RESEARCH ARTICLE

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# The Spontaneous Combustion Potency of Lignite Coal Based on FTIR

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**ABSTRACT**

**To understand the role of functional groups in the spontaneous combustion of lignite coal, the distribution of functional groups in the lignite coal of the Sajau Formation in the Berau Basin, Indonesia, was studied. The functional group characterization was carried out using the Fourier Transform Infra Red (FTIR) method. The results revealed the presence of four functional groups, namely hydroxyl structures, aliphatic structures, oxygen-containing structures, and aromatic structures. The lignite contained more hydroxyl and oxygen-bearing functional groups, from which aliphatic and aromatic; therefore, spontaneous combustion becomes easy in lignite coal.**

**Keywords:** Coal, Lignite, FTIR, Functional Spontaneous Combustion.

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## I. Introduction

Mining activities are subject to various hazards, including spontaneous combustion [1], [2]. Adverse consequences of the spontaneous combustion of coal include environmental problems [3], [4], economic losses [5], and safety- and work-related problems [6]. An assessment of the potential tendency for spontaneous combustion is, hence, extremely important in order to reduce economic, social, and environmental risks [7].

Several characteristics of coal can trigger spontaneous combustion, such as oxygen concentration, moisture content, maceral composition, coal pore properties, activity and content of each chemical functional group, and inherent coal property [8]-[11].

Several chemical processes that occur during the oxidation process involve oxygen adsorption, the formation of stable compounds and gases, decomposition of unstable intermediates, and the formation of peroxides, hydro-peroxides, and hydroxyl species [12]-[17]. The Fourier Transform Infra Red (FTIR) method is often employed for identifying functional groups and micro-chemical transformation in coal. During the drying process of lignite in air, which produces ester compounds, functional groups containing oxygen will increase and then decrease due to decomposition or by reacting with hydroxyl groups [18]. During the oxidation process in coal, carboxyl, carbonyl, and hydroxyl compounds can be formed from peroxy acid [19]. Due to changes in temperature and coal rank, oxygen species compounds, such as carboxyl, carbonyl, hydroxyl, ethers, and methoxy groups, in coal look distinct reaction [12]. Thus, the overall coal oxidation process involves an increase in the oxygen functional group, which is accompanied simultaneously by a reduction in the aliphatic content [20], [21].

Coal in the Sajau Formation located in the Berau Basin in the northern part of Kalimantan Island, Indonesia, is a typical low-rank coal with a measured reserve of 1 ×109 MT, which can be used as an energy source or for other industrial purposes. However, being a typical low-rank form of coal, the potential for self-combustion in Sajau coal is quite large. The present research was conducted to study the micro-chemical changes of lignite coal using FTIR with the aim of revealing the oxidizing characteristic of coal and the tendency for spontaneous combustion to occur.

## II. Experimental Study

### A. Materials

Five lignite coals from Berau Basin, North Kalimantan, were used in this research. To identify the characterization of the functional groups of coals by FTIR analysis, proximate and ultimate measurements were carried out.

### B. Methods

#### 1) Proximate, and Ultimate Measurements

The proximate analysis measured moisture, volatile matter, fixed carbon, and ash of coals. The ASTM standard of D-3173, D-3174, D-388, and D-3175 was used as a reference for moisture, ash, fixed carbon, and volatile matter, respectively. The standard reference used in identifying elements in coal through ultimate analysis is as follows: ASTM D-3178 for carbon and hydrogen, ASTM D-3179 for nitrogen, ASTM D-3177 for sulphur, and oxygen (%) by difference: 100 - (%C + %H + %N + %S organic). The result of proximate and ultimate measurements is tabulated in Table I.

*2) FTIR Spectroscopy*

In the pre-treatment of the FTIR investigation, coal samples were treated with acid to remove the impurities within. In the acid treatment experiment, coal was crushed to powder size (200 mesh), resulting in as much as 50 grams. It was then kept in 300 ml of an acid mixture consisting of 120 ml of hydrochloride acid and 180 ml of hydrofluoric acid for 1 day at a temperature of 600 ºC. Furthermore, to ensure that the coal sample remained in a neutral state, the sample was washed with deionized water and filtered. In this study, the potassium bromide pellet (KBr pellet) technique was used in the FTIR measurement. Scans were carried out with a 4 cm-1 resolution scanning of 4000–400 cm-1 from 32 scans per spectrum FTIR interferogram. Bruker FT Infrared spectrometer was used for this process. The FTIR peak assignments were used from previous studies [22]–[27]. Table II presents a list of the band assignments used in this study.

## III. Result And Discussion

### *A. Proximate and Ultimate Measurements*

Table-I shows the result of the proximate and ultimate measurements of lignite from Berau Basin, North Kalimantan. The arithmetic mean of H/C = 1.08 and O/C = 0.37. All the coals show the presence of moderate moisture and ash at 17.16–22.58 wt. % and 10.01–20.40 wt. %, respectively. The coals have moderate volatile matter (38.37%–40.77%) and fixed carbon (28.85%–33.40%). The samples have low sulphur (1.07–2.03 wt. %). The measurement of C-H-N-S-O elements in coals indicated that carbon had the highest presence, compared to the other elements. It was followed by oxygen and hydrogen, while elemental nitrogen was present in the least quantity (Table I). Based on the H/C vs. O/C ratios [23] and a heating value of 7,277.42–7,747.42 Btu/Lb., these coals are lignite-A in rank.

### *B. Fourier Transform Infra-Red*

Fig. 2 shown the representative FTIR spectra of lignite as received samples.

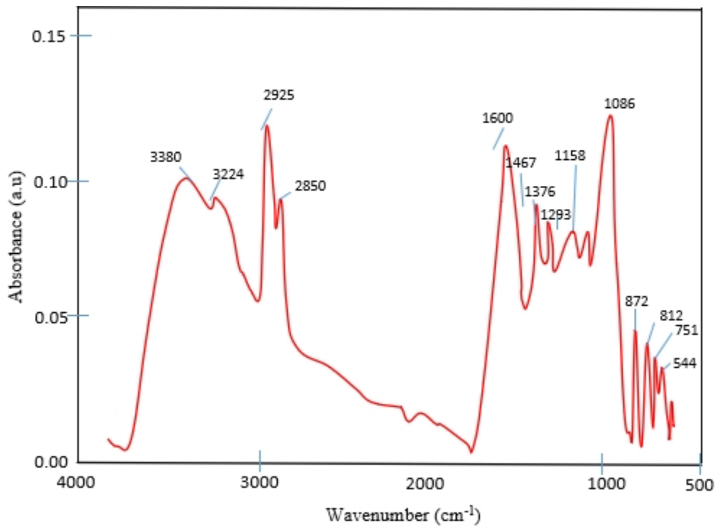


Fig. 1. FTIR spectra of representative lignite samples.

TABLE I: Proximate and Ultimate Analysis of Coals

| Parameters | SJ-1 | SJ-10 | SJ-12 | SJ-17 | SJ-21 |
|---|---|---|---|---|---|
| | | Proximate (wt.%; ad) | | | |
| Moisture | 18.43 | 21.39 | 18.48 | 17.16 | 22.58 |
| Ash | 20.40 | 10.35 | 10.01 | 15.25 | 7.42 |
| Volatile Matter | 38.37 | 40.06 | 40.77 | 39.35 | 39.96 |
| Fixed Carbon | 28.85 | 28.21 | 30.47 | 28.24 | 33.40 |
| | | Ultimate (wt.%; daf) | | | |
| Carbon | 60.81 | 60.45 | 64.12 | 59.25 | 62.15 |
| Hydrogen | 5.15 | 5.17 | 4.18 | 6.12 | 5.11 |
| Nitrogen | 0.92 | 0.87 | 0.96 | 0.98 | 0.74 |
| Sulfur | 1.75 | 2.03 | 1.07 | 1.84 | 1.68 |
| Oxygen | 31.35 | 31.51 | 29.67 | 31.81 | 30.32 |
| H/C | 0.98 | 0.97 | 1.27 | 0.81 | 1.01 |
| O/C | 0.38 | 0.38 | 0.39 | 0.32 | 0.37 |
| High Heating Value (Btu/Lb) | 7277 | 7769 | 7747 | 7385 | 7763 |

TABLE II: Band Assignments Of Ftir From Coals

| Wave number (cm-1) | Peak Assignment |
|---|---|
| 3500–3200 | O–H stretch, hydrogen bonded |
| 2925 | Aliphatic stretch vibrations–methylene - $CH_2$ (A) |
| 2850 | Aliphatic stretch vibrations–methylene -$CH_2$ (S) |
| 1600 -1595 | Aromatic ring C=C stretching (S) |
| 1467 | Aliphatic bending $CH_2$ (symmetrical) |
| 1376 | C-H Alkane bending |
| 1293 | C-O stretching of lignin-gualacyl ring |
| 1158 | R–O–R Ethers |
| 1086 | Si-O-Si(s) stretching vibration |
| 900-700 | C-H out-of-plane vibration of aromatic ring structure |
| 872 | Isolated aromatic hydrogen |
| 818 | Two adjacent aromatic hydrogen |
| 751 | Four adjacent aromatic hydrogen |
| 544 | Si-O-$Al^{VI}$ vibrations of clay minerals |

A: Asymmetric; S : Symmetric.

The FTIR spectra of functional group from the lignite coals is shown in Fig. 2. The presence of broad and strong hydroxyl absorption at the wavenumber 3380 cm-1 in lignite coal indicates the moisture content in the coal. Other researchers [28], [29] have made similar observations, noting the wavenumber range to be 3400–3200 cm-1; this indicates the existence of -OH stretching vibrations from the hydrogen hydroxyl group of the water absorbed from clay minerals and the -OH group of phenol [30].

A sharp and strong absorption peak of the aliphatic functional group -$CH_2$ was identified at 2925 cm-1 (asymmetrical) and at 2850 cm-1 (symmetrical). A similar research study concluded that the wavenumber 2920 cm-1 and 2851 cm−1, related to the suberin aliphatic chain, are responsible for asymmetric and symmetric CH2 stretching vibrations, respectively [32]. Another study conducted on lignite coals in NW Greece identified an association between the wavenumber 2925 cm-1 and ~2855 cm-1 and the asymmetric and symmetric aliphatic functional group -$CH_2$ stretching vibrations [32].

The wavenumber range of 1600–1595 cm-1 indicates the existence of aromatic ring stretching vibrations of C=O or C=C; other researchers have found the peak at 1610 cm-1 [3].

Similarly, the wavenumber range of 1509–1371 cm-1 is known to be aliphatic bending. The aliphatic bending CH compound was identified at the peak of 1376 cm-1.

The wavenumber range of 1300–1000 cm-1 is ascribed as a region of cellulose and lignin. The 1294 cm-1 peak was probably formed by the stretch vibration of C-O in the lignin-gualacyl ring. This is consistent with the findings of a previous study, which identified the peak at 1266 cm-1. The carbon−oxygen functional groups in lignite coal was identified in C-O-C group ethers at a peak of 1158 cm-1.

The wavenumber range of 900–700 cm-1 identified C-H out-of-plane vibration of aromatic ring structure; peaks at 870 cm-1, 818 cm-1, and 751 cm-1 were ascribed to isolated aromatic hydrogens, two close in aromatic hydrogens, and four close in aromatic hydrogens, respectively [26].

Thus, four main functional groups were identified in the lignite coal: hydroxyl structures, aliphatic structures, oxygen-containing structures, and aromatic structures. The intensity of the hydroxyl functional group indicates that the amount of moisture content in lignite coal is high. (This is also shown by proximate analysis, where the moisture content reached 22 %.)

In the process of spontaneous combustion in coal, moisture is one of the important factors to be considered [33]-[37]. Similarly, in the formation of water–hydrogen peroxide complex and free radicals in coal, moisture content will accelerate oxidation, which eventually causes spontaneous combustion to occur [38]. The increase in ignition corresponds to an increase in combustion temperature; this is due to the increased moisture content in coal. The heat released during low temperature coal oxidation is affected by the presence of moisture [39]. The high moisture content (proximate analysis results) and the development of O-H hydroxyl functional groups, as revealed by the results of the present study, indicates that the tendency for spontaneous combustion is very high in the lignite coal of Sajau Formation.

The same is indicated by the high intensity of oxygen-bearing functional compounds -C-O-O−, -OH, and C=O, where it exists as an unstable element and is reactive to spontaneous combustion [40].

As the initial oxidation degree increases, the amount of aliphatic hydrocarbons shows a decreasing trend, while the content of functional groups containing oxygen (–COO–, C=O, COOH) and that of hydroxyl groups will result in a significantly increased concentration of free radicals. During oxidation at a low temperature, the presence of sulphur and the oxidation of the C-H and C-O/C-O-C bonds increase the chemical activity of the coal's molecular structure, thereby causing spontaneous combustion.

## IV. Conclusion

The current study examined the Sajau lignite coal deposits in the Berau basin, North Kalimantan, Indonesia, by FTIR spectroscopy methods and derived the following conclusions:

- Hydroxyl and oxygen-bearing functional groups were found to be more functional groups than aromatic and aliphatic functional groups.
- High content of hydrogen and oxygen-bearing functional groups indicates that these coals are prone to spontaneous combustion.
- Lignite coal has a great potential for spontaneous combustion.

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## Conflict of Interest

The author declares no competing financial interest.

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