

STRUCTURAL CHARACTERIZATION OF THE KEROGEN FROM  
PUMPHERSTON OIL SHALE

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ABSTRACT

In order to contribute to structural characterization of the kerogen from Pumpherston (Scotland) oil shale, a twenty-nine step alkaline permanganate degradation of this kerogen was carried out. According to atomic H/C and O/C ratios, 1.64 and 0.10, respectively, this kerogen was classified as type I kerogen. The Pumpherston shale kerogen was of somewhat higher maturity, its vitrinite reflectance being 0.59%.

A moderate total yield of oxidation products was obtained, 65.14% based on original kerogen, the yields of neutrals and bases, ether-soluble acids, acids from aqueous solutions and precipitated acids being 3.73%, 35.94%, 3.33% and 22.14%, respectively. The non-degraded residue was very high, 18.66% relative to initial kerogen. Precipitated acids were further degraded in thirty-one step yielding 58.44% of neutrals and bases, ether-soluble acids and acids from aqueous solutions. The yield of "non-degradable" residual precipitated acids was relatively high, 12.16% relative to starting acids.

Detailed capillary GC-MS analysis of the oxidation products revealed the presence of saturated unbranched  $C_9$ - $C_{36}$  monocarboxylic and  $C_6$ - $C_{33}$   $\alpha, \omega$ -dicarboxylic acids,  $C_{15}$  and  $C_{17}$  branched monocarboxylic acids,  $C_3$ - $C_9$  alkane-tricarboxylic,  $C_6$ ,  $C_8$ - $C_{13}$  alkane-tetracarboxylic,  $C_{10}$  and  $C_{11}$  branched alkane-tetracarboxylic acids, and various aromatic mono-, di- tri- and tetracarboxylic acids. Normal monocarboxylic and  $\alpha, \omega$ -dicarboxylic acids were by far the most abundant fractions of the acidic products, 54.32%

and 36.75%, respectively. The participation of aromatic and alkane-polycarboxylic acids, 3.79% and 5.04%, respectively, was much less important.

The dominance of saturated aliphatic acids in the oxidation products suggested a prevailing aliphatic cross-linked structure of Pumpherson oil shale kerogen. A relatively low participation of aromatic acids in the oxidation products was observed in spite of somewhat higher maturity of this kerogen, compared to other examined type I kerogens. The small proportion of alkane-polycarboxylic acids suggested a smaller participation of alicyclic and/or heterocyclic precursor structures.

The predominance of n-monocarboxylic over  $\alpha, \omega$ -dicarboxylic acids and also an exceptionally low ratio of precipitated versus ether-soluble acids (0.62) suggested that the kerogen core network was highly cross-linked and that substitution at its periphery, branching in the matrix and substitution of ring structures were abundant. The high non-degraded residues indicated the presence of highly resistant, presumably aliphatic, nucleus in the kerogen structure.

The degradation of the kerogen from Pumpherson oil shale, shown as example, will serve as basis for demonstration of the feasibilities of an optimized alkaline permanganate oxidation method for structural characterization and classification of kerogens.