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ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois 60439

**USERS HANDBOOK FOR THE
ARGONNE PREMIUM COAL SAMPLES**

by
Karl S. Vorres
Chemistry Division

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USERS HANDBOOK FOR THE ARGONNE PREMIUM COAL SAMPLES

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1. ABSTRACT

This Users Handbook for the Argonne Premium Coal Samples provides the recipients of those samples with information that will enhance the value of the samples, to permit greater opportunities to compare their work with that of others, and aid in correlations that can improve the value to all users. It is hoped that this document will foster a spirit of cooperation and collaboration such that the field of basic coal chemistry may be a more efficient and rewarding endeavor for all who participate.

The different sections are intended to stand alone. For this reason some of the information may be found in several places.

The handbook is also intended to be a dynamic document, constantly subject to change through additions and improvements. Please feel free to write to the editor with your comments and suggestions.

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2. THE EIGHT COALS IN THE ARGONNE PREMIUM COAL SAMPLE PROGRAM*

(adapted from a paper in Energy & Fuels 4, 420-426 (1990))

* Work performed under the auspices of the Office of Basic Energy Sciences, Division of Chemical Sciences, U. S. Department of Energy, under contract number W-31-109-ENG-38.

ABSTRACT

The full set of eight coals for the Premium Coal Sample Program includes a lignite, subbituminous, high volatile, medium volatile and low volatile bituminous, as well as a liptinite-rich, an inertinite rich and a coking coal. The coals were selected on the basis of C, H, S and O contents as well as maceral content and geological age. Ampoules containing 5 grams of -100 mesh or 10 grams of -20 mesh material from each sample are available. Some analytical information is available. The methods of selection, collection, transportation, processing, packaging, distribution and characterization are summarized. The eight samples were each collected in about 1 to 1 1/2 ton quantities, placed in steel drums, purged with argon and taken to Argonne National Laboratory (ANL) for processing. After transfer to a nitrogen-filled enclosure, they were crushed, pulverized, mixed and packaged in sealed amber borosilicate ampoules. Five-gallon carboys hold about 80% of the batch in reserve for filling more ampoules after the original samples (about 5,000 of -20 mesh or 10,000 of -100 mesh) are depleted. More than 350 researchers in various groups are or have been participating in the research with these samples. Over 760 shipments totalling over 20,000 ampoules have been made by October 1993 to more than 110 different organizations for a range of programs in basic coal research.

2.1. Introduction

The Premium Coal Sample Program is intended to provide the basic coal research community with the highest quality samples of a limited number (8) of coals for basic research. The availability of the ampoules is the result of the cooperation of many individuals within a number of organizations whose efforts made the high quality of the samples possible.

The need for a Premium Coal Sample Program was expressed on a number of occasions, culminating in the Coal Sample Bank Workshop held March 27 and 28, 1981 in Atlanta, Georgia. Funding was later made available from the Division of Chemical Sciences of the Office of Basic Energy Sciences of the U. S. Department of Energy for the program. The premium coal samples produced from each coal and distributed through this program are chemically and physically as identical as possible, have well-characterized chemical and physical properties, and will be stable over long periods of time. To achieve these goals, coals have been mined, transported, processed into the desired particle and sample

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sizes, packaged in humid nitrogen environments as free of oxygen as possible, and carefully characterized by a variety of techniques.

One of the reasons for preparing these samples was to permit workers to determine if the apparent difference in results between two laboratories was due to the samples or the experimental technique.

The premium coal reference splits produced from each coal sample and distributed through this program are chemically and physically as identical as possible, have well-characterized chemical and physical properties, and will be stable over long periods of time. To achieve these goals, coal samples were mined, transported, processed into the desired particle and sample sizes, packaged in humid nitrogen environments as free of oxygen as possible, and carefully characterized by a variety of techniques.

2.2. Selection of the Coals

It was decided to include a set of eight coals in the program. The selection of these eight coal samples was based on those parameters which would represent significant differences among the available coal types mined in the United States and maximize our understanding of the fundamental properties of coal. A cluster analysis of whole coal seam data from the Pennsylvania State Coal Sample Data Base was carried out with data from 200 samples to establish desirable choices in terms of the significant compositional parameters, C, H, O and S. Using increasing carbon and decreasing oxygen on one axis and hydrogen and sulfur content on the other, the cluster analysis provided identification of compositional characteristics for eight coal samples. These composition characteristics are listed in Table I and were used to select the set of initial sample choices.

The list was then examined to consider the variety of maceral contents which exist in U. S. coal types. There are three important maceral groups, vitrinite, liptinite and inertinite.

With help from the U. S. Geological Survey, individual coals were identified for collection. The compositional characteristics, primarily carbon content, were used to guide the selection of five of the coals. These provided a rank range from lignite through low volatile bituminous. Anthracites were not included because of their low reactivity and relative scarcity. The other three were selected to give a range of sulfur contents, a larger content of macerals other than vitrinite, and a range of bituminous coals with varied paleobotanical source material. Within the compositional constraints from the cluster analysis one of the samples was selected for its known coking properties. A short description of the source of the samples is given in a later section. Table II gives the identity of these samples and some of their characteristics. Samples #1,2,3,5 and 8 were

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selected to give a range of compositional parameters, primarily carbon, hydrogen and oxygen, which vary with the degree of coalification of the sample. In addition #3 provides a sample with a relatively high sulfur content. Coal #4 was also selected for its known good coking properties, coal #6 was selected for high liptinite and #7 for high sporinite and inertinite contents.

2.3. Collection of Mine Samples

The actual collection of coal samples began by identifying the potential sources of coal samples and seeking permission to acquire the samples. At least one staff geologist from the U. S. Geological Survey was present at each site for supervision of the actual collection of the sample and to document the seam for later description in USGS Circulars which will provide a permanent, referenceable description of the sample.

For a typical underground sample, an initial meeting with the mine operator both clarified the plan and minimized the time that the coal sample was exposed to the air. On the morning of the collection, the coal bed face was freshly exposed, by cutting back through about 8' of coal, to provide a block of coal the entire thickness of the coal bed, about 12-18" wide and long enough to provide for the 1 ton sample. The bed was exposed with a continuous miner, and a roof bolter immediately followed to secure the seam roof. The loose coal was scraped away from the sample block, and several layers of plastic were placed on the mine floor. After measuring and calculating the amount needed for the sample, the block was marked for removal by the USGS representative. The block was then removed by the collection crew with hand picks from the roof to the floor to provide a channel-type sample. Particular care was taken to avoid contamination of the sample with nearby material. When the bed thickness exceeded four feet (Illinois #6, Pittsburgh, Pocahontas, Blind Canyon and Lewiston-Stockton), stainless steel drums were taken into the mine for sample collection. For the first sample (Upper Freeport) only, double plastic bags were used to transport the coal to the surface. In all cases, the coal samples were loaded into 55-gallon stainless steel drums from 1/2 to 5 hours after collection and then the drums were purged with argon. An additional supply of chunks of coal in a 15 gallon container was obtained from each coal bed for experimenters who need larger pieces for their work.

The subbituminous sample was collected as a 6" core sample from the Wyodak-Anderson seam that was about 120' thick at the sample site. The drilling contractor also obtained two additional 3" cores, one for the USGS, and the other for long-term storage of the sample. All cores were rinsed with distilled, deaerated water immediately after they were released from the core barrel and loaded into the stainless steel drums for purging and shipment.

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The lignite sample was obtained as a series of 3" core-type samples drilled through the 18 foot thick seam at about 20' intervals over a freshly exposed top surface. Cold weather limited reactions at the surface. This approach provided channel-type samples representative of a sample area of about one acre. The samples were also quickly loaded into the drums and purged with argon.

2.4. Sample Descriptions

The first sample is an Upper Freeport seam, medium-volatile bituminous coal which was collected from an underground mine near Homer City (Indiana County) Pennsylvania in January 1985. The seam was 4' thick where it was sampled. The sample was collected in special double-plastic bags and transferred to the stainless steel drums at the surface.

The second sample is from the Wyodak-Anderson seam, a sub-bituminous coal collected about 6 miles northeast of Gillette, (Campbell County) Wyoming in October 1985. The seam was about 120' thick at the collection site. The sample for processing consisted of a 6" core sample through the entire seam.

The third sample is a high-volatile bituminous coal, from the Illinois #6 or Herrin seam, and was collected about 60 miles southeast of St. Louis in St. Clair County in Illinois in December 1985. The 55-gallon drums were taken into the underground mine for this and all subsequent underground mines because the seam was 7' thick at the Illinois site and at least 6' thick for all other underground samples. The original sample was a block which weighed at least 4 tons. The initial 3 tons were mechanically mined (resulting in a higher mineral matter content) and became the Illinois Basin Coal Sample 105 (fifth in a series of samples). This sample was processed in the nitrogen-filled glove box to provide -20 mesh material which was placed in sealed 5 gallon, one-gallon and one-pint (pound) containers. The final ton was hand-picked in the usual fashion for the premium samples.¹

The fourth sample (high-volatile bituminous) was obtained underground from the Pittsburgh seam (sometimes referred to as Pittsburgh #8) and was collected about 60 miles south of Pittsburgh in Greene County, Pennsylvania in March 1986. This seam was 6' thick at the collection site. The sample drums were taken into the mine for loading.

The fifth sample is a low-volatile bituminous from the Pocahontas #3 seam, collected underground in Buchanan County, Virginia in June 1986. This seam was 6' thick at the collection site and the drums were loaded in the mine.

1. Information on price and availability of these samples may be obtained from the Illinois State Geological Survey, 615 E. Peabody Drive, Champaign, IL 61820.

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The sixth sample (high-volatile bituminous) is an underground Blind Canyon seam sample collected in Emery County, Utah about 150 miles southeast of Salt Lake City in August 1986. The seam was about 7' thick at the collection site. Drums were loaded in the mine.

The seventh sample (high-volatile bituminous) is from the Lewiston-Stockton seam of the Kanawha formation. This was collected underground about 20 miles east of Charleston in Kanawha County, West Virginia in October 1986. The seam was about 6' thick at the collection site and the drums were loaded in the mine.

The eighth sample is a lignite from the Beulah-Zap seam collected in Mercer County, North Dakota, about 8 miles northwest of Beulah in November 1986. The seam was about 18' thick at the collection area. Collection was done by accumulating about 50 3" core samples spaced about 20' apart in each direction. Samples were immediately placed in the stainless steel drums.

2.5. Purging and Transportation of Mine Samples

The 55 gallon drums were fitted with "quick-connect" fittings on the side which led to a steel tube terminating about 1" from the bottom of the inside of the drum. The top of the drum was fitted with a welded tee attached to a valve and a pressure gauge. The drum top was fitted with a special high density gasket to maintain a gas tight seal (2). The purging of the air was done by attaching several drums in series and connecting them to a cylinder of 99.999% argon gas. The gas flow path was in through the fitting to the bottom of the drum and around the coal to exit at the valve. The argon was passed through the drums for at least the volume required to convert air in empty drums to 100 ppm of oxygen assuming perfect mixing during the purging. Following the purging the drums were tested for holding pressure at 6 psig and transported to ANL. Purging typically required 1-2 hours.

All samples were transported by the same truck and driver. The truck was loaded at ANL with stainless steel drums, argon cylinders and tools and then driven to the mine site. The sealed drums were then transported in a refrigerated semitrailer at temperatures of 40-45° F to prevent freezing and limit chemical reactions on the way to the processing facility at ANL. The samples arrived at the laboratory within one-half to two days of the collection and argon purging, and were immediately unloaded.

2.6. Preparation of Research Samples

The drums were unloaded from the truck, weighed and placed into an airlock in a nitrogen-filled processing and packaging facility. This facility is a large enclosure in two parts, each of which was constructed of sheets of aluminum and clear plastic

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windows. Seventy pairs of long rubber gloves mounted in the windows permit manipulation of the samples and equipment during the processing. The dimensions of the facility are about 5-6' wide, 13' high and the equivalent of 40' long. The processing and packaging sections are separated by a sealed mixer-blender. Oxygen control is part of the gas-handling system design which includes a cyclone separator, high-efficiency particulate filter, industrial blower and cooling coils, as well as steam supply for humidity control. A part of the gas stream is passed over a palladium-on-alumina catalyst with a slow stream of hydrogen to react with and convert the trace amounts of oxygen to steam. The oxygen content of the facility was maintained below 100 ppm, and typically was about 30 ppm. Gas concentrations were monitored with an oxygen fuel-cell type analyzer (Teledyne Trace Oxygen Analyzer), hydrogen (Control Instruments) and hydrocarbon monitor (Beckman Hydrocarbon Analyzer). Separate temperature and humidity indicators were used for each of the two enclosures.

The processing consisted of several steps starting with the crushing and pulverizing the coal to -20 mesh, and mixing the entire ton-sized batch. This batch was then placed into containers. Half of the batch was placed in sealed 5 gallon pails for regrinding to -100 mesh and subsequent packaging. Each half ton was sealed partly (about 80%) in 5 gallon glass carboys for long term storage and the balance in ampoules for distribution to researchers. Details of the processing follow.

After the airlock was purged with nitrogen, the drums were opened, and the contents were transferred to a rotating bar crusher (Jacobsen) using a hydraulic drum dumper (Tubar). The sample was reduced to pieces that would pass between bars with 1/2" openings. The flow of crushed coal to the elevator was regulated with an adjustable gate. The sample was raised with a vibrating lift (FMC Syntron) to the pulverizer (Fitzmill model D) where it was initially ground to pass through a 20-mesh screen. With the exception of the lignite, the entire one-ton batch used for processing was ground and accumulated in a 2000-liter mixer-blender (Littleford). After thorough (established by previous testing program) four-minute mixing the sample was transferred by a tubular conveyer (Dynamet) to a second nitrogen-filled enclosure. This tubular conveyor was used for the last 7 samples. Difficulty with transporting fine material on a second vibrating lift necessitated the equipment substitution. About half the batch was transferred to 5-gallon leverlock pails for transfer back to the initial airlock for later repulverizing to -100 mesh. About 80% of the balance was placed into 5-gallon borosilicate glass carboys for long-term storage. About 5,000 ampoules containing 10 grams of -20 mesh samples were sealed with a hydrogen-oxygen torch. The flame was kept at the stoichiometric composition with a mass flow controller (Linde mass flowmeter/flow controller). The half batch that was transferred to the initial airlock was pulverized to pass a 100-mesh screen and accumulated again in the mixer-blender. After mixing, the -100 mesh material was transferred to the second enclosure

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for placing into 5-gallon borosilicate carboys and into 10,000 ampoules of 5 grams of -100 mesh material. The ampoule filling-sealing system was built by Kuchar Industrial Service and Supply of Joliet, Illinois. The control system was extensively modified by ANL personnel to provide computer control for ease of changing control parameters. Filling of the ampoules was done with a Mateer-Burt system which uses computer control for the amount of pulverized coal dispensed to each ampoule. The carboys were stoppered with special stopcock assemblies to retain the nitrogen atmosphere after removal from the nitrogen-filled enclosure. The ANL glassblower sealed the carboys for long-term storage. Samples were taken during the processing for homogeneity analyses to establish the uniformity of the samples during the processing and sealing.

The North Dakota Beulah-Zap sample was obtained as a series of channel type samples in each drum. The high moisture content of this coal precluded processing through two successive stages of grinding. The moist material would have accumulated on the pulverizer screen and prevented the final grinding. Instead, one half of the batch was processed for -20 mesh material and the other half batch was ground just once to provide the -100 mesh sample. The high moisture content of the Wyodak sample led to limited production of the -100 mesh material and processing of the material from carboys of -20 mesh with a small pulverizer after the lignite sample. This activity resulted in the production of 4,000 of the -100 mesh ampoules.

Additional processing during the summer of 1991 of material in the carboys provided an additional 8,000 of the -100 mesh Wyodak and 2,000 of the -100 mesh Illinois #6 samples.

2.7. Sample Storage

The samples and borosilicate carboys are kept in racks in a dark storage room that is kept close to 72°F year round. The borosilicate carboys can be used to replenish supplies of the ampoules whenever needed to sustain the inventory for shipments. It is expected that about 75,000 ampoules can be provided from each sample. This quantity of ampoules can meet requests for 30 ampoules per work day of each coal for the next decade and is expected to meet the actual demand for a substantially longer period.

2.8. Analysis of Samples

Three types of analyses were made. These were to indicate homogeneity of mixing, elemental and proximate analysis data, and stability of the samples as well as integrity of the seals.

Homogeneity Analyses

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For the homogeneity analyses, a series of 39 samples was taken during the processing of each coal sample to determine whether there were any differences in composition during the processing and packaging of the thoroughly-mixed material. The as-received moist samples to be tested for homogeneous mixing were irradiated by neutrons at the University of Illinois TRIGA reactor and the induced radioactivity of several species was counted at the ANL Analytical Chemistry Laboratory to indicate the relative content of selected elements in each sample. The radioactive species that were counted varied from sample to sample depending on the relative abundance of the inorganic constituents in the sample. The species included ^{24}Na , ^{42}K , ^{46}Sc , ^{76}As , and ^{140}La . Results were calculated in terms of disintegrations per minute per gram (DPM/g) of sample. The multiplier gives the factor by which the DPM/g should be multiplied. Table III gives the results of the analyses.

As a further test of homogeneity the last three irradiated samples were also analyzed for percent S, gross calorific value, moisture, and ash at the ANL Analytical Chemistry Laboratory. The values are given in Table IV.

The samples for the analyses reported in Table IV were not kept in a vessel at constant humidity, resulting in significant differences in the measured moisture content from fresh samples, but were expected to be consistent within the sample set.

The values given for the standard deviation/average value provide a useful measure of the consistency of the homogeneity of the samples for the given analyses.

Proximate and Elemental Analyses

Additional samples were submitted for a range of analyses including: proximate, ultimate, major and minor elements in the ash, heat content, forms of sulfur, and maceral analysis. A large number of laboratories participated in the analytical studies. The analytical data are given in Table V.

The data from the analyses can be used to calculate empirical formulae based on the organic material in the coal and on the basis of 100 carbon atoms per "formula weight". The formulae for the samples in order of increasing H/C are given below:

	Carbon	Hydrogen	Oxygen	Nitrogen	Sulfur
Pocahontas	100	58.5	2.0	1.2	0.2
Upper Freeport	100	66.0	6.6	1.6	0.3
Lewiston-St.	100	76.3	8.9	1.6	0.3
Pittsburgh	100	76.7	8.0	1.7	0.4
Illinois #6	100	77.3	13.1	1.5	1.2
Beulah-Zap	100	79.5	20.9	1.4	0.4
Wyodak-And.	100	85.6	18.0	1.3	0.2
Blind Canyon	100	85.7	10.8	1.7	0.2

Integrity of Seals and Long Term Stability

In order to establish the integrity of the seals, additional work is being done at the Analytical Chemistry Laboratory of the ANL which includes the evaluation of the gas atmosphere inside the ampoules initially at approximately six month intervals (3) and later at annual or longer intervals. Particular attention is given to the oxygen content to ascertain potential oxidation. Ampoules were placed in an evacuable chamber, evacuated and the glass containers broken to release the contained gases. Until 1991 these gases were analyzed with a CEC mass spectrometer to indicate the content of different gases. Starting in 1991 data were taken with a VG Gas Analysis mass spectrometer model 30-01. Analytical data were given for nitrogen, oxygen, methane, moisture, hydrogen, carbon dioxide, argon and heavier hydrocarbons. Data for carbon monoxide were not given initially because the CEC mass spectrometer cannot differentiate it from nitrogen. The results indicated that the oxygen is always at or below the limits of detection (30-50 ppm). The carbon monoxide is usually at or below the limits of detection (.05%). The carbon dioxide content has increased in the low rank coals and the Pittsburgh as well as the Pocahontas sample over a multiyear period. The methane content has increased for the higher rank coals. The hydrogen content was substantial in the Pittsburgh and Pocahontas samples.

2.9. Reproducibility of Analytical Data

Samples are distributed as 5-gram ampoules of -100 mesh or 10-gram ampoules of -20 mesh material.

The importance of sample mixing must be stressed. All coal samples are subject to segregation on standing. It is necessary to remix the sample before opening the ampoule. The recommended method is to turn the ampoule so that the coal alternately falls into the top and then the body of the ampoule. This should be repeated a number of times (at least 10). Rolling the ampoule on its side is not as effective and should not be relied upon for thorough mixing.

The standard deviations and reproducibilities of the analytical data as reported by Commercial Testing and Engineering Company are given in Table VI. These represent the results from evaluation of the data from as many as 60 different laboratories which are part of the Company.

The samples are intended to be used immediately after opening for all work involving air-sensitive properties. Any unused portion should be discarded, as the original properties may change on further storage.

2.10. Long Term Supply

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One of the important characteristics of a sample supplier is the ability to make the samples available over a long period of time. The preparation of sample material was planned to provide for the equivalent of 50,000 of 5 gram ampoules and 25,000 of the 10 gram ampoules. This is accomplished by the initial preparation of 10,000 of the 5 gram ampoules and 5,000 of the 10 gram ampoules. The balance of the ampoules will be prepared by placing an appropriate number of the 5 gallon carboys into the nitrogen filled enclosure. Each carboy holds about 10 kilograms. The carboys will be opened in the nitrogen filled environment, remixed and sealed into more ampoules to replenish the inventory. At the time of the writing the inventory of sealed ampoules is expected to be at least 15 years for the most-ordered samples (Illinois #6 and Wyodak-Anderson -100 mesh).²

2.11. Information Dissemination

Newsletters and Users Handbooks (1) are sent without charge to recipients of Argonne Premium Coal Samples and individuals who have asked to be included in the mailing list.³

2.12. Microbes in the Samples

The observation of carbon dioxide in some ampoules and methane in others led to an effort to examine the samples for the presence of microbes which might have produced these gases. Samples of each coal in each particle size were placed in anaerobic conditions with culture media selected to allow the growth of bacteria which may have been present. After suitable times the samples were examined and some growth was observed in the three lowest rank samples (Beulah-Zap, Wyodak-Anderson and Illinois #6). The samples were checked and sent to the Anaerobic Microbiology Department at Virginia Polytechnic Institute. Cultures prepared from these samples were found to belong to the genus Clostridium and were of a previously unidentified species. It is believed that these samples belonged to the same species. It is possible that some of the bacteria were introduced with the sample #2 (Wyodak-Anderson) and inoculated the processing equipment which led to the observation of these bacteria in some, but not all, of the later samples. The equipment was thoroughly cleaned, but not sterilized, under aerobic conditions between the processing of successive coals.

2.13. Acknowledgments

2. Information on the price and availability of the samples may be obtained from the author.

3. Individuals who wish to be placed on the mailing list or receive a copy of the Handbook should write the author.

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The sponsorship of the U. S. Department of Energy, Office of Basic Energy Sciences, Chemical Sciences Division is gratefully appreciated. The work was performed under contract number W-31-109-ENG-38. The efforts of many who made the program work as effectively as it has must also be mentioned. These include the original planners: Phil Horwitz, John Unik, Randall Winans, Gary Dyrkacz and John Young; the Advisory Board, who met with the manager and sponsor, C. Blaine Cecil, USGS; John Larsen, Lehigh University; Marvin Poutsma, Oak Ridge National Laboratory; Ronald Pugmire, University of Utah; William Spackman, Pennsylvania State University; Leon Stock, University of Chicago; Irving Wender, University of Pittsburgh; Randall Winans and John Young, Argonne National Laboratory; the staff of the U. S. Geological Survey, who supervised and participated in the sample collection: C. Blaine Cecil, Brenda Pierce, Ron Stanton and Peter Warwick; the coal companies who generously made samples available: Rochester and Pittsburgh Mining Company, Peabody Coal Company, Coteau Properties, Inc. and others; many individuals involved in the design and construction of the processing facility: Herbert Brown, K. Michael Myles, Gale Teats, Kurt Schultz, Ed Lewandowski, Mike Slawacki, Rich Graczyk, Pat Doolin; the sample collection crew from the Pittsburgh Testing Laboratory: David Allen, Tim Graham, Ron Lowman; the truck driver: Randy Engelhart; those who assisted with the coal processing: Gale Teats, Kurt Schultz, Don Piatak, Wally Czyz, Stuart Janikowski, Freddie Morris, Dmitry Silversteyn, Bart Beals, David Clow, James Krizek, and Mark Kopciewski; the glassblower: Joe Gregar; cluster analysis: Paul Neill; homogeneity analyses: Bob Heinrich; chemical analyses: Peter Lindahl and Toni Engelkemeir; computer programming: Paul Day and Miriam Bretscher.

Appreciation is expressed to Butterworth-Heinemann and to the American Chemical Society for permission to publish tables and graphs in the Analytical Data section.

2.14. References

- (1) Vorres, K.S. Users Handbook for the Argonne Premium Coal Sample Program, **1989** ANL/PCSP-89/1, Oct., available from the National Technical Information Service.
- (2) Harvey, R.D.; Kruse, C.W. J. Coal Qual. **1988** 7 109
- (3) Vorres, K.S. Proc. 1989 Intl. Conf. Coal Science, **1989** II 1083

Additional references from the "Bibliography on Work with the Argonne Premium Coal Samples" (see Section 5) providing general information on the Argonne Premium Coal Sample Program include numbers: 4, 12, 13, 34 (Illinois Basin Coal Sample Program), 43, 62, 75, 76, 77, 78, 79 (model for biomass), 81.

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Table I. Results of Cluster Analysis For Selection of Samples

Group	% Carbon	% Hydrogen	% Sulfur*	% Oxygen**
1	73.6 $\pm$ 1.5	4.9 $\pm$ 0.2	0.5 $\pm$ 0.2	20.0 $\pm$ 1.5
2	74.5 $\pm$ 1.9	5.6 $\pm$ 0.5	1.1 $\pm$ 0.4	17.5 $\pm$ 2.0
3	79.0 $\pm$ 1.7	5.5 $\pm$ 0.4	4.4 $\pm$ 0.3	10.0 $\pm$ 1.5
4	79.2 $\pm$ 2.0	5.6 $\pm$ 0.4	0.9 $\pm$ 0.6	12.8 $\pm$ 2.0
5	82.7 $\pm$ 2.0	5.7 $\pm$ 0.4	1.3 $\pm$ 0.6	8.1 $\pm$ 1.8
6	85.4 $\pm$ 1.4	5.4 $\pm$ 0.3	0.8 $\pm$ 0.3	6.8 $\pm$ 1.4
7	89.6 $\pm$ 1.0	4.9 $\pm$ 0.3	0.8 $\pm$ 0.3	3.2 $\pm$ 1.0
8	91.3 $\pm$ 0.5	4.3 $\pm$ 0.2	0.7 $\pm$ 0.2	2.3 $\pm$ 0.6

* Organic

** By difference

Table II. Argonne Premium Coal Samples and Some Characteristics

#	Seam	State	Rank	C	H	O	S	Ash
1	Upper Freeport	PA	Med. Vol. Bit.	86	4.7	8	2.3	13
2	Wyodak-Anderson	WY	Subbituminous	75	5.4	18	0.6	9
3	Illinois #6	IL	High Vol. Bit.	78	5.0	14	4.8	15
4	Pittsburgh (#8)	PA	High Vol. Bit.	83	5.3	9	2.2	9
5	Pocahontas #3	VA	Low Vol. Bit.	91	4.4	2	0.7	5
6	Blind Canyon	UT	High Vol. Bit.	81	5.8	12	0.6	5
7	Lewiston-Stockton	WV	High Vol. Bit.	83	5.3	10	0.7	20
8	Beulah-Zap	ND	Lignite	73	4.8	20	0.8	10

The coal samples are listed in the order collected. The weight % C, H and O values are given on the moisture and ash-free basis, while S and ash are on the dry basis. The data were provided by Commercial Testing and Engineering, Inc., Lombard, IL from the results of analyses at 55 laboratories in their organization.

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Table III. Homogeneity Analyses of Coal Samples by Irradiation

Coal #1: Upper Freeport

Species Counted	Na	K	As
Multiplier:	10^6	10^6	10^5
Average:	3.870	4.430	3.987
Maximum:	4.286	4.853	4.267
Minimum:	3.631	4.131	3.748
Std. Dev.	0.1216	0.1526	0.1095
Std. Dev./Ave:	0.0314	0.0345	0.0275

Coal #2: Wyodak-Anderson

Species Counted	Na	As	La	Sc
Multiplier:	10^7	10^4	10^4	10^4
Average:	1.742	10.164	8.201	4.890
Maximum:	1.892	12.880	9.026	5.317
Minimum:	1.622	8.811	7.630	4.498
Std. Dev.	0.0504	0.8586	0.2792	0.1782
Std. Dev./Ave:	0.0289	0.0845	0.0340	0.0364

Coal #3: Illinois #6

Species Counted	Na	K	Sc	As	La
Multiplier:	10^7	10^6	10^4	10^5	10^5
Average:	2.236	6.189	1.028	1.828	1.382
Maximum:	2.469	6.984	1.114	2.058	1.500
Minimum:	2.010	5.465	0.931	1.625	1.250
Std. Dev.	0.122	0.370	0.049	0.118	0.073
Std.Dev./Ave:	0.0544	0.0598	0.0476	0.0647	0.0525

Coal #4: Pittsburgh

Species Counted	Na	K	Sc	As	La
Multiplier:	10^6	10^6	10^3	10^5	10^5
Average:	7.196	3.336	10.165	3.310	1.304
Maximum:	8.668	3.634	10.910	3.668	1.424
Minimum:	6.755	2.931	9.567	2.901	1.178
Std. Dev.	0.330	0.137	0.318	0.133	0.049
Std. Dev/Ave:	0.0458	0.0410	0.0313	0.0402	0.0376

Coal #5: Pocahontas #3

Species Counted	Na	Sc	As	La
Multiplier	10^7	10^3	10^5	10^5
Average:	1.160	4.583	2.752	0.960
Maximum:	1.411	4.900	2.993	1.017
Minimum:	1.006	4.142	2.284	0.898
Std. Dev.	0.084	0.189	0.167	0.029
Std. Dev/Ave:	0.0725	0.0413	0.0584	0.0295

Coal #6: Blind Canyon

Species Counted	Na	K	Sc	La
Multiplier:	10^7	10^5	10^3	10^4
Average:	1.390	3.493	1.531	3.166
Maximum:	1.520	5.108	1.703	3.438
Minimum:	1.29	2.389	1.398	2.882

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Std. Dev.	0.056	0.516	0.057	0.132
Std. Dev/Ave:	0.0404	0.1476	0.0372	0.0418

Coal #7: Lewiston-Stockton

Species Counted:	Na	K	Sc	As	La
Multiplier:	10^6	10^6	10^4	10^4	10^5
Average:	2.806	5.427	1.207	9.480	1.748
Maximum:	3.291	6.539	1.347	11.507	1.979
Minimum:	2.095	3.758	0.891	6.925	1.319
Std. Dev.	0.206	0.499	0.077	0.882	0.112
Std. Dev/Ave:	0.0736	0.0919	0.0636	0.0931	0.0643

Coal #8: Beulah-Zap

Species Counted:	Na	La	Sc
Multiplier:	10^7	10^4	10^3
Average:	3.461	1.847	1.129
Maximum:	4.218	2.370	1.318
Minimum:	3.021	1.671	0.968
Std. Dev.	0.256	0.153	0.075
Std. Dev/Ave:	0.0738	0.0828	0.0662

The calculated uncertainties (in percent) of the weighted average values for the DPM/g were 1.8% or less for counts with multipliers of up to 10^5 and equal to or less than 0.4% for multipliers of 10^6 or 10^7 .

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Table IV. Homogeneity Analyses for Last Three Coals from Sulfur, Gross Calorific Value, Moisture and Ash Data (as-received)

Analysis:	S (wt %)	GC Value (Btu/lb)	Moisture (wt %)	Ash (wt %)
Coal: Blind Canyon				
Average:	0.585	13,559	2.87	4.73
Maximum:	0.652	13,665	3.47	5.06
Minimum:	0.544	13,438	2.45	4.59
Std. Dev:	0.0212	49.9	0.24	0.124
SD/Ave:	0.0361	0.0037	0.0847	0.0263
Coal: Lewiston-Stockton				
Average:	0.699	11,549	1.46	19.62
Maximum:	0.800	11,630	1.86	19.99
Minimum:	0.645	11,387	1.04	19.40
Std. Dev:	0.0277	52.8	0.19	0.11
SD/Ave:	0.0396	0.0046	0.1278	0.0057
Coal: Beulah-Zap				
Average:	0.572	9,864	27.19	9.48
Maximum:	0.658	10,507	34.89	9.82
Minimum:	0.508	9,307	17.15	9.11
Std. Dev:	0.0395	300	4.645	0.148
SD/Ave:	0.0691	0.0304	0.171	0.0156

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Table V. Elemental and Proximate Analyses

Calculation of As-received, maf and Dmmf values from Dry Data from Commercial Testing and Engineering								
Coal	UF	WY	IL	PITT	POC	UT	WV	ND
AR H2O	1.13	28.09	7.97	1.65	0.65	4.63	2.42	32.24
AR Ash	13.03	6.31	14.25	9.10	4.74	4.49	19.36	6.59
AR VM	27.14	32.17	36.86	37.20	18.48	43.72	29.44	30.45
AR S	2.29	0.45	4.45	2.15	0.66	0.59	0.69	0.54
AR Btu	13315	8426	10999	13404	14926	13280	11524	7454
Dry Ash	13.18	8.77	15.48	9.25	4.77	4.71	19.84	9.72
Dry VM	27.45	44.73	40.05	37.82	18.60	45.84	30.17	44.94
Dry S	2.32	0.63	4.83	2.19	0.66	0.62	0.71	0.80
Dry Btu	13467	11717	11951	13629	15024	13925	11810	11001
Dry C	74.23	68.43	65.65	75.50	86.71	76.89	66.20	65.85
Dry H	4.08	4.88	4.23	4.83	4.23	5.49	4.21	4.36
Dry N	1.35	1.02	1.16	1.49	1.27	1.50	1.25	1.04
Dry Cl	0.00	0.03	0.05	0.11	0.19	0.03	0.10	0.04
Dry F	below detection levels for all samples							
Pyritic S	1.77	0.17	2.81	1.37	0.15	0.24	0.16	0.14
Sulfate S	0.01	0.03	0.01	0.01	0.03	0.03	0.03	0.03
Organic S	0.54	0.43	2.01	0.81	0.48	0.35	0.52	0.63
MAF C	85.50	75.01	77.67	83.20	91.05	80.69	82.58	72.94
MAF H	4.70	5.35	5.00	5.32	4.44	5.76	5.25	4.83
MAF N	1.55	1.12	1.37	1.64	1.33	1.57	1.56	1.15
MAF Org S	0.74	0.47	2.38	0.89	0.50	0.37	0.65	0.70
MAF Cl	0.00	0.03	0.06	0.12	0.20	0.03	0.12	0.04
MAF O	7.51	18.02	13.51	8.83	2.47	11.58	9.83	20.34
MAF Btu	15511	12843	14140	15018	15777	14613	14733	12185
Dmmf C	88.08	76.04	80.73	84.95	91.81	81.32	85.47	74.05
Dmmf H	4.84	5.42	5.20	5.43	4.48	5.81	5.44	4.90
Dmmf N	1.60	1.13	1.43	1.68	1.34	1.59	1.61	1.17
Dmmf Org	0.76	0.48	2.47	0.91	0.51	0.37	0.67	0.71
Dmmf Cl	0.00	0.03	0.06	0.12	0.20	0.03	0.13	0.04
Dmmf O	4.72	16.90	10.11	6.90	1.66	10.88	6.68	19.13
Dmmf Btu	15980	13020	14696	15336	15908	14728	15247	12370

Modified Parr Formula (used)

MM(dry) = 1.13 Ash + 0.47 Pyritic S(dry) + 0.50 Cl (dry)

Parr Formula (not used)

MM(dry) = 1.08 Ash(dry) + 0.55 S (total dry)

Abbreviations: UF = Upper Freeport seam; WY = Wyodak Anderson seam; IL = Illinois #6 seam; PITT = Pittsburgh seam; POC = Pocahontas #3 seam; UT = Blind Canyon seam; WV = Lewiston-Stockton seam; ND = Beulah-Zap seam; AR = As received; VM = volatile matter; MAF = moisture and ash-free; Dmmf = dry, mineral matter free

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Table VI.

Analysis Data with Standard Deviations, Reproducibilities
as Reported by C. T. & E.

Coal Analysis	Value	S.D.	Reproducibility
Upper Freeport			
Moisture	1.13	0.0725	0.205
Ash	13.03	0.1509	0.427
Volatile	27.14	0.5156	1.458
Sulfur	2.29	0.0428	0.121
Btu	13,315	56.5602	160.0
Carbon	74.23	0.6190	
Hydrogen	4.08	0.0503	
Nitrogen	1.35	0.0270	
Wyodak-Anderson			
Moisture	28.09	0.7043	1.99
Ash	6.31	0.1093	0.31
Volatile	32.17	1.2241	3.46
Sulfur	0.45	0.0225	0.06
Btu	8,426	66.9858	189
Carbon	68.43	.3606	
Hydrogen	4.88	0.0283	
Nitrogen	1.02	.0424	
Illinois #6			
Moisture	7.97	0.0656	0.185
Ash	14.25	0.2628	0.743
Volatile	36.86	0.7566	2.140
Sulfur	4.45	0.1773	0.501
Btu	10,999	35.2414	99.7
Carbon		---	
Hydrogen		---	
Nitrogen		---	
Pittsburgh			
Moisture	1.65	0.1094	0.310
Ash	9.10	0.1825	0.516
Volatile	37.20	0.4274	1.209
Sulfur	2.15	0.0703	0.199
Btu	13,404	45.4765	128.6
Carbon		---	
Hydrogen		---	
Nitrogen		---	

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Pocahontas			
Moisture	0.65	0.1111	0.31
Ash	4.74	0.0695	0.20
Volatile	18.48	0.6508	1.84
Sulfur	0.66	0.0347	0.10
Btu	14,926	16.1909	46
Carbon	86.71	.1273	
Hydrogen	4.23	.0771	
Nitrogen	1.27	.0490	
Blind Canyon			
Moisture	4.63	0.1215	0.34
Ash	4.49	0.1123	0.32
Volatile	43.72	0.8061	2.28
Sulfur	0.59	0.0225	0.06
Btu	13,280	41.3476	117
Carbon	76.89	.0775	
Hydrogen	5.49	.3667	
Nitrogen	1.5	.0778	
Lewiston-Stockton			
Moisture	2.42	0.1990	0.56
Ash	19.36	0.1220	0.35
Volatile	29.44	0.3539	1.00
Sulfur	0.69	0.0234	0.07
Btu	11,524	25.1364	71
Carbon	66.20	.6773	
Hydrogen	4.21	.0495	
Nitrogen	1.25	.0316	
Beulah-Zap			
Moisture	32.24	0.8672	2.45
Ash	6.59	0.1292	0.37
Volatile	30.45	2.4189	6.84
Sulfur	0.54	.0417	0.12
Btu	7,454	82.2394	233
Carbon	65.85	1.9445	
Hydrogen	4.36	.2332	
Nitrogen	1.04	.0707	

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3. ANALYTICAL DATA

3.1. Ultimate (Elemental) and Proximate Analyses

Calculation of As-received, maf and Dmmf values from Dry Data from CT&E

Coal	UF	WY	IL	PITT	POC	UT	WV	ND
AR H2O	1.13	28.09	7.97	1.65	0.65	4.63	2.42	32.24
AR Ash	13.03	6.31	14.25	9.10	4.74	4.49	19.36	6.59
AR VM	27.14	32.17	36.86	37.20	18.48	43.72	29.44	30.45
AR S	2.29	0.45	4.45	2.15	0.66	0.59	0.69	0.54
AR Btu	13315	8426	10999	13404	14926	13280	11524	7454
Dry Ash	13.18	8.77	15.48	9.25	4.77	4.71	19.84	9.72
Dry VM	27.45	44.73	40.05	37.82	18.60	45.84	30.17	44.94
Dry S	2.32	0.63	4.83	2.19	0.66	0.62	0.71	0.80
Dry Btu	13467	11717	11951	13629	15024	13925	11810	11001
Dry C	74.23	68.43	65.65	75.50	86.71	76.89	66.20	65.85
Dry H	4.08	4.88	4.23	4.83	4.23	5.49	4.21	4.36
Dry N	1.35	1.02	1.16	1.49	1.27	1.50	1.25	1.04
Dry Cl	0.00	0.03	0.05	0.11	0.19	0.03	0.10	0.04
Dry F	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Pyritic S	1.77	0.17	2.81	1.37	0.15	0.24	0.16	0.14
Sulfate S	0.01	0.03	0.01	0.01	0.03	0.03	0.03	0.03
Organic S	0.54	0.43	2.01	0.81	0.48	0.35	0.52	0.63
MAF C	85.50	75.01	77.67	83.20	91.05	80.69	82.58	72.94
MAF H	4.70	5.35	5.00	5.32	4.44	5.76	5.25	4.83
MAF N	1.55	1.12	1.37	1.64	1.33	1.57	1.56	1.15
MAF Org S	0.74	0.47	2.38	0.89	0.50	0.37	0.65	0.70
MAF Cl	0.00	0.03	0.06	0.12	0.20	0.03	0.12	0.04
MAF F	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MAF O	7.51	18.02	13.51	8.83	2.47	11.58	9.83	20.34
MAF Btu	15511	12843	14140	15018	15777	14613	14733	12185
Dmmf C	88.08	76.04	80.73	84.95	91.81	81.32	85.47	74.05
Dmmf H	4.84	5.42	5.20	5.43	4.48	5.81	5.44	4.90
Dmmf N	1.60	1.13	1.43	1.68	1.34	1.59	1.61	1.17
Dmmf Org	0.76	0.48	2.47	0.91	0.51	0.37	0.67	0.71
Dmmf Cl	0.00	0.03	0.06	0.12	0.20	0.03	0.13	0.04
Dmmf F	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Dmmf O	4.72	16.90	10.11	6.90	1.66	10.88	6.68	19.13
Dmmf Btu	15980	13020	14696	15336	15908	14728	15247	12370

Modified Parr Formula (used)

MM(dry) = 1.13 Ash + 0.47 Pyritic S(dry) + 0.50 Cl (dry)

Parr Formula (not used)

MM(dry) = 1.08 Ash(dry) + 0.55 S (total dry)

Abbreviations: UF = Upper Freeport seam; WY = Wyodak Anderson seam; IL = Illinois #6 seam; PITT = Pittsburgh seam; POC = Pocahontas #3 seam; UT = Blind Canyon seam; WV = Lewiston-Stockton seam; ND = Beulah-Zap seam; AR = As received; VM = volatile matter; MAF = moisture and ash-free; Dmmf = dry, mineral matter free

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3.2. Coal "Formulae"

The Ultimate analysis data were used to calculate the relative amounts of carbon compared to hydrogen, oxygen, nitrogen, and organic sulfur using the MAF and Dmmf data. The results are given below.

MAF					
Coal	C	H	O	N	S
Pocahontas #3	100	58.5	2.03	1.25	.21
Upper Freeport	100	66.0	6.59	1.55	.32
Pittsburgh	100	76.7	7.96	1.69	.40
Lewiston-Stockton	100	76.3	8.93	1.62	.30
Blind Canyon	100	85.7	10.8	1.67	.17
Illinois #6	100	77.3	13.0	1.51	1.15
Wyodak-Anderson	100	85.6	18.0	1.28	.23
Beulah-Zap	100	79.5	20.9	1.35	.36

Dmmf					
Coal	C	H	O	N	S
Pocahontas #3	100	58.6	1.36	1.25	.21
Upper Freeport	100	65.9	4.02	1.56	.32
Pittsburgh	100	76.7	6.09	1.70	.40
Lewiston-Stockton	100	76.4	5.86	1.61	.29
Blind Canyon	100	85.7	10.0	1.68	.17
Illinois #6	100	77.3	9.39	1.52	1.15
Wyodak-Anderson	100	85.5	16.7	1.27	.24
Beulah-Zap	100	79.4	19.4	1.35	.36

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Laboratories which participated in the different analyses indicated in this section include:

Alberta Research Council

Argonne National Laboratory Analytical Chemistry Laboratory

Argonne National Laboratory Basic Coal Chemistry Group

CANSPECS, a Canadian round robin of international laboratories

Commercial Testing and Engineering, Inc. **

Illinois State Geological Survey

Massachusetts Institute of Technology Energy Laboratory

University of North Dakota Energy and Mineral Research Center

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3.3. Major, Minor and Trace Elements in Ash

Major and Minor Elements in Ash (%)

	UF	WY	IL	PITT	POC	UT	WV**	ND**
Al ₂ O ₃	24.1	15.5	18.3	25.2	20.1	16.6	31.35	10.22
BaO	0.05	0.5					.02	.84
CaO	4.2	15.1	7.9	2.6	12.8	9.9	.38	24.72
Fe ₂ O ₃	17.3	10.2	18.0	19.5	15.8	10.0	2.89	8.00
K ₂ O	2.7	0.8	2.9	2.1	0.6	1.2	2.92	.94
MgO	1.6	3.6	1.2	1.3	2.0	1.5	0.73	7.48
MnO	0.05	0.04					0.04*	0.14*
Na ₂ O	0.0	1.5	0.0	0.0	2.0	3.6	0.34	7.76
P ₂ O ₅	0.1	1.2	0.2	0.0	0.4	0.3	0.20	0.48
SO ₃	3.9	22.0	6.8	2.0	12.4	9.8	0.32	17.55
SiO ₂	44.8	28.7	43.7	45.9	32.0	45.9	58.26	18.40
SrO	0.05	0.4					0.05	1.12
TiO ₂	1.3	1.2	1.0	1.2	1.9	1.2	1.86	0.48
Undetermined							0.64	1.87

* = Mn₃O₄

The tables on the next three pages are taken from Ref. 317 to give a compilation of major and minor concentrations in the whole coal, and also the trace elements in the whole coal. To obtain the values of the major and minor elements in the ash, the following values of ash at 550°C from Appendix 1 of the Open File Report for Ref. 317 should be used:

Coal	Ash
UF	13.5
WY	8.5
IL	16.2
PITT	9.2
POC	5.3
UT	4.6
WV	19.4
ND	9.5

The techniques used include:

DCAES = direct current atomic emission spectroscopy

ICAP-AES = inductively coupled argon plasma atomic emission spectroscopy

FAAS = flame atomic absorption spectroscopy

GFAAS = graphite furnace atomic absorption spectroscopy

WDXRF = wavelength dispersive x-ray fluorescence spectrometry

EDXRF = energy dispersive x-ray fluorescence spectrometry

INAA = instrumental neutron activation analysis

Abbreviations: UF = Upper Freeport seam; WY = Wyodak Anderson seam; IL = Illinois #6 seam; PITT = Pittsburgh seam; POC = Pocahontas #3 seam; UT = Blind Canyon seam; WV = Lewiston-Stockton seam; ND = Beulah-Zap seam

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Major and Minor Elements in Ash (%) Data from Ref. 317

Table 1. Average concentrations of major elements in weight percent based on triplicate analyses except values in brackets are averages of 2 analyses and numbers in parentheses are based on only one analysis. Complete data set is given in Appendix 1. Material analyzed: (A)=ash (C)=whole coal.

Sample	UF PC-1	WY PC-2	IL PC-3	PITT PC-4	POC PC-5	UT PC-6	WV PC-7	ND PC-8
Technique								
Si								
DCAES(A)	3.1	1.4	3.6	2.7	0.95	0.86	5.2	0.60
DCAES(C)	3.3	0.77	3.3	2.3	0.88	---	---	---
WDXRF(A)	[2.67]	[1.24]	[3.04]	[1.96]	[0.804]	(0.893)	(4.90)	(0.768)
Al								
WDXRF(A)	[1.54]	[0.672]	[1.21]	[0.981]	[0.548]	(0.370)	(3.17)	(0.45)
ICAP-AES(A)	1.60	0.699	1.25	1.00	0.549	[0.347]	3.16	0.400
DCAES(A)	2.4	0.53	2.0	2.1	0.71	0.32	3.9	0.23
DCAES(C)	2.0	0.48	2.0	1.7	0.85	---	---	---
Fe								
INAA(C)	1.78	0.366	2.67	1.35	0.509	0.317	0.397	0.547
WDXRF(A)	[1.93]	[0.33]	[2.70]	[1.44]	[0.52]	(0.29)	(0.37)	(0.45)
ICAP-AES(A)	1.86	0.367	2.72	1.32	0.507	[0.282]	0.385	0.472
DCAES(A)	1.6	0.27	2.4	1.9	0.50	0.24	0.40	0.37
DCAES(C)	2.3	0.29	2.3	1.3	0.69	---	---	---
Mg								
WDXRF(A)	[0.079]	[0.26]	[0.09]	[0.03]	[0.067]	(0.048)	(0.08)	(0.42)
ICAP-AES(A)	0.082	0.239	0.077	0.038	0.0548	[0.030]	0.094	0.398
DCAES(A)	0.15	0.37	0.12	0.073	0.11	0.041	0.097	0.51
DCAES(C)	0.099	0.20	0.098	0.048	0.077	---	---	---
Ca								
WDXRF(A)	[0.40]	[1.12]	[0.90]	[0.20]	[0.443]	(0.401)	(0.06)	(1.54)
ICAP-AES(A)	0.445	1.19	0.96	0.206	0.456	[0.409]	0.058	1.54
DCAES(A)	0.64	1.2	1.6	0.41	0.58	0.29	0.078	1.3
DCAES(C)	0.58	1.0	1.7	0.29	0.80	---	---	---
Na								
INAA(C)	0.0341	0.115	0.102	0.0343	0.0782	0.146	0.0388	0.529
ICAP-AES(A)	0.032	0.119	0.097	0.032	0.0826	[0.126]	0.034	0.466
WDXRF(A)	[0.03]	[0.092]	[0.11]	[0.03]	[0.071]	(0.13)	(0.05)	(0.50)
DCAES(A)	0.045	0.13	0.15	0.036	0.13	0.072	0.036	(0.25)
K								
INAA(C)	0.227	0.0292	0.195	0.110	0.029	[0.022]	0.506	[0.029]
WDXRF(A)	[0.27]	[0.03]	[0.20]	[0.11]	[0.03]	(0.02)	(0.46)	(0.03)
ICAP-AES(A)	0.283	0.028	0.194	0.110	0.028	[0.014]	0.495	0.014
DCAES(A)	0.30	0.033	0.26	0.13	0.036	0.017	0.36	0.037
Ti								
WDXRF(A)	0.080	[0.051]	[0.07]	[0.059]	[0.040]	(0.02)	(0.24)	(0.02)
ICAP-AES(A)	0.079	0.056	0.070	0.056	0.038	[0.023]	0.260	0.020
DCAES(A)	0.053	0.036	0.066	0.057	0.028	0.019	0.18	0.018
DCAES(C)	0.10	0.044	0.092	0.091	0.082	---	---	---
P								
WDXRF(C)	---	0.03	---	0.009	---	---	---	0.02
WDXRF(A)	[0.006]	[0.03]	[0.004]	[0.010]	[0.002]	(0.001)	(0.007)	(0.02)
ICAP-AES(A)	0.0079	0.025	0.0059	0.011	0.0022	[0.00094]	0.0084	0.012
DCAES(A)	---	0.026	---	---	---	(0.00074)	(0.017)	0.011
Mn								
WDXRF(A)	---	---	---	---	---	---	---	(0.007)
ICAP-AES(A)	0.0041	0.0020	0.0076	0.0018	0.0016	[0.00041]	0.0015	0.0080
DCAES(A)	0.0055	0.0033	0.0011	0.0036	0.0024	0.00061	0.0020	0.010
DCAES(C)	0.0053	0.0013	0.0016	0.0020	0.0019	---	---	---

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Trace Elements (ppm) Data from Ref. 317

Table 2. Average concentrations of trace elements in micrograms per gram based on triplicate analyses except bracketed values, are averages of 2 analyses and numbers in parentheses are based on only one analysis. Complete data set is given in Appendix 1. Material analyzed: (A)=ash (C)=whole coal.

Sample	UF PC-1	WY PC-2	IL PC-3	PITT PC-4	POC PC-5	UT PC-6	WV PC-7	ND PC-8
Technique								
Be								
ICAP-AES(A)	1.5	0.25	0.76	0.77	0.80	[0.13]	1.9	[0.18]
DCAES(A)	1.4	0.14	0.97	1.2	0.67	0.20	3.0	0.28
Sc								
INAA(C)	4.06	1.68	2.59	2.57	1.79	0.813	7.62	0.846
DCAES(A)	2.1	1.3	2.6	1.9	1.3	0.69	6.4	0.90
V								
ICAP-AES(A)	26	14	32	15	11	[4.0]	44	3.5
DCAES(A)	16	9.0	24	13	7.1	3.7	32	3.6
DCAES(C)	41	[14]	52	24	18	---	---	---
Cr								
INAA(C)	20.3	6.1	33.1	14.8	9.1	5.3	35.8	2.23
EDXRF(A)	26.0	8.2	43.2	17.9	12.3	---	45.9	2.6
ICAP-AES(A)	20	6.2	31	14	9.2	[4.8]	40	2.4
EDXRF(C)	19	[4]	35	8	5	---	49	---
DCAES(A)	19	5.7	38	19	8.8	4.8	39	2.4
DCAES(C)	32	7	52	24	16	---	---	---
Co								
INAA(C)	5.33	1.68	4.39	2.62	4.07	1.00	7.74	0.778
FAAS(A)	5.0	1.6	4.3	2.4	3.8	[0.83]	8.1	---
DCAES(A)	3.5	1.3	3.7	2.6	2.6	0.64	6.3	0.55
DCAES(C)	5.0	---	---	---	5.0	---	---	---
Ni								
INAA(C)	14.5	4.9	21.0	[10.3]	8.6	[3.4]	15.4	---
EDXRF(A)	14	3.9	18	9.3	7.91	---	17	1.9
ICAP-AES(A)	14	4.9	18	8.5	6.7	[3.3]	16	1.3
EDXRF(C)	23	8	32	13	11	5	18	6
DCAES(A)	14	5.2	22	13	6.5	4.0	21	1.8
DCAES(C)	25	---	33	12	[11]	---	---	---
Cu								
EDXRF(A)	20.4	12.9	9.6	6.2	12.5	---	23.6	3.3
ICAP-AES(A)	19	12	10	5.5	12	[3.8]	19	4.7
EDXRF(C)	18	17	14	10	17	8	31	9
DCAES(A)	17	13	11	6.5	19	2.9	16	4.9
DCAES(C)	18	7	9	6	19	---	---	---
Zn								
INAA(C)	19.7	11.3	220	9.1	6.4	6.4	13.5	5.69
EDXRF(A)	20.5	10.6	107	8.4	4.8	---	12	5.4
ICAP-AES(A)	19	10	180	7.8	4.0	[6.2]	13	4.8
EDXRF(C)	33	25	140	15	14	---	10	5
DCAES(C)	33	---	280	27	---	---	---	---
Ga								
DCAES(A)	6.2	2.4	4.7	4.7	2.3	1.2	12	1.7
DCAES(C)	10	3	7	5	4	---	---	---
Ge								
DCAES(A)	3.6	---	8.9	1.2	0.46	---	[1.1]	---
DCAES(C)	4	---	9	(3.0)	---	---	---	---
As								
INAA(C)	17.1	3.6	4.7	8.42	10.3	0.48	6.2	2.63
DCAES(A)	30	---	---	17	15	---	---	---

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Trace Elements (ppm) Data from Ref. 317

Table 2 (continued)

Sample	UF PC-1	WY PC-2	IL PC-3	PITT PC-4	POC PC-5	UT PC-6	WV PC-7	ND PC-8
Technique								
Rb								
INAA(C)	19.5	---	16	7.7	---	[1.02]	29.7	[0.93]
EDXRF(A)	21.2	3.5	15	9.1	2.3	---	43.6	---
EDXRF(C)	21	13	20	8	5	3	42	4
Sr								
INAA(C)	49	252	39	61	105	70	60	590
EDXRF(A)	60	260	29.9	68	110	---	78.0	640
ICAP-AES(A)	59	150	29	64	85	[60]	49	500
EDXRF(C)	62	294	33	63	85	63	86	780
DCAES(A)	63	220	40	91	110	89	70	630
Y								
EDXRF(A)	10	3.6	4.1	4.9	6.89	---	21.2	---
ICAP-AES(A)	9.3	3.8	4.2	4.3	6.2	2.0	11	[1.8]
EDXRF(C)	---	---	---	---	---	(2)	19	---
DCAES(A)	4.7	3.0	4.7	3.1	4.6	1.8	9.1	2.4
Zr								
EDXRF(A)	27.3	22.7	22.3	20.5	16.9	---	80.5	6.5
EDXRF(C)	23	19	23	17	10	18	103	18
DCAES(A)	11	17	17	12	12	11	34	13
DCAES(C)	33	---	21	24	30	---	---	---
Nb								
EDXRF(A)	2.5	1.0	[2.1]	1.9	0.85	---	8.3	---
EDXRF(C)	---	---	---	---	---	---	[13]	---
DCAES(A)	1.7	1.4	2.5	1.8	1.1	0.51	3.6	0.58
Ba								
INAA(C)	61	310	94	47	198	36	133	680
EDXRF(A)	52	270	74.5	35.7	180	---	110	460
EDXRF(C)	60	410	121	30	140	29	210	1030
ICAP-AES(A)	55	15	81	41	16	31	120	420
DCAES(A)	41	320	60	38	210	36	130	580
DCAES(C)	81	250	120	66	450	---	---	---
La								
INAA(C)	10.1	5.35	6.10	6.15	6.76	3.31	21.5	2.82
EDXRF(A)	8.2	---	---	[4.4]	2.2	---	17	---
EDXRF(C)	16	6	15	9	5	10	16	8
DCAES(A)	6.9	6.1	9.3	5.8	7.2	2.9	14	3.7
Ce								
INAA(C)	18.3	9.4	12.6	11.3	11.6	4.81	35.8	4.45
EDXRF(A)	17.0	[5.2]	7.2	9.0	7.6	---	29.9	---
EDXRF(C)	40	25	40	17	10	15	55	19
DCAES(A)	(10)	9	(28)	---	12	6.9	26	---
Nd								
INAA(C)	(8.0)	---	---	---	---	[2.0]	11.7	[2.3]
DCAES(A)	8	---	(6.5)	3.9	6.0	(2.9)	19	---
Sm								
INAA(C)	1.97	0.978	1.20	1.09	1.22	0.508	3.52	0.41
DCAES(A)	---	---	---	---	0.76	0.37	[1.7]	(0.47)
Yb								
INAA(C)	0.88	0.42	0.52	0.470	0.555	0.20	1.61	0.287
DCAES(A)	0.84	0.29	0.61	0.54	0.45	0.21	1.5	0.20
Pb								
GFAAS(A)	7.4	2.9	6.5	2.9	2.4	[1.6]	12	1.5
DCAES(A)	10	3.4	14	7.3	11	1.9	16	2.6
DCAES(C)	8	---	8	4	5	---	---	---

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3.4. Mineral Matter Analysis

Data from Illinois State Geological Survey, Richard Harvey
November 15, 1988

Results of Mineral Analyses (dry coal basis)

Coal	1	2	3	4	5	6	7	8
	UF	WY	IL	PIT	POC	UT	WV	ND
Total mineral matter (%LTA)	15.3	8.7	18.1	10.9	5.5	5.3	21.6	8.7
Quartz	1.5	2.0	3.4	1.7	0.3	0.8	2.6	0.6
Pyrite	3.4	0.1	5.5	2.4	0.1	0.5	0.3	0.3
Calcite	1.0	0.4	1.9	0.5	1.7	1.3	0.3	1.7
Total clay (diff.)	9.4	6.2	7.3	6.3	3.4	2.7	18.4	6.1
Illite	p	?	p	p	?	?	p	?
Expandable	p	?	p	p	p	?	p	?
Kaolinite	p	p	p	p	p	?	p	p
Gypsum	m	m				m		major
Marcasite	tr		tr	tr				
Siderite					tr?			
Analcime						tr-m		
Rutile						tr		
Ca/Na feldspar							tr	
Unknown					tr?			

p = present, analysis in progress; m = minor amount; tr = trace amount; blank = not detected

.....
Mineral Constituents as a Percentage of Total Mineral Matter

Coal	1	2	3	4	5	6	7	8
	UF	WY	IL	PIT	POC	UT	WV	ND
Total mineral matter (%LTA)	15.3	8.7	18.1	10.9	5.5	5.3	21.6	8.7
Quartz	10	23	19	16	5	15	12	7
Pyrite	22	1	30	22	2	9	1	3
Calcite	7	5	10	5	31	24	1	20
Total clay (diff.)	61	71	41	57	62	52	86	70

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3.5. Maceral Analyses

Data are given on a mineral-matter free basis in %.

	UF	WY	IL	PITT	POC	UT	WV	ND
Lipt.	1	<1	5	7	1	5	12	-
Vitr.	91	89	85	85	89	87	73	-
Inert.	8	11	10	8	10	8	15	-

Abbreviations: UF = Upper Freeport seam; WY = Wyodak Anderson seam; IL = Illinois #6 seam; PITT = Pittsburgh seam; POC = Pocahontas #3 seam; UT = Blind Canyon seam; WV = Lewiston-Stockton seam; ND = Beulah-Zap seam

3.6. Optical Reflectance Measurements

The data are reported in terms of two types of measurements: The mean average and mean maximum reflectance. The procedure involves the measurement of the reflectance of a particular small spot on the sample using an oil immersion technique and light of a specified wavelength (546 nm). Because coals are anisotropic the reflectance values depend on the orientation of the light beam to the orientation of the particle. Rotation of the particle will result in variation of the measured reflectance. Thus, some workers report the average values as the mean average of the measurements, while others determine the maximum reflectance for each spot and report the mean maximum reflectance.

The data and comments from the University of Kentucky are given below. The values were obtained from -20 mesh samples prepared for reflected light microscopic analyses as per ASTM D2797. Mean-maximum reflectance readings were acquired utilizing a Leitz MPV Compact microscope photometer, in compliance with ASTM D2798 guidelines.

Table 1. Mean Maximum Vitrinite Reflectance

Coal	Reflectance	Std. Dev.	Rank
Beulah-Zap	0.25	.04	lignite
Wyodak	0.32	.05	subbit.
Illinois #6	0.46	.05	subbit.
Blind Canyon	0.57	.04	hvBb
Pittsburgh	0.81	.05	hvAb
Lew.-Stockton	0.89	.05	hvAb
Upper Freeport	1.16	.05	m vb
Pocahontas #3	1.68	.05	lvb

The workers indicate that there is actually no division between lignite and subbituminous coal based on the vitrinite (huminite) reflectivity; coals with measured reflectances of less than 0.47% are considered to be of subbituminous rank or lower (Davis, 1984). They correlated the reflectivity ranges with the ASTM coal-rank classes in accordance with Davis.

They also indicate that despite the apparent subbituminous rank, the microscopic appearance of the Illinois #6 coal is more consistent with a rank level in the high volatile bituminous range.

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Reference: Davis, A. 1984, Coal Petrology and Petrographic Analysis, In Coal Geology and Coal Technology (Ed. by C. R. Ward) Blackwell Scientific, Melbourne, pp. 74-112.

The data from Woods Hole Oceanographic Institute are given below as the mean average vitrinite reflectance in oil (n_o 1.518) @ 546 nm. The method involved mounting in a cold set epoxy resin, grinding and polishing to standard procedures (ICCP, 1963, 1971, 1975). The samples were examined in reflected and fluorescence light. Reflectance measurements in oil were determined on a Leitz MPV 3 microscope system, using a 50x oil immersion objective and mineral standards for photometer calibration. Vitrinite particles were carefully selected and measured using a 5 micron measuring diaphragm to give the mean reflectance (% R_o). Fluorescence examination was performed on all samples using a Zeiss Axiophot microscope fitted with a x40 oil immersion objective, a 100w HBO mercury bulb, and an LP520 BP450-90 filter set.

Table 2. Mean Average Vitrinite Reflectance

Coal	Reflectance Mean % R_o	# Readings	Std. Dev.	Spore Fluorescence Color
Beulah-Zap	0.28	49	.04	yellow (about 0.3 % R_o)
Wyodak	0.31	50	.08	yellow/yellow orange (about 0.35 % R_o)
Illinois #6	0.46	24	.05	yellow/yellow orange (about 0.45 % R_o)
Blind Canyon	0.50	50	.05	light orange/light-mid orange (about 0.5-0.6 % R_o)
Pittsburgh	0.72	50	.04	mid orange (about 0.6-0.75 % R_o)
Lew.-Stockton	0.77	50	.05	mid orange, moderate intensity (about 0.7-0.8 % R_o)
Upper Freeport	0.99	50	.07	dark red brown trace weak intensity (about ≥ 1.0 % R_o)
Pocahontas #3	1.42	50	.06	spores no longer fluoresce (≥ 1.1 % R_o)

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The University of Kentucky workers provided reflectance distributions for each sample, reported as vitrinoid type (V-type) histograms. A vitrinoid-type of 1 represents reflectance values in the range of 0.10 to 0.19%, while V-Type 18 includes reflectances of 1.80 to 1.89%. These are given on the next page page.

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Vitrinoid (V-type) Histograms of Reflectance of the Coals Courtesy of University of Kentucky Center for Applied Energy Research

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3.7. Ash Fusion Properties

		Temperatures in ° F.							
		UF	WY	IL	PITT	POC	UT	WV	ND
Reducing	Initial	2191	2050	1952	2039	2183	2012	2700+	2246
	h = w	2250	2120	1996	2098	2240	2079	2700+	2310
	h = 1/w	2321	2185	2043	2190	2310	2154	2700+	2349
	fluid	2433	2230	2153	2416	2407	2202	2700+	2394
Oxidizing									
Initial	-	2140	2341	2517	2400	2149	2700+	2329	
	h = w	2170	2375	2554	2414	2194	2700+	2393	
	h = 1/w	2200	2425	2578	2422	2240	2700+	2425	
	fluid	2225	2510	2610	2487	2309	2700+	2460	

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3.8. Particle Size Measurements

-100 mesh								
Size	UF	WY	IL	PITT	POC	UT	WV	ND
(microns)	wt. %	wt. %	wt. %	wt. %	wt. %	wt. %	wt. %	wt. %
500+	3.00E-02	0.00E+00	1.80E-01	3.77E-01	1.17E-01	1.69E-02	5.50E-02	2.27E-01
500-425	1.92E-02	0.00E+00	1.29E-01	9.57E-02	1.02E-01	3.58E-02	6.89E-02	1.92E-01
425-355	6.87E-02	6.40E-03	2.27E-01	1.13E-01	1.72E-01	8.20E-02	1.52E-01	3.72E-01
355-300	9.86E-02	7.73E-03	3.64E-01	1.51E-01	3.21E-01	1.75E-01	2.24E-01	4.64E-01
300-250	1.63E-01	8.26E-03	4.21E-01	2.02E-01	3.65E-01	3.06E-01	2.65E-01	5.20E-01
250-212	2.53E-01	6.45E-02	5.61E-01	5.27E-01	6.00E-01	7.52E-01	5.57E-01	7.36E-01
212-180	3.18E-01	5.01E-02	5.43E-01	3.07E-01	4.19E-01	1.07E+00	4.69E-01	8.48E-01
180-150	1.20E+00	5.29E-01	7.29E-01	1.52E+00	6.26E-01	3.19E+00	2.00E+00	2.89E+00
150-125	3.30E+00	1.96E+00	4.08E+00	4.54E+00	9.44E-01	7.61E+00	5.28E+00	5.15E+00
125-106	5.77E+00	5.01E+00	6.09E+00	5.74E+00	1.69E+00	7.94E+00	6.87E+00	7.03E+00
106-90	8.08E+00	1.00E+01	1.02E+01	9.19E+00	3.56E+00	1.07E+01	8.64E+00	7.60E+00
90-75	1.03E+01	1.18E+01	9.36E+00	1.14E+01	5.96E+00	1.16E+01	9.97E+00	7.47E+00
75-63	6.33E+00	8.00E+00	6.22E+00	6.67E+00	5.01E+00	6.14E+00	6.00E+00	4.91E+00
63-53	7.99E+00	1.55E+01	1.21E+01	1.18E+01	1.01E+01	8.75E+00	9.07E+00	8.14E+00
53-45	1.31E+01	1.05E+01	7.25E+00	7.21E+00	7.99E+00	5.59E+00	6.19E+00	5.09E+00
45-38	6.25E+00	6.28E+00	1.04E+01	9.19E+00	7.87E+00	5.59E+00	5.27E+00	4.80E+00
38-	3.67E+01	3.03E+01	3.12E+01	3.09E+01	5.42E+01	3.05E+01	3.89E+01	4.36E+01
TOTAL	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0

-20 mesh								
Size	UF	WY	IL	PITT	POC	UT	WV	ND
(microns)	wt. %	wt. %	wt. %	wt. %	wt. %	wt. %	wt. %	wt. %
1000+	1.43E-02	6.75E-03	9.71E-03	9.89E-01	0.00E+00	0.00E+00	1.51E-02	2.28E-01
1000-850	6.48E-03	9.31E-02	4.01E-02	2.77E-01	2.19E-02	1.14E-02	4.85E-02	1.11E-01
850-710	3.31E-02	4.33E-01	2.12E-01	4.64E-01	3.79E-02	8.83E-02	1.39E-01	2.15E-01
710-600	3.64E-02	1.64E+00	7.85E-01	6.98E-01	2.75E-01	3.97E-01	6.39E-01	7.00E-01
600-500	1.26E-01	4.30E+00	2.41E+00	1.28E+00	8.44E-01	1.41E+00	1.86E+00	2.89E+00
500-425	1.82E-01	4.81E+00	3.61E+00	1.79E+00	1.83E+00	3.07E+00	3.28E+00	4.34E+00
425-355	4.12E-01	7.17E+00	4.83E+00	2.48E+00	2.87E+00	4.85E+00	5.12E+00	6.76E+00
355-300	8.59E-01	8.22E+00	6.97E+00	4.71E+00	4.35E+00	7.45E+00	7.13E+00	9.34E+00
300-250	1.41E+00	8.29E+00	6.96E+00	4.93E+00	5.21E+00	8.20E+00	7.14E+00	8.00E+00
250-212	2.96E+00	1.03E+01	9.37E+00	7.08E+00	7.99E+00	1.08E+01	9.63E+00	8.86E+00
212-180	2.79E+00	5.44E+00	5.86E+00	5.90E+00	4.49E+00	6.27E+00	5.42E+00	4.75E+00
180-150	4.72E+00	6.51E+00	7.46E+00	7.82E+00	6.27E+00	4.71E+00	8.00E+00	7.30E+00
150-125	6.39E+00	5.83E+00	7.36E+00	7.91E+00	6.89E+00	1.11E+01	7.69E+00	5.72E+00
125-106	5.51E+00	4.90E+00	5.82E+00	6.23E+00	7.72E+00	7.01E+00	5.70E+00	4.30E+00
106-90	7.27E+00	4.54E+00	5.54E+00	6.01E+00	4.86E+00	5.77E+00	5.21E+00	3.72E+00
90-75	7.09E+00	2.45E+00	5.08E+00	7.35E+00	8.20E+00	5.79E+00	5.20E+00	3.90E+00
75-63	5.83E+00	2.66E+00	3.03E+00	2.74E+00	3.51E+00	3.66E+00	3.28E+00	3.11E+00
63-53	8.49E+00	3.28E+00	5.93E+00	3.66E+00	4.27E+00	3.86E+00	3.93E+00	2.28E+00
53-45	6.00E+00	3.34E+00	3.29E+00	6.13E+00	1.03E+01	3.86E+00	2.58E+00	2.40E+00
45-38	6.40E+00	1.72E+00	2.23E+00	3.63E+00	3.24E+00	2.32E+00	3.92E+00	2.24E+00
38-	3.35E+01	1.41E+01	1.32E+01	1.79E+01	1.69E+01	9.37E+00	1.41E+01	1.88E+01
TOTAL	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0

Particle sizes are given in microns. Data courtesy of Alan Sayre at M. I. T.

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3.9. Surface Area Measurements

BET Multipoint Analysis for Six Premium Coals in the Concentration Range $0.05 \leq P/P_0 \leq 0.35$ for Nitrogen Adsorption

Coal	Mesh	Weight	BET eq params			wt. monol. N ₂ , g	surface area	sp. area
			slope	inter cept	corr coeff			
UF	-100	.6978	1697.3	64.89	.9994	5.675	1.98	2.48
WY	-20	.5013	1096.9	24.22	.9995	8.919	3.11	6.20
IL	-100	.5388	270.8	4.04	.9998	36.38	12.68	23.53
PITT	-100	.6559	2128.4	104.74	.9968	4.478	1.56	2.38
POC	-100	.5276	2294.6	92.53	.9993	4.189	1.46	2.77
ND	-100	.6690	2717.0	95.12	.9997	3.556	1.24	1.85

Temperature = 77 K, measurements with a Quantasorb apparatus. Wyodak and Illinois #6 samples were dried at 110 C under vacuum for 24 h; Beulah-Zap lignite was dried at 80-90 C. Samples were outgassed with heating for 2 h at the temperature at which they had been dried or by repetitive adsorption and desorption of N₂.

Data from Ref. 63, Gumkowski, M.; Liu, Q. and Arnett, E. M., Energy & Fuels, 2 (3) 299 (1988)

Coal	Mesh	CO ₂	N ₂	m ² /g
WY	-200/+230	206	5.0	
	-325/+400	208	5.0	
PITT	-200/+230	119	1.3	
	-325/+400	117		
ND	-200/+230	229	0.5	
	-325/+400	250	1.0	

Values for Pittsburgh -200/+230 fraction:

Pore volume by Hg porosimetry: 0.43 m³/g; N₂: 0.012 and H₂O: 0.031

Helium pycnometer density: 1.39 +/- 0.01 g/cm³

Data from Ref. 46, Bartholomew, C. H. et al, Preprints, Fuel Chemistry Div. Am. Chem. Soc. 33 (3) 24 (1988)

Surface areas of Illinois #6 coal

Adsorbate	Ads temp. K	Cross-sec. area Sq. Angstroms	BET surface m ² /g
Ar	77	16.2	14,15
CO ₂	178	25.3	132,132
Cyclopropane	203	25.2	36,31

Data from Ref. 15, Larsen, J. W. and Wernett, P., Preprints, Fuel Chemistry Div., AM. Chem. Soc., 32 (4) 232-236 (1987)

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3.10. Free-Swelling Indices

	UF	WY	IL	PITT	POC	UT	WV	ND
FSI	8.5	0	2-4	-	8.0	1.5	3.5	-

Data courtesy of Commercial Testing & Engineering Co.

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3.11. Plasticity and Dilatometry

Gieseler Plastometer Composite Data

Coal	DDPM*	Fluid Temp.	Initial Soft.	Solid.	Range
UF	30,000	450 C	373 C	497 C	124 C
WY	Broke Free	--	--	--	--
IL	86	417	367	444	77
PITT	29,267	430	381	472	91
POC	44	474	460	509	49
UT	3	409	396	438	42
WV	to be measured				

Courtesy of Commercial Testing and Engineering Co.

Arnu Dilatometer Composite Data

Coal	Contract	Expan	Init Soft	Max Cont	Max Exp
UF	-30	250	350	405	450
WY	-10	--	360	--	--
IL	-20	-5	355	402	425
PITT	-30	175	350	400	455
POC	-30	30	408	453	500
UT	-36	--	375	--	--
WV	to be measured				
ND	to be measured				

Data courtesy of Commercial Testing and Engineering, Inc.

UF = Upper Freeport, WY = Wyodak-Anderson, IL = Illinois #6, PITT = Pittsburgh, POC = Pocahontas #3, UT = Blind Canyon seam, WV = Lewiston-Stockton, ND = Beulah-Zap seam

* DDPM = dial divisions per minute

USERS HANDBOOK FOR THE ARGONNE PREMIUM COAL SAMPLES

Gieseler Plastometer Fluidities, Courtesy of David Bodily, Fossil Fuel Characterization Laboratory, University of Utah

COAL SAMPLE	INITIAL SOFTENING TEMPERATURE °C	MAXIMUM FLUIDITY TEMPERATURE °C	RESOLIDIFI- CATION TEMPERATURE °C	MAXIMUM FLUIDITY DDPM
BLIND CANYON	NONE	NONE	NONE	NONE
ILLINOIS NO. 6	395	420	436	45
PITTSBURGH NO. 8	397	432	468	27,262
LEWISTON STOCKTON	419	442	460	106
UPPER FREEPORT	393	442-462	497	MAXIMUM OF MACHINE 30,000
POCOHONTAS	460	482	504	39

USERS HANDBOOK FOR THE ARGONNE PREMIUM COAL SAMPLES

Gieseler Plastometer Fluidities, Courtesy of David Bodily, Fossil Fuel Characterization Laboratory, University of Utah

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Gieseler Plastometer Fluidities, Courtesy of David Bodily, Fossil Fuel Characterization Laboratory, University of Utah

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Gieseler Plastometer Fluidities, Courtesy of David Bodily, Fossil Fuel Characterization Laboratory, University of Utah

USERS HANDBOOK FOR THE ARGONNE PREMIUM COAL SAMPLES

Gieseler Fluidities of Samples Rechecked Over 3 Years

Data Courtesy Penn State, Coal & Organic Petrology Labs, D. Glick

GIESELER FLUIDITY OF ARGONNE COALS STORED IN AMPOULES Penn State - Coal & Organic Petrology Labs - D. Glick

	As Rec'd at PSU	Stored 8 Months	Stored 2 Years
ANL-101, Upper Fr., mvb	8/22/89	4/19/90	7/26/91
max. fluidity, ddpm	29910	29934	30001
initial fluidity T, C	381	376	374
max. fluidity T, C	456	456	452
solidification T, C	507	502	496
fluid range, C	126	126	122
ANL-301, Ill. #6, hvBb	8/21/89	4/12/90	8/02/91
max. fluidity, ddpm	72	54	70
initial fluidity T, C	368	367	374
max. fluidity T, C	418	413	412
solidification T, C	447	444	442
fluid range, C	79	77	68
ANL-401, Pitt., hvAb	8/23/89	4/11/90	8/01/91
max. fluidity, ddpm	25055	17093	28816
initial fluidity T, C	386	384	378
max. fluidity T, C	438	430	434
solidification T, C	475	473	472
fluid range, C	89	89	94
ANL-501, Pocahontas, lvb	8/17/89	4/20/90	7/29/91
max. fluidity, ddpm	46	39	42
initial fluidity T, C	453	444	443
max. fluidity T, C	486	480	479
solidification T, C	515	511	513*
fluid range, C	62	67	70*
ANL-601, Bl. Cy., HvBb	8/18/89	4/17/90	8/03/91
max. fluidity, ddpm	2	2	2
initial fluidity T, C	404	398	401
max. fluidity T, C	424	415	417
solidification T, C	446	438	441
fluid range, C	41	40	40
ANL-701, Lew.-St., hvAb	8/21/89	4/13/90	7/31/91
max. fluidity, ddpm	112	12	158
initial fluidity T, C	410	406	406
max. fluidity T, C	445	422	438
solidification T, C	469	431	465
fluid range, C	53	25	59

* equipment problems at end of run; results shown are from extrapolation

3.12. Structure and Lattice Parameters of Coal Samples

Structural and Lattice Parameters of Coal Samples
Data courtesy of Ronald J. Pugmire, see Refs. 390 & 86

Coal	f_a	$f_{a'}$	f_a^C	f_a^H	f_a^N	f_a^P	f_a^S	f_a^B	f_{al}	f_{al}^H	f_{al}^*	f_{al}^O
ND ^a	.65	.55	.10	.22	.33	.09	.15	.09	.35	.26	.09	.11
WY	.63	.55	.08	.17	.38	.08	.14	.16	.37	.27	.10	.10
UT ^a	.62 ₅	.60 ₅	.02	.21 ₅	.39	.06 ₅	.14	.18 ₅	.37 ₅	.27	.10 ₅	.05
IL	.72	.72	.00	.26	.46	.06	.18	.22	.28	.19	.09	.05
PITT ^a	.71	.70	.01	.27	.43	.06	.15	.22	.29	.21	.08	.04
WV	.75	.75	.00	.27	.48	.05	.21	.22	.25	.17	.08	.04
UF	.81	.81	.00	.28	.53	.04	.20	.29	.19	.11	.08	.02
POC	.86	.86	.00	.33	.553	.02	.17	.34	.14	.09	.05	.01

Coal	X_b	C	o+1	P_o	B.L.	S.C.	MW	M_o
ND ^a	.16	9	3.9	.63	2.5	1.4	269	40
WY	.29	14	5.6	.55	3.1	2.5	408	42
UT ^a	.31	15	5.1	.49	2.5	2.6	368	36
IL	.31	15	5.0	.63	3.2	1.8	321	27
PITT ^a	.31	15	4.5	.62	2.9	1.6	310	28
WV	.29	14	4.8	.69	3.3	1.5	270	20
UF	.36	18	5.3	.67	3.6	1.7	310	17
POC	.40	20	4.4	.74	3.3	1.1	307	13

^a Averaged over two or more ampules

f_a = fraction of sp^2 -hybridized carbon; f_a = total carbon; $f_{a'}$ = in an aromatic ring; f_a^C = carbonyl; f_a^H = protonated and aromatic; f_a^N = nonprotonated and aromatic; f_a^P = phenolic or phenolic ether; f_a^S = alkylated aromatic; f_a^B = aromatic bridgehead. Fraction of sp^3 hybridized carbon: f_{al}^H = total carbon; f_{al}^O = bonded to oxygen; f_{al}^* = CH or CH_2 ; f_{al}^* = CH_3 or non-protonated;

X_b = mole fraction of aromatic C at bridgehead; C = ave. number of C per cluster; o+1 = coordination number of cluster (side chains and bridges); P_o = fraction of bridges that are intact; B.L. = number of bridges and loops/cluster; S.C. = number of side chains/cluster; MW = mol. wt./cluster using maf C.; M_o = mass of side chain/cluster

USERS HANDBOOK FOR THE ARGONNE PREMIUM COAL SAMPLES

3.13. Survey of Carbon Aromaticities

MEAN VALUES OF CARBON AROMATICITY AND STANDARD DEVIATIONS
(No. of MEASUREMENTS) FOR ARGONNE PREMIUM COALS

COAL	CP/MAS		CP/MAS at 2.3T		SPE	
	f_a	S.D.	f_a	S.D.	f_a	S.D.
Pocahontas	0.85	0.01(12)	0.85	0.01 (5)	0.86	0.05 (3)
Upper Freeport	0.80	0.02(10)	0.82	0.01 (4)	0.81	0.02 (3)
Lewiston-Stockton	0.75	0.02 (9)	0.76	0.02 (4)	0.76	0.04 (3)
Blind Canyon	0.63	0.03(11)	0.64	0.02 (5)	0.66	0.02 (4)
Pittsburgh #8	0.72	0.03(11)	0.73	0.01 (4)	0.75	0.03 (3)
Illinois #6	0.71	0.02(10)	0.72	0.00 (4)	0.73	0.04 (3)
Wyodak-Anderson	0.62	0.04(11)	0.65	0.02 (4)	0.74	0.03 (3)
Beulah-Zap	0.69	0.05(12)	0.67	0.05 (5)	0.76	0.03 (4)

Data from Ref. 500

f_a = Carbon aromaticity

S. D. = standard deviation

CP/MAS = cross polarization/magic angle spinning

2.3 T = 2.3 Tesla, which is 25 megahertz carbon frequency

SPE = single pulse excitation

USERS HANDBOOK FOR THE ARGONNE PREMIUM COAL SAMPLES

3.14. EPR Values

Data and Reference Numbers from Ref. 496

SURVEY OF EPR CARBON RADICAL INTENSITIES (In Units of Spins/Gram-Organic)

Coal Type:	Reference						Mean Values
	3	5*	6	7	8	11	
Pocahontas	3.10	1.10	0.21	2.33	3.4	1.54	1.95p1.22
Upper Freeport	2.17	0.84	0.74	0.74	--	0.87	1.07p0.62
Pittsburgh	1.91	0.82	0.53	1.80	1.0	1.00	1.17p0.55
Lewiston- Stockton	3.78	0.83	0.88	--	--	1.64	1.78p1.38
Blind Canyon	3.02	0.85	0.56	--	0.8	1.36	1.32p1.00
Illinois #6	1.43	0.42	0.19	--	0.9	1.00	0.79p0.49
Wyodak- Anderson	2.41	0.39	0.76	3.29	--	1.54	1.68p1.19
Beulah- Zap	3.35	0.34	0.39	2.52	1.5	1.51	1.60p1.18

*Reported as spins/cm³ in Ref. 5.

USERS HANDBOOK FOR THE ARGONNE PREMIUM COAL SAMPLES

3.15. XPS Surface Densities of Oxygen Functional Groups

Data Courtesy of G. Gibbon, A. W. Wells, Pittsburgh Energy Technology Center. See Ref. 399

XPS SURFACE DENSITIES (PERCENT)*

	PITTSBURGH #8	BLIND CANYON	ILLINOIS #6
CARBON - CARBON	86.8	89.6	78.5
HYDROXYL	2.9	0.4	7.5
ETHER	8.2	9.2	8.5
CARBONYL	0.4	1.2	2.2
CARBOXYL	1.6	N.D.	3.2
PHENOL	1.3	0.4	4.3

SILYLATION FOR TOTAL HYDROXYL**

3.28	0.26	4.72
------	------	------

GAS PHASE SILYLATION FOR SURFACE HYDROXYL**

0.065	0.152	0.76 ± 0.02
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TOTAL CARBOXYL - SCHAFER METHOD**

0.0753	0.1000	0.1085
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PERCENT CARBON - ACID WASHED, AND VACUUM DRIED

75.9	76.1	66.6
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HYDROXYL DISTRIBUTION (PERCENT)

CARBOXYLIC ACID	2	28	2
PHENOLS	98	72	98
SURFACE HYDROXYL	2	58	16
TOTAL HYDROXYL	98	42	83

*XPS densities are the average values from several analyses, and where not normalized to 100%. The phenol density is the difference between the hydroxyl and carboxyl densities. The ether density was obtained by subtracting the hydroxyl density from the C-O bond density. The hydroxyl density was obtained from a separate XPS analysis for TMS ethers in gas phase silylated coal.

**In hydroxyl or carboxyl groups per 100 carbon atoms.

3.16. Heats of Immersion of Coals in Bases

Data from Ref. 56

 Table I. Heats of Immersion (ΔH_{imm}) of Six Premium Coals, Three Coals Reported in Previous Study and Three Prototype Solids (Dowon, Silica and Carbo-pack F) in Twelve Liquid Bases.

Bases	ΔH_{imm} of Wyodak (cal/g)	ΔH_{imm} of Wyoming ^a Residue (cal/g)	ΔH_{imm} of Illinois #6 (cal/g)	ΔH_{imm} of Illinois #6 ^b (cal/g)	ΔH_{imm} of Texas ^a (cal/g)	ΔH_{imm} of Pittsburgh #8 (cal/g)	ΔH_{imm} of Pocahontas #3 (cal/g)	ΔH_{imm} of North Dakota (cal/g)	ΔH_{imm} of Upper Freeport (cal/g)	ΔH_{imm} of Dowon MP-50 (kcal/equiv of acid)	ΔH_{imm} of Silica ^b (cal/g)	G. C. of Heats of Carbo-pack-F ^c (kcal/mole)
Pyridine	-35.90 ± 2.70	-32.14 ± 0.90	-30.49 ± 0.80	-41.30 ± 0.40	-29.46 ± 0.17	-20.20 ± 1.09	-7.30 ± 0.65	-24.99 ± 0.62	-6.82 ± 0.34	-15.90 ± 0.003	-24.95 ± 0.40	-8.92 ± 0.00
Dimethyl Sulfonide	-41.70 ± 0.70	-41.05 ± 0.37	-26.43 ± 1.67	-35.90 ± 1.00	-36.81 ± 0.17	-17.47 ± 1.13	-4.17 ± 1.06	-44.00 ± 1.11	-3.47 ± 0.99	-9.87 ± 0.19	-22.81 ± 1.40	-9.69 ± 0.20
4-Methyl Pyridine	-17.96 ± 1.35	-35.15 ± 0.10	-32.76 ± 1.21	-43.70 ± 1.17	-21.27 ± 0.74	-26.11 ± 0.62	-4.23 ± 0.56	-5.40 ± 0.80		-16.62 ± 0.09	-23.82 ± 0.52	-11.29 ± 0.25
Toluene	-3.44 ± 0.86		-6.69 ± 0.90			-0.86 ± 0.09	-2.05 ± 0.40	-2.05 ± 0.94	-0.45 ± 0.62	-1.51 ± 0.13	-12.27 ± 1.20	-10.49 ± 0.20
Cyclohe- xanone	-1.50 ± 1.10	-2.00 ± 0.59	-6.83 ± 1.10	-11.30 ± 0.30		+0.96 ± 2.17	-0.74 ± 1.42	+0.63 ± 0.56		-27.63 ± 0.21	-10.41 ± 1.00	-9.65 ± 0.19
n-Butyl- amine	-59.06 ± 2.61	-80.60 ± 3.27	-82.42 ± 1.17			-49.09 ± 0.06	-3.03 ± 0.69	-16.14 ± 1.30		-20.07 ± 0.20	-34.10 ± 0.63	-11.62 ± 0.29
2,6-Dimethyl Pyridine	-4.52 ± 0.25	-8.70 ± 0.60	-26.15 ± 1.00			-9.92 ± 0.007	-0.64 ± 0.12	-1.30 ± 0.57		-17.06 ± 0.003	-23.67 ± 1.82	-12.82 ± 0.10
2,4,6-Trimethyl Pyridine	-2.30 ± 0.43	-2.47 ± 0.19	-17.05 ± 0.45			-2.95 ± 1.44	-1.36 ± 0.42	+0.41 ± 0.31		-17.23 ± 0.030	-21.89 ± 0.70	-13.51 ± 0.32
n-Butyl- amine	-101.66 ± 3.10		-70.55 ± 0.35			-50.90 ± 2.51	-4.24 ± 0.40	-94.35 ± 2.46		-29.27 ± 0.25	-37.76 ± 0.85	-8.56 ± 0.14
Propylene Carbonate	-1.23 ± 0.71	+2.52 ± 1.20	-6.67 ± 0.95			-0.27 ± 0.04	-0.90 ± 0.16	-0.90 ± 0.24		-3.36 ± 0.04	-17.40 ± 1.16	-9.96 ± 0.40
Ethylene- diamine	-101.74 ± 0.80	-105.50 ± 1.96	-66.26 ± 3.07	-86.11 ± 1.90	-93.35 ± 1.42	-34.13 ± 2.60	-12.89 ± 0.50	-103.60 ± 0.94	-14.33 ± 2.82			
Acetoni- trile	-13.27 ± 1.20	-3.25 ± 0.76	-12.20 ± 0.74	+0.92 ± 0.55	-7.33 ± 0.40	-3.15 ± 1.01	-6.01 ± 1.13	-14.94 ± 0.70				

a. Reference (12)

b. Obtained by E. F. Cassidy

c. Obtained by D. J. Hutchinson

3.17. Heats of Immersion of Coals in Acids

Data from Ref. 443

 Table 3 Heats of immersion (ΔH_{imm}) of coals and polyvinylpyridine in acid solutions (0.65 M) in acetonitrile

Acids	pK_a^a	$-\Delta H_{imm}$ (cal g ⁻¹)				
		PVP	Exxon Rawhide	Wyodak	Illinois no. 6	Pittsburgh no. 8
Ethanesulfonic	-1.68	148.33 ± 17.0	37.35 ± 0.84	44.62 ± 1.56	22.86 ± 0.48	21.28 ± 2.13
Methanesulfonic	-1.92	147.55 ± 1.47	37.99 ± 1.46	44.79 ± 2.00	21.56 ± 0.24	21.98 ± 1.19
Triflic	-5.90	130.54 ± 9.54 ^c	59.16 ± 2.85	60.16 ± 1.61	45.08 ± 2.36	29.39 ± 1.47
Trifluoroacetic	0.54	85.75 ± 0.72	32.19 ± 0.86	35.69 ± 1.15	18.53 ± 0.48	12.62 ± 0.60
Trichloroacetic	0.69	80.82 ± 1.40	28.17 ± 0.03	23.89 ± 0.88	14.71 ± 0.72	08.07 ± 0.70
Difluoroacetic	1.30	74.99 ± 1.89	29.73 ± 0.56	31.55 ± 0.66	16.44 ± 0.45	10.03 ± 0.66
Dichloroacetic	1.36	70.56 ± 0.82	29.06 ± 0.22	26.52 ± 0.49	16.38 ± 0.38	09.90 ± 1.50
4-Toluenesulfonic	-6.55	66.89 ± 1.99	24.81 ± 1.02	24.81 ± 0.95	20.39 ± 0.41	08.92 ± 1.25
Benzenesulfonic	-2.70	62.08 ± 0.53	30.55 ± 0.94	29.30 ± 0.22	23.79 ± 1.87	18.58 ± 0.24
Chloroacetic		60.00 ± 0.82	27.25 ± 0.07	26.72 ± 0.94	16.75 ± 0.59	07.60 ± 0.66
4-Chlorobenzenesulfonic		53.26 ± 1.37	24.89 ± 0.94	24.09 ± 1.21	19.14 ± 0.98	10.82 ± 0.66
4-Nitrobenzenesulfonic	-4.00		23.24 ± 0.27	26.23 ± 1.00	20.81 ± 0.79	07.13 ± 0.71
Boron trichloride ^b			24.10 ± 1.79	26.18 ± 2.40	33.78 ± 2.23	16.94 ± 0.27

^a Acidic dissociation constants of sulfonic acids in water at 25°C from References 27 and 36 which describe the unusual difficulties of comparing the strengths of very strong acids

^b Hexane as solvent

^c See text

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3.18. Capillary Gas Chromatograms of the Aliphatic Fraction of Pyridine Extracts of Coal Samples

Data courtesy of M. L. Lee & H. K. Chang, Brigham Young Univ.
Ref. 108

Figure 4-1. Capillary gas chromatograms of the aliphatic fractions of (A) North Dakota lignite and (B) Wyodak subbituminous coal extracts. Chromatographic conditions: temperature programmed from 60°C to 300°C at 4°C min⁻¹ after a 1-min isothermal period.

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Capillary Gas Chromatograms of the Aliphatic Fraction of Pyridine Extracts of Coal Samples

Data courtesy of M. L. Lee & H. K. Chang, Brigham Young Univ.
Ref. 108

Figure 4-2. Capillary gas chromatograms of the aliphatic fractions of (A) Illinois #6 and (B) Pittsburgh #8 coal extracts. Chromatographic conditions are given in Figure 4-1. Peaks that are marked "o" represent the n -alkanes.

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Capillary Gas Chromatograms of the Aliphatic Fraction of Pyridine Extracts of Coal Samples

Data courtesy of M. L. Lee & H. K. Chang, Brigham Young Univ.
Ref. 108

Figure 4-3. Capillary gas chromatograms of the aliphatic fractions of (A) Upper Freeport and (B) Pocahontas #3 coal extracts. Chromatographic conditions are given in Figure 4-1. Peaks that are marked "o" represent the *n*-alkanes.

3.19. Capillary Gas Chromatograms of the Neutral Polycyclic Aromatic Fraction of Pyridine Extracts

Data courtesy of M. L. Lee & H. K. Chang, Brigham Young Univ.
Ref. 108

Figure 4-5. Capillary gas chromatograms of the neutral polycyclic aromatic fractions of (A) North Dakota lignite and (B) Wyodak subbituminous coal extracts. Chromatographic conditions: temperature programmed from 60°C to 290°C at 4°C min⁻¹ after a 1-min isothermal period.

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Capillary Gas Chromatograms of the Neutral Polycyclic Aromatic Fraction of Pyridine Extracts of Coal Samples

Data courtesy of M. L. Lee & H. K. Chang, Brigham Young Univ.
Ref. 108

Figure 4-6. Capillary gas chromatograms of the neutral polycyclic aromatic fractions of (A) Illinois #6 and (B) Pittsburgh #8 coal extracts. Chromatographic conditions are given in Figure 4-5.

USERS HANDBOOK FOR THE ARGONNE PREMIUM COAL SAMPLES

Capillary Gas Chromatograms of the Neutral Polycyclic Aromatic Fraction of Pyridine Extracts of Coal Samples

Data courtesy of M. L. Lee & H. K. Chang, Brigham Young Univ.
Ref. 108

Figure 4-7. Capillary gas chromatograms of the neutral polycyclic aromatic fractions of (A) Upper Freeport and (B) Pocahontas #3 coal extracts. Chromatographic conditions are given in Figure 4-5.

3.20. Capillary Gas Chromatograms of the Sulfur-Bearing Polycyclic Aromatic Fraction of Pyridine Extracts

Data courtesy of M. L. Lee and H. K. Chang, Brigham Young Univ.
Ref. 108

Figure 4-10. Gas chromatograms of (A) A-2, (B) P-2, and (C) P-3 fractions of a Wyodak subbituminous coal. Chromatographic conditions: (A) temperature programmed from 85°C to 290°C at 6°C/min after a 1-min isothermal period; (B) and (C) temperature programmed from 85°C to 300°C at 5°C/min after a 1-min isothermal period. Peak numbers are identified in Table 4-6.

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Capillary Gas Chromatograms of the Sulfur-Containing Polycyclic Aromatic Fraction of Pyridine Extracts of Coal Samples

Data courtesy of M. L. Lee & H. K. Chang, Brigham Young Univ.
Ref. 108

Figure 4-11. Gas chromatograms of (A) A-2, (B) P-2, and (C) P-3 fractions of an Illinois #6 coal. Chromatographic conditions are given in Figure 4-10.

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Capillary Gas Chromatograms of the Sulfur-Containing Polycyclic Aromatic Fraction of Pyridine Extracts of Coal Samples

Data courtesy of M. L. Lee and H. K. Chang, Brigham Young Univ.
Ref. 108

Figure 4-12. Gas chromatograms of (A) A-2, (B) P-2, and (C) P-3 fractions of a Pittsburgh #8 coal. Chromatographic conditions are given in Figure 4-10.

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Capillary Gas Chromatograms of the Sulfur-Containing Polycyclic Aromatic Fraction of Pyridine Extracts of Coal Samples

Data courtesy of M. L. Lee and H. K. Chang, Brigham Young Univ.
Ref. 108

Figure 4-14. Gas chromatograms of (A) A-2, (B) P-2, and (C) P-3 fractions of a Pocahontas #3 coal. Chromatographic conditions are given in Figure 4-10.

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Capillary Gas Chromatograms of the Sulfur-Containing Polycyclic Aromatic Fraction of Pyridine Extracts of Coal Samples

Data courtesy of M. L. Lee and H. K. Chang, Brigham Young Univ.
Ref. 108

Figure 4-13. Gas chromatograms of (A) A-2, (B) P-2, and (C) P-3 fractions of an Upper Freeport coal. Chromatographic conditions are given in Figure 4-10.

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3.21. Photoacoustic FTIR Spectra of Coal Samples

Data courtesy of H. L. C. Meuzelaar & Huai Huaying, Univ. of Utah

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Photoacoustic Fourier Transform Infrared Spectra of Coal Samples

Data courtesy of H. L. C. Meuzelaar & Huai Huaying, Univ. of Utah

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Photoacoustic Fourier Transform Infrared Spectra of Coal Samples

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USERS HANDBOOK FOR THE ARGONNE PREMIUM COAL SAMPLES

Photoacoustic Fourier Transform Infrared Spectra of Coal Samples

Data courtesy of H. L. C. Meuzelaar & Huai Huaying, Univ. of Utah

3.22. Thermogravimetric-Fourier Transform Infrared (TG-FTIR) Data on Coal Samples

Courtesy P. R. Solomon, Advanced Fuel Research, Inc., Ref. 130

Figure 5. TG-FTIR Analysis of Pocahontas Coal during the Pyrolysis Cycle. a) Weight Loss (solid), Sum of Evolved Products (dashed), and Temperature Profile. b) Tar Evolution Rate and Integrated Amount Evolved. c) Methane Evolution Rate and Integrated Amount Evolved. d) H₂O Evolution Rate and Integrated Amount Evolved. e) CO₂ Evolution Rate and Integrated Amount Evolved. f) CO Evolution Rate and Integrated Amount Evolved.

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Thermogravimetric-Fourier Transform Infrared (TG-FTIR) Data on Coal Samples

Courtesy P. R. Solomon, Advanced Fuel Research, Inc., Ref. 130

Figure 6. TG-FTIR Analysis of Upper Freeport Coal during the Pyrolysis Cycle. a) Weight Loss (solid), Sum of Evolved Products (dashed), and Temperature Profile. b) Tar Evolution Rate and Integrated Amount Evolved. c) Methane Evolution Rate and Integrated Amount Evolved. d) H₂O Evolution Rate and Integrated Amount Evolved. e) CO₂ Evolution Rate and Integrated Amount Evolved. f) CO Evolution Rate and Integrated Amount Evolved.

Thermogravimetric-Fourier Transform Infrared (TG-FTIR) Data on Coal Samples

Courtesy P. R. Solomon, Advanced Fuel Research, Inc., Ref. 130

Figure 7. TG-FTIR Analysis of Pittsburgh No. 8 Coal during the Pyrolysis Cycle. a) Weight Loss (solid), Sum of Evolved Products (dashed), and Temperature Profile. b) Tar Evolution Rate and Integrated Amount Evolved. c) Methane Evolution Rate and Integrated Amount Evolved. d) H₂O Evolution Rate and Integrated Amount Evolved. e) CO₂ Evolution Rate and Integrated Amount Evolved. f) CO Evolution Rate and Integrated Amount Evolved.

USERS HANDBOOK FOR THE ARGONNE PREMIUM COAL SAMPLES

Thermogravimetric-Fourier Transform Infrared (TG-FTIR) Data on Coal Samples

Courtesy P. R. Solomon, Advanced Fuel Research, Inc., Ref. 130

Figure 8. TG-FTIR Analysis of Stockton Seam Coal during the Pyrolysis Cycle. a) Weight Loss (solid), Sum of Evolved Products (dashed), and Temperature Profile. b) Tar Evolution Rate and Integrated Amount Evolved. c) Methane Evolution Rate and Integrated Amount Evolved. d) H₂O Evolution Rate and Integrated Amount Evolved. e) CO₂ Evolution Rate and Integrated Amount Evolved. f) CO Evolution Rate and Integrated Amount Evolved.

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Thermogravimetric-Fourier Transform Infrared (TG-FTIR) Data on Coal Samples

Courtesy P. R. Solomon, Advanced Fuel Research, Inc., Ref. 130

Figure 9. TG-FTIR Analysis of Illinois No. 6 Coal during the Pyrolysis Cycle. a) Weight Loss (solid), Sum of Evolved Products (dashed), and Temperature Profile. b) Tar Evolution Rate and Integrated Amount Evolved. c) Methane Evolution Rate and Integrated Amount Evolved. d) H₂O Evolution Rate and Integrated Amount Evolved. e) CO₂ Evolution Rate and Integrated Amount Evolved. f) CO Evolution Rate and Integrated Amount Evolved.

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Thermogravimetric-Fourier Transform Infrared (TG-FTIR) Data on Coal Samples

Courtesy P. R. Solomon, Advanced Fuel Research, Inc., Ref. 130

Figure 10. TG-FTIR Analysis of Utah Blind Canyon Coal during the Pyrolysis Cycle. a) Weight Loss (solid), Sum of Evolved Products (dashed), and Temperature Profile. b) Tar Evolution Rate and Integrated Amount Evolved. c) Methane Evolution Rate and Integrated Amount Evolved. d) H₂O Evolution Rate and Integrated Amount Evolved. e) CO₂ Evolution Rate and Integrated Amount Evolved. f) CO Evolution Rate and Integrated Amount Evolved.

USERS HANDBOOK FOR THE ARGONNE PREMIUM COAL SAMPLES

Thermogravimetric-Fourier Transform Infrared (TG-FTIR) Data on Coal Samples

Courtesy P. R. Solomon, Advanced Fuel Research, Inc., Ref. 130

Figure 11. TG-FTIR Analysis of Wyodak Subbituminous Coal during the Pyrolysis Cycle. a) Weight Loss (solid), Sum of Evolved Products (dashed), and Temperature Profile. b) Tar Evolution Rate and Integrated Amount Evolved. c) Methane Evolution Rate and Integrated Amount Evolved. d) H₂O Evolution Rate and Integrated Amount Evolved. e) CO₂ Evolution Rate and Integrated Amount Evolved. f) CO Evolution Rate and Integrated Amount Evolved.

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Thermogravimetric-Fourier Transform Infrared (TG-FTIR) Data on Coal Samples

Courtesy P. R. Solomon, Advanced Fuel Research, Inc.. Ref. 130

Figure 12. TG-FTIR Analysis of Zap Lignite during the Pyrolysis Cycle. a) Weight Loss (solid), Sum of Evolved Products (dashed), and Temperature Profile. b) Tar Evolution Rate and Integrated Amount Evolved. c) Methane Evolution Rate and Integrated Amount Evolved. d) H₂O Evolution Rate and Integrated Amount Evolved. e) CO₂ Evolution Rate and Integrated Amount Evolved. f) CO Evolution Rate and Integrated Amount Evolved.

USERS HANDBOOK FOR THE ARGONNE PREMIUM COAL SAMPLES

3.23. Photoacoustic FTIR Spectra of LTA (Low Temperature Ash) from Coal Samples

Data Courtesy of H. L. C. Meuzelaar, University of Utah

USERS HANDBOOK FOR THE ARGONNE PREMIUM COAL SAMPLES

Photoacoustic Fourier Transform Infrared Spectra of LTA (Low Temperature Ash) from Coal Samples

Data Courtesy of H. L. C. Meuzelaar, University of Utah

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Photoacoustic Fourier Transform Infrared Spectra of LTA (Low Temperature Ash) from Coal Samples

Data Courtesy of H. L. C. Meuzelaar, University of Utah

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Photoacoustic Fourier Transform Infrared Spectra of LTA (Low Temperature Ash) from Coal Samples

Data Courtesy of H. L. C. Meuzelaar, University of Utah

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3.24. Solvent Diffusion in Coals

Kinetic Constants for Solvent Diffusion in Coals

Data from Ref. 113

Sample	Solvent	Q	$(Q-1)/V^a$	E(kJ/mol)	n	k
PITT	pyridine	2.14	1.4	58-66	0.84	27.9
	BA	1.93	0.9	25-27	0.72	48.5
	HA	2.28	0.9	44	1.17	1.9
	THF	1.41	0.5	41-44	0.87	6.2
IL	pyridine	2.23	1.5	41-42	0.37	392
UT	pyridine	2.22	1.5	62-64	0.69	48.4

n = roughly 0.5 for Fickian diffusion, about 1 for relaxation controlled diffusion

k = constant

Q = solvent swelling ratio at equilibrium

V = molar volume of solvent

BA = butyl amine

HA = hexyl amine

THF = tetrahydrofuran

All entries in units of $(10^{-2} \text{ mol/cm}^3)$

3.25. Coal Solubility in Pyridine

Coal	Solubility, %
------	---------------

UF	20.9
WY	6.1
IL	27.1
PITT	25.0
POC	1.2
UT	29.4
WV	12.4

Data Courtesy of David Buchanan,
derived from Energy Fuels **1988** 2 163-170

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3.26. Sulfur in Coal as a Percentage of Total Organic S

Aliphatic/non-thiophenic sulfur in coal as a percentage of total organic sulfur.

Coal	C, wt %	flash pyrol.	TPR	CAPTO	XPS	XANES 3rd deriv.	XANES least squares	DEIHRMS
Beulah-Zap, ND	74.05	39		35	45	35	45	31-41
Wyodak, WY	76.04	36	25	28	37	33	40	20-36
Illinois #6, IL	80.73		25	28	31	33	37	22-37
Bl. Canyon, UT	81.32			11	35	24	26	12-19
Pittsburgh, PITT	84.95			18	25	22	41	8-13
L. Stockton, WV	85.47			13	14	19	22	9-14
U. Freeport, UF	88.08		5-10	28	19	13	5	5-7
Pocahontas, POC	91.81			16	0	13	0	3-4

flash pyrol. = flash pyrolysis, TPR = temperature programmed reduction, CAPTO = controlled atmosphere programmed temperature oxidation, XPS = x-ray photoelectron spectroscopy, XANES = x-ray absorption near-edge structure, DEIHRMS = desorption electron impact high-resolution mass spectroscopy

Data from: Davidson, Robert M., IEACR/60 IEA Coal Research, London, August, 1993, 79 pp.

3.27. High Resolution Mass Spectrometric Analysis of Extracts
Data courtesy of Randall E. Winans, see Refs. 402, 409, 427

High Resolution Mass Spectrometric Analysis of Extracts
Data courtesy of Randall E. Winans, see Refs. 402, 409, 427

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High Resolution Mass Spectrometric Analysis of Extracts

Data courtesy of Randall E. Winans, see Refs. 402, 409, 427

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High Resolution Mass Spectrometric Analysis of Extracts
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High Resolution Mass Spectrometric Analysis of Extracts
Data courtesy of Randall E. Winans, see Refs. 402, 409, 427

High Resolution Mass Spectrometric Analysis of Extracts
Data courtesy of Randall E. Winans, see Refs. 402, 409, 427

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3.28. Additional Analytical Data for Some Coals

The additional data which have been received are summarized below. The order of the data is the same as the sequence of sample availability:

The results may represent a mean of the results of a round-robin analysis.

Coal Sample 1, Upper Freeport medium volatile bituminous

Maceral Analysis

		with ash	MMF
Vitrinite	%	78.7	89.7
Liptinite	%	0.7	0.8
Semifusinite	%	1.3	1.5
Fusinite	%	6.7	7.6
Other Inertinites	%	0.3	0.3
Mineral Matter	%	12.3	

Pore Size - Cumulative Pore Area (sq. m/g) 1.081

BET Surface Area (sq. m/g) 1.25

Coal 2, Wyodak Subbituminous

Capacity Moisture 29.37%

Density 1.410 g/ml

Specific Surface Area in Nitrogen 2.9 m²/gm

Coal 7, West Virginia, Stockton Lewiston Seam, High Volatile Bituminous Coal

Maceral Analysis, volume %

Vitrinites	72.8	
Inertinites	15.6	
		Semifusinites 10.9
		Micrinites 1.1
		Indeterminate 1.7
		Fusinite 1.9
Exinites	11.5	
		Sporinite 10.2
		Resinite 1.0
		Cutinite 0.3

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2	—	X	—	—	—	—	—	—	52	—	—	—	X	—	—	—	—
3	X	—	—	—	—	—	—	—	53	—	X	X	X	—	—	—	X
4	X	X	X	X	X	X	X	X	54	X	X	X	X	X	X	X	X
5	—	—	X	—	—	—	—	—	55	X	X	X	X	X	X	X	X
6	—	—	X	—	—	—	—	—	56	X	X	X	X	X	—	—	X
7	X	—	—	—	—	—	—	—	57	X	X	X	—	—	X	—	X
8	X	X	X	—	—	—	—	—	58	—	—	X	—	—	—	—	—
9	X	X	X	X	X	X	X	X	59	—	—	—	—	—	—	X	—
10	X	—	—	—	—	—	—	—	60	X	X	X	X	X	X	X	X
11	X	—	—	—	—	—	—	—	61	X	—	—	—	—	—	—	—
12	X	X	X	X	X	X	X	X	62	X	X	X	X	X	X	X	X
13	X	X	X	X	X	X	X	X	63	X	X	X	X	X	—	—	X
14	—	—	—	X	—	—	—	—	64	—	—	—	X	—	—	—	—
15	—	—	X	—	—	—	—	—	65	—	—	—	X	—	—	—	—
16	X	—	—	X	—	—	—	—	66	—	X	X	X	X	—	—	—
17	X	X	X	X	X	X	—	—	67	—	—	X	—	—	—	—	—
18	X	X	X	—	X	X	X	X	68	—	—	X	—	—	—	—	—
19	X	X	X	X	X	X	X	X	69	—	—	X	—	—	—	—	—
20	X	—	X	—	X	—	—	—	70	—	—	—	X	—	—	—	X
21	—	—	—	X	—	X	—	—	71	X	—	—	—	—	—	—	—
22	X	X	X	X	X	X	X	X	72	X	—	—	—	—	—	—	—
23	—	—	X	—	—	—	—	—	73	X	—	—	—	—	—	—	—
24	X	X	X	X	X	—	—	—	74	X	—	X	X	—	X	X	—
25	X	X	X	X	X	X	X	X	75	X	X	X	X	X	X	X	X
26	—	—	—	—	—	—	—	—	76	X	X	X	X	X	X	X	X
27	—	—	X	—	—	—	—	—	77	X	X	X	X	X	X	X	X
28	—	X	X	X	X	—	—	—	78	X	X	X	X	X	X	X	X
29	X	X	X	X	X	—	—	—	79	X	X	X	X	X	X	X	X
30	—	X	—	—	—	—	—	—	80	X	X	X	X	X	X	X	X
31	X	X	X	X	X	X	—	—	81	—	—	X	—	—	—	—	—
32	—	—	X	—	—	—	—	—	82	—	—	X	—	—	—	—	—
33	X	X	X	—	X	—	—	—	83	—	X	—	—	—	—	—	—
34	—	—	X	—	—	—	—	—	84	—	—	X	—	—	—	—	—
35	—	—	X	—	—	—	—	—	85	—	X	X	X	X	—	—	—
36	X	X	X	X	X	X	X	X	86	X	X	X	X	X	X	X	X
37	X	X	X	X	X	X	X	X	87	X	—	X	X	X	—	X	—
38	X	X	X	X	—	—	—	X	88	X	X	X	X	X	X	X	X
39	X	X	X	X	X	X	X	X	89	X	X	X	X	X	—	—	—
40	—	—	X	—	—	—	—	—	90	—	X	X	—	X	—	—	X
41	—	—	—	—	—	—	—	—	91	X	X	—	X	X	X	X	—
42	—	—	X	—	—	—	—	—	92	—	—	—	X	—	—	—	—
43	X	X	X	X	X	X	X	X	93	—	—	—	X	X	—	—	X
44	—	X	X	—	—	X	—	—	94	X	—	X	X	X	—	X	X
45	X	X	X	X	X	X	X	X	95	—	—	X	X	—	—	—	X
46	—	X	—	X	—	—	—	X	96	X	X	X	X	X	X	X	X
47	—	—	X	X	—	X	—	—	97	—	—	X	—	—	—	—	X
48	X	X	X	X	X	X	X	—	98	—	—	X	—	—	—	—	—
49	X	X	—	—	—	—	—	—	99	—	—	X	—	—	—	—	—
50	X	X	X	—	X	—	—	X	100	—	X	X	—	—	—	—	—

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102	—	—	X	—	—	—	—	—	152	—	X	X	—	X	—	—	—
103	X	—	X	X	X	X	X	—	153	—	—	—	X	—	—	—	—
104	—	X	—	X	—	—	—	—	154	—	—	X	—	—	—	—	—
105	—	—	X	—	—	—	—	—	155	—	X	—	X	—	—	X	—
106	—	—	—	—	—	X	X	—	156	—	—	—	X	—	—	—	—
107	—	—	—	—	X	—	—	—	157	—	—	—	X	—	—	—	X
108	X	X	X	X	X	X	X	X	158	—	—	X	X	—	—	—	—
109	X	X	X	X	X	—	—	X	159	—	X	—	—	—	—	—	X
110	—	—	—	X	—	—	—	—	160	—	—	X	—	—	—	—	—
111	—	—	—	X	—	—	—	—	161	—	X	X	—	X	—	—	—
112	—	X	—	—	—	—	—	—	162	—	X	X	—	—	—	—	X
113	—	—	X	X	—	X	—	—	163	—	X	—	—	—	—	—	—
114	X	X	X	X	X	X	X	X	164	X	X	X	—	—	—	—	—
115	X	X	X	X	X	X	X	X	165	—	X	—	—	—	—	—	—
116	X	—	—	—	—	—	—	—	166	X	X	X	X	X	X	X	X
117	X	—	—	—	—	—	—	—	167	X	X	X	X	X	X	X	—
118	X	X	X	X	X	X	X	X	168	—	—	—	—	—	—	—	X
119	X	X	X	X	—	X	X	X	169	—	—	X	—	—	—	—	—
120	X	X	X	X	X	X	X	X	170	—	—	X	—	—	—	—	—
121	—	—	—	X	—	—	—	—	171	—	—	X	—	—	—	—	—
122	—	—	—	X	—	—	—	X	172	X	X	X	X	X	X	X	X
123	X	—	X	X	X	—	X	—	173	—	—	X	—	—	—	—	—
124	—	X	X	—	—	—	—	X	174	—	—	X	X	X	X	—	X
125	—	—	—	—	—	—	—	X	175	—	—	—	X	—	—	—	—
126	—	—	X	—	—	—	—	—	176	—	X	X	—	—	—	—	—
127	X	X	X	X	X	X	X	X	177	—	—	X	—	—	—	—	—
128	X	X	X	X	X	X	X	X	178	—	X	—	—	—	—	—	—
129	—	—	X	X	—	X	—	—	179	—	X	X	—	—	—	—	—
130	X	X	X	X	X	X	X	X	180	X	—	X	X	X	—	X	—
131	X	—	X	—	X	—	—	—	181	—	X	X	—	—	—	—	—
132	X	—	X	—	X	—	—	—	182	—	—	—	—	—	—	—	—
133	—	X	—	—	—	—	—	X	183	—	X	—	—	—	—	—	—
134	—	—	—	—	—	—	X	—	184	X	X	X	X	X	X	X	X
135	—	—	X	X	X	X	—	X	185	X	X	X	X	X	X	X	X
136	X	X	X	X	X	—	—	X	186	X	X	X	X	X	X	X	X
137	—	—	—	—	—	—	—	X	187	—	—	X	—	—	—	—	—
138	—	X	—	—	—	—	—	X	188	—	—	X	—	—	—	—	—
139	—	—	—	X	—	—	—	X	189	X	X	X	X	X	X	X	X
140	—	—	—	X	—	—	—	X	190	X	X	X	X	X	X	X	X
141	—	—	—	X	X	X	—	X	191	—	X	X	—	X	—	X	X
142	—	X	X	X	—	X	X	—	192	—	X	—	—	—	—	—	—
143	—	X	—	—	—	—	—	X	193	X	X	X	X	X	X	X	X
144	X	—	—	—	—	—	—	—	194	X	X	X	X	X	X	X	X
145	—	X	X	X	—	—	—	—	195	X	X	X	X	X	X	X	X
146	X	—	—	—	—	—	—	—	196	—	—	X	—	—	—	—	—
147	—	—	—	—	—	X	—	—	197	—	—	X	—	—	—	—	—
148	—	X	—	—	—	—	—	—	198	—	X	—	X	—	—	—	—
149	—	X	—	—	—	—	—	X	199	—	—	—	X	X	—	—	X

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150 | _ | _X | _X | _ | _ | _ | _ | 200 | _ | _X | _ | _X | _ | _ | _ | _

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201	_X		_X	_X				X	251		_X						
202		_X						X	252								X
203			X						253	_X	X	X	_X	_X	_X	X	X
204			X						254		X	X					
205				X					255		X	X		X			X
206			X						256								X
207			X						257	X		X	X	X	X	X	
208						X			258	X	X	X	X	X	X	X	X
209	X	X	X	X	X	X	X	X	259	X	X	X	X		X	X	X
210	X	X	X	X	X	X	X	X	260			X					
211	X	X	X	X	X	X	X	X	261			X					
212	X	X	X	X	X	X	X	X	262	_X	_X	X	_X	_X	_X	_X	_X
213	X	X	X	X	X	X	X	X	263			X					
214	X	X	X	X	X	X	X	X	264	X	X	X	X	X	X	X	X
215		X	X	X		X	X	X	265	X	X	X	X	X	X	X	X
216	X	X	X	X	X	X	X	X	266	X	X	X	X	X	X	X	X
217	X	X	X	X	X	X	X	X	267	X	X	X	X	X	X	X	X
218		X		X				X	268	X	X	X	X	X	X	X	X
219	X	X	X	X	X	X	X	X	269	X	X	X	X	X	X	X	X
220			X						270						X		
221	X	X	X	X	X	X	X	X	271	X		X	X	X	X		
222	X		X	X	X	X	X		272							X	
223	X	X	X	X	X	X	X	X	273	X	X	X	X	X	X	X	X
224			X	X		X			274		X	X		X			
225						X			275						X		
226		X	X	X					276			X					
227	X	X	X						277		X	X	X				
228			X						278	X	X	X	X	X			X
229	X	X	X	X	X	X	X	X	279			X				X	X
230		X	X					X	280				X		X		X
231		X	X					X	281	X							
232	X	X	X	X	X	X	X	X	282								X
233			X						283	X	X	X	X	X	X	X	X
234			X					X	284	X	X	X	X	X	X	X	X
235								X	285	X	X	X	X		X	X	X
236	X		X	X				X	286			X					
237	X	X	X	X	X	X	X	X	287				X		X		X
238	X		X	X	X			X	288		X						X
239	X	X	X	X	X	X	X	X	289	X	X	X		X	X	X	X
240					X				290	X	X	X	X	X	X	X	X
241			X						291		X	X		X		X	X
242			X						292				X				X
243	X	X	X	X	X	X	X	X	293				X				
244		X	X						294			X					
245				X					295		X	X					X
246	X	X	X						296			X					
247	X	X	X	X	X	X	X	X	297			X					

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248	X	X		X	X			298		X				X		
249	X	X		X	X			299		X						
250	X	X	X	X	X			300		X						X

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301	—	—	X	—	—	—	—	—	351	X	—	X	—	—	—	—	—
302	—	—	—	—	—	—	—	X	352	—	—	—	X	—	—	—	—
303	X	—	X	X	—	—	—	—	353	X	X	X	X	X	X	X	X
304	X	X	X	X	X	—	—	X	354	X	—	X	X	—	—	—	—
305	X	X	X	—	X	—	—	—	355	X	X	X	X	X	X	X	X
306	X	X	X	X	X	X	X	X	356	X	X	X	X	X	X	X	X
307	—	—	X	—	—	—	—	—	357	X	—	—	X	X	X	—	—
308	—	—	X	—	—	—	—	—	358	X	X	X	X	X	X	X	X
309	—	—	X	—	—	—	—	—	359	X	X	X	X	X	X	X	X
310	X	—	—	—	—	—	—	—	360	—	—	—	—	—	X	—	X
311	X	X	X	—	—	—	—	—	361	—	X	—	X	X	X	—	X
312	X	X	X	X	X	X	X	X	362	X	—	X	—	—	—	—	—
313	—	—	—	—	—	—	X	—	363	—	—	X	—	—	—	—	—
314	X	X	X	X	X	X	X	X	364	—	—	X	—	—	—	—	—
315	—	—	—	—	X	—	—	—	365	X	X	X	X	X	X	X	X
316	—	—	X	—	—	—	—	—	366	X	X	X	X	X	X	X	X
317	X	X	X	X	X	X	X	X	367	—	X	—	—	—	—	—	X
318	—	—	X	—	—	—	—	—	368	—	—	—	—	—	—	—	X
319	—	—	X	—	—	X	—	X	369	X	X	X	X	X	X	X	X
320	—	X	X	X	—	—	—	X	370	—	—	—	X	—	—	—	—
321	—	X	—	—	—	—	—	—	371	—	—	—	X	—	—	—	—
322	—	—	X	X	—	—	—	X	372	—	X	—	—	—	—	—	—
323	—	—	—	X	—	—	—	—	373	—	X	X	X	—	—	—	X
324	—	—	—	—	—	—	X	—	374	X	X	X	X	X	X	X	X
325	—	—	X	—	—	—	—	—	375	—	—	—	X	—	—	—	—
326	X	X	X	X	X	X	X	X	376	—	—	—	X	—	—	—	X
327	—	—	X	—	—	—	—	X	377	X	X	X	X	X	X	X	X
328	—	—	X	—	—	—	—	—	378	—	—	X	X	—	X	—	X
329	—	X	—	X	—	X	—	—	379	—	—	—	—	—	—	X	—
330	—	—	X	—	—	—	—	—	380	—	—	—	—	—	—	X	—
331	X	X	X	X	X	X	X	X	381	—	X	—	—	—	—	—	X
332	X	—	X	—	X	X	—	—	382	X	X	X	X	X	—	—	—
333	X	X	X	X	X	—	—	—	383	X	X	X	X	X	X	X	X
334	X	—	X	—	—	—	—	—	384	—	—	—	X	—	—	—	—
335	—	—	X	—	—	—	—	—	385	X	X	X	X	X	X	X	X
336	—	—	—	X	—	—	—	—	386	—	—	X	X	—	—	—	—
337	—	—	X	—	—	—	—	—	387	X	—	X	X	X	X	—	X
338	—	—	—	—	—	—	—	X	388	X	X	X	X	X	X	X	X
339	—	—	X	—	—	—	—	—	389	X	X	X	—	—	—	—	—
340	X	X	X	X	X	X	X	X	390	X	X	X	X	X	X	X	X
341	—	—	X	—	—	X	X	X	391	—	—	X	—	—	—	X	—
342	—	—	—	—	—	—	—	X	392	—	—	X	—	—	—	X	—
343	X	—	X	X	X	X	—	X	393	X	X	X	X	X	X	X	X
344	—	—	X	X	—	—	—	X	394	—	X	—	—	—	—	—	—
345	X	—	X	X	X	X	X	—	395	—	X	—	—	—	X	—	—
346	—	X	—	—	—	—	—	—	396	—	X	X	X	—	X	X	—
347	X	X	X	X	X	X	X	X	397	—	—	—	—	—	—	—	—
348	—	—	X	—	—	—	—	—	398	X	—	—	X	—	—	—	—
349	—	—	—	—	—	—	—	X	399	—	—	X	—	—	—	—	—
350	—	—	X	—	—	—	—	—	400	—	—	X	—	X	—	—	—

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401	X	X	X	X	X	X	X	X	451	X							
402	X				X		X	X	452				X				
403			X						453		X	X					
404	X	X	X	X	X	X	X	X	454		X						
405	X	X	X	X	X	X	X	X	455	X	X	X	X	X	X	X	X
406	X			X					456			X		X			
407		X							457	X		X					
408	X	X	X	X	X	X	X	X	458				X		X		X
409	X	X	X	X	X	X	X	X	459				X				
410		X							460				X		X		
411		X						X	461	X							
412		X						X	462	X	X						
413	X	X	X	X	X	X	X	X	463	X	X	X	X	X	X	X	X
414	X								464				X				
415				X					465	X	X	X	X	X	X	X	X
416					X	X		X	466		X						X
417	X	X	X	X	X	X	X	X	467	X			X				X
418	X		X	X	X				468			X					
419			X						469								X
420	X	X	X	X	X	X	X	X	470				X				
421								X	471			X		X			X
422	X	X	X	X	X			X	472	X	X	X	X	X	X	X	X
423			X		X			X	473	X	X	X	X	X	X	X	X
424	X	X	X	X	X	X	X	X	474	X	X	X	X	X	X	X	X
425	X	X	X	X	X	X	X	X	475			X		X		X	
426	X	X	X	X	X	X	X	X	476		X	X	X	X	X		X
427	X	X	X	X	X	X	X	X	477	X	X	X		X	X	X	X
428	X		X						478					X			
429	X			X					479	X	X	X	X	X	X	X	X
430	X		X		X			X	480	X	X	X	X	X	X	X	X
431	X	X	X	X	X	X	X	X	481		X	X					
432		X							482	X	X	X	X	X	X	X	X
433		X						X	483	X	X	X	X	X	X	X	
434		X							484	X	X	X	X	X	X	X	X
435						X			485	X	X	X	X	X	X	X	X
436			X						486	X	X	X	X	X	X	X	X
437				X					487	X	X	X	X	X	X	X	X
438	X			X					488	X	X	X	X	X		X	X
439			X						489	X		X		X			
440	X	X	X	X	X	X	X	X	490	X	X	X	X	X	X	X	X
441	X	X	X	X	X	X	X	X	491		X	X	X	X	X		X
442			X						492			X	X	X	X		X
443		X	X	X					493	X	X	X	X	X	X	X	X
444	X		X	X	X	X	X	X	494	X	X	X	X	X	X	X	X
445	X	X	X	X	X	X	X	X	495						X		X
446	X		X	X	X				496	X	X	X	X	X	X	X	X
447			X						497	X	X	X	X	X	X	X	X
448					X		X	X	498	X	X	X	X	X	X	X	X
449								X	499				X	X	X		X
450								X	500	X	X	X	X	X	X	X	X

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501							X		551								
502	X	X	X	X	X	X	X	X	552								
503	X	X	X	X	X	X	X	X	553								
504	X	X	X	X	X	X	X	X	554								
505	X	X	X	X	X	X	X	X	555								
506	X	X	X	X	X	X	X	X	556								
507	X	X	X	X	X	X	X	X	557								
508	X	X	X	X	X	X	X	X	558								
509	X	X	X	X	X	X	X	X	559								
510	X	X	X	X	X	X	X	X	560								
511	X	X	X	X	X			X	561								
512		X			X		X		562								
513	X	X	X	X	X	X	X	X	563								
514	X	X	X	X	X	X	X	X	564								
515	X	X	X	X	X	X	X	X	565								
516		X	X		X			X	566								
517	X	X	X	X	X	X	X	X	567								
518	X								568								
519			X	X					569								
520		X							570								
521			X						571								
522	X		X		X		X		572								
523	X	X	X	X	X	X	X	X	573								
524		X	X					X	574								
525		X		X				X	575								
526		X	X						576								
527		X		X					577								
528	X	X	X	X	X	X	X	X	578								
529	X	X			X	X		X	579								
530		X	X	X				X	580								
531		X	X					X	581								
532		X	X						582								
533			X						583								
534		X				X		X	584								
535	X	X	X	X	X	X	X	X	585								
536	X								586								
537									587								
538									588								
539									589								
540									590								
541									591								
542									592								
543									593								
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549									599								
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GENERAL INFORMATION

4.6. Ampoule Label Information

The labels on each ampoule have five lines of printed information on them.

The first line reads "Premium Coal Sample Program".

The second line indicates the seam name for the coal, for example, "Upper Freeport seam."

The third line indicates the rank of the coal, for example, "Medium Volatile Bituminous"

The fourth line has two parts. The first part is the "COAL ID". This is a three digit number, such as 701. The 7 stands for the seventh coal in the series of Argonne Premium Coal Samples (Lewiston-Stockton seam from West Virginia). The 1 stands for the first processing of this coal. If additional ampoules are filled from carboys, then that filling would be the second processing and the labels for the new set of ampoules would have a COAL ID of 702. The last part of the fourth line is the serial number for the ampoule, for example, 00441. This is the 441st ampoule that was labeled. The serial numbers are not exactly the sequence in which the ampoules were sealed. In the processing, lots of about 150 ampoules were placed on trays and later transferred to boxes for labeling. The serial numbers are typically within 150 of the exact number of their sequence of sealing. A typical batch of -20 mesh ampoules is about 5,000 ampoules, whereas the batch of -100 mesh ampoules has about 10,000 ampoules.

The fifth line also has two parts. The first part indicates the contents as either 5 grams -100 mesh or 10 grams -20 mesh material. The second part indicates the date that the ampoule was sealed, as for example, 12/02/86.

4.7. Ampoule Considerations

SUGGESTED PROCEDURE FOR OPENING GLASS AMPOULES

There are two types of glass ampoules, (1) standard and (2) "easy-break". The standard type has a gradually sloping shoulder between the top and body. The "easy-break" type has an expansion and then a contraction in going from the top to the body. Also, the area of the contraction has been scored to permit easy breaking.

The suggested procedure for the standard ampoules involves two steps. First, score the ampoule with a glass tubing knife around the shoulder, about 3/4"-1" from the top. Do this so that the two ends of the scoring come together. Second, apply a white hot glass rod to the moistened scratch to form a break around the scoring. You should hear a small snapping sound as the crack propagates around the ampoule. The tip should be easily removed from the body of the ampoule. If not, then use a short piece of conduit (pipe) with a few layers of paper towel inside to slide over the tip. Wrap the body of the ampoule in protective toweling or use a leather glove, moisten the scratch and snap it like glass tubing while holding it away from you.

The glass-tubing knife is better than a file, since it has a tungsten carbide cutting edge. It is available with a wooden handle from laboratory supply houses.

For the "easy-break" ampoules, moisten the scoring, and cover the ampoule with protective toweling, or use leather gloves. Snap the ampoule like glass tubing while holding it away from you.

SUGGESTED PROCEDURE FOR MIXING SAMPLES IN AMPOULES

Since coal samples tend to segregate in containers over a period of time it is necessary to remix the sample before opening the ampoule. The recommended method is to turn the ampoule so that the coal alternately falls into the top and then the body of the ampoule. This should be done continuously for at least 10 times. The method of rolling the ampoule on its side is not effective in mixing and is to be discouraged.

COMMENTS ON RE-USE OF THE CONTENTS OF AMPOULES

Many precautions have been taken to protect the contents from atmospheric oxidation. After the ampoule has been opened, there is no assurance that it will be the same for a future experiment. It is strongly recommended that any surplus sample be discarded, and that fresh ampoules be used for future experiments.

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4.8. Ordering Argonne Premium Coal Samples

ARGONNE NATIONAL LABORATORY

PREMIUM COAL SAMPLE PROGRAM ANNOUNCEMENT

January 19, 1988

Eight coals have been processed. Samples have been prepared and tested for homogeneity. They are being characterized and offered in sealed ampoules to coal researchers. Ampoules of either 5 grams of -100 mesh or 10 grams of -20 mesh can be provided.

The coals are listed in the order collected. Data describing the samples are given below. The moisture and ash-free values are given in %, except for sulfur and ash which are in dry %.

#	Seam	State	Rank	C	H	O	S	Ash
1	Upper Freeport	PA	Med. Vol. Bit.	85.5	4.70	7.5	2.32	13.2
2	Wyodak-Anderson	WY	Subbituminous	75.0	5.35	18.0	0.63	8.8
3	Illinois #6	IL	High Vol. Bit.	77.7	5.00	13.5	4.83	15.5
4	Pittsburgh (#8)	PA	High Vol. Bit.	83.2	5.32	8.8	2.19	9.2
5	Pocahontas #3	VA	Low Vol. Bit.	91.1	4.44	2.5	0.66	4.8
6	Blind Canyon	UT	High Vol. Bit.	80.7	5.76	11.6	0.62	4.7
7	Lewiston-Stockton	WV	High Vol. Bit.	82.6	5.25	9.8	0.71	19.8
8	Beulah-Zap	ND	Lignite	72.9	4.83	20.3	0.80	9.7

Analytical data will be sent separately as soon as they are available. The amber borosilicate glass ampoules have been flame sealed under nitrogen. Instructions for opening the ampoules will be included. The samples are intended to be used immediately after opening. Any unused portion should be discarded, as the original properties may change on further storage.

One of the purposes of the Argonne Premium Coal Sample Program is to further the basic understanding of the properties and behavior of coal. In order to maximize the benefit to all researchers, each request implies an agreement to provide the manager of the Premium Coal Sample Program with a reference to each journal article or public report describing the research results. This bibliographic information and analytical data will be available to other researchers through periodic reports. This program is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, which provides for this suite of eight coals.

The cost of the ampoules is

set of six 5-gram ampoules of -100 mesh: \$48.00
set of six 10-gram ampoules of -20 mesh: \$96.00

Shipments will be made by UPS blue label within the United States. International Shipments will be made by Express Mail, and an additional charge of \$20.00 per set of six ampoules will be made.

To order send a check in U.S. dollars payable to Argonne National Laboratory with the attached order/invoice to:

Assistant Controller, OCF/201
Argonne National Laboratory, 9700 South Cass Ave.
Argonne, IL 60439 USA

For technical questions, please contact the Coal Chemistry Group, Chemistry Division, Building 200, Argonne National Laboratory at (708) 252-3655 or FAX (708) 252-9288.

ARGONNE NATIONAL LABORATORY

Assistant Controller
OCF, Building 201
Argonne National Laboratory
Argonne, IL 60439, USA

_____ (PLEASE INDICATE A STREET
ADDRESS, UPS DOES NOT
DELIVER TO A POST OFFICE
BOX)

[illegible]

These samples will be used in a research program to (please, indicate project nature, such as determine functional group concentration of a series of coals): _____

(signed) _____
date _____
phone () _____

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G. Maciel, Colorado State University, Fort Collins, CO
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 I. G. Meighan, The Queen's University of Belfast, Belfast, Northern Ireland
 M. Melchior, Exxon Research and Engineering Co., Annandale, NJ
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 K. A. Nater, SBN European Center for Coal Specimens, Eysgelshoven, The Netherlands
 D. Netzel, Western Research Institute, Laramie, WY
 D. S. Newman, Bowling Green State University, Bowling Green, KY
 M. Nishioka, BCR National Laboratory, Pittsburgh, PA
 M. Nomura, Osaka University, Osaka, Japan
 J. Obst, U.S. Department of Agriculture, Madison, WI
 E. Ogata, University of Tokyo, Tokyo, Japan
 E. S. Olson, Universal Fuel Development Associate, Grand Forks, ND
 R. Owens, Auburn University, Auburn, AL
 C. Palmer, Principia College, Elmhurst, IL
 J. H. Penn, West Virginia University, Morgantown, WV
 F. Pfeifer, Exxon Research and Engineering Co., Annandale, NJ
 B. Pierce, U.S. Geological Survey, Reston, VA
 D. Pieta, Polish Academy of Sciences, Gliwice, Poland
 M. L. Poutsma, Oak Ridge National Laboratory, Oak Ridge, TN
 A. Prakash, Viking Systems International, Pittsburgh, PA
 R. Prokopuk, CANMET Energy Research Labs., Ottawa, Ontario, Canada
 M. Pruski, Iowa State University, Ames, IA
 R. J. Pugmire, University of Utah, Salt Lake City, UT
 K. Qin, Petroleum University, Beijing, China
 R. Rathbone, University of Kentucky, Lexington, KY
 H. Resing, Naval Research Laboratory, Washington, D.C.
 J. T. Riley, Western Kentucky University, Bowling Green, KY
 J. M. Rincon, Universidad Nacional de Colombia, Bogota, Columbia
 J. Ripmeester, National Research Council of Canada, Ottawa, Ontario, Canada
 G. Robbins, Consol Inc., Library, PA
 T. L. Robl, University of Kentucky, Lexington, KY
 P. Rohar, Pittsburgh Energy Technology Center, USDOE, Pittsburgh, PA
 L. M. Ross, Amoco Production Co., Tulsa, OK
 M. Rostem-Abodi, Illinois State Geological Survey, Champaign, IL
 R. R. Ruch, Illinois State Geological Survey, Champaign, IL

K. Runnion, J. K. Research, Bozeman, MT
 D. Ryan, University of Michigan, Ann Arbor, MI
 F. S. Sadek, Costech Analytical Technologies, Winston-Salem, NC
 V. Sahajwalla, CSIRO, North Ryde, NSW, Australia
 Y. Sanada, Hokkaido University, Sapporo, Japan
 K. T. Schroeder, Pittsburgh Energy Technology Center, USDOE, Pittsburgh, PA
 H.-R. Schulten, Fachhochschule Fresenius, Wiesbaden, Germany
 P. C. Scott, Office of Fossil Energy, USDOE, Washington, D.C.
 C. G. Scouten, Amoco Oil Co., Naperville, IL
 E. Sebestova, Czech Academy of Sciences, Praha, Czech Republic
 M. S. Seehra, West Virginia University, Morgantown, WV
 S. Serenellini, Enirecherche, Milan, Italy
 M. A. Serio, Advanced Fuel Research, East Hartford, CT
 J. S. Shabtai, University of Utah, Salt Lake City, UT
 N. Shah, University of Kentucky, Lexington, KY
 A. G. Sharkey, University of Pittsburgh, Pittsburgh, PA
 R. Shores, Research Triangle Institute, Research Triangle Park, NC
 B. G. Silbernagel, Exxon Research and Engineering Co., Annandale, NJ
 M. Siskin, Exxon Research and Engineering Co., Annandale, NJ
 L. D. Smoot, Brigham Young University, Provo, UT
 C. E. Snape, University of Strathclyde, Glasgow, Scotland, UK
 P. R. Solomon, Advanced Fuel Research, East Hartford, CT
 M. S. Solum, University of Utah, Salt Lake City, UT
 D. A. Sommerfeld, University of Utah, Salt Lake City, UT
 C. Song, Pennsylvania State University, University Park, PA
 R. Spangler, Geotech, Inc., Grand Junction, CO
 R. Spears, U.S. Bureau of Mines, Tuscaloosa, AL
 R. Sprecher, Pittsburgh Energy Technology Center, USDOE, Pittsburgh, PA
 T. G. Squires, Associated Western Universities, Inc., Salt Lake City, UT
 K. C. Srivastava, ARCTECH, Inc., Chantilly, VA
 M. Steele, Delta State University, Cleveland, MS
 H. Stephens, Sandia National Laboratory, Albuquerque, NM
 F. D. Stevenson, Office of Basic Energy Sciences, USDOE, Washington, D.C.
 F. Stohl, Sandia National Laboratory, Albuquerque, NM
 E. Suuberg, Brown University, Providence, RI
 T. Suzuki, Kyoto University, Kyoto, Japan
 K. Swapan, University of Nevada, Reno, NV
 B. J. Sword, British Coal Corp., Gloucestershire, England, UK
 T. Takanohashi, Tohoku University, Sendai, Japan
 G. H. Taylor, The Australian National University, Canberra, Australia
 S. C. Teerman, Chevron Petroleum Technology Co., La Habra, CA
 H. Thomann, Exxon Research and Engineering Co., Annandale, NJ
 L. T. Thompson, University of Michigan, Ann Arbor, MI
 J. S. Thrasher, University of Alabama, Tuscaloosa, AL
 R. Timpe, University of North Dakota, Grand Forks, ND
 W. Trahanovsky, Iowa State University, Ames, IA
 Y. D. Tsvetkov, Institute of Chemical Kinetics and Comb., Novosibirsk, Russia
 P. C. Uden, University of Massachusetts, Amherst, MA
 B. R. Utz, Pittsburgh Energy Technology Center, USDOE, Pittsburgh, PA
 G. Variali, The University of Rome, Rome, Italy
 A. M. Vassallo, CSIRO, North Ryde, NSW, Australia
 A. M. van der Veen, SBN, European Center for Coal Specimens, Eygelshoven, The Netherlands
 M. I. Venkatesan, University of California at Los Angeles, Los Angeles, CA
 J. G. Verkade, Iowa State University, Ames, IA

J. Volkwein, U.S. Bureau of Mines, Bruceton, PA
W. P. Vorkink, Brigham Young University, Provo, UT
P. F. van Bergen, Delft University of Technology, Delft, The Netherlands
Y. Wang, East China Normal University, Shanghai, People's Republic of China
B. Ward, University of Mississippi, University, MS
R. P. Warzinski, Pittsburgh Energy Technology Center, USDOE, Pittsburgh, PA
P. R. Watson, Oregon State University, Corvallis, OR
C. L. Weitzsacker, Kansas State University, Manhattan, KS
A. Wells, Pittsburgh Energy Technology Center, USDOE, Pittsburgh, PA
I. Wender, University of Pittsburgh, Pittsburgh, PA
P. C. Wernett, Pfizer, Inc., Bethlehem, PA
C. A. Wert, University of Illinois, Urbana, IL
D. L. Wertz, University of Southern Mississippi, Hattiesburg, MS
J. T. Westrich, Shell Development Company, Houston, TX
R. A. Winschel, Consol Inc., Library, PA
R. Wolny, Mobil R & D Corp., Paulsboro, NJ
A. S. Wong, University of Kentucky, Lexington, KY
K. Wood, Purdue University, Lafayette, IN
A. Wroblweski, Technical University, Zwirki, Poland
X. Wu, East China Normal University, Shanghai, People's Republic of China
Y. Yamada, National Institute for Resources and Environment, Ibaraki, Japan
X. Yang, Exxon Research and Engineering Co., Annandale, NJ
C. Ye, Wuhan Institute of Physics, Wuhan, Hubei, People's Republic of China
Y. Yun, Brown University, Providence, RI
P. Zhang, Institute of Coal Chemistry, Taiyuan, Shanxi, People's Republic of China
Y. Zhang, University of Utah, Salt Lake City, UT
K. W. Zilm, Yale University, New Haven, CT
J. Zondlo, West Virginia University, Morgantown, WV

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