

Metalloporphyrins in coal. 4 TLC-NMR of iron porphyrins from coal: the direct characterization of coal hemes using paramagnetically Shifted¹ H NMR spectroscopy.

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A new approach to the identification of iron porphyrins in coal is described that involves their separation from other porphyrins by preliminary thin-layer chromatography (TLC) followed by repeated TLC to separate the iron porphyrins. The repeated TLC involves both redevelopment with a given solvent (multiple development) and with a sequence of solvent systems (sequential development). Homologous polyalkylporphyrins are separated in some cases; isomers generally are not. Hemes from Colorado coal are thus split into 22 fractions, with carbon numbers ranging from C32 (most mobile on silica gel) to C[^] (least mobile); these fractions are then examined by mass spectrometry and by paramagnetically shifted NMR spectroscopy of the corresponding low spin iron(III) dicyanide complexes. The latter spectra are particularly useful in providing direct structural information about the hemes extracted from coal. Etioheme III (C32) is confirmed as the most mobile component, while mixed suites of monodemethylation products (C31, formed both by benzylic cleavage and by aromatic protodesubstitution) and of monodeethylation (C30) products are isolated from and identified in coal porphyrins for the first time. The importance of these findings in relation to current theories of heme catagenesis is outlined.

Adres publiczny

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