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Mineralogical and Geochemical Compositions of the No. 5 Coal in Chuancaogedan Mine, Junger Coalfield, China

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Abstract: This paper reports the mineralogy and geochemistry of the Early Permian No. 5 coal from the Chuancaogedan Mine, Junger Coalfield, China, using optical microscopy, scanning electron microscopy (SEM), Low-temperature ashing X-ray diffraction (LTA-XRD) in combination with Siroquant software, X-ray fluorescence (XRF), and inductively coupled plasma mass spectrometry (ICP-MS). The minerals in the No. 5 coal from the Chuancaogedan Mine dominantly consist of kaolinite, with minor amounts of quartz, pyrite, magnetite, gypsum, calcite, jarosite and mixed-layer illite/smectite (I/S). The most abundant species within high-temperature plasma-derived coals were SiO_2 (averaging 16.90%), Al_2O_3 (13.87%), TiO_2 (0.55%) and P_2O_5 (0.05%). Notable minor and trace elements of the coal include Zr (245.89 mg/kg), Li (78.54 mg/kg), Hg (65.42 mg/kg), Pb (38.95 mg/kg), U (7.85 mg/kg) and Se (6.69 mg/kg). The coal has an ultra-low sulfur content (0.40%). Lithium, Ga, Se, Zr and Hf present strongly positive correlation with ash yield, Si and Al, suggesting they are associated with aluminosilicate minerals in the No. 5 coal. Arsenic is only weakly associated with mineral matter and Ge in the No. 5 coals might be of organic and/or sulfide affinity.

Keywords: early Permian coals; minerals; trace elements; Junger Coalfield

1. Introduction

Coal is responsible for about 65% of electricity generation in China. The large abundance of coal makes it a reliable, long-term fuel source for both in China and in other coal-rich countries like Australia, Turkey and South Africa. With the increasing use of coal, a large amount of pollutants are produced, not only gas emissions (SOx, NOx and CO_2) but also ash residues. Environmental impact of coal and coal combustion are generally associated with the minerals and the trace elements in coal. Studies on the mineralogy and geochemistry of coal are the basic work for researching environmental impact of coal and coal combustion. Dai *et al.* [1,2], Gürdal [3], Yang [4] Wang [5], Kolker [6], Finkelman [7] and Tang *et al.* [8] have done much research on mineralogical and geochemical characteristics of the coal in many areas. The Ordos basin is the most important energy base in China. Late Paleozoic coals from the Ordos basin have attracted much attention. Dai *et al.* [9–11], and Wang *et al.* [12] have studied the geochemistry and mineralogy of the coal and its coal combustion products from the Heidaigou, Guanbanwusu, and Haerwusu Surface Mines in the Junger Coalfield. The previous studies mostly focused on the No. 6 coals in Junger Coalfield. In this paper, we report the data on the mineralogy and elemental geochemistry of the No. 5 Coals in the Chuancaogedan mine, Junger coalfield, China.

2. Geological Setting

The Junger Coalfield is located on the northeastern margin of the Ordos Basin. The coalfield is 65-km long (N–S) and 26-km wide (W–E), with a total area of 1700 km^2. The geological setting of the area has been described in detail by Dai *et al.* [9]. The Chuancaogedan Mine is situated in the southeastern part of the Junger Coalfield (Figure 1).

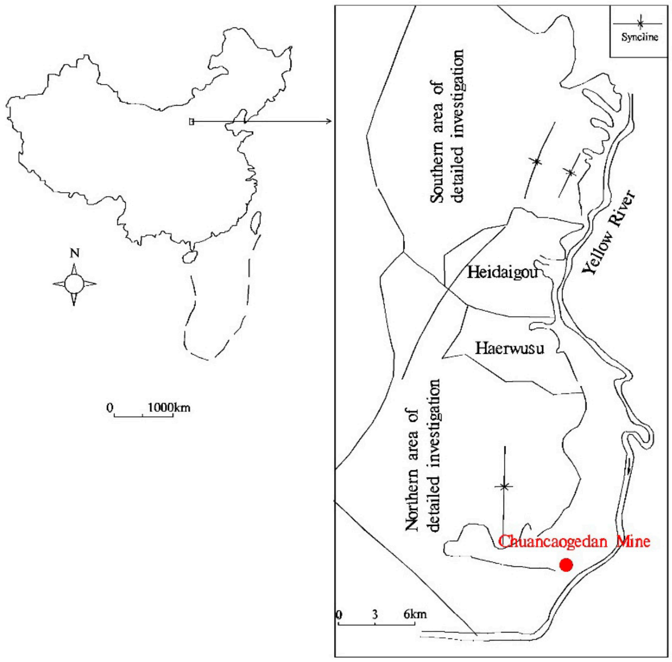

Figure 1. Location of the Chuancaogedan Mine in the Junger Coalfield, northern China (modified after Dai *et al.* [10]).

The coal-bearing sequences include Benxi Formation and Taiyuan Formation (both Pennsylvanian) and the Shanxi Formation (Lower Permian) with a collective thickness of 134 m; 110–150 m of which is mainly the Taiyuan and Shanxi formation (Figure 2). The Taiyuan Formation, with a thickness of 52 m, is mainly made up of sandstone, mudstone and coals. In the Shanxi Formation, which has a thickness of 67 m, there are five coal seams, named No. 1, No. 2, No. 3, No. 4 and No. 5 Coals in order from top to bottom.

3. Samples and Analytical Procedures

Fifteen bench samples of the No. 5 Coal were collected from the Chuancaogedan Mine, Junger Coalfield following the Chinese Standard Method GB 482-2008 [13], the cumulative thickness of the No. 5 Coal is about 4.0 m. From bottom to top, the fifteen bench samples are ZG501 to ZG517. All samples were air-dried, sealed in polyethylene bags to prevent oxidation, and parts of them were ground to pass 200 mesh, and stored in brown glass bottles for chemical analyses.

Proximate analyses were measured in accordance with ASTM standards (ASTM D3173-11 [14], ASTM D3175-11 [15], and ASTM D3174-11 [16], respectively). Total sulfur was determined following the ASTMD 3177-02 [17].

Mineralogical analyses of the coal samples were performed by means of Powder X-ray diffraction (XRD), optical microscopy and scanning electron microscopy (SEM).

Low-temperature ashing of the powdered coal samples was carried out using an EMITECH K1050X plasma asher (Quorum, Lewes, UK) prior to XRD analysis. XRD analysis of the low-temperature ashes was performed on a D/max-2500/PC powder diffractometer (Rigaku, Tokyo, Japan) with Ni-filtered Cu-Kα radiation and a scintillation detector. Each XRD pattern was recorded over a 2θ interval of 2.6°–70°, with a step size of 0.01°. X-ray diffractograms of the Low-temperature ashings (LTAs) and non-coal samples were subjected to quantitative mineralogical analysis using the Siroquant™ interpretation software system (Sietronics, Mitchell, Australia). More analytical details are given by Dai *et al.* [18,19] and Wang *et al.* [20].

X-ray fluorescence (XRF) spectrometry (ARL ADVANT'XP+, ThermoFisher, Waltham, MA, USA) was used to determine the major element oxides in high-temperature ashed coal samples, including SiO_2, Al_2O_3, CaO, K_2O, Na_2O, Fe_2O_3, MnO, MgO, TiO_2 and P_2O_5. Trace elements within acid-digested ashed coal samples, except for As, Se, Hg and F, were determined by conventional inductively coupled plasma mass spectrometry (ICP-MS). For its analysis, samples were digested using an UltraClave Microwave High Pressure Reactor (Milestone, Sorisole, Italy). The basic load for the digestion tank was composed of 330-mL distilled H_2O, 30-mL 30% H_2O_2, and 2-mL 98% H_2SO_4. Initial nitrogen pressure was set at 50 bars and the highest temperature was set at 240 °C that lasted for 75 min. The reagents for 50-mg sample digestion were 5 mL 40% HF, 2 mL 65% HNO_3 and 1 mL 30% H_2O_2. Multi-element standards were used for calibration of trace element concentrations. More details are given by Dai *et al.* [21] Arsenic and Sewere analyzed by more advanced ICP-MS which utilized collision/reaction cell technology (ICP-CCT-MS) as outlined by Li *et al.* [22]. Fluorine was determined by an ion-selective electrode (ISE) method. Mercury was determined using a Milestone DMA-80 Hg analyzer (Milestone, Sorisole, Italy).

The quantitative analysis of minerals and determinations of elements were completed at the State Key Laboratory of Coal Resources and Safe Mining of China University of Mining and Technology (Beijing, China).

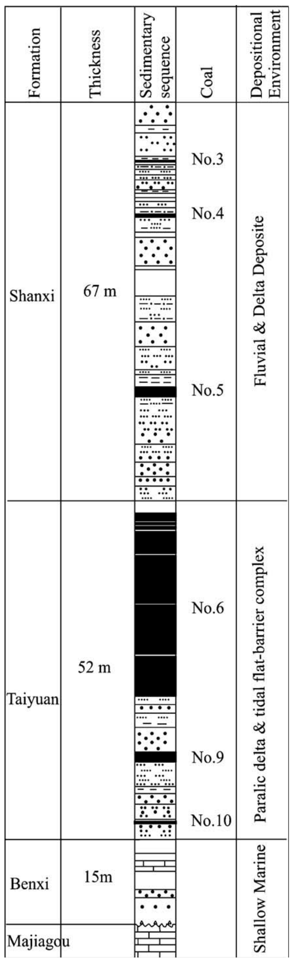

Figure 2. Stratigraphic sequence of the Junger Coalfield [9].

4. Results and Discussion

4.1. Coal Chemistry

The results of the total sulfur and proximate analysis of samples from the No. 5 coal are presented in Table 1. Ash yields of the Chuancaogedan No. 5 coal range from 5.95% to 60.70% (Figure 3), with an average of 32.69%, indicating a high ash coal according to Chinese National Standard (GB/T 15224.1-2004, 10.01% to 16.00% for low ash coal, 16.01% to 29.00% for medium ash coal, and >29.00% for high ash coal) [23]. The ash yields tend to increase from the bottom to the top in the coal seam.

The contents of volatile matter of the No. 5 coal varies from 32.57% to 50.30% through the coal-seam section (Figure 3), with a mean of 37.22%, suggesting that the Chuancaogedan coals are medium-high volatile bituminous coals based on MT/T 849-2000 (28.01% to 37.00% for medium-high volatile coal, 37.01% to 50.00% for high volatile coal and >29.00% for super high volatile coal) [24].

The No. 5 coals have a moisture content of 2.22% to 5.61% (Figure 3), with an average of 3.81%, indicating a low-medium rank coal in accordance of MT/T 850-2000 (⩽5% for low moisture coal, 5% to 15% for medium moisture coal, and >15% for high moisture coal) [25].

The total sulfur of No. 5 coals changes from 0.12% to 0.83% (Figure 3), averaging 0.40%, which corresponds to ultra-low-sulfur coal according to Chinese National Standard (GB/T 15224.2-2010) (<0.5% for super low sulfur coal, 0.51% to 0.9% for low sulfur coal and 0.9% to 1.50% for medium sulfur coal) [26].

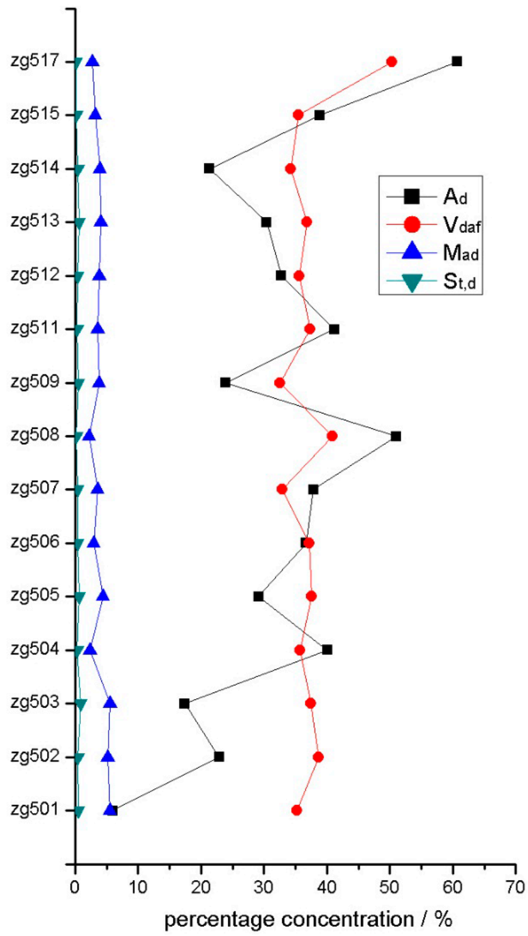

Figure 3. Variation of total sulfur and proximate analysis through the No. 5 Coal section.

Table 1. Proximate analysis and total sulfur in the No. 5 Coal (%).

Sample	Proximate Analysis			$S_{t,d}$
	M_{ad}	V_{daf}	A_d	
ZG517	2.78	50.3	60.7	0.12
ZG515	3.19	35.52	38.9	0.18
ZG514	3.91	34.3	21.38	0.40
ZG513	4.14	36.9	30.46	0.61
ZG512	3.86	35.59	32.79	0.35
ZG511	3.64	37.39	41.16	0.30
ZG509	3.82	32.57	23.9	0.47
ZG508	2.22	40.84	51.02	0.21
ZG507	3.54	32.91	37.88	0.36
ZG506	2.94	37.23	36.66	0.36
ZG505	4.39	37.61	29.17	0.64
ZG504	2.42	35.75	40.04	0.29
ZG503	5.61	37.47	17.41	0.83
ZG502	5.2	38.63	22.89	0.46
ZG501	5.52	35.29	5.95	0.48
Average	3.81	37.22	32.69	0.40

M, moisture; V, volatile matter; A, ash yield; S_t, total sulfur; ad, air-dry basis; d, dry basis; daf, dry and ash-free basis.

4.2. Minerals in the No. 5 Coal

The mineral phase percentages were calculated to a coal ash basis from the XRD results obtained on the low temperature ashes and are reported in Table 2. The results show that minerals in the No. 5 coal are mainly made up of kaolinite, followed by gypsum (averaging 0.99%), magnetite (0.85%), calcite (0.33%), quartz (0.31%), pyrite (0.26%) and mixed-layer I/S (0.01%).

Table 2. Mineral contents in coal samples from the Chuancaogedan Mine measured by Low-temperature ashing X-ray diffraction (LTA-XRD) (%).

Samples	Kaolinite	Quartz	Magnetite	Pyrite	Gypsum	Calcite	Jarosite	I/S
ZG517	55.42	0.97	4.31	-	-	-	-	-
ZG515	38.32	-	0.58	-	-	-	-	-
ZG514	21.38	-	-	-	-	-	-	-
ZG513	30.46	-	-	-	-	-	-	-
ZG512	32.79	-	-	-	-	-	-	-
ZG511	41.16	-	-	-	-	-	-	-
ZG509	23.57	0.07	-	0.26	-	-	-	-
ZG508	50.76	-	0.26	-	-	-	-	-
ZG507	37.77	0.11		-	-	-	-	-
ZG506	36.22	-	0.44	-	-	-	-	-
ZG505	29.11	-	0.06	-	-	-	-	-
ZG504	39.72	0.08	0.24	-	-	-	-	-
ZG503	15.32	-	-	-	1.15	0.33	0.61	-
ZG502	22.07	-	-	-	0.82	-	-	-
ZG501	5.89	-	0.05	-	-	-	-	0.01

I/S: mixed-layer illite/smectite.

Kaolinite is common in coal [27,28]. As presented in Table 2, kaolinite is the most abundant mineral in the Chuancaogedan coal seam, with abundance within the ash varying from 5.89% to 55.42% (average 32.00%). Kaolinite occurs as infillings of cells or fractures (Figure 4A–C). In addition, kaolinite presents as thin-layered or flocculent forms (Figure 5A,B) in the No. 5 Coal.

Pyrite is only observed in ZG509 (0.26 wt %) (Figure 6), occurring as fracture-fillings (Figure 4D) or as pyrite aggregates (Figure 5C).

Magnetite presents in seven samples; the content varies from 0.05% to 4.31%. Other minerals, such as quartz, calcite, jarosite, mixed-layer illite/smectite (I/S) and gypsum, are only present in a few samples. Gypsum occurs in columnar form as shown by SEM scans (Figure 5D).

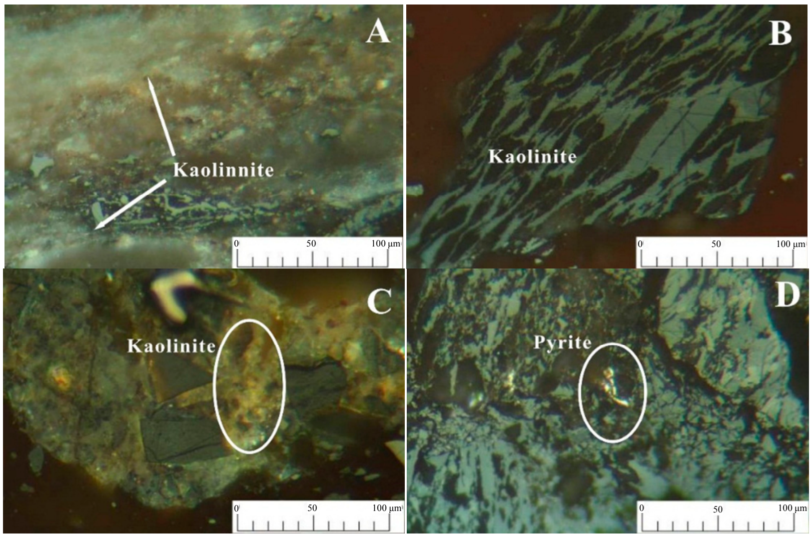

Figure 4. Minerals in the No. 5 Coal (reflected light): (**A**) kaolinite in dispersed form; (**B**) kaolinite in-filling cells; (**C**) kaolinite with organic matter; and (**D**) pyrite in vitrinite.

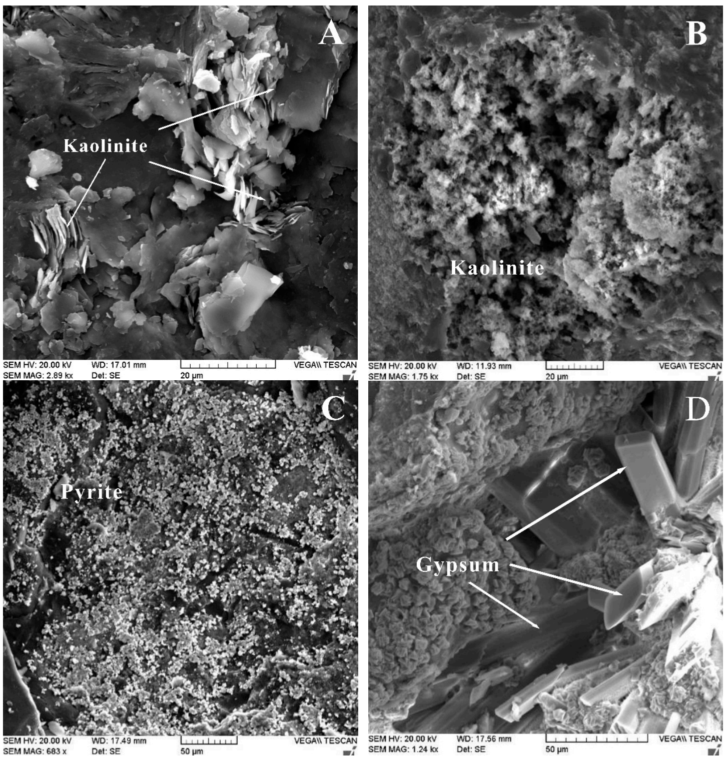

Figure 5. Minerals in the No. 5 Coal (SEM, secondary electron images): (**A**) kaolinite as thin-layered forms; (**B**) flocculent kaolinite; (**C**) pyrite aggregates; and (**D**) columnar gypsum.

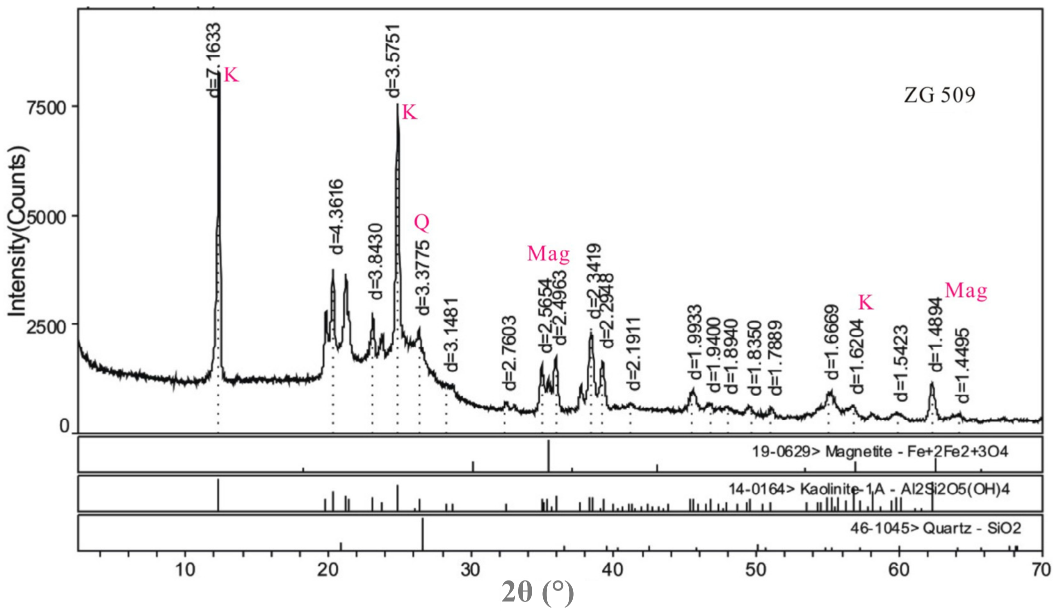

Figure 6. X-ray diffraction (XRD) patterns of coal samples (ZG509).

4.3. Geochemistry of the No. 5 Coals

4.3.1. Major Elements

The major elements in coals from the Chuancaogedan Mine are dominated by SiO_2, Al_2O_3, and Fe_2O_3 (Table 3), which conform to major mineral compositions of the coals (kaolinite, magnetite and pyrite). Average values for high-temperature plasma No. 5 coal samples are as follows: SiO_2 (16.90 wt %), Al_2O_3 (13.87 wt %), Fe_2O_3 (0.70 wt %), TiO_2 (0.55 wt %), CaO (0.26 wt %), K_2O (0.06 wt %), MgO (0.04 wt %), Na_2O (0.02 wt %), and P_2O_5 (0.05 wt %). Coals from Chuancaogedan Mine contain higher proportions of SiO_2, Al_2O_3, TiO_2, P_2O_5, and lower proportions of Fe_2O_3, Na_2O than the average values for Chinese coals reported by Dai *et al.* [29].

The SiO_2/Al_2O_3 ratios range from 1.17 to 1.27, with an average of 1.22 for the No.5 coal. This is higher than those of other Chinese coals (1.42) [29] and also higher than the theoretical SiO_2/Al_2O_3 ratio of kaolinite (1.18), suggesting quartz or amorphous silica occurs in the mineral matter portion of the coal. The ash has a TiO_2 content of 0.88% to 2.93%, much higher than the proportion within ash of other Chinese coals, and this is mainly affiliated with magnetite in No. 5 coal. Iron may be isomorphic replaced by Ti in magnetite (Fe_3O_4). The average contents of K_2O and Na_2O are 0.18% and 0.05%, respectively. K_2O and Na_2O are probably attributed to mixed-layer I/S. The concentration of Fe_2O_3 varies from 0.27% to 1.66%, with an average of 0.70%. The positive relation coefficient between Fe_2O_3 and $S_{t,d}$ (rFe_2O_3-$S_{t,d}$ = 0.66) suggest that Fe is mainly associated with sulfide (pyrite).

4.3.2. Trace Elements

In contrast with the common Chinese coals [29], the No. 5 coals are slightly enriched in Li (averaging 78.54 mg/kg), Se (6.69 mg/kg), Zr (245.89 mg/kg), Hg (65.42 mg/kg), Pb (38.95 mg/kg), and U (7.85 mg/kg), with CC between 2 and 5 (CC, concentration coefficient, is the ratio of element concentration in investigated coals *vs.* Chinese coals or world hard coals [30]), while As (averaging 0.28 mg/kg), Co (3.44 mg/kg), Sr (93.10 mg/kg), Sb (0.36 mg/kg), and Tl (0.16 mg/kg) are depleted (with CC lower than 0.5), and the remaining elements (CC are between 0.5 and 2) are close to the average values for Chinese coals [29].

As stated above, elements including Li, Se, Zr and Hf are higher than that for Chinese average coals [29], and F and Ga are close to the average values. The correlation coefficients between F, Ga and ash are 0.81 and 0.78, respectively, and the main mineral in coals is kaolinite, so they are probably related to the kaolinite (Figures 4 and 5). The high trace elements and boehmite in the No. 6 coals were derived from the weathered and oxidized bauxite in the exposed crust of the older Benxi Formation (Missisippian) situated to the northeast of the coal basin [11]. Benxi Formation bauxite; was an important terrigenous source for most Late Paleozoic coals in Junger coalfield, China [9]. During peat accumulation, the Junger Coalfield was in the low lying area between the Yinshan Oldland to the N and W and the upwarped Benxi Formation to the N and E. The paleo rivers ran dominantly in the N and E directions from these sediment-source regions to the Junger Coalfield [31].

4.3.3. Evaluated Li, Ga, Se, Zr, Hf, As, and Ge in the No. 5 Coal

Lithium: The content of Li in the No. 5 coals varies from 17.76 to 157.83 mg/kg (average 78.54 mg/kg), which is much higher than that of the No. 6 coals (average 37.80 mg/kg) [9] and Chinese coals (average 14 mg/kg) [29]. Lithium in coal samples is positively correlated with ash yield, Si, and Al, with correlation coefficients of 0.88, 0.69 and 0.62, respectively (Table 4), suggesting that Li is associated with aluminosilicate minerals.

Gallium: The Chuancaogedan coals have a Ga content close to the Chinese coal average [26], ranging from 6.34 to 27.10 mg/kg, with an average of 13.98 mg/kg. Gallium is generally related to clay minerals in coal [1,32]. The correlation coefficient between Ga and ash yield, Si and Al are 0.78, 0.51 and 0.24, respectively (Table 4). This strongly suggests that kaolinite may contain (but is not high in) Ga, and Ga mainly occurs in inorganic association.

Selenium: The concentration of Se in the No. 5 coals ranges from 2.02 to 19.07 mg/kg, with a mean of 6.69 mg/kg. The correlation between Se and ash yield, Si, and Al (correlation coefficient = 0.60, 0.37, 0.11 (Table 4)) suggest that only part of total Se exists in minerals.

Zirconium and Hafnium: Zr and Hf are enriched in the No. 5 coals, with average concentration of 245.89 mg/kg and 6.93 mg/kg, respectively. The correlation coefficient of Zr-Hf is 0.99 (Table 4), showing that they have similar occurrence. They are both positively correlated with ash yield, Si, and Al (rZr-ash = 0.76, rZr-Si = 0.59, rZr-Al = 0.62, rHf-ash = 0.81, rHf-Si = 0.64, rHf-Al = 0.67 (Table 4)), identifying the occurrence of Zr and Hf in association with aluminosilicate minerals. Zircon is the most common zirconium mineral, therefore the Zr is believed to be at least partly due to the probable presence of this heavy mineral these samples [10].

Arsenic: The content of As in the No. 5 coals was below the ICP-MS detection limit for three samples, but otherwise varies from 0.15 up to 0.64 mg/kg (average 0.28 mg/kg), which is lower than that of both the No. 6 coals (average 0.56 mg/kg) [9] and Chinese coals (average 5.00 mg/kg) [29]. A wide variety of As-bearing phases has been observed in high-As coals from southwestern Guizhou; for example: pyrite; Fe–As oxide; K–Fe sulfate; and As-bearing clays [33,34]. Occurrences of organically associated As have also been reported in Guizhou coal [34]. Arsenic in the Chongqing coal correlates with Fe_2O_3, suggesting a pyrite affinity [35]. The correlation coefficient between As and ash yield, Si, and Al in Chuancaogedan coals are 0.34, 0.54 and 0.22, respectively, which indicates that only a small part of the total As occurs in minerals. Arsenic has a negative correlation with Fe_2O_3 (correlation coefficient of −0.36), which suggests that As may not be affiliated with pyrite occurrence in the No. 5 coals.

Germanium: The Chuancaogedan coals have a Ge content of close to the average for Chinese coals [29], ranging from 0.35 to 4.21 mg/kg, with an average of 1.74 mg/kg. In the Tongda coal mine, Yimin coalfield, Ge occurs with major organic affinity, and partial sulfide affinity was observed also. As, Fe, and S show similar trends to Ge, though with a markedly higher sulfide affinity (mainly in pyrite) [36]. The correlation coefficients of Ge and ash yield, major elements and selected trace elements in the No. 5 coals range from −0.53 to 0.40, which means Ge may presents organic and/or sulfide affinity in these coals.

Table 3. Elemental concentrations in the No. 5 Coal from Chuancaogedan Mine (oxides in %, elements in mg/kg, Hg in ng/g).

Elemental Concentrations	Sample															
	ZG517	**ZG515**	**ZG514**	**ZG513**	**ZG512**	**ZG511**	**ZG509**	**ZG508**	**ZG507**	**ZG506**	**ZG505**	**ZG504**	**ZG503**	**ZG502**	**ZG501**	**Average**	**Coal [a]**
SiO_2	32.55	20.7	11.13	15.98	17.15	21.82	12.32	27.33	19.57	19.55	15.1	20.24	7.94	11.63	2.98	16.9	8.47
Al_2O_3	25.71	16.72	9.08	13	13.97	17.8	10.2	22.47	16.28	16.03	12.37	17.3	6.55	9.45	2.5	13.87	5.98
Fe_2O_3	1.66	0.33	0.27	0.56	0.31	0.34	0.46	0.37	0.51	0.34	0.75	0.42	1.3	0.86	0.22	0.7	4.85
TiO_2	1.11	0.73	0.52	0.45	0.96	0.76	0.5	0.47	0.73	0.36	0.45	0.77	0.24	0.2	0.07	0.55	0.33
CaO	0.33	0.14	0.12	0.13	0.11	0.16	0.12	0.09	0.17	0.1	0.12	0.2	0.69	0.37	0.08	0.26	1.23
K_2O	0.14	0.05	0.02	0.04	0.03	0.04	0.02	0.08	0.09	0.06	0.09	0.17	0.04	0.03	0.01	0.06	0.19
MgO	0.1	0.04	0.02	0.03	0.03	0.02	0.03	0.04	0.05	0.03	0.04	0.06	0.06	0.04	0.01	0.04	0.22
Na_2O	0.02	0.01	0.01	0.01	0.01	0.01	0.01	0.02	0.02	0.01	0.01	0.03	0.03	0.02	0	0.02	0.16
P_2O_5	0.02	0.02	0.01	0.01	0.02	0.02	0.02	0.02	0.18	0.01	0.02	0.47	0.01	0.01	0	0.05	0.09
Li	114.2	83.99	46.99	72.25	82.51	120.42	75.33	157.83	83.09	103.42	56.04	79.12	35.33	49.82	17.76	78.54	14
Be	7.75	12.28	6.43	4.16	2.75	1.7	1.97	1.56	3.42	1.41	1.07	2.79	1.78	2.31	3.65	3.67	2
F	345.88	251.06	156.83	193.14	214.15	263.93	159.81	279.3	291.42	208.39	204.84	385.27	137.27	124.31	59.85	218.37	140
Sc	12.79	7.62	4.61	4.57	6.87	9.09	3.62	12.95	14.82	11.47	9.23	10.36	6.51	5.74	3.75	8.27	3
V	64.73	32.79	31.86	28.11	37.3	39.77	44.09	19.05	30.68	27.24	23.07	31.78	11.74	10.8	11.35	29.63	21
Cr	18.61	8.41	12.87	7.89	10.26	7.7	10.48	3.83	8.86	6.49	7.66	13.05	4.43	2.64	1.65	8.32	12
Co	4.98	2.9	4.86	5.4	2.69	2.03	3.23	1.23	1.13	1.7	1.89	0.86	5.99	5.61	7.05	3.44	7
Ni	10.37	10.74	11.54	12.64	6.9	5.13	7.35	4.35	4.63	3.71	5.21	4.16	13.59	17.47	16.9	8.98	14
Cu	18.84	22.08	19.63	20.61	17.23	10.95	17.78	9.13	13.36	16.73	12.42	22.44	7.06	8.36	8	14.97	13
Zn	14.85	7.12	16.37	19.96	17.08	16.39	14.62	11.81	19.36	35.83	30.03	25.94	54.71	35.57	13.6	22.22	35
Ga	27.1	15.62	9.51	13.58	18.24	16.19	13.34	12.89	14.7	13.36	17.16	12.3	10.34	9.05	6.34	13.98	9
As	0.64	0.42	0.36	0.62	0.23	0.18	0.42	0.15	0.24	0.19	0.41	0	0	0.31	0	0.28	5
Se	19.07	4.41	5.64	5.94	10.35	11.07	8.83	3.83	6.51	4.31	5.28	5.09	4.45	3.62	2.02	6.69	2
Rb	5.81	1.92	0.37	1.41	0.73	1	0.25	2.65	2.59	1.84	2.21	4.04	0.28	1.01	0.2	1.75	8
Sr	20.8	12.34	15.2	14.31	11.25	11.54	14.68	14.97	321.07	14.08	24.89	849.94	35.48	18.81	17.13	93.1	423
Y	0.19	0.22	0.29	0.2	0.27	0.18	0.38	0.21	0.28	0.08	0.12	0.3	3.77	0.27	5.43	0.81	20.76
Zr	450.76	241.43	165.49	292.81	303.95	354.05	272.13	221.16	270.52	262.09	326.43	202.89	139.76	150.53	34.28	245.89	52
Ge	1.41	1.15	3.49	4.21	2.74	1.72	1.66	0.77	0.43	1.39	1.67	0.35	1.33	1.4	2.4	1.74	2.78
Mo	1.45	1.77	2.11	2.31	2.72	1.6	1.77	0.72	1.52	1.69	3.14	1.69	3.05	1.9	3.13	2.04	4
Cd	0.35	0.17	0.12	0.21	0.19	0.22	0.18	0.32	0.37	0.39	0.63	0.29	0.22	0.21	0.06	0.26	0.2
Sn	5.21	1.11	0.06	0.77	1.02	1.75	0	2.98	3.01	2.29	1.94	3.08	1.17	2.84	0.63	1.86	2
Sb	0.34	0.28	0.49	0.52	0.38	0.31	0.4	0.22	0.15	0.3	0.64	0.13	0.2	0.57	0.43	0.36	2
Cs	0.72	0.25	0.07	0.31	0.13	0.15	0.06	0.31	0.25	0.14	0.23	0.3	0.04	0.09	0.02	0.2	1
Ba	424.52	13.3	11.1	18.23	17.36	9.69	14.36	11.76	38.57	7.68	23.79	235.07	20.29	10.21	12.67	57.91	56.03
La	0.11	0.16	0.73	0.64	0.57	0.22	0.63	0.28	0.76	0.05	0.08	2.7	4.87	1.22	4.6	1.17	25.78
Ce	1.5	3.96	20.77	17.15	8.1	2.46	8.88	2.57	12.33	1.25	2.33	41.7	25.28	13.79	20.11	12.15	49.11
Nd	0.11	0.2	1.1	0.66	0.58	0.15	0.75	0.19	0.5	0.06	0.15	1.75	6.42	1.03	4.95	1.24	21.5
Sm	0.02	0.04	0.2	0.1	0.09	0.03	0.14	0.03	0.09	0.01	0.03	0.36	1.33	0.13	1.02	0.24	4.3

Table 3. *Cont.*

Elemental Concentrations	Sample																
	ZG517	**ZG515**	**ZG514**	**ZG513**	**ZG512**	**ZG511**	**ZG509**	**ZG508**	**ZG507**	**ZG506**	**ZG505**	**ZG504**	**ZG503**	**ZG502**	**ZG501**	**Average**	**Coal [a]**
Eu	0.05	0	0.02	0.01	0.01	0	0.02	0.01	0.02	0	0.01	0.07	0.24	0.02	0.21	0.05	0.87
Yb	0.04	0.03	0.05	0.02	0.03	0.02	0.05	0.03	0.04	0.02	0.02	0.04	0.45	0.04	0.59	0.1	2.12
Hf	13.5	6.96	4.41	7.82	8.16	10.04	7.51	6.61	7.54	8.11	8.94	5.88	3.43	4.03	1.01	6.93	2.4
Ta	3.86	0.95	0.5	0.73	0.97	1.21	0.48	0.77	0.86	0.61	0.38	0.72	0.46	0.82	0.11	0.89	0.7
W	2.5	1.42	0.7	0.65	1.69	1.43	0.67	0.9	1.16	0.42	0.02	1.21	0.66	0.61	1.2	1.02	2
Hg	29	20	44	54	81	17	129	38	45	90	145	52	87	83	66	65.42	15
Tl	0.37	0.36	0.45	0.28	0.02	0.03	0.03	0.02	0.03	0.11	0.27	0.05	0.13	0.14	0.14	0.16	0.4
Pb	55.82	52.08	42.78	40.99	57.31	55.41	54.81	36.74	38.99	32.3	37.3	30.22	20.5	20.03	8.95	38.95	13
Bi	0.77	0.66	0.36	0.44	0.5	0.51	0.39	0.51	0.74	0.42	0.37	0.56	0.36	0.33	0.1	0.47	0.8
Th	1.71	1.32	1.54	1.06	1.09	0.79	2.02	1.17	1.1	0.81	1.41	0.67	2.51	0.65	0.29	1.21	6
U	5.93	18.41	17.64	22.3	8.55	4.8	6.16	4.92	8.73	5.32	5.15	5.1	1.75	2.1	0.91	7.85	3

[a] Coal, Chinese average coals value by Dai *et al.* [29] or world hard coals [37].

Table 4. Correlation coefficients between the content of each element in coal and ash yield, major elements.

	Ad	**SiO_2**	**Al_2O_3**	**TiO_2**	**Fe_2O_3**	**CaO**	**K_2O**	**MgO**	**Na_2O**	**P_2O_5**	**Li**	**Ga**	**Se**	**Zr**	**Hf**	**As**	**Ge**
Ad	1																
SiO_2	0.66 **	1															
Al_2O_3	0.51	0.89 **	1														
TiO_2	0.09	0.15	0.12	1													
Fe_2O_3	−0.66 **	−0.92 **	−0.93 **	−0.37	1												
CaO	−0.52 *	−0.92 **	−0.96 **	−0.29	0.96 **	1											
K_2O	0.22	−0.30	−0.13	−0.15	0.14	0.14	1										
MgO	−0.51	−0.91 **	−0.91 **	−0.27	0.92 **	0.92 **	0.33	1									
Na_2O	−0.47	−0.95 **	−0.91 **	−0.34	0.93 **	0.96 **	0.34	0.91 **	1								
P_2O_5	0.15	−0.19	0.15	0.16	−0.14	−0.09	0.74 **	0.05	0.11	1							
Li	0.88 **	0.69 **	0.62 *	−0.02	−0.67 **	−0.56 *	−0.07	−0.66 **	−0.51 *	−0.01	1						
Ga	0.78 **	0.51	0.24	0.37	−0.47	−0.39	0.13	−0.30	−0.41	−0.10	0.55 *	1					
Se	0.60 *	0.37	0.11	0.48	−0.37	−0.24	−0.07	−0.18	−0.30	−0.12	0.41	0.87 **	1				
Zr	0.76 **	0.59 *	0.36	0.35	−0.55 *	−0.51	0.05	−0.47	−0.50	−0.11	0.62 *	0.93 **	0.81 **	1			
Hf	0.81 **	0.64 *	0.41	0.29	−0.59 *	−0.53 *	0.07	−0.49	−0.52 *	−0.10	0.67 **	0.94 **	0.81 **	0.99 **	1		
As	0.34	0.54 *	0.22	0.20	−0.36	−0.41	−0.23	−0.32	−0.51	−0.41	0.16	0.58 *	0.51	0.63 *	0.61 *	1	
Ge	−0.40	0.09	−0.06	0.26	0.01	−0.06	−0.53 *	−0.09	−0.22	−0.47	−0.35	−0.13	0.03	−0.04	−0.10	0.40	1

** Correlation is significant at the 0.01 level (two-tailed); * Correlation is significant at the 0.05 level (two-tailed).

5. Conclusions

Based on mineralogical and geochemical investigation of the No. 5 coal from Chuancaogedan Mine, Junger Coalfield, the conclusions are summarized below.

The No. 5 coal at the Chuancaogedan Mine has a high-ash yield (averages of 32.69%) and an ultra-low-sulfur content (0.40%), while the mean contents of volatile matter and moisture are 37.22% and 3.81%, respectively.

The mineral component of the No. 5 coal mainly consists of kaolinite, followed by magnetite, quartz, gypsum, mixed-layer I/S, pyrite, and calcite. Kaolinite is characteristically abundant and may have been derived from the weathered surface of the Benxi Formation bauxite during peat accumulation in the coal swamp.

Compared with common Chinese coals, the No. 5 coal is slightly enriched in SiO_2 (averaging 16.90%), Al_2O_3 (13.87%), TiO_2 (0.55%), P_2O_5 (0.55%), Li (78.54 mg/kg), Se (6.69 mg/kg), Zr (245.89 mg/kg), Hg (65.42 mg/kg), Pb (38.95 mg/kg) and U (7.85 mg/kg), and has a lower concentration of Fe_2O_3, Na_2O, As, Co, Sr, Sb and Tl, while others are close to averages for Chinese coals. The SiO_2/Al_2O_3 ratios (average of 1.22) are higher than that of the Chinese coals (1.42) and the theoretical SiO_2/Al_2O_3 ratio of kaolinite (1.18), suggesting quartz occurs in the mineral matter.

The modes of occurrence of Li, Ga, Se, Zr, Hf, As and Ge in the No. 5 coal were preliminarily investigated by correlation analysis. The correlation coefficients of Li, Ga, Se, Zr and Hf and ash yield are 0.88, 0.78, 0.60, 0.76 and 0.81, respectively, suggesting they occur in inorganic association. Li, Zr and Hf present positive correlation with Si and Al (rLi-Si = 0.69, rLi-Al = 0.62, rZr-Si = 0.59, rZr-Al = 0.62, rHf-Si = 0.64, rHf-Al = 0.67), indicating they are associated with aluminosilicate minerals in the No. 5 coal. Arsenic may be associated with organic and/or inorganic components of the tested coal samples, given that it is only moderately correlated with ash yield, Si, Al, and Fe_2O_3. Germanium may have organic and/or sulfide affinity in the No. 5 coals.

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