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Development of a Macromolecular Model for Yangdong Coal Via NMR, FTIR, and XPS Spectroscopy

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Abstract

The molecular structure of coal is a critical factor determining its physicochemical properties and serves as a key bridge connecting macroscopic coal characteristics with microscopic molecular evolution. In this study, Yangdong coal (YD) was analyzed using a combination of techniques including proximate and ultimate analysis, Fourier transform infrared spectroscopy (FTIR), X-ray photoelectron spectroscopy (XPS), and solid-state nuclear magnetic resonance (13C NMR) spectroscopy to systematically determine its elemental composition, surface functional groups, aromatic structure configuration, and aliphatic structure distribution of the coal sample. The results indicated that the YD coal had a bridge/peripheral carbon ratio of 0.20 and an aromaticity of 77.98%. The aromatic structures were predominantly composed of benzene, naphthalene, and phenanthrene, while the aliphatic carbon structures were mainly in cyclic form. Based on the analytical data, the molecular formula of the coal was determined as $C_{200}H_{147}O_{22}N_3$, with a molecular weight of 2944.38. The constructed macromolecular model showed that the aromatic structural units consisted of six benzene rings, five naphthalene rings, two phenanthrene (or anthracene) rings, and one pyrene ring. Nitrogen atoms were present in the forms of pyridine and pyrrole. Using these findings, a molecular structure model was constructed and optimized through simulation, providing key insights into the molecular structure of coal and offering important guidance for its efficient utilization.

Keywords

Molecular Structure Model, ^{13}C NMR, XPS, FTIR.

1. Introduction

As a vital driver of China's economic development, the coal industry requires a comprehensive understanding of coal's fundamental structure and properties, particularly for supporting the modern industries that depend on this resource[1]. Coal is primarily utilized in thermal power generation, coke production, iron and steel smelting, and the development of new materials. As a complex and heterogeneous organic rock, it consists mainly of a macromolecular network structure and various inorganic minerals[2]. The physicochemical properties and utilization potential of coal are fundamentally governed by its molecular structure. Therefore, elucidating coal's structural characteristics at the molecular level is crucial for enhancing its efficient utilization and advancing clean conversion technologies.

Over the past few decades, researchers have made sustained efforts to elucidate the macromolecular structure of coal, leading to the proposal of approximately 140 structural models of coal and its derivatives[3]. Early studies primarily relied on chemical experimental methods such as pyrolysis and polycondensation to derive structural information, which was

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then used to construct planar molecular models. Among these, the models proposed by Krevelen, Given, Fuchs, Wiser, and Shinn are particularly representative[4]. The Krevelen model macroscopically characterized the coalification pathway and rank based on H/C and O/C atomic ratios. The Given model, which emphasized hydrogenated aromatic structures, effectively explains the liquefaction behavior of coal but underestimated its aromaticity. In contrast, the Fuchs model depicted a highly cross-linked three-dimensional polymer network, highlighting the physical rigidity of coal. The Wiser model, as a more balanced two-dimensional representation, integrated aromatic rings of varying sizes, bridging bonds, and heteroatoms, thereby laying the foundation for the modern understanding of coal structure. The Shinn model, reconstructed from experimental products, offered both quantitative insights and practical applicability[5].

In recent years, modern analytical techniques and computer-aided molecular design have been widely applied to construct molecular structure models of coal. Researchers have systematically investigated the microstructural characteristics of coal using a combination of techniques, including scanning electron microscopy (SEM)[6], X-ray diffraction (XRD)[7], X-ray photoelectron spectroscopy (XPS)[8, 9], Fourier-transform infrared spectroscopy (FTIR)[10], and nuclear magnetic resonance (NMR)[11, 12]. Research by Liu et al.[13], using optical profilometry and atomic force microscopy on multi-scale rough samples, demonstrated that lower surface porosity in coal enhances its hydrophobicity and wettability. At the molecular level, Jiang et al.[14] established systematic correlations between molecular parameters and vitrinite reflectance (R^o) in medium- to high-rank coals. While Yan et al.[15] identified the ubiquitous presence of amorphous and disordered carbon in coals of varying metamorphic degrees, observing progressive graphitization of aromatic layers with advancing metamorphism. To advance quantitative modeling, Ni and Zhang et al.[16, 17] comprehensively applied techniques including ultimate analysis, solid-state ^{13}C NMR, XPS, FTIR, and GC/MS to characterize aromatic structures, heteroatoms, and aliphatic carbon distributions in coal. Furthermore, Hu et al.[18] employed FTIR, ^{13}C NMR, and XPS to analyze functional groups and carbon skeleton structures, thereby validating the reliability of the molecular model in predicting wettability behavior.

However, due to the high heterogeneity of coal and its strong dependence on coalification history and geological conditions, the evolution of Yangdong coal has been significantly influenced by regional magmatic-thermal metamorphism, making existing generalized structural models inadequate. To overcome the limitations of relying on a single analytical technique, this study adopts an integrated approach combining ^{13}C NMR, XPS, and FTIR spectroscopy to construct a comprehensive two-dimensional molecular structure model for Yangdong coal. The specific objectives are: (1) to precisely determine aromaticity and the ratio of bridgehead to peripheral aromatic carbon using ^{13}C NMR; (2) to identify and semi-quantify key functional groups, particularly hydroxyl and carbonyl groups, via FTIR; (3) to quantitatively characterize the chemical speciation of carbon, oxygen, and nitrogen by XPS; and (4) to integrate multi-source structural parameters to propose a representative average two-dimensional molecular structure of Yangdong coal.

2. Materials and Methods

2.1. Samples and Sample Preparation

This study focuses on coal samples from the Yangdong Coal Mine (coded YD) in the Hanfeng coalfield. Following the deposition of the Carboniferous-Permian coal-bearing strata, this region has undergone multiple phases of intense tectonic movements, including the Indosinian, Yanshanian, and Himalayan orogenies[19, 20]. Consequently, the microstructure of YD coal is particularly complex. Investigating its microstructure will not only enhance the understanding of coal structural evolution under complex geological settings but also provide a critical

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structural basis for revealing the occurrence and migration patterns of gas in this mining area, thereby elucidating the mechanisms of coal and gas outbursts.

2.2. Proximate and Ultimate Analysis

The coal samples underwent proximate and ultimate analysis following the procedures outlined in GB/T212-2008 and GB/T476-2008. The test results provided basic parameters of the coal samples, and coal quality analysis was subsequently conducted.

Table 1. Property analyses of coal samples.

Sample	Proximate analysis (wt.%)					Ultimate analysis (wt.%)						
	M_{ad}	A_{ad}	V_{daf}	F_c		C	H	O	N	S	H/C	R_0
YD	1.28	12.26	19.83	66.63		80.02	3.76	14.47	1.30	0.45	0.56	1.73

As shown in Table 1, the YD coal sample was classified as medium-rank coal. Normalization of the data yielded atomic ratios of H/C, O/C, N/C, and S/C as 0.5639, 0.1356, 0.0139, and 0.0021, respectively, for its molecular structure. These elemental ratios, determined from the compositional analysis, provided essential constraints for constructing the molecular model of YD coal.

2.3. FTIR Spectroscopy Analysis

FTIR tests are effective for investigating the functional groups and molecular structure of coal. The in-situ DFTIR spectra were obtained using an FTIR spectrometer (Nicolet™ iS20, Thermo Fisher Scientific™, USA)[21]. The demineralized coal samples were first dried, then mixed with KBr in a 1:99 ratio, and milled for two hours to ensure complete mixing. An infrared lamp was used during the milling process in the agate mortar to prevent moisture absorption. The mixture was then placed into a small crucible and dried in a vacuum oven for about 10 hours. After drying, the coal samples were transferred to the testing instrument, where 16 scans were performed in the spectral range of 4000–650 cm^{-1} with a resolution of 4 cm^{-1}, generating the in-situ DFTIR spectra.

2.4. XPS Spectroscopy

XPS analysis was conducted using a Thermo Scientific K-Alpha spectrometer (ThermoFisher) under an analysis chamber vacuum of approximately 5×10^{-9} mbar. A monochromated Al Kα X-ray source (hν = 1486.6 eV) was employed with an accelerating voltage of 12 kV and a filament current of 6 mA. Spectra were acquired in constant analyzer energy (CAE) mode with a pass energy of 100 eV and a step size of 1.0 eV, using an instrument work function of 4.2 eV. High-resolution spectra of C1s, O1s, N1s, and S2p were collected, and all binding energies were calibrated relative to the C1s peak at 284.8 eV.

2.5. 13C-NMR Spectroscopy

Solid-state ^{13}C Nuclear Magnetic Resonance (NMR) spectroscopy was conducted using an Avance NEO 400WB wide-bore solid-state spectrometer (Bruker, Germany). Samples were packed into 4 mm ZrO_2 rotors and analyzed using a complete sideband suppression technique at a spinning rate of 10 kHz. The detection was carried out at a resonance frequency of 100.62 MHz, with an acquisition time of 2 ms and a recycle delay of 4 s, each sample was scanned 1024 times.

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3. Results and Discussion

3.1. ^{13}C-NMR Spectroscopy Analysis

Fig. 1 displays the deconvoluted ^{13}C NMR spectrum of YD coal, revealing three distinct chemical shift regions: aliphatic carbon (0-90 ppm), aromatic carbon (90-170 ppm), and carboxyl/carbonyl carbon (170-240 ppm). The aromatic carbon peak in the 90-170 ppm region showed the most prominent absorption signal, suggesting that the carbon atoms in the molecular structure primarily existed as protonated aromatic carbon and alkyl-substituted aromatic carbon.

The ^{13}C NMR spectroscopy was deconvoluted using PeakFit software, with carbon functional groups assigned based on their characteristic chemical shifts. The relative areas of the deconvoluted subpeaks were calculated to determine the proportional distribution of carbon skeletal structures and derive structural parameters for constructing the molecular model of YD coal. As summarized in Table 2, the carbon skeletal structure of YD coal was dominated by aromatic carbon (67.57%), significantly higher than aliphatic carbon (22.34%) and carbonyl/carboxyl carbon (10.09%). The bridgehead carbon ratio (X_{BP}), an indicator of aromatic condensation degree, was further introduced to characterize the backbone structure of YD coal.

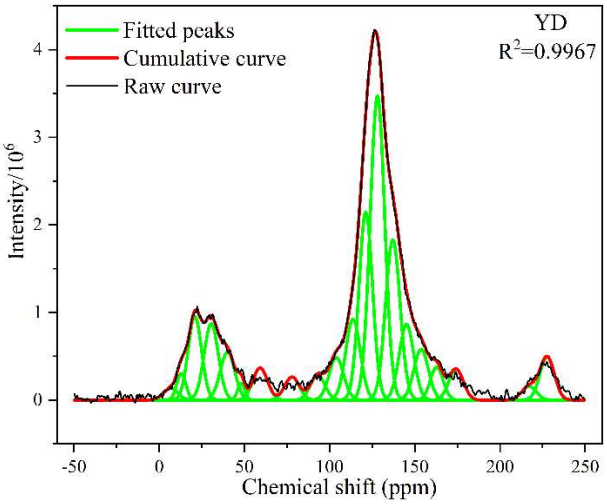

Fig. 1 ^{13}C NMR spectroscopy of YD coal.

Table 2. The ^{13}C NMR parameters of the coal sample.

Sample	f_{al}^*	f_{al}^H	f_{al}^O	f_a^H	f_a^B	f_a^S	f_a^P	f_a^N	f_a^C	$f_{a`}$	fa	f_{al}
YD	7.97	9.87	4.18	47.45	12.13	5.73	6.04	23.9	6.63	71.35	77.98	22.02

$$X_{BP} = \frac{f_a^B}{f_a^S + f_a^P + f_a^H} \quad (1)$$

The structural parameter XBP for YD was calculated to be 0.20 using Equation (1). According to the definition of bridgehead carbon ratio, the reference values for typical aromatic structures are: 0 for benzene, 0.25 for naphthalene, 0.4 for anthracene/phenanthrene, and 0.4 for pyrene. These results indicated that the aromatic structure of YD coal was dominated by benzene and naphthalene rings, with three- and four-ring aromatic units present in relatively lower proportions.

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3.2. FTIR Spectroscopy Analysis

Infrared spectroscopy is a powerful tool for studying the chemical structure of coal and can be widely used for characterizing coal structures. The infrared absorption peaks can be divided into four categories: hydroxyl groups (3000~3600 cm^{-1}), aliphatic hydrocarbon structures (2700~3000 cm^{-1}), oxygen-containing functional groups (1000~1800 cm^{-1}), and aromatic hydrocarbon structures (700~900 cm^{-1}). Based on previous studies and in accordance with functional group assignments, the FTIR spectral fitting results for YD coal are presented in Fig. 2.[22, 23]

The infrared spectral fitting results indicated that the absorption peaks within the range of 700~900 cm^{-1} (Fig. 2 (d)) were relatively continuous, confirming the presence of aromatic benzene ring structures. Among them, the absorption peak near 810 cm^{-1} was the most intense, indicating that the substitution pattern of the benzene ring is mainly 1,2,4-trisubstituted. Meanwhile, the distinct absorption peaks at 720 cm^{-1} and 732 cm^{-1} suggested that the coal also contains a certain amount of 1,2-disubstituted and 1,2,3-trisubstituted structures. Additionally, the absorption peak at 710 cm^{-1} reflected the skeletal vibration of $(CH_2)n$ on the normal alkyl side chain. The oxygen element in YD coal mainly existed in the form of carboxyl, hydroxyl, ether bonds, and carbonyl groups. A small absorption peak observed near 1270 cm^{-1} can be attributed to the contribution of aromatic C=C skeletal vibrations and methyl deformation vibrations. A sharp absorption peak at 1400 cm^{-1} was characteristic of Si-O-Si bond stretching vibrations. The distinct absorption peaks at 1550 cm^{-1} and 1650 cm^{-1} indicated the presence of ester, ketone, and aldehyde type C=O bonds in the molecular structure (Fig. 2 (c)).

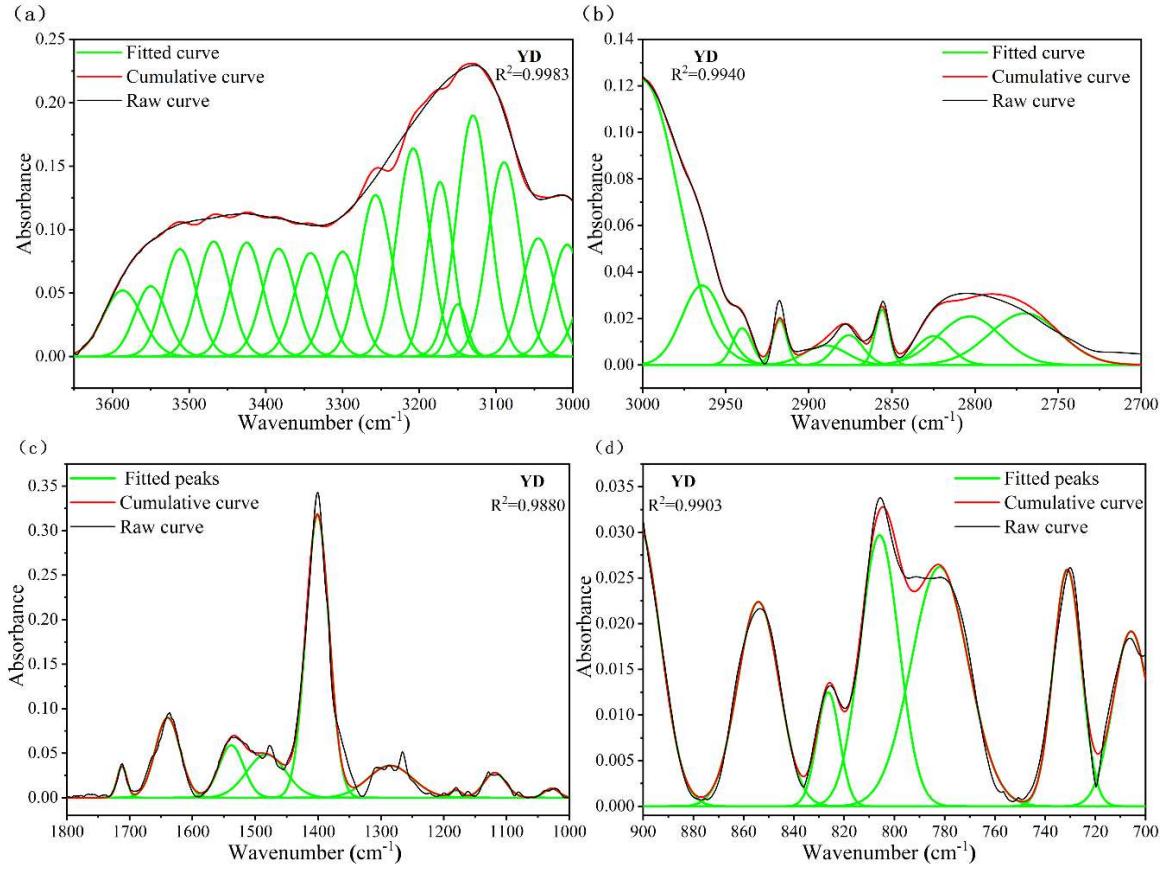

Fig. 2 Curve-fitting of the FTIR pattern of YD coal.

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The absorption peaks in the 2700–3000 cm^{-1} range were primarily attributed to aliphatic hydrocarbons. In particular, the fitting results around 2795, 2855, 2917, and 2995 cm^{-1} were satisfactory, and these peaks corresponded to the symmetric stretching of CH_2, symmetric stretching of CH_3, asymmetric stretching of CH_2, and asymmetric stretching of CH_3, respectively (Fig. 2 (b)). Quantitative analysis revealed that in the molecular structure of YD coal, the proportions of methyl, methylene, and methine groups were 28.46%, 43.72%, and 27.83%, respectively, indicating that the alkyl side chains were predominantly composed of methylene, supplemented by methyl and methine groups. These aliphatic structural characteristics provided an important basis for constructing the molecular structure model of YD coal. As shown in Fig. 2 (a), a broad absorption band was observed in the 3000–3600 cm^{-1} region, which was characteristic of abundant free hydroxyl groups, suggesting the possible presence of phenolic and alcoholic compounds, with the maximum absorption peak located near 3140 cm^{-1}.

3.3. XPS Spectroscopy Analysis

XPS was employed to characterize the chemical states of elements such as C, O, N, and S in coal and their relative abundances, making it a widely used technique for investigating coal molecular structures. The results obtained from the analysis and fitting of the test data for YD coal are shown in Fig. 3, with the detailed data summarized in Table 3. The C1s spectrum was deconvoluted into three characteristic peaks: the peak at a binding energy of 284.8 eV was assigned to C–C/C–H bonds in aromatic structures and substituted alkanes, with a relative content of 80.34%; the peak at 286.0 eV was attributed to C–O structures in ether and hydroxyl groups, accounting for 14.35%; and the peak at 289.13 eV was assigned to COO– groups in carboxyl functionalities, contributing 5.31% (Fig. 3 (a)). These results indicated that aromatic carbon was the predominant form of carbon in the YD coal molecular structure, while the content of carboxyl carbon was very low.

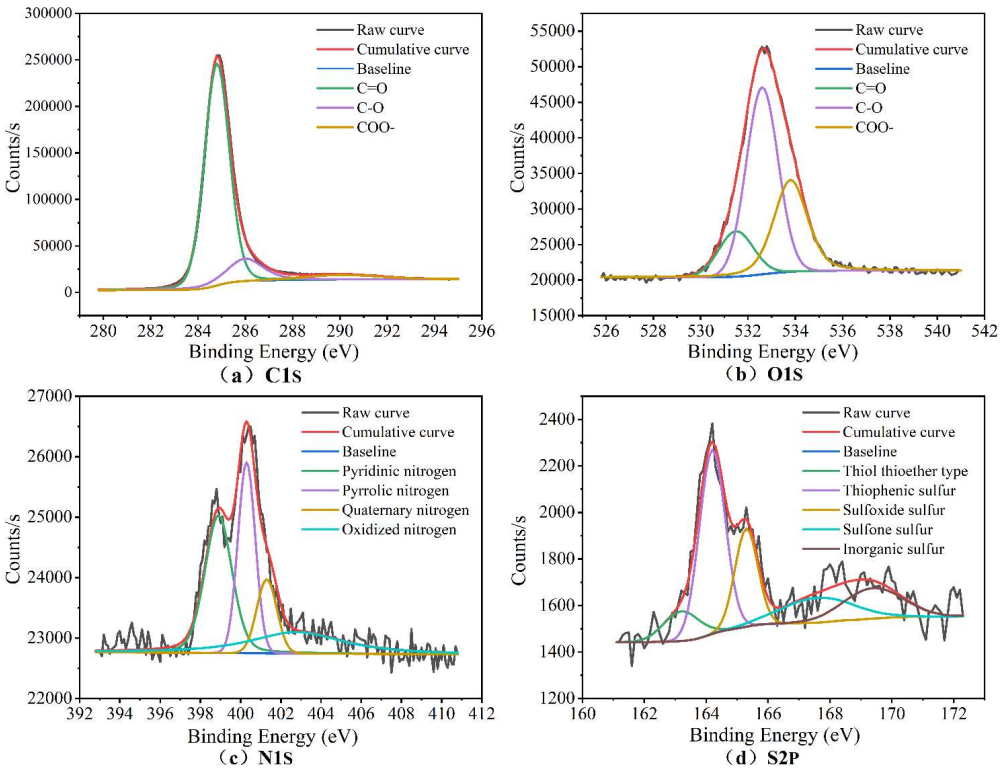

Fig. 3 XPS spectra and fitted curves of YD coal.

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As shown in Fig. 3 (b), peak fitting of the O1s XPS spectrum for YD coal revealed three distinct oxygen species. These were identified as carbonyl oxygen (C=O) at 531.5 eV, ether oxygen (C–O) at 532.6 eV, and carboxyl oxygen (COO–) at 533.80 eV, with relative contents of 14.26%, 34.94%, and 31.70%, respectively. The distribution shows that organic oxygen is primarily present as C–O and COO– bonds, with a small proportion existing as C=O bonds.

Table 3. XPS C1s , O1s , N1s, and S2p data of YD coal components.

Elemental peak	Center gravity /eV	Functionality	Relative area percentage /%
C1s	284.8	C—C, C—H	80.34
	286.0	C—O—	14.35
	290.0	COO—	5.31
O1s	531.5	C=O	14.26
	532.6	C—O	54.04
	533.8	COO—	31.70
N1s	398.9	Pyridinic nitrogen	35.28
	400.3	Pyrrolic nitrogen	28.54
	401.3	quaternary nitrogen	12.70
	402.8	oxidized nitrogen	23.49
S2p	163.2	Thiol thioether type	9.01
	164.2	Thiophenic sulfur	40.82
	165.3	Sulfoxide sulfur	19.23
	167.6	Sulfone sulfur	15.17
	169.4	Inorganic sulfur	15.76

According to Fig. 3 (c), peak fitting of the N1s XPS spectrum for YD coal revealed four types of nitrogen functionality: pyridinic (398.9 eV, 35.28%), pyrrolic (400.3 eV, 28.54%), quaternary (401.3 eV, 12.70%), and oxidized nitrogen (402.8 eV, 23.49%). The prevalence of pyridinic and pyrrolic nitrogen species indicates that nitrogen atoms are primarily incorporated into aromatic structures such as pyridine and pyrrole rings, suggesting a high stability for the nitrogen forms in this anthracite. The peak-fitting analysis of the S2p spectrum identified five sulfur species in YD coal. The distribution was dominated by organic sulfate (a doublet at 165.28/166.68 eV, totaling 43.94%), followed by thiophenic sulfur (164.2 eV, 40.82%). The remaining spectral components were assigned to other sulfur forms.

3.4. The Molecular Structure of Coal

Through calculation and structural optimization, a molecular structure model of YD coal was obtained. The bridge carbon/peripheral carbon ratio (X_{BP}) of this model was adjusted iteratively until the calculated value reached 0.20, matching the experimental measurement. The aromatic structural units in the model consisted of benzene (6), naphthalene (5), anthracene (1), phenanthrene (1), pyrene (1), pyridine (2), and pyrrole (1), totaling 144 aromatic carbon atoms as can be seen in Table 4. Based on the aromatic carbon rate (Fa = 77.98%) determined by nuclear magnetic resonance, the total number of carbon atoms was calculated to be 202, which included 58 aliphatic carbon atoms.

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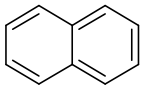
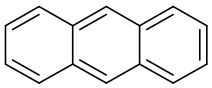
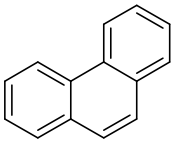
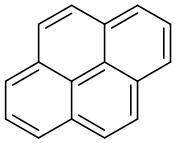
Table 4. Types of aromatic structure units in the chemical structural model of group components.

Types							
YD	6	5	1	1	1	2	1

According to the elemental analysis of YD coal, oxygen accounted for 14.47% of the total element content. Based on the O/C atomic ratio, it was estimated that there were approximately 27 oxygen atoms in the molecular structure of YD coal. FTIR analysis indicated that the coal contained oxygen-containing functional groups such as hydroxyl, carboxyl, ether, and carbonyl groups. Combined with the fitting results of the O1s XPS spectrum, it was further inferred that the numbers of carboxyl, ether, and carbonyl groups were approximately 5, 5, and 6, respectively.

In addition, elemental analysis showed that nitrogen accounted for only 1.30% of the total elements. Based on the N/C atomic ratio, it was estimated that there were approximately three nitrogen atoms in the molecular structure of YD coal. The N1s XPS spectra indicated that nitrogen atoms existed predominantly as pyridinic and pyrrolic nitrogen, followed by protonated pyridine and nitrogen oxides. Based on the above analysis, two pyridinic nitrogen atoms and one pyrrolic nitrogen atom were incorporated into the two-dimensional molecular model of YD coal to reflect the dominant nitrogen forms. Although organic sulfur was primarily present as thiophenic sulfur, elemental analysis showed that sulfur accounted for only 0.45% of the total elements, with an S/C atomic ratio of 0.0021. Due to the extremely low content, corresponding to fewer than one sulfur atom in the model, no sulfur atoms were included in the final two-dimensional molecular structure of YD coal.

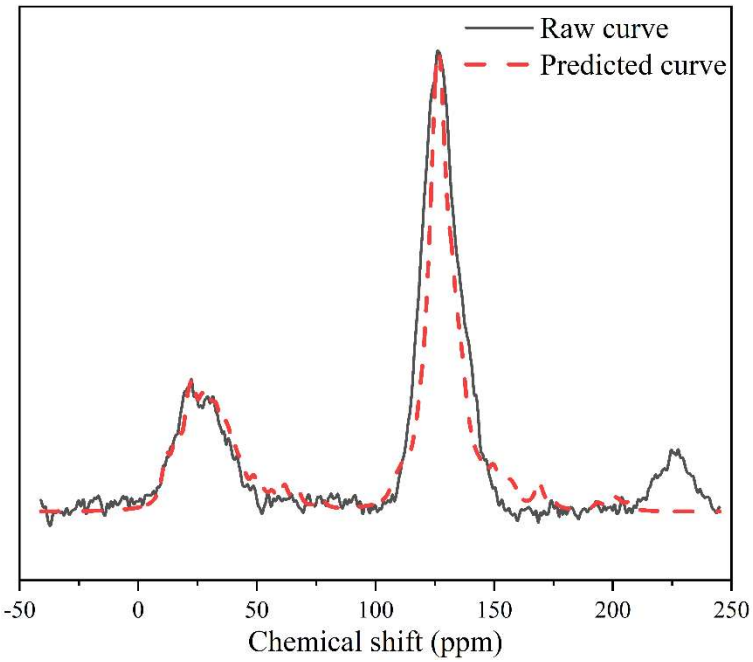


Fig. 4 Chemical structural model of YD coal.

The initial planar model of the YD coal macromolecule was drafted using ChemDraw. The ^{13}C NMR spectrum was then simulated with MestreNova software. By repeatedly comparing the calculated spectrum with the experimental one, the molecular structure and functional group

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positions were progressively adjusted and optimized until satisfactory agreement was achieved (Fig. 4). The final macromolecular structure model of YD coal, shown in Fig. 5, was established with a molecular formula of $C_{200}H_{147}N_3O_{22}$ and a molecular weight of 2944.38.

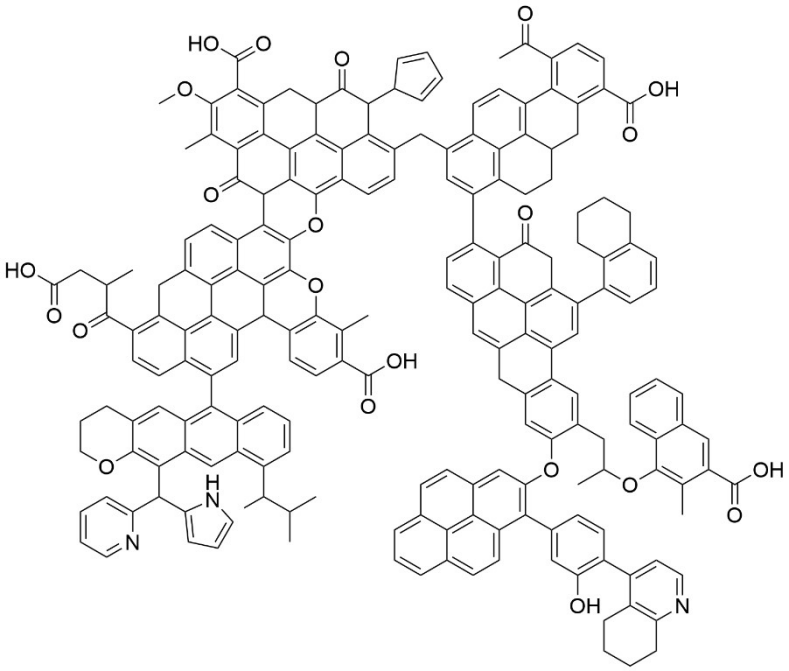

Fig. 5 Chemical structural model of YD coal.

4. Conclusion

In this study, modern characterization techniques were combined with molecular simulation to analyze coal samples from the Yangdong Coal Mine (Hanfeng coalfield), leading to the construction of a representative molecular structure model. The main conclusions are as follows:

(1) ^{13}C NMR characterization revealed the molecular structural features of YD coal: its bridge-peripheral ratio is 0.20, and the aromatic carbon content is 77.98%; aromatic carbon dominates the carbon skeleton (67.57%), significantly higher than aliphatic carbon (22.34%) and carbonyl carbon (10.09%). Further analysis indicates that the aromatic structure is mainly composed of units such as benzene, naphthalene, and phenanthrene, while the aliphatic carbon is primarily cyclic.

(2) XPS and FTIR analyses indicated that oxygen in YD coal existed primarily in three forms: carbonyl oxygen (C=O, 531.5 eV; 14.26%), ether oxygen (C–O, 532.6 eV; 34.94%), and carboxyl oxygen (COO–, 533.80 eV; 31.70%). Regarding nitrogen speciation, pyrrolic nitrogen was identified as the most abundant form, followed by pyridinic nitrogen. In addition, the alkyl side chains were found to be dominated by methylene groups, with methyl and methine groups serving as secondary constituents.

(3) A coal molecular model demonstrating strong spectral consistency and structural validity was successfully constructed. The distribution of its functional groups and the configuration of its carbon framework were characterized using ^{13}C NMR, FTIR, and XPS. A two-dimensional molecular structure with the formula $C_{200}H_{147}N_3O_{22}$ was developed, and the structural reliability of the model was confirmed by the agreement between simulated and experimental spectral data.

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