Application of FTIR spectrometry on studying thermal simulation of brown coal: Implications for its hydrocarbon generation

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Fourier Transform infrared spectrometry (FTIR) is one of the most powerful and convenient technique for the characterization of coal, kerogen and other sediments in organic geochemistry. This paper describes the use of FTIR spectrometer to study the chemical structures of residue from thermal simulation experiment of brown coal. The coal was collected from Tengchong-Lianghe basin, Yunnan Province, SW China. The method of curve-fitting analysis was used in order to more precisely quantify peak areas of different chemical structures. Analytical results indicate that variation of FTIR spectra corresponds to the stage of hydrocarbon generation relatively well.

In the first stage, when simulation temperature is from room temperature (24°C) to 200°C, FTIR spectra area around 1705cm^{-1} which represents stretching vibration of oxygenous groups in coal descends fastly. In the meanwhile, we observed there are a lot of CO_2 generated. Area around 2950cm^{-1} and 2920cm^{-1} represents asymmetric stretching vibration of methyl (A_{CH3}) and methylene (A_{CH2}) changes unconspicuously. The yield of total hydrocarbon is from 20.9mg/gTOC to 41.0mg/gTOC. The HI and S_1+S_2 of coal show slight change. In the second stage (200-350°C), the sum of A_{CH3} and A_{CH2} diminishes, accompanying generation of oil and gas in experiment. The yield of total hydrocarbon is from 41.0mg/gTOC to174.9 mg/gTOC. The HI and S_1+S_2 is from 172mg/gTOC to 10mg/gTOC and 95.04mg/g to 34.39mg/g, respectively. The ratio of A_{CH3} and A_{CH2} increases as a result of the break of long aliphatic chains. In the last stage (>350°C), area around 1600cm^{-1} which presents stretching vibration of aromatic ring increases because of condensation of aromatic rings. The sum of A_{CH3} and A_{CH2} decreases to zero almostly. The yield of total hydrocarbon reaches 238.2 mg/gTOC. The HI and S_1+S_2 descreases to 4mg/gTOC and 3.69mg/g, respectively.

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Geochemical characteristics of Longqiao iron deposit, Anhui, China

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Longqiao iron deposit located in the north margin of Luzong basin, Anhui Province, China, is a large, high-grade layered magnetite deposit. Iron mineralization is strictly controlled by the stratum of DongMaanshan Group of Middle Triassic. The principal intrusive rocks related to the mineraliztion are plutonic syenite (monzonite) and hypabyssal syenite porphyry.

The main ore mineral in Longqiao iron deposit is magnetite and less hematite. The magnetite decrepitated temperature have two obvious ranges of 360~390°C and 410~450°C.Chemically these different magnetite are characterized by magnetite contains very low V and Ti contents, generally about hundreds ppm, lower about one order of magnitude than that in porphyritic iron ores, Ti/TFe ratios are also declining. Na_2O,K_2O, MgO and CaO in magnetite and hematite are relatively high comparing with porphyritic ones. The ∑REE, LREE/HREE, $(La/Yb)_N$, $(La/ Sm)_N$ and $(La/Lu)_N$ ratios have a wide range, and obvious Eu and Ce anomaloes. The magnetite mineralization process can be divided into thermal metamorphic stage and magmatic hydrothermal reworked stage.

Hydrogen- and oxygen-isotope data suggested that the ore-forming fluids in Longqiao iron deposit mostly consisted of magmatic water, mixed in various proportions of meteoric water. The variation of sulfur isotopic composition of the pyrite and anhydrite were not resulted from changes of physicochemical conditions, but rather due to compositional variation of sulfur at the sources. Lead isotopic composition provides similar results.

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[1] Wu *et al.* (1996) Special Publication.