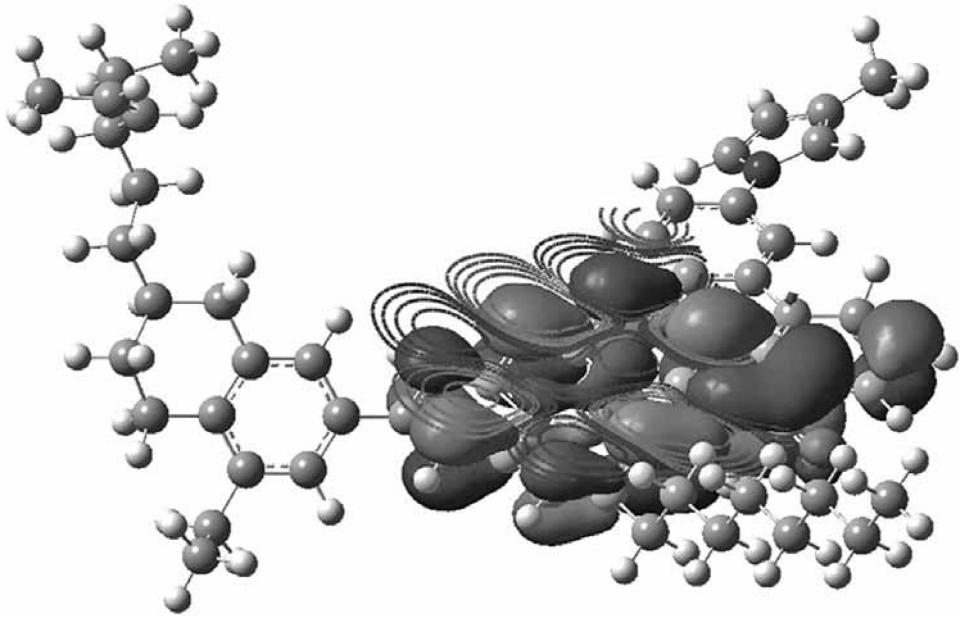

Fig. 3. Uppermost occupied molecular orbital in the structural model of bitumen.

In Fig. 3, we show the uppermost occupied orbital of the structural model of bitumen. The uppermost occupied molecular orbital includes the π-conjugate system of the model's aromatic fragment. This conjugate system is very thermostable. It is able to form donor–acceptor bonds with heavy-metal ions, thereby acting as a sorbent. The ionization potential is $I = 6.93$ eV, according to the Koopmans theorem.

To investigate the thermochemical transformation of bitumen, we need to know the thermodynamic functions of this heavy organic residue. Quantum-chemical calculations of the model molecule yield the following results:

1. The null-vibration energy $E_0 = 659.77130$ kcal/mol.

2. The thermal energy $E = 699.71$ kcal/mol.

3. The isochoric specific heat $C_V = 243.45$ cal/mol K.

4. The entropy $S = 379.455$ cal/mol K.

5. The enthalpy $H = E + R \cdot T = 699.71 + (0.00198726 \times 298.15) = 700.30$ kcal/mol.

6. The Gibbs free energy $G = H - TS = 587.17$ kcal/mol.

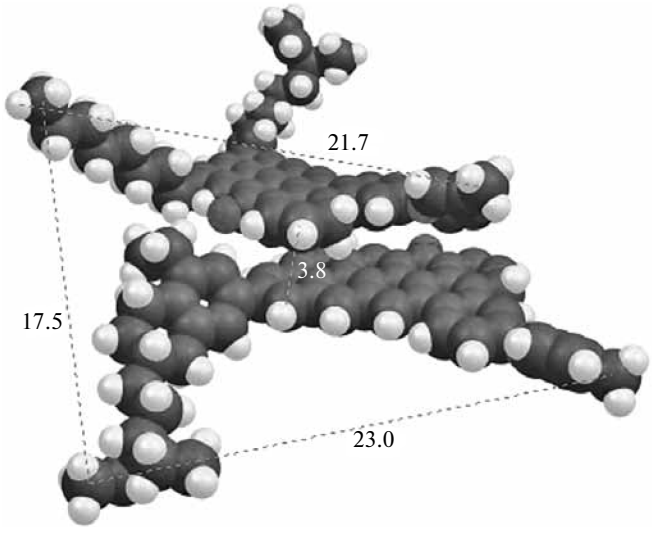

Fig. 4. Optimized structure of two structural models in the supermolecule approximation.

In Fig. 4, we show the optimized structure of two structural models in the supermolecule approximation. We see that the molecules are oriented so that the condensed aromatic fragments are parallel. The interplane distance in this case is 3.8 Å, which is close to the experimental value (3.7 Å). In Fig. 4, we also show the distance between the carbon atoms (Å) characterizing different dimensions of the complex. The interaction energy of the two molecules is

$$\Delta E = E(\text{complex}) - 2E(\text{molecule})$$

$$= 9.95 \text{ kcal/mol}.$$

Thus, the structural and chemical characteristics of the mean hypothetical bitumen molecule show that, in combination with quantum-chemical calculation of the electron structure, the proposed method—based on the experimental elementary composition, degree of aromatic content, and mean molecular mass—may be successfully used in developing processing technology for high-molecular materials.