EPR studies on petrographic constituents of bituminous coals, chars of brown coals group components, and humic acids 600 °C char upon oxygen and solvent action.

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Streszczenie

Free radicals were characterized in petrographic constituents of bituminous coals and in chars from brown coal components by EPR. The change in free radical concentration on oxidation of humic acid 600 °C char from humodetritous brown coal with gaseous 10% oxygen at 330 °C was evaluated. Spin concentration in the petrographic constituents from a bituminous coal increases in the order liptinite < vitrinite ≪ inertinite. Increasing maturity of each petrographic constituent correlates with an increase in spin concentration and decrease i n *g*-value. Heat treatment of brown coal group components (bitumens, cellulose, lignin, humic acids, and residual coal) leads to the formation of free radicals up to a temperature of about 550 °C and to their sharp disappearance at higher temperatures. Strongly marked maxima in the spin concentration of the chars are observed at atomic H/C ratios in the range 0.40−0.42 and O/C ratios in the range 0.08−0.10. Increasing heat treatment temperature causes a steady decrease in *g*-value from about 2.0040 to 2.0025. Treatment of the 600 and 700 °C chars with organic solvents resulted in an increase in their spin concentration. This effect was particularly strong in the case of treatment with tetralin and naphthalene. Burning off humic acid 600 °C char with 10% oxygen at 330 °C leads to a decrease in spin concentration in oxidized products. Structural units associated with elevated char free radicals density were more prone to oxidation and presumably are peripheral polyaromatic skeletons of lower structural ordering.

Słowa kluczowe

Aromatic compounds, Coal, Electron paramagnetic resonance spectroscopy, Hydrocarbons, Quantum mechanics

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