



OPEN Structural characterization and macromolecular structure construction of non-caking coal in Chicheng Mine

Jinzhang Jia^{1,2}, Qiang Yang^{1,2,3}, Baogang Liu^{1,2} & Dongming Wang^{1,2}

Given that coal is not a homogeneous substance, it is of great significance to identify and quantify the structural characteristics thereof for comprehensive analysis. In this paper, the non-caking coal in Chicheng Coal Mine was selected as the research object. The C, H, O, N, and S contents in the coal samples were obtained by proximate/ultimate analysis experiments. The structural characteristics of aromatic, aliphatic hydrocarbons, and oxygen-containing functional groups in the experimental coal samples were obtained by Fourier transform infrared spectroscopy (FT-IR) experiments. X-ray photoelectron spectroscopy (XPS) experiments were performed to obtain the occurrence state of N and S elements in coal samples. Nuclear magnetic resonance (¹³C NMR) experiments provided the carbon skeleton structural information of the coal samples. The macromolecular structure model of non-caking coal in the Chicheng Coal Mine was established on this basis. The molecular formula of non-caking coal in Chicheng Coal Mine was determined to be C₂₀₀H₁₈₁O₁₂N₃S. The ¹³C NMR-predicted spectrum of the model showed good consistency with the ¹³C NMR-experimental spectrum obtained from the experiments, providing researchers with reference to the construction ideas and methods of molecular structure models of different coal samples.

The macromolecular structure of coal is complex, and significant molecular structure and morphological differences exist for coals at different metamorphic degrees¹. As such, it is imperative to build an accurate macromolecular structure model when studying the adsorption-diffusion of coal bed methane in coal. The structure of coal is closely related to its adsorption and reactivity properties, therefore coal structure is one of the main topics in coal chemistry research. The correct understanding of the occurrence status and microcrystalline structure parameters of the main elements in coal is of practical significance for constructing macromolecular structure models, studying the inherent properties of coal, achieving the “dual carbon” goal, and achieving high-quality development of the coal industry.

Initially, Picher² established the first macromolecular structure model of lignite by structural statistical analysis, which could quantitatively describe the aromatic and fatty clusters in coal structure. This provided the foundation for experimental research and theoretical analysis for developing the macromolecular structure model of coal. Given³ used infrared spectroscopy and X-ray diffraction methods to evaluate the ratio of aromatic hydrogen to aliphatic hydrogen and the composition of functional groups. The molecular structure model of bituminous coal with condensed aromatic structure mainly composed of benzene and naphthalene was constructed on this basis. However, the deficiency of this model was that the existence of S atoms and ether bonds was not considered, so it could not accurately reflect the chemical properties of low metamorphic bituminous coal.

Wiser⁴ constructed a coal macromolecular structure model with an aromatic structure (aromatic rings were cross linked by weak bonds such as ether bond, thioaldehyde bond, and short burning bond) and added the S element to the model. The Wiser model is considered a modern coal model that can comprehensively reflect the fundamental structure of coal molecules. Honda model⁵ was based on the aromatic structure of phenanthrene and naphthalene. Short bonds such as -CH₂ and -CH were used as cross linking structures to construct the Honda macromolecular structure model, which considers the existing forms of small molecular compounds and macromolecular compounds in coal molecular structure. Shinn⁶ constructed the Shinn bituminous coal macromolecular structure model based on the functional groups and bridge bond types on the coal's surface. The

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