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上湾煤及其惰质组富集物的结构表征与模型构建

蔺华林, 李克健, 章序文

中国神华煤制油化工有限公司上海研究院, 上海 201108

Structure characterization and model construction of Shangwan coal and it’s inertinite concentrated

LIN Hua-lin, LI Ke-jian, ZHANG Xu-wen

China Shenhua Coal to Liquid and Chemical Shanghai Research Institute, Shanghai 201108, China

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摘要 对神东上湾煤(SDR)及其岩相分离所得惰质组富集物(SDI)分别进行核磁(^{13}C-NMR)、红外光谱(FT-IR)和X射线光电子能谱(XPS)表征,得到煤结构单元信息,与元素分析数据相结合构建了SDR和SDI的结构模型,用ACD/CNMR predictor软件计算结构模型的 ^{13}C化学位移。结果表明,SDR芳香结构主要是缩合程度为2的萘,SDI主要是菲和萘,SDI较SDR结构芳香度较高,两个结构中氧主要以羰基氧和羟基氧的形式存在,氮主要以吡咯和吡啶形式存在,两个结构模型计算得到核磁谱图与实验谱图吻合较好,结构式分别为$C_{181}H_{136}N_2O_{24}$和$C_{186}H_{148}N_2O_{22}$。

关键词: 煤 惰质组富集物 ^{13}C-NMR 芳香度 模型构建

Abstract: Shendong Shangwan coal (SDR) and its inertinite concentrated(SDI)from petrographical separation were characterized by ^{13}C-CP/MAS NMR, FT-IR and XPS and their structure unit information was obtained. Based on structure parameters and elemental analysis, macromolecular structure models of SDR and SDI were constructed and ^{13}C chemical shift of the two models was calculated by ACD/CNMR predictor. The results indicate that naphthalene with condensation degrees of 2 is the main form of aromatic carbon in SDR, naphthalene and phenanthrene are those in SDI. The aromaticity of SDI is greater than that of SDR. For SDR and SDI, oxygen atoms are present as carbonyl groups and nitrogen atoms exist in the forms of pyridine and pyrrole. The calculated chemical shift spectrogram of model is well consistent with that of the experimental results. The structural formulas calculated for SDR and SDI are $C_{181}H_{136}N_2O_{24}$ and $C_{186}H_{148}N_2O_{22}$, respectively.

Key words: coal inertinite concentrated ^{13}C-NMR aromaticity model construction

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通讯作者: 蔺华林, Tel: 13482272609, E-mail: linhualin@csclc.com。 E-mail: linhualin@csclc.com

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