Report on Micro-FTIR characterization of different rank coals Working Group (2012-2013)

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Introduction

FTIR has been widely studied to characterize coal macerals (Lin et al., 1993; Mastalerz et al., 1993, 1995, 1996; Bustin et al, 1999; Guo et al., 1996, 1998; Liu et al., 1998; Li et al., 1998; Wang et al., 2011; Chen et al., 2012). However, considering the sample preparation and individual maceral determination, in situ reflectance micro-FTIR has more advantages than FTIR techniques. Unfortunately, the study on the application of micro-FTIR on coal and maceral is not very common, especially for coal of different ranks.

Activities

Samples selected. Eight samples, from lignite to anthracite, were collected from various coal mines in China. Details are listed in Table 1, along with the maximum vitrinite reflectance values. The samples were prepared as polished blocks for Micro-FTIR analysis.

Table 1 General information of coal samples used

Samples #ID	Sources	coal rank	Ro (%)
JS	Jinsuo coal mine	lignite	0.32
W-C6	Wulantuga coal mine	Subbituminous coal	0.45
J6-6	Zhungeer coal mine	high volatile C bituminous coal	0.59
HD-XG-8	Hedongcoalfield	high volatile B bituminous coal	0.75
HZ-CC-2	Caocun coal mine	high volatile A bituminous coal	1.03
SHT-13-3	Wuhai coal mine	medium volatile bituminous coal	1.12
A-18	Adaohai coal mine	low volatile bituminous coal	1.59
JC-WTP-4	Jinchen coal mine	anthracite	3.81

Micro-FTIR analysis. Measurements were made with a Nicolet model 6700 Fourier-transform infrared spectrometer equipped with the Nicolet Continuμm microscopy, as well as the OMNIC 8 software. Spectra were recorded by co-adding 300 scans at a resolution of 4 cm^{-1}.For each test, telocollinite was chosen and spectra were Kramers-Kronig transformed to obtain an absorbance spectrum. The Peak separation and semiquantitative calculation of Micro-FTIR were done using the curve-fitting program of PeakFit software.

Results and discussion

Micro-FTIR characteristics of coals

The standard Micro-FTIR spectra of different coal ranks are presented in Figure 1; the identified functional groups include aromatic CHx, aliphatic CHx, aromatic carbon, oxygenated groups, and aromatic CHx out-of-plane deformation. As rank increase the peak intensities of aliphatic CHx decrease, corresponding that of aromatic carbon increase. This indicates that the results obtained by Micro-FTIR method in this study is the same with the general conclusion in previous works.

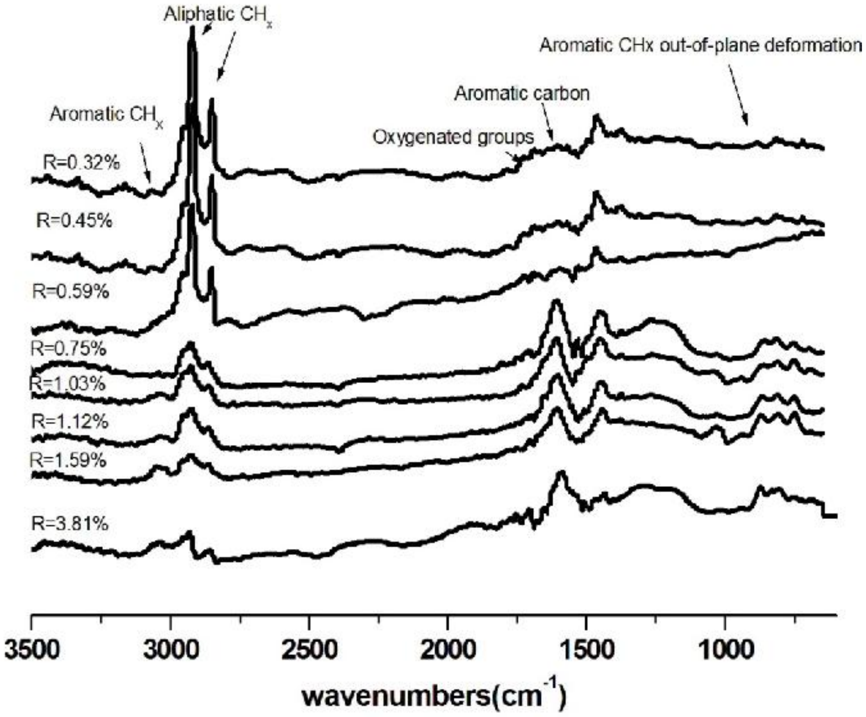

Figure 1.Micro-FTIR spectra of samples used.

The peaks selected for Mirco-FTIR by curve fitting analysis in this work are the relatively more intense and stable absorption peaks. The band area (not peak intensity) was used. The curve-fitting analyses of sample W-C6 in the region of 3000-2800 cm^{-1} and of sample SHT-13-3 for the region of 900-700 cm^{-1}, are shown in Figures 2 and 3, respectively.

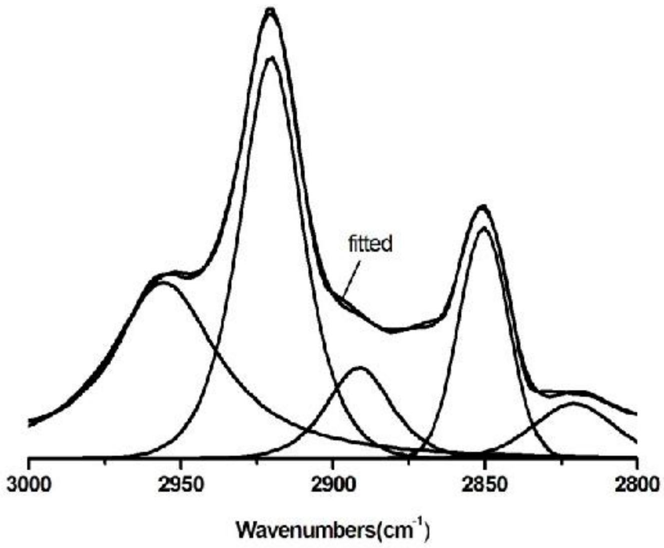

Figure 2. Curve-fitted micro-FTIR spectra between 3000-2800 cm^{-1} for coal sample W-C6.

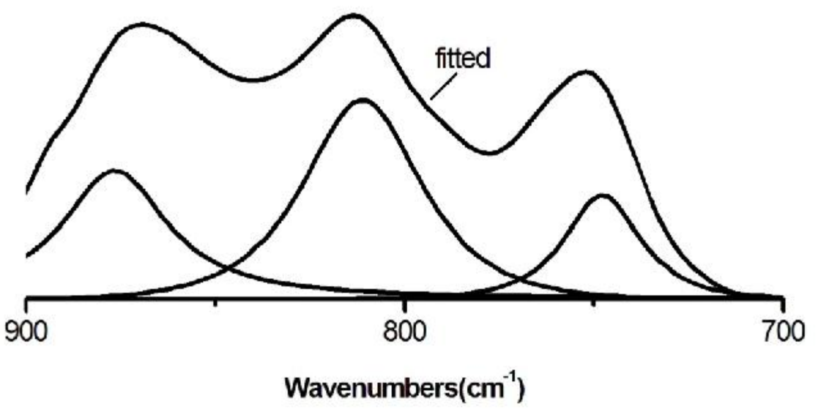

Figure 3. Curve-fitted micro-FTIR spectra between 900-700 cm-1 for coal sample SHT-13-3.

Structural parameters of Micro-FTIR analysis

Some structural parameters were selected to evaluate the chemical characteristics of coals used. The CH_2/CH_3 (2920 cm^{-1} / 2950 cm^{-1}) ratio is used to estimate the length and degree of branching aliphatic side chains. The integrated area of H_{AL} (3000-2700 cm^{-1}) might be considered to estimate the concentration of aliphatic hydrogen. The ratio of integrated areas of 3000-2800 cm^{-1} to 900-700 cm^{-1} (I_2) can be used to compare the relative abundance of aliphatic and aromatic functional groups.

Figure 4 shows the relationship between the CH_2/CH_3 ratio and the coal rank for the samples used. Although the correlation coefficient is 0.812, the relation between the CH_2/CH_3 ratio and the coal rank is obvious. With the coal rank increase, the CH_2/CH_3 ratio decrease.

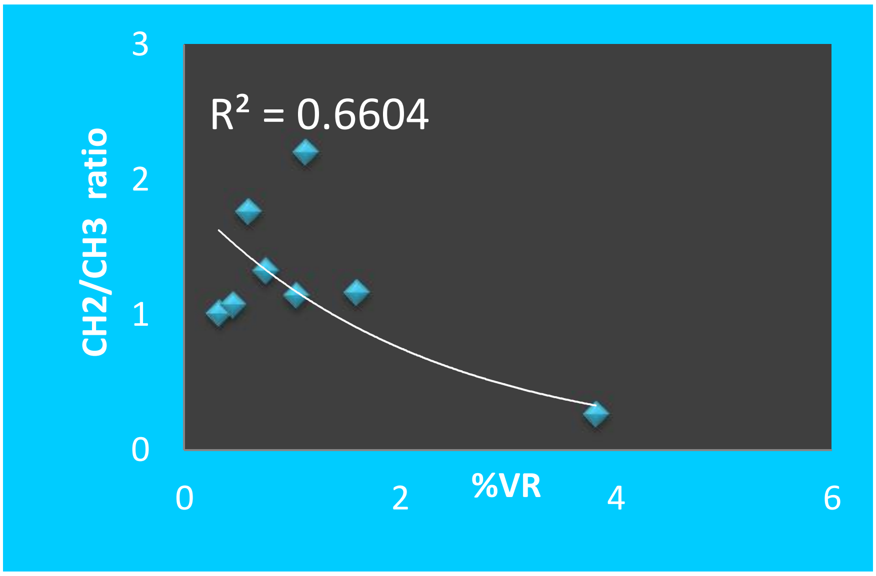

Figure 4.The relation between CH_2/CH_3 ratio and coal rank.

In order to study the relationship between coal rank and relative abundance of aliphatic and aromatic functional groups, the I2 index was plotted against rank (Figure 5). It should be noted that the correlation coefficient between those two parameters is low when all the samples were considered. The reason should be further studied. When the samples JS and J6-6 were taken out, the correlation coefficient is up to 0.84.

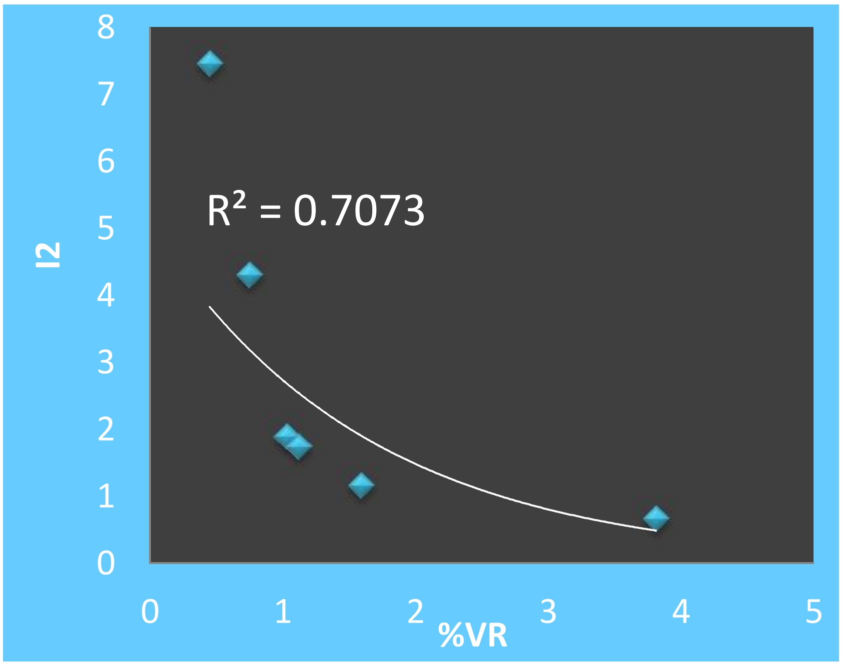

Figure 5.The relation between $I_2$and coal rank.

Meanwhile, the relationship between coal rank and the concentration of aliphatic hydrogen was also studied (Figure 6).The Hal steadily decreased from VR=0.32% to 1.59%, followed increase when almost VR>2.4%. In Figure 1, the weaknesses of the aliphatic CHx stretching signal around 3000-2700 cm^{-1} for the JC-WTP-4 sample that is high rank coal. It is difficult to obtain the value of the concentration of aliphatic hydrogen for JC-WTP-4. Therefore, it seems to be reasonable to study the relationship between the coal rank and the concentration of aliphatic hydrogen for coals when VR<1.5%.

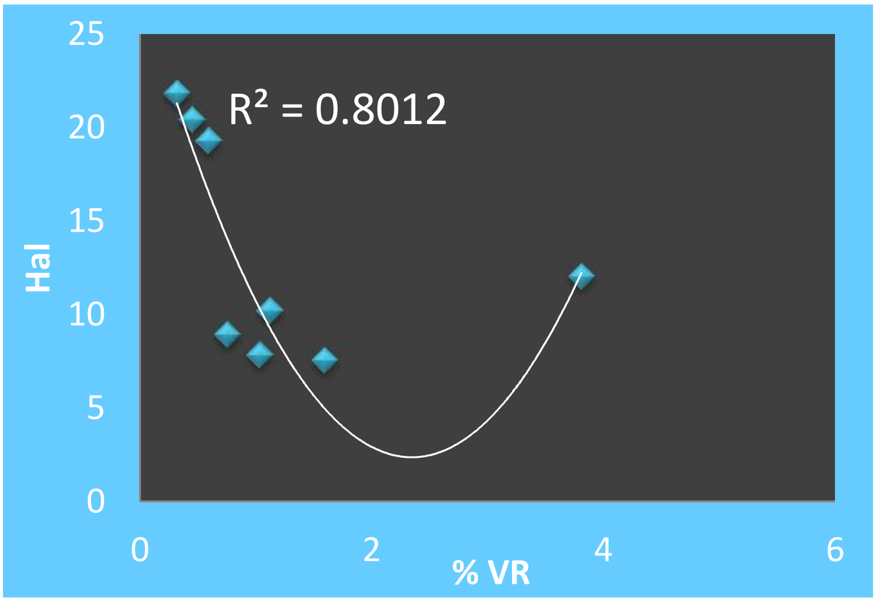

Figure 6.The relation between aliphatic hydrogen(Hal) and coal rank.

Conclusions

1. The peak characterization of coals from peat to anthracite using Micro-FTIR techniques can be obtained.
2. Preliminary studies show the correlations between coal rank and the CH_2/CH_3 ratio and the concentration of aliphatic hydrogen for the samples used, respectively.

Main References

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