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COAL

Structure and Properties of Heavy Organic Residue from Coal Hydrogenation

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Abstract—On the basis of elementary analysis and ^{13}C NMR spectroscopy, as well as the mean molecular mass and the degree of aromatic content, a structural model of bitumen (coal oil) that satisfies experimental data is formulated. The fragmentary composition of the model is determined: alkyl, naphthene, and aromatic components are present. On the basis of the PM6 quantum-chemical method, with geometric optimization of the electronic structure of a hypothetical bitumen molecule from coal hydrogenation, the interatomic distances and ionization potential are calculated. The IR spectrum is proposed. The uppermost occupied molecular orbital is identified. In the approximation of a supermolecule consisting of two molecules, the interplane distances and molecular-interaction energy are determined. The proposed method of investigating the structure and properties of complex organic systems may be used in the development of processing technologies for carbon-bearing materials.

Keywords: bitumen, coal hydrogenation, prediction of properties, structural model, quantum-chemical calculations

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Catalytic hydrogenation to convert high-molecular compounds within the organic mass of coal into gaseous and liquid products is accompanied by the formation of slurry, consisting of liquid products and a solid residue (a mixture of high-boiling hydrocarbons). Further processing of the residue yields additional liquid products or artificial bitumen, depending on the technology employed. The bitumen formed, thanks to its adhesive and hydrophobic properties is a valuable structural material and may also be used for the production of resins, glue, paints, and plastics.

Thus, the production of bitumen and bitumen composites may be of great economic and environmental benefit in coal producing regions. However, the development of effective methods of bitumen utilization is constrained by inability to predict their chemical composition and structure and hence their properties and reactivity. There has been intermittent research in this area. For example, the physicochemical properties of coal bitumen and petroleum bitumen were compared in [1, 2].

In the present work, we find methods of predicting the physicochemical properties of coal-based bitumen (coal oil) on the basis of structural and chemical analysis and identify effective thermochemical and physical processing methods.

The bitumen considered is a byproduct of the catalytic hydrogenation of Karazhyra lignite (Eastern Kazakhstan). Its basic characteristics are as follows: $W^a = 8.0\%$; $A^a = 7.2\%$; $V^{daf} = 45.4\%$; $C^{daf} = 69.7\%$; $H^{daf} = 5.7\%$; $N^{daf} = 1.41\%$; and $O^{daf} = 22.03\%$. Its elementary composition and structural parameters are as follows:

Elementary composition, wt %, *daf*:	
C	87.20
H	7.38
S	1.10
N	1.55
O	2.77
Carbon content in structural fragments, wt %, *daf*:	
CH_{ar}	19.4
CH_2	19.2
CH_3	10.9
C=O	1.8
C_{con}	48.7
Mean molecular mass *Mr*;	900
Aromatic index f_a	0.69