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**STUDY OF THE INTERRELATIONSHIPS AMONG CHEMICAL AND
PETROGRAPHIC VARIABLES OF UNITED STATES COALS**

Technical Report 9

By
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U. S. DEPARTMENT OF ENERGY

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ABSTRACT

Multivariate statistical techniques, using data from the computerized data base being developed by the Coal Research Section of The Pennsylvania State University, are used in a study of the interrelationships among various coal properties. The properties chosen for study are the components of the ultimate analysis (carbon, hydrogen, organic sulfur, nitrogen and oxygen); moisture; volatile matter; calorific value; maximum reflectance of the vitrinite-group macerals; and the relative proportions of the vitrinite-, liptinite-, and inertinite-group macerals. The coals included in the study are from four coal provinces (Eastern, Interior, Rocky Mountain, and Northern Great Plains) and range in rank from lignite to anthracite.

A coal's characteristics, properties, and utilization behavior are determined by the maceral and mineral materials composing the coal. This study supports the idea that the level of coalification achieved by the maceral materials is of critical importance in fixing the properties that a specific seam will display in a particular area.

A factor analysis performed on all data together indicates that most variation in the data set is correlated with changes in rank (variables which vary with rank include carbon, oxygen, calorific value, moisture, volatile matter, and reflectance).

Hydrogen is not recognized by the analysis as a rank-dependent element when all coals are studied because of its curvilinear response to rank increase. The maceral groups account for the next greatest amount of variation. Nitrogen and sulfur are each independent of all other variables. A cluster analysis indicates that the data set represents a continuum with no distinct groups. The data set may be dissected into four groups distinguished from each other on the basis of rank, on the relative proportions of the maceral groups, and on the organic sulfur content. Factor analyses of the individual groups provide insights into coalification at various stages of rank. Carbon, oxygen, and calorific value vary together and are strongly affected by coalification for most levels of rank. Reflectance, moisture and volatile matter usually vary together, except for high levels of high volatile bituminous rank. Hydrogen content increases with rank until the middle levels of high volatile bituminous rank, then decreases. At rank levels of medium volatile bituminous and higher, a distinct change is observed in the response of variables to coalification: reflectance, volatile matter and hydrogen are strongly correlated with rank; carbon, oxygen and calorific value no longer vary strongly with rank and they behave independently of one another.

The coals of individual provinces are studied as a comparison of properties of different geographic areas. Eastern province coals are highest in rank; Western coals (Rocky Mountain and Northern Great Plains coal provinces) are lowest in rank. The results of

factor analyses for these provinces indicate that properties of their coals are consistent with that expected of their position along the rank continuum. Interior province coals are intermediate in rank and are highest in organic sulfur content which is usually associated with a strongly marine-influenced environment of deposition. The results of factor analysis indicate that the Interior province coals have properties which are unusual when compared with the other coals; they seem to be higher in moisture content and lower in reflectance than expected of their levels of rank.

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I. INTRODUCTION AND OBJECTIVES OF STUDY

A computerized coal data base is being developed by the Coal Research Section at The Pennsylvania State University. This data base contains quantitative and qualitative data on coals from throughout the United States. The samples cover the entire range of rank and include the major types of coal represented in this country. The Pennsylvania State University is now under contract with the Energy Research and Development Administration Fossil Energy Division (ERDA contract number EX-76-C-01-2030) to expand this data base to a total of 1600 coal samples by August, 1979. Although as yet incomplete, this collection of coals presents an opportunity for a preliminary investigation of the interrelationships among select properties of coals from the United States.

The main objective of this study is to evaluate statistically the interrelations among components of the organic portion of coals. Variables chosen are those that are commonly used to characterize the organic portion of coal, and to classify coals according to rank. The chemical parameters included in the study are components of the proximate and ultimate analyses, and calorific value. Petrographic parameters included are reflectance and maceral composition. Since coal is a complex material, multivariate analyses are utilized in this study.

Another goal of this study is to gain insight into the nature of coalification, or metamorphism, of coals of this country. Many models of coalification have been proposed by various researchers.

This study involves the statistical analysis of variables representing the organic portion of coals from a wide range of rank. Therefore, the results of coalification may be observed and may be checked against the expected results of the models of coalification.

A final objective is to investigate whether natural groupings exist within coals of this country. The coals of this study are from many geographic regions and from several geologic periods; they were deposited in various environments of deposition; and they have been subjected to different types and degrees of post-depositional alteration. These questions may be asked: To what extent do these many variations affect the ultimate nature of coal? For coals of this country, are there natural groupings based on, for example, geographic region or age of the coal? Also, are there distinct divisions of coal based on rank? To approach these questions of natural groupings, a multivariate classification method is used. This allows the variables to be analyzed simultaneously, and objectivity in the study is increased.

II. PREVIOUS RESEARCH

Coal has been defined as "a compact stratified mass of mummified plants which have been modified chemically in varying degree, interspersed with smaller amounts of inorganic matter" (Francis, 1954).

There are three major factors which control the properties of coal. One is the proportion and type of maceral material present. A second is the amount of coalification achieved by the maceral material since deposition. A third factor is the varying amount and kinds of mineral matter which enter the coal system either at the time of deposition or later. In this study, only the organic portion of the coal is considered, and the level of coalification achieved is the primary factor of variation within the data to be examined.

A. Rank

The extent of alteration (coalification) that the plant material has undergone since time of deposition influences many of the properties of a coal. The rank of a coal is a measure of this alteration. Discussions of the processes and results of coalification are given by many authors, including Francis (1954), White (1925), Schopf (1948), Dulhunty (1954), van Krevelen (1961), Stach (1968), and Teichmüller and Teichmüller (1966, 1968, 1976). It is generally accepted that coalification occurs in two stages. The first stage involves biological-bacterial processes and is termed biochemical coalification. This is primarily a diagenetic process. The second stage begins at the formation of lignite and is termed geochemical coalification.

The results of early geochemical coalification are said to be primarily "physico-structural" changes due to overburden pressure associated with increasing depth of burial (Teichmüller and Teichmüller, 1968). The main process acting at this stage is dewatering due to decreasing porosity. Chemical changes also occur and these include decarboxylation ($-\text{COOH}$), dehydroxylation ($-\text{OH}$), and loss of other edge groups rich in oxygen from the chemical structures of coal. These processes result in an enrichment of carbon, an increase in calorific value, and a decrease in both moisture content and oxygen. The second phase of geochemical coalification begins in the high volatile bituminous rank range. Most of the oxygen of the coal molecules is said to have been lost by the time this stage is reached, leaving mainly hydrogen-rich edge groups. The loss of hydrogen in the form of methane becomes the main process of coalification. The results of coalification at this stage are a decrease of hydrogen and volatile matter, and an increase in reflectance.

It has long been recognized that the amount of coalification of a coal significantly influences the properties of that coal. Therefore, many systems developed for classifying coals are based primarily on determining the rank of a coal.

One approach to studying and classifying coals by rank is based on components of the elemental analysis. Seyler (1938) developed a classification for coals based on carbon and hydrogen. Lines of equal volatile matter and equal calorific value were superimposed on his plots of carbon versus hydrogen so that elemental

properties could be graphically related to behavioral properties. He also developed quantitative methods for predicting calorific value and volatile matter from the components of elemental analyses. Van Krevelen (1961) used a diagram plotting atomic ratios of H/C versus O/C to indicate chemical processes of coalification. Many other approaches to the use of elemental analyses for studying properties of coals have been devised, including those by Campbell (1906), Grout (1907), Ralston (1915) and White (1933).

Another group of rank classification is aimed primarily at evaluating the behavior of coals for industrial purposes from results of proximate analyses and other tests of behavior. The current American Society of Testing and Materials (ASTM, 1976, Standard D-388) classification is based on volatile matter and calorific value; agglomerating properties are used as a basis of subclassification. The International Standards Organization (see van Krevelen, 1961) proposed a three-part classification scheme based on 1) volatile matter (dry, ash-free) and calorific value (moist, ash-free) as rank indicators; 2) caking properties to indicate behavior in a grate; and 3) coking properties to evaluate the suitability of coal for coking. The National Coal Board of England used volatile matter and caking properties to classify coal behavior in solid-fuel burning appliances (Moffat, Hicks, and Matthews, 1950). Some other early studies of coal based on proximate and behavioral properties were carried out by Ashley (1928), Parr (1932), Mott (1948), Spooner (1951), and King (1944).

Reflectance has been used as a measure of coal rank and thus as an indicator of the properties of coal. The percent of incident light which is reflected from the polished surface of vitrinite particles is the reflectance value of a coal. The amount of reflectance of vitrinite increases with increased coalification. Seyler (1938, 1943) was an early advocate of reflectance measurements of coal and believed that reflectance increased in a discontinuous, step-wise manner. Broadbent and Shaw (1955), with the help of the photomultiplier of measuring reflectance, established that reflectance of vitrinite increases in a continuous manner. Benedict and Berry (1964) related reflectance measurements of vitrinite to certain coal properties, namely volatile matter, calorific value, free-swelling index, oxidation, and yields of carbonization products. Teichmüller and Teichmüller (1968) and McCartney and Teichmüller (1972) referred to the range of rank for which they believed reflectance to be a good measure of rank. Marshall (1976) recently proposed a method of classifying coals based on reflectance and results of dilatometer analyses. Other classification systems have been developed using reflectance as a rank parameter with petrographic composition as the second parameter; these will be discussed later. The variation of reflectance and its use as an indicator of rank has been the subject of many other papers (see van Krevelen, 1961).

B. Maceral composition

The development of coal petrology in recent years has added a new approach to studying and classifying coals. Stopes (1919, 1935)

was the first to classify coals on the basis of microscopic and petrographic composition, and to relate composition to chemical and physical properties. She proposed the term "maceral" as the organic counterpart of "mineral" to designate the organic components of coal. Cady (1942) also discussed fundamental chemical differences in the three kinds of coalified materials: vitrinite, fusinite and "waxy-resinoid phytals" (liptinite). He suggested that the chemical differences in the petrographic components may be important in coal utilization. This three-component classification of macerals is useful for many purposes. The basic chemical differences in the three groups are that the liptinite-group macerals are relatively rich in hydrogen and are the most aliphatic in chemical structure; the inertinite-group macerals are relatively rich in carbon and are highly aromatic in chemical structure; and the vitrinite-group macerals are relatively enriched in oxygen and are intermediate in degree of aromaticity and aliphatic structure. Van Krevelen (1961) uses the atomic H/C versus O/C ratios for the maceral groups to indicate different lines of development during coalification. Given and others (1960), also studying the chemistry of macerals, cite experimental evidence that the macerals of the liptinite group are more aliphatic than are the vitrinite-group macerals, and that the macerals of the vitrinite group are enriched in hydroxyl groups. The three maceral groups are known to behave differently from one another in certain technological processes. Under coking conditions, vitrinite and exinite groups are considered

reactive macerals because they become plastic, and volatilize, respectively. The degree to which these macerals are reactive depends on the rank of the coal. The inertinite macerals (fusinites, macrinite, micrinite, and sclerotinite) receive their name because they are inert to the coking process. Discussions of maceral properties and of systems developed for predicting coke strength are given by Ammosov and others (1957), Spackman and others (1960), Schapiro and Gray (1960), Schapiro and others (1961), Thompson and others (1966), Benedict and others (1968b), Harrison and others (1964), Brown, Cook, and Taylor (1964), and Brown, Hesp and Waters (1964a,b). Studies relating maceral composition and conversion yields in liquefaction processes indicate that macerals of the vitrinite and liptinite groups are probably reactive in liquefaction processes, and the inertinite-group macerals are probably inert in the processes (Fisher and others, 1942; Davis and others, 1976; Mitchell and others, 1976).

Several systems have been developed for classifying the organic constituents of coal. Thiessen (1920) developed a method for use with transmitted-light microscopy. The classification schemes most widely in use today are adaptations of the Stoper-Heerlen system (International Committee of Coal Petrology, 1971) for reflected light microscopy which is based on morphology, reflectance and behavior in technological processes. In this system, coal macerals are classified into three main classes as discussed above, and each component is composed of macerals with unique identifying characteristics of morphology, texture,

and reflectance. Some modifications have been made to the classification scheme. For instance, Benedict and others (1968) have subdivided vitrinite into "reactive" vitrinite and "pseudovitrinite" based on slight differences in reflectance, morphology, and behavior (pseudovitrinite is more inert in the coking process than the reactive vitrinite). Brown, Cook, and Taylor (1964) also subdivide vitrinite into two components: vitrinite A and B. M. Teichmüller (1974a,b) has added three new members to the liptinite maceral group based on observations of fluorescence in blue light. Spackman and others (1976) discuss the possible relation of these "new" macerals to conversion yields in liquefaction processes. Several other classification systems other than the Stopes-Heerlen system have been suggested for incident-light microscopy, including those by Hacquebard (1950) and Spackman (1958).

III. SAMPLING DESCRIPTION

The Penn State/ERDA coal data base contains data on several kinds of gross sample types, including channel, lithotype, and run-of-mine samples. This study is limited to channel samples. They are considered to provide the best descriptive data of properties of whole seams of coal. Ideally, a fresh, vertical face was sampled by making a cut perpendicular to the bedding. Width and depth of the cut varied with the height of the seam to give approximately 500 to 600 pounds of coal. The samples were coned and quartered until a sample size of about 35 pounds was obtained. This smaller sample size was crushed to $\frac{1}{4}$ inch. Five pounds of $\frac{1}{4}$ inch coal were ground to -20 mesh (0.84 millimeters) and riffled to give about 80 grams of sample for chemical and petrographic analyses.

A total of 119 channel samples are included in this study. The coals considered are those which had complete chemical and petrographic data in the computerized data base as of September, 1976. Four coal provinces are represented, including the Eastern province (64 samples), the Interior province (25 samples), the Rocky Mountain province (19 samples) and the Northern Great Plains province (11 samples). Figure 1 is a map of the four basins and the location of channel samples. Table 1 gives a classification of the samples according to apparent ASTM rank*. The coals include 5 lignites, 8 subbituminous coals, 86 high volatile bituminous coals, 4 medium volatile bituminous coals, 6 low volatile

* ASTM requires equilibrium moisture analyses for determining rank; an as-received moisture basis is used here because equilibrium moisture analyses are not available for all coals.

Figure 1. LOCATIONS OF PROVINCES AND SAMPLING SITES

Table 1. Distribution of channel samples by region and by ASTM rank classification

	lig- nite	subbituminous			high volatile bituminous			medium volatile bituminous	low volatile bituminous	semi-anthra- cite to anthracite	Total
		C	B	A	C	B	A				
Eastern Province					1	3	40	4	6	10	64
Interior Province					6	11	8				25
Northern Great Plains Province	4		5				2				11
Rocky Mountain Province	1		1	2	9	4	2				19
Total	5		6	2	16	18	52	4	6	10	119

bituminous coals and 10 semianthracites and anthracites. All coals above the low volatile bituminous rank are excluded from statistical computations because of the low number of samples for this wide range of rank. Some plots include these samples to give an indication of trends of properties in the extremely high rank coals. Complete information regarding location, seam name, and rank for all the samples is found in Appendix I.

Obtaining a complete set of statistically random samples from the total population of American coals is difficult to achieve. The results of this study must be viewed with this limitation in mind.

IV. DESCRIPTION OF VARIABLES

Variables chosen for this study are those that express the organic composition of coals. They include the common chemical and petrographic components of coal analyses. The chemical analyses included were determined by Commercial Testing and Engineering Company. Carbon, hydrogen, and oxygen have been used by various authors to determine coal rank and to predict other coal properties such as volatile matter and calorific value. Nitrogen and organic sulfur are also components of the ultimate analysis and they complete the conventional elemental description of a coal. Variables of a proximate analysis include determinations of ash, moisture, and volatile matter. Ash is not included in this study. However, the ash value is used to calculate other variables to a mineral-free basis. The moisture, volatile matter, and calorific value are included because they have also been used to indicate rank. Moisture is not an organic constituent, but the moisture-holding capacity of a coal reflects changes in the organic portion of coal during metamorphism. These changes are both physical due to compression by overburden pressure, and chemical. The moisture value is also used to calculate other variables to a dry basis. To be consistent with the other variables of this study, moisture is converted to the mineral-free basis. Calorific value is included because it is a commonly used measure of rank. The percent reflectivity of vitrinite ("reflectance") is included because it is a petrographic measure of rank. The volume percent of the three maceral-group components - vitrinite, liptinite, and inertinite - complete the data set.

Appendix II contains the data matrix of coals and the variables that are included in this study.

A. Variables of the ultimate analysis

1. Carbon and hydrogen

Carbon and hydrogen percentages are determined according to ASTM Standard D-3178. A weighed quantity of coal ground to pass a 250 μ sieve is burned in a closed system and the combustion products are fixed in absorption trains (carbon dioxide absorption train for carbon; water absorption train for hydrogen). The results must be corrected for inorganic carbon from carbonate mineral matter, and inorganic hydrogen from free moisture and water of hydration of clays. Differences in results of repeated analyses must not exceed 0.3 percent for carbon, or 0.07 percent for hydrogen.

2. Nitrogen

ASTM Standard D-3179 explains methods for determining the percent of nitrogen present in a coal; the method commonly used for the Penn State/ERDA samples is presented here. Approximately one gram of a sample crushed to pass a 250 μ sieve is converted to ammonium salts by destructive digestion of the sample with a hot, catalyzed mixture of concentrated sulfuric acid and potassium sulfate, the salts are decomposed, the ammonia content is determined and is used to calculate the percentage of nitrogen. Differences in results of repeated analyses must not exceed 0.05 percent.

3. Organic sulfur

The total sulfur content of a coal is determined by the Eschka method as described in ASTM Standard D-3177. A sample ground to pass a 250 μ sieve is ignited with an Eschka mixture

(two parts by weight of light calcined magnesium oxide and one part anhydrous sodium carbonate). The sulfur is precipitated as barium sulfate which is filtered, ashed, and weighed. Differences in results of repeated analyses must not exceed 0.05 percent for coals with less than two percent total sulfur, and 0.10 percent for greater than two percent total sulfur. Organic sulfur is determined by subtracting from the percent of total sulfur the sum of pyritic and sulfatic sulfur, determined according to ASTM Standard D-2492. Sulfate sulfur is determined by extracting a weighed sample of coal with dilute hydrochloric acid followed by precipitation with barium chloride and weighing as barium sulfate. Differences in results of reported analyses must not exceed 0.02 percent. Pyritic sulfur is determined by extracting a weighed sample of coal with dilute nitric acid followed by titrimetric determination of iron in the extract as a measure of pyritic sulfur. Differences in results of repeated analyses must not exceed 0.05 percent for coals with pyritic sulfur less than two percent, or 0.10 percent for coals with two percent or more total sulfur.

4. Oxygen

Oxygen is determined by subtracting from 100 the total percentages of ash, carbon, hydrogen, total sulfur, and nitrogen, all calculated to the dry basis. This is in accordance with ASTM Standard D-3176.

B. Variables of the proximate analysis

1. Moisture

Moisture is determined according to ASTM Standard D-3172. The amount of weight loss is measured when approximately one gram of coal, crushed to pass a 250 μ sieve, is dried by air passing through an oven preheated to 104 to 110°C. Differences in results of repeated analyses must not exceed 0.2 percent for coals with less than five percent moisture and 0.3 percent for coals containing greater than five percent moisture.

2. Ash

Ash is determined according to ASTM Standard D-3174. One gram of coal ground to pass a 250 μ sieve is heated gradually to 500°C in one hour and to 750°C in two hours. The coal is burned at 700 to 750°C until a constant weight (± 0.001 gram) is obtained and the remaining inorganic residue is weighed. Differences in results of repeated analyses must not exceed 0.2 percent for coals with no carbonates, 0.3 percent for coals containing carbonates, and 0.5 percent for coals with greater than 12 percent ash and with carbonates and pyrites. The percent of ash is used in this study to convert other variables to a mineral-matter-free basis.

3. Volatile matter

Volatile matter is determined according to ASTM Standard D-3175. One gram of coal ground to pass a 250 μ sieve is rapidly heated to 950 $\pm$ 20°C and held at that temperature for seven minutes. The percent volatile matter is then determined by measuring the amount of weight loss corrected for loss due to moisture content.

Differences in results of repeated analyses must not exceed 0.3 percent for anthracites, 0.5 percent for semianthracites and bituminous coals, 0.7 percent for subbituminous coals, and 1.0 percent for lignites and peats.

C. Calorific value

Gross calorific value is defined by ASTM Standard-407 as the heat produced by combustion of unit quantity at constant volume, in an oxygen bomb calorimeter under specific conditions. Gross calorific value is determined according to ASTM Standard D-2015. One gram of sample ground to pass a 250 μ sieve is burned in oxygen in a calibrated isothermal jacket bomb calorimeter, and calculations are made with temperature readings taken before, during, and after combustion. Differences in results of repeated analyses must not exceed 50 British thermal units per pound (Btu/lb).

D. Calculations to dry, mineral-matter-free basis

Values of proximate and ultimate analyses are converted to dry, mineral-matter-free values. In this way only the organic portion of the coal is considered.

Moisture corrections are made for all variables except hydrogen according to the following formula:

$$V_d = V_{ad} \times \frac{100}{100 - M_{ad}} \quad (1)$$

where V_d is the variable on a dry basis, V_{ad} is the variable on an as-determined basis, and M_{ad} is the moisture on an as-determined basis.

Hydrogen reported on the as-determined basis includes hydrogen to a dry basis and including the correction for free-moisture hydrogen is as follows:

$$H_d = (H_{ad} - 0.119 M_{ad}) \times \frac{100}{100 - M_{ad}} \quad (2)$$

The mineral matter is calculated using the Modified Parr formula (Given and others, 1975) which is a modification of the Parr formula for mineral-matter (Parr, 1932). The Modified Parr mineral-matter formula is

$$MM = 1.13 \text{ Ash} + 0.47 S_{\text{pyr}} + Cl \quad (3)$$

where MM is mineral matter, S_{pyr} is pyritic sulfur, and Cl is chlorine. The ash term corrects for water lost by decomposition of clays in the ash determination; the average water of constitution of clays is assumed to be 11.2 percent. The sulfur term allows for loss in weight of pyritic sulfur when pyrite is burned to ferric oxide. The Parr determination assumes that all sulfur is pyritic sulfur and thus includes sulfatic and organic sulfur in the mineral-matter calculation. When information on the forms of sulfur is available, the Modified Parr formula may be used to give a better approximation of the percent of inorganic material present. Given and Yarzab (1975)

state that chlorine is usually very small for United States coals and can be omitted from the calculation. Chlorine contents are usually determined for coals in the Penn State/ERDA data base and are included in calculating to the mineral-matter-free basis.

The actual mineral-matter free variables used in the analyses are calculated in the following manner:

$$C_{\text{dmmf}} = (C_{\text{dry}} - C_{\text{carbonates}}) \times \frac{100}{100 - \text{MM}} \quad (4)$$

$$H_{\text{dmmf}} = (H_{\text{dry}} - H_{\text{clay water}}) \times \frac{100}{100 - \text{MM}} \quad (5)$$

$$S_{\text{org, dmmf}} = S_{\text{org, dry}} \times \frac{100}{100 - \text{MM}} \quad (6)$$

$$N_{\text{dmmf}} = N_{\text{dry}} \times \frac{100}{100 - \text{MM}} \quad (7)$$

$$O_{\text{dmmf}} = 100 - C_{\text{dmmf}} - H_{\text{dmmf}} - S_{\text{org, dmmf}} - N_{\text{dmmf}} \quad (8)$$

where $C_{\text{carbonates}}$ is a correction for carbonate carbon and $H_{\text{clay water}}$ is an approximate correction for the hydrogen present in water of constitution of the clays.

In addition, before they are converted to a mineral-matter-free basis, the calorific value is corrected for the heat of combustion of pyrite, and the volatile matter is approximately corrected for loss of carbonate, clay water, and chlorine. The actual formulae are discussed in detail in Given and Yarzab (1975).

E. Petrographic variables

1. Reflectance

The mean maximum reflectance in oil of vitrinite is determined in accordance with ASTM Standard D-2798. An MPV1 photometer is attached to a Leitz Ortholux incident-light microscope and the percent reflectance of vitrinite is measured in monochromatic light with a wavelength of 546 nm. The microscope substage is rotated 360° to determine the maximum reflectance for each vitrinite particle. One hundred readings are taken on two pellets (50 readings per pellet) of coal ground to minus 20 mesh and the readings are averaged. Differences between the averages of the two pellets must not exceed 0.02% reflectance.

2. Maceral composition

The maceral classification used at Penn State is a modification of the Stopes-Heerlen classification (International Handbook of Coal Petrology, 1971). Table 2 lists the maceral groups, the individual macerals comprising each group, and some of the maceral properties. The groups are described as follows.

a. Macerals of the vitrinite group

The vitrinite group is conventionally considered to be composed of telinite and collinite (ICCP, 1971), or vitrinite and pseudovitrinite (Benedict and others, 1968a). It may also be considered as a more comprehensive "suite" of materials which include the vitrinitic-related macerals in lignites, brown coals, and anthracites (Spackman and Thompson, 1964). It is in this latter sense that the term is employed here. Vitrinite is derived from

Table 2. Modified Stoper-Heerlen maceral classification

Maceral Group	Maceral	Origin		Appearance		Chemistry	Technological Behavior	
		Source	Process	Thin Section	Reflected Light		Carbonization	Liquefaction
VITRINITE	Telinite (cell walls) Collinite (cell fillings, structureless vitrinite)	Woody tissues, bark, leaves, etc.	Mummification	Red-brown	Intermediate grey	Intermediate hydrogen content and volatiles	Principal reactive constituent in coking coal	Susceptible to Liquefaction
LIPTINITE (OR EXINITE)	Resinite	Resins	Resistant remains	Yellow	Dark grey	Higher hydrogen content and volatiles; more aliphatic	Reactive during carbonization	Susceptible to Liquefaction
	Sporinite	Spore exines						
	Cutinite	Cuticles						
	Alginite	Algae						
	Fluorinite	Plant Oils, Fats			Black			
	Bituminite	Bacterial lipoids, Fats, Proteins	Migration		Between Vitrinite & Sporinite			
	Exudatinite	Exudates from liptinite & Vitrinites		Black				
INERTINITE	Micrinite (massive & granular)	Plant materials	Degradation products	Opaque	White, yellowish, light grey	Lower hydrogen content and volatiles; more aromatic	Generally inert during carbonization	Generally resistant to liquefaction
	Fusinite	Woody tissues, etc.	Fire; biochemical oxidation					
	Semifusinite	Woody tissues, etc.	Intermediate between vitrinite and fusinite					
	Sclerotinite	Fungal sclerotia, hyphae	Resistant remains					

plant particles such as the woody tissues, bark, and parts of leaves. They are preserved by rapid burial and mummification in the peat stage. Pseudovitrinite is an addition to the original classification system (Benedict and others, 1968a). It is derived from the same plant particles as vitrinite but may have been subjected to slightly more intense oxidation in the peat stage prior to mummification (Teichmüller and Teichmüller, 1975); or pseudovitrinite may be derived from different plant species than is normal vitrinite (Koch, 1970). The macerals of the vitrinite group are the principal reactive components in the carbonization process and are susceptible to liquefaction, with pseudovitrinite being slightly less reactive than normal vitrinite.

b. Macerals of the liptinite group

The liptinite group is composed of plant particles which are resistant to alteration during the peat stage and early coalification processes. Therefore, in coals they are similar in morphology to their plant precursors. The liptinite-group macerals consist of resinite (coalified resin), sporinite (coalified spore and pollen exines), cutinite (coalified cuticle tissue) and alginite (fossilized algae). Of the maceral groups, the liptinites are the most aliphatic in chemical structure, the most enriched in hydrogen, and the most volatile in technological processes. They are volatile in the coking process and are thought to be reactive in liquefaction processes.

c. Macerals of the inertinite group

The inertinite group of macerals consist of micrinite, macrinite, fusinite, semifusinite, and sclerotinite. Micrinite

(previously termed granular micrinite), and macrinite (previously termed massive micrinite), are considered to be degradation products of plant materials formed during diagenesis and early stages of coalification (Teichmüller and Teichmüller, 1975). Fusinite (fusinite and semifusinite) is derived from the same plant tissues as is vitrinite but fusinite has had a different mode of preservation. Some ideas for the origin of fusinite are that it has been charred by fires in the peat swamp, or it has been subjected to intense biochemical oxidation prior to burial. Vitrinite, semifusinite, and fusinite may be considered as a continuum with semifusinite intermediate in the resulting properties. Sclerotinite is derived from fungal sclerotia and hyphae. Inertinite macerals have the most aromatic molecular structure of the maceral groups and are the most enriched in carbon and have the lowest hydrogen content of the maceral groups. Inertinite macerals are relatively unreactive in carbonization and liquefaction processes.

In the Penn State system of maceral analyses, a Leitz GmbH Wetzlar Ortholux microscope is used to determine the maceral composition of a coal. Polished pellets containing minus 20 mesh coal are examined on a grid system at a magnification of 600x. The grid spacing is one millimeter on the X-axis and two millimeters on the Y-axis. A ten point graticule inserted in one of the eyepieces allows ten counts to be made at each grid intersection. A total of 1,000 points are counted on two pellets (500 counts per pellet). At the Penn State Coal Research Section, differences in repeated results must be within ± 2 percent.

V. COALS FROM THROUGHOUT THE UNITED STATES

The purpose of this study is to analyze the interrelationships among select chemical and petrographic variables of United States coal. The 109 samples included in the statistical computations are channel samples ranging in rank from lignite through low volatile bituminous. (Anthracites are included in bivariate plots in section VIIIA.) In following sections of this report, the coals will be analyzed for natural groupings which may exist in the data set. However, the first step is to evaluate all the coals together as one sampling population. This will provide a "reconnaissance" investigation of variable interaction over a wide range of rank.

A systematic approach is followed for the statistical analysis of the data in all phases of study. First, the frequency distribution of each variable is analyzed and, when appropriate, mathematical transformations are performed to achieve normality. Next, factor analyses are performed to study the interrelationships among variables. Finally, results of factor analyses are discussed allowing interpretation of the underlying factors of variation within a given set of coals.

A. Univariate analyses

1. Tests of frequency distribution for normality

To perform tests of significance and set up confidence limits for statistical analyses, multivariate joint normality is an ideal to achieve (Griffiths, 1967). NORMSTAT, a statistical program written for the IBM 370 computer, is used to test the frequency distribution

for normality. There are two types of normality tests in the program. The first test is concerned with the shape of the curve as described by the skewness and kurtosis. Skewness is a measure of departure from symmetry. The curve for random samples of a normally distributed population is symmetrical about the mean; that is, the curve is not skewed (skewness $\sqrt{\beta_1}$ is equal to zero). In this study, if the mean of a variable is greater than the mode, such that a long tail of the distribution extends toward the high values, then the distribution is termed positively skewed. If the mean is less than the mode, and a long tail extends toward the low values, the distribution is termed negatively skewed. Kurtosis is a measure of the "peakedness" of the curve and a normally distributed curve has a kurtosis (β_2) equal to 3.0. The calculated skewness and kurtosis of a sample frequency distribution may be tested against the expected values of a normally distributed population (Pearson and Hartley, 1954) at a selected probability level for the sample size. Tabulated values of kurtosis are not given for sample sizes less than 200 since the test is unstable for smaller sample sizes. Therefore, for this study the values of kurtosis are tested against a sample size of 200, as a conservative test. If the calculated values of either skewness or kurtosis are within the accepted limits given by the tabulated values, then there is no evidence that the distribution is more skewed or peaked than expected for a normally distributed population.

The second test for normality is the Chi-square (χ^2) "goodness-of-fit" test. It tests the fit of a set of observations, class by class, to an expected normal distribution with the same mean and

variance (Griffiths, 1967). The calculated χ^2 is checked against the tabulated χ^2 (Selby, 1975) with the correct degrees of freedom and probability level desired. If the calculated χ^2 is less than the tabulated χ^2 at a given probability level, then there is no evidence for a significant departure from normality.

Skewness, kurtosis, and χ^2 are all checked at the five and one percent probability levels. If the distributions tested are found to deviate from a normal distribution, the appropriate mathematical transformation is performed to achieve normality (Griffiths, 1967), or to obtain the distribution closest to a normal distribution. Table 3 gives summary statistics for the variables and lists the transformations that were performed.

Frequency distributions of the untransformed variables are found in Figure 2 and are discussed below. Care must be taken in interpreting the frequency distribution of a variable. Within a homogeneous population, a variable has a set variance. However, non-random sampling of a population will superimpose a variance which may not reflect the true variance of the population. As the ERDA project progresses and the sample size of the data base increases, the sample frequency distributions should become better estimators of the population frequency distributions.

2. Analysis of frequency distributions of the variates

The distribution of reflectivity of vitrinite in oil (hereafter called "reflectance") is positively skewed and values greater than 1.10 percent are widely spaced. Reflectance is considered a sensitive indicator of rank changes in all ranges of bituminous coals, especially in the high levels of bituminous rank

Table 3. Summary statistics for variables of U.S. coals

	Low	High	Mean	St. Dev.	Skewness	Kurtosis [†]	χ^2 ^{††}	Transfor- mation	Skewness	Kurtosis [†]	χ^2 ^{††}
Reflectance	0.30	1.80	0.75	0.31	1.343**	4.851**	30.9**	log x	0.322	2.959	20.7
Carbon	71.52	91.56	82.88	4.37	-0.321	2.722	23.4				
Hydrogen	4.26	6.61	5.46	0.39	-0.573**	3.982**	30.8**				
Oxygen	1.61	21.45	8.92	4.43	0.857**	3.346	23.4	log x	-0.511	3.304*	21.0
Sulfur	0.10	4.01	1.11	0.76	1.499**	5.122**	113.8**	log x	0.114	3.131	45.8**
Nitrogen	0.13	2.55	1.62	0.42	-0.933**	5.118**	14.8				
Volatile matter	18.10	53.61	39.68	7.18	-1.447**	5.055**	54.0**				
Moisture	0.70	38.04	7.54	7.54	2.142**	8.150**	58.2**	log x	0.010	2.291**	22.3
Btu/lb	11902	16113	14794	888	-1.162**	4.042**	41.8**	$\log \frac{x}{1-x}$	-0.110	2.735	13.5
Vitrinites	46.2	92.5	78.0	9.0	-0.981**	3.881*	25.5*	$\log \frac{x}{1-x}$	-0.288	2.928	16.8
Inertinites	5.0	36.1	16.2	6.8	0.907**	3.652*	25.6*	log x	-0.129	2.732	6.4
Liptinites	0.0	33.6	5.8	5.7	2.186**	8.762**	75.9**	$\sqrt{x}$	0.662	4.047*	38.7**

*Significant at the 5 percent probability level (109 samples)

**Significant at the 1 percent probability level

†Kurtosis tested at sample size of 200

††d.f. = 40

Figure 2. FREQUENCY DISTRIBUTIONS FOR VARIABLES OF UNITED STATES COALS

Figure 2 (continued). FREQUENCY DISTRIBUTIONS FOR VARIABLES OF UNITED STATES COALS

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Figure 2 (continued). FREQUENCY DISTRIBUTIONS FOR VARIABLES OF UNITED STATES COALS

(McCartney and Teichmüller, 1972). If the coal samples are representative of a single, homogeneous population, then the long tail towards the high values is an aspect of the sensitivity of reflectance in high levels of rank; that is, a small increase in rank results in a relatively large increase in reflectance as compared to low levels of rank. The skewed distribution is also due to a small sample size (ten samples) of medium and low volatile bituminous coals.

The carbon distribution has a slight negative skew. Carbon is an especially sensitive rank indicator for high volatile bituminous and lower rank coals, so a wider spread in the lower carbon values would be expected. The distribution of oxygen content is skewed to the high values. Oxygen content is inversely related to carbon content; oxygen decreases as rank increases. The content of oxygen is especially affected by changes in the early stages of coalification, over the same range where carbon is a sensitive rank parameter.

The frequency distribution of calorific value is negatively skewed. Calorific value changes with coalification over the same range of rank as do carbon and oxygen. In levels of rank lower than medium volatile bituminous, the calorific value of a coal increases progressively with coalification, and the skewed distribution is what would be expected if this were true.

The moisture content distribution is strongly skewed to the right. Moisture content decreases considerably with increased rank in low-rank coals, and then changes little with continued coalification. The four coals with greater than 30 percent moisture are all lignites.

The frequency distribution for volatile matter is highly skewed to the low values and may be at least bimodal. Values greater than 30 percent volatile matter appear to be approximately normally distributed. The ten coals with volatile matter less than 30 percent are of low and medium volatile bituminous rank. In these high-rank bituminous coals the amount of volatile products of pyrolysis is most greatly decreased by coalification. The skewness is again due in part to the small sample size of medium and low volatile bituminous coals.

The distribution of hydrogen content has a slight negative skew. Losses of hydrogen accompanying rank increases are most pronounced at medium volatile bituminous and higher ranks. The extended tail to the lower values is again partly a result of few samples of the high rank bituminous coals.

The above parameters are considered to be dependent on rank; that is, their content in a coal is altered by the processes of coalification. The shapes of the frequency distributions are consistent with the models of coalification (for example, Teichmüller and Teichmüller, 1966; van Krevelen, 1961). At low levels of rank, the main effects of coalification are the loss of moisture and oxygen and the increase in carbon and calorific value; reflectance increases slightly. In high volatile bituminous coals, oxygen continues to decrease and carbon and calorific value increase; reflectance also increases significantly. For medium and low volatile bituminous coals, reflectance increases and volatile matter and hydrogen decrease strongly with coalification; carbon continues

to increase but at a slower rate than for earlier levels of coalification; oxygen and calorific value are not increased significantly with further coalification in this range of rank. The processes of coalification and their effects will be further discussed in later sections of this report. A summary of the model is presented here in explanation of the observed frequency distribution. The skewed distributions of all the rank-dependent factors result from mixed sampling of coals of different levels of rank where different processes are the primary causes of coalification.

The contents of organic sulfur and nitrogen do not appear to be altered significantly by the processes of coalification, so their frequency distributions are not considered to be a function of rank. The distribution of sulfur values is highly skewed to the right and appears to be at least bimodal. Coals very high in pyritic sulfur usually result from marine-influenced environments of deposition due to the availability of sulfate ions and iron on clays or organic complexes. The relative abundances of pyritic and organic sulfur in a coal are generally similar (Cady, 1935). Therefore, the organic sulfur content is also primarily a function of the original conditions of deposition. The highly skewed frequency distribution of organic sulfur results from mixed populations of marine-influenced and non-marine coals. Coals of the western United States are generally low in sulfur content; the sampled Western coals have a mean sulfur content of 0.60 percent. In contrast, the sampled Illinois Basin coals have a mean sulfur content of 2.02 percent. Sampled coals of the Eastern province

have an intermediate mean sulfur content of 0.97 percent. The statistics of sulfur values for the four provinces of this study are given in Table 4.

The frequency distribution of nitrogen has a slight negative skew. Again, nitrogen is a function of early environmental conditions (Teichmüller and Teichmüller, 1974). The distribution of nitrogen approaches normality and the extended tail towards the low values is due perhaps to a small sample size of low-nitrogen coals. Nitrogen content of coal is very difficult to measure (Rees, 1966), so the very low values (less than 0.8 percent) could also be attributed to experimental error.

The three maceral groups represent the petrographic component of the coal. Together these three groups sum to 100 percent. As the proportions of one maceral group increases, that of one or perhaps both of the other groups decreases. Therefore, pseudo-correlations will exist among these three parameters in many of the statistical analyses. The same is true for components of the ultimate analysis. Carbon, oxygen, hydrogen, nitrogen, and sulfur sum to 100 percent.

The distribution of vitrinite is negatively skewed. Coals of the United States are generally high in vitrinite content. The mean vitrinite content of sampled coals is 78 percent, with a standard deviation of nine percent. Only one coal contains less than 50 percent vitrinite. This coal, PSOC-122, is a channel sample composed of several lithotypes, including one cannel coal which is high in liptinite-group macerals and low in vitrinite-group macerals.

Table 4. Comparison of the content of organic sulfur
in coals of different provinces

	Low	High	Mean	St. dev.
Eastern province	0.10	2.77	0.97	0.52
Interior province	0.42	4.01	2.02	0.86
Rocky Mountain province	0.31	1.16	0.62	0.20
Northern Great Plains province	0.26	1.18	0.57	0.24

The distribution of the inertinite-group macerals has a slight positive skew with a mean of 16 percent. Only four coals have inertinite-group contents greater than 30 percent (See Figure 2).

The frequency distribution of liptinite-group macerals has a strong positive skew. The mean content of liptinite-group macerals is six percent, but the mode is closer to four percent. Only twenty coals, or 18 percent of the samples, have liptinite content greater than ten percent (See Figure 2). Nine coals are reported with less than one percent liptinite-group macerals and these are all medium or low volatile bituminous coals. At these high ranks, liptinite-group macerals are so similar in reflectance to vitrinite-group macerals that it is difficult or impossible to distinguish between the two groups of macerals.

8. Factor analysis

The variables used in this study are those that describe the organic portion of coals. The values of some variables are determined very early in the history of a coal (for instance, the proportion of the inertinite group macerals), and are not altered significantly

through most levels of rank. However, the values of other variables (for instance, calorific value) are altered during the processes of coalification. To complicate the matter further, the processes of coalification change at different levels of rank such that the rate of change of any variable, and the variables subjected to major changes are not constant at all levels of rank. The nature of the development and alteration of coal as a dynamic system is such that the properties are interacting and varying together. Therefore, to detect any underlying pattern of interaction, it is essential to study all the selected variables simultaneously. This can be done with the aid of factor analysis. CORFAN, a program compiled by Ondricks and Srivastava (1970) and run on the IBM 370 computer, is used for factor analyses in the R-mode to study variable interaction. Discussions of the theory are given by Davis (1973), Nie and others (1975), and Rummell (1970), and readers are referred to these authors for more detailed explanations of the analysis.

The first step in a factor analysis is the determination of interdependence among variables. The degree of linear correlation between two variables is measured by the correlation coefficient r . This is a measure of the association between two variables. Correlation coefficients range from -1.0 to +1.0. A zero correlation indicates total linear independence of two variables; +1.0 or -1.0 indicates a total linear dependence, that is, a perfect relationship. The sign of r indicates the type of relationship: a negative correlation indicates an inverse relationship between variables and a positive correlation indicates a direct relationship.

Table 5. Correlation matrix for variables of U.S. coals

	Reflectance (log x)	Carbon	Hydrogen	Oxygen (log x)	Sulfur (log x)	Nitrogen	Volatile Matter	Moisture (log x)	Btu/lb (log x/1-x)	Vitrinites (log x/1-x)	Inertinites (log x)
Carbon	0.871**										
Hydrogen	-0.292**	-0.194									
Oxygen (log x)	-0.349**	-0.954**	0.281**								
Sulfur (log x)	-0.185	0.021	0.132	-0.071							
Nitrogen	0.126	0.155	0.194	-0.197	0.016						
Volatile Matter	-0.390**	-0.761**	0.589**	0.791**	0.248**	-0.011					
Moisture (log x)	-0.857**	-0.842**	0.057	0.781**	0.048	-0.115	0.648**				
Btu/lb (log x/1-x)	0.846**	0.961**	-0.095	-0.952**	0.070	0.157	-0.702**	-0.847**			
Vitrinites (log x/1-x)	-0.172	-0.166	-0.012	0.095	0.071	-0.012	0.061	0.278**	-0.193		
Inertinites (log x)	0.197*	0.165	-0.224*	-0.149	-0.044	0.068	-0.188	-0.257**	0.165	-0.804**	
Liptinites ($\sqrt{x}$)	-0.112	-0.055	0.423**	0.165	-0.007	-0.048	0.327**	-0.045	-0.004	-0.573**	0.016

*Significant at the 5 percent probability level (d.f. = 107; $r = 0.195$)

**Significant at the 1 percent probability ($r = 0.254$)

Table 5 is a correlation matrix for the variables and indicates the significance of correlation at the five and one percent probability have been standardized (transformed such that their means are equal to zero and variances are equal to unity). This removed any biases due to differences in units of measurement.

The correlation matrix is used as input into the second step of factor analysis. (Use of the correlation (r) matrix leads to the term R-mode factor analysis). In this step, the variables are grouped according to their mutual correlations into principal components, or factors. Variables which are grouped under a component are those that behave similarly, or that are affected by the same process. The variables grouped under the first component of a factor analysis are those accounting for the greatest amount of variance within the data set. The second component contains a set of correlated variables accounting for the greatest amount of variance not explained by the first component; that is, component two is linearly independent of component one. Each remaining component is linearly independent of the previous components and accounts for variance not explained by all the preceding components. The factor analysis reduces the original number of variables to, usually, a fewer number of mutually uncorrelated underlying components (Davis, 1973). It is these components which are the source of variance within the variables of the data set. The variables which are grouped, or "loaded", under a given component are those which are being controlled by the same forces (factors). Therefore, these variables are providing the same information and one may be used to predict the others. Also, reduction of the parameters into a smaller number of components allows the

sources of variance, or the processes contributing to change, to be identified.

Table 6 shows the principal components for variables of all the coals considered in the study. Six components were extracted and together they explain approximately 96 percent of the total data variance. A problem in factor analyses is deciding the best number of components to extract. Each component extracted is a linearly independent source of information. A common practice is to extract those components with eigenvalues ($\sum \lambda_i^2$; see Table 6) greater than one (Davis, 1973). These are the components which explain at least as much variance as any of the standardized variables. (Each variable is "standardized" such that its variance is equal to one. Therefore, the total amount of variance to explain in the data set is equal to the number of variables; that is, the trace of the correlation matrix.) A second consideration in deciding on the number of principal components to extract is based on the "communalities" of each variable. If the loading of a variable on each component is squared and summed, the total is the amount of variance of that variable retained in the extracted components (Davis, 1973). A communality of 1.00 indicates that the total variance of a variable is accounted for. In this study, components were extracted until at least 85 percent (communality = 0.85) of each variable was retained in the components. In Table 6 the six components were extracted to raise the communality of each variable to at least 0.85. However, the first five components are considered the most significant sources of variance based on the eigenvalues ($\sum \lambda_i^2$ are approximately one).

Table 6. Original matrix of factor loadings for
J.S. coals

	C ₁	C ₂	C ₃	C ₄	C ₅	C ₆	Communalities (h_i^2)
Carbon	-0.953						0.952
Reflectance (log x)	-0.950						0.931
Oxygen (log x)	0.947						0.952
Btu/lb (log x/1-x)	-0.933						0.957
Moisture (log x)	0.880						0.883
Volatile matter	0.876						0.941
Vitrinites (log x/1-x)		-0.906					0.968
Liptinites ($\sqrt{x}$)		0.767				0.374	0.996
Inertinites (log x)		0.651	0.556	0.412			0.994
Hydrogen		0.387	-0.719			-0.395	0.974
Sulfur (log x)			-0.428	0.733	0.496		0.982
Nitrogen					-0.815		0.997
Sum λ_i^2	5.424	2.053	1.570	1.039	0.995	0.469	
% Variation Explained	45.20	17.11	13.08	8.70	8.29	3.91	
Cumulative %	45.20	62.31	75.39	84.09	92.38	96.29	

C. Analysis of factor components

The first component in Table 6 contains six of the twelve variables and accounts for approximately 45 percent of the total variance in the data set. The parameters loading on this component are those whose values are altered by the processes of coalification. The proportions of carbon, oxygen, and moisture of a coal are altered in early stages of coalification, as is the calorific value of a coal. The values of reflectance and volatile matter are also affected by the processes of coalification, especially in the high-rank bituminous coals. The major factor controlling the value of each of these variables is the degree of coalification or the rank of the coal. Therefore, the factor controlling this component is identified as coalification, as measured by rank. Since coalification accounts for 45 percent of the variance, much more than any other single factor (see Table 6), it is considered the major factor effecting variation in the coals of this study.

The second component accounts for approximately 17 percent of the total variance and is composed of the three maceral groups. The proportion of the maceral groups is generally controlled by the original environment of deposition and by alteration early in the peat stage. This proportion is not subsequently altered by the processes of coalification, although individual macerals undergo chemical and physical alterations (Spackman, 1958; Teichmüller and Teichmüller, 1975). Therefore, the proportion of the three maceral groups would be expected to contribute an independent source of information to the data set, and, therefore, to be a principal component of variation.

The third component accounts for 13 percent of the total variance. The variable loading most strongly is hydrogen. The content of hydrogen in a coal is altered by coalification in the upper levels of rank represented by this group of coals. However, hydrogen does not load on the first component with the other rank-dependent variables. One possible explanation is that the content of hydrogen is not significantly altered until the highest levels of rank, so its variation is not as rank dependent for the entire range of rank as that of the variables loading on component one. However, volatile matter is also sensitive to rank over only the higher levels represented in this study, and volatile matter does load on the first component. An alternative explanation for the loading of hydrogen is that it does not have a linear response to the processes of coalification over this entire range of rank (lignites through low volatile bituminous coals). To illustrate the response of hydrogen to rank increases, hydrogen is plotted against a variable which loads on the first component and is rank dependent for this range of rank. Figure 3 is a plot hydrogen and reflectance, which increases with rank. The response of hydrogen to increasing coalification is curvilinear. In the early stages of coalification, there appears to be a general increase in hydrogen content and the curve peaks at approximately 0.57 percent reflectance. With continued coalification, hydrogen decreases. The curvilinear response of hydrogen through rank is discussed further in Section IA2a of this report. The basic mathematical procedure of factor analyses is to separate the linearly independent sources of information. However, hydrogen response is

Figure 3. PLOT ILLUSTRATING CURVILINEAR RESPONSE OF HYDROGEN TO INCREASES IN RANK

curvilinear through rank and does not behave like other rank variables. This suggests that hydrogen content may be controlled by rank in part, and also by some other factor. Therefore, hydrogen is not grouped with the other rank-dependent factors.

Two other variables have slight loadings on component three with hydrogen. These are the inertinite-group macerals and sulfur. The loading of the inertinite-group macerals ($r=0.556$) is inverse to that of hydrogen ($r=-0.719$) indicating that as the proportion of these macerals increases, the proportion of hydrogen decreases. Of the three maceral groups, the inertinites are lowest in their characteristic hydrogen content (van Krevelen, 1961). The inverse grouping of hydrogen and inertinite on the factor analysis suggests a relationship, although slight, between maceral composition and hydrogen content. The very slight loading ($r=-0.428$, or 16 percent variance common among the two variables) of sulfur on this component suggests that hydrogen and sulfur are also controlled in part by a common factor. Teichmüller and Teichmüller (1974) make a strong point that marine-influenced coals are enriched in both hydrogen and sulfur. This will be discussed in more detail in Section IXB4. The correlation coefficient between sulfur and hydrogen is very low ($r=0.132$) and is not significantly different from zero correlation. However, results of this factor analysis suggest that sulfur and hydrogen may be responding at least in part to a common factor. Figure 4 is a plot of hydrogen and sulfur, and a very slight trend is observed. For high levels of sulfur, there is a tendency for high levels of hydrogen. However, hydrogen values are also associated

Figure 4. PLOT OF HYDROGEN VERSUS SULFUR FOR U.S. COALS

with rank. Coals from the Interior province are high in sulfur. They also have relatively high hydrogen contents owing to their level of rank. Therefore, the positive correlation between sulfur and hydrogen is interpreted as a pseudocorrelation. Component three is interpreted as the "hydrogen factor" which is controlled in part by the processes of coalification and in part by the environment of deposition.

The fourth component accounts for approximately nine percent of the total variance in the data set and its only loading is by organic sulfur. Component five accounts for approximately eight percent of the total variance. Nitrogen is strongly loaded ($r=-0.815$) on the sixth component and sulfur has a slight inverse loading ($r=0.496$). Teichmüller and Teichmüller (1974) observed that along with hydrogen and sulfur, nitrogen is also enriched in marine-influenced coals. However, for the coals represented in this study, nitrogen content does not seem to be controlled by the same processes as hydrogen content, as seen in Figure 5. Also, nitrogen does not vary directly with sulfur content, as seen in Figure 6.

In summary, the twelve variables used to characterize samples ranging in rank from lignites through low volatile bituminous coals may be reduced, through factor analysis, to five principal components, indicating five independent sources of variation. These five components are rank, maceral composition, the hydrogen factor, sulfur content, and nitrogen content. Together the components explain approximately 92 percent of the total variance. The results are similar to those found in a study of 35 coals, ranging in rank from lignite to anthracite, by Fleuckinger and others (1972).

Figure 6. PLOT OF SULFUR VERSUS NITROGEN FOR U.S. COALS

VI. CLASSIFICATION OF U.S. COALS

In the previous factor analysis, all 109 coals of this study were analyzed together. However, these coals include lignites, subbituminous, and bituminous coals of four provinces, and from several geologic ages. Therefore, these samples may not be from a single population, but they may be samples of several populations. The skewed distributions of many of the variables may be the result of sampling from several populations. However, skewed distributions can also result from non-random sampling of a single population. The next step in this study is to attempt to classify coals. This will provide insight into whether more than one population exists. If natural groupings are detected, the variable interactions within a single population may be determined.

A. Cluster analysis of U.S. coals

In this study, the classification of the coals into their most natural groupings or clusters, according to the chosen variables, was accomplished by the computer program CLUS (Rubin and Friedman, 1967). In this way, all the variable interactions may be used simultaneously to determine the groupings, and the possibility of operator bias in grouping the data is kept to a minimum.

The CLUS procedure of classification allows many options to the approach of classification. For this study, the first step was to perform an R-mode factor analysis so that the linearly independent sources of variation could be identified. As discussed, the variables of U.S. coals were reduced to five components, or linearly independent sources of variation. These five components are then used for the cluster analysis.

The CLUS algorithm offers five criteria which may be used to find the natural clusterings of the samples. All of the criteria are based on the relationship that the total variation (T) in a set of data is equal to the variation between groups (B) plus the variation within each group (W), or $T = B + W$ (Siegal and Griffiths, 1974). For any given data set, T is fixed. The best classification is one that minimizes the variation within a group (W) such that samples in that group are all similar. Also, the classification should maximize the variation between the groups (B) so that the groups are well separated and easy to distinguish.

Two criteria of classification were chosen for this study. One criterion is $\log |T|/|W|$. The equation

$$T = B + W \quad (9)$$

is transformed to

$$\log \frac{|T|}{|W|} = \log |B + W| + 1 \quad (10)$$

and the logarithm of the ratio is used for convenience of calculation. Maximizing $\log |T|/|W|$ is the basis of the criterion. After the samples have been clustered according to the maximum $\log |T|/|W|$, the generalized distance between the multivariate means of the clusters is calculated. This distance is the Mahalanobis distance, or D^2 , and it is a measure of the separation between clusters. (A large D^2 indicates a large separation.) The other classification criterion used in this study is the approximation to the maximum $\log |T|/|W|$, and D^2 calculated from the classification.

The first cluster analysis was performed on all 109 samples, using the five principal components identified by the R-mode

factor analysis. Table 7 and Figure 7 are values of the maximum and approximate $\log |T|/|W|$ and D^2 calculated from each. As with factor analyses, there are no significance tests to help in deciding the best number of clusters of data. One indication of the best number of classes is a change in slope of the curve obtained by plotting the values of a partitioning criterion against the number of groups, as in Figure 7. For the curve of approximate $\log |T|/|W|$, there is a change in slope at 4 groups. The biggest increases in the value of the criterion are from two to three, and from three to four groups. After four groups, the value increases at a slower rate. The plot of D^2 from approximate $\log |T|/|W|$ shows the same deflection, but it is more pronounced than that of the approximate $\log |T|/|W|$. The curve of maximum $\log |T|/|W|$ has a change in slope at five groups. D^2 calculated from the maximum $\log |T|/|W|$ classification has a deflection at both four and five groups. For a given number of groups, the spread of values of the partitioning criteria are also helpful in deciding the number of groups to choose. At two, three and four groups, the values plot closely together (see Figure 7). However, at five groups, the values are widely spaced. Therefore, a classification of the coals into four groups is suggested.

Plots may be obtained of the classification achieved by CLUS. The plot obtained when only two groups are requested is given in Figure 8. The plot illustrates that the coals represent a continuum and that there is no distinct break in the clusters of samples.

Figure 7. PLOT OF PARTITIONING CRITERIA OF U.S. COALS
BASED ON FIVE PRINCIPAL COMPONENTS

Figure 8. PLOT OF CLUSTER ANALYSIS OF U.S. COALS WHEN TWO GROUPS ARE REQUESTED

Table 7. Values of partitioning criteria for the cluster analysis of U.S. coals

No. of Groups	approx. log. $\left \frac{T}{W} \right $	D^2	max. log $\left \frac{T}{W} \right $	D^2
2	1.1	3.6		
3	2.3	6.5	2.6	5.4
4	3.4	9.9	3.8	9.6
5	4.1	10.2	4.7	14.4
6	4.4	12.0	5.2	16.7

Therefore, these samples are interpreted as being non-random samples from a single, continuous population; further subdivision of this continuum is somewhat arbitrary. However, the continuum may be "dissected" into groups of greatest similarity (Kendall, 1966).

The plot of four groups obtained from the cluster analysis is given in Figure 9. In this plot, one group of coals (group B) splits out as a separate cluster. By examining results of the cluster analysis, the X-axis of this plot is identified as representing rank, with coalification increasing toward the right. Therefore, these coals which split out separately are the coals of the highest rank in this study. The Y-axis is identified as representing maceral composition, with the proportion of vitrinite increasing upwards. The group B coals are also very high in vitrinite. On the basis of the position on the plot, the group of coals is recognized as the medium and low volatile bituminous coals or very high levels of high volatile A bituminous rank. At these very high levels of bituminous rank, liptinite is so similar to vitrinite in reflectance that the two groups are

Figure 9. PLOT OF CLUSTER ANALYSIS OF U.S. COALS WHEN FOUR GROUPS ARE REQUESTED

very difficult or impossible to distinguish from one another. Therefore, the proportion of the vitrinite group of macerals appears to increase with rank.

The other coals again represent a continuum which is varying along both the X and Y axes. This indicates that both rank and maceral composition are contributing to variation. An interesting trend is that the proportion of vitrinite has a tendency to decrease with increased rank. This is interpreted as a pseudocorrelation between rank and vitrinite content. The lowest rank coals in this study are the Cretaceous and Tertiary coals of the western states. The highest rank coals are Pennsylvanian in age. According to Spackman (personal communication, 1977), the seeming correlation between vitrinite content and rank is attributable in part to a changing floral assemblage through time. The plants of the Carboniferous, including such plants as the seed ferns, ferns, lycopods, and sphenopsids, were commonly prolific producers of thick-walled mega- and microspores which were locally deposited in the accumulating peat, serving as a diluent with respect to the concentration of vitrinite. This diluent effect is further increased by the formation of exinite-micrinite rich durains in the eastern Paleozoic coals. In the Cretaceous, these plants became less important members of the floral complex, many becoming extinct, with angiosperms rapidly assuming an important status in the swamp communities. The gymnosperms became the dominant member of the plant community. Gymnosperms produce smaller, thinner-walled palynomorphs than did the Carboniferous plants. Also, the Gymnosperm palynomorphs

are equipped with bladders that assist in wind dispersal such that the local concentration of exines is reduced. Owing to the small size and thin walls, the proportion of liptinitic material is less than that contributed by larger, thicker-walled spore and pollen common in the Carboniferous. An even more important factor is the change to the habit of reducing the production of megaspores to four, with three of these aborting and then being retained in the megasporangium without developing an exine of liptinitic source material. The angiosperms have been important members of the swamp and marsh communities from the Tertiary to the present. All of these retain the megaspore in the ovule with no production of liptinitic source material and with a reduction in total pollen production when compared with many gymnosperms. Therefore, from the Carboniferous to the Tertiary there has been a decrease in the contribution of liptinitic material to the coal-forming swamps and a change from large, thick-walled palynomorphs to small, thin-walled palynomorphs.

The plot of reflectance versus the proportion of the liptinite-group macerals (Figure 10) shows the association between increasing rank (increasing reflectance) and increasing proportions of the liptinite-group macerals. All of the coals with a very high content of macerals of the liptinite group are from the Eastern and Interior provinces and are Pennsylvanian in age. The western coals, which are younger, generally have a low content of macerals of the liptinite group. For coals with a reflectance greater than about 1.10, the content of liptinite-group macerals again decreases; in the higher levels of rank these macerals cannot be distinguished from the

Figure 10. PLOT OF REFLECTANCE VERSUS THE LIPTINITE-GROUP MACERAL CONTENT FOR U.S. COALS

vitritine-group macerals. Figure 11 is a plot of reflectance and vitritine-group macerals. All of the coals with the low content of macerals of the vitritine group are from the Interior and Eastern provinces.

From the cluster analysis of the 109 coal samples, twelve high-rank coals were grouped together distinctly within the continuum. The next step in the classification procedure is to remove this group of coals from the data matrix and to attempt to classify remaining samples.

B. Cluster analysis of coals lower in rank than medium volatile bituminous

1. Factor analysis

The frequency distributions of the variables of the remaining coals were checked for normality and eight of the twelve variables were found to deviate from the distribution expected of a normally-distributed population. Oxygen, moisture, sulfur, liptinite and inertinite are log-normally distributed. The distributions of carbon, calorific value, and vitritine are normalized by the transformation $\log x/1-x$.

The correlation matrix generated as input into the factor analysis is given in Table 8. The original matrix of factor loadings is given in Table 9. Seven components were extracted to raise the communalities of all the variables to greater than 0.85. Only the first four components are considered significant, linearly independent sources of variation in the data set and these four components account for 83 percent of the total variance.

The first component contains eight variables and accounts for 48 percent of the total variance. Six of the eight variables are

Figure 11. PLOT OF REFLECTANCE VERSUS THE VITRINITE-GROUP MACERAL CONTENT FOR U.S. COALS

Table 8. Correlation matrix for coals lower in rank than medium
volatile bituminous

	Reflectance	Carbon (log x/1-x)	Hydrogen	Oxygen (log x)	Sulfur (log x)	Nitrogen	Volatile Matter	Moisture (log x)	Btu/lb (log x/1-x)	Vitrinites (log x/1-x)	Inertinites (log x)
Carbon (log x/1-x)	0.827**										
Hydrogen	0.104	0.149									
Oxygen (log x)	-0.785**	-0.972**	-0.153								
Sulfur (log x)	-0.116	0.141	0.006	-0.287**							
Nitrogen	0.292**	0.287**	0.206*	-0.367**	0.018						
Volatile Matter	-0.868**	-0.717**	0.159	0.654**	0.184	-0.218*					
Moisture (log x)	-0.890**	-0.853**	-0.219*	0.830**	-0.042	-0.271**	0.703**				
Btu/lb (log x/1-x)	0.812**	0.966**	0.272**	-0.965**	0.226*	0.306**	-0.640**	-0.877**			
Vitrinites (log x/1-x)	-0.410**	-0.348**	0.162	0.318**	0.085	-0.033	0.412**	0.384**	-0.345**		
Inertinites (log x)	0.224*	0.177	-0.230*	-0.186	0.006	0.108	-0.228*	-0.260*	0.184	-0.811**	
Liptinites	0.489**	0.410**	0.036	-0.345**	-0.152	-0.109	-0.434**	-0.387**	0.395**	-0.608**	0.067

*Significant at the 5 percent probability level (d.f. = 94; $r = 0.205$)

**Significant at the 1 percent probability level ($r = 0.267$)

Table 9. Original matrix of factor loadings from the R-mode analysis for coals
lower in rank than medium volatile bituminous

	C ₁	C ₂	C ₃	C ₄	C ₅	C ₆	C ₇	Communalities (h_i^2)
Carbon (log x/1-x)	0.944							0.987
Btu/lb (log x/1-x)	0.937							0.985
Reflectance	0.923							0.964
Oxygen (log x)	-0.922							0.988
Moisture (log x)	-0.919							0.911
Volatile matter	-0.804							0.994
Inertinites (log x)		-0.690	-0.526					0.942
Vitrinites (log x/1-x)	-0.531	0.751						0.990
Sulfur (log x)			-0.720	0.524				0.999
Nitrogen				0.712		0.436		0.998
Hydrogen		0.570			-0.708			0.986
Liptinites (log x)	0.528		0.423		-0.387	0.430		0.995
Sum λ_i^2	5.779	1.877	1.284	1.050	0.954	0.542	0.253	
% Variation Explained	48.16	15.64	10.70	8.75	7.95	4.52	2.10	
Cumulative %	48.16	63.80	74.50	83.25	91.21	95.72	97.83	

strongly loaded on this factor. These include carbon, calorific value, and reflectance which are inverse of oxygen, moisture, and volatile matter. Again, these are the variables whose proportion is altered through the processes of coalification. Carbon, calorific value and reflectance increase, while oxygen, moisture, and volatile matter decrease as a result of the coalification processes. The loadings of vitrinite and liptinite on this component are due to a changing floral community from the Carboniferous to the Tertiary, an induced correlation with rank as discussed in Section VIA. This first component is interpreted as the rank factor controlling data variance.

The second component contains three variables and accounts for 16 percent of the data variance. Vitrinite and inertinite are inversely loaded on this component and this is interpreted as the maceral composition factor. Hydrogen also has a small loading ($r=0.570$) on this component. It varies directly with vitrinite and indirectly with inertinite. This indicates that hydrogen is in part controlled by maceral composition.

The third component also contains three variables. Sulfur has the strongest loading ($r=-0.720$). The inertinite-group macerals have a slight loading ($r=-0.526$) and the liptinite-group macerals are inversely loaded ($r=0.423$). The relationship between sulfur and the two maceral groups again could be a pseudocorrelation. The youngest coals of this study, and the coals lowest in rank, are those from the western states. These coals are low in liptinite (Figure 10). Since the coals were deposited in non-marine environments, they are also low in sulfur. Figure 12 is a plot of carbon and sulfur showing that the lowest rank coals (western coals) have low sulfur content.

Figure 12. PLOT OF CARBON VERSUS SULFUR FOR U.S. COALS

The fourth component contains two variables and accounts for 10 percent of the data variance. The variable with the strongest loading is nitrogen. This factor is interpreted as the nitrogen component, and it is probably controlled by the conditions of deposition.

The fifth component contains hydrogen, but it is not interpreted as a major, linearly independent source of variance. The response of hydrogen is curvilinear over the range of rank, so although the value of hydrogen is altered by coalification processes, it is not grouped with the variables of the first component. Liptinite has a very slight loading on this factor with hydrogen, indicating again that the amount of hydrogen present in a coal is partly related to the maceral composition of the coal.

In summary, four principal components were recognized in this data set. These components represent factors which control the variation expressed in the variables. These factors are identified as:

Factor 1: Rank

Factor 2: Maceral composition

Factor 3: Organic sulfur

Factor 4: Nitrogen

2. Cluster analysis

A cluster analysis was performed on this set of coals using the above four principal components to group the samples into the best classification possible. The values of the partitioning criteria used to classify the coals are given in Table 10 and Figure 13. The curve of the value of approximate $\log |T|/|W|$ in Figure 13 shows the greatest increase in value from two to three

Figure 13. PLOT OF PARTITIONING CRITERIA FOR CLASSIFYING COALS LOWER IN RANK THAN MEDIUM VOLATILE BITUMINOUS

Table 10. Values of partitioning criteria for classifying coals lower in rank than medium volatile bituminous

No. of Groups	Approximate $\log \frac{ T }{ W }$	D^2	Max. $\log \frac{ T }{ W }$	D^2
2	1.2	3.1	1.1	2.0
3	2.2	4.4	2.6	5.5
4	3.0	5.4	3.3	9.3
5	3.5	7.3	3.9	11.2
6	3.9	8.1		

groups, which agrees with the maximum of four groups in the previous set. (One group has been removed from this set.) D^2 from approximate $\log |T|/|W|$ shows slight slope changes at three, four, and five groups. Maximum $\log |T|/|W|$ shows a change in slope in the curve at three groups, and the D^2 calculated from maximum $\log |T|/|W|$ shows a slope change at four groups. The spread in partitioning values is small for 2 or 3 groups, and is large for greater than 3 groups. Therefore, division or dissection of the coals into four groups is suggested.

Another tool which is helpful in determining the number of groups for the best classification of a set of samples is a table comparing the groupings of samples when different numbers of groups are requested. Table 11 is a comparison of the clusters established by the approximate $\log |T|/|W|$ criterion when three and four groups are requested. Most of the coals are contained in three groups even when four groups are requested. Also, the groupings of the coals are stable for requests of three or four clusters. This

Table 11. Comparison of classification into 3 and 4 groups of coals lower in rank than medium volatile bituminous. Maximum log $|T|/|W|$ criterion was used for grouping the coals

CLASSES	1	2	3	4
1			2162 2273 2284 1308 2242 1275 2285 4309 4249 1275 2286 1326 2251 1277 2287 1329 2252 1278 2290 2356 1267 2279 1305 1270 2281 1306 2272 2283 1307	2024 2163 2164 2165
2		2022 4234 4248 4056 4055 4238 2285 4059 4239 4310 3065 3241 4311 4068 3242 4312 3230 2243 4313 3231 3246 4314 4233 3247 4315		2026 3086 4097 2166 3245
3	1001* 1299 1345 1363 1005 1300 1349 1367 1011 1302 1353 1371 1102 3128 1354 1375 2107 1331 1355 1268 1332 1357 1269 1337 1361 1271 1341 1362	1330	3150 3250 1265	3105

* The first digit of each sample number is a code for provinces: 1 = Eastern Province, 2 = Interior Province, 3 = Northern Great Plains Province, 4 = Rocky Mountain Province.

indicates that three is the optimum number of groups to use when separating the coals into groups of similarity. Little is gained by going to four groups.

Discriminant equations. Once the samples have been separated into groups of similarity, it is important to understand the basis of the groupings, or to know what makes the groups different from one another. This information is achieved by examining the discriminant (Z) equations separating each pair of groups. This equation gives the relative importance of each principal component in separating the groups. The components used in CLUS are rank (F_1), maceral composition (F_2), organic sulfur (F_3) and nitrogen (F_4).

The discriminant equation separating groups C and B is

$$Z_{CB} = 0.293 F_1 - 0.060 F_2 - 0.032 F_3 - 0.129 F_4 \quad (11)$$

Groups C and B are separated mainly on the basis of rank and nitrogen content. The discriminant equation separating groups C and A is

$$Z_{AC} = 0.132 F_1 - 0.087 F_2 - 0.463 F_3 + 0.000 F_4 \quad (12)$$

Groups A and C are separated mainly on the basis of organic sulfur content, and rank plays a minor role. The discriminant equation separating groups B and A is

$$Z_{BA} = 0.161 F_1 - 0.027 F_2 - 0.431 F_3 + 0.129 F_4 \quad (13)$$

Again, organic sulfur is the primary basis for separating group A from group B, and rank plays a secondary role in the clustering of group A from the other coals.

Figure 14 is a plot of coals classified into three groups by the approximate $\log |T|/|W|$ criterion. The axes are identified as rank along the X-axis and sulfur content along the Y-axis. This represents the importance of both rank and environment of deposition

Figure 14. PLOT OF CLUSTER ANALYSIS OF U.S. COALS LOWER IN RANK THAN MEDIUM VOLATILE BITUMINOUS WHEN THREE GROUPS ARE REQUESTED

as the primary factors controlling variation in any coal. The coals have been classified into three fairly distinct groups. Group C (referred to as Group III in further analyses) contains coals which are relatively high in rank and which have moderate to low sulfur contents. These are primarily Eastern province coals. Group B (referred to as Group I in further analyses) contains coals which are relatively low in rank and have moderate to low sulfur contents. These are primarily western coals from the Rocky Mountain and Northern Great Plains coal provinces. Group A (referred to as Group II in further analyses) contains coals which are intermediate in rank and are moderate to high in their sulfur contents. These primarily are coals of the Interior province but this group also contains some Eastern province coals. Although the coals are fairly distinct with few overlaps between groups, the clusters are not widely separated from one another. This is because the coals represent a continuum and the classification is somewhat arbitrary. In addition to the three groups discriminated here, the previous cluster analysis separated the medium and low volatile bituminous coals into a group of similar coals. These will be termed Group IV coals for the rest of this report.

Table 12 is a summary of the distribution of coals by rank into the most natural groupings determined by the cluster analysis of U.S. coals. The next step in this study will be to analyze the groups to determine the significant factors of variation within each set of coals.

Table 12. Distribution of rank in groups of U.S. coals,
as determined by cluster analysis

	Lignite	Subbituminous	High Volatile Bituminous				
			C	B	A	mvb	lbv
Group I	5	5	13	5	3		
Group II			4	11	16		
Group III				4	30		
Group IV					2	4	6

VII. ANALYSIS OF GROUPS OF COALS SEPARATED BY CLUS

A. Group I from CLUS

Group I from the cluster analysis contains 30 coal samples, including five from the Interior province, nine from the Northern Great Plains province, and 16 from the Rocky Mountain province. The data matrix for Group I is in Appendix III. The ASTM rank of these samples ranges from lignite to high volatile A bituminous. Only three of the 30 coals are high volatile A in rank and the remaining coals are of lower levels of rank. Group I is discriminated from Group III primarily by rank. It is discriminated from Group II primarily by the content of organic sulfur and partially by rank. The mean sulfur content of Group I is 0.81 percent.

1. Univariate analyses

Summary statistics of variables for coals of this group are given in Table 13. Three variables are lognormally distributed at the five percent probability level. These variables are sulfur, moisture, and the liptinite-group macerals. The volatile matter distribution has a positive skew and is very peaked. The proportion of volatile products is not considered to vary predictably with coalification at these low levels of rank. The highly peaked distribution is an aspect of the small variance through low levels of rank. The values for volatile matter range from 40 to 54 percent with a mean of 45 percent. These high values for volatile matter are characteristic of low-rank coals. Both nitrogen and the vitrinite-group macerals have negatively skewed distributions; transformations did not achieve a normal distribution.

Table 13. Summary statistics for variables of Group I of CLUS

	Low	High	Mean	St. Dev.	Skewness	Kurtosis [†]	χ^2 ^{††}	Transfor- mation	Skewness	Kurtosis [†]	χ^2 ^{††}
Reflectance	0.30	0.70	0.50	0.50	-0.482	2.673	11.0				
Carbon	71.52	82.74	77.78	2.96	-0.263	2.132**	11.1				
Hydrogen	4.76	6.15	5.56	0.41	-0.400	2.160**	25.4*				
Oxygen	8.35	21.45	14.34	3.74	0.259	1.898**	20.0*				
Sulfur	0.26	2.51	0.81	0.58	1.798**	5.430**	31.7**	log x	0.812*	3.004	14.8
Nitrogen	0.13	2.01	1.51	0.45	-1.366**	4.532**	17.4				
Volatile matter	39.77	53.61	44.77	3.89	0.887*	4.252**	9.6				
Moisture	4.02	38.04	15.58	9.61	1.012**	3.254	16.9	log x	-0.180	2.366*	15.7
Btu/lb	11902	14863	13717	836	-0.470	2.123**	16.4				
Vitrinites	67.2	92.1	83.1	5.5	-0.833*	3.559	7.6				
Inertinites	5.1	22.1	12.7	5.1	0.420	2.101**	11.0				
Liptinites	1.6	11.9	4.3	2.6	1.913**	6.202**	25.6**	log x	0.656	3.417	13.6

*Significant at the 5 percent probability level (30 samples)

**Significant at the 1 percent probability level

†Kurtosis tested at sample size of 200

††d.f. = 10

2. Factor analysis

The correlation matrix generated as input into the factor analysis is given in Table 14. Table 15 is the original matrix of factor loadings from the R-mode factor analysis. Six factors were extracted to account for at least 85 percent of the variance of each variable. The six factors explain 96 percent of the total data variance. Based on the eigenvalues ($\sum \lambda_i^2$) for the components, only the first three and perhaps four components are significant, linearly independent sources of information in the data set.

The first component contains nine variables and accounts for 51 percent of the total variance. Six variables have loadings greater than 0.75 on this component. These include calorific value, carbon, hydrogen, and reflectance with positive loadings, and oxygen and moisture with negative loadings. Component one is interpreted as the rank factor for low-rank coals. Also loading on this factor are the vitrinite-group macerals ($r=0.610$) and the inertinite-group macerals ($r=-0.686$). This indicates a slight tendency for the macerals of the vitrinite group to increase with rank, and a slight tendency for liptinites to decrease through rank. Nitrogen has a slight loading ($r=0.589$) on this factor, which suggests a correlation between rank increase and nitrogen content. However, when nitrogen is plotted against carbon (Figure 15) no obvious dependence of nitrogen on rank is apparent.

Since nine of the twelve variables are loaded on this first component, it is difficult to interpret the underlying factors controlling data variation. Therefore, the factor matrix is rotated mathematically so that the variables are grouped more closely based

Table 14. Correlation matrix for variables of Group I from CLUS

	Reflectance	Carbon	Hydrogen	Oxygen	Sulfur (log x)	Nitrogen	Volatile Matter	Moisture (log x)	Btu/lb	Vitrinites	Inertinites
Carbon	-0.696**										
Hydrogen	-0.562**	0.774**									
Oxygen	-0.692**	-0.988**	-0.797**								
Sulfur (log x)	-0.024	0.359	0.169	-0.436*							
Nitrogen	0.672**	0.485**	0.389*	-0.525**	-0.123						
Volatile Matter	-0.566**	-0.266	0.022	0.267	0.109	-0.507*					
Moisture (log x)	-0.724**	-0.773**	-0.750**	0.754**	-0.031	-0.423*	0.189				
Btu/lb	0.661**	0.946**	0.842**	-0.953**	0.444*	0.375*	-0.176	-0.776**			
Vitrinites	0.234	0.414*	0.556**	-0.467**	0.192	0.311	-0.046	-0.405*	0.471**		
Inertinites	-0.251	-0.518**	-0.623**	0.567**	-0.286	-0.285	-0.017	0.467**	-0.571**	-0.891**	
Liptinites (log x)	0.064	0.183	0.064	-0.168	0.215	-0.112	0.163	-0.084	0.175	-0.315	-0.128

*Significant at the 5 percent probability level (d.f. = 27; $r = 0.367$)

**Significant at the 1 percent probability level ($r = 0.470$)

Table 15. Original matrix of factor loadings from the
R-mode factor analysis of Group I from CLUS

	C ₁	C ₂	C ₃	C ₄	C ₅	C ₆	Communalities (h_i^2)
Oxygen	-0.958						0.976
Btu/lb	0.940						0.970
Carbon	0.939						0.942
Hydrogen	0.861						0.897
Moisture (log x)	-0.838						0.891
Reflectance	0.767	-0.500					0.882
Inertinites	-0.686						0.997
Vitrinites	0.610		0.726				0.991
Nitrogen	0.589	-0.570				-0.486	0.989
Volatile Matter		0.742					0.972
Sulfur (log x)		0.601		0.658			0.960
Liptinites (log x)			-0.728		-0.545		1.000
Sum λ_i^2	6.095	1.887	1.460	0.906	0.702	0.416	
% Variation Explained	50.79	15.73	12.16	7.55	5.85	3.47	
Cumulative %	50.79	66.52	78.68	86.23	92.08	95.55

Figure 15. PLOT OF CARBON VERSUS NITROGEN FOR U.S. COALS

on similarity and the factors are easier to interpret. The rotated matrix of factor loadings is given in Table 16. The complete matrix of factor loadings for both the original and the rotated matrix are given in Appendix IV.

The first component contains variables that are dependent on rank. These variables are the six with the highest loadings on the first component of the original matrix; calorific value, carbon, hydrogen, and reflectance are positively loaded, and moisture and oxygen are negatively loaded on this component.

The second component contains two variables. Volatile matter has a strong loading ($r=0.953$) and reflectance has a slight loading ($r=-0.483$).

The third component contains inertinite and vitrinite in an inverse loading. This component is recognized as the maceral factor.

The last three components each contain one variable. These are sulfur, the liptinite-group macerals, and nitrogen.

3. Interpretation of coalification processes active in Group I coals

The first component on the rotated factor matrix contains six variables whose values are altered by the chemical and/or physical processes of coalification at low levels of rank. According to Teichmüller and Teichmüller (1968), the major chemical reactions active in early stages of coalification involve loss of hydroxyl (-OH), carboxyl (-COOH), carbonyl (C=O), and methoxyl (-OCH₃) functional groups and the loss of ring oxygen. In these reactions, oxygen is the element being lost in the greatest proportion resulting in the enrichment of carbon and, to a lesser degree, hydrogen. This relative

Table 16. Rotated matrix of factor loadings from the
R-mode factor analysis of Group I coals from CLUS

	C ₁	C ₂	C ₃	C ₄	C ₅	C ₆	Communalities (h_i^2)
Moisture (log x)	-0.897						0.891
Btu/lb	0.891						0.970
Carbon	0.875						0.942
Oxygen	-0.846						0.976
Hydrogen	0.842						0.897
Reflectance	0.720	-0.483					0.882
Volatile Matter		0.953					0.972
Inertinites			0.907				0.997
Vitrinites			-0.918				0.991
Sulfur (log x)				0.948			0.960
Liptinites (log x)					-0.981		0.999
Nitrogen						-0.866	0.989
Sum λ_i^2	4.646	1.347	2.026	1.282	1.116	1.049	
% Variation Explained	38.72	11.22	16.89	10.68	9.30	8.74	
Cumulative %	38.72	49.94	66.83	77.51	86.81	95.55	

behavior of oxygen to carbon and hydrogen is observed in the factor analysis. The change in the proportion of these elemental components results in a change in the heating value of the coal. The combustible substances of a coal which release heat when oxidized are carbon, hydrogen, nitrogen, and sulfur; oxygen consumes heat during the combustion process (Mackowsky, 1975). Therefore, as the amount of oxygen decreases and the proportion of the other chemical components increases, the heating value of a coal - measured on the dry, mineral-matter-free basis - must also increase. In summary, one primary factor active in the lower stages of coalification for U.S. coals (up to high volatile A bituminous) is identified as the chemical reactions which result in a loss of oxygen and an enrichment of carbon and hydrogen; calorific value also increases as a result of this alteration of the proportion of the elemental components.

A second result of the chemical reactions of coalification which is often reported is an increase in aromaticity of the molecular structure of vitrinite (Teichmüller and Teichmüller, 1975). Aromaticity is defined as the fraction of aromatic carbon divided by total carbon within the coal structure (see van Krevelen, 1961). An increase in aromaticity effects a change in the optical properties of the coal structure. Reflectance measurements of the vitrinite-group macerals are reported to increase as aromaticity increases (McCartney and Teichmüller, 1972). Reflectance is a function of both the refractive index and the absorptive index of a coal as defined by Beer's equation (van Krevelen, 1961):

$$\text{reflectance (\%)} = \frac{(n-N)^2 + n^2 K^2}{(n+N)^2 + n^2 K^2} \times 100\% \quad (11)$$

where

n = refractive index of the reflecting medium
 N = refractive index of the surrounding medium
 (1.518 for immersion oil)
 K = absorption index of the reflecting medium

According to McCartney and Teichmüller (1972), both refractivity and absorption depend in part on aromaticity. The absorption index depends on the boility of delocalized electrons which absorb electromagnetic wave energy of the incident light. Electron mobility increases with size of the aromatic complex and with condensation (McCartney and Teichmüller, 1972). Refractive index is a function of atomic density; it also increases with degree of aromaticity. Van Krevelen (1961) reported refractivity and absorption of coals, calculated from reflectance measurements in two media, and found that refractivity increases significantly and steadily in low and medium stages of coalification up to about 92.5 percent carbon (dmmf). The absorption index in their studies was found not to change significantly until high stages of coalification, around 92 percent carbon. Reflectance begins to change with increased coalification at low levels of rank when aromaticity and refractive index are increasing. However, in low-rank coals, the dependence of reflectance values on rank is not as great as in high rank coals. The relatively moderate loading ($r=0.720$) of reflectance on the rank component and the fact that reflectance is split on two components suggests that reflectance is not totally a function of coalification for Group I coals.

Recent studies of the chemical structure of coal suggest that the loss of functional groups from the vitrinite structural units play a role in affecting the reflectance of low-rank coals (P.H. Giver personal communication, 1977). Loss of functional groups occurs with

coalification and this may in some way be affecting reflectance. However, the true chemical structure of vitrinite is not understood, and attributing variation in reflectance to that structure is, of course, speculative. It seems certain that alteration in the chemical structure of coal occurs as a result of coalification. Reflectance is an optical analysis, and its variation must be associated in some way with chemico-structural changes.

The loading of reflectance on the factor matrix is split between the first component with rank parameters and the second component with volatile matter. The plot of reflectance and volatile matter for the 109 samples lower in rank than anthracite (Figure 31) shows a strong linear relationship with a correlation coefficient of $r = -0.890$. This indicates that approximately 79 percent of the variation is common to both variables ($r^2 = 0.792$), and that 21 percent is not explained with the association. Volatile matter does not load on the rank component, so volatile matter does not appear to vary with rank for Group I coals. Reflectance is split between the rank component and the component with volatile matter. This suggests that reflectance variations for Group I coals (low levels of rank) are associated in part with rank changes, and in part with a different factor which also affects volatile matter.

Another aspect of coalification to be recognized in Group I coals is suggested by the change in moisture content through increased rank. Teichmüller and Teichmüller (1975) attribute the moisture content of a coal primarily to the porosity of coal. Porosity in low-rank coals decreases with increasing depth of burial, so the

moisture-holding capacity also decreases. Therefore, the moisture content of a coal decreases with increased rank. In very early stages of coalification, the loss of moisture is also due to the decomposition of hydrophylic functional groups, especially the -OH groups (Teichmüller and Teichmüller, 1975).

A fourth possible aspect of coalification must be considered for these low levels of rank. This is the process of bituminization, or the generation of petroleum-like substances. Teichmüller (1974) proposes the origin of petroleum-like substances in coal as a result of the temperatures associated with rank increases, and her ideas are presented here. Bituminization is said to begin in the subbituminous coal stage at temperatures around 65 to 110° C, depending on length of heating (Teichmüller and Teichmüller, 1975). Bituminization is said to be especially strong during the high volatile C to high volatile B bituminous stage, and to continue until the medium volatile bituminous stage. The petroleum precursors in coal are reported to be mainly hydrogen rich, aliphatic edge groups of the vitrinitic structures, and macerals of the liptinite group. As a result of bituminization, the precursors are converted to relatively mobile bitumen which is adsorbed onto the submicroscopic pore structure of the vitrinites. Bitumen also may be chemically combined within the vitrinite structure.

If the process of bituminization is indeed associated with coalification, it may affect the value of several variables included in this data set. If the hydrogen-rich bitumen products are trapped within the coal structure, the hydrogen content of the coal is not

decreased. This is consistent with enrichment of hydrogen for the low-rank coals of Group I. Migration of the bitumen into the pore structure could be a minor factor in the decreasing moisture-holding capacity of coal with increased rank. If enough bitumen is produced, the vitrinitic structures become so impregnated with petroleum-like substances that they have a dull fluorescence when observed under blue-light excitation. Also, their reflectance is decreased below that expected of the rank of the coal. The moisture-holding capacity for high-bitumen coals is reportedly reduced and the volatility of the coal is increased (Teichmüller, 1974). The results of the factor analysis do not disagree with the supposed results of bituminization. Therefore, bituminization is proposed as a possible aspect of coalification in the range of rank represented by Group I coals.

In summary, there are at least four coalification factors identified for coals ranging in rank from lignite to early stages of high volatile A bituminous. One is a chemical factor, resulting in decreases in the contents of oxygen and moisture, and increases in the proportions of carbon and hydrogen; therefore, calorific value is increased. The second factor is characterized by changes in reflectance and, in part, volatile matter, perhaps caused by changes in the chemical structure of the coal. The third coalification factor is a physical factor as measured by moisture. With increased overburden and, therefore, increased rank, the porosity of a coal is reduced and its moisture-holding capacity is also reduced. The fourth possible factor is bituminization which may affect volatile matter, moisture-holding capacity, reflectance, and hydrogen.

B. Group II from CLUS

Thirty coals were grouped into Group II by the cluster analysis of coals lower in rank than medium volatile bituminous. The data matrix for Group II coals is included in Appendix III. These coals cover the entire range of high volatile bituminous rank (high volatile C through high volatile A bituminous). Therefore, these coals are intermediate in rank between Groups I and III. The group includes 11 coals from the Eastern province, 18 coals from the Interior province and one coal from the Rocky Mountain province. Group II was separated from Group I and III primarily on the basis of organic sulfur content, and partially on the basis of rank. The mean value of sulfur in Group II is 1.83 percent compared to 0.81 percent from Group I and 0.79 percent for Group III.

1. Univariate analyses

Summary statistics of the variables of Group II are found in Table 17. On the basis of X^2 , none of the variables have distributions which are significantly different from a normal distribution. Reflectance and liptinite contents have distributions which are positively skewed at the one percent confidence level. The nitrogen distribution has a strong negative skew owing to one coal with an unusually low reported value (0.19 percent nitrogen). No transformations were performed on the variables.

2. Factor analysis

The correlation matrix for variables of this group of coals is given in Table 18 and is used as input into the factor analysis. The original matrix of factor loadings from the factor analysis is in Table 19. Seven components were extracted, and at

Table 17. Summary statistics for variables of Group II of CLUS

	Low	High	Mean	St. Dev.	Skewness	Kurtosis [†]	χ^2 ^{††}
Reflectance	0.36	1.01	0.63	0.14	0.723*	3.710	8.8
Carbon	79.33	85.64	82.69	2.12	-0.278	1.813**	12.8
Hydrogen	5.10	5.98	5.53	0.20	-0.082	2.904	9.5
Oxygen	4.62	12.50	8.18	2.03	0.149	2.400*	9.6
Sulfur	0.63	4.01	1.83	0.77	0.517	3.331	9.9
Nitrogen	0.19	2.55	1.76	0.44	-1.306**	6.979**	13.8
Volatile matter	35.29	47.92	42.86	2.90	-0.330	3.354	7.3
Moisture	1.39	12.64	6.28	3.03	0.386	2.231**	5.4
Btu/lb	14241	15620	14929	392	0.063	2.010**	13.9
Vitrinites	61.9	88.6	77.8	7.8	-0.709	2.670	6.8
Inertinites	9.2	35.6	18.6	6.9	0.667	2.578	14.4
Liptinites	1.4	7.5	3.6	1.6	0.942*	3.419	11.2

*Significant at the 5 percent probability level (30 samples)

**Significant at the 1 percent probability level

†Kurtosis tested at sample size of 200

††d.f. = 10

Table 18. Correlation matrix for variables of Group II from CLUS

	Reflectance	Carbon	Hydrogen	Oxygen	Sulfur	Nitrogen	Volatile Matter	Moisture	Btu/lb	Vitrinites	Inertinites
Carbon	0.515**										
Hydrogen	0.134	-0.134									
Oxygen	-0.547**	-0.923**	0.048								
Sulfur	-0.048	-0.294	0.009	-0.028							
Nitrogen	0.066	0.004	-0.057	-0.135	-0.208						
Volatile Matter	-0.754**	-0.451*	0.401*	0.434*	0.048	-0.099					
Moisture	-0.805**	-0.491**	-0.267	0.519**	0.004	0.089	0.390*				
Btu/lb	0.593**	0.874**	0.231	-0.878**	-0.142	0.006	-0.283	-0.649**			
Vitrinites	-0.239	-0.036	-0.312	0.017	0.244	-0.191	0.103	0.213	-0.217		
Inertinites	0.180	0.001	0.263	0.028	-0.253	0.197	-0.100	-0.129	0.148	-0.985**	
Liptinites	0.403	0.178	0.403*	-0.207	-0.102	0.091	-0.076	-0.491**	0.444*	-0.671**	0.535**

*Significant at the 5 percent probability level (d.f. = 23; $r = 0.361$)

**Significant at the 1 percent probability level ($r = 0.463$)

Table 19. Original matrix of factor loadings from the
R-mode factor analysis of Group II from CLUS

	C ₁	C ₂	C ₃	C ₄	C ₅	C ₆	C ₇	Communalities (h_i^2)
Btu/lb	0.880							0.969
Reflectance	0.834							0.978
Moisture	-0.792							0.875
Oxygen	-0.791			-0.547				0.991
Carbon	-0.790							0.996
Liptinites	-0.600	-0.570						0.963
Volatile Matter	-0.567							0.952
Vitrinites		0.827						0.997
Inertinites		-0.812						0.990
Hydrogen		-0.529	0.642					0.929
Nitrogen			-0.575					0.997
Sulfur			0.497	0.508	-0.740			1.000
Sum λ_i^2	4.459	2.568	1.437	1.168	0.851	0.734	0.411	
% Variation Explained	37.16	21.40	12.39	9.73	7.10	6.11	3.42	
Cumulative %	37.16	58.56	70.95	80.68	87.78	93.89	97.32	

least 87 percent of the variation of each variable is explained. The first four components have eigenvalues greater than 1.0 and are considered the most significant, linearly independent sources of information in the data set. The factor matrix was rotated to help in identifying the underlying factors. The rotated matrix is given in Table 20. The complete matrix of factor loadings for both the original and the rotated matrix is given in Appendix IV.

The first component contains three variables. These are carbon and calorific value with a positive loading and oxygen with a negative loading. This is identified as a continuation of the chemical rank factor which was identified in the Group I data set. The most important chemical reactions of this factor involve loss of oxygen and the enrichment of carbon. As a consequence, the heating value of the coal also increases.

The second component contains inertinite and vitrinite contents in an inverse loading. Liptinite has a minor loading ($r = -0.484$) on this component which is identified as the maceral composition factor.

The third factor contains hydrogen. In the factor analysis of Group I coals, hydrogen loaded on the same factor as carbon, oxygen, and calorific value. The coals of Group II are in the range of rank where the hydrogen curve through rank reaches a peak and begins to decrease with further rank increases. For Group I coals, hydrogen increases owing to the coalification process. Since the response of hydrogen to coalification is not linear in this range of rank, hydrogen is an individual variable on a component in the components analysis.

Table 20. Rotated matrix of factor loadings from the
R-mode factor analysis of Group II from CLUS

	C ₁	C ₂	C ₃	C ₄	C ₅	C ₆	C ₇	Communalities (h_i^2)
Oxygen	-0.947							0.991
Carbon	0.933							0.996
Btu/lb	0.905							0.969
Inertinites		-0.979						0.990
Vitrinites		0.956						0.997
Hydrogen			0.954					0.969
Reflectance				0.898				0.978
Volatile Matter				-0.819				0.952
Moisture				-0.671				0.875
Nitrogen					-0.986			0.997
Sulfur						-0.979		0.999
Liptinites		-0.484					0.800	0.963
Sum λ_i^2	2.953	2.221	1.321	2.129	1.035	1.054	0.966	
% Variation Explained	24.61	18.50	11.01	17.74	8.62	8.79	8.05	
Cumulative %	24.61	43.11	54.12	71.86	80.48	89.27	97.32	

The fourth component contains three variables. These are reflectance with a positive loading ($r=0.898$), and volatile matter ($r=-0.819$) and moisture ($r=-0.671$) with negative loadings.

The last three components are not considered significant sources of variance within the data set. Each of these three components contains a single variable: nitrogen on component five, sulfur on component six, and liptinite on component seven.

3. Interpretation of coalification processes active in coals of medium rank

The first component contains three variables which are influenced by chemical reactions of coalification. These reactions involve loss of oxygen and enrichment of carbon, and result in an increase in the heating value of the coal. This coalification factor was identified in the lower levels of rank represented by Group I coals. However, in the lower rank coals the loss of oxygen resulted in enrichment in hydrogen as well as carbon. For Group II coals, hydrogen is not enriched and, in fact, does not load at all with oxygen and carbon in the factor analysis. This is interpreted to be the result of the curvilinear behavior of hydrogen for this range of rank. At levels of coalification in the range of high volatile A bituminous rank, chemical reactions of coalification begin to involve the loss of methane (Teichmüller and Teichmüller, 1975). Therefore, hydrogen decreases with further coalification. Evidently Group II covers a range of rank where the equilibrium of the chemical system is changing (Teichmüller, 1974) such that hydrogen is released during the reactions of coalification.

A second coalification process active for this set of data is interpreted as an alteration of the vitrinitic structure and/or

chemical composition. This results in an increase in reflectivity of the coal as discussed above. Volatile matter is increasing more directly with reflectance for Group II coals than for the lower rank Group I coals. Volatile matter and reflectance are more strongly correlated for Group II coals ($r=-0.754$) than for those of Group I ($r=-0.566$). The common cause of the variance in reflectance and volatile matter is not obvious. They load on a separate factor from carbon, oxygen, and calorific value. Therefore, their variation might be controlled by a separate factor. If increase in aromaticity is an aspect of coalification for high volatile coals, reflectance and volatile matter may be associated with this increase as suggested by McCartney and Teichmüller (1972).

The moisture content is still decreasing in response to coalification for the high volatile bituminous coals represented in Group II. However, the behavior of moisture content is not related to the chemical coalification pattern represented by the loss of oxygen. Instead, moisture varies with the same factor which causes alteration of reflectance and volatile matter. This association could indicate that loss of moisture with increased rank in the volatile bituminous range of rank may not be due to chemical losses such as the removal of hydrophylic groups. Instead, the moisture-holding capacity may depend on the microporosity of the coal structure. The association of moisture with reflectance and volatile matter suggests that they all may be varying owing to some alteration of the chemical structure of the coal. More research is needed into the actual chemical structure of coal in order to support or disprove this idea.

In summary, coalification results in at least two major sources of variation in Group II coals. One is the chemical factor resulting in decrease in oxygen content and increase in carbon and calorific value. A second factor results in an increase in the reflectance; a change in the amount of volatile products; and a decrease in moisture content, perhaps due to a decrease in submicroscopic porosity.

C. Group III from CLUS

Thirty-four coals comprise Group III from the cluster analysis of coals lower in rank than medium volatile bituminous. The data matrix of Group III is given in Appendix III. Thirty of the coals of this group are high volatile A bituminous and four are high volatile B bituminous in rank. One high volatile B coal, PSOC-105, was dropped from further statistical analysis of this group. This coal has a very low reported nitrogen content of 0.40 percent compared to the mean of 1.69. The purpose of the study of individual groups of coal is to analyze variable interaction within a homogeneous data set, not to explain unusual variance contributed by misclassified samples. Therefore, 33 coals are retained in Group III. These include 30 Eastern province samples, two samples from the Northern Great Plains province, and one from the Interior province.

Group III was separated from Group I primarily on the basis of rank, and from Group II on the basis of rank and organic sulfur content. Group III represents coals of the upper levels of high volatile rank. These coals are moderate to low in their organic sulfur content ranging from 0.42 to 1.66 percent, and they have a mean organic sulfur value of 0.79 percent.

1. Univariate analyses

Summary statistics of the variables of Group III are given in Table 21. Three variables are lognormally distributed: sulfur, moisture, and inertinite. The frequency distribution of vitrinite is significantly skewed at the one percent probability level, but does not deviate from normality on the basis of kurtosis or χ^2 ; no transformation was performed. The hydrogen distribution departs from normality on the basis of χ^2 , but not on the basis of skewness or kurtosis; no transformation was performed. The distribution of other variables are not significantly different from normality on the basis of skewness or χ^2 .

2. Factor analysis

The correlation matrix generated as input into the factor analysis is given in Table 22. The original matrix of factor loadings for Group III coals is given in Table 23. Six components were extracted to account for at least 85 percent of the variation of each variable. Based on the eigenvalues, the first four components are considered as the most important linearly independent sources of data variance in this group of coals.

The first component contains six variables. The variables are reflectance, carbon, and calorific value with negative loadings, and moisture, volatile matter, and oxygen with positive loadings. Since the values of these variables are known to be affected by coalification, this is recognized as the rank factor and changes in rank account for at least 41 percent of the total variance.

The matrix is rotated so that the underlying factors may be more easily interpreted. The rotated matrix is given in Table 24.

Table 21. Summary statistics for variables of Group III of CLUS

	Low	High	Mean	St. Dev.	Skewness	Kurtosis [†]	χ^2 ^{††}	Transfor- mation	Skewness	Kurtosis [†]	χ^2 ^{††}
Reflectance	0.64	1.07	0.86	0.11	0.372	2.116**	15.9				
Carbon	81.97	88.91	85.22	1.58	0.316	2.555	11.2				
Hydrogen	4.99	5.96	5.54	0.21	-0.168	3.336	22.0*				
Oxygen	3.15	11.25	6.75	1.66	0.199	3.134	9.9				
Sulfur	0.42	1.66	0.79	0.34	1.497**	4.100**	32.8*	log x	0.842*	3.281	29.7
Nitrogen	1.14	2.46	1.69	0.28	0.656*	3.207	16.1				
Volatile matter	33.47	42.59	37.91	2.63	-0.161	2.188*	7.9				
Moisture	1.08	10.63	3.4	2.3	1.300*	4.282**	28.5**	log x	0.332	1.960**	10.5
Btu/lb	14796	15853	15285	284	-0.075	2.333**	12.0				
Vitrinites	54.8	86.1	73.5	8.4	-0.863**	2.992	16.7				
Inertinites	8.4	36.1	16.6	6.2	1.208**	4.602**	18.1	log x	0.297	2.672	9.6
Liptinites	2.4	23.5	9.9	5.7	0.795*	2.810	11.2				

*Significant at the 5 percent probability level (33 samples)

**Significant at the 1 percent probability level

†Kurtosis tested at sample size 200

††d.f. = 10

Table 22. Correlation matrix for variables of Group III from CLUS

	Reflectance	Carbon	Hydrogen	Oxygen	Sulfur (log x)	Nitrogen	Volatile Matter	Moisture (log x)	Btu/lb	Vitrinites	Inertinites (log x)
Carbon	0.785**										
Hydrogen	-0.500**	-0.213									
Oxygen	-0.656**	-0.945**	-0.021								
Sulfur (log x)	-0.311	-0.059	0.413*	-0.204							
Nitrogen	0.178	0.160	0.115	-0.336	0.055						
Volatile Matter	-0.898**	-0.665**	0.624**	0.464**	0.548**	-0.093					
Moisture (log x)	-0.815**	-0.686**	0.251	0.620**	0.169	-0.202	0.642**				
Btu/lb	0.667**	0.904**	0.016	-0.911**	0.154	0.168	-0.445*	-0.698**			
Vitrinites	-0.135	-0.051	0.220	0.003	0.190	-0.123	0.218	0.199	0.001		
Inertinites (log x)	0.292	0.111	-0.169	-0.071	-0.290	0.301	-0.331	-0.433*	0.093	-0.692**	
Liptinites	-0.107	-0.101	-0.162	0.154	-0.007	-0.246	0.024	0.190	-0.147	-0.672**	-0.044

*Significant at the 5 percent probability level (d.f. = 31; $r = 0.349$)

**Significant at the 1 percent probability level ($r = 0.449$)

Table 23. Original matrix of factor loadings from the
R-mode factor analysis of Group III from CLUS

	C ₁	C ₂	C ₃	C ₄	C ₅	C ₆	Communalities (h_i^2)
Reflectance	-0.937						0.932
Carbon	-0.907						0.959
Moisture (log x)	0.864						0.845
Volatile Matter	0.837						0.930
Oxygen	0.812	0.478					0.969
Btu/lb	-0.812						0.943
Vitrinites		-0.708	-0.647				0.994
Sulfur (log x)		-0.634					0.980
Hydrogen		-0.580				0.505	0.958
Inertinites (log x)		0.516	0.464	0.464			0.964
Liptinites		0.519		-0.714			0.979
Nitrogen				0.591	0.580		0.990
Sum λ_i^2	4.963	2.422	1.546	1.323	0.653	0.525	
% Variation Explained	41.36	20.18	12.89	11.03	5.52	4.37	
Cumulative %	41.36	61.54	74.43	85.46	90.98	95.35	

Table 24. Rotated matrix of factor loadings from the
R-mode factor analysis of Group III from CLUS

	C ₁	C ₂	C ₃	C ₄	C ₅	C ₆	Communalities (h_i^2)
Carbon	-0.965						0.959
Btu/lb	-0.960						0.943
Oxygen	0.947						0.969
Reflectance	-0.771	0.482					0.932
Moisture (log x)	0.747						0.845
Volatile Matter	0.585	-0.560				0.497	0.930
Hydrogen		-0.949					0.958
Inertinites (log x)			0.948				0.964
Vitrinites			-0.649	0.742			0.994
Liptinites				-0.970			0.979
Nitrogen					0.963		0.990
Sulfur (log x)						0.951	0.980
Sum λ_i^2	4.289	1.584	1.640	1.554	1.048	1.327	
% Variation Explained	35.74	13.20	13.66	12.95	8.74	11.06	
Cumulative %	35.74	48.94	62.61	75.56	84.30	95.35	

The complete matrix of factor loadings for both the original and the rotated matrix is given in Appendix IV.

The first component in the rotated matrix of factor loadings contains the same six variables as the original matrix. Carbon, calorific value and oxygen are strongly loaded on this component indicating that they are being controlled by a common factor. Again, this factor is the set of chemical reactions primarily involving the loss of oxygen or oxygen-rich groups. The loadings of reflectance ($r=-0.771$) and moisture ($r=0.747$) are moderate and volatile matter is only slightly loaded in this factor ($r=0.585$). These last three variables are responding in part to the same factor effecting variation in carbon.

The second component contains hydrogen with a strong negative loading. Volatile matter and reflectance have minor loadings on this component. This is also considered a chemical coalification factor but it involves loss of hydrogen in the chemical reactions. Reflectance and volatile matter are responding in part to this factor as well as to the first factor.

The third factor contains the inertinite- and vitrinite-group macerals in inverse loadings. The fourth component contains vitrinite- and liptinite-group macerals. Together these two components account for the maceral composition of Group III coals.

The last two components each contain a single variable. Nitrogen loads on the fifth and sulfur loads on the sixth component. These are not considered significant factors controlling variation in the data set.

3. Interpretation of coalification processes active in the high levels of high volatile bituminous rank

The chemical processes involving the loss of oxygen-containing components continues to be an important factor of coalification for these high levels of high volatile bituminous rank.

A second factor of coalification is the release of hydrogen. This is considered to be due primarily to the release of methane (Teichmüller and Teichmüller, 1974). The release of hydrogen is reported to be associated with the "coalification jump" of the liptinitic macerals (Stach, 1968). At about the beginning of the high volatile A bituminous rank, the reflectance of liptinite begins to increase with further coalification as the macerals lose hydrogen-rich aliphatic units. Hydrogen is also lost from the vitrinite structural units. Both reflectance and volatile matter are varying with the factors of carbonization and dehydrogenation.

D. Group IV from CLUS

In the cluster analysis of all the coals considered in this study, twelve samples were grouped together as a distinct population. The data matrix for this set of coals is in Appendix III. This population was characterized as being high in rank and as having a large proportion of the macerals of the vitrinite-group, or conversely, a low proportion of the liptinite-group macerals. The group was identified as the medium and low volatile bituminous coals. All the samples in this group are from the Eastern province. The twelve samples include six low volatile, four medium volatile and two high volatile bituminous coals on the basis of ASTM rank classification.

One coal, PSOC-301, has been eliminated from further statistical analyses of this group. From the plot of the cluster analysis given in Figure 9 (page 59), this coal is identified as a misclassification. On the basis of maceral composition, PSOC-301 is more similar to the continuum of coals lower in rank than to this group of medium and low volatile bituminous samples. PSOC-301 is a high volatile bituminous coal according to ASTM classification and contains 3.1 percent liptinite-group macerals compared to 0.4 percent for the other eleven samples. This coal is at the level of rank where the liptinite-group macerals are still darker in reflected light than macerals of the vitrinite group. For medium and low volatile bituminous coals, the liptinite macerals have increased in reflectance enough that they are difficult or impossible to distinguish from the vitrinites, so the proportion of macerals identified as vitrinite decreases. Since PSOC-301 is interpreted as a misclassification, it is omitted from this group and the remaining eleven samples will be analyzed to determine properties of medium and low volatile bituminous coals.

1. Univariate analyses

Summary statistics of variables of Group IV coals are given in Table 25. The shape of the curves are difficult to test for normality due to the small sample size. The distribution of three variables have a significant positive skew, including that of volatile matter, moisture, and the liptinite group macerals. Transformation of the liptinite group macerals gives a distribution which is not as different from normality as is the untransformed distribution. However, even after transformation, the curve is

Table 25. Summary statistics for variables of Group IV from CLUS

	Low	High	Mean	St. Dev.	Skewness	Kurtosis [†]	χ^2_{++}	Transfor- mation	Skewness	Kurtosis [†]	χ^2_{++}
Reflectance	1.17	1.80	1.45	0.22	0.126	1.600**	7.5				
Carbon	88.09	91.56	90.00	0.94	-0.532	3.262	11.8				
Hydrogen	4.44	5.31	4.81	0.27	0.232	2.200**	3.2				
Oxygen	1.61	4.34	2.98	0.95	0.192	1.688**	4.7				
Sulfur	0.10	1.40	0.78	0.40	0.197	2.291**	4.5				
Nitrogen	0.85	2.27	0.14	0.40	0.448	2.904	2.3				
Volatile matter	18.10	32.78	22.25	4.46	1.136**	3.703*	20.5*				
Moisture	0.70	6.15	2.05	1.56	1.718**	5.379**	19.2				
Btu/lb	16113	15565	15816	167	0.030	2.097**	6.8				
Vitrinites	65.0	92.5	81.4	9.6	-0.652	2.194**	8.4	log x/1-x	0.494	1.918**	10.7
Inertinites	7.4	35.0	18.2	9.9	0.578	2.132**	9.6	log x	-0.048	1.748	9.0
Liptinites	0.0	2.5	0.4	0.8	2.029**	5.668**	45.4**	$\sqrt{x}$	1.506**	3.930*	28.6**

*Significant at the 5 percent probability level (11 samples)

**Significant at the 1 percent probability level

†Kurtosis tested at sample size of 200

††d.f. = 40

significantly different from normality at the five percent probability level.

2. Factor analysis

The correlation coefficient generated as input into the factor analysis is given in Table 26. The original matrix of factor loadings is given in Table 27. Five components were extracted to account for at least 85 percent of the variance of each variable. On the basis of eigenvalues, the first four are considered to be the significant linearly independent sources of variation in the data set. All but two of the variables load on the first and second components, and together these components account for 68 percent of the data variance. This suggests that the number of factors contributing to variation in the chemical and petrographic variables of coals are decreasing in these high levels of bituminous rank.

The matrix of factor loadings is rotated in order to simplify interpretation of the underlying factors. The rotated matrix of the factor loadings is given in Table 28. The first component contains volatile matter and hydrogen with positive loadings and reflectance with a negative loading. This is interpreted as the rank factor with reflectance increasing and volatile matter and hydrogen decreasing in response to coalification in high levels of bituminous rank.

The second component contains nitrogen and oxygen in inverse loadings. The fourth component contains sulfur and carbon in inverse loadings. The five components of the elemental analysis of coals sum to 100 percent. Therefore, components two and four together

Table 26. Correlation matrix for variables of Group IV from CLUS

	Reflectance	Carbon	Hydrogen	Oxygen	Sulfur	Nitrogen	Volatile Matter	Moisture	Btu/lb	Vitrinites (log x/1-x)	Inertinites (log x)
Carbon	0.262										
Hydrogen	-0.773**	-0.570									
Oxygen	0.192	-0.726*	0.165								
Sulfur	-0.242	-0.543	0.413	-0.046							
Nitrogen	-0.283	0.396	-0.179	-0.781**	0.075						
Volatile Matter	-0.848**	-0.423	0.878**	0.168	0.121	-0.154					
Moisture	-0.529	0.108	0.283	-0.576	0.431	0.499	0.153				
Btu/lb	-0.419	0.484	0.138	-0.653*	-0.031	0.392	0.110	0.780**			
Vitrinites (log x/1-x)	-0.399	-0.229	0.613*	-0.101	0.341	0.003	0.509	0.154	0.124		
Inertinites (log x)	0.432	0.241	-0.638*	0.107	-0.360	-0.004	-0.533	-0.209	-0.161	-0.997**	
Liptinites ($\sqrt{x}$)	-0.591	-0.246	0.601	-0.089	0.370	-0.011	0.531	0.757**	0.525	0.393	-0.458

*Significant at the 5 percent probability level (d.f. = 9; $r = 0.602$)

**Significant at the 1 percent probability level ($r = 0.735$)

Table 27. Original matrix of factor loadings from the
R-mode factor analysis of Group IV from CLUS

	C ₁	C ₂	C ₃	C ₄	C ₅	Communalities (h_i^2)
Hydrogen	0.879					0.980
Reflectance	-0.841					0.923
Liptinites ($\sqrt{x}$)	0.798					0.916
Volatile Matter	0.785					0.971
Inertinites ($\log x$)	-0.762					0.992
Vitrinites ($\log x/1-x$)	0.724		-0.614			0.993
Moisture	0.611	0.640				0.986
Oxygen		0.919				0.949
Carbon		-0.780				0.954
Nitrogen		-0.763				0.930
Btu/lb		-0.760				0.915
Sulfur				0.742		0.935
Sum λ_i^2	4.826	3.322	1.269	1.198	0.828	
% Variation Explained	40.22	27.58	10.57	9.99	6.90	
Cumulative %	40.22	67.90	78.48	88.46	95.37	

Table 28. Rotated matrix of factor loadings from the
R-mode factor analysis of Group IV from CLUS

	C ₁	C ₂	C ₃	C ₄	C ₅	Communalities (h_i^2)
Volatile Matter	0.920					0.971
Reflectance	-0.896					0.980
Hydrogen	0.782					0.923
Nitrogen		-0.956				0.930
Oxygen		0.869				0.949
Vitrinites (log x/1-x)			-0.952			0.993
Inertinites (log x)			0.938			0.992
Sulfur				0.915		0.935
Carbon				-0.694		0.954
Moisture					-0.843	0.986
Btu/lb					-0.822	0.915
Liptinites ($\sqrt{x}$)					-0.801	0.916
Sum λ_i^2	2.784	2.402	2.192	1.676	2.389	
% Variation Explained	23.20	20.01	18.27	13.97	19.91	
Cumulative %	23.20	43.22	61.49	75.46	95.37	

account for the variation of elemental composition which is not explained by hydrogen.

The third component contains the vitrinite- and inertinite-group macerals with inverse loadings. This is the factor which accounts for maceral composition. Since the liptinitic macerals are difficult or impossible to distinguish in these high levels of rank, almost the entire maceral composition is composed of the vitrinite- and inertinite-group macerals

The fifth component contains three variables, all with negative loadings. These are moisture, calorific value, and the liptinite-group macerals. This component is not interpreted as a significant source of information. For these high levels of rank, the values of moisture, calorific value, and liptinite do not vary predictably or significantly with rank.

3. Interpretation of the coalification processes active in high levels of bituminous rank

The first component contains hydrogen, volatile matter, and reflectance. The loading of these variables and the absence of carbon, oxygen, and calorific value on the first component indicate a major change in response to coalification for medium and low volatile bituminous coals. The loss of oxygen is no longer as significant an aspect of coalification as it was for all the lower stages of rank. In contrast, the loss of hydrogen is a major result of coalification. Teichmüller and Teichmüller (1975) state that hydrogen is lost primarily in the form of methane. Methane is reportedly released from the vitrinitic structure and from the liptinite. It is accompanied by decrease in volatile matter, and an increase in the reflectance of vitrinite.

According to the bituminization model proposed by Teichmüller (1974) the loss of hydrogen in medium and low volatile bituminous coals also results from a decomposition of the petroleum-like products of bituminization. In this model, the hydrocarbons of the bitumen which formed at lower stages of rank are thermally cracked into hydrocarbons of smaller molecular size, leaving strongly reflecting, polycondensed residues. This is said to contribute to the overall decrease in the amount of volatile products of pyrolysis. The thermal conditions necessary for the cracking of petroleum-like substances in coal are considered to be the same as those required for converting petroleum into gases. Therefore, the medium volatile bituminous stage is said to correspond with the "deadline" for important economic petroleum occurrences (Teichmüller, 1974). The results of factor analysis for medium and low volatile bituminous coals do not contradict the expected results of bituminization.

The above results of coalification involving loss of hydrogen and volatile matter and an increase in reflectance are considered the most significant results of coalification in the upper stages of bituminous rank. Carbon and oxygen are no longer responding significantly to the processes of coalification as they were for lower levels of rank. The fact that calorific value is not varying with carbon and oxygen is also unique to these high levels of bituminous rank. The correlation coefficient between calorific value and oxygen ($r = -0.653$) is significant at the five percent

probability level. However, only 43 percent of variation is common between the two variables, and 57 percent of the variance is not common. The correlation between carbon and calorific value ($r=0.484$) is not significant at the 5 percent probability level.

VIII. DISCUSSION OF VARIABLES AFFECTED BY RANK

A. Bivariate plots of rank parameters

The preceding discussions of individual groups separated by cluster analysis make it clear that the particular interactions among several variables of this study depend on the stage of rank being considered. These variables are the ones whose values are altered by the processes of coalification. In order to better understand the behavior of rank-dependent variables through coalification, it is helpful to observe binary plots of these rank parameters. The untransformed data are used in the plots.

The ASTM rank classification is used in the United States and elsewhere to classify coal according to rank. This classification is reproduced in Table 29. For low-rank coals, the classification is based on calorific value on a moist, mineral-matter-free basis (mmmf). For high-rank coals, it is based on volatile matter on the dry, mineral-matter-free basis (dmmf). In the ASTM classification scheme, rank parameters are corrected to the mineral-free basis by the Parr mineral-matter formula. In this study, variables are corrected to the mineral-matter-free basis by the Modified Parr formula because data on the forms of sulfur are available (see Section IV D). Also, since only the organic portion of coal is considered in this study, calorific value is corrected to the dry basis rather than the moist basis used by ASTM. The limits of rank parameters for a given rank on this basis have been estimated and are given in Table 30. These limits were obtained by plotting a variable corrected for mineral matter by the Parr

Table 29. ASTM Rank Classification

Class	Group	Fixed Carbon Limits, percent (Dry, Mineral-Matter-Free Basis)		Volatile Matter Limits, Percent (Dry, Mineral-Matter-Free Basis)		Calorific Value Limits, Btu per pound (Moist ² Mineral-Matter-Free Basis)		Agglomerating Character
		Equal or Greater Than	Less Than	Greater Than	Equal or Less Than	Equal or Greater Than	Less Than	
I. Anthracitic	1. Meta-anthracite	98	--	--	2	--	--	non-agglomerating
	2. Anthracite	92	98	2	8	--	--	
	3. Semianthracite ³	86	92	8	14	--	--	
II. Bituminous	1. Low volatile bituminous coal	78	86	14	22	--	--	commonly agglomerating ⁵
	2. Medium volatile bituminous coal	69	78	22	31	--	--	
	3. High Volatile A bituminous coal	--	69	31	--	14 000 ⁴	--	
	4. High Volatile B bituminous coal	--	--	--	--	13 000 ⁴	14 000	agglomerating
	5. High Volatile C bituminous coal	--	--	--	--	11 500	13 000	
III. Subbituminous	1. Subbituminous A coal	--	--	--	--	10 500	11 500	non-agglomerating
	2. Subbituminous B coal	--	--	--	--	9 500	10 500	
	3. Subbituminous C coal	--	--	--	--	8 300	9 500	
IV. Lignitic	1. Lignite A	--	--	--	--	6 300	8 300	non-agglomerating
	2. Lignite B	--	--	--	--	--	6 300	

¹ This classification does not include a few coals, principally nonbanded varieties, which have unusual physical and chemical properties and which come within the limits of fixed carbon or calorific value of the high-volatile bituminous and sub-bituminous ranks. All of these coals either contain less than 48 percent dry, mineral-matter-free fixed carbon or have more than 15,500 moist, mineral-matter-free British thermal units per pound.

² Moist refers to coal containing its natural inherent moisture but not including visible water on the surface of the coal.

³ If agglomerating, classify in low-volatile group of the bituminous class.

⁴ Coals having 69 percent or more fixed carbon on the dry, mineral-matter-free basis shall be classified according to fixed carbon regardless of calorific value.

⁵ It is recognized that there may be nonagglomerating varieties in these groups of the bituminous class, and there are notable exceptions in high volatile C bituminous group.

Table 30. Rank classification using Modified Parr mineral matter formula to correct variables to the mineral-free basis

Class	Group	Volatile Matter Limits, percent		Calorific Value Limits, Btu per pound		Carbon Limits, percent		Reflectance Limits, percent	
		>	≤	≥	<	≥	<	≥	<
I. Anthracite	Meta-anthracite								
	Anthracite		7					(3.00)	
	Semianthracite	7	13			(915)*		2.05	(3.00)
II. Bituminous	Low volatile A bituminous	13	21				(91.5)	1.50	2.05
	Medium volatile bituminous	21	30			(89)		1.10	1.50
	High volatile A bituminous	30	(39)	14900		83	(89)	0.71	1.10
	High volatile B bituminous			14400	14300	80	83	0.57	0.71
	High volatile C bituminous			13700	14400	78	80	0.47	0.57
III. Subbituminous	Subbituminous A			13200	13700	76	78	(0.43)	(0.47)
	Subbituminous B			12800	13200	74	76	(0.39)	(0.43)
	Subbituminous C			12200	12300	72	74	(0.34)	(0.39)
IV. Lignite	Lignite A				12200				
	Lignite B								(0.34)

* Values in parenthesis are questionable

formula against that variable corrected by the Modified Parr formula. For calorific value, plots of moist calorific value against dry calorific value were also obtained. These limits of rank are used in the present study only as guidelines for plotting rank divisions using the Modified Parr mineral-matter formula to correct variables to the mineral-free basis. More coals must be considered to firmly establish the particular limits of each variable for a given rank.

In the plots that do not include anthracites, symbols are used for designating coals of different provinces. The individual provinces will be considered in more detail in the next section of this study. However, it is informative to see where the coals of a given province fit into the rank scheme. In general, the level of rank represented by the provinces increases in the following order: Northern Great Plains province (lowest rank), Rocky Mountain province, Interior province, and Eastern province. In the plots that do include anthracite, symbols for provinces are not used because all anthracites in this study are from the Eastern province. The numbers on the plots with anthracite indicate the number of coals which plot at a given point.

The first bivariate plot of rank parameters is reflectance versus carbon (Figure 16). Both of these parameters are often used to indicate rank, and rank divisions have been marked along both the reflectance and the carbon axes. In this study, the strong enrichment of carbon with increased rank has been observed for all levels of rank lower than medium volatile bituminous. Reflectance has been observed to increase through most levels of rank, especially

Figure 16. PLOT OF REFLECTANCE VERSUS CARBON FOR U.S. COALS

in the upper stages of rank (high volatile bituminous and above). These trends are observed in the bivariate plot of reflectance and carbon. For levels of rank lower than about the high volatile C/B boundary, the values of reflectance are not strongly increasing with rank. In this rank range, there is a wide spread in carbon values. In the medium and low volatile bituminous coals, the values of reflectance are widely spaced. In contrast, there is little variation on the carbon axis for these high levels of rank. Since reflectance and carbon are most sensitive to coalification at opposite ends of rank represented in this study, both will be used as indices of rank in plots against the other rank parameters.

The spread in values is greatest at about the high volatile B to A bituminous range based on carbon. This is due to the plotting of six coals of the Interior province. Although these coals would be high volatile B to A bituminous based on carbon content, they would be classified as subbituminous to high volatile B bituminous based on reflectance. This "underclassification" of Interior province coals, based on reflectance, will be discussed further in Section IX B4. The plot of reflectance and carbon values of anthracites are included in Figure 17. This plot shows that carbon is most strongly enriched in low levels of rank. At high levels of rank where carbon content is greater than 90 percent, the further enrichment of carbon is difficult and the rate of enrichment with coalification is decreased.

During the processes of coalification, losses of oxygen and increases in carbon occur simultaneously. The plot of carbon against oxygen is given in Figure 18, and the strong negative

Figure 17. PLOT OF REFLECTANCE VERSUS CARBON FOR U.S. COALS, INCLUDING ANTHRACITES

Figure 18. PLOT OF CARBON VERSUS OXYGEN FOR U.S. COALS

correlation ($r=-0.974$) between the variables is observed. The relation between variables is particularly strong for the lowest levels of rank. These are from the Northern Great Plains and Rocky Mountain provinces. Again, there is a large scatter in the lower rank high volatile bituminous coals. At this level, the carbon and oxygen values of some Interior province coals do not appear to be responding to coalification as predictably as do the other samples. The curve is not completely linear. In fact, there are two possible places where the slope may change. One is approximately in the high volatile C bituminous rank range; the other is within the high volatile A bituminous rank range. There is a strong negative correlation between variables at all levels of rank indicating that as oxygen is lost, carbon is enriched. However, the change in slope at various stages of rank may be due to a change in the chemical reactions which accompany rank increase. If the changes in slope are real, they are only minor. Hickling (1932) found coals of the carbon and oxygen plot to lie within a narrow band of continuous variation in composition from lignites to anthracites. He noted a change in slope at the anthracite end of the curve where oxygen losses are a less important and hydrogen losses are a more important result of coalification than for lower levels of rank.

The plot of reflectance and oxygen is given in Figure 19; it is nearly a mirror image of the plot of reflectance and carbon. This is expected considering the strong negative correlation between carbon and oxygen. The plot of reflectance and oxygen illustrates the small amount of variation of oxygen in medium and low volatile bituminous coals. At this stage of coalification, the major processes of rank

Figure 19. PLOT OF REFLECTANCE VERSUS OXYGEN FOR U.S. COALS

Figure 20. PLOT OF REFLECTANCE VERSUS OXYGEN FOR U.S. COALS, INCLUDING ANTHRACITES

increase are no longer the loss of oxygen-rich chemical units. The departure of Interior province coals to the low-reflectance side of the curve of the remaining coals again is observed. Figure 20 is a plot of reflectance and oxygen including anthracites. The variation in oxygen for high levels of rank is relatively small. This is because most of the oxygen has been lost from the coal in earlier levels of coalification.

The calorific value of coal varies directly with increasing carbon for most levels of rank. The plot of carbon and calorific value is given in Figure 21; the strong correlation ($r=0.950$) between these variables is observed. The curve is not linear through all levels of rank, but appears to change slope at two points. One change is around the high volatile C and B bituminous boundary. The other is at the upper levels of high volatile A bituminous rank. This second change in slope is at the level of rank where the loss of hydrogen results from coalification. At lower levels of rank, both hydrogen and carbon are enriched with rank increases; calorific value also increases. When hydrogen is lost as a result of coalification, calorific value does not increase as strongly with rank increases as for lower rank coals. The plot of reflectance and calorific value (Figure 22) shows similar trends as the plot of reflectance and carbon for all levels of rank lower than anthracite. However, when the anthracites are included (Figure 23), the plots are seen to differ. There is a tendency for calorific value to decrease slightly with increased coalification for these high levels of rank. Again, this is associated with the loss of hydrogen.

Figure 21. PLOT OF CARBON VERSUS CALORIFIC VALUE FOR U.S. COALS

Figure 22. PLOT OF REFLECTANCE VERSUS CALORIFIC VALUE FOR U.S. COALS

Another aspect of coalification with low-rank coals is the decrease of moisture content with increase in rank. For all except the lowest levels of rank, this is due primarily to a decrease in porosity associated with increased overburden pressure. The plot of carbon versus moisture (Figure 24) shows this approximate trend of moisture through rank. In the high volatile B to A bituminous rank range, several Interior province coals have higher moisture contents than expected. This suggests that these Interior province coals may be more porous than other coals of the same rank. When reflectance is plotted against moisture (Figure 25), a stronger correlation is observed. The moisture content of coals is seen to decrease sharply up through the lower levels of rank, until about the high volatile C bituminous stage. Moisture decreases at a lesser rate from high volatile C to the high volatile A bituminous rank. At higher levels of rank shown in this plot, there is little variation in moisture content and most coals have less than four percent moisture. The plot of reflectance and moisture for coals including anthracites is given in Figure 26. The moisture content of coals is reported to increase to some degree at levels of rank greater than low volatile bituminous (Teichmüller and Teichmüller, 1975). This is reportedly due to chemico-structural alterations of the vitrinite structure at these high levels of rank. The plot of reflectance and moisture in Figure 26 does not include enough data for anthracites to either support or disprove the idea that moisture content increases in extremely high levels of rank.

Figure 25. PLOT OF REFLECTANCE VERSUS MOISTURE FOR U.S. COALS

Figure 26. PLOT OF REFLECTANCE VERSUS MOISTURE FOR U.S. COALS, INCLUDING ANTHRACITES

The curvilinear behavior of hydrogen through rank has been discussed in Section V C. It is observed in Figure 27 in which carbon and hydrogen are plotted. The general trend observed in this study is for hydrogen to be enriched at low levels of rank until about the high volatile bituminous rank boundary. At approximately the middle of high volatile A bituminous rank, the hydrogen content of coals begins to decrease with further rank increase. One Interior province coal falls well below the trend of the other coals. This coal is PSOC 164. It was classified with Group II by the cluster analysis, but was dropped from the group as a misclassification because of its unusually low hydrogen content. The plot of hydrogen and reflectance (Figure 28) again shows the curvilinear response of hydrogen through rank. The decrease of hydrogen content at high levels of rank is obvious in this plot. When anthracites are included in the plot (Figure 29), the loss of hydrogen associated with high levels of coalification is obvious.

In factor analyses, volatile matter was found not to vary directly with coalification at low levels of rank. This is illustrated in Figure 30 in which volatile matter is plotted against carbon. The amount of volatile matter begins to decrease with rank at the start of high volatile A bituminous rank. As can be seen in the plot, volatile matter does not vary with coalification at low levels of rank. When reflectance and volatile matter are plotted (Figure 31), a strong negative correlation is observed ($r=-0.942$). However, in low levels of rank, there is more scatter in the plot than for high levels of rank. The variance begins to decrease

Figure 27. PLOT OF CARBON VERSUS HYDROGEN FOR U.S. COALS

Figure 28. PLOT OF REFLECTANCE VERSUS HYDROGEN FOR U.S. COALS

Figure 29. PLOT OF REFLECTANCE VERSUS HYDROGEN FOR U.S. COALS, INCLUDING ANTHRACITES

Figure 30. PLOT OF CARBON VERSUS VOLATILE MATTER FOR U.S. COALS

Figure 31. PLOT OF REFLECTANCE VERSUS VOLATILE MATTER FOR U.S. COALS

at about the middle stages of high volatile A bituminous rank. At all levels of rank, volatile matter decreases as reflectance increases.

For the medium and low volatile bituminous coals, both hydrogen and volatile matter decrease as reflectance increases. When volatile matter and hydrogen are plotted (Figure 32), a negative correlation between the two variables for high levels of rank is apparent. Below about the middle stages of high volatile A bituminous rank, there is no predictable relation between the two variables.

B. Analysis of the effect of rank parameters on the cluster analysis

The discriminant equations for cluster analysis indicate that the groups of coals were separated partly on the basis of rank (see Section VI B2). However, it was not possible to determine which variables were causing the groupings at various rank levels. The study of bivariate plots of rank parameters provides insight into how various parameters are varying through the series of coalification. The plots also provide suggestions as to why the particular groups were chosen by the cluster analysis.

First, the bivariate plots illustrate why no groups were strongly discriminated from one another. Most plots are a continuous series of coals with no distinct separation along the series. The only exceptions are the breaks observed in plots which include volatile matter or moisture. For example, the plot of reflectance and volatile matter (Figure 31) has a distinct gap between volatile matter values of about 25 to 33 percent. This is probably due to the few number of samples rather than to a real break within the continuous series of volatile matter through rank. This gap probably

Figure 32. PLOT OF VOLATILE MATTER VERSUS HYDROGEN FOR U.S. COALS

contributes to the relatively distinct grouping of medium and low volatile coals. The coals lower in rank are a continuum in the cluster analysis. The plot of reflectance and moisture (Figure 25) also has a break at low levels of rank. Again, this is interpreted as due to the small sampling of low rank coals.

In discussing the plots of rank parameters, it was mentioned that several plots exhibit at least one distinct change in slope at some level of rank. Past researchers have commented on this phenomenon and have attributed it to changes in equilibrium in the chemical processes at different stages of coalification. One such change is firmly established in the literature of coal petrology and is termed "coalification jump". This is said to occur at the boundary between high volatile and medium volatile bituminous coals (Stach and Michels, 1955) and is reported as the point at which the release of methane becomes more important and the losses of oxygen-rich compounds and water become less important than in earlier reactions of coalification. The plots of rank parameters presented here support this coalification break. Carbon and oxygen do not vary as strongly with rank in high-rank coals as they do in lower levels of rank. Hydrogen and volatile matter are seen to decrease strongly for high levels of bituminous rank. The variation in calorific value with rank declines at medium volatile bituminous rank and actually decreases in anthracites in association with loss of hydrogen and volatile matter. The medium and low volatile bituminous coals were grouped by the cluster analysis as a separate population of coal samples.

For the data of this study, there appear to be at least two other stages of "breaks", or positions in the coalification process where several parameters exhibit simultaneous changes in slope. The first "break" occurs at approximately the boundary between high volatile B and C bituminous rank. Up until this stage, the moisture content decreases strongly with coalification (Figure 24), and hydrogen content is enriched (Figure 27). A change in the slope at this point also is found in the curves of carbon (Figure 16), oxygen (Figure 19) and calorific value (Figure 22). The values of all three variables are strongly altered by processes of coalification in levels of rank below this break, and are less strongly altered in higher levels of rank. This break is thought to control the clustering of Group I. The factor analysis of Group I indicates that moisture and oxygen are strongly decreasing with rank, and calorific value, carbon, and hydrogen are strongly increasing. The mean carbon content of Group I is 78 percent (about subbituminous A rank), and only six of the 29 coals analyzed are higher than high volatile C bituminous rank.

The second "break" occurs roughly at the middle stage of high volatile A bituminous rank. At this break, the slopes of moisture (Figure 25), and hydrogen (Figure 27) through rank are altered. In the stages of rank intermediate between the first and second breaks, moisture is seen to decrease although at a smaller rate than for the lowest levels of rank. After the second coalification break, the moisture content becomes somewhat stabilized, suggesting that porosity in coal has reached a minimum. At the second break,

volatile matter begins to decrease with increase in rank. Between the first and second breaks, the hydrogen curve through rank has stopped increasing and is beginning to decrease in response to coalification. This range of rank is where hydrogen ceases to be enriched and begins to be decreased through coalification. At levels of rank above the second break, the hydrogen content decreases significantly with rank. A slight change in slope of the linear relation between carbon and oxygen may also be observed at this second break. This is probably due to the loss of hydrogen from the chemical structure, as well as the loss of oxygen. Therefore, the carbon content is enriched due to loss of both hydrogen- and oxygen-rich groups, and the correlation between carbon and oxygen is altered slightly.

The break at the middle stage of high volatile A bituminous rank may be contributing to the discrimination between Group II and Group III coals. The mean carbon content of Group III is 85 percent, which is in the medium levels of high volatile A bituminous rank. The mean carbon content of Group II is 83 percent, which is at about the high volatile B/A bituminous boundary. Therefore, Group II is midway between Group I and Group III in rank, and contains coals mainly in the rank range between the first and second breaks. The results of factor analyses for all groups support these ideas about the basis of splitting the groups.

The discriminant equations for the clustering of coals lower in rank than medium volatile bituminous make it clear that the organic sulfur content is significant in separating Group II from

Groups I and III. The strong influence of sulfur in discriminating this group is probably the result of the level of rank of Interior province coals. Most of the coals of Group II are from the Interior province. Many coals of this province were deposited under marine-influenced conditions. As a result, the total sulfur and often the organic sulfur contents are high. The fact that coals of Group I and III have lower sulfur contents is a result of many western coals (low rank) and Eastern province coals (high rank) being deposited under conditions which are generally less marine-influenced than were Interior province coals (medium rank).

IX. ANALYSIS OF COALS FROM INDIVIDUAL COAL PROVINCES

A. Eastern province coals

1. Geologic setting

The Eastern province is a major area of coal-bearing rocks that includes three regions: the Appalachian region, the Anthracite region, and the Atlantic Coast region. Only the Appalachian and Anthracite regions are involved in this study. They are located in the plateau and ridge and valley physiographic provinces of the Appalachian Mountains. Summaries of the environments of deposition, geology, and occurrences of coal-bearing strata of the province are given by Stearns and Mitchum (1962), Arndt and Averitt (1968), Branson (1962a), Wanless and others (1969), Arkle (1974), Donaldson (1974), and Ferm (1974).

The coal-bearing rocks were deposited in an area which at times extended as far west as the Western region of the Interior province (eastern parts of Kansas, Nebraska, and Oklahoma, and into central Texas) and at least as far east as the anthracite fields found in eastern Pennsylvania. The original basin of the Eastern province was asymmetrical with units thicker toward the east. The strata are commonly non-marine sandstones, conglomerates, shales, and coals derived from an eastern source. Marine-influenced coals are more common in the older coals and toward the southwest. Donaldson (1974) cites evidence that the major environments of deposition changed through time from primarily "extensive sea (Pottsville time) to relatively small bay (Allegheny-lower Conemaugh time) to entirely river-influenced low-salinity bay-lake (Conemaugh-Monogahele

time) to relatively small lakes of fluvial plain (Dunkard time)." Many coal units are laterally widespread while others can only be traced for a matter of miles. Cyclic repetition of strata, including coal units, is common in most of the province. These reported sequences are best developed in the western part of the province and are poorly developed nearest the source area. At the time of deposition, the western margin of the basin was farthest removed from the topographic highs contributing sediments, and sedimentation was slower. Close to the sedimentary source, the idealized cyclical development was interrupted by rapid and irregular influx of sedimentary material (Arndt and Averitt, 1968).

The coal-bearing units of the Eastern province are today preserved in structural basins resulting from post-depositional uplift and folding associated with the post-Pennsylvanian Alleghenian Orogeny. Rank usually increases with increases in the degree of deformation within this province. The anthracites occur in the intensely folded and faulted regions of northeast Pennsylvania. The dips of beds in the Appalachian region are greatest on the eastern edge of the basin. Common dips are 20° with local steepening; ranks are as high as medium and low volatile bituminous (Arndt and Averitt, 1968). The dips decrease toward the west; in the Allegheny plateau coal-bearing units are essentially flat lying. Coals in the western parts of the basin are high volatile bituminous.

The Appalachian region contains coals ranging from Early Mississippian to Early Permian in age. Coals of Early Mississippian age are generally anthracite or semianthracite, and are found in Virginia, West Virginia, and Alabama. The coal-bearing rocks of

Pennsylvanian age are divided into four stratigraphic units (Table 31). The lowest unit stratigraphically is the Pottsville Group which occurs throughout the region. The next unit is the Allegheny Group which occurs in western Pennsylvania, eastern Ohio, West Virginia, Maryland, and Kentucky. The next unit is the Conemaugh Group found in western Pennsylvania, Maryland, Ohio, and northern West Virginia. The last unit is the Monongahela Group of western Pennsylvania, Maryland, West Virginia, and Ohio. Lower Permian coals are found in the Dunkard Group in Pennsylvania, Ohio, West Virginia and Maryland.

The Anthracite region of eastern Pennsylvania contains two coal-bearing units of Early and Middle Pennsylvanian age (Arkle, 1974). The lowest unit stratigraphically is the Pottsville Group. Above the Pottsville Group is the Llewellyn Formation which may be correlative with the Allegheny and Conemaugh Groups of the Appalachian Bituminous region.

The 54 coal samples from the Appalachian region used in this study represent all four series of Pennsylvanian coal-bearing strata and are from the following states: Alabama (3 samples), Ohio (8 samples), Pennsylvania (24 samples), Tennessee (2 samples), Virginia (6 samples), and West Virginia (1 sample). The coals range in rank, based on ASTM rank classification, from high volatile C bituminous through low volatile bituminous. Forty of the 54 samples are of high volatile A bituminous rank. All of the low and medium volatile bituminous coals in this study are from the Appalachian region. The seven coals in this study with a rank of semianthracite or higher are from the Anthracite region of the Eastern province. These coals are not included in the statistical computations because the properties

Table 31. Classification of Pennsylvanian rocks in the Appalachian Basin, the Eastern Interior Basin (Indiana, Western Kentucky and Illinois) and the Western Interior Basin

APPALACHIAN	INDIANA		WESTERN KENTUCKY	ILLINOIS	MID-CONTINENT	
Waynesburg coal			HENSHAW	McLEANSBORO	French Creek sh.	VIRGINIA
MONONGAHELA					WABAUNSEE	
Pittsburgh coal					Tooeke ls. SHAWNEE Oread ls.	
CONEMAUGH			Dixon ss.		DOUGLAS Stranger ss.	
	LISMAN	PEDEE	Stanton ls. LANSDOWN Plattsburg ls.		MISSOURI	
		WABASH	KANSAS Hertha ls.			
		Inglefield ss.	PLEASANTON			
		DITNEY	Holdenville sh.			
WEST FRANKLIN		MARMATON				
Upper Freeport coal	SHELBURN Coal VII	Anvil Rock ss.	Anvil Rock ss.		DES MOINES	
ALLEGHENY	DUGGER Coal VI	CARBONDALE	CARBONDALE			
	PETERSBURG Coal V	Sebree ss.	Isabel ss.			
	LINTON Coal III	TRADEWATER	TRADEWATER			Blackjack Creek ls.
	STAUNTON Minshall ls.			CABANISS		
Brookville coal	BRAZIL	POTTSVILLE	POTTSVILLE	Seville ls. KREBS Riverton member		
KANAWHA	Lower Black coal			Upper cgl.	Grindstaff ss.	ATOKA
	MANSFIELD	POTTSVILLE	CASEYVILLE	CASEYVILLE	Hale ss. MORROW	
					Hindustan	SPRINGER
Squire Jim coal						

(from Wanless, 1962, p. 2)

of anthracites are different from lower rank coals and because the sample size of anthracites is small. They have been included in some plots to illustrate trends of variables at high levels of rank.

2. Univariate analyses

Summary statistics of the variables of coals from the Eastern province are given in Table 32. The coal samples from this province range in rank from high volatile C through low volatile bituminous. Samples from the Eastern province are primarily in the upper ranks of bituminous coals, with only four samples lower in rank than high volatile A bituminous. Therefore, the frequency distributions of rank-dependent variables reflect the sampling of high-rank bituminous coals and the absence of low-rank coals. The samples were separated by the cluster analysis into three of the four coal groups; only Group I (lowest rank coals) does not include Eastern province coals.

Frequency distributions of variables of Eastern province coals are given in Figure 33. The scale of the distributions is the same scale used for plotting the frequency distributions of all 109 samples of this study. Therefore, the relative value of variables from the Eastern province may be compared to the variable distributions of the samples representative of the entire country. This practice will be followed for discussions of other provinces.

The distributions of carbon, oxygen, and calorific value are normally distributed. Moisture is lognormally distributed, with all values lower than ten percent. Sulfur is skewed toward the high values, with the most frequent value around 0.65 to 0.75 percent. The frequency distribution of nitrogen shows no evidence against a normal distribution.

Table 32. Summary statistics for variables of Eastern province coals

	Low	High	Mean	St. Dev.	Skewness	Kurtosis [†]	χ^2 ^{††}	Transfor- mation	Skewness	Kurtosis [†]	χ^2 ^{††}
Reflectance	0.47	1.80	0.96	0.30	1.188**	3.875*	33.0**	log x	0.512	3.103	20.3
Carbon	79.56	91.56	86.03	2.66	0.149	2.787	23.4*				
Hydrogen	4.59	6.61	5.42	0.40	-0.474	4.306**	33.5**				
Oxygen	1.61	11.52	5.88	2.16	0.006	2.661*	9.9	log x	0.658*	3.856*	37.1**
Sulfur	0.10	2.77	0.97	0.52	0.464*	5.421**	44.6**				
Nitrogen	0.85	2.55	1.68	0.33	0.136	3.606*	11.0				
Volatile matter	18.10	48.01	35.54	7.81	-0.972**	3.074	28.7*	log x	0.063	1.862**	17.7
Moisture	0.70	9.21	3.18	2.10	0.992**	2.967	28.6*				
Btu/lb	14460	16113	15395	355	-0.201	2.552*	13.5				
Vitrinites	46.2	92.5	75.1	9.9	-0.744*	3.302	15.7	$\log \frac{x}{1-x}$	-0.010	3.050	19.6
Inertinites	7.4	36.1	17.7	7.5	0.929**	3.250	18.6	log x	0.081	2.432*	12.0
Liptinites	0.0	33.6	7.2	6.6	1.584**	6.335**	34.5**	$\sqrt{x}$	0.043	2.840	18.1

*Significant at the 5 percent probability level (54 samples)

**Significant at the 1 percent probability level

†Kurtosis tested at sample size 200

††d.f. = 12

Figure 33. FREQUENCY DISTRIBUTIONS FOR VARIABLES OF COALS FROM THE EASTERN PROVINCE

Figure 33 (continued). FREQUENCY DISTRIBUTIONS FOR VARIABLES OF COALS FROM THE EASTERN PROVINCE

Figure 33 (continued). FREQUENCY DISTRIBUTIONS FOR VARIABLES OF COALS FROM THE EASTERN PROVINCE

Figure 33 (continued). FREQUENCY DISTRIBUTIONS FOR VARIABLES OF COALS FROM THE EASTERN PROVINCE

Figure 33 (continued). FREQUENCY DISTRIBUTIONS FOR VARIABLES OF COALS FROM THE EASTERN PROVINCE

Figure 33 (continued). FREQUENCY DISTRIBUTIONS FOR VARIABLES OF COALS FROM THE EASTERN PROVINCE

Hydrogen and reflectance both have skewed frequency distributions. The distribution of hydrogen is skewed toward the lower values but the normality of the distribution is not improved by transformation. Reflectance is skewed toward high values and is lognormally distributed. Both reflectance and hydrogen are highly sensitive to rank changes in the upper levels of rank represented in this group of coals, resulting in the skewed distributions. The frequency distribution of volatile matter is highly skewed toward low values. Actually, the distribution is at least bimodal. As discussed, volatile matter is not responsive to rank changes until the upper levels of bituminous rank when it becomes extremely sensitive to rank changes.

The frequency distributions of all the groups of macerals are significantly skewed. The distribution of vitrinite is skewed toward the low values with a mean of approximately 75 percent. The distribution of inertinite-group macerals is skewed toward the high values with a mean of approximately 18 percent. The distribution of liptinite-group macerals is "J" shaped because many coals have liptinite values less than one percent. This results from an inability to distinguish petrographically the liptinite-group macerals from the vitrinite-group macerals in low volatile and many medium volatile coals. The distribution is normalized by taking the square root of the original values.

3. Factor analysis

The correlation matrix for variables of Eastern province coals is given in Table 33 and is used as input for the components analysis.

Table 33. Correlation matrix for variables of Eastern province coals

	Reflectance (log x)	Carbon	Hydrogen	Oxygen	Sulfur (log x)	Nitrogen	Volatile Matter	Moisture (log x)	Btu/lb	Vitrinites (log x/1-x)	Inertinites (log x)
Carbon	0.908**										
Hydrogen	-0.815**	-0.748**									
Oxygen	-0.837**	-0.948**	0.634**								
Sulfur (log x)	-0.394**	-0.445**	0.348*	0.214							
Nitrogen	-0.289*	-0.234	0.212	0.046	0.216						
Volatile Matter	-0.953**	-0.883**	0.913**	0.797**	0.387**	0.256					
Moisture (log x)	-0.696**	-0.586**	0.392**	0.557**	0.285*	0.216	-0.521**				
Btu/lb	0.766**	0.894**	-0.465**	-0.926**	-0.225	-0.195	-0.682**	-0.603**			
Vitrinites (log x/1-x)	0.190	0.230	-0.292	-0.211	0.047	-0.184	-0.257	0.130	0.105		
Inertinites (log x)	0.097	0.004	-0.130	-0.016	-0.013	0.207	-0.090	-0.260	0.015	-0.762	
Liptinites	-0.574**	-0.514**	0.745**	0.483**	0.007	0.126	0.678**	0.178	-0.307	-0.598	-0.012

*Significant at the 5 percent probability level (d.f. = 52; $r = 0.273$)

**Significant at the 1 percent probability level ($r = 0.351$)

Six components were extracted to account for at least 85 percent of the variance of each variable. The six components account for 99 percent of the variance of the data. However, four components account for 87 percent of the total variance and are interpreted as the most significant, linearly independent components affecting variation in the data set.

The rotated matrix is given in Table 34 and is used to interpret the components analysis. Six factors were rotated to raise the communalities of all variables to greater than 85 percent.

Two components of the rotated matrix contain rank parameters. Carbon, oxygen, and calorific value load heavily on the first component; these variables are measures of the process of carbonization. Hydrogen and the percent of observable liptinite load heavily on the fourth component and these are affected by the process of demethanation associated with high levels of coalification. Reflectance and volatile matter are about equally split between the two components.

The second component contains inertinite and vitrinite in an inverse relation and is a measure of maceral composition.

The third component contains nitrogen.

The last two components are not considered significant sources of information based on their eigenvalues (less than one). The fifth contains sulfur. The sixth component contains moisture. For early stages of high volatile coals, moisture decreases with rank as the porosity decreases. However, for higher stages of high volatile coals and for low and medium volatile coals, the moisture content is fairly constant. Since accurate measurements of moisture are

Table 34. Rotated matrix of factor loadings from the
R-mode factor analysis of Eastern province coals

	C ₁	C ₂	C ₃	C ₄	C ₅	C ₆	Communalities (h_i^2)
Btu/lb	-0.958						0.966
Oxygen	0.929						0.985
Carbon	-0.861						0.988
Reflectance (log x)	-0.695			0.529			0.951
Volatile Matter	0.632			-0.676			0.953
Inertinites (log x)		0.956					0.968
Vitrinites (log x/1-x)		-0.888					0.983
Nitrogen			-0.975				0.997
Liptinites ($\sqrt{x}$)				-0.916			0.936
Hydrogen				-0.826			0.927
Sulfur (log x)					0.963		0.976
Moisture (log x)						-0.850	0.997
Sum λ_i^2	3.848	1.798	1.063	2.740	1.221	0.957	
% Variation Explained	32.07	14.98	8.86	22.83	10.17	7.98	
Cumulative %	32.07	47.05	55.91	78.74	88.91	98.89	

seldom obtained because of variations in the conditions of humidity, and since moisture is such a small portion of high rank coals, it contributes little information about coals in this data set.

4. Interpretation of coalification processes important for Eastern province coals

The components containing rank parameters indicate that at least two and perhaps three processes are involved in coalification for the range of rank represented in Eastern province coals. One may be thought of as the process of carbonization, or the loss of oxygen, which accounts for coalification within the lower levels of bituminous rank. The second is loss of hydrogen in the higher levels of bituminous rank. The fact that reflectance and volatile matter load on two components indicates that they are affected by both of the major factors of chemical coalification. Reflectance and volatile matter have been described as functions of the molecular arrangement of coal and this in turn is affected by both the loss of oxygen-rich compounds (and increase in carbon) and by the loss of methane.

B. Interior province coals

1. Geologic setting

The Interior province is a major coal-bearing area in the stable interior region of the United States. The coal-bearing units are primarily of Pennsylvanian age and are approximately time-correlative with the Eastern province units (see Table 31). The province is divided into four regions. Two minor regions are the Southwestern region, located in north central Texas, and the Northern region, located in Michigan within the Michigan basin.

These regions are not represented in this study. The Eastern region is located in Illinois, Indiana, and western Kentucky with small outliers in Missouri and Iowa. The Western region is located in Iowa, Missouri, Oklahoma, the eastern parts of Kansas and Nebraska, and in western Arkansas. Summaries of the geology and occurrence of coal-bearing units of the last two regions are given in Wanless (1955, 1962), Wanless and others (1969), Branson (1962), Bristol and Howard (1971), and Clegg (1972).

Coal-bearing units in the Eastern and Western regions are generally flat-lying strata characteristic of a gently downwarped area. Broad arches and basins are common due to epeirogenic movement. The Arkoma basin in Oklahoma and Arkansas is the only area which was rapidly subsiding in the otherwise stable Interior province. Coals are primarily high volatile bituminous in rank with some medium volatile bituminous coals. The Arkoma basin also contains coals of medium and low volatile bituminous rank.

The coal units are usually members of cyclical sedimentary deposits consisting of alternations of coal, marine limestone, shale, sandstone, and underclay. The cyclic sedimentation is better developed in the Eastern region than in the Western region. In both regions, the older coals are discontinuous and are of variable thickness due to pre-depositional topography. The younger coals are usually very persistent laterally. Individual seams are usually 10 to 12 feet in thickness, although some are less than one foot thick.

This study includes 25 coals from the Interior province. All are Pennsylvanian in age. The Western region is represented by eight

coals from the Des Moines Series of Middle Pennsylvanian age. They are from the following states: Missouri (5 samples), Iowa (2 samples), and Kansas (2 samples). The Eastern region is represented by 17 samples. The five samples from Indiana are from the Pottsville Group (2 samples) and the Allegheny Group (3 samples). The remaining samples are all approximately Alleghenian in age and are from Illinois (8 samples) and Kentucky (4 samples). The coals are all high volatile bituminous in rank and include 6 high volatile C, 12 high volatile B and 7 high volatile A bituminous coals.

2. Univariate analyses

Summary statistics of the untransformed and transformed data on the Interior province coals are given in Table 35 and the frequency distributions are in Figure 34. The distributions of most variables show no evidence against being normally distributed. This data set does not contain samples of either very high or very low levels of rank, so rank parameters are not highly skewed. Most of the Interior province coals were assigned to Group II (medium rank) by the cluster analysis. Moisture is slightly skewed toward the low values and is lognormally distributed. Hydrogen and nitrogen are slightly skewed towards low values but transformations do not normalize the distributions. Vitrinite is skewed toward the low values with a mean of 80 percent. Exinite is skewed toward the high values due to two samples with greater than 20 percent exinite. Transformations normalized the distribution of vitrinite and improved the normality of the liptinite distribution.

3. Factor analysis

The correlation matrix of variables of Interior province

Table 35. Summary statistics for variables of Interior province coals

	Low	High	Mean	St. Dev.	Skewness	Kurtosis [†]	χ^2_{++}	Transfor- mation	Skewness	Kurtosis [†]	χ^2_{++}
Reflectance	0.36	0.80	0.57	0.10	0.553	3.026	8.7				
Carbon	78.92	85.64	82.04	1.88	0.204	2.250**	11.6				
Hydrogen	4.26	6.12	5.48	0.36	-1.050*	6.408**	12.4				
Oxygen	5.17	11.27	8.87	1.70	-0.377	2.503	12.8				
Sulfur	0.42	4.01	2.02	0.86	0.354	3.276	11.2				
Nitrogen	0.19	2.48	1.60	0.53	-0.874*	3.890*	6.4				
Volatile matter	37.12	48.25	43.13	2.88	0.008	2.774*	9.5				
Moisture	2.69	19.61	8.59	3.96	0.749*	3.599*	11.1	log x	-0.426	2.708	11.5
Btu/lb	14241	15539	14778	339	0.701	2.907	13.4				
Vitrinites	61.7	92.1	80.4	8.2	-0.975*	3.009	14.5	$\log \frac{x}{1-x}$	-0.456	2.611	8.3
Inertinites	5.1	26.9	14.5	5.7	0.570	2.916	8.2				
Liptinites	1.4	23.0	5.1	5.5	2.669**	8.894**	59.0**	log x	1.340**	4.662**	13.5

*Significant at the 5 percent probability level (25 samples)

**Significant at the 1 percent probability level

†Kurtosis tested at sample size 200

††d.f. = 10

Figure 34. FREQUENCY DISTRIBUTIONS FOR VARIABLES OF COALS FROM THE INTERIOR PROVINCE

Figure 34 (continued). FREQUENCY DISTRIBUTIONS FOR VARIABLES OF COALS FROM THE INTERIOR PROVINCE

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Figure 34 (continued). FREQUENCY DISTRIBUTIONS FOR VARIABLES OF COALS FROM THE INTERIOR PROVINCE

Table 36. Correlation matrix for variables of Interior province coals

	Reflectance	Carbon	Hydrogen	Oxygen	Sulfur	Nitrogen	Volatile Matter	Moisture (log x)	Btu/lb	Vitrinites (log x/1-x)	Inertinites
Carbon	0.178										
Hydrogen	-0.018	-0.288									
Oxygen	0.024	-0.862**	0.203								
Sulfur	-0.310	-0.348	-0.240	-0.028							
Nitrogen	-0.189	-0.022	0.078	-0.234	-0.141						
Volatile Matter	-0.508**	-0.097	0.476*	-0.224	0.235	0.548					
Moisture (log x)	-0.600**	-0.441*	0.027	0.402*	0.028	0.213	0.064				
Btu/lb	0.287	0.819**	0.084	-0.735**	-0.351	-0.012	0.152	-0.639**			
Vitrinites (log x/1-x)	-0.170	-0.053	0.185	-0.147	0.187	0.226	0.177	0.197	-0.178		
Inertinites	-0.052	0.121	-0.085	-0.135	-0.004	0.068	0.198	-0.270	0.294	-0.795**	
Liptinites (log x)	0.318	-0.200	-0.032	0.479*	-0.221	-0.440*	-0.336	0.005	-0.079	-0.595**	0.048

*Significant at the 5 percent probability level (d.f. = 23; $r = 0.396$)

**Significant at the 1 percent probability level ($r = 0.505$)

coals is given in Table 36 and is used as input into the factor analysis. In the original matrix of factor analysis, eight components were extracted and they account for 98 percent of the data variance. However, the first five components account for 86 percent of the variance, and these are considered to be the most significant sources of information in the data matrix.

The rotated matrix is given in Table 37. The matrix was rotated on eight factors to raise the communalities of each variable to greater than 85 percent.

The first component contains carbon, oxygen, and calorific value which are measures of the process of carbonization.

The second component contains volatile matter. The loading of reflectance on this component is slight ($r=0.574$). There is an inverse relationship between reflectance and volatile matter. Reflectance is split between this component and the fifth component.

The third component contains inertinite and vitrinite and accounts for the maceral compositions of the coals.

The fourth component contains hydrogen. The content of this variable is neither increased nor decreased significantly or predictably by coalification in the range of rank represented by the Interior province samples. This is the rank range where hydrogen ceases to be enriched due to coalification and begins to decrease with further coalification.

The fifth component contains moisture and reflectance. During coalification, moisture is significantly decreased in the low levels of bituminous coals of this data set.

The last three components were extracted to raise the communalities to greater than 90 percent for each variable. The components contain

Table 37. Rotated matrix of factor loadings from the
R-mode factor analysis of Interior province coals

	C ₁	C ₂	C ₃	C ₄	C ₅	C ₆	C ₇	C ₈	Communalities (h_i^2)
Carbon	0.933								0.992
Oxygen	-0.928								0.990
Btu/lb	0.850								0.954
Volatile Matter		-0.799							0.963
Inertinites			0.974						0.993
Vitrinites (log x/1-x)			-0.875						0.991
Hydrogen				-0.949					0.988
Moisture (log x)					-0.855				0.977
Reflectance		0.574			0.737				0.991
Nitrogen						0.952			0.991
Liptinites (log x)							0.900		0.994
Sulfur								-0.940	0.997
Sum λ_i^2	2.717	1.111	1.820	1.200	1.499	1.121	1.183	1.140	
% Variation Explained	22.64	9.26	15.17	10.00	12.49	9.34	9.86	9.50	
Cumulative %	22.64	31.90	47.07	57.07	69.56	78.90	88.76	98.26	

nitrogen, exinite, and organic sulfur, respectively. However, they are not considered significant, linearly independent sources of information for explaining the total data variance. It is interesting to note, however, that sulfur for the Interior province coals of this study ranges from 0.42 to 4.01 percent with a mean of 2.02 percent. This is higher than for the Eastern province coals which range from 0.10 to 2.77 percent sulfur with a mean of 0.97 percent. The high sulfur content is a result of the strong marine influence for the Interior province coals.

4. Discussion of principal components

The carbonization factor, found to be highly significant for all but for the highest rank group of coals, is a major factor of coalification of the Interior province samples.

Volatile matter and reflectance are inversely related. Volatile matter has the strongest loading on component two ($r=-0.799$). Reflectance is split between this factor and component five. This indicates that reflectance is varying with volatile matter and also with some factor that does not affect volatile matter.

In the factor analysis, the strong loading of reflectance and moisture on a component, and the fact that reflectance does not load on the rank component, is unique to Interior province coals. Based on ASTM rank classification (calorific value for low rank coals), the coals of this data set range in rank from high volatile C through high volatile A bituminous. Carbon content ranges from 79 to 86 percent with a mean of 82 percent, and this range is consistent with the ASTM classification. However, reflectance varies from 0.36 to 0.80 with a mean of 0.57 percent. The coals would be roughly

classified (by reflectance criteria) as subbituminous (C?) through high volatile A bituminous with a mean rank of high volatile C bituminous. This "under-classification" of Interior province coals is observed in the plot of carbon and reflectance (Figure 16).

One possible explanation for the above correlation between moisture and reflectance, and the poor correlation between reflectance and other rank parameters in this province, may be related to the porosity of the Interior province coals. A study was conducted by Gan and others (1972) on the porosity of American coals. In their study, the four coals of the Interior province had open porosities ranging from 11.9 to 23.2 percent. The porosity of the coals from the Eastern province ranged from 4.1 to 9.5 percent. Only ten coals were included in the study and they ranged from lignites to anthracites. Even so, these results suggest that Interior province coals are more porous than those from the Eastern province. The list of coals, their rank, and percent open porosity are given in Table 38.

The plot of carbon versus moisture (Figure 24) indicates that the moisture content of many Interior province coals is greater than expected for a given carbon content. Harrison (1965) studied the relationship between moisture and reflectance of coals. He found that an increase in moisture of a coal results in a decrease in the reflectance of the coal. It is a common practice to keep coal samples in a dessicator before measuring their reflectance. If Interior province coals have unusually high porosities, and as a result have high moisture contents, the reflectance would be affected; this

Table 38. Porosity data for American coals
(from Gan, Nandi and Walker, 1972)

	Province	Rank	% Carbon, daf	Total open pore vol. cc/g	% Open porosity
PSOC-089	Northern Great Plains	lig	63.3	0.073	9.6
PSOC-190	Interior	hvCB	75.8	0.232	23.2
PSOC-197	Eastern	hvCB	76.5	0.105	11.9
PSOC-026	Interior	hvCb	77.3	0.158	16.7
RAND sample	Interior	hvCb	79.9	0.083	9.5
PSOC-105A	Interior	hvCb	81.3	0.144	15.5
PSOC-004	Eastern	hvAb	83.8	0.033	4.1
PSOC-135	Eastern	myb	88.4	0.042	5.3
PSOC-127	Eastern	lvb	89.6	0.052	6.5
PSOC-080	Eastern	anth	90.8	0.076	10.4

reflectance would tend to indicate a lower rank level than the coal has actually achieved.

Another explanation for the lowered reflectance values of many Interior province coals may be associated with the chemical structure of the coals. In a study by Abdel-Baset and others (1977), the hydroxyl content of Interior province coals was found to be higher than for coals of the same rank from the Eastern and Rocky Mountain provinces. This was interpreted by the authors to be convincing evidence of differences in structural characteristics which result from differences in origin and history of coalification. The amount of light that is reflected from the surface of a piece of vitrinite is associated with the chemical structure of the vitrinite. Therefore, structural differences could affect the reflectance of coal.

A third possible explanation for the seemingly unpredictable behavior of reflectance with rank may involve the conditions of the original depositional environment. Teichmüller (1974) has proposed a model for marine-influenced coals and it is briefly presented here. In this model, marine-influenced coals often have a decreased reflectance. According to the model, marine-influenced coals, as compared to non-marine coals of the same section, are relatively rich in hydrogen and sulfur, and the vitrinite precursors are abundant in hydrogen-rich, aliphatic edge groups. By process of bituminization discussed in Section VII A3, these hydrogen-rich edge groups of the vitrinite precursors are converted to mobile petroleum-like substances which are adsorbed onto the vitrinite structures. This should result in perhydrous vitrinite with a

decreased reflectance and a dull reddish fluorescence when observed under blue-light excitation. Also, in Teichmüller's model, the moisture content is usually relatively low since the internal pore system is partially or totally filled by the bitumen. According to Teichmüller these bitumen-rich coals have special coking properties. During coking, they soften at lower temperatures and exhibit higher fluidities than would be expected for their level of geochemical coalification.

The above hypothesis of marine-influenced coals in some ways is consistent with observed properties of coals from the Interior province. Many of these coals were deposited in marine-influenced environments. The average amount of organic sulfur is greater in the Interior province coals than for those of other coal provinces (see Table 4); this is consistent with the strong marine influence in the depositional environment. As reported above, reflectance often indicates lower levels of rank than those based on ASTM rank classification. This may be due to the bitumen adsorbed onto the vitrinite structure. This idea is supported by the fact that the vitrinite of many Interior province coals has been observed to exhibit dull reddish brown fluorescence when excited with blue light. Teichmüller suggests that the reflectivity of vitrinite of a given seam generally decreases with decreasing amounts of oxidation during the early peat-forming stage. Anaerobic environments are said to produce the hydrogen-rich vitrinite. In slightly more aerobic environments, where oxygen is available but still restricted, the humic acids produced are said to be relatively deficient in hydrogen and enriched in oxygen. These, according to

Teichmüller's hypothesis, would lead to subhydrous vitrinite which is lacking in adsorbed bitumens and thus would have higher reflectances than the perhydrous vitrinite. Therefore, pseudovitrinite, which is more strongly reflecting than normal vitrinite, may have formed in slightly more oxidizing conditions than the normal vitrinite. Koch (1970) proposes that pseudovitrinite originates from different parent material than normal vitrinite and is not related to varying oxidizing conditions. However, the fact that pseudovitrinite has not been observed to fluoresce under blue light excitation, even in coals where some vitrinite is strongly fluorescent, tends to support the idea of varying reflectance/fluorescence properties based on the amount of oxygen available in the original environment.

In some ways, however, the interrelations of variables of the Interior province are not consistent with the model of marine-influenced environments. Teichmüller (1974) makes a strong point that, together with sulfur and hydrogen, the nitrogen content is greater in coals deposited in marine-influenced environments of deposition. On the original factor matrix, however, sulfur has inverse loadings with both hydrogen (component 4) and nitrogen (component 5), suggesting that as sulfur increases, both hydrogen and nitrogen decrease. However, the correlation coefficients for sulfur versus nitrogen and for sulfur versus hydrogen are not significant for $\alpha=0.05$. It does not appear that hydrogen and nitrogen are increasing significantly with sulfur as would be expected from Teichmüller's model of marine-influenced coals. Also, the variation of moisture is not as expected. Interior province coals

have high moisture instead of low moisture contents for their level of rank.

In Teichmüller's model, a very interesting effect of marine-influence on coals has to do with the coking properties of coals. Because the vitrinite has large amounts of adsorbed bitumen, the coals are said to have lower softening temperatures and higher fluidities than would be expected at a given rank level. Walter and others (1963) have compiled data on the plastic, agglutinating and swelling properties of American coals. Their reported values of plasticity for Illinois and Pennsylvania coals of similar carbon content do not support the idea of increased fluidity in the Interior province. In fact, they seem to indicate that fluidities are lower for Illinois coals than for Pennsylvania coals. However, plasticity data are given for only four Illinois coals, and therefore the interpretation is indeed tenuous.

It has long been recognized that coals of the Interior province behave differently in the coking process than expected from empirical methods of predicting coke strength. These methods were first developed for use with American coals by U.S. Steel (Schapiro, Gray, and Eusner, 1961). The data used by U.S. Steel in developing the empirical method are from low sulfur (and therefore non-marine) coals from the Eastern province. The method uses reflectance as a measure of rank. According to Teichmüller's model, the reflectance of the vitrinite may be a function of, among other things, the environment of deposition. In marine-influenced coals the reflectance is lower than that of non-marine-influenced coals of the

same rank. If this is true, the same predictive formula developed for Eastern province coals may not apply directly to the coals of the Interior province.

The factor analyses of Eastern and Interior province coals support the idea that reflectance varies differently in coals from the two provinces. For Eastern province coals, reflectance varies with carbon through rank. For Interior province coals carbon and reflectance do not vary together. In both provinces, reflectance varies with moisture and volatile matter. Three possible explanations are presented above to explain these differences. These are based on porosity, on chemical structure of the vitrinite, and on the environment of deposition. More research is required to determine the actual cause of the unusual variance of reflectance for Interior province coals.

C. Western Coals

1. Geologic setting

The coals discussed from the Interior and Eastern provinces are all Paleozoic (Pennsylvanian) in age. The remainder of the samples of this study are from the Northern Great Plains and the Rocky Mountain coal provinces. These samples are younger in age, ranging from Late Cretaceous to Paleocene. Because of the small total number of samples, the coals have been grouped together and are termed Western coals for the purpose of this study.

The Rocky Mountain province is a major coal-bearing area of Cretaceous, Paleocene, and Eocene sediments. The province is divided into eight major regions from the following areas:

1. Bighorn Basin region - northern Wyoming and southern Montana
2. Green River region - southwestern Wyoming and northwestern Colorado
3. Uinta region - western Colorado and eastern Utah
4. Wind River Basin region - central Wyoming
5. San Juan River region - southwestern Colorado, northwestern New Mexico, northwestern Utah
6. Hams Fork region - western Wyoming
7. Hanna Field - southeastern Wyoming
8. Southwestern Utah region - Utah

The Rocky Mountain province is represented in this study by 19 samples. Eighteen are Late Cretaceous in age, and one is Paleocene in age. The coals are from the following regions: Green River region (five samples), Uinta region (six samples), San Juan region (six samples), Hams Fork region (one sample), and Hanna Field region (one sample). Summaries of the geology of the coal-bearing rocks of the area or of the regions included in this study are given by Weimer (1960), Hale and van de Graff (1964), Landes (1957), Berryhill and others (1950), Schell (1964), and Read and others (1950).

The coal-bearing units of Cretaceous age were deposited in association with a large sea extending from the Gulf of Mexico to the Arctic Ocean (Weimer, 1969). The Cretaceous coal-bearing sediments of the Northern Great Plains also were deposited in environments related to this inland sea. The sedimentary units are much thicker in the western parts of the original depositional basin than in the eastern parts. The eastern part of the basin overlaps the western edge of the stable interior craton region. The sediments consist of inter-tonguing marine and non-marine units. The westernmost sediments are

primarily marine. The central area of the basin is characterized by a complex interfingering of the marine and non-marine units resulting from minor transgressions and regressions of the ancient strandline. The major trend of Late Cretaceous time was an eastward regression of the sea.

The coal-bearing units today are preserved in isolated intermontane structural basins resulting from the post-Cretaceous Laramide Orogeny. The isolated basins vary from broad, structurally simple downwarps to narrow, highly folded and faulted basins. Even the broad basins are locally complex due to igneous intrusions and faults and folds associated with the post-depositional deformation. Coal rank in the province tends to increase with the age of the coal and with the degree of deformation. Reported ranks vary from lignite through anthracite, with low-rank bituminous and subbituminous ranks most common. The anthracites are relatively rare and are the result of thermal alterations adjacent to igneous intrusions. Coals of this study range in rank from subbituminous through high volatile A bituminous. Individual seams range up to 100 feet in thickness. The seams are lenticular and are traceable laterally only a few miles to tens of miles.

The Northern Great Plains province is a major region of coal-bearing sediments preserved in North Dakota, South Dakota, Montana, Wyoming, Colorado, and New Mexico east of the Rocky Mountain Front. The coals are primarily Late Cretaceous to Eocene in age, with some Jurassic coals present. Of the eleven samples from this province, three are Cretaceous in age and are from the Raton Mountain and Denver regions. Descriptions of the geology of the regions

represented in this study are given by Landes (1957), Berryhill and others (1950), Matson (1969), Carter (1956), Read and others (1950), Weimer (1960), and Mapel (1958).

The coal-bearing units are primarily clastic sediments eroded from the nearby uplifts of the Laramide Orogeny or deposited in association with the Cretaceous and Tertiary inland sea environments. Both the Denver region and the Raton Mesa region are on the western margin of the Northern Great Plains province. They are asymmetrical north-trending structural basins with gentle dips on the east and steeply dipping to overturned beds on the west next to the Rocky Mountain Front. Their structures are locally complex due to folding, faulting and igneous intrusions. Sedimentary thicknesses are greatest on the west and rank increases regionally with increased depth of burial or locally with increased degree of deformation. In the Denver Basin region, Cretaceous coals are generally subbituminous to high volatile C, and Tertiary coals are generally lignite to subbituminous in rank. Cretaceous coal seams average around 2 to 11 feet in thickness and are more laterally extensive than are the Tertiary coal seams which are generally lenticular. In the Raton Mesa region, rank increases to the north and to the west and generally varies from high volatile C to high volatile B bituminous.

All the Paleocene coal samples of the Northern Great Plains in this study are from the Fort Union region and are from Wyoming, North Dakota, and Montana. Coal-bearing units are also in Upper Cretaceous and Eocene strata. The region is an asymmetrical syncline with gentle slopes (less than five degrees) on the east and steeper, more irregular dips on the west where the basin is upturned against

the Bighorn Mountains. Rank in the southwest and extreme western parts of the basin is subbituminous. Seams are 10 to 20 feet thick, lenticular, and have dips which are relatively steep. The rest of the region contains primarily lignites and subbituminous C coals with seams 20 to 40 feet in thickness, but ranging up to 200 feet thick. The seams are more persistent than in the western and southwestern parts of the basin.

2. Univariate analyses

Summary statistics of untransformed and transformed data of Western coals are given in Table 39. The coals range in rank from lignite through high volatile A bituminous. Most of the coals were classified with Group I by the cluster analysis but Groups II and III each contain two Western coals. Frequency distributions (Figure 35) of most variables are not significantly different from a normal distribution. Sulfur, volatile matter, moisture, and liptinite-group macerals all have distributions which are slightly skewed toward the high values; all are lognormally distributed.

3. Factor analysis

Table 40 is the correlation matrix of the variables for Western coals. This matrix is generated as input for components analysis. Six components were extracted in the original components analysis, and they account for at least 85 percent of the variance of each variable. The first four components account for approximately 90 percent of the total data variance and are considered the most significant, linearly independent sources of information in the data set. The rotated matrix is given in Table 41 and is used to interpret the principal components.

Table 39. Summary statistics for variables of Western coals

	Low	High	Mean	St. Dev.	Skewness	Kurtosis [†]	χ^2_{++}	Transfor- mation	Skewness	Kurtosis [†]	χ^2_{++}
Reflectance	0.30	0.84	0.52	0.12	0.130	3.196	9.8				
Carbon	71.52	83.83	77.89	3.15	-0.072	2.215**	12.7				
Hydrogen	4.76	6.15	5.53	0.40	-0.300	2.181**	9.8				
Oxygen	7.91	21.45	14.43	3.70	0.185	2.040**	14.9				
Sulfur	0.26	1.18	0.60	0.21	1.217**	4.505**	7.3	log x	0.168	3.380	6.3
Nitrogen	0.13	2.33	1.55	0.47	-1.251**	4.588**	11.2				
Volatile matter	39.47	53.61	44.26	3.17	0.730*	3.832*	12.4	log x	0.497	3.220	11.5
Moisture	1.63	38.04	14.51	10.19	1.003**	3.152	28.4**	log x	-0.401	2.698	34.5
Btu/lb	11902	15405	13725	870	-0.229	2.300**	10.3				
Vitrinites	67.2	90.6	81.1	6.0	-0.451	2.349**	10.3				
Inertinites	5.6	26.7	15.0	5.8	0.318	2.018**	18.1				
Liptinites	1.3	11.9	3.9	2.5	2.135**	7.288**	29.6**	log x	0.629	3.560	9.0

*Significant at the 5-percent probability level (30 samples)

**Significant at the 1 percent probability level

†Kurtosis tested at sample size of 200

††d.f. = 10

Figure 35. FREQUENCY DISTRIBUTIONS FOR VARIABLES OF COALS FROM THE WESTERN STATES

Figure 35 (continued). FREQUENCY DISTRIBUTIONS FOR VARIABLES OF COALS FROM THE WESTERN STATES

Figure 35 (continued). FREQUENCY DISTRIBUTIONS FOR VARIABLES OF COALS FROM THE WESTERN STATES

Figure 35 (continued). FREQUENCY DISTRIBUTIONS FOR VARIABLES OF COALS FROM THE WESTERN STATES

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Table 40. Correlation matrix for variables of Western coals

	Reflectance	Carbon	Hydrogen	Oxygen	Sulfur (log x)	Nitrogen	Volatile Matter (log x)	Moisture (log x)	Btu/lb	Vitrinites	Inertinites (log x)
Carbon	0.815**										
Hydrogen	0.506**	0.711**									
Oxygen	-0.821**	-0.992**	-0.757**								
Sulfur (log x)	-0.057	0.114	0.001	-0.122							
Nitrogen	0.644**	0.493**	0.345	-0.562**	-0.238						
Volatile Matter (log x)	-0.686**	-0.467**	-0.035	0.461*	0.282	-0.592**					
Moisture (log x)	-0.824**	-0.916**	-0.712**	0.914**	-0.061	-0.446*	0.405*				
Btu/lb	0.806**	0.969**	0.810**	-0.978**	0.112	0.513**	-0.406*	-0.929**			
Vitrinites	-0.045	-0.056	0.398*	-0.010	-0.279	0.210	0.176	-0.063	0.050		
Inertinites (log x)	0.092	0.052	-0.416*	0.010	0.231	-0.150	-0.284	0.054	-0.048	-0.910**	
Liptinites (log x)	-0.046	0.018	0.024	0.004	0.154	-0.218	0.284	-0.006	-0.006	-0.236	-0.164

*Significant at the 5 percent probability level (d.f. = 28; $r = 0.361$)

**Significant at the 1 percent probability level ($r = 0.463$)

Table 4i. Rotated matrix of factor loadings from the
R-mode factor analysis of Western coals

	C ₁	C ₂	C ₃	C ₄	C ₅	C ₆	Communalities (h_i^2)
Btu/lb	0.975						0.984
Carbon	0.955						0.966
Oxygen	-0.954						0.981
Moisture (log x)	-0.937						0.928
Hydrogen	0.845						0.931
Reflectance	0.757					-0.509	0.909
Inertinites (log x)		-0.966					0.993
Vitrinites		0.966					0.955
Sulfur (log x)			-0.963				0.997
Liptinites (log x)				0.988			0.998
Nitrogen					-0.854		0.995
Volatile Matter (log x)						0.792	0.940
Sum λ_i^2	5.181	2.112	1.034	1.112	0.997	1.182	
% Variation Explained	43.17	17.60	8.62	9.26	8.31	9.85	
Cumulative %	43.17	60.77	69.39	78.66	86.97	96.82	

The first component contains variables affected by rank. In the original matrix, this accounts for 48 percent of the total variance. The parameters affected by rank for this set of Western coals are calorific value, carbon, oxygen, moisture, hydrogen, and reflectance.

The second component contains vitrinite and inertinite in an inverse relation. This component accounts for most of the maceral composition of the coals and is independent of rank.

The third and fourth components contain sulfur and liptinite, respectively.

Components five and six are not considered significant sources of data variance. Component five contains nitrogen. Component six contains volatile matter, and reflectance has a slight loading.

4. Discussion of principal components

The results of this factor analysis are almost identical to that of Group I from the cluster analysis. This is expected since Group I contains most of the Western coals. Coalification results in enrichment in carbon and hydrogen due largely to loss of oxygen-rich compounds. Moisture is decreased, probably due to both decrease in porosity and loss of hydrophillic functional groups. Reflectance is increased; this may be due to loss of functional groups, increase in aromaticity, or both. It is concluded that the behavior of variables of Western coals are consistent with their degree of coalification.

X. CONCLUSIONS

On the basis of cluster analysis, it is concluded that the coals of this data set are from a continuous population insofar as the parameters measured are concerned.

Through the cluster analysis technique, the coals may for convenience be subdivided into groups of greatest similarity, although the groups are not strongly discriminated from one another. Four groups of similar coals were separated.

1. Group I includes the lowest rank coals of the data set (lignite to high volatile A bituminous). It is primarily composed of coals from the western U.S. and also includes coals from the Interior province. The strongest results of coalification are the increase in carbon, calorific value, and hydrogen, and the decrease of moisture. Reflectance increases, although not as strongly as do the other rank-dependent variables for this group.
2. Group II includes high volatile bituminous coals. The range of rank overlaps with the upper range of Group I coals, and the lower range of Group III coals. The group is primarily composed of Interior province coals (19 samples) and Eastern province coals (10 samples), and also includes 2 samples from the Rocky Mountain province. Group II is mainly discriminated by sulfur content. Some results of coalification are the increase in carbon and calorific value and the decrease in oxygen. Hydrogen

is no longer increasing with rank. Reflectance, moisture, and volatile matter are responding together, and their variance is independent of that of carbon, oxygen, and calorific value.

3. Group III includes high volatile A and B bituminous coals. It is primarily composed of Eastern province coals (30 samples) but also includes 1 sample from the Interior province and 2 samples from the Rocky Mountain province. This group is discriminated from Group II by sulfur content. The variables most strongly affected by coalification are carbon and calorific value which are increased, and oxygen which is decreased. Reflectance and moisture content are affected by rank, but not as strongly as are the other rank-dependent variables from Group II. Volatile matter varies slightly due to coalification.
4. The medium and low volatile bituminous coals are the most distinct group within the set of coals. All the samples in this group are from the Eastern province. Results of factor analysis suggest a major change in the results of coalification at the beginning of the medium volatile bituminous rank. The variables most strongly affected in this rank range are volatile matter which decreases, and reflectance which increases. Hydrogen losses are also associated with coalification. Calorific value, oxygen, and carbon no longer vary strongly with the coalification

factor as they did for lower rank coals. Also, the three parameters vary independently of one another.

The results of cluster analysis suggest that there are natural subgroups of U.S. coals, based on the variables included in this study. Because only 109 samples were included in the cluster analysis, it is premature to propose a new classification based on these results. However, because these are natural groupings, they may prove useful as a basis for subdividing U.S. coals for research into various types of coal utilization. When the Penn State/ERDA data base contains more coal samples and a wider range of variables, the cluster analysis technique should be used to verify the groupings found in the present study. At that time, it may be appropriate to propose a new classification of U.S. coals.

The sulfur and nitrogen contents of coals are each interpreted as providing independent sources of information. The content of each is thought to be determined in the early stages of deposition and diagenesis, and not to alter significantly due to the processes of coalification.

The Eastern province coals are the highest rank coals represented in this data set. The coals of the Rocky Mountain and Northern Great Plains provinces are the lowest rank coals of the data set. Variation of properties in all these provinces is thought to be consistent with their level of rank.

Variation among parameters of the Interior province coals is the most inconsistent with what is expected for their level of rank. They are unusually high in organic sulfur content. This is consistent

with the idea that Interior province coals were deposited in a marine-influenced environment. Also, the moisture content of these coals seems to be unusually high for their level of rank if carbon is used as a rank measure. Reflectance values are often lower than expected for their rank based on ASTM rank classification. This suggests that variances in their properties from those of other coals from the same rank may be due to a different depositional history and/or post-depositional history than other coals have experienced.

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APPENDIX I.

Location, ASTM rank, and seam information

APPENDIX I. Location, ASTM rank, and seam information

EASTERN PROVINCE

SAMPLE	REGION	STATE	RANK	AGE	SEAM
PSOC-001	APPALACHIAN	KY	HVA	PENNSYL.	UPPER ELKHORN #3
PSOC-005	APPALACHIAN	KY	HVA	PENNSYL.	UPPER ELKHORN #3
PSOC-011	APPALACHIAN	KY	HVA	PENNSYL.	KENTUCKY C
PSOC-102	APPALACHIAN	PA	HVA	PENNSYL.	PITTSBURGH
PSOC-113	APPALACHIAN	PA	LOW VCL	PENNSYL.	LOWER KITTANNING
PSOC-114	APPALACHIAN	PA	LOW VCI	PENNSYL.	UPPER KITTANNING
PSOC-116	APPALACHIAN	PA	LOW VOL	PENNSYL.	LOWER FREEPORT
PSOC-122	APPALACHIAN	WV	HVA	PENNSYL.	LOWER KITTANNING
PSOC-125	APPALACHIAN	PA	HVA	PENNSYL.	LOWER FREEPORT
PSOC-126	APPALACHIAN	PA	LOW VCL	PENNSYL.	LOWER KITTANNING
PSOC-134	APPALACHIAN	AL	MED VCL	PENNSYL.	PRATT
PSOC-265	APPALACHIAN	VA	HVA	PENNSYL.	JAWBONE
PSOC-267	APPALACHIAN	VA	HVA	PENNSYL.	CLINTWOOD
PSOC-268	APPALACHIAN	VA	HVA	PENNSYL.	LYCNS
PSOC-269	APPALACHIAN	VA	HVA	PENNSYL.	IMBODEN
PSOC-270	APPALACHIAN	AL	HVA	PENNSYL.	AMERICAN
PSOC-271	APPALACHIAN	AL	HVA	PENNSYL.	MARY LEE
PSOC-273	APPALACHIAN	OH	HVA	PENNSYL.	CHIO #6A
PSOC-276	APPALACHIAN	OH	HVA	PENNSYL.	CHIO #8
PSOC-277	APPALACHIAN	OH	HVA	PENNSYL.	OHIO #9
PSOC-278	APPALACHIAN	OH	HVA	PENNSYL.	OHIO #9
PSOC-299	APPALACHIAN	TN	HVA	PENNSYL.	SEWANEE
PSOC-300	APPALACHIAN	TN	HVA	PENNSYL.	PFE WEE
PSOC-301	APPALACHIAN	VA	HVA	PENNSYL.	SPLASHDAM
PSOC-302	APPALACHIAN	VA	HVA	PENNSYL.	LOWER FANNER
PSOC-305	APPALACHIAN	OH	HVE	PENNSYL.	OHIO #11
PSOC-306	APPALACHIAN	OH	HVA	PENNSYL.	OHIO #12
PSOC-307	APPALACHIAN	OH	HVA	PENNSYL.	OHIO #12A
PSOC-308	APPALACHIAN	OH	HVE	PENNSYL.	OHIO #5
PSOC-317	APPALACHIAN	PA	LOW VCL	PENNSYL.	LOWER FREEPORT
PSOC-319	APPALACHIAN	PA	LOW VCL	PENNSYL.	UPPER KITTANNING
PSOC-320	APPALACHIAN	PA	MED VOL	PENNSYL.	PITTSBURGH
PSOC-323	APPALACHIAN	PA	MED VCL	PENNSYL.	BRICKVILLE
PSOC-324	APPALACHIAN	PA	MED VOL	PENNSYL.	MIDDLE KITTANNING
PSOC-326	APPALACHIAN	PA	HVA	PENNSYL.	UPPER KITTANNING
PSOC-328	APPALACHIAN	PA	HVA	PENNSYL.	UPPER FREEPORT
PSOC-329	APPALACHIAN	PA	HVA	PENNSYL.	BROOKVILLE
PSOC-330	APPALACHIAN	PA	HVE	PENNSYL.	MIDDLE KITTANNING
PSOC-331	APPALACHIAN	PA	HVA	PENNSYL.	BRICKVILLE
PSOC-332	APPALACHIAN	PA	HVA	PENNSYL.	LOWER KITTANNING
PSOC-337	APPALACHIAN	PA	HVA	PENNSYL.	LOWER KITTANNING
PSOC-341	APPALACHIAN	PA	HVA	PENNSYL.	CLARION
PSOC-345	APPALACHIAN	PA	HVA	PENNSYL.	LOWER KITTANNING
PSOC-349	APPALACHIAN	PA	HVA	PENNSYL.	LOWER CLARION
PSOC-353	APPALACHIAN	PA	HVA	PENNSYL.	UPPER CLARION
PSOC-354	APPALACHIAN	PA	HVA	PENNSYL.	LOWER KITTANNING
PSOC-355	APPALACHIAN	PA	HVA	PENNSYL.	LOWER KITTANNING
PSOC-357	APPALACHIAN	KY	HVA	PENNSYL.	LOWER ELKHORN
PSOC-361	APPALACHIAN	KY	HVA	PENNSYL.	LOWER ELKHORN
PSOC-362	APPALACHIAN	KY	HVA	PENNSYL.	LOWER ELKHORN
PSOC-363	APPALACHIAN	KY	HVA	PENNSYL.	HAZARD #5A
PSOC-367	APPALACHIAN	KY	HVA	PENNSYL.	HAZARD #7
PSOC-371	APPALACHIAN	KY	HVA	PENNSYL.	IMBODEN
PSOC-375	APPALACHIAN	KY	HVA	PENNSYL.	HAZARD #9
PSOC-080	ANTHRACITE	PA	AN	PENNSYL.	BUCK MOUNTAIN
PSOC-083	ANTHRACITE	PA	SEMI-AN	PENNSYL.	PENNSYLVANIA #8 1/2
PSOC-084	ANTHRACITE	PA	SEMI-AN	PENNSYL.	PENNSYLVANIA #8
PSOC-085	ANTHRACITE	PA	AN	PENNSYL.	PENNSYLVANIA #8--LEADER
PSOC-379	ANTHRACITE	PA	SEMI-AN	PENNSYL.	P&M 'B'
PSOC-383	ANTHRACITE	PA	SEMI-AN	PENNSYL.	P&M 'A'
PSOC-384	ANTHRACITE	PA	SEMI-AN	PENNSYL.	P&M 'B'

APPENDIX I (continued). Location, ASTM rank, and seam information

INTERIOR PROVINCE

SAMPLE	REGION	STATE	RANK	AGE	SEAM
PSOC-022	EASTERN	IL		PENNSYL.	ILLINOIS #6
PSOC-024	EASTERN	IL	HVA	PENNSYL.	ILLINOIS #2
PSOC-026	EASTERN	IL	BVC	PENNSYL.	ILLINOIS #6
PSOC-105	EASTERN	IN	HVE	PENNSYL.	INDIANA #1 BLOCK
PSOC-107	EASTERN	IN	HVE	PENNSYL.	BRASIL BLOCK--TOP VEIN
PSOC-162	WESTERN	MO	HVE	PENNSYL.	UPPER RICH HILL
PSOC-163	WESTERN	MO	EVA	PENNSYL.	EASTER
PSOC-164	WESTERN	MO	HVE	PENNSYL.	TEPO
PSOC-165	EASTERN	KY	HVE	PENNSYL.	KENTUCKY #9
PSOC-166	EASTERN	KY	HVE	PENNSYL.	KENTUCKY #11
PSOC-243	WESTERN	IA	BVC	PENNSYL.	IOWA BOTTOM
PSOC-244	WESTERN	IA	BVC	PENNSYL.	LOWER CHEROKEE
PSOC-251	WESTERN	KS	BVA	PENNSYL.	MINEFAL
PSOC-252	EASTERN	IL	HVA	PENNSYL.	ILLINOIS #5
PSOC-272	EASTERN	KY	EVE	PENNSYL.	KENTUCKY #9
PSOC-273	EASTERN	KY	HVE	PENNSYL.	KENTUCKY #11
PSOC-279	EASTERN	IN	HVE	PENNSYL.	INDIANA #3
PSOC-280	EASTERN	IN	HVC	PENNSYL.	INDIANA #6
PSOC-281	EASTERN	IN	HVE	PENNSYL.	INDIANA #7
PSOC-283	EASTERN	IL	EVA	PENNSYL.	TOP DEKOVEN
PSOC-284	EASTERN	IL	HVA	PENNSYL.	LOWER DEKOVEN
PSOC-286	WESTERN	MO	HVE	PENNSYL.	TEFO
PSOC-287	WESTERN	MO	HVE	PENNSYL.	BEVIER
PSOC-290	EASTERN	IL	HVE	PENNSYL.	ILLINOIS #4
PSOC-356	EASTERN	IL	HVE	PENNSYL.	ILLINOIS #6

WESTERN

Northern Great Plains Province

PSOC-065	PORT UNION	WY	SUEFIT B	PALEO.	DEITZ
PSOC-086	PORT UNION	ND	LIGNITE	PALEO.	ZAP
PSOC-150	RATON MOUNTAIN	NM	HVA	CRET.	YANKEE
PSOC-230	PORT UNION	MT	SUEFIT B	PALEO.	ROSEBUD
PSOC-231	DENVER	CO	SUEFIT B	CRET.	LARAMIE #3
PSOC-241	PORT UNION	WY	SUEFIT B	PALEO.	MONARCH
PSOC-242	PORT UNION	WY	SUEFIT B	PALEO.	DEITZ
PSOC-245	PORT UNION	ND	LIGNITE	PALEO.	UPPER GASCOYNE
PSOC-246	PORT UNION	ND	LIGNITE	PALEO.	HAGEL
PSOC-247	PORT UNION	ND	LIGNITE	PALEO.	NOGNAN
PSOC-250	RATON MOUNTAIN	NM	HVA	CRET.	YORK CANYON

Rocky Mountain Province

PSOC-055A	SAN JUAN RIVER	NM	HVC	CRET.	NEW MEXICO #8
PSOC-056	SAN JUAN RIVER	AZ	HVC	CRET.	ARIZONA #2
PSOC-059	GREEN RIVER	CO	HVC	CRET.	WADGE
PSOC-068	UINTA	UT	HVB	CRET.	LOWER SUNNYSIDE
PSOC-097	HANNA FIELD	WY		PALEO.	EEI #80
PSOC-233	GREEN RIVER	CC	HVC	CRET.	WADGE
PSOC-234	GREEN RIVER	CO	HVC	CRET.	WADGE
PSOC-238	UINTA	UT	HVA	CRET.	UTAH A
PSOC-239	UINTA	UT	HVA	CRET.	UTAH B
PSOC-248	HAMS FORK	WY		CRET.	ACAVILLE #1
PSOC-249	UINTA	UT	HVE	CRET.	ROCK CANYON
PSOC-309	SAN JUAN RIVER	NM	BVC	CRET.	NEW MEXICO #8
PSOC-310	SAN JUAN RIVER	NM	HVC	CRET.	NEW MEXICO #7
PSOC-311	SAN JUAN RIVER	NM	HVC	CRET.	NEW MEXICO #6
PSOC-312	SAN JUAN RIVER	AZ	HVC	CRET.	RED
PSOC-313	UINTA	UT	HVE	CRET.	HIAWATHA
PSOC-314	UINTA	UT	HVA	CRET.	BLIND CANYON
PSOC-315	GREEN RIVER	CC	HVC	CRET.	WADGE
PSOC-316	GREEN RIVER	CO	HVC	CRET.	FISH CREEK

APPENDIX II.

Data matrices by provinces

LIST OF ABBREVIATIONS

Maximum reflectance, % in oil	R_o
Carbon, % dmmf (Modified Parr)	C
Hydrogen, % dmmf (Modified Parr)	H
Oxygen, % dmmf (Modified Parr)	O
Sulfur, % dmmf (Modified Parr)	S
Nitrogen, % dmmf (Modified Parr)	N
Volatile matter, % dmmf (Modified Parr)	VM
Moisture, % mmf	M
Vitrinite-group macerals, volume % mmf	VIT
Inertinite-group macerals, volume % mmf	IN
Liptinite-group macerals, volume % mmf	LIP

APPENDIX II.1. Data matrix for Eastern province coals

SAMPLE	R _o	C	H	O	S	N	VM	M	Btu/lb	VIT	IN	LIP
PSOC-001	0.87	84.19	5.40	8.16	0.71	1.54	37.91	1.83	15118.	54.8	21.7	23.5
PSOC-005	0.83	84.50	5.66	7.40	0.82	1.62	39.03	1.98	15154.	62.4	26.1	11.5
PSOC-011	0.94	84.83	5.59	7.65	0.42	1.51	36.87	1.54	15238.	77.5	16.3	6.2
PSOC-102	0.85	84.42	5.16	8.38	0.89	1.14	38.55	1.79	15184.	82.5	13.6	3.9
PSOC-113	1.80	90.56	4.59	2.62	1.05	1.18	18.44	0.93	15678.	86.9	13.1	0.0
PSOC-114	1.69	89.55	4.69	3.92	0.63	1.22	18.71	1.15	15605.	65.4	34.4	0.2
PSOC-116	1.47	88.09	4.89	4.32	1.38	1.32	21.43	1.35	15565.	85.8	14.2	0.0
PSOC-122	0.75	84.46	6.61	6.73	0.80	1.39	48.01	1.20	15789.	46.2	20.2	33.6
PSOC-125	1.17	88.98	5.31	4.34	0.52	0.85	32.78	1.32	15784.	91.4	7.4	1.3
PSOC-126	1.68	90.23	4.75	3.60	0.48	0.94	19.07	0.70	15877.	86.0	14.0	0.0
PSOC-134	1.31	90.02	4.74	3.87	0.64	1.53	24.94	0.80	15690.	78.6	21.4	0.0
PSOC-265	0.96	86.72	5.38	4.76	0.68	2.46	35.52	1.43	15473.	56.0	36.1	7.9
PSOC-267	1.01	85.26	5.55	4.62	2.03	2.55	36.99	1.39	15427.	66.2	29.1	4.7
PSOC-268	1.07	86.50	5.42	4.41	1.53	2.15	34.09	1.28	15594.	75.9	19.1	5.0
PSOC-269	1.03	86.95	5.40	5.43	0.57	1.67	35.53	1.36	15503.	79.0	16.9	4.1
PSOC-270	0.98	85.15	5.44	4.85	2.77	1.79	35.29	1.54	15620.	71.3	22.9	5.8
PSOC-271	0.99	86.54	5.37	5.60	0.58	1.91	33.92	2.01	15351.	74.4	19.3	6.3
PSOC-275	0.78	83.06	5.96	8.12	0.80	2.07	40.79	3.49	15093.	74.1	19.3	6.6
PSOC-276	0.65	83.54	5.53	7.75	1.36	1.82	43.69	4.62	14928.	80.7	15.6	3.7
PSOC-277	0.68	82.76	5.45	8.48	1.27	2.05	41.94	4.52	14922.	58.8	35.6	5.6
PSOC-278	0.57	79.56	5.98	10.15	2.63	1.68	46.93	4.03	14761.	77.1	20.5	2.4
PSOC-299	0.86	86.86	5.45	4.81	0.76	2.12	37.97	1.89	15523.	81.9	10.9	7.2
PSOC-300	0.88	84.40	5.61	7.21	0.76	2.01	38.75	3.02	15050.	73.6	16.3	10.1
PSOC-301	1.05	88.85	5.30	3.16	0.62	2.07	31.88	1.04	15801.	79.7	17.2	3.1
PSOC-302	1.01	88.91	5.35	3.15	0.60	1.95	34.51	1.08	15853.	55.5	30.4	14.1
PSOC-305	0.67	84.32	5.57	6.78	1.44	1.89	40.75	6.35	15073.	86.2	12.0	1.8
PSOC-306	0.70	84.42	5.74	6.69	1.25	1.90	40.77	5.25	15342.	61.9	30.6	7.5
PSOC-307	0.76	83.76	5.71	7.23	1.41	1.89	42.67	5.07	15074.	87.0	10.1	2.9
PSOC-308	0.47	79.85	5.53	11.52	1.30	1.81	45.96	9.21	14460.	79.8	15.1	5.1
PSOC-317	1.57	90.47	4.44	2.88	0.58	1.64	18.10	2.39	15939.	65.0	35.0	0.0
PSOC-319	1.55	91.56	4.44	2.18	0.10	1.71	18.57	2.33	15907.	77.5	22.4	0.1
PSOC-320	1.30	90.40	4.94	1.61	0.78	2.27	23.45	2.47	15874.	92.5	7.4	0.1
PSOC-323	1.24	90.36	5.05	2.14	1.01	1.44	24.75	2.94	15949.	77.3	22.5	0.2
PSOC-324	1.18	89.74	5.07	2.08	1.40	1.70	24.47	6.15	16113.	89.6	7.9	2.5
PSOC-326	0.78	85.49	5.71	5.71	1.55	1.54	43.49	2.79	15502.	77.0	18.5	4.5
PSOC-328	0.78	85.38	5.59	6.76	0.63	1.63	39.44	6.34	15179.	86.1	10.6	3.3
PSOC-329	0.68	84.99	5.62	6.71	1.04	1.63	41.96	6.02	15249.	74.9	20.4	4.7

APPENDIX II.1.(continued). Data matrix for Eastern province coals

SAMPLE	R _o	C	H	O	S	N	VM	M	Btu/lb	VIT	IN	LIP
PSOC-330	0.76	83.49	5.40	8.54	0.73	1.86	39.74	6.64	14796.	84.2	12.4	3.4
PSOC-331	0.77	84.57	5.59	7.45	0.75	1.63	39.40	5.62	15035.	80.5	13.6	5.9
PSOC-332	0.76	84.36	5.79	7.45	0.74	1.66	39.77	6.66	15194.	76.3	15.8	7.9
PSOC-337	0.89	86.15	5.76	5.77	0.71	1.61	37.32	2.53	15382.	75.1	8.4	16.4
PSOC-341	0.75	86.01	5.79	5.29	1.46	1.45	42.59	4.08	15613.	68.1	13.3	18.5
PSOC-345	0.79	85.17	5.71	5.96	1.45	1.71	41.01	2.84	15379.	75.0	8.9	16.0
PSOC-349	0.77	84.28	5.80	6.60	1.66	1.66	42.92	3.55	15390.	84.6	10.3	5.5
PSOC-353	0.73	84.94	5.76	6.29	1.55	1.45	41.21	8.12	15354.	77.2	12.6	10.0
PSOC-354	0.82	84.65	5.58	7.28	0.62	1.86	37.46	5.84	15169.	75.3	9.4	15.4
PSOC-355	0.80	84.65	5.65	7.14	0.71	1.84	39.03	4.29	15187.	79.0	10.4	10.6
PSOC-357	1.04	87.77	5.45	4.72	0.55	1.52	33.73	1.55	15665.	76.6	16.8	6.7
PSOC-361	1.01	87.08	5.42	5.48	0.61	1.41	33.68	1.32	15627.	72.6	16.7	10.7
PSOC-362	1.03	87.65	5.44	5.03	0.42	1.46	33.47	1.40	15634.	71.2	16.8	11.9
PSOC-363	0.80	83.90	5.48	8.28	0.76	1.58	38.73	4.23	14983.	60.3	21.1	18.7
PSOC-367	0.84	84.10	5.45	8.36	0.55	1.53	37.99	3.53	14910.	68.3	19.1	12.6
PSOC-371	1.04	87.04	5.38	5.39	0.72	1.47	34.71	1.41	15687.	81.2	12.3	6.6
PSOC-375	0.80	84.47	5.52	7.69	0.81	1.50	38.25	3.28	15073.	75.8	12.2	12.0
ANTHRACITES												
PSOC-080	4.17	92.74	2.45	3.41	0.63	0.78	4.35	2.95	14960.	96.3	3.7	0.0
PSOC-083	3.04	91.75	3.59	1.92	1.35	1.38	6.54	1.48	15523.	80.3	19.7	0.0
PSOC-084	2.15	94.03	3.50	0.21	0.84	1.42	5.85	1.44	15700.	70.8	29.2	0.0
PSOC-085	2.82	92.36	3.81	2.38	0.84	0.61	6.47	1.38	15598.	97.5	2.5	0.0
PSOC-147	2.47	91.67	4.40	1.60	0.72	1.62	18.15	1.45	15923.	87.7	12.3	0.0
PSOC-148	2.39	90.30	4.12	3.21	0.86	1.51	16.59	1.64	15580.	87.7	12.3	0.0
PSOC-159	3.10	92.30	3.33	1.97	0.82	1.58	10.12	1.14	15328.	92.4	7.6	0.0
PSOC-379	2.80	93.20	3.74	1.41	0.55	1.10	7.77	1.97	16142.	82.7	17.3	0.0
PSOC-383	2.57	92.59	3.83	1.88	0.63	1.08	8.72	2.20	15643.	82.8	17.2	0.0
PSOC-384	2.70	94.17	3.58	0.62	0.62	1.00	6.77	2.18	15711.	83.4	16.6	0.0

APPENDIX II.2. Data matrix for Interior province coals

SAMPLE	R _o	C	H	O	S	N	VM	M	Btu/lb	VIT	IN	LIP
PSOC-022	0.49	80.03	5.81	10.73	1.85	1.58	41.76	19.61	14329.	88.4	7.2	4.4
PSOC-024	0.70	82.37	5.52	8.69	2.32	1.10	40.56	5.66	14844.	85.3	11.6	3.1
PSOC-026	0.54	80.27	5.76	10.36	2.43	1.18	44.58	13.83	14627.	85.8	6.2	8.1
PSOC-105	0.56	81.93	5.53	11.08	1.06	0.40	37.55	7.09	14734.	61.7	16.1	22.1
PSOC-107	0.78	81.97	4.99	11.25	0.42	1.37	37.12	10.63	14654.	62.4	14.6	23.0
PSOC-162	0.57	82.31	5.53	7.57	2.38	2.21	42.57	6.07	14708.	79.6	16.9	3.5
PSOC-163	0.73	84.44	5.59	7.55	2.23	0.19	41.95	2.69	15190.	79.8	16.3	3.9
PSOC-164	0.49	83.07	4.26	7.48	3.90	1.29	42.30	8.77	14562.	76.4	17.4	6.2
PSOC-165	0.59	79.92	5.29	10.96	2.56	1.27	42.85	6.76	14241.	88.6	9.2	2.2
PSOC-166	0.53	79.39	5.52	11.27	2.51	1.31	42.14	6.76	14433.	87.2	9.2	3.6
PSOC-243	0.52	80.84	6.12	9.69	1.46	1.88	48.25	13.71	14437.	86.7	9.5	3.8
PSOC-244	0.50	78.92	5.78	9.73	4.01	1.55	46.71	10.10	14462.	75.0	20.8	4.2
PSOC-251	0.80	84.60	5.46	6.96	1.40	1.59	41.08	2.90	15438.	80.8	15.9	3.3
PSOC-252	0.65	82.26	5.36	8.37	2.18	1.83	41.69	4.52	14823.	82.1	14.7	3.2
PSOC-272	0.63	81.43	5.51	8.77	1.81	2.48	42.67	6.88	14858.	82.7	14.3	3.0
PSOC-273	0.62	79.33	5.34	10.52	2.48	2.32	42.18	7.75	14409.	85.7	10.9	3.4
PSOC-279	0.46	80.48	5.81	9.92	2.04	1.75	47.74	8.24	14784.	69.9	26.1	4.0
PSOC-280	0.50	82.74	5.68	8.35	1.28	1.95	43.97	13.51	14863.	92.1	5.1	2.8
PSOC-281	0.50	84.89	5.14	7.20	0.63	2.14	40.85	11.62	14788.	83.6	15.0	1.4
PSOC-283	0.58	82.72	5.81	8.67	0.88	1.92	47.92	4.10	15378.	67.9	24.6	7.5
PSOC-284	0.60	85.64	5.73	5.17	1.56	1.90	46.38	4.11	15539.	87.1	10.1	2.8
PSOC-286	0.43	85.09	5.10	5.51	2.53	1.78	44.61	8.46	15147.	83.5	14.3	2.2
PSOC-287	0.53	82.20	5.48	8.85	1.51	1.96	43.25	10.73	14854.	71.2	26.9	1.9
PSOC-290	0.36	82.46	5.28	8.43	2.41	1.42	45.64	9.56	14777.	82.5	15.6	1.9
PSOC-356	0.53	81.79	5.48	8.61	2.59	1.52	41.95	10.70	14762.	85.0	13.0	2.0

APPENDIX II.3. Data matrix for Western coals

SAMPLE	R _o	C	H	O	S	N	VM	M	Btu/lb	VIT	IN	LIP
PSOC-055A	0.62	78.62	6.15	12.94	0.66	1.62	45.52	15.02	14264.	83.5	12.8	3.7
PSOC-056	0.57	77.42	5.82	14.98	0.44	1.34	47.18	7.66	13636.	83.9	12.8	3.3
PSOC-059	0.59	76.52	5.72	15.34	0.46	1.96	43.67	11.92	13967.	82.6	13.5	3.9
PSOC-065	0.35	73.82	5.62	19.53	0.26	0.77	45.32	18.66	12776.	86.4	11.3	2.3
PSOC-068	0.70	81.96	5.72	10.29	0.55	1.48	41.29	4.55	14613.	81.2	15.3	3.5
PSOC-086	0.31	73.28	4.76	20.40	0.73	0.83	45.86	34.71	12428.	67.2	21.1	11.7
PSOC-097	0.30	76.10	5.44	16.93	0.95	0.59	53.61	14.77	13435.	88.6	7.9	3.5
PSOC-150	0.64	82.96	5.94	8.96	0.68	1.47	40.47	4.13	14962.	74.4	22.0	3.6
PSOC-230	0.51	76.28	5.04	17.10	0.47	1.11	42.05	21.67	13037.	78.2	18.1	3.7
PSOC-231	0.56	76.61	5.00	16.26	0.40	1.74	39.77	20.71	13217.	76.1	20.7	3.2
PSOC-233	0.61	78.28	5.42	13.89	0.47	1.94	41.45	8.34	13792.	88.8	6.5	4.7
PSOC-234	0.61	78.55	5.45	13.41	0.58	2.01	41.66	8.47	13889.	86.8	9.0	4.2
PSOC-238	0.58	80.67	6.09	10.39	1.16	1.70	45.18	4.02	14640.	85.2	11.9	2.9
PSOC-239	0.60	81.56	6.13	10.10	0.44	1.77	46.25	4.12	14712.	83.9	8.7	7.4
PSOC-241	0.48	73.90	5.26	18.99	0.40	1.45	43.37	18.86	12798.	85.7	12.5	1.8
PSOC-242	0.43	74.45	5.43	17.98	0.46	1.68	45.93	20.19	13033.	90.6	5.6	3.8
PSOC-245	0.34	73.39	5.03	20.27	1.18	0.13	49.58	38.04	12329.	75.1	20.7	4.2
PSOC-246	0.38	71.52	4.82	21.45	0.63	1.57	48.65	36.78	11902.	78.7	17.2	4.1
PSOC-247	0.45	75.53	4.84	17.61	0.50	1.51	45.08	33.33	12462.	75.0	20.8	4.2
PSOC-248	0.47	75.44	5.13	17.06	0.63	1.74	44.68	19.70	13097.	76.3	22.1	1.6
PSOC-249	0.67	81.27	5.37	11.07	0.76	1.53	40.13	4.29	14446.	70.2	26.7	3.0
PSOC-250	0.84	83.83	5.64	7.91	0.54	2.08	39.47	1.63	15405.	74.7	22.9	2.4
PSOC-309	0.48	79.52	5.61	12.50	0.61	1.76	44.73	12.64	14274.	73.4	24.8	1.8
PSOC-310	0.49	78.65	5.65	13.24	0.79	1.67	43.15	12.05	13942.	83.5	14.5	2.0
PSOC-311	0.49	78.86	5.72	13.07	0.52	1.82	43.12	10.87	13928.	80.9	16.3	2.8
PSOC-312	0.44	78.39	5.72	14.17	0.31	1.41	45.65	11.42	13774.	85.9	11.7	2.4
PSOC-313	0.57	81.13	6.04	10.40	0.59	1.85	44.96	7.54	14545.	78.9	9.3	11.9
PSOC-314	0.59	81.35	6.05	10.28	0.67	1.66	46.97	4.59	14735.	81.8	12.0	6.2
PSOC-315	0.55	77.86	5.76	13.73	0.63	2.01	42.34	12.04	13859.	87.6	10.4	2.0
PSOC-316	0.54	79.07	5.48	12.64	0.48	2.33	40.57	12.67	13850.	87.1	11.6	1.3

APPENDIX III.

Data matrices for groups from CLUS

LIST OF ABBREVIATIONS

Maximum reflectance, % in oil	R _o
Carbon, % dmmf (Modified Parr)	C
Hydrogen, % dmmf (Modified Parr)	H
Oxygen, % dmmf (Modified Parr)	O
Sulfur, % dmmf (Modified Parr)	S
Nitrogen, % dmmf (Modified Parr)	N
Volatile matter, % dmmf (Modified Parr)	VM
Moisture, % mmf	M
Vitrinite-group macerals, volume % mmf	VIT
Inertinite-group macerals, volume % mmf	IN
Liptinite-group macerals, volume % mmf	LIP

APPENDIX III.1. Data matrix for Group I from CLUS

SAMPLE	R _o	C	H	O	S	N	VM	M	Btu/lb	VIT	IN	LIP
PSOC-022	0.49	80.03	5.81	10.73	1.85	1.58	41.76	19.61	14329.	88.4	7.2	4.4
PSOC-026	0.54	80.27	5.76	10.36	2.43	1.18	44.58	13.83	14627.	85.8	6.2	8.1
PSOC-055A	0.62	78.62	6.15	12.94	0.66	1.62	45.52	15.02	14264.	83.5	12.8	3.7
PSOC-056	0.57	77.42	5.82	14.98	0.44	1.34	47.18	7.66	13636.	83.9	12.8	3.3
PSOC-059	0.59	76.52	5.72	15.34	0.46	1.96	43.67	11.92	13967.	82.6	13.5	3.9
PSOC-065	0.35	73.82	5.62	19.53	0.26	0.77	45.32	18.66	12776.	86.4	11.3	2.3
PSOC-068	0.70	81.96	5.72	10.29	0.55	1.48	41.29	4.55	14613.	81.2	15.3	3.5
PSOC-086	0.31	73.28	4.76	20.40	0.73	0.83	45.86	34.71	12428.	67.2	21.1	11.7
PSOC-097	0.30	76.10	5.44	16.93	0.95	0.59	53.61	14.77	13435.	88.6	7.9	3.5
PSOC-166	0.53	79.39	5.52	11.27	2.51	1.31	42.14	6.76	14433.	87.2	9.2	3.6
PSOC-230	0.51	76.28	5.04	17.10	0.47	1.11	42.05	21.67	13037.	78.2	18.1	3.7
PSOC-231	0.56	76.61	5.00	16.26	0.40	1.74	39.77	20.71	13217.	76.1	20.7	3.2
PSOC-233	0.61	78.29	5.42	13.89	0.47	1.94	41.45	8.34	13792.	88.8	6.5	4.7
PSOC-234	0.61	78.55	5.45	13.41	0.58	2.01	41.66	8.47	13889.	86.8	9.0	4.2
PSOC-238	0.58	80.67	6.09	10.39	1.16	1.70	45.19	4.02	14640.	85.2	11.9	2.9
PSOC-239	0.60	81.56	6.13	10.10	0.44	1.77	46.25	4.12	14712.	83.9	8.7	7.4
PSOC-241	0.48	73.90	5.26	18.99	0.40	1.45	43.27	18.86	12798.	85.7	12.5	1.8
PSOC-242	0.43	74.45	5.43	17.98	0.46	1.68	45.93	20.19	13033.	90.6	5.6	3.8
PSOC-243	0.52	80.84	6.12	9.69	1.46	1.88	48.25	13.71	14437.	86.7	9.5	3.8
PSOC-245	0.34	73.39	5.03	20.27	1.18	0.13	49.58	38.04	12329.	75.1	20.7	4.2
PSOC-246	0.38	71.52	4.82	21.45	0.63	1.57	48.65	36.78	11902.	78.7	17.2	4.1
PSOC-247	0.45	75.53	4.84	17.61	0.50	1.51	45.08	33.33	12462.	75.0	20.8	4.2
PSOC-248	0.47	75.44	5.13	17.06	0.63	1.74	44.68	19.70	13097.	76.3	22.1	1.6
PSOC-280	0.50	82.74	5.68	8.35	1.28	1.95	43.97	13.51	14863.	92.1	5.1	2.8
PSOC-310	0.49	78.65	5.65	13.24	0.79	1.67	43.15	12.05	13942.	83.5	14.5	2.0
PSOC-311	0.49	78.86	5.72	13.07	0.52	1.82	43.12	10.87	13928.	80.9	16.3	2.8
PSOC-312	0.44	78.39	5.72	14.17	0.31	1.41	45.65	11.42	13774.	85.9	11.7	2.4
PSOC-313	0.57	81.13	6.04	10.40	0.59	1.85	44.96	7.54	14545.	78.9	9.3	11.9
PSOC-314	0.59	81.35	6.05	10.28	0.67	1.66	46.97	4.59	14735.	81.8	12.0	6.2
PSOC-315	0.55	77.86	5.76	13.73	0.63	2.01	42.34	12.04	13859.	87.6	10.4	2.0

APPENDIX III.2. Data matrix for Group II from CLUS

SAMPLE	R _o	C	H	O	S	N	VM	M	Btu/lb	VIT	IN	LIP
PSOC-024	0.70	82.37	5.52	8.69	2.32	1.10	40.56	5.66	14844.	85.3	11.6	3.1
PSOC-162	0.57	82.31	5.53	7.57	2.38	2.21	42.57	6.07	14708.	79.6	16.9	3.5
PSOC-163	0.73	84.44	5.59	7.55	2.23	0.19	41.95	2.69	15190.	79.8	16.3	3.9
PSOC-164	0.49	83.07	4.26	7.48	3.90	1.29	42.30	8.77	14562.	76.4	17.4	6.2
PSOC-165	0.59	79.92	5.29	10.96	2.56	1.27	42.85	6.76	14241.	88.6	9.2	2.2
PSOC-244	0.50	78.92	5.78	9.73	4.01	1.55	46.71	10.10	14462.	75.0	20.8	4.2
PSOC-249	0.67	81.27	5.37	11.07	0.76	1.53	40.13	4.29	14446.	70.2	26.7	3.0
PSOC-251	0.80	84.60	5.46	6.96	1.40	1.59	41.08	2.90	15438.	80.8	15.9	3.3
PSOC-252	0.65	82.26	5.36	8.37	2.18	1.83	41.69	4.52	14823.	82.1	14.7	3.2
PSOC-267	1.01	85.26	5.55	4.62	2.03	2.55	36.99	1.39	15427.	66.2	29.1	4.7
PSOC-270	0.98	85.15	5.44	4.85	2.77	1.79	35.29	1.54	15620.	71.3	22.9	5.8
PSOC-272	0.63	81.43	5.51	8.77	1.81	2.48	42.67	6.88	14658.	82.7	14.3	3.0
PSOC-273	0.62	79.33	5.34	10.52	2.48	2.32	42.18	7.75	14409.	85.7	10.9	3.4
PSOC-276	0.65	83.54	5.53	7.75	1.36	1.82	43.69	4.62	14928.	80.7	15.6	3.7
PSOC-277	0.68	82.76	5.45	8.48	1.27	2.05	41.94	4.52	14922.	58.8	35.6	5.6
PSOC-278	0.57	79.56	5.98	10.15	2.63	1.68	46.93	4.03	14761.	77.1	20.5	2.4
PSOC-279	0.46	80.48	5.81	9.92	2.04	1.75	47.74	8.24	14784.	69.9	26.1	4.0
PSOC-281	0.50	84.89	5.14	7.20	0.63	2.14	40.85	11.62	14788.	33.6	15.0	1.4
PSOC-283	0.58	82.72	5.81	8.67	0.88	1.92	47.92	4.10	15378.	67.9	24.6	7.5
PSOC-284	0.60	85.64	5.73	5.17	1.56	1.90	46.38	4.11	15539.	87.1	10.1	2.8
PSOC-285	0.64	84.49	5.48	7.16	0.89	1.98	43.84	4.29	15349.	43.6	50.6	5.8
PSOC-286	0.43	85.09	5.10	5.51	2.53	1.78	44.61	8.46	15147.	83.5	14.3	2.2
PSOC-287	0.53	82.20	5.48	8.85	1.51	1.96	43.25	10.73	14854.	71.2	26.9	1.9
PSOC-290	0.36	82.46	5.28	8.43	2.41	1.42	45.64	9.56	14777.	82.5	15.6	1.9
PSOC-306	0.70	84.42	5.74	6.69	1.25	1.90	40.77	5.25	15342.	61.9	30.6	7.5
PSOC-307	0.76	83.76	5.71	7.23	1.41	1.89	42.67	5.07	15074.	87.0	10.1	2.9
PSOC-308	0.47	79.85	5.53	11.52	1.30	1.81	45.96	9.21	14460.	79.8	15.1	5.1
PSOC-309	0.48	79.52	5.61	12.50	0.61	1.76	44.73	12.64	14274.	73.4	24.8	1.8
PSOC-326	0.78	85.49	5.71	5.71	1.55	1.54	43.49	2.79	15502.	77.0	18.5	4.5
PSOC-329	0.68	84.99	5.62	6.71	1.04	1.63	41.96	6.02	15249.	74.9	20.4	4.7
PSOC-356	0.53	81.79	5.48	8.61	2.59	1.52	41.95	10.70	14762.	85.0	13.0	2.0
PSOC-305	0.67	84.32	5.57	6.78	1.44	1.89	40.75	6.35	15073.	86.2	12.0	1.8

APPENDIX III.3. Data matrix for Group III from CLUS

SAMPLE	R _O	C	H	O	S	N	VM	M	Btu/lb	VIT	IN	LIP
PSOC-001	0.87	84.19	5.40	8.16	0.71	1.54	37.91	1.83	15118.	54.80	21.70	23.50
PSOC-005	0.83	84.50	5.66	7.40	0.82	1.62	39.03	1.98	15154.	62.40	26.10	11.50
PSOC-011	0.94	84.83	5.59	7.65	0.42	1.51	36.87	1.54	15238.	77.50	16.30	6.20
PSOC-102	0.85	84.42	5.16	8.38	0.89	1.14	38.55	1.79	15184.	82.50	13.60	3.90
PSOC-107	0.78	81.97	4.99	11.25	0.42	1.37	37.12	10.63	14654.	62.40	14.60	23.00
PSOC-150	0.64	82.96	5.94	8.96	0.68	1.47	40.47	4.13	14962.	74.40	22.00	3.60
PSOC-250	0.84	83.81	5.64	7.91	0.54	2.08	39.47	1.63	15405.	74.70	22.90	2.40
PSOC-265	0.96	86.72	5.38	4.76	0.68	2.46	35.52	1.43	15473.	56.00	36.10	7.90
PSOC-268	1.07	86.50	5.42	4.41	1.53	2.15	34.09	1.28	15594.	75.90	19.10	5.00
PSOC-269	1.03	86.95	5.40	5.43	0.57	1.67	35.53	1.36	15503.	79.00	16.90	4.10
PSOC-271	0.99	86.54	5.37	5.60	0.58	1.91	33.92	2.01	15351.	74.40	19.30	6.30
PSOC-275	0.78	83.06	5.96	8.12	0.80	2.07	40.79	3.49	15093.	74.10	19.30	6.60
PSOC-299	0.66	86.86	5.45	4.81	0.76	2.12	37.97	1.89	15523.	81.90	10.90	7.20
PSOC-300	0.88	84.40	5.51	7.21	0.76	2.01	38.75	3.02	15050.	73.60	16.30	10.10
PSOC-302	1.01	88.91	5.39	3.15	0.60	1.95	34.51	1.08	15853.	55.50	30.40	14.10
PSOC-328	0.78	85.38	5.59	6.76	0.63	1.63	39.44	6.34	15179.	86.10	10.60	3.30
PSOC-330	0.76	83.48	5.10	8.54	0.73	1.86	39.74	6.64	14796.	84.20	12.40	3.40
PSOC-331	0.77	84.57	5.59	7.45	0.75	1.63	39.40	5.62	15035.	80.50	13.60	5.90
PSOC-332	0.76	84.36	5.79	7.45	0.74	1.66	39.77	6.66	15194.	76.30	15.80	7.90
PSOC-337	0.89	86.15	5.76	5.77	0.71	1.61	37.32	2.53	15382.	75.10	8.40	16.40
PSOC-341	0.75	86.01	5.79	5.29	1.46	1.45	42.59	4.08	15613.	68.10	13.30	18.50
PSOC-345	0.79	85.17	5.71	5.96	1.45	1.71	41.01	2.84	15379.	75.00	8.90	16.00
PSOC-349	0.77	84.23	5.80	6.60	1.66	1.66	42.92	3.55	15390.	84.60	10.30	5.50
PSOC-353	0.73	84.94	5.76	6.29	1.55	1.45	41.21	8.12	15354.	77.20	12.60	10.00
PSOC-354	0.82	84.65	5.58	7.28	0.62	1.86	37.46	5.84	15169.	75.30	9.40	15.40
PSOC-355	0.80	84.65	5.65	7.14	0.71	1.84	39.03	4.29	15187.	79.00	10.40	10.60
PSOC-357	1.04	87.77	5.45	4.72	0.55	1.52	33.73	1.55	15665.	76.60	16.80	6.70
PSOC-361	1.01	87.08	5.42	5.48	0.61	1.41	33.68	1.32	15627.	72.60	16.70	10.70
PSOC-362	1.03	87.65	5.44	5.03	0.42	1.46	33.47	1.40	15634.	71.20	16.80	11.90
PSOC-363	0.80	83.90	5.48	8.28	0.76	1.58	38.73	4.23	14983.	60.30	21.10	18.70
PSOC-367	0.84	84.10	5.45	8.36	0.55	1.53	37.99	3.53	14910	68.30	19.10	12.60
PSOC-371	1.04	87.04	5.38	5.39	0.72	1.47	34.71	1.41	15687.	81.20	12.30	6.60
PSOC-375	0.80	84.47	5.52	7.69	0.81	1.50	38.25	3.28	15073.	75.80	12.20	12.00

APPENDIX III.4. Data matrix for Group IV from CLUS

SAMPLE	R _O	C	H	O	S	N	VM	M	Btu/lb	VIT	IN	LIP
PSOC-113	1.80	90.56	4.59	2.62	1.05	1.18	18.44	0.93	15678.	86.9	13.1	0.0
PSOC-114	1.69	89.55	4.69	3.92	0.63	1.22	18.71	1.15	15605.	65.4	34.4	0.2
PSOC-116	1.47	88.09	4.89	4.32	1.38	1.32	21.43	1.35	15565.	85.8	14.2	0.0
PSOC-125	1.17	88.98	5.31	4.34	0.52	0.85	32.78	1.32	15784.	91.4	7.4	1.3
PSOC-126	1.68	90.23	4.75	3.60	0.48	0.94	19.07	0.70	15877.	86.0	14.0	0.0
PSOC-134	1.31	90.02	4.74	3.07	0.64	1.53	24.94	0.80	15690.	78.6	21.4	0.0
PSOC-317	1.57	90.47	4.44	2.88	0.58	1.64	18.10	2.39	15939.	65.0	35.0	0.0
PSOC-319	1.55	91.56	4.44	2.18	0.10	1.71	18.57	2.33	15907.	77.5	22.4	0.1
PSOC-320	1.30	90.40	4.94	1.61	0.78	2.27	23.45	2.47	15874.	92.5	7.4	0.1
PSOC-323	1.24	90.36	5.05	2.14	1.01	1.44	24.75	2.94	15949.	77.3	22.5	0.2
PSOC-324	1.18	89.74	5.07	2.08	1.40	1.70	24.47	6.15	16113.	89.6	7.9	2.5

APPENDIX IV.

Complete matrices of factor analyses

Table IV-1. Original matrix of factor loadings of the R-mode component analysis of United States coals

	F 1	F 2	F 3	F 4	F 5	F 6	h_i^2
Reflectance, % in oil	-0.95029	-0.04875	0.00414	0.15385	0.04373	-0.01767	0.93134
Carbon, % dmmf	-0.95300	-0.00073	-0.19495	0.00573	-0.07225	0.01498	0.95169
Hydrogen, % dmmf	0.33536	0.38679	-0.71391	0.16440	0.11194	-0.39488	0.97439
Oxygen, % dmmf	0.24717	0.10334	0.16512	0.09632	0.04767	-0.06864	0.95166
Sulfur, % dmmf	0.08017	0.02000	-0.42792	-0.73270	-0.49548	0.09872	0.98203
Nitrogen, % dmmf	-0.15234	0.08546	-0.37464	-0.33116	0.81537	0.22762	0.99717
Volatile matter, % dmmf	0.87628	0.27234	-0.28205	-0.09923	-0.02029	-0.09410	0.94070
Moisture, % mmf	0.87967	-0.17068	0.17064	-0.10140	0.04298	0.19843	0.88358
Btu/lb, % dmmf	-0.93252	0.05946	-0.26969	-0.00517	-0.09677	-0.02816	0.95605
Vitrinite, vol. % mmf	0.23889	-0.90639	-0.32063	0.06946	0.02013	-0.05891	0.99012
Inertinite, vol. % mmf	-0.29576	0.60525	0.55576	-0.40182	0.12433	-0.23335	0.99404
Liptinite, vol. % mmf	0.12946	0.76685	-0.26535	0.38222	-0.18818	0.37370	0.99638
Sum λ_i^2	5.42306	2.05214	1.56940	1.03905	0.99516	0.46933	
% Variation explained	45.19217	17.10947	13.07833	8.65875	8.29301	3.91111	
Cumulative %	45.19217	62.30164	75.37996	84.03870	92.33170	96.24280	

Table IV-2. Original matrix of factor loadings of the R-mode component analysis of coals lower in rank than medium volatile bituminous

	F 1	F 2	F 3	F 4	F 5	F 6	F 7	h_i^2
Reflectance, % in oil	0.92723	-0.00189	0.20875	0.07263	0.12844	-0.07054	0.18498	0.96431
Carbon, % dmmf	0.94236	0.18973	-0.03049	-0.10503	0.07268	-0.04220	-0.20917	0.98684
Hydrogen, % dmmf	0.13086	0.57500	0.19355	0.16645	-0.72737	-0.17146	0.11047	0.98555
Oxygen, % dmmf	-0.92098	-0.25737	0.17348	0.10127	-0.06628	-0.02632	0.16764	0.98798
Sulfur, % dmmf	0.05681	0.35378	-0.74300	-0.48998	-0.03761	0.17280	0.21965	0.99960
Nitrogen, % dmmf	0.33698	0.31847	-0.22627	0.73207	0.02570	0.44222	0.00766	0.99837
Volatile matter, % dmmf	-0.81276	0.17323	-0.22396	-0.07022	-0.37957	0.00808	-0.22281	0.94218
Moisture, % mmf	-0.91874	-0.11500	-0.03610	-0.01442	0.01254	0.20289	-0.10173	0.91049
Btu/lb, % dmmf	0.93531	0.25582	-0.08336	-0.11045	-0.05790	-0.06118	-0.13296	0.98502
Vitrinite, vol. % mmf	-0.54036	0.74262	0.17353	-0.02410	0.32702	-0.08814	0.00885	0.99072
Inertinite, vol. % mmf	0.33806	-0.67029	-0.52265	0.27009	-0.17490	-0.23186	0.00521	0.99407
Liptinite, vol. % mmf	0.53046	-0.36382	0.42066	-0.35268	-0.31508	0.42510	0.00634	0.99512
Sum λ_i^2	5.79700	1.90127	1.25125	1.04552	0.94174	0.54948	0.24396	
% Variation explained	48.30835	15.84389	10.51040	8.71269	7.84780	4.57904	2.03298	
Cumulative %	48.30835	64.15224	74.66263	83.37531	91.22310	95.80212	97.83510	

Table IV-3a. Original matrix of factor loadings of the R-mode component analysis of Group I from cluster analysis

	F 1	F 2	F 3	F 4	F 5	F 6	h_i^2
Reflectance, % in oil	0.76670	-0.50010	-0.19580	-0.05123	-0.00939	0.05835	0.88236
Carbon, % dmmf	0.93897	0.03306	-0.20306	0.04808	0.11644	-0.01529	0.94215
Hydrogen, % dmmf	0.86117	0.16978	0.08500	-0.29867	0.15537	-0.07984	0.89737
Oxygen, % dmmf	-0.95827	-0.06471	0.16731	-0.11521	-0.08548	0.06965	0.97589
Sulfur, % dmmf	0.30515	0.60067	-0.23091	0.65817	0.10240	-0.09360	0.95967
Nitrogen, % dmmf	0.58886	-0.57016	0.11350	0.05600	-0.25516	-0.48617	0.98934
Volatile matter, % dmmf	-0.29620	0.74170	0.05920	-0.44672	0.17719	-0.31545	0.97182
Moisture, % mmf	-0.83777	0.10080	0.06583	0.33719	-0.15710	-0.18942	0.89062
Btu/lb, % dmmf	0.93983	0.16312	-0.16499	0.03910	0.16925	0.04723	0.96952
Vitrinite, vol. % mmf	0.61033	0.23042	0.72615	0.08343	-0.15474	0.08436	0.99091
Inertinite, vol. % mmf	-0.68553	-0.39604	-0.43009	0.01440	0.41885	-0.09925	0.99727
Liptinite, vol. % mmf	0.10179	0.34709	-0.72752	-0.20145	-0.54484	0.03857	0.99903
Sum λ_i^2	6.09496	1.39738	1.45966	0.90628	0.70164	0.41606	
% Variation explained	50.79134	15.72918	12.16384	7.55233	5.84702	3.46716	
Cumulative %	50.79134	66.51950	78.68333	86.23566	92.08267	95.54982	

Table IV-3b. Rotated matrix of factor loadings of the R-mode component analysis of Group I from cluster analysis

	F 1	F 2	F 3	F 4	F 5	F 6	h_i^2
Reflectance, % in oil	0.71964	-0.48301	0.00954	-0.12601	-0.05148	-0.33553	0.88239
Carbon, % dmmf	0.87458	-0.15425	0.18281	0.27410	-0.09396	-0.18996	0.94214
Hydrogen, % dmmf	0.84256	0.18727	0.36010	0.00418	0.01981	-0.14935	0.89737
Oxygen, % dmmf	-0.84553	0.14681	-0.23515	-0.34291	0.07987	0.24289	0.97589
Sulfur, % dmmf	0.15274	0.05761	0.12234	0.94835	-0.10236	0.09056	0.95967
Nitrogen, % dmmf	0.32707	-0.30761	0.15052	-0.10350	0.06675	-0.86597	0.98933
Volatile matter, % dmmf	-0.11279	0.95344	0.02767	0.02776	-0.09460	0.19892	0.97181
Moisture, % mmf	-0.89706	0.11150	-0.20311	0.17891	0.03138	0.02082	0.89061
Btu/lb, % dmmf	0.89107	-0.08062	0.24300	0.31596	-0.07033	-0.07196	0.96951
Vitrinite, vol. % mmf	0.27009	-0.01130	0.90664	0.07779	0.28714	-0.08567	0.99091
Inertinite, vol. % mmf	-0.33262	-0.02864	-0.91769	-0.11918	0.15207	0.07954	0.99726
Liptinite, vol. % mmf	0.11192	0.07996	-0.07464	0.10418	-0.98079	0.04165	0.99903
Sum λ_i^2	4.64613	1.34697	2.02614	1.28242	1.11559	1.04865	
% Variation explained	38.71777	11.22475	16.88454	10.68683	9.29656	8.73877	
Cumulative %	38.71777	49.94252	66.82706	77.51387	86.81042	95.54919	

Table IV-4a. Original matrix of factor loadings of the R-mode component analysis of Group II from cluster analysis

	F 1	F 2	F 3	F 4	F 5	F 6	F 7	h_i^2
Reflectance, % in oil	0.83401	0.12636	0.01619	0.40813	-0.02505	0.29793	-0.10061	0.97789
Carbon, % dmmf	0.78959	0.43025	-0.10873	-0.36341	0.13834	-0.15365	-0.02381	0.99570
Hydrogen, % dmmf	0.18150	-0.52919	0.64206	-0.20447	-0.15680	0.29004	-0.30572	0.96921
Oxygen, % dmmf	-0.79113	-0.43083	-0.01474	0.24530	0.19640	0.26178	0.06552	0.99111
Sulfur, % dmmf	-0.20071	0.21572	0.49713	0.50762	-0.43804	-0.46300	-0.04197	0.99964
Nitrogen, % dmmf	0.11639	-0.18210	-0.57474	-0.17595	-0.73995	0.20271	0.02689	0.99734
Volatile matter, % dmmf	-0.56754	-0.33571	0.44357	-0.54753	-0.08730	-0.05687	0.10144	0.95249
Moisture, % mmf	-0.79199	-0.05106	-0.33041	-0.22126	-0.02205	-0.27131	-0.11066	0.97545
Etu/lb, % dmmf	0.88006	0.16917	0.19510	-0.33289	-0.01849	-0.12852	-0.02214	0.96935
Vitrinite, vol. % mmf	-0.45110	0.82738	0.19117	-0.08999	-0.03151	0.23073	0.06975	0.99730
Inertinite, vol. % mmf	0.37690	-0.81186	-0.26122	0.08903	0.10460	-0.25515	-0.19075	0.94976
Liptinite, vol. % mmf	0.59863	-0.56976	0.19024	0.05501	-0.05550	-0.02846	0.48576	0.96273
Sum λ_i^2	4.45944	2.56763	1.43696	1.16786	0.85144	0.73365	0.41104	
% Variation explained	37.16196	21.39691	12.39132	9.73221	7.09537	6.11379	3.42531	
Cumulative %	37.16196	58.55887	70.95018	80.68237	87.77774	93.89153	97.31683	

Table IV-4b. Rotated matrix of factor loadings of the R-mode component analysis of Group II from cluster analysis

	F 1	F 2	F 3	F 4	F 5	F 6	F 7	h_1^2
Reflectance, % in oil	0.34948	-0.10844	0.11016	0.89846	-0.03641	0.00532	0.15250	0.97787
Carbon, % dmmf	0.93300	0.01391	-0.14315	0.22896	0.04650	0.22324	0.01285	0.99577
Hydrogen, % dmmf	0.00649	-0.19855	0.95449	-0.01631	0.03537	-0.02275	0.12885	0.96920
Oxygen, % dmmf	-0.94730	-0.02982	0.05514	-0.24414	0.12371	0.11907	-0.02650	0.99110
Sulfur, % dmmf	-0.08525	0.15401	0.01907	0.00694	0.09744	-0.97914	-0.00491	0.99964
Nitrogen, % dmmf	0.02482	-0.11379	-0.03763	0.01573	-0.98647	0.02406	0.01150	0.99733
Volatile matter, % dmmf	-0.21618	0.11414	0.45045	-0.81870	0.06182	-0.00005	0.12544	0.95248
Moisture, % mmf	-0.39775	0.01198	-0.28038	-0.67109	-0.12517	0.00678	-0.41581	0.87544
Btu/lb, % dmmf	0.90506	-0.10831	0.19455	0.23026	0.03436	0.05863	0.20731	0.96934
Vitrinite, vol. % mmf	-0.02792	0.95622	-0.11260	-0.08792	0.07148	-0.09134	-0.21975	0.99729
Inertinite, vol. % mmf	-0.00665	-0.97871	0.08708	0.06426	-0.07366	0.19168	0.06599	0.98976
Liptinite, vol. % mmf	0.17272	-0.48436	0.18186	0.15307	-0.03644	0.00671	0.89026	0.96272
Sum λ_j^2	2.95268	2.22071	1.32120	2.12875	1.03469	1.05434	0.96555	
% Variation explained	24.60565	18.50554	11.01001	17.73958	8.62245	8.78615	8.04628	
Cumulative %	24.60565	43.11159	54.12160	71.86118	80.48361	89.26974	97.31602	

Table IV-5a. Original matrix of factor loadings of the R-mode component analysis of Group III from cluster analysis

	F 1	F 2	F 3	F 4	F 5	F 6	h_i^2
Reflectance, % in oil	-0.93745	0.09161	-0.19594	-0.01377	0.04814	0.06099	0.93182
Carbon, % dmmf	-0.90674	-0.26892	-0.00741	-0.22360	0.01947	-0.11751	0.95874
Hydrogen, % dmmf	0.38667	-0.57979	0.44028	0.12503	-0.29933	-0.41613	0.95791
Oxygen, % dmmf	0.81196	0.47754	-0.20242	0.16041	-0.09256	0.07603	0.96875
Sulfur, % dmmf	0.24134	-0.63375	0.43239	-0.27259	0.06335	0.50451	0.97969
Nitrogen, % dmmf	-0.27522	-0.15365	0.44516	0.59137	0.57999	-0.07778	0.98968
Volatile matter, % dmmf	0.83661	-0.34192	0.31808	-0.01112	-0.09406	0.06279	0.92964
Moisture, % mmf	0.86354	0.00658	-0.05161	-0.10917	0.25715	-0.13762	0.84540
Btu/lb, % dmmf	-0.81163	-0.44494	0.14710	-0.21206	-0.12806	-0.05447	0.94270
Vitrinite, vol. % mmf	0.22162	-0.70754	-0.64702	0.15692	0.03698	0.01377	0.99455
Inertinite, vol. % mmf	-0.38780	0.51599	0.46424	0.46438	-0.30857	0.14572	0.96425
Liptinite, vol. % mmf	0.12449	0.51913	0.36011	-0.71450	0.18345	-0.14306	0.97930
Sum λ_i^2	4.96314	2.42181	1.54643	1.32333	0.66287	0.52479	
% Variation explained	41.35951	20.18173	12.88594	11.02815	5.52389	4.37328	
Cumulative %	41.35951	61.54124	74.42818	85.45631	90.98019	95.35347	

Table IV-5b. Rotated matrix of factor loadings of the R-mode component analysis of Group III from cluster analysis

	F 1	F 2	F 3	F 4	F 5	F 6	h_i^2
Reflectance, % in oil	-0.77084	0.48172	0.17349	0.06861	0.05755	-0.25972	0.93182
Carbon, % dmmf	-0.96506	0.12572	-0.02311	-0.01953	0.05310	-0.08684	0.95873
Hydrogen, % dmmf	0.05291	-0.94882	-0.06266	0.11838	0.06785	0.17973	0.95790
Oxygen, % dmmf	0.94739	0.04566	0.04334	-0.01046	-0.22236	-0.13297	0.96875
Sulfur, % dmmf	-0.05708	-0.21831	-0.15034	0.00883	0.03853	0.95111	0.97969
Nitrogen, % dmmf	-0.14541	-0.05014	0.16933	0.09695	0.96285	0.02944	0.98968
Volatile matter, % dmmf	0.58484	-0.56028	-0.15862	0.01913	-0.03706	0.49678	0.92964
Moisture, % mmf	0.74712	-0.21920	-0.45040	-0.16628	0.02176	0.09041	0.84540
Btu/lb, % dmmf	-0.95998	-0.07449	0.03449	0.04549	0.00513	0.11087	0.94269
Vitrinite, vol. % mmf	0.02534	-0.08099	-0.64905	0.74247	-0.09535	0.07563	0.99454
Inertinite, vol. % mmf	-0.08079	0.07295	0.94843	-0.05004	0.16520	-0.15192	0.96424
Liptinite, vol. % mmf	0.09785	0.06937	-0.04327	-0.97026	-0.14564	0.02037	0.97929
Sum λ_i^2	4.28881	1.58457	1.43989	1.55395	1.04021	1.32692	
% Variation explained	35.74007	13.20471	13.66572	12.94956	8.73512	11.05766	
Cumulative %	35.74007	48.94476	62.61047	75.56003	84.29515	95.35281	

Table IV-6a. Original matrix of factor loadings of the R-mode component analysis of medium and low volatile bituminous coals

	F 1	F 2	F 3	F 4	F 5	h_i^2
Reflectance, % in oil	-0.84098	0.10241	-0.12078	0.32479	-0.37672	0.97973
Carbon, % dmmf	-0.37981	-0.78012	-0.34526	-0.24045	-0.15584	0.95414
Hydrogen, % dmmf	0.87875	0.34381	0.02197	-0.15200	0.09516	0.92304
Oxygen, % dmmf	-0.14962	0.91892	0.21981	-0.13241	-0.12763	0.94894
Sulfur, % dmmf	0.50947	0.12072	0.31458	0.74725	0.05721	0.93474
Nitrogen, % dmmf	0.11241	-0.76331	-0.06385	0.21814	0.53238	0.93037
Volatile matter, % dmmf	0.78476	0.31586	-0.05582	-0.45328	0.21666	0.97113
Moisture, % mmf	0.61077	-0.64015	0.40411	0.13403	-0.14698	0.98570
Btu/lb, % dmmf	0.42072	-0.76021	0.68950	-0.24345	-0.30476	0.91511
Vitrinite, vol. %, mmf	0.72400	0.14956	-0.61430	0.22871	-0.13036	0.99333
Inertinite, vol. % mmf	-0.76243	-0.13395	0.56714	-0.21686	0.15604	0.99227
Liptinite, vol. % mmf	0.79799	-0.12313	0.33119	-0.08054	-0.38395	0.91554
Sum λ_i^2	4.82644	3.32197	1.26876	1.19844	0.82843	
% Variation explained	40.22031	27.68311	10.57296	9.93699	6.60359	
Cumulative %	40.22031	67.90341	78.47636	88.46335	95.36693	

Table IV-6b. Rotated matrix of factor loadings of the R-mode component analysis of medium and low volatile bituminous coals

	F 1	F 2	F 3	F 4	F 5	h_i^2
Reflectance, % in oil	-0.89566	0.24839	0.13412	-0.10234	0.29556	0.97973
Carbon, % dmmf	-0.41210	-0.50956	0.05201	-0.69457	-0.19879	0.95414
Hydrogen, % dmmf	0.78151	0.19430	-0.40599	0.26613	-0.19718	0.92304
Oxygen, % dmmf	0.13700	0.85885	0.13560	0.17479	0.35542	0.94893
Sulfur, % dmmf	0.03644	-0.07910	-0.23139	0.91531	-0.18925	0.93474
Nitrogen, % dmmf	0.04239	-0.95602	0.06783	0.06928	-0.07197	0.93036
Volatile matter, % dmmf	0.92033	0.16488	-0.29612	-0.01415	-0.09505	0.97112
Moisture, % mmf	0.16501	-0.41442	-0.00746	0.27610	-0.84287	0.98569
Btu/lb, % dmmf	0.09755	-0.38413	-0.07047	-0.27803	-0.82205	0.91511
Vitrinite, vol. % mmf	0.25688	-0.02861	-0.95254	0.12388	-0.06195	0.99333
Inertinite, vol. % mmf	-0.27770	0.01309	0.93822	-0.13909	0.12341	0.99227
Liptinite, vol. % mmf	0.39090	0.14030	-0.22403	0.22620	-0.80103	0.91553
Sum λ_i^2	2.78435	2.40156	2.19254	1.67650	2.38902	
% Variation explained	23.20288	20.01297	18.27116	13.97095	19.90852	
Cumulative %	23.20288	43.21585	61.48701	75.45786	95.36638	

Table IV-7a. Original matrix of factor loadings of the R-mode component analysis of Eastern Province coals

	P 1	P 2	P 3	P 4	P 5	P 6	h_i^2
Reflectance, % in oil	-0.96739	0.08679	-0.02216	0.03909	-0.03986	0.06374	0.95104
Carbon, % dmmf	-0.96609	0.04235	-0.07479	-0.15230	0.10537	-0.12463	0.99054
Hydrogen, % dmmf	0.84713	0.08768	-0.22714	-0.37988	-0.06477	0.03602	0.92671
Oxygen, % dmmf	0.89726	-0.06233	-0.09809	0.38582	-0.05751	0.12290	0.98585
Sulfur, % dmmf	0.40583	-0.18367	0.54045	-0.36391	-0.59182	-0.05419	0.97613
Nitrogen, % dmmf	0.28789	0.21457	0.63777	-0.34348	0.55414	0.19049	0.99699
Volatile matter, % dmmf	0.95340	0.01633	-0.09796	-0.16954	-0.03679	0.06500	0.95316
Moisture, % mmf	0.64675	-0.42297	0.19736	0.12319	0.24792	-0.53319	0.99707
Btu/lb, % dmmf	-0.82461	0.14830	-0.11504	-0.46509	-0.07057	-0.17120	0.96580
Vitrinite, vol. % mmf	-0.28752	-0.93024	0.04073	-0.05931	0.04440	0.16765	0.98327
Inertinite, vol. % mmf	-0.04300	0.83339	0.38738	0.30992	-0.13933	-0.07531	0.96759
Liptinite, vol. % mmf	0.64917	0.41273	-0.48822	-0.29639	0.11348	-0.07041	0.93581
Sum λ_i^2	6.15261	2.03208	1.21799	1.01594	0.77957	0.43178	
% Variation explained	51.27173	16.93399	10.14989	8.46619	6.49643	3.59814	
Cumulative % variation	51.27173	68.20572	78.35561	86.82179	93.31821	96.91634	

Table IV-7b. Rotated matrix of factor loadings of the R-mode component analysis of Eastern province coals

	F 1	F 2	F 3	F 4	F 5	F 6	h_i^2
Reflectance, % in oil	-0.69473	0.03212	-0.15735	0.52908	0.22783	0.33281	0.95103
Carbon, % dmmf	-0.86130	-0.05417	-0.08954	0.38548	0.26254	0.14219	0.99054
Hydrogen, % dmmf	0.40823	-0.04691	0.09569	-0.82581	-0.24889	-0.06919	0.92670
Oxygen, % dmmf	0.92985	0.05304	-0.07854	-0.30390	-0.03403	-0.13685	0.98584
Sulfur, % dmmf	0.16377	-0.01956	0.09531	-0.06887	-0.96297	-0.08819	0.97613
Nitrogen, % dmmf	0.07565	0.12673	0.57545	-0.08630	-0.09618	-0.08364	0.99699
Volatile matter, % dmmf	0.63209	-0.02503	0.13091	-0.67604	-0.24482	-0.13745	0.95315
Moisture, % mmf	0.45103	-0.18063	0.11438	-0.11178	-0.11759	-0.84947	0.99707
Btu/lb, % dmmf	-0.95800	-0.01655	-0.09498	0.08271	0.01741	0.17775	0.96580
Vitrinite, vol. % mmf	-0.04684	-0.88863	-0.03899	0.42558	-0.08552	-0.03820	0.98327
Inertinite, vol. % mmf	0.01312	0.95546	0.11580	0.16582	-0.04067	0.10934	0.96758
Liptinite, vol. % mmf	0.19985	0.19161	0.00637	-0.91637	0.13296	-0.04123	0.93581
Sum λ_i^2	3.35132	1.79823	1.06291	2.73973	1.22121	0.95648	
% Variation explained	32.09433	14.98521	8.85755	22.83107	10.17678	7.97068	
Cumulative %	32.09433	47.07953	55.93707	78.76814	88.94492	96.91559	

Table IV-8a. Original matrix of factor loadings of the R-mode component analysis of Interior Province coals

	F 1	F 2	F 3	F 4	F 5	F 6	F 7	F 8	h_i^2
Reflectance, % in oil	0.43423	0.53835	-0.39945	-0.26503	0.17203	0.44557	0.08389	-0.13347	0.96116
Carbon, % dmmf	0.88398	-0.19993	-0.19966	0.12075	-0.21066	-0.26771	-0.01328	-0.02215	0.99255
Hydrogen, % dmmf	-0.17266	-0.18722	0.18570	-0.85839	0.29981	-0.09556	-0.12837	-0.19018	0.98784
Oxygen, % dmmf	-0.75754	0.56165	0.07329	-0.21791	0.02615	0.09577	-0.11640	0.15574	0.98984
Sulfur, % dmmf	-0.33388	-0.23685	0.11126	0.63517	0.59098	0.10352	0.15625	-0.17051	0.99685
Nitrogen, % dmmf	-0.04218	-0.57265	0.16513	-0.18094	-0.50162	0.53295	0.25544	-0.01417	0.99083
Volatile matter, % dmmf	-0.07475	-0.65854	0.54749	-0.25133	0.27848	-0.12088	0.22092	0.14247	0.96344
Moisture, % mmf	-0.74315	-0.15379	0.05696	0.04905	-0.50779	-0.29221	0.01156	-0.22826	0.97705
Btu/lb, % dmmf	0.91948	-0.14663	0.05959	-0.20792	0.07043	-0.17367	0.06570	-0.02124	0.95375
Vitrinite, vol. % mmf	-0.30035	-0.65822	-0.65452	-0.11754	0.14884	0.00289	-0.00524	0.05675	0.99108
Inertinite, vol. % mmf	0.38225	0.16529	0.84098	0.16603	-0.04939	0.19139	-0.20991	-0.04592	0.99350
Liptinite, vol. % mmf	-0.06785	0.83549	0.11713	-0.14115	-0.02252	-0.25746	0.43699	-0.00431	0.99405
Sum λ_i^2	3.33114	2.70176	1.73483	1.47543	1.13088	0.81635	0.41534	0.18620	
% Variation explained	27.75948	22.51462	14.45688	12.29523	9.42399	6.80289	3.46119	1.55167	
Cumulative %	27.75948	50.27409	64.73096	77.02618	86.45016	93.25304	96.71422	98.26588	

Table IV-8b. Rotated matrix of factor loadings of the R-mode component analysis of Interior Province coals

	F 1	F 2	F 3	F 4	F 5	F 6	F 7	F 8	h_i^2
Reflectance, % in oil	0.06226	0.57430	-0.03644	-0.07240	0.73700	0.02163	0.24355	0.13387	0.96114
Carbon, % dmmf	0.93347	0.07628	0.02246	0.20247	0.09949	-0.06564	-0.07820	0.23138	0.99254
Hydrogen, % dmmf	-0.13118	-0.19395	-0.08626	-0.94890	0.03571	0.00864	-0.02487	0.16397	0.98783
Oxygen, % dmmf	-0.92836	0.08261	0.01879	-0.09424	-0.06792	-0.17509	0.22853	0.15627	0.98983
Sulfur, % dmmf	-0.16964	-0.16832	-0.04093	0.15482	-0.03139	-0.10385	-0.13738	-0.93992	0.99684
Nitrogen, % dmmf	0.03393	-0.13536	-0.01399	-0.02293	-0.10830	0.95175	-0.20803	0.09892	0.99082
Volatile matter, % dmmf	0.11474	-0.79882	0.06185	-0.42298	-0.09363	0.24657	-0.10514	-0.21872	0.96343
Moisture, % mmf	-0.36736	0.03368	-0.16890	-0.01403	-0.88481	0.15893	0.05333	0.03501	0.97704
Btu/lb, % dmmf	0.55032	-0.09775	0.17533	-0.16463	0.34754	-0.03602	0.04328	0.19835	0.95373
Vitrinite, vol. % mmf	0.50772	-0.09472	-0.87489	-0.11215	-0.06219	0.12397	-0.41441	-0.11425	0.99107
Inertinite, vol. % mmf	0.11327	-0.11912	0.97399	0.00309	0.08044	0.06562	-0.07485	-0.03778	0.99349
Liptinite, vol. % mmf	-0.22019	0.12864	0.17660	0.03240	0.06103	-0.24945	0.89982	0.14540	0.99404
Sum λ_i^2	2.71677	1.11147	1.81587	1.19987	1.49921	1.12138	1.18320	1.14001	
% Variation explained	22.63974	9.26223	15.16554	9.99892	12.49339	9.34479	9.86004	9.50012	
Cumulative %	22.63974	31.90196	47.06750	57.06642	69.55980	78.90459	88.76462	98.26474	

Table IV-9a. Original matrix of factor loadings of the R-mode component analysis of Western coals

	F 1	F 2	F 3	F 4	F 5	F 6	h_i^2
Reflectance, % in oil	0.89704	-0.17555	0.15352	0.13232	-0.08644	-0.15208	0.90874
Carbon, % dmmf	0.95746	-0.12317	-0.16762	-0.01772	0.07921	-0.00099	0.96658
Hydrogen, % dmmf	0.75483	0.43492	-0.29349	-0.10510	0.20595	0.17304	0.93143
Oxygen, % dmmf	-0.97495	0.05897	0.15050	0.04096	-0.01224	-0.04631	0.98063
Sulfur, % dmmf	-0.00385	-0.32477	-0.67327	-0.44367	-0.47950	-0.10512	0.99660
Nitrogen, % dmmf	0.65468	0.11095	0.48403	0.10089	-0.43798	0.34291	0.99479
Volatile matter, % dmmf	-0.55835	0.35180	-0.62863	-0.14796	0.11014	0.26198	0.94050
Moisture, % mmf	-0.93105	0.00948	0.16036	0.01459	-0.12439	0.14048	0.92807
Btu/lb, % dmmf	0.96830	-0.00596	-0.18794	-0.06314	0.07667	0.03593	0.98411
Vitrinite, vol. % mmf	0.09079	0.94826	0.15685	-0.17174	-0.09238	-0.15811	0.99506
Inertinite, vol. % mmf	-0.06268	-0.96003	0.08137	-0.14284	0.16060	0.12266	0.99344
Liptinite, vol. % mmf	-0.06728	-0.01595	-0.62428	0.76517	-0.13531	-0.01529	0.99854
Sum λ_i^2	5.80322	2.30853	1.72970	0.89904	0.56418	0.31379	
% Variation explained	48.36014	19.23770	14.41420	7.49204	4.70151	2.61494	
Cumulative %	48.36014	67.59784	82.01202	89.50406	94.20555	96.82048	

Table IV-9b. Rotated matrix of factor loadings of the R-mode component analysis of Western coals

	F 1	F 2	F 3	F 4	F 5	F 6	h_i^2
Reflectance, % in oil	0.75728	-0.06677	0.54836	0.01378	-0.26377	-0.50862	0.90873
Carbon, % dmmf	0.95522	-0.08424	-0.04927	0.01622	-0.13348	-0.16288	0.96657
Hydrogen, % dmmf	0.84488	0.36327	0.06153	-0.01451	-0.06879	0.27732	0.93142
Oxygen, % dmmf	-0.95378	0.02064	0.07189	0.00216	0.21430	0.13933	0.98063
Sulfur, % dmmf	0.09414	-0.17362	-0.96296	0.06517	0.09284	0.13204	0.99659
Nitrogen, % dmmf	0.37260	0.13778	0.12749	-0.11900	-0.85440	-0.27667	0.99478
Volatile matter, % dmmf	-0.30365	0.22257	-0.22466	0.18526	0.29301	0.79158	0.94049
Moisture, % mmf	-0.93715	-0.04857	0.01942	-0.01088	0.01741	0.21600	0.92807
Btu/lb, % dmmf	0.97465	0.01923	-0.05246	-0.01347	-0.15124	-0.08932	0.98410
Vitrinite, vol. % mmf	0.03333	0.96570	0.10467	-0.21381	-0.04598	0.05084	0.99505
Inertinite, vol. % mmf	-0.03618	-0.96645	-0.09174	-0.18416	0.05367	-0.11357	0.99344
Liptinite, vol. % mmf	0.02533	-0.02049	-0.06400	0.98829	0.08196	0.09970	0.99853
Sum λ_i^2	5.18057	2.11235	1.03433	1.11154	0.99741	1.18218	
% Variation explained	43.17142	17.60294	8.51940	9.26285	8.31178	9.85152	
Cumulative %	43.17142	60.77435	69.39375	78.65660	86.96837	96.81989	