

**SUPRAMOLECULAR STRUCTURE OF ACTIVATED CARBONS PREPARED
BY HEAT-SHOCK ALKALI ACTIVATION OF COALS**

Sabierova V. O.

L. M. Litvinenko Institute of Physical-Organic and Coal Chemistry NAS of Ukraine, Kyiv
Sabierova@nas.gov.ua

Coals of different coal rank (CR) are easily converted to highly porous adsorbents upon alkaline (KOH) activation with heat shock – rapid introducing samples into a reactor zone preheated up to 800 °C. At a low KOH/coal ratio (1 g/g), activated carbons (ACs) are formed with a developed specific surface area *S*, depending on the CR (table). All ACs are microporous materials; the micropore (≤ 2 nm) surface fraction is dominant (≥ 90 %).

The aim of this work is to study the supramolecular structure of ACs prepared from different rank coals by heat-shock alkali activation.

Supramolecular structure was studied by X-ray diffraction method (Bruker D8, CuK α , $\lambda = 0.154$ nm). Interlayer distances (d_{002}), heights (L_c) and average diameters (L_a) of ACs crystallites were determined and compared with the same characteristics of coals (table).

Table. The crystallite characteristics of coals and activated carbons

C ^{daf} , %	Coals			Activated carbons (ACs)			
	d_{002} , nm	L_c , nm	L_a , nm	<i>S</i> , m ² /g	d_{002} , nm	L_c , nm	L_a , nm
70.4	0.412	0.802	1.46	2012	0.355	0.651	3.73
80.0	0.407	0.872	1.68	1950	0.346	1.154	3.53
81.0	0.403	0.891	1.54	1955	0.358	1.053	3.80
83.5	0.395	0.893	1.59	1728	0.356	1.045	3.57
85.0	0.393	0.928	1.68	1749	0.360	1.158	3.38
86.4	0.388	0.927	1.61	1548	0.367	1.163	3.78
88.6	0.383	0.966	1.53	1422	0.359	1.327	3.80
89.4	0.377	1.039	1.51	1304	0.361	1.260	3.58
90.0	0.375	1.152	1.57		0.358	1.302	3.88
90.8	0.370	1.156	1.56	1255	0.363	1.450	4.00
91.2	0.369	1.157	1.74	1237	0.357	1.547	3.76
94.6	0.370	1.421	1.87	990	0.356	1.530	4.51
95.2	0.367	1.550	1.92		0.358	1.472	5.22
95.6	0.368	1.512	1.91	818	0.350	1.601	5.34

The ACs crystallites are more structured, have a higher height, diameter, volume and number of graphene layers, but a smaller interlayer distance. That is, crystallites formed in heat-shock alkali activation are closer to graphite structure. The total crystallite content of ACs is less than in the coals. The activant KOH does not prevent the growing of graphene layers due to thermoinitiated condensation reactions, and this effect is more evident in the heat shock. It can be assumed that KOH molecules and K⁺ ions are spatially fixed on the layer planes due to interaction of K⁺ with the π - system of graphenes. The combined action of alkali and heat shock disorders crystallites by transforming them from a pseudocrystalline state to an amorphous one. Only the most structurally organized crystallites are stored in the final ACs. They are connected in a rigid framework by single graphenes being chaotically oriented in space relative to each other.

The fulfillment of two conditions – the presence of covalent linking between single graphenes and their spatial disordering, makes it necessary to recognize the existence of single C_{ar}-C_{ar} bonds between graphene structural fragments. They cross-link crystallites and graphenes into porous spatial framework.