

油页岩的¹³C-NMR特征及FLASHCHAIN热解模拟研究

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Characterization of oil shales by ¹³C-NMR and the simulation of pyrolysis by FLASHCHAIN

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摘要 采用固体 ¹³C-NMR核磁共振技术表征了甘肃窑街矿区油页岩的碳骨架结构, 分析并计算了油母质团簇化学结构参数, 包括团簇平均碳原子数、芳碳原子数、脂碳原子数及芳环数。在热重红外分析仪 (TG-FTIR) 上进行了油页岩的热解实验, 得到了热解产物的生成规律。结合样品的团簇化学结构参数, 采用基于油页岩结构的FLASHCHAIN模型模拟其热解产物的生成过程; 模拟结果与TG-FITR实验数据符合较好, 印证了模型预测的合理性。

关键词: 核磁共振 热重红外 油页岩 热解 结构参数 FLASHCHAIN

Abstract: The carbon skeleton structure of oil shales from Gansu Yaojie mine was characterized by the ¹³C solid-state NMR; the chemical structure parameters of cluster in the oil shales, such as average number of carbons, aromatic carbons, aliphatic carbons and aromatic rings, were determined. TG-FTIR tests were used to obtain the yields of pyrolysis products. Considering the cluster chemical structure parameters determined by ¹³C solid-state NMR, the release of pyrolysis products was simulated by FLASHCHAIN. The simulation results are in good agreement with the TG-FTIR tests, proving the rationality of the model proposed.

Key words: ¹³C-NMR TG-FTIR oil shales pyrolysis structural parameters FLASHCHAIN

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