

ARTICLES

THE RESULT OF INVESTIGATION OF COAL FROM
CHANDGANA TAL DEPOSIT*Tsatsral G.*, Narangerel J. and Purevsuren B.**Institute of Chemistry and Chemical Technology, Mongolian Academy of Sciences,
Ulaanbaatar, Mongolia*

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Abstract: Proximate and ultimate analyses showed that Chandgana Tal coal has the following properties; W^h -13.29%, A^d -12.43%, V^{daf} -44.98%, Q^{daf} -5914 kcal/kg, C-67.56%, H-5.79%, S-1.67%, N-1.18% and O-23.8%. Pyrolysis of coal was performed at 200-700°C using small quartz reactor. With increasing temperature of pyrolysis, the yield of hard residue decreased, while the yield of tar and pyrolytic water increased. The yield of coal tar was maximum at 700°C, and reached 4.8%. At this stage, coal was pyrolyzed in a bigger scale retort of laboratory. The tar was separated from water and analysed by FT-IR and organic composition.

Thermolysis experiments were also performed in order to explore the possibility of obtaining liquid products under mild condition. The results show that 23.5% of liquid product can be obtained at 450°C with coal to tetralin ratio (1:1.8).

Keywords: Coal, pyrolysis, thermolysis, tar, FT-IR spectra;

INTRODUCTION

Coal is an organic sedimentary rock that is formed from the accumulation and preservation of plant materials, usually in a swampy environment. Coal is one of the world's most important sources of energy, fueling almost 40% of electricity production worldwide. In many countries, this figure is much higher: Poland relies on coal for more than 94% of its electricity generation, South Africa - 92%, China - 77%, and Australia - 76%. Coal has been the world's fastest growing energy source in recent years - faster than natural gas,

oil, nuclear and hydro energy, and renewables. It has played this important role for centuries not only in providing electricity but also as an essential fuel for steel and cement production as well as other industrial production. The world currently consumes over 6 billion tons of coal annually. Coal is used in a variety of sectors, including in power generation, iron and steel production, cement manufacturing, and it is also used as a liquid fuel[1].

Mongolia has limited oil reserves but a relatively large reserve of coal.

*corresponding author: tsatsaa1007@gmail.com



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Proven coal reserves were estimated at 34 billion tons in 2015. The Chandgana Tal coal deposit is located in Nyalga-Choir basin, in Mörön soum of Khentii (aimag) Province in east Mongolia. The deposit has geological reserves amounting to 1.17 billion tons of low rank coal, one of the largest coal reserves in Asia. The mine has an annual production capacity of 3 million tons of coal.

When coal is heated under air-free conditions, the organic matter undergoes a series of changes as the temperature increases, forming gaseous (coal gas), liquid (tar), and solid (semi-coke or coke) products. Solvent extraction involves coal dissolution with hydrogen donor solvent containing hydro-aromatic compounds. Hydrogenated aromatic compounds easily donate hydrogen to the coal. Solvent extract liquefaction includes the solvent refinery process, extraction with

a hydrogendonating solvent, liquid solvent extraction, and supercritical gas extraction[2]. Processes for direct coal liquefaction by solvent extraction are considered along with the structure and properties of coal and the mechanism of coal liquefaction, heteroatom removal during liquefaction, kinetic models for donor-solvent coal liquefaction, the design of coal liquefaction reactors, and the refining of coal liquids. Attention is given to the catalytic hydrogenation of coal in the presence of a solvent, the origin and character of coal, laboratory reactors for rate measurements, reaction networks based on lumped fractions, free-radical reaction models, reactor types, the compatibility of coal-derived liquids and petroleum fuels, the stability of coal liquids, thermal cracking, catalytic hydrotreating, catalytic cracking, and catalytic reforming[3].

MATERIALS AND METHODS

Sample preparation, proximate and ultimate of coal from the Chandgana Tal deposit were performed according to the Mongolian National Standard MNS 656-79 (moisture content), MNS 652-79 (ash yield), MNS 654-79 (volatile matter yield), MNS 669-87 (gross calorific value), and MNS 895-79 (sulphur content).

The pyrolysis experiments of coal samples were performed in a laboratory vertical cylindrical retort made of stainless steel with 1000g of sample. The retort was placed in an electric furnace with a maximum temperature of 950°C. A chrome-alumel thermocouple was immersed in the coal bed to measure the actual heating temperature. The retort was connected with air-cooled iron tube and water-cooled laboratory glass condenser and a vessel for collecting the condensate of liquid product (pitch and pyrolysis water). The non-condensable gaseous product shall be removed and isolated by passing it through a thin glass tube located in between the condenser and liquid collecting vessel. The experiments were

carried out at a temperature of 900°C and the heating rate was 20°C min⁻¹. The yields of product including solid residue (coal char), tar and pyrolysis water determined by weighing, and the yield of gases was determined by the difference[4] obtained.

The thermolysis of coal samples was carried out in a stainless steel autoclave using tetralin as a hydrogen donor solvent. Prior to the treatment, coal samples were air dried for 24 hours, powdered to a particle size of <0.2 mm. Then 1g of coal sample was mixed with 1.8g of tetralin (mass ratio 1:1.8), sealed in the autoclave and heated in a laboratory furnace for 2 hours to temperatures of 350°C, 400°C and 450°C respectively. After completion of each experiment, the autoclave was cooled to room temperature and all uncondensed gas was released. And the resulting liquid products were removed, filtered, and the solid residue from the filter was subjected to sequential extraction with chloroform in a Soxhlet apparatus. Liquid products of thermal dissolution of coal in tetralin was distilled by

a laboratory rotary evaporation apparatus for complete removal of chloroform. The degree of coal conversion was determined by the loss of the coal organic matter (COM) after extraction and also change in the ash contents of the initial coal samples and the insoluble residue. The yields of pyrolysis products including solid residue (coal char), tar and pyrolysis water were determined by weighing, and the yield of gases calculated by difference[4].

The FT-IR spectra of the samples were obtained on an Interspec 200-X series of FT-

IR spectrometers with PIKE Diffution IR accessories using a KBr disc containing 1% finely ground samples. All the spectra were measured in the frequency range of 4000 to 400 cm^{-1} , and 32 scans were taken per sample.

Sample survey: The study was carried out on select coal sample from Chandgana Tal deposit, which is located on the territory Khentii aimag, about 53 km to the east of Undurkhan. The proven reserves of the Chandgana Tal deposit are 124 million tons[5].

RESULTS AND DISCUSSION

Analytical sample of Chandgana Tal coal was prepared by a standard method. The results of

proximate and ultimate analyses of the samples are shown in Table 1.

Table 1. The results of proximate and ultimate analysis of the Chandgana Tal coal

Moisture, W^a	Ash, %		Yield of volatile matter, %		Caloric value, Q^{daf} kcal/kg	Elemental analysis, %					H/C
	A^a	A^d	V^a	V^{daf}		C^{daf}	H^{daf}	N^{daf}	S^{daf}	O^{daf}	
13.29	10.78	12.43	34.15	44.98	5914	67.56	5.79	1.18	1.67	23.8	1.03

Results of the proximate and ultimate analysis indicate that coal from Chandgana Tal deposit is brown coal containing volatile matter ($V^{daf}=44.98\%$), and carbon ($C^{daf}=67.56\%$). The value is usually between $V^{daf}=45-55\%$ in

brown coal[4]. The ratio of hydrogen to carbon was 1.03%. The sulfur content of the coal sample is $S^{daf}=1.67\%$, which is considered as medium sulfur. The results of FT-IR analysis of coal samples are shown in Figure 1.

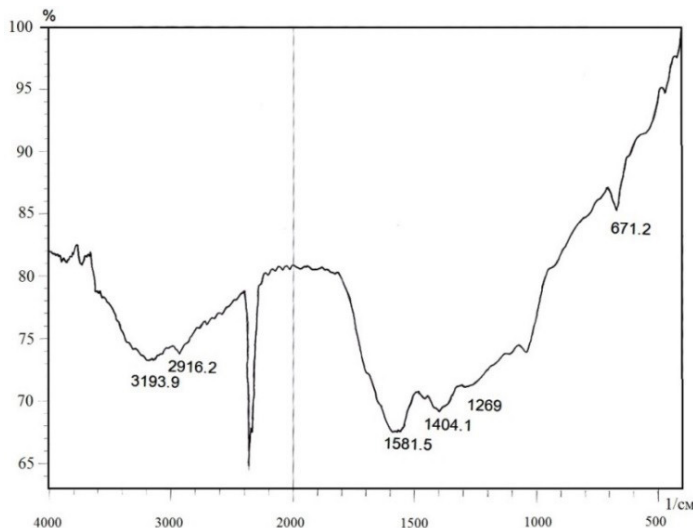


Figure 1. The FT-IR spectra of coal from Chandgana Tal deposit

In the FT-IR spectra, Chandgana Tal coals, wavelengths can be observed, such as 671 cm^{-1} wavelength for low intensity absorbance of aromatic rings -CH; 1269 cm^{-1} wavelength for low intensity absorbance of C-O- ether groups, 1404 cm^{-1} wavelength for medium intensity absorbance of aromatic C=C, 1582 cm^{-1} wavelength for low intensity absorbance

of ester >C=O group in carboxyl, 2916 cm^{-1} wavelength for high intensity absorbance of aliphatic -CH, - CH_2 , - CH_3 groups, and 3194 cm^{-1} wavelength for low intensity absorbance of -OH groups[6,7].

The results of FT-IR analysis of coal ash samples are shown in Figure 2.

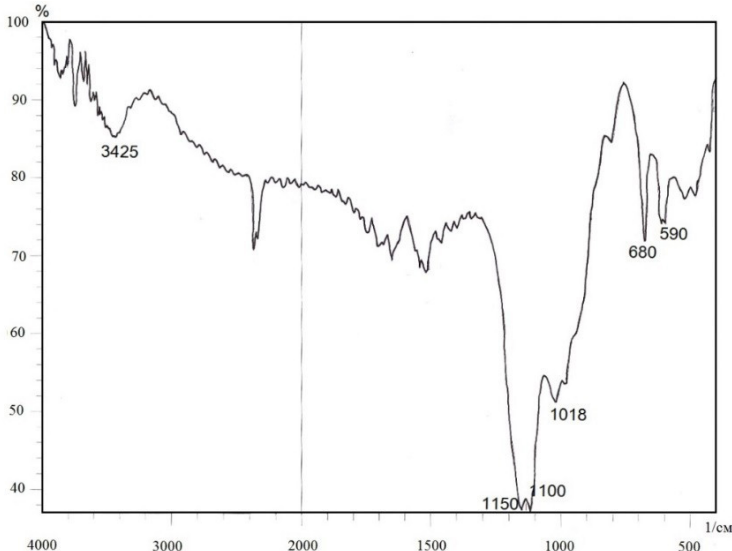


Figure 2. The FT-IR spectra of ash of coal from Chandgana Tal deposit

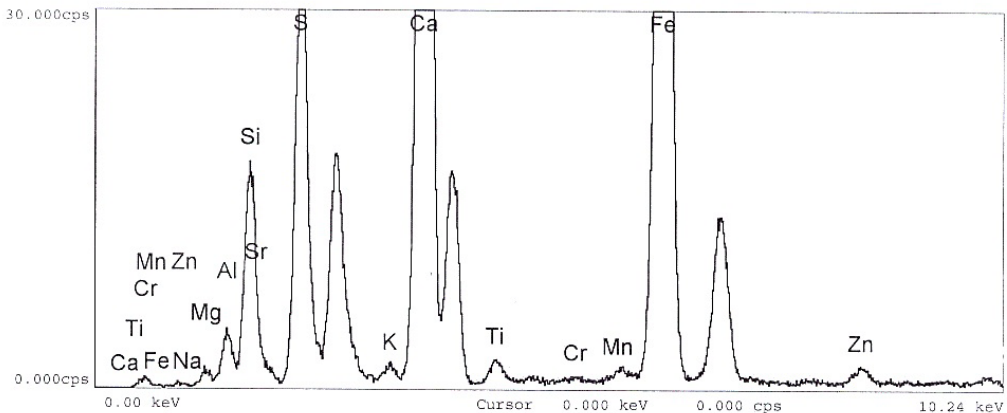


Figure 3. The x-ray fluorescence spectrogram of coal ash of Chandgana Tal deposit

The result of FT-IR analysis of coal ash of Chandgana Tal deposit shows the following wavelengths[6,7] - 590-680 cm^{-1} wavelength for absorbances of -Si-O-Al-, -Si-O-Fe-, -Si-O-Mg, 1018 cm^{-1} wave range for intensity

absorbance of Ca-O- group, 1100-1150 cm^{-1} wave range for high intensity absorbance of -S-O- and -Si-O-, and 3425 cm^{-1} wavelength range for low intensity absorbance of hydroxyl group.

The mineral component of ash in the coal ash of Chandgana Tal deposit investigated by the x-ray fluorescence spectroscopy, is shown in Table 2.

Table 2. Composition of coal ash of Chandgana Tal deposit, %

Elements, %		Oxides, %	
Na	n.d	Na ₂ O	n.d
Mg	7.83	MgO	12.98
Al	6.23	Al ₂ O ₃	11.78
Si	11.34	SiO ₂	24.25
S	6.04	SO ₃	15.07
K	0.2	K ₂ O	0.24
Ca	16.47	CaO	23.05
Ti	0.26	TiO ₂	0.43
Cr	0.01	Cr ₂ O ₃	0.02
Mn	0.05	Mn ₂ O ₃	0.07
Fe	8.16	Fe ₂ O ₃	11.67
Zn	0.13	ZnO	0.16
Sr	0.26	SrO	0.31

n.d- not detected

As shown in Table 2 and Figure 3, magnesium (MgO-12.98%), aluminum (Al₂O₃-11.78%), silica (SiO₂-24.25%), calcium (CaO-23.05%) and iron (Fe₂O₃-11.67%) oxides, are detected as macro elements of more than 1%. Therefore, the coal ash can be classified as carbonate types of ash. The composition of carbonate ash is SiO₂-15-40%, Al₂O₃-5-20%, Fe₂O₃-5-20%, CaO-20-40% [4]. The Chandgana Tal coal ash

contained Fe₂O₃<CaO+MgO (11.67<36.03), which means that the coal ash is lignite type ash with a high content of basic oxides.

Coal and their ash included kaolinite, apatite, montmorillonite, chalcopryrite, sulfates, barytes, dolomite, calcite and other minerals. The results of x-ray phase analysis for mineral contained in coal ash are shown in Figure 4 and Table 3.

Table 3. Analysis of x-ray phase in coal ash of Chandgana Tal

Substances detected in the analysis	Chemical formula
Anhydrite	CaSO ₄
Hematite	Fe ₂ O ₃
Magnetite	Fe ₃ O ₄
Quartz	SiO ₂

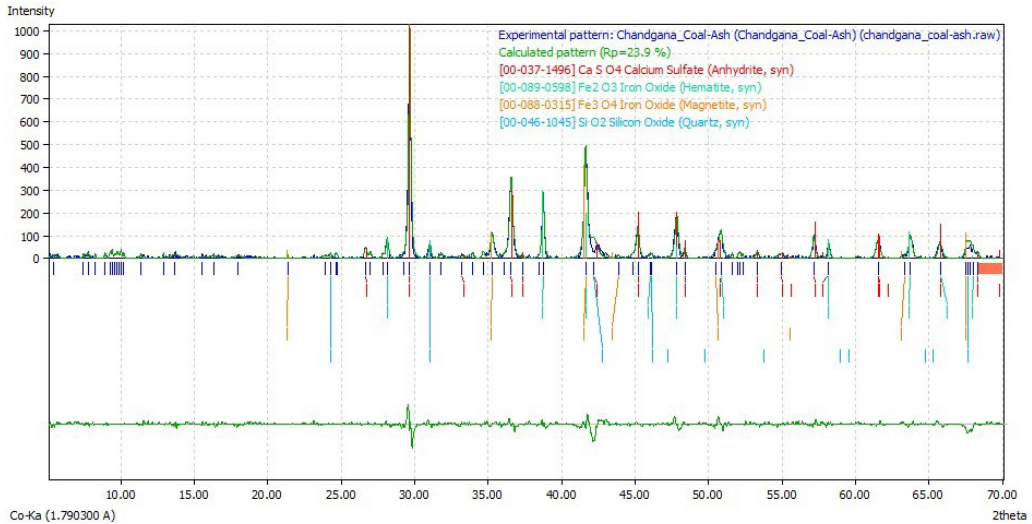


Figure 4. The x-ray phase spectrogram of coal ash of Chandgana Tal

The analysis of x-ray phase has detected hematite and quartz in coal ash, confirming the result of x-ray fluorescence and FT-IR analysis.

The pyrolysis experiments of Chandgana

Tal coal sample with 0.0-0.2mm size have been carried out in a standard quartz retort of laboratory at 200-7000C temperature. The yield of pyrolysis products including char, tar, pyrolytic water and gas are shown in Figure 5.

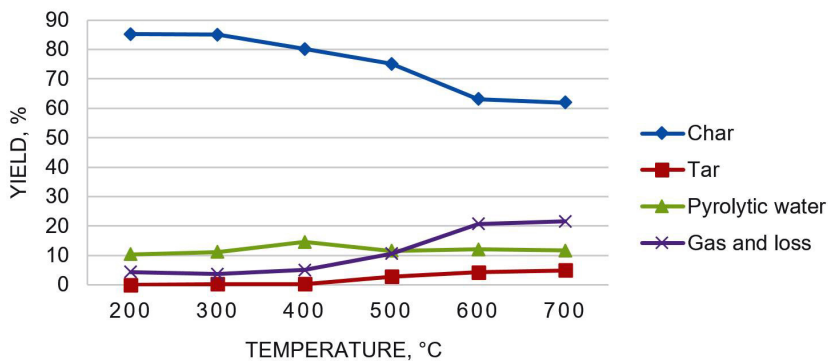


Figure 5. Yeild of pyrolysis product and pyrolysis temperature

As shown in figure 5, the yield of products such as tar, pyrolytic water and gas, was very low at a low temperature (200-300°C), confirming the start of coal organic mass decomposition.

With the increase of temperature, the yield of char decreased, while the yield of liquid

product and pyrolysis gas increased. The yield of tar is maximum at 700°C, or 4.8%. This temperature was selected for pyrolysis in a bigger scale retort. The yield of pyrolysis product are shown in Table 4.

Table 4. The result of pyrolysis experiments of Chandgana Tal coal (in bigger scale retort), wt%

Temperature of pyrolysis, °C	Char	Tar+pyrolytic water	Gas and loss
700	60.34	16.37	23.29

If we compare the result of a bigger scale retort (Table 4) and result of a standard quartz retort of laboratory (Figure 5), the yields of liquid product are similar and the yield of gas product is low in small scale experiment, showing that coal pyrolysis performed well in larger space. The high yield of all liquid and gas products (39.66%) shows an intensive thermal

decomposition of the organic coal mass with a higher degree of conversion.

The high yield of char could be suitable for the production of smokeless fuel. And low yield of tar shows that this coal is not suitable for liquefaction by pyrolysis. The result of proximate analysis of initial coal sample and char after pyrolysis are given Table 5.

Table 5. The result of proximate analysis of initial coal sample and char after pyrolysis, wt%

Sample	Moisture W ^a , %	Ash		Volatile matter	
		A ^a	A ^d	V ^a	V ^{daf}
Initial coal sample	13.29	10.78	12.43	34.15	44.98
Char after pyrolysis	0.87	25.6	25.82	5.38	7.32

The yield of volatile matter reduced by about 6 times and the yield of ash almost doubled as compared with that of initial coal.

The tar obtained by pyrolysis was separated from water. The composition of tar was

determined by organic compound group. These are free carbon, organic bases, organic acids, phenols, asphaltene, and neutral oil. The result of organic compound groups of tar is shown in Table 6.

Table 6. The result of organic compound groups of tar of Chandgana Tal coal, wt %

Free carbon	Organic bases	Organic acids	Phenols	Asphaltenes	Neutral oil
8.83	0.6	0.03	5.31	20.85	64.38

The table shows that neutral oil is a major group. Asphaltenes, which is the second largest part of tar, has high molecular mass compounds, insoluble in hexane. Organic

bases and organic acids had very low content. The result of FT-IR analysis of coal tar is shown in Figure 6.

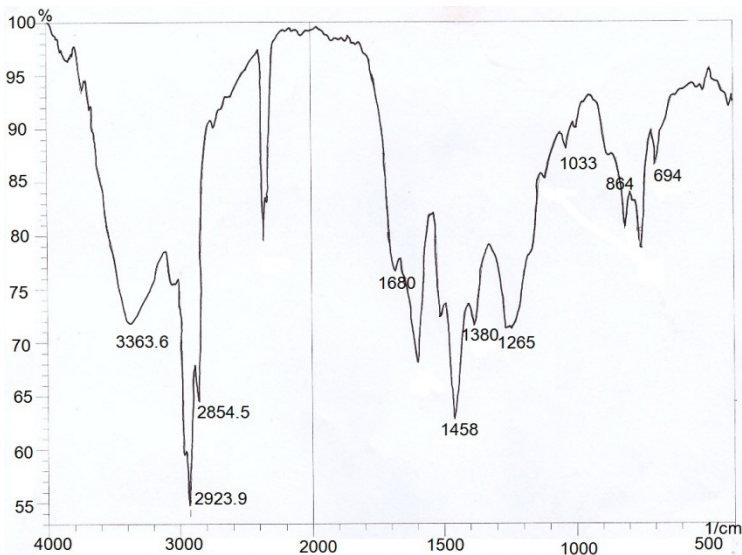


Figure 6. The FT-IR spectra of coal tar from Chandgana Tal deposit

In the FT-IR, the spectra of tar can be recognized as follows: 694-864 cm⁻¹ for absorption of -CH groups of cyclo aromatic, 1033-1265 cm⁻¹ for absorption of C-O- groups of ether, 1380 cm⁻¹ and 1458 cm⁻¹ for -CH₂, -CH₃ groups, 1680 cm⁻¹ for >C=O group of carbon acid and ester, 2854.5 cm⁻¹ and 2923.9 cm⁻¹ for -CH, -CH₂, -CH₃ groups, 3363.6 cm⁻¹ for -OH groups[6,7].

Coal consisted of complex and high molecular components, which can be converted into liquid product. The coal liquefaction

technology is classified as direct and indirect. The direct liquefaction process is divided into two types, thermal dissolution and catalytic hydrogenation.

Using this method, the thermolysis (thermal dissolution) experiments of Chandgana Tal coal in the tetralin (hydrogen donor solvent) have been carried out in a laboratory scale autoclave at 350-450°C and determined the yield of thermolysis products including hard residue, tar and gas as shown in Table 7.

Table 7. The results of thermolysis experiments of Chandgana Tal coal, wt %

Donor solvent, g	Coal:solvent	Temperature, °C	Hard residue	Tar	Gas and loss
Tetralin	1:1.8	350	60.00	6.85	33.15
		400	30.00	13.70	56.30
		450	25.00	23.50	51.50

Table 7 shows that the yield of hard residue (char) decreases intensively and the yield of tar and gas increase intensively with the increase in heating temperature. The highest yield (23.5%) of tar was obtained at 450°C. At this condition, the yield all liquid and gas products reached 75%, demonstrating that there was

an intensive thermolysis of coal organic mass with a higher degree of conversion (almost 1.9 times higher than that of pyrolysis).

The next step of our work was to investigate the characteristics of the obtained char after thermolysis with the initial coal sample given in Table 8.

Table 8. Characteristics of char after thermolysis and initial coal of Chandgana Tal, wt%

Name of coal deposit	Temperature, °C	Ash	Volatile matter
Initial coal sample	-	12.43	44.98
Char after thermolysis	350	25.90	30.05
	400	50.91	45.97
	450	49.49	21.44

Compared to the initial coal sample, ash content increased and the content of volatile matter decreased. This is an indication of intensive thermal decomposition of coal organic mass by

thermolysis.

Char obtained from coal is activated by water steam to obtain absorbent material. The result of char activation is shown in Table 9.

Table 9. Absorption properties of char and activated char

Sample	Iodine absorption, %	Methylene blue absorption, mg/g
Char of pyrolysis (hard residue)	10.45	15.6
Activated hard residue	22.71	120

The result in Table 9 shows the absorption ability (iodine and methylene blue adsorption) of activated char. Iodine and methylene blue absorption by activated char are 2 and 8 times

higher than that of initial char respectively. Therefore, the Chandgana Tal coal char could be used for the production of absorption materials with a high level of absorption.

CONCLUSIONS

1. The yield of volatile matter ($V^{daf}=44.98\%$), carbon content ($C^{daf}=67.56\%$) and sulfur content ($S^{daf}=1.67\%$) of Chandgana Tal coal showed that the coal belongs to the lignite type of coal with medium content of sulfur.
2. In the FT-IR, the spectra of Chandgana Tal coal can be recognized as $-CH$ of aromatic rings, $C-O$ -ether group, $C=C$ in aromatic, $>C=$ of ester of carboxyl, $-CH$, $-CH_2$, $-CH_3$ in aliphatic structures, and $-OH$ groups.
3. The ash of Chandgana Tal coal ($MgO-12.98\%$, $Al_2O_3-11.78\%$, $SiO_2-24.25\%$, $CaO-23.05\%$, $Fe_2O_3-11.67\%$) can be classified as carbonate type ash with basic character.
4. With the increase of temperature, the yield of char decreases, while the yields of liquid product and pyrolysis gas increase. The yield of tar is maximum at $700^\circ C$, or 4.8% .
5. The results show that neutral oil is a major group of coal tar. Asphaltenes, which is the second largest part of tar, has high molecular compounds, insoluble in hexane. Organic bases and organic acids had relatively low content.
6. The result of thermolysis of Chandgana Tal coal in tetralin with constant mass ratio coal/tetralin (1:1.8) at $450^\circ C$ shows that 23.5% of liquid product can be obtained by way of thermal decomposition of the coal.

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