Table 1. Structural parameters of bitumen according to X-ray structural analysis

Bitumen	Structural parameters				
	L_a, Å	L_c, Å	d_{002}, Å	d_r, Å	number of layers in bundle
Coal-based bitumen	17.1	9.5	3.73	4.75	4.5

Here L_a is the diameter of the coal layer; L_c is the packet thickness; d_{002} is the interplane distance; d_r is the number of bitumen rings.

From the C, H, N, O, and S content of bitumen per 100 g of organic mass, we determine the degree of unsaturation of the structure [2, 3]

$$n_{at} = \frac{C}{12} + H + \frac{N}{14} + \frac{O}{16} + \frac{S}{32}, \quad (1)$$

$$n_{bo} = \frac{C}{6} + \frac{H}{2} + \frac{3N}{28} + \frac{O}{16} + \frac{S}{32}, \quad (2)$$

$$\delta = 2(n_{bo} - n_{at}). \quad (3)$$

Here n_{at} is the total number of gram atoms of all the elements; n_{bo} is the number of chemical bonds in the molecule per 100 g of bitumen.

We calculate the structural and chemical characteristics of the bitumen for mean molecular mass on the basis of the method in [3, 4].

Table 1 presents X-ray structural analysis of bitumen [1].

Table 2. Structural parameters of bitumen for molecular mass M

Structural parameters	$M = 900, f = 0.69$
C	**65.4**
C_{al}	20.27
C_{ar}	45.13
H	**66.42**
H_{al}	40.55
H_{ar}	25.87
N	0.96
O	1.56
S	0.32
Number of atoms	134.67
Number of rings	**11.11**
Number of bonds	167.34
Σ-bonds	144.77
Π-bonds	**22.56**
δ	**7.26**

We see that the supermolecular structure of the bitumen is partially formed, and the interplane distance $d_{002} = 3.73$ Å is close to $d_{002} = 3.35$ Å for graphite [3]. The number of layers in a bundle is 4.5, which indicates the formation of condensed aromatic structures.

Table 2 presents numerical values of the structural parameters for the molecular mass, calculated by the method of [3, 4].

A hypothetical structural model of the bitumen molecule is based on experimental data for the elementary composition, the degree of aromatic content, and the mean molecular mass. Obviously, this is not the only possible model, since there are several degrees of freedom (the type of condensation, isomers, etc.) These may be limited by taking account of the ^{13}C and ^{1}H NMR spectra. However, the proposed model permits description of the bitumen structure consistent with the experimental data and provides the basis for identifying effective processing methods.

In Fig. 1, we show an optimized structural model of bitumen according to the semiempirical PM6 quantum-chemical method [5]. The model contains alkyl, naphthene, and aromatic structural fragments. That is in good agreement with experimental data. This structural model of the bitumen molecule indicates that thermochemical processing in the presence of appropriate catalysts yields liquid products consisting mainly of saturated hydrocarbons.

The proposed model is of interest for effective selection of the parameters in physical treatment of bitumen—for example, treatment by ultrasound of specific frequency or an accelerated electron flux.

At present, ultrasound technology is widely used in processing heavy organic fractions [6]. To reach resonance, we need to adjust the ultrasound frequency to a specific vibrational frequency in the compound's IR spectrum.

In Fig. 2, we show the theoretical IR spectrum of the structural model of bitumen, in terms of the wave number (cm^{-1}) and frequency (Hz). The spectrum consists of two main absorption bands: 2500–3000 cm^{-1} (absorption by C–H bonds); and 500–1700 cm^{-1} (absorption by C–C bonds and deformational oscillations). Thus, the structural model permits selection of the ultrasound frequency for use on the bitumen.