Structural identification of paramagnetic iron porphyrins from Colorado coal with use of 1D and 2D ^{1}H NMR spectroscopy: geochemical implications on their origin from heme.

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Streszczenie

A fraction of iron porphyrins from Colorado coal constituting one major and one minor C28 isomer was analysed with the use of 1D and 2D ^{1}H nuclear magnetic resonance spectroscopy. 2D ^{1}H COSY and NOESY experiments in a low viscosity solvent (CD_3 OD) led to the structrural identification of the major component. Assignment of the hyperfine shifted resonances, of all the peripheral substituents on the porphyrin macrocycle, resulted in an unambiguous identification of iron(III) 2,7,12,18-tetramethyl-13,17-diethyl porphyrin. Reliability of the 2D ^{1}H NMR method used was confirmed by analyzing a related structure, i.e. deuteroheme-IX in the same way. The minor constituent of the analysed fraction was identified by reproducing the ^{1}H NMR spectrum with its synthetic counterpart: low-spin iron(III) 2,7,12,18-tetramethyl-3,8-diethyl porphyrin. Both identified coal iron porphyrins represent products derived from a common protoheme-IX related precursor, selectively degraded via different routes during coal diagenesis.