	—	—
36	15.8	18.6	16.7	8.6	12.0					
37	2.8	—	2.7	1.3	3.8	11.0	—	10.9	6.7	9.4
47	6.5	7.6	6.6	—	15.2	1.5	—	1.9	1.3	—
51	6.6	7.1	—	—	5.6					
54	1.3	1.9	1.7	1.0	1.4	6.4	8.6	7.5	6.8	9.5
57	7.0	—	—	4.3	7.0	2.0	8.7	7.4	6.3	—
59	4.7	5.7	—	6.1	—	23.6	30.0	27.7	18.6	26.0
65	5.7	6.1	—	3.0	4.2	5.8	7.1	—	—	4.0
68	7.6	8.6	6.2	4.4	6.2	1.6	—	1.4	—	—

chloroform insoluble fraction. The same sample was found to have a relatively high content of heavy hydrocarbon gases ($C_2 + C_3$, Table 8) of which the saturated ones are much in excess of the unsaturated ones (sat./unsat.=55.6).

The paraffin-naphthene fraction has a relatively high percentage of paraffin hydrocarbons (58.4%) among which n-alkanes with the odd number of carbon atoms in a molecule are much in excess of n-alkanes with the even number of carbon atoms (odd/even=2.47), and a low percentage of naphthenes (38.9%) with the predominance of mono- and tricyclic structures.

According to the infrared spectra, benzene and alcohol-benzene resins of Sample 47 contain small amounts of oxygen-containing groups which are associated, as a rule, with the aliphatic structures. Benzene resins have the major content of the aromatic structures and the latter, based on the UV spectroscopic data, are represented primarily by benzene and naphthalene derivatives. Polynuclear aromatic structures have not been detected.

The organic matter in Sample 47 is likely to be rich in the lipid components. Its transformation evidently proceeded in the reducing environment.

Sample 1 taken from a depth of 0-7 m, i.e., from the intensive fermentation-microbial activity zone, stands noticeably apart based on the bituminological characteristics. A comparatively high percentage of β_{chl} is noted (3.13) (Table 2) together with an organic matter content of 0.84%. The bitumoid "A", as in the rest of the samples, is represented mainly by resins in which alcohol-benzene resins dominate over benzene ones. Asphaltenes are absent in A_{chl} . In A_{alb} they comprise 21.05%. However, Sample 1 differs considerably from the others in the composition and structure of some of the fractions. The greatest amount of "hydrocarbons", comprising 0.91% of the organic matter, has been found in this sediment. Among the

"hydrocarbons," n-alkanes are predominant (59.2%) of which low carbon number ($C_{17}-C_{24}$) ones amount to over 50% (Tables 6 and 7). Paraffin hydrocarbons contain almost equal amounts ($[i C_{19}]/[i C_{20}]=0.93$) of pristane and phytane. The ratio of odd to even n-alkanes is 1.08.

The IR spectra of the samples show no sharp difference between the benzene and the alcohol-benzene resin fractions: oxygen-containing groups play a significant part in the composition of both fractions. These groups are represented mainly by acids, ethers, and ketones associated with the aliphatic structures. Carbonyl associated with the aromatic structures are contained in a greater proportion in benzene resins than in alcohol-benzene resins.

A rather high content of the naphthene-aromatic and aromatic structures is noted in benzene and alcohol-benzene resins (Table 4). The aromatic fragments, based on the UV spectroscopic data, are represented mainly by benzene and naphthalene derivatives and, to a much lesser extent and not in all the samples, by anthracene and phenanthrene derivatives. More condensed aromatic structures were not found.

The established value of the odd coefficient close to zero (as in oil), as well as the high content of paraffins in the paraffin-naphthene fraction, can serve as evidence of the biochemical process of the formation of paraffin hydrocarbons at the sedimentogenesis and early diagenesis stages.

SIMULATION OF THE TRANSFORMATION OF DISPERSED ORGANIC MATTER

The reproduction of the natural geochemical processes, especially of oil and gas formation, in the laboratory entails certain difficulties. The kinetics of these processes are such that to reproduce them to the full extent in short experimental times is impossible. For instance, an intensive temperature effect may

TABLE 7
Composition of Paraffin-Naphthene Fraction of Hydrocarbons
(based on mass spectrometry data, ratio in %)

Sample	Paraffin Hydrocarbons	Naphthene Hydrocarbons						Alkylbenzenes
		one-ring	two-ring	three-ring	four-ring	five-ring	six-ring	
1	59.2	10.2	7.4	11.3	4.0	3.1	3.3	1.5
5	52.8	14.0	5.3	12.1	5.3	3.2	2.2	5.1
7	32.7	23.7	7.3	22.9	3.1	3.3	2.3	4.5
20	12.4	49.2	4.3	22.4	3.1	3.4	1.2	4.0
25	37.7	14.6	12.4	17.6	6.2	4.7	2.0	4.8
27	36.6	25.4	8.1	20.3	4.4	1.2	1.0	2.9
29	54.7	5.9	8.5	18.4	3.3	1.5	1.2	6.5
34 (cc)	42.0	11.65	13.1	20.9	3.8	2.7	1.6	4.4
34 (3)	45.8	8.3	25.1	6.5	5.2	5.5	2.4	1.2
35	49.0	19.6	5.4	14.2	3.5	3.1	1.6	3.6
36	26.5	20.4	9.8	15.6	4.2	3.8	1.9	11.8
37	50.1	14.1	6.0	16.9	3.8	3.8	1.4	3.9
47	28.4	16.2	5.1	22.3	4.9	3.5	3.8	15.8
51	48.3	20.2	5.3	1.3	4.2	3.9	1.6	5.2
54	28.9	15.5	11.3	24.7	9.4	4.2	2.6	3.4
57	25.3	33.8	3.8	11.3	10.3	6.4	5.5	3.6
59	40.7	6.4	14.2	20.3	11.0	4.4	2.0	1.0
65	42.8	13.6	11.2	18.1	4.2	3.1	1.9	5.3
68	36.9	8.3	8.0	15.2	12.4	6.5	5.3	7.4

TABLE 8
Composition of Gases Liberated During the Experiment

Sample	Condi-tions	CO ₂ cm ³ /kg of sediment	Hydrocarbonic Gases, (cm ³ /kg of sediment X 10 ⁻⁴)							Σ satur.		Σ unsatur.
			CH ₄	C ₂ H ₆	C ₂ H ₄	C ₃ H ₈	C ₃ H ₆	heavy HC	satur.	unsat.		
5	before ^a	3.74	51.3	—	—	—	—	—	—	—	—	—
5	I	17.40	2885.9	15.58	12.88	2.20	10.91	41.57	17.78	23.79	0.75	—
5	III	298.59	19752.3	145.05	205.08	58.50	159.40	568.03	263.55	364.48	0.56	—
35	before ^a	40.90	2083.5	12.65	366.90	tr	29.30	408.85	12.65	396.20	0.03	—
35	II	167.82	5016.1	34.52	310.40	tr	20.73	365.65	34.52	331.13	0.10	—
35	III	733.75	14251.8	187.50	669.56	34.70	45.18	936.88	222.20	714.74	0.31	—
47	before ^a	11.59	423.9	72.90	3.90	705.60	10.11	792.50	778.50	14.00	55.60	—
47	II	47.07	1360.3	42.16	7.30	306.80	tr	356.26	348.96	7.30	47.80	—
47	III	20.80	1445.1	87.07	221.02	321.10	tr	629.19	408.17	221.02	1.85	—
57	before ^a	0.92	228.8	—	—	—	—	—	—	—	—	—
57	I	23.62	624.4	3.24	13.10	tr	—	26.34	3.24	13.10	0.24	—
57	III	302.05	2501.3	20.68	45.10	tr	—	65.78	20.68	45.10	0.46	—
68	before ^a	3.04	199.5	—	—	—	—	—	—	—	—	—
68	II	178.47	1957.2	16.50	23.30	4.85	tr	44.65	21.35	23.30	0.92	—
68	III	352.98	4804.1	56.50	60.73	47.74	tr	164.97	104.24	60.73	1.72	—

^a Gas composition determined immediately after the attainment of the device of the predetermined thermobaric conditions (3-4 hours after the commencement of the experiment) is arbitrarily taken as pre-experimental. It is assumed that during this time mainly the desorption processes have been completed.

having an output through the plunger channel into the sampling system.

The experimental methods allow for a relatively fast (2-2.5 hours) attainment of the chamber with the sample to the predetermined thermobaric conditions and an exposure of the sample to these conditions during 76 hours. The connecting branches to the plunger and the trap for liquid are prefilled with helium. However, about 1.3 ml of the air which was not removable from the sand and from the chamber remained in the system. The liquid liberated during the experiment accumulates in the trap, and gas after the displacement of mercury fills up the accumulator. Gas and liquid volumes are continuously recorded. The first gas sampling for the chromatographic analysis is made

TABLE 9
Conditions of Simulation Experiments

Conditions	H (km)	t (°C)	P (kg/cm ²)
I	3.5	105	770
II	5	154	1100
III	6.5	216	1430

3.5-4 hours after the commencement of the experiment, the second one 50 hours, and the third one 77 hours after it. The total duration of the experiment is 78 hours.

On the completion of the experiment, the fluorine plastic chamber is cut and the sample is taken out of it

for the analysis. Figure 3 shows the cut chamber and the general view of the sample and Figure 4 shows the sample in section.

Chromatographic Studies of Gases Liberated During the Experiment

The volumes of gas and liquid liberated in the experiment are presented in Table 10.

The analyses of O_2 , N_2 , and CO_2 were made on two experimental models of the HL-14 gas chromatograph with a thermal conductivity detector. The analysis of hydrocarbon gases was accomplished on the Tsvet-4 gas chromatograph with an ionization-flame detector. The separation of CO_2 and hydrocarbon gases was performed on an analytical silica gel column.

The concentrations of individual gases are given in Table 8.

Since the air was not removed completely from the chamber, it was impossible to estimate O_2 and N_2 quantitatively, although the two gases were undoubtedly present.

As seen from Table 8, the gaseous phase of the initial samples (without O_2 and N_2) consists principally of

CO_2 (~99%) and methane. Ethane, ethylene, propane, and propylene are found only in Samples 35 and 47. Heavier gases (C_4 - C_5) were discovered in no sample.

The experimental conditions, I, II, and especially III showed a sharp increase in amounts of CO_2 and CH_4 , as shown in Figure 5. A simultaneous appearance of heavy hydrocarbon gases was noted. The concentration of the latter increased mainly at the expense of unsaturated hydrocarbons. In contrast, in the experiments with Sample 47, the content of propane decreased by nearly one-half relative to the initial amount.

Thus, the thermocatalytic transformation of organic matter is accompanied by an intensive CO_2 liberation with a simultaneous formation of hydrocarbon gases. The concentrations of the gases and their relationships are determined to a large extent by the individual peculiarities of the initial organic matter.

Results of the Bituminological Studies of the Samples

The same series of the analyses by the same experimental methods were made for the samples before and after the simulation experiments.

Table 11 shows the data of the bituminological studies. From this table it is obvious that the total amount of bitumoids under experimental conditions I and II increases to a greater or lesser degree. Under the more severe conditions III, the content of bitumoids continues to grow, yet much more slowly. An increase of both A_{chl} and A_{alb} occurs.

It should be noted that the experiment reveals a trend in the reaction of bitumoids: the ratio A_{chl}/A_{alb} increases considerably. In some of the samples the maximum increase of this ratio corresponds to relatively mild thermobaric conditions (Sample 35, condition II; Sample 68, condition II), in other samples—(5, 47, 57)—to the severe experimental conditions (III). Similar changes are noticed for β_{chl} (Figure 6).

The fractions of A_{chl} and A_{alb} in the samples before the experiment, as indicated previously, are represented principally by the resins among which the alcohol-benzene resins are far in excess of the benzene ones. During the experiment the relationship between the fractions in both A_{chl} and A_{alb} changes (Figure 7).

The content of the "hydrocarbon" fraction changes in both extracts, and these changes are of a dissimilar character in different samples (Table 12). However, in all the samples a distinct trend is apparent toward an increase of "hydrocarbons" in organic matter. A decrease in the content of "hydrocarbons" of A_{chl} and A_{alb} in some of the samples is probably accounted for by conversion of the solid C_{17} - C_{34} , hydrocarbons present initially, under the influence of temperature and pressure into lower molecular weight liquid and gaseous molecules which are lost during the extraction.

It is believed that a decrease in the amount of hydrocarbons, especially in A_{chl} of Sample 47, is related to the presence of long-chain paraffin hydrocarbons in the "hydrocarbon" fraction of the initial sample.

A sharp increase of the content of the alcohol-benzene resins compared to the benzene ones in A_{chl} of

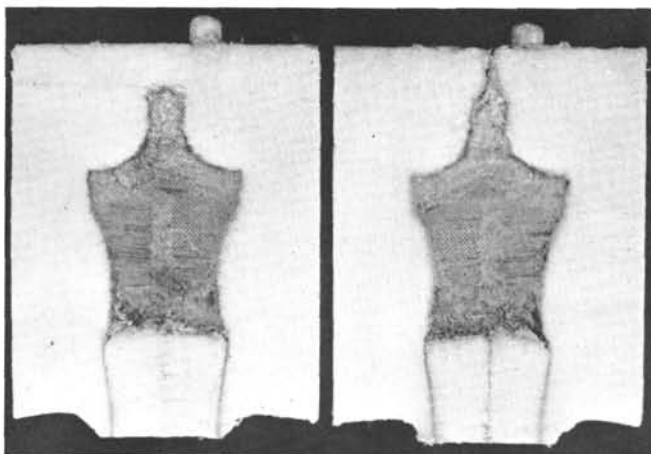


Figure 3. General view of the sample in the chamber after the experiment.

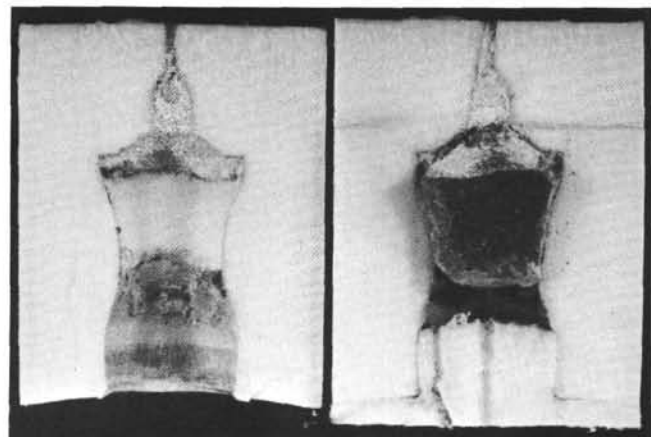


Figure 4. Sample in the chamber after the experiment in section.

TABLE 10
Volumes of Gases and Liquids Liberated During the Experiments (ml)

Sample	Condi- tions	Volume of Upper Sand	Volume of Gas Before Experiment	Volume of Gas of				Volume of Gas of Sample III before Sampling	Total Volume of Gas Genera- ated	Volume of Liquid Generated
				Sample I		Sample II				
				before Sampling	after Sampling	before Sampling	after Sampling			
5	I	1.06	22.11	26.70	18.55	20.7	16.65	16.65	6.54	5.40
5	III	1.06	22.93	40.30	28.00	28.1	16.10	14.40	15.77	6.10
35	II	2.15	15.05	22.70	13.20			14.70	9.15	3.50
35	III	3.22	24.01	37.60	31.20	29.7	21.70	17.60	8.00	3.80
47	II	1.06	14.51	20.00	12.30			12.50	5.70	4.60
47	III	5.37	25.08	30.10	23.10			18.70	0.60	2.20
57	I	1.06	29.00	26.17	17.56	22.96 with add V=6.12	15.00	14.46	2.00	1.80
57	III	0.53	33.00	40.84	29.28	28.82	16.82	17.30	8.60	4.10
68	II	1.07	25.02	27.79	20.87	23.64	13.34	12.52	4.72	4.40
68	III	0.54	31.92	40.53	31.33	31.23	21.99	19.84	6.36	4.10

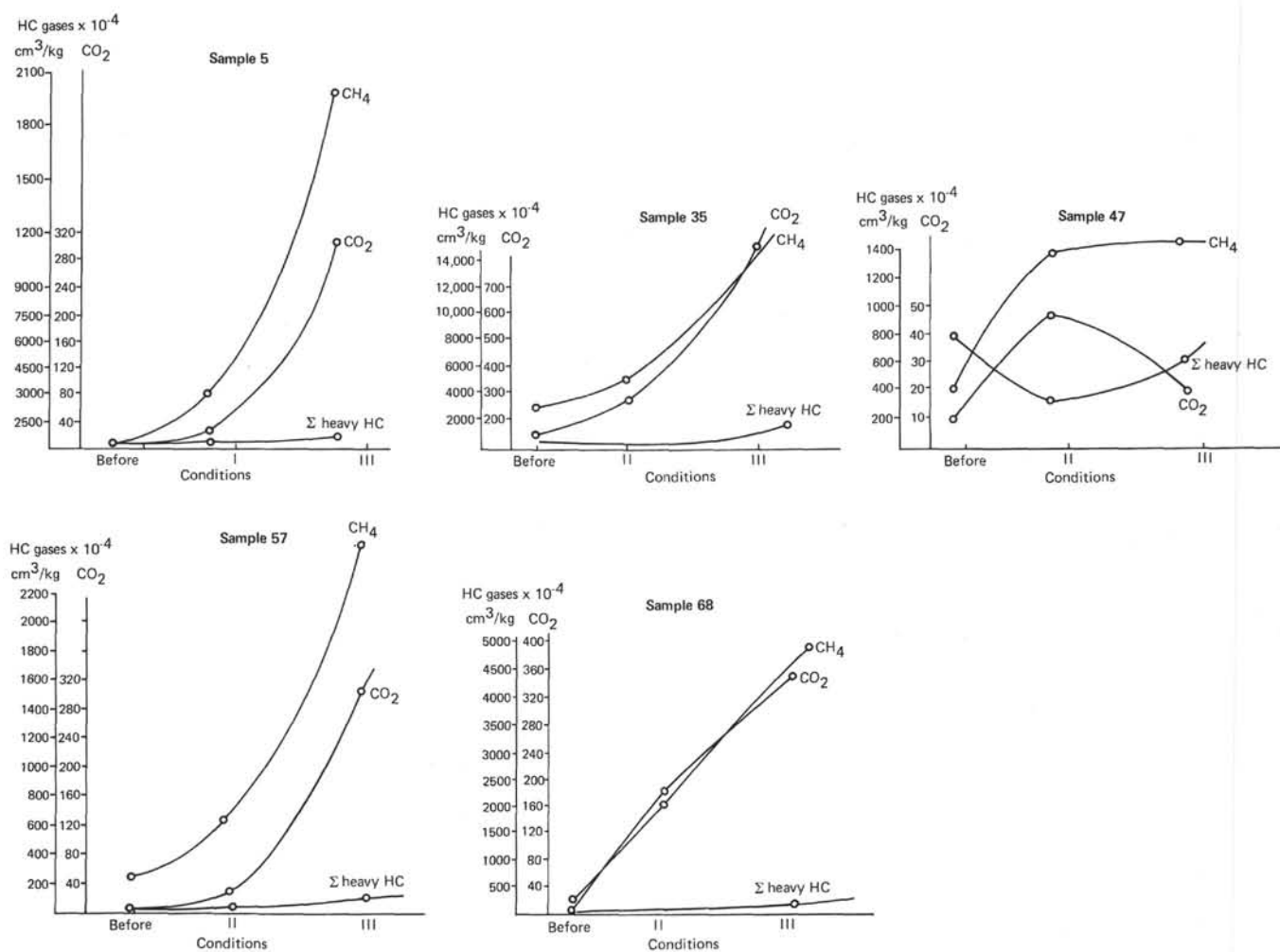


Figure 5. Distribution of gases as dependent on experimental conditions.

all the samples, except for Sample 68, can be attributed only to the presence of the atmospheric oxygen remains in the simulating chamber.

A relatively large amount of asphaltenes enters into the composition of A_{alb} of the samples. Their content under the mild experimental conditions (I and II) decreases in Samples 5, 37, and 47 and increases in Samples 57 and 68.

A decrease in the abundance of asphaltenes is accompanied mainly by an increase of "hydrocarbons" and benzene resins. Such a distribution of the fractions under the experimental conditions is probably related to the fact that asphaltenes of the sediments under study are represented chiefly by the saturated (naphthenic and aliphatic) fragments and in much smaller quantities by the aromatic blocks. Under

TABLE 11
Bituminological Characteristics of Organic Matter of Simulating Samples (%)

Sample	Condi- tions	Corg	Org. Matter	Achl in OM	Aalb in OM	Achl+ Aalb	Achl Aalb	β chl	β alb	HCchl in OM	HCalb in OM	HC in OM	HC in sedim.(%)
5	before	0.50	0.88	0.11	2.27	2.38	0.50	2.00	4.00	0.01	0.05	0.06	0.0005
5	I			5.45	6.82	12.27	0.80	9.60	12.00	0.40	0.12	0.52	0.0045
5	III			8.64	7.84	16.58	1.10	15.20	13.80	0.42	0.08	0.50	0.0044
35	before	0.42	0.74	0.68	2.30	2.98	0.29	1.19	4.05	0.11	0.17	0.28	0.0021
35	II			9.46	3.24	12.70	2.92	16.67	5.71	0.79	0.23	1.02	0.0075
35	III			8.38	4.19	12.57	2.00	14.76	7.38	0.51	0.28	0.79	0.0021
47	before	0.44	0.77	1.56	1.96	3.51	0.80	2.73	3.41	0.41	0.10	0.51	0.0039
47	II			1.56	2.85	4.41	0.55	2.73	5.00	0.17	0.23	0.40	0.0031
47	III			1.25	3.38	4.63	1.31	7.73	5.91	0.14	0.14	0.28	0.0022
57	before	0.45	0.79	2.15	3.42	5.57	0.63	3.78	6.00	0.18	0.13	0.31	0.0024
57	I			2.26	4.68	6.94	0.49	4.00	8.22	0.36	0.30	0.66	0.0052
57	III			2.28	2.15	4.43	1.06	4.00	3.78	0.26	0.21	0.47	0.0037
68	before	0.81	1.43	2.80	1.82	4.62	1.54	4.94	3.21	0.19	0.09	0.28	0.0040
68	II			2.59	1.40	3.99	1.85	4.56	2.47	0.37	1.40	0.37	0.0053
68	III			2.80	4.90	7.70	0.57	4.94	8.64	0.34	4.90	0.34	0.0049

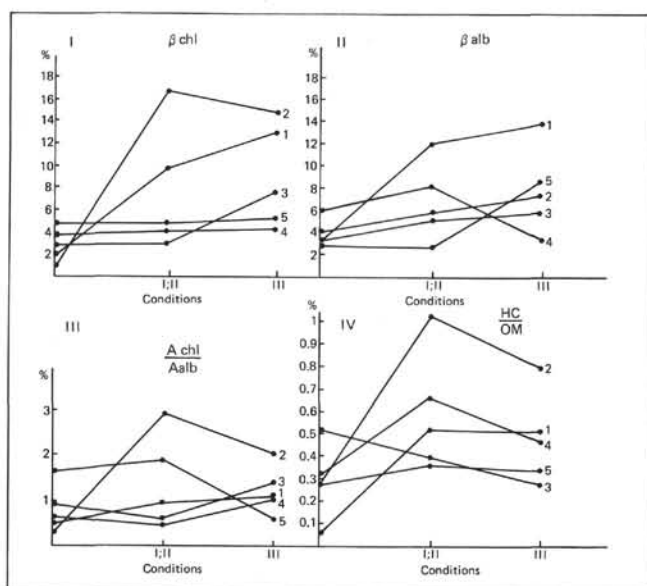


Figure 6. Distribution of separate parameters of bitumoid "A" as dependent on experimental conditions. (I) Sample 5; (II) Sample 35; (III) Sample 47; (IV) Sample 57; (V) Sample 68.

relatively mild thermobaric conditions, separate structures apparently break off with a resulting increase of the hydrocarbon and benzene fractions.

Under more severe experimental conditions (III) when some increase of the content of asphaltenes occurs, the perization processes are apt to prevail over the destructive processes. Such a trend holds for all the samples, with the difference that in some samples these processes occur under milder thermobaric conditions, and, in others, under more severe conditions.

The experimental conditions being equal, the above-mentioned differences may be related to the different composition of the initial organic matter and, as a consequence, to the different character of the structures and molecular relationships within individual fractions.

During the heating experiments, not only the quantitative relationships between individual fractions

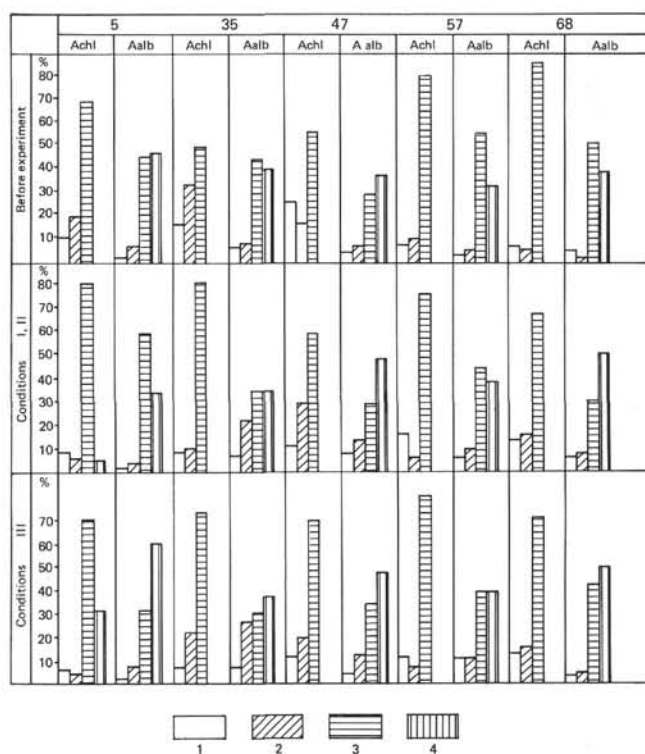


Figure 7. Fractional composition of bitumoid "A" under different experimental conditions. (1) hydrocarbons; (2) benzene resins; (3) alcohol-benzene resins; (4) asphaltenes.

of the bitumoid β are noted to change but the structure of these fractions is found to change substantially. Gas-liquid chromatography and mass spectrometry show that an insignificant decrease of the content of paraffin hydrocarbons (Sample 68 excluded) in the paraffin-naphthene fraction (Table 13) is accompanied by a 1.5-2 times increase in C_{17} - C_{24} hydrocarbons and isomeric forms. The maxima are found to be somewhat shifted towards the molecules with a smaller number of carbon atoms (C_{21} - C_{25}) (Figure 8). The concentrations of naphthene hydrocarbons and, among the, those of mono-, bi-, and tricyclic structures also increases.

TABLE 12
Fractional Composition of Bitumoid "A" (simulating samples)

Sample	Condi- tions	Achl (%)						Aalb (%)						
		HC	Benz resins	Alc-benz resins	Asph	Σ resins	B. res A-b. res	HC	Benz res.	Alc-benz resins	Asph	Σ res- ins	Benz. res A-b. res	Σ res asph
5	before	10.00	20.00	70.00	—	90.00	0.29	2.00	7.00	45.00	46.00	52.00	0.16	1.13
5	I	7.32	6.10	81.70	4.88	87.80	0.07	1.74	3.48	60.00	34.78	63.48	0.06	1.83
5	III	4.85	3.89	71.16	30.10	75.05	0.05	1.01	7.07	32.32	60.61	39.39	0.22	0.65
35	before	16.67	33.33	50.00	—	83.33	0.67	7.35	7.35	44.12	41.18	51.47	0.17	1.25
35	II	8.33	10.18	81.49	—	91.67	0.12	6.98	23.26	34.88	34.88	58.14	0.67	1.67
35	III	6.12	20.41	73.47	—	93.88	0.28	6.67	26.67	29.62	37.04	56.29	0.90	1.52
47	before	26.19	16.67	57.14	—	73.81	0.29	5.00	6.67	30.00	58.33	36.67	0.22	0.63
47	II	11.11	29.63	59.26	—	88.89	0.50	8.16	14.29	28.57	48.98	42.86	0.50	0.88
47	III	11.29	19.35	69.36	—	88.71	0.28	4.08	12.24	34.70	48.98	46.94	0.35	0.96
57	before	8.22	10.96	80.82	—	93.78	0.14	3.90	4.68	57.04	34.38	61.72	0.08	1.80
57	I	16.13	6.45	77.42	—	83.87	0.08	6.25	9.38	43.74	40.63	53.12	0.21	1.31
57	III	11.43	8.57	80.00	—	88.57	0.11	10.00	10.00	40.00	40.00	50.00	0.25	1.25
68	before	6.94	6.25	86.81	—	93.06	0.07	4.81	2.88	51.93	40.38	54.81	0.06	1.36
68	II	14.10	16.67	69.23	—	85.90	0.24	6.78	8.47	32.21	52.54	40.68	0.26	0.77
68	III	12.12	16.67	71.21	—	87.88	0.23	2.60	4.27	42.70	50.43	46.97	0.10	0.93

It is interesting to note that in all the samples at different experimental conditions a trend towards a decrease of the odd coefficient is apparent (Figure 8), i.e., n-alkanes show more structures with an even number of carbon atoms in a molecule.

Tables 14 and 15 present the results of the IR and UV spectroscopic analyses. As may be seen from the results, during the heating experiments, especially under the severe conditions, there occurs an appreciable increase of aromatic structures in the benzene resins and alcohol-benzene resins represented mainly by naphthalene and anthracene derivatives. Simultaneously, the benzene derivatives become considerably less abundant. A simultaneous increase of the amount of the naphthene-aromatic fragments is noted. Thus, as temperature and pressure grow, the degree of cyclicity and aromaticity in the molecules also grows. These changes are undoubtedly a consequence of the dehydrogenation and dehydrocyclization processes.

The observed increase of the oxygen-containing groups represented mainly by ketones, acids, and ethers of the aliphatic character can apparently be accounted for only by the presence of oxygen from the air in the simulating chamber. However, it is interesting to note that under more severe experimental conditions, the carbonyl groups associated with the aromatic rings appear in the structures of the benzene resins and alcohol-benzene resins.

Based on the UV-spectroscopic data, the initial samples contain rather large amounts of sulfurous organic compounds in the form of sulfides and thiophenes. Their content in the samples under study is dissimilar (Table 15). Under the experimental conditions, their abundance somewhat increases.

CONCLUSION

The samples studied were found to contain all the constituents encountered in rocks, i.e., hydrocarbons, resins, asphaltenes, insoluble matter. The relationship

TABLE 13
Composition of the Methane-Naphthene Fraction of Hydrocarbons
in Experimental Samples (ratio in %, based on mass spectrometry)

Sample	Experimental Conditions	Paraffin Hydro- carbons	Naphthene Hydrocarbons						Alkylbenzenes
			one-ring	two-ring	three-ring	four-ring	five-ring	six-ring	
5	before	52.8	14.0	5.3	12.1	5.3	3.2	2.2	5.1
5	I	41.8	30.4	1.0	17.1	1.5	1.3	1.0	5.9
5	III	51.5	10.6	7.9	19.0	1.2	2.1	1.4	5.3
35	before	59.0	9.6	5.4	14.2	3.5	3.1	1.6	3.6
35	II	46.9	6.2	17.8	15.3	4.1	3.3	1.4	5.0
35	III	46.6	14.7	8.0	17.1	5.0	2.1	1.4	5.1
47	before	58.4	6.2	5.1	12.3	4.9	3.5	3.8	5.8
47	II	44.2	10.6	13.5	15.2	4.1	2.6	1.2	8.6
47	III	48.4	13.5	8.2	18.0	3.8	2.3	1.2	4.6
57	before	25.3	33.8	3.8	11.3	10.3	6.4	5.5	3.6
57	I	20.1	35.2	3.5	15.8	7.1	3.4	2.5	12.4
57	III	19.8	48.4	3.4	17.0	4.1	2.9	1.7	3.7
68	before	36.9	8.3	8.0	15.2	12.4	6.5	5.3	7.4
68	II	52.9	9.0	5.1	16.7	5.8	4.8	2.1	4.6
68	III	38.1	13.1	11.1	24.7	8.2	2.2	1.9	1.7

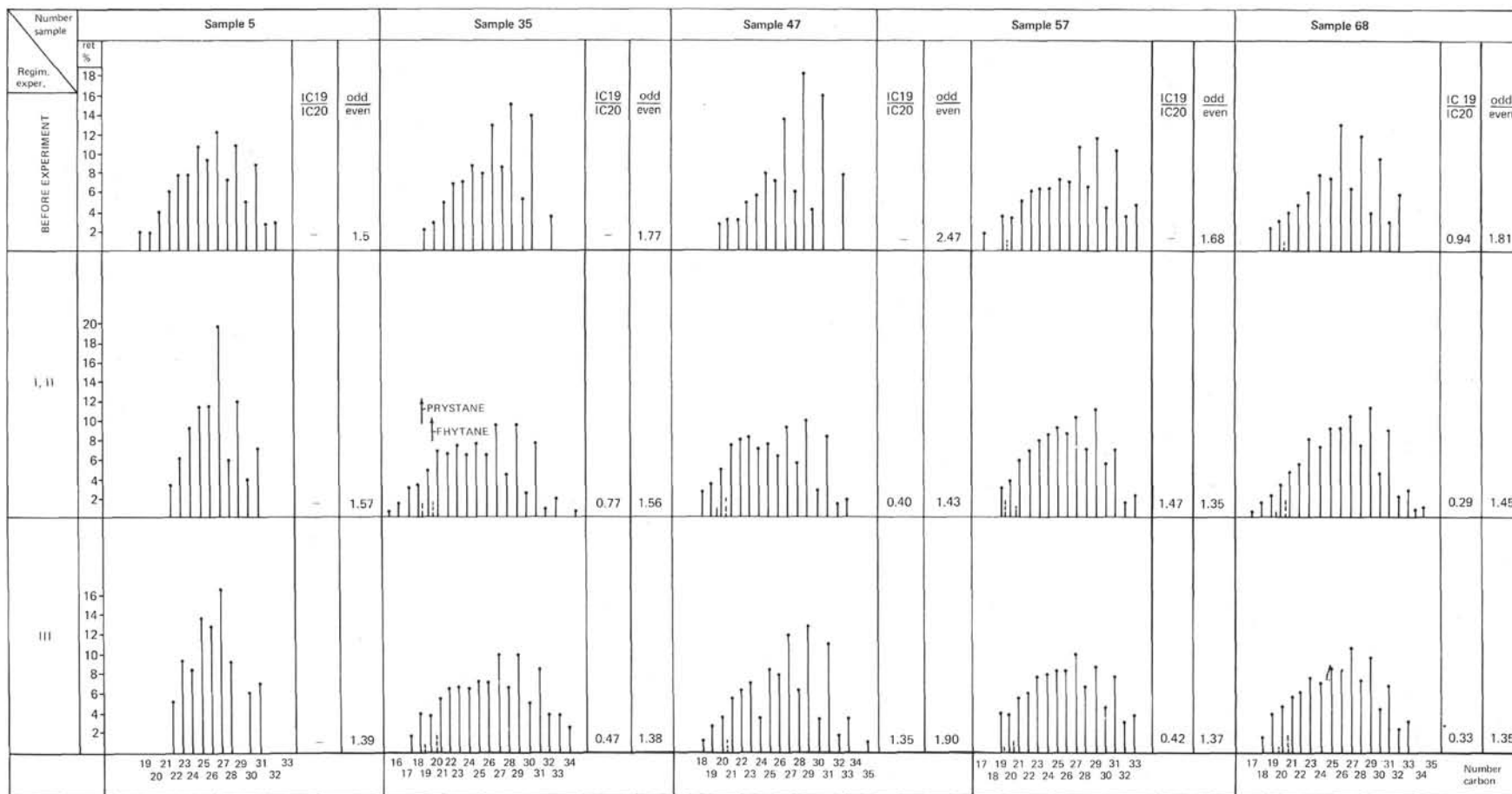


Figure 8. Distribution of normal paraffin hydrocarbons in the methane-naphthene fraction as dependent on experimental conditions.

TABLE 14
Molar Relationships of Functional Groups in Chromatographic Fractions of Bitumoid Achl (simulating samples)

Sample	Conditions	Benzene Resins								Alcohol-Benzene Resins							
		Absorption (cm ⁻¹)															
		1740	1710	1670	1600	1470	1380	1115	1030	1740	1710	1670	1600	1470	1380	1115	1030
5	before	0.90	1.26	—	8.60	6.70	6.30	8.30	9.20	1.43	1.79	0.46	8.21	6.71	10.27	5.00	60.44
5	I	4.50	5.93	2.90	5.90	25.10	36.50	12.15	73.60	—	3.90	0.60	17.50	73.70	5.90	2.45	—
5	II	2.17	3.04	—	20.50	16.00	15.10	5.50	21.13	2.70	4.30	0.70	5.80	62.90	7.30	3.65	6.20
35	before	2.35	3.30	0.75	4.30	15.14	24.07	8.80	46.20	2.07	2.64	0.79	17.70	7.29	16.47	2.83	42.70
35	II	1.90	4.50	1.30	35.20	14.30	26.20	7.70	50.40	1.60	2.10	1.00	19.50	7.10	13.20	4.80	26.40
35	III	3.00	5.60	1.10	23.80	12.80	17.30	6.35	30.10	1.10	3.25	0.50	9.10	6.00	9.60	2.10	9.70
47	before	2.90	3.40	1.46	44.87	14.29	20.13	4.60	48.00	3.30	2.00	0.70	17.60	8.80	6.70	4.20	27.70
47	II	2.10	3.39	1.50	29.80	12.60	20.10	6.70	46.90	0.70	4.50	1.00	—	7.70	16.00	8.10	—
47	III	3.20	4.00	1.25	44.90	17.60	27.70	6.50	63.30	0.60	1.80	0.34	—	5.00	6.20	16.00	89.20
57	before	2.75	5.01	1.25	56.62	18.90	28.30	7.00	6.00	1.00	1.40	0.30	3.60	4.10	5.70	1.30	5.00
57	I	3.00	5.70	0.95	23.80	17.10	28.00	3.60	44.60	2.75	3.60	1.00	15.90	9.40	14.70	6.00	36.40
57	III	0.50	0.75	0.35	11.70	3.40	5.00	3.10	59.70	5.10	7.25	1.80	31.60	19.60	27.60	12.30	61.70
68	before	1.28	1.60	1.67	20.90	8.40	—	6.60	22.40	0.75	1.20	0.35	6.40	3.00	5.20	0.90	4.90
68	II	2.10	1.70	0.80	15.50	9.60	12.70	4.20	16.60	0.80	1.10	0.35	8.90	3.10	5.10	2.10	10.60
68	III	2.80	3.25	1.30	31.10	13.40	18.40	6.00	39.30	1.20	2.50	0.45	8.60	4.30	7.10	2.90	17.90

TABLE 15
Relative Content of Aromatic Structures in Resins of Bitumoid "A"
Based on UV-Spectroscopic Data (internal standard) (simulating samples)

Sample	Conditions	Benzene Resins					Alcohol-Benzene Resins				
		Sulfides	Achl Thio-phenes	Naphthalenes	Benzenes	Anthracenes	Sulfides	Thio-phenes	Aalb Naphthalenes	Benzenes	Anthracenes
5	before	1	1	1	1	1	1	1	1	1	1
5	I	2.5	—	2.5	2.8	2.8	1.7	—	1.8	1.75	1.75
5	III	7.5	—	5.0	7.3	7.3	2.1	—	1.3	1.4	1.3
35	before	1	1	6.0	—	1	1	—	1	—	1
35	II	0.3	0.6	0.5	—	1.3	0.55	—	0.8	—	2.2
35	III	0.06	0.2	0.09	—	1.4	0.8	—	0.7	—	2.1
47	before	1	1	1	1	1	1	—	1	—	1
47	II	1.2	1	0.75	—	1.1	10	—	7	—	4.8
47	III	0.56	0.4	0.4	—	0.4	14	—	8.6	—	3.5
57	before						1	1	1	1	1
57	I						0.8	—	0.3	0.2	0.65
57	III						0.8	—	0.4	0.4	1.4
68	before						1	—	—	—	—
68	II						0.6	—	0.7	—	—
68	III						0.9	—	0.7	—	—

between these constituents, their structure and properties depend to a great extent on the initial organic matter, on the conditions, and the degree of its transformation.

The experimental simulation revealed that accumulation of the light hydrocarbon fraction and heavy hydrocarbon gases occurs simultaneously with the formation of condensed aromatic and naphthene-

aromatic structures resulting from hydrogen disproportionation.

The general picture of the evolution in the formation of hydrocarbons as a result of the catagenic transformation of organic matter based on the natural material corroborates the major existing concepts and is indicative of the organic origin of oil and gas in nature.