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论文

两种褐煤的13C-NMR特征及CPD高温快速热解模拟研究

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摘要：

采用 13C-NMR固体核磁表征元宝山褐煤及白音华褐煤的碳骨架结构参数，分析两种褐煤团簇化学结构参数，元宝山褐煤团簇中平均碳原子数为16.21，其中芳碳原子数为9.24，脂碳原子数为6.97，芳环数为1.81；白音华褐煤团簇中平均碳原子数为17.14，其中芳碳原子数为9.43，脂碳原子数为7.71，芳环数为1.86。两种褐煤均以桥键及环状链接为主，元宝山褐煤团簇中桥键及环状链接多于白音华褐煤，而白音华褐煤则侧支链稍多。结合两种褐煤团簇化学结构参数，采用基于煤结构的CPD热解模型，模拟这两种褐煤的高温快速热解过程，模拟结果合理可靠。

关键词： 褐煤；固体 13C-NMR；CPD；高温快速热解

The 13C-NMR measurements of two types of lignite and the CPD simulation of lignite rapid pyrolysis at high temperature

Abstract:

Two types of lignite from Yuanbaoshan and Baiyinhua coal mines were examined using the 13C solid state NMR technique.The parameters relating to the carbon skeletal structure of the two type of lignite were derived from the 13C-NMR spectrum, which shows the chemical structure of each lignite cluster.The average number of carbon atoms in the Yuanbaoshan cluster is found to be 16.21, among which the aromatic carbon number is 9.24, and the fat carbon number is 6.97.The aromatic ring is 1.81.The average number of carbon atoms in the Baiyinhua cluster is 17.14, with a aromatic carbon number of 9.43, and a fat carbon number of 7.71.The aromatic ring measures 1.86.The attachments on the clusters of both lignites are mainly by bridges and loops.The difference between the two is more bridges and loops found in the Yuanbaoshan cluster, and more side chains in the Baiyinhua cluster.The CPD (Chemical Percolation Devolatilization) model based on the structure of coal, together with the parameters of the cluster chemical structure, were used to simulate the rapid pyrolysis process of the two type of lignite at a high temperature.The simulation results are rational and reliable.

Keywords: lignite; solid-state 13C-NMR; CPD; high-temperature rapid pyrolysis

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