

## Comparative analysis of the structure of coals of different stages of metamorphism according to $^{13}\text{C}$ NMR data

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### Abstract

In this paper, the method of cross-polarization with magic angle rotation and decoupling from protons (CPMAS)  $^{13}\text{C}$  NMR spectroscopy obtained quantitative data on the distribution of carbon over structural fragments and calculated the degree of aromaticity ( $f_a$ ) of some coal samples from various Siberian deposits of a wide range of metamorphism. All the coals used in the work were characterized by standard methods (proximate and ultimate analysis). The optimal parameters of the pulse program for recording the spectra of coals have been determined. To obtain quantitative data, the spectra were simulated. The spectrum model included from 9 to 13 components, depending on the stage of coal metamorphism. The dependences of the degree of aromaticity and the sum of oxygen-containing functional groups on the stage of coal metamorphism were constructed. The results obtained show that the structure of coals regularly changes depending on the stage of their metamorphism. The revealed relationships of the structure and properties of coals, together with the parameters of their reactivity, can ensure the safe behavior of coals in the processes of mining and processing, as well as in determining possible ways of using the studied coal samples as a valuable chemical raw material.

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