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The Hunt Institute for Botanical Documentation, a research division of Carnegie Mellon University, specializes in the history of botany and all aspects of plant science and serves the international scientific community through research and documentation. To this end, the Institute acquires and maintains authoritative collections of books, plant images, manuscripts, portraits and data files, and provides publications and other modes of information service. The Institute meets the reference needs of botanists, biologists, historians, conservationists, librarians, bibliographers and the public at large, especially those concerned with any aspect of the North American flora.

Hunt Institute was dedicated in 1961 as the Rachel McMasters Miller Hunt Botanical Library, an international center for bibliographical research and service in the interests of botany and horticulture, as well as a center for the study of all aspects of the history of the plant sciences. By 1971 the Library's activities had so diversified that the name was changed to Hunt Institute for Botanical Documentation. Growth in collections and research projects led to the establishment of four programmatic departments: Archives, Art, Bibliography and the Library.

THE PENNSYLVANIA STATE UNIVERSITY

INTER-OFFICE CORRESPONDENCE

Date: February 21, 1985

From: P. H. Given

To: A. Traverse, 435 Deike

I enclose herewith a copy of a memo I sent you on 29 November last, which contains most of the information you asked for. I also enclose a copy of the Letter of Award, which gives the grant number. In the proposed budget the funds provided in support of your salary were described as covering 3% of your time for 9 academic and 3 summer months.

P.H.G.

THE PENNSYLVANIA STATE UNIVERSITY

INTER-OFFICE CORRESPONDENCE

Date: November 29, 1984

From: P. H. Given

To: A. Traverse, 435 Deike

This is to advise you that we have now had the formal letter from the National Science Foundation announcing the award to the University of $61,740 in support of the project "The Chemical Structure of Sporopollenins". The budget makes provision for a contribution of $1639 towards your salary, to be used in the period 1 November 1984 to 31 October 1985. I should be grateful if you would pass this information to the appropriate person in your Department.

The budget,"NSF Sporopollenin", is kept by Karen Copenhaver in Coal Research. The budget number is 424-04, and the fund number, 6804.

PHG

NATIONAL SCIENCE FOUNDATION
WASHINGTON D C 20550
NOV 16 1984

PI COPY

Grant No. EAR-8408992
Proposal No. EAR-8408992

Dr. Bryce Jordan
President
Pennsylvania State University
201 Old Main
University Park, PA 16802

Dear Dr. Jordan:

The National Science Foundation hereby awards a grant of $61,740 to Pennsylvania State University for support of the project described in the proposal referenced above.

This project, under the direction of Peter H. Given, Department of Materials Science and Engineering, is entitled:

"The Chemical Structure of Sporopollenins (Geology)."

This award is effective November 1, 1984 and expires April 30, 1986. A 6 month unfunded flexibility period is included in this award.

This grant is awarded pursuant to the authority of the National Science Foundation Act of 1950 (42 U.S.C. 1861 et seq.) and is subject to FL200 Grant General Conditions (Apr/83).

The budget indicates the amounts, by categories, on which NSF has based its support.

The cognizant NSF program official for this grant is John A. Maccini (202) 357-7866. The cognizant NSF grants official is Altie H. Metcalf (202) 357-9626.

Sincerely yours,

Stephen R. Williams
Grants Officer

Enclosures

WDM:tlk 11/26/84

cc: A. Muan
P. H. Given

THE PENNSYLVANIA STATE UNIVERSITY
408 WALKER BUILDING
UNIVERSITY PARK, PENNSYLVANIA 16802

College of Earth and Mineral Sciences
Fuel Science Section
Material Sciences Department

Area Code 814
865-1662

September 13, 1984

Ms. Elizabeth D. White
Greer Laboratories Inc.
P.O. Box 800
Lenoir, N.C. 28645

Dear Madam,

You recently sent to my colleague, Dr. Alfred Traverse, a catalog of the pollens you sell. The enquiry was in fact made on my behalf, since I have a research project calling for specimens of both spores and pollens from a variety of plants. I note from your letter that you have specimens from more species than are listed in your catalog, and am writing to ask if you can supply spores/pollens from any of the following:

Lilium henryii or other species
Spartina alternifolia
Juncus roemerianus
Lycopodium spp.
or *Selaginella*
or *Achrosticum* spp.
Equisetum arvense or other species.

Please quote prices for any of these that are available, and indicate delivery times. I take it that all of the items in your catalog are available from stock?

Yours faithfully,

P. H. Given

file

Peter H. Given
Professor of Fuel Science

PHG/jk

THE PENNSYLVANIA STATE UNIVERSITY

INTER-OFFICE CORRESPONDENCE

Date: September 13, 1984

From: Peter H. Given

To: A. Traverse, 435 Deike

My plans in the sporopollenin project call for spores from 2 or 3 pre-Gymnospermous plants, and I regard these as essential. I had in mind Lycopodium sp., a fern and Equisetum sp.: hence my letter (copy attached) to Greer Laboratories. Also, two Gymnosperms: *Taxodium distichum* and *Pinus strobus* or *Pinus ponderosa* seem suitable from the Greer list. Finally, a dicotyledonous Angiosperm (*Quercus rubra*?) and one or two monocotyledons. The grasses listed by Greer are not what I had in mind, but *Elymus condensatus* or *Arrhenatherum elatius* might be suitable if either *Spartina* nor *Juncus* nor *Lilium* are available. I am not sure which of the "weeds" are monocots. - all?

I think that I should order 5-10 grams of most specimens, but 15-20 gram of the sample selected for preliminary trial experiments (Lycopodium?)

P. H. G.

THE PENNSYLVANIA STATE UNIVERSITY

DEPARTMENT OF CHEMISTRY

INTER-OFFICE CORRESPONDENCE

Date: July 8, 1983

From: L. M. Jackman

To:

Proposal for NMR Spectrometer for Solids

Our NSF proposal is still under consideration. In the meantime, DOE has announed an Energy Research Instrumentation Program and I think we should submit the proposal to them.

Enclosed are copies of your submission for the NSF proposal. Would you please bring them up to date and return them to me as soon possible.

I believe that it is important to submit our proposal to DOE at the earliest opportunity. Would you therefore let me have your sections on or before July 25th.

LJM:ds

Enclosures

P. H. Given, W. Spackman, P. C. Painer, A. Davis, and A. Traverse: Coal Research Projects

Introductory Remarks

We are anxious to apply information from CP-MAS ^{13}C nmr spectra as contributions to the solution of several problems arising in researches on the applied chemistry and pure organic geochemistry of coals. Coals are a very diverse set of materials, of very considerable interest in their own right as complex natural products, and their study is a highly interdisciplinary endeavor. In addition, sooner or later, fuels for industrial process heat, transportation and as a source for chemical production will have to be based on the conversion of coal to clean gaseous and liquid fuels. A much greater understanding of basic coal science than is now available will be essential in the development of new processes.

Unlike crude petroleum, coals are mostly insoluble in the usual organic solvents. However, to a greater or lesser degree, their solid structure contains, in fossilized form, various kinds of cellular tissue, reproductive cells and cell inclusions that clearly demonstrate an origin of the "maceral" components of coals in organs of the higher plants. Chemical structural study of an insoluble, involatile, non-crystalline, three-dimensional macromolecular network (a fair description of most macerals in coals) is obviously difficult. Integration of data from a number of experimental techniques shows that the vitrinitic macerals* in coals are predominantly of aromatic character. The macromolecular network is built up from alkyl aromatic structures each containing 1-3 fused rings, frequently substituted with phenolic OH groups and linked to hydroaromatic rings[1-5]. Some oxygen as ether, and some heterocyclic O, N and S structures are thought to be present. CP-MAS ^{13}C nmr studies by a number of authors have contributed significantly to this picture[2,3,6,7].

*Vitrinite is the most abundant maceral (60-90%) in most coals, and is thought to be derived mostly from cellulosic and lignified cell walls in woody tissues.

The distribution of the above structural features varies with the degree of metamorphism or rank of the coal, in a manner not yet well-defined. Also, the widely differing geological histories of the sets of coals in the seven major coal basins or "provinces" of the U.S. have resulted in chemical differences between coals even at the same apparent level of rank[8-10]. Hence one must study a rather large sample base if one wishes to make generalizations about the chemistry of coals.

The nmr technique is of great value for obtaining structural information about solid coal macerals, but its potential has not yet been fully realized. The spectra obtained for coals are poorly resolved compared with those obtainable for pure substances in solution, and in most published work the aromaticity $[f_a - C_{ar}/(C_{ar} + C_{al}]$ is the only information extracted. In very recent work (some completed but not yet in print), a time-resolved spectroscopic technique is used for following the dipolar dephasing mode of relaxation of the excited nuclei; the dephasing time depends partly on the number of near-neighbor protons and hence the amount of information obtainable is greatly increased[11-13]. Thus four environments of aromatic carbon atoms (bridgehead, bonded to O, etc.) and two-three of aliphatic, can be distinguished with some confidence[12-13].

The problems we wish to address with the aid of CP-MAS ^{13}C nmr and following the dipolar dephasing will now be indicated. The funding status of these projects is indicated in an Appendix.

1. Relation of Structural Characteristics of Coals to Liquefaction Behavior, (Given, Painter, Spackman, Davis)

In published work, we empirically related the conversion of 104 coals (to liquids + gases) to such basic compositional parameters as contents of C, S and reactive macerals, H/C ration, and optical reflectance of vitrinite, using cluster, principal components, and multiple regression analyses[9]. In effect, a new classification of coals was developed, with a geological/geochemical basis[8,9]. We have now shown that the distribution of structures in the liquid

products varies with the coal used[14-16] (this, of course, is important inasmuch as composition determines the characteristics of liquid products as fuels).

We are now anxious to relate important aspects of liquefaction behavior and product composition to more fundamental chemical characteristics of the coals. We are currently using FTIR, and a selective oxidation procedure with GC/MS product analysis, to identify structural features of a relatively homogeneous set of 22 well-characterized coals whose liquefaction behavior is being examined. The FTIR and ^{13}C nmr on the same samples is a powerful approach to elucidating structural features is already apparent in published work in a differnt set of coals (even though dipolar dephasing was not followed)[2,17]. The structural information obtained in the proposed combined study will not only assist the understanding of liquefaction behavior, but also will contribute a fundamental route to understanding the geochemical basis of the new coal classification.

2. Contributions of Cellulose and Lignin to Coal Formation (Given, Spackman, Painter)

It will obviously not be easy to interpret the structural features identified above in terms of their function in the marcromolecular network. One would expect to receive valuable assistance in this interpretation from a much deeper understanding of the input to coalification than is now available. This input presumably includes as major constitutents microbially altered lignin, cellulose and other plant polymers. The chemical evidence on survival of cellulose in peats is paradoxical and conflicting[18-20]. However, microscopic study of thin-sections shows that tissues and organs containing mostly unlignified cell walls to very commonly survive in altered form in some peats[21], and coalified cell walls in the lignite from Brandon, Vermont are birefringent, indicating the survival of some partly crystalline cellulose[22]. Evidence on whether and how polymeric lignin is structurally altered before burial of the peat is virtually non-existent.

We have started to address these problems by comparing structural features of peats from four different environments in the Everglades of Florida with the

characteristics of ploymers in the plants from which the peats were derived, now growing at the surface. Remanent fragments of organs and tissues are separated first by wet-sieving, and identified and described botanically before chemical study. The techniques we are using are FTIR with computerized subtraction of spectra, pyrolysis/mass spectrometry, and a selective oxidation reaction with GC/MS product analysis. We have been able to obtain some ^{13}C nmr spectra of plant polymers and peat materials through the kindness of a colleague in another university, but we are very anxious that the technique should take its place in the experimental design as a principal research tool, and for this we obviously need access to an instrument on this campus. Cellulose[23] and lignin[24] both give well-defined CP-MAS ^{13}C nmr spectra in which the resonances have been indentified with structrual features in the polymers.

Some useful contributions to the study of humic acids and other peat components, and of young coalified wood, have already been published, using ^{13}C nmr[7,25-28]. However, the many features of our approach that distinguish it from the approach of others include the use of several techniques in parallel, and a reliance on botanical studies to identify the source of peats at different depths in a core and to define the nature of the tissues or organs selected for chemical work.

3. The Earliest Stages of Coal Formation (Spackman, Given, Painter)

This proposed project, not yet funded, is an extension of the research outlined in the previous section. It is proposed to apply the same methodologies to the study of certain samples that, in preservation of plant tissues and, presumably, chemistry, are not too far removed from peats but have started the transformation into mature coals. Such samples include the Brandon lignite, from Vermont (of Oligocene age, about 15 million years), and the peat buried some 300 feet below Trail Ridge in Okefenokee Swamp, Georgia. The research strategy combining botanical and chemical components will be specially important here (and again will distinguish our work from that of others).

4. The Nature of Sporopollenin (Given, Traverse)

Sporopollenin is the name given to the resistant outer-wall material of spores and pollen grains, and it is the presumed precursor of sporinite, a common hydrogen-rich maceral in coals. It is said to be an oxidative co-polymer of β-carotene and a long-chain fatty acid ester of antheraxanthin (a hydroxylated carotenoid)[28], i.e., or predominantly isoprenoid character. The chemistry of sporinite macerals, so far as it is known, is not in accord with this view[29], nor are the results of pyrolysis/mass spectrometry[30] or FTIR spectroscopy of sporopollenin samples[31]. A problem is that it is difficult to remove the cellulose inner wall (intine) from the sporopollenin (exine), and so interpretation of spectra is not clean. We propose to try to remove the cellulose with cell-free cellulase enzymes or by dissolution in Schweitzer's solution. ^{13}C nmr combined with FTIR will then be invaluable not merely in testing the supposed carotenoid origin, but in proposing an alternative origin, if that proves necessary, and a structure.

5. Determination of Coal Structural Parameters (Painter, Davis)

In recent work, we have developed FTIR procedures for measuring aliphatic C-H, aromative C-H, and hydroxyl groups in coal. These procedures have been applied to a set of vitrinite concentrates[32,33]. Our aim in this work has been to determine various structural parameters, but without measurements of quantities such as f_a (aromaticity), the data obtained from FTIR alone are limited. We have been able to obtain CP-MAS ^{13}C nmr data for certain samples by cooperating with other groups (particularly Professor Pugmire's and Professor Koening's), but if we are to systematically study a large number of coals and macerals, we clearly need ready access to an instrument located at Penn State. Our goal is to combine the data obtained from FTIR and nmr with the methods of statistical structural analysis, developed more than twenty years ago, by van Krevelen[34] and Dryden[35], to determine quantities associated with a mean structural unit. In previous work, a range of values for parameters such as f_a were inferred, with considerable ambiguity, from various measurements. With modern spectroscopic instrumentation, such quantities can now be

directly determined. Furthermore, the use of pulse sequences to distinguish carbon resonances (bridgehead, etc.) should allow us to greatly extend previous work in providing measurements of quanities such as average aromatic ring size, and degree and type of substitution of a mean structural unit.

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Traverse, A. (Professor of Palynology)	Date and Place of Birth	September 7, 1924 Port Hell, Prince Edward Is., Canada
	Degrees and Date	S.B., 1946; A.M. 1948; Ph.D. 1951 Harvard
Additional Experience	Head of Fuels Microscopy Lab.	U.S. Bureau of Mines 1951-1955
	Palynologist	Shell Development Co. 1955-1962
	Consultant, Palynology	Austin, Texas 1962-1965
	Asst. Professor of Geology	University of Texas 1965-1966
Date of Initial Appointment to Penn State		1966

1980-1982 Publications

Litwin, R. J., Traverse, A. and Ash, S. R. (1980), Abstract. Spores from compressed fern megafossils of the Chinle Formation - a preliminary report, Amer. Assoc. Strat. Palynologists, Program & Abstracts, October 14-18, 1980, p. 23.

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Robbins, E. I. and Traverse, A. (1982), Abstract. Processes of natural resource accumulation in ancient lake sediments in the Newark Rift System (eastern North America), CIMP-AASP Meeting, Dublin, Abstracts:21.

THE PENNSYLVANIA STATE UNIVERSITY

INTER-OFFICE CORRESPONDENCE

Date: 16 November 1982

From: P. H. Given

To: W. Spackman
A. Davis
P. C. Painter
A. Traverse

The attached document was prepared for inclusion in a proposal that Lloyd Jackman, Professor of Chemistry, is submitting this month both to DOD and the National Science Foundation, Chemistry Division. The proposal requests funds for a new nuclear magnetic resonance system, which would have a multi-element capability, and also facilities for cross-polarization and magic-angle spinning for solid samples. The document will be added to others prepared by faculty in Chemistry, Polymer Science, etc., outlining a number of other projects in which the instrumentation would be useful. I thought that you would like to be informed of what is being done.

P. H. G.

PHG:djm
Enclosure

Coal Research Projects Proposed by P. H. Given, W. Spackman, P. C. Painter, A. Davis and A. Traverse

Introductory Remarks

We are anxious to apply information from CP-MAS ^{13}C nmr spectra as contributions to the solution of several problems arising in researches on the applied chemistry and pure organic geochemistry of coals. Coals are a very diverse set of materials, of very considerable interest in their own right as complex natural products, and their study is a highly interdisciplinary endeavor. In addition, sooner or later, fuels for industrial process heat, transportation and as a source for chemical production will have to be based on the conversion of coal to clean gaseous and liquid fuels. A much greater understanding of basic coal science than is now available will be essential in the development of the new processes.

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*Vitrinite is the most abundant maceral (60-90%) in most coals, and is thought to be derived mostly from cellulosic and lignified cell walls in woody tissues.

by a number of authors have contributed significantly to this picture[2,3,6,7].

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The nmr technique is of great value for obtaining structural information about solid coal macerals, but its potential has not yet been fully realized. The spectra obtained for coals are poorly resolved compared with those obtainable for pure substances in solution, and in most published work the aromaticity ($f_a = C_{ar}/(C_{ar}+C_{al})$) is the only information extracted. In very recent work (some completed but not yet in print), a time-resolved spectroscopic technique is used for following the dipolar dephasing mode of relaxation of the excited nuclei; the dephasing time depends partly on the number of near-neighbor protons and hence the amount of information obtainable is greatly increased[11-13]. Thus four environments of aromatic carbon atoms (bridgehead, bonded to O, etc.) and two-three of aliphatic, can be distinguished with some confidence[12-13].

The problems we wish to address with the aid of CP-MAS ^{13}C nmr and following the dipolar dephasing will now be indicated. The funding status of these projects is indicated in an Appendix.

1. Relation of Structural Characteristics of Coals to Liquefaction Behavior (Given, Painter, Spackman, Davis)

In published work, we empirically related the conversion of 104 coals (to liquids + gases) to such basic compositional parameters as contents of C, S and reactive macerals, H/C ratio, and optical reflectance of vitrinite, using

cluster, principal components, and multiple regression analyses[9]. In effect, a new classification of coals was developed, with a geological/geochemical basis[8,9]. We have now shown that the distribution of structures in the liquid products varies with the coal used[14-16] (this, of course, is important inasmuch as composition determines the characteristics of liquid products as fuels).

We are now anxious to relate important aspects of liquefaction behavior and product composition to more fundamental chemical characteristics of the coals. We are currently using FTIR, and a selective oxidation procedure with GC/MS product analysis, to identify structural features of a relatively homogeneous set of 22 well-characterized coals whose liquefaction behavior is being examined. That FTIR and ^{13}C nmr on the same samples is a powerful approach to elucidating structural features is already apparent in published work on a different set of coals (even though dipolar dephasing was not followed)[2,17]. The structural information obtained in the proposed combined study will not only assist the understanding of liquefaction behavior, but also will contribute a fundamental route to understanding the geochemical basis of the new coal classification.

2. Contributions of Cellulose and Lignin to Coal Formation (Given, Spackman, Painter)

It will obviously not be easy to interpret the structural features identified above in terms of their function in the macromolecular network. One would expect to receive valuable assistance in this interpretation from a much deeper understanding of the input to coalification than is now available. This input presumably includes as major constitutents microbially altered lignin, cellulose and other plant polymers. The chemical evidence on survival of cellulose in peats is paradoxical and conflicting[18-20]. However, microscopic study of thin-sections shows that tissues and organs containing mostly

unlignified cell walls do very commonly survive in altered form in some peats[21], and coalified cell walls in the lignite from Brandon, Vermont are birefringent, indicating the survival of some partly crystalline cellulose[22]. Evidence on whether and how polymeric lignin is structurally altered before burial of the peat is virtually non-existent.

We have started to address these problems by comparing structural features of peats from four different environments in the Everglades of Florida with the characteristics of polymers in the plants from which the peats were derived, now growing at the surface. Remanent fragments of organs and tissues are separated first by wet-sieving, and identified and described botanically before chemical study. The techniques we are using are FTIR with computerized subtraction of spectra, pyrolysis/mass spectrometry, and a selective oxidation reaction with GC/MS product analysis. We have been able to obtain some ^{13}C nmr spectra of plant polymers and peat materials through the kindness of a colleague in another university, but we are very anxious that the technique should take its place in the experimental design as a principal research tool, and for this we obviously need access to an instrument on this campus. Cellulose[23] and lignin[24] both give well-defined CP-MAS ^{13}C nmr spectra in which the resonances have been identified with structural features in the polymers.

Some useful contributions to the study of humic acids and other peat components, and of young coalified wood, have already been published, using ^{13}C nmr[7,25-28]. However, the many features of our approach that distinguish it from the approach of others include the use of several techniques in parallel, and a reliance on botanical studies to identify the source of peats at different depths in a core and to define the nature of the tissues or organs selected for chemical work.

3. The Earliest Stages of Coal Formation (Spackman, Given, Painter)

This proposed project, not yet funded, is an extension of the research outlined in the previous section. It is proposed to apply the same methodologies to the study of certain samples that in preservation of plant tissues and, presumably, chemistry are not too far removed from peats but have started the transformation into mature coals. Such samples include the Brandon lignite, from Vermont (of Oligocene age, about 15 million years), and the peat buried some 300 feet below Trail Ridge in Okefenokee Swamp, Georgia. The research strategy combining botanical and chemical components will be specially important here (and again will distinguish our work from that of others).

4. The Nature of Sporopollenin (Given, Traverse)

Sporopollenin is the name given to the resistant outer-wall material of spores and pollen grains, and it is the presumed precursor of sporinite, a common hydrogen-rich maceral in coals. It is said to be an oxidative co-polymer of β-carotene and a long-chain fatty acid ester of antheraxanthin (a hydroxylated carotenoid)[28], i.e., of predominantly isoprenoid character. The chemistry of sporinite macerals, so far as it is known, is not in accord with this view[29], nor are the results of pyrolysis/mass spectrometry[30] or FTIR spectroscopy of sporopollenin samples[31]. A problem is that it is difficult to remove the cellulose inner wall (intine) from the sporopollenin (exine), and so interpretation of spectra is not clean. We propose to try to remove the cellulose with cell-free cellulase enzymes or by dissolution in Schweitzer's solution. ^{13}C nmr combined with FTIR will then be invaluable not merely in testing the supposed carotenoid origin, but in proposing an alternative origin if that proves necessary, and a structure.

5. Determination of Coal Structural Parameters (Painter, Davis)

In recent work, we have developed FTIR procedures for measuring aliphatic C-H, aromatic C-H, and hydroxyl groups in coal. These procedures have been applied to a set of vitrinite concentrates[32,33]. Our aim in this work has been to determine various structural parameters, but without measurements of quantities such as f_a (aromaticity), the data obtained from FTIR alone are limited. We have been able to obtain CP-MAS ^{13}C nmr data for certain samples by cooperating with other groups (particularly Professor Pugmire's and Professor Koenig's), but if we are to systematically study a large number of coals and macerals, we clearly need ready access to an instrument located at Penn State. Our goal is to combine the data obtained from FTIR and nmr with the methods of statistical structural analysis, developed more than twenty years ago, by van Krevelen[34] and Dryden[35], to determine quantities associated with a mean structural unit. In previous work, a range of values for parameters such as f_a were inferred, with considerable ambiguity, from various measurements. With modern spectroscopic instrumentation, such quantities can now be directly determined. Furthermore, the use of pulse sequences to distinguish carbon resonances (bridgehead, etc.) should allow us to greatly extend previous work in providing measurements of quantities such as average aromatic ring size, and degree and type of substitution of a mean structural unit.

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Other Research Support

The projects listed above as items 1, 2 and 5 are already in progress with support as follows:

Projects 1 and 5

A. Davis, W. Spackman, P. L. Walker, P. H. Given, P. C. Painter and N. Suhr, "A Data Base for the Analysis of Compositional Characteristics of Coal Seams and Macerals", $1,381,322, 1 February 1980 to 31 January 1983, U. S. Department of Energy, Contract No. DE-AC22-80PC-30013.

P. H. Given, W. Spackman, A. Davis, H. L. Lovell, P. C. Painter and J. L. Duda, "The Relation of Coal Characteristics to Coal Liquefaction Behavior", $329,306 for 2 years, terminating 2 March 1983, U. S. Department of Energy, Contract No. DE-AC22-81PC40784.

Cooperative Program in Coal Research (supported by a number of industrial companies).

Project 2

P. H. Given, P. C. Painter and W. Spackman, "The Nature of the Contribution of the Polymers of Cell Walls of the Higher Plants to Coal Formation", $61,600, 1 September 1981 to 31 December 1982, U. S. Department of Energy, Contract No. DE-AC02-81ER10988.

Grant from Exxon Education Foundation to P. H. Given, $8,000 for 1 year, from 1 October 1982.

Some Relevant Facilities Already Available

1. Finnigan Model 4010 gas chromatograph/mass spectrometer/data system.

2. Waters ALC/GPC 244 high performance liquid chromatograph with refractive index and absorption detectors.

3. Varian Series 3700 gas chromatograph with both flame ionization and thermal conductivity detectors.

4. Digilab FTS/15B Fourier Transform Infrared Spectrometer.

5. Digilab FTS/15E FTIR integrated into GC/FTIR system.

6. Biological and petrographic microscopes, with facilities for U.V. fluorescence and polarized light studies.

7. Boats and coring equipment for field work in southern Florida.

8. Bench-scale test equipment for coal liquefaction studies.

9. Penn State/DOE Coal Sample and Data Base (over 1000 samples from all major U.S. coal fields, extensively characterized and data stored on magnetic tape, selective retrieval and manipulation through the University's IBM 370 computer).

Personnel

Brief biographies of the faculty members involved now follow, together with a one-page selection of recent publications for each. Members of the group, representing several different disciplines, work closely together, with the result that many of their publications have multiple authorship. In spite of the repetition involved, it has been thought clearest and fairest to all concerned to list multi-author papers in the bibliography of each member of the group who was a co-author.

Vita of Dr. P. H. Given

Professor of Fuel Science

Dr. Peter H. Given obtained his B.A. in Chemistry from the University of Oxford; his studies included much natural product organic chemistry and a year of biochemistry taken as a special subject. He obtained his M.A. and D.Phil. from the same University, his thesis research, on Carbonium Ion Reactions of Aromatic Hydrocarbons on Cracking Catalysts, being supervised by Dr. D. Ll. Hammick and Professor Sir Robert Robinson. From 1945 to 1960, he was employed by the British Coal Utilisation Research Association, being Head of the Organic Chemistry Section from 1950. He was responsible in this Section for basic research on catalytic reactions, the chemical structure of coal macerals, and the polarographic reduction of aromatic substances in non-aqueous solvents.

He was appointed Associate Professor of Fuel Science at The Pennsylvania State University in 1961, Professor in 1962, and served as Department Chairman from 1965-69. His main research interests are the organic geochemistry and biogeochemistry of peats, and the applied chemistry and geochemistry of coal. Since 1974, he has been responsible for directing a major program on the relation of coal characteristics to liquefaction behavior, supported at a rate varying between $200,000 and $350,000 per year, first by the RANN Division of the National Science Foundation, and then by the Fossil Energy Division of the Department of Energy. He has recently obtained a grant ($60,000) from the Basic Energy Science Division of DOE, to investigate the roles of cellulose and lignin in contributing to coal formation.

He is a member of the American Chemical Society and its Fuel Chemistry Division, the Chemical Society (London), the Geochemical Society (Councillor, 1975-78) and its Organic Geochemistry Division (of which he was Chairman, 1972-73), the Geological Society of America and its Coal Geology Division, and Sigma Xi.

Selected Recent Publications of P. H. Given

Phenols as chemical fossils in coals, J. Bimer, P. H. Given and S. Raj, *in* ACS Symposium Series No. 71, Organic Chemistry of Coal, ed. J. W. Larsen, pp. 86-99 (1978).

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Vita of Dr. W. Spackman

Professor of Paleobotany

Dr. WILLIAM SPACKMAN is Director of the Coal Research Section in the College of Earth and Mineral Sciences at The Pennsylvania State University. He has held this position since the creation of the Section in 1957. In addition, he holds joint appointments in the Departments of Geosciences and Biology as Professor of Paleobotany.

Dr. Spackman was graduated from the University of Illinois in 1942 with a B.S. degree, having majored in Botany and minored in entomology and chemistry. He received his M.A. degree in 1947 and his Ph.D. in 1949 in Biology, from Harvard University. Dr. Spackman joined the staff of The Pennsylvania State University in 1949 as a member of the faculty in the Department of Geology.

He began his research in the field of coal petrology in 1951 with an investigation into the anomolous coking behavior of certain Kentucky coals. With the sponsorship of the steel and coal industries, the work was broadened to include a search for relationships between coal composition and coal behavior during carbonization, with a view to predicting coke quality from a knowledge of composition of the feedstock coal.

Currently, Dr. Spackman directs and participates in major research efforts, under contract with DOE, aimed at characterizing the Nation's coal resources and relating compositional characteristics to preparation, liquefaction and gasification behavior. He also directs and participates in a research program sponsored by the National Science Foundation concerned with modern coal-forming environments. He also directs Penn State's recently created Cooperative Program in Coal Research.

Dr. Spackman is a member of four international coal commissions (relating to coal petrology) and is Past-President of the International Commission for Coal Petrographic Nomenclature. He is a member of the Geological Society of America, The Botanical Society of America, the American Society for Testing Materials and the American Association of Stratigraphic Palynologists.

In 1976 Dr. Spackman was awarded the Joseph Becker Award of the Ironmaking Division of the Iron and Steel Society of AIME for contributions to the steel industry. In 1977 he was chosen as the recipient of the Gilbert H. Cady Award of the Geological Society of America for contributions to coal geology.

Selected Recent Publications of W. Spackman

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Cohen, A. D. and Spackman, W. (1981), Phytogenic organic sediments and sedimentary environments in the Everglades-mangrove complex, Part III. The alteration of plant material in peats and the origin of coal macerals, Palaeontographica, Abt. B, Bd. 172, 125-149.

Vita of Dr. P. C. Painter

Associate Professor of Polymer Science

EDUCATION:

1972 - 1975 - Ph.D. in Macromolecular Science, Case Western Reserve University, Cleveland, Ohio

1969 - 1970 - M.S. in Biochemical Engineering, University College, University of London, London, England

1965 - 1968 - B.S. in Chemical Engineering, University College, University of London, London, England.

PROFESSIONAL EXPERIENCE:

1968 - 1969 - High School Teacher as part of V.S.O. (English Equivalent of Peace Corps), Happy Grove School, Portland, Jamaica.

1970 - 1972 - Research Scientist, J. Lyons & Co., London, England.

1975 - 1976 - Research Associate, Macromolecular Science Department, Case Western Reserve University, Cleveland, Ohio.

1977 - 1980 - Assistant Professor, Polymer Science Section, College of Earth and Mineral Sciences, The Pennsylvania State University.

1980 -Present Associate Professor, Polymer Science Section, College of Earth and Mineral Sciences, The Pennsylvania State University.

PROFESSIONAL ASSOCIATIONS:

American Physical Society
High Polymer Physics (APS)
American Chemical Society
Society for Applied Spectroscopy

RESEARCH INTERESTS:

The general application of vibrational spectroscopy to structural characterization. Present research involves studies of the structure of coal by FTIR; the low-frequency Raman modes of biopolymers; characterization of the gel form of crystallizable polymers.

Selected Recent Publications of P. C. Painter

Books

"Theory of Vibrational Spectroscopy and its Application to Polymeric Materials", P. C. Painter, M. M. Coleman and J. L. Koenig, John Wiley & Sons (1982).

Journals

"Fourier transform infrared study of mineral matter in coal. A novel method of mineralogical analysis", P. C. Painter, M. M. Coleman, R. G. Jenkins, P. W. Whang and P. L. Walker, Jr., Fuel, 57, 337-344 (1978).

"Concerning the putative presence of nitrate in lignites", P. C. Painter, J. Youtcheff and P. H. Given, Fuel, 59, 523 (1980).

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"Concerning the application of FTIR to the study of coal. A critical assessment of band assignments and the application of spectral analysis programs, P. C. Painter, R. W. Snyder, M. Starsinic, M. M. Coleman, D. J. Kuehn and A. Davis, Applied Spectroscopy, 35, 475 (1981).

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Vita of Dr. A. Davis

Professor of Geology, Assistant Director of Coal Research Section

EDUCATION

1956 B.Sc., A.R.C.S.	Imperial College of Science and Technology, London University (Geology)
1961 M.S.	The Pennsylvania State University (Geology)
1965 Ph.D.	University of Durham (Geology)

EXPERIENCE

1956	Geologist, John Taylor & Sons, New Consolidated Goldfields, England
1957	Prospecting Officer, National Coal Board, Open-cast Executive, England
1958	Scientist, National Coal Board, Coal Survey, England
1958 - 1961	Graduate Assistant, The Pennsylvania State University
1961 - 1965	Senior Research Associate, The University of Newcastle-upon-Tyne, England
1965 - 1973	Senior Geologist, Geological Survey of Queensland, Australia
1973 - Present	Professor, The Pennsylvania State University, Assistant Director, Coal Research Section; Director, Anthracite Division, Coal Research Section

SOCIETY MEMBERSHIP AND OTHER ACTIVITIES

Geological Society of America - Hon Secretary, Queensland Division, 1971
Hon Treasurer, Queensland Division, 1972

Geological Society of America - Member

American Society for Testing and Materials - Member

International Committee for Coal Petrology - Member
- Commission on Industrial Applications - President, 1981

Selected Recent Publications of A. Davis

Davis, A., Spackman, W. and Given, P. H. (1976), The influence of the properties of coal on their conversion into clean fuels, Energy Sources, 3, 55.

Mitchell, G. D., Davis, A. and Spackman, W. (1977), A petrographic classification of solid residues derived from the hydrogenation of bituminous coals, *in* Liquid Fuels from Coal (R. T. Ellington, ed.), p. 255, Academic Press, New York.

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Davis, A. (in preparation), Coal petrology, Chapter 3 *in* A Handbook of Coal Geology (C. Ward, ed.), Blackwells, England.

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Vita of Dr. A. Traverse

Professor of Palynology

EDUCATION

1946 S.B., *magna cum laude*, Harvard University (Biology)
Phi Beta Kappa, Sigma Xi

1947 Certificate, King's College, Cambridge, England (Botany)

1948 A.M., Harvard University (Paleobotany)

1951 Ph.D., Harvard University (Paleobotany)

EXPERIENCE - INDUSTRIAL AND ACADEMIC

1951-1955 Coal Technologist and Head of Fuels Microscopy Laboratory, U.S. Bureau of Mines

1955-1962 Palynologist--Research, Shell Development Company

1962-1965 Consultant, Palynology, Austin, Texas

1965-1966 Assistant Professor of Geology, University of Texas

1966-1970 Associate Professor of Geology and Biology, The Pennsylvania State University

1970-Present Professor of Geology and Biology (title now: Professor of Palynology), The Pennsylvania State University

SOCIETY MEMBERSHIPS (AND OTHER ACTIVITIES) (Partial List)

American Association for the Advancement of Science (Fellow)

American Association of Stratigraphic Palynologists
Secretary-Treasurer, 1967-1970
President, 1970-1971
Councillor, 1971-1972

Botanical Society of America
(Paleobotanical Section)
Secretary-Treasurer, 1957-1960
Acting Chairman, 1958
Chairman, 1960-1961

Catalog of Fossil Spores and Pollen
Member, Editorial Board, 1957-1966
Editor, 1966-1977

Geological Society of America (Fellow)

International Association for Plant Taxonomy
Committee for Fossil Plants, 1959-Present
Secretary, 1969-Present

International Commission for Palynology
Member of Council for U.S.A., 1973-1976
President, 1976-1980
Past-President, Councillor, 1980-Present

PERTINENT HONORS

Selected as on-board palynologist, "Glomar Challenger", Leg 42B, Black Sea, May-June 1975

Appointed Adjunct (i.e., honorary) Professor of Geobiology, Juniate College, Huntingdon, Pennsylvania, August 1977, continuing to present

Presided at 5th International Palynological Conference, Cambridge, England, June-July 1980

Guest Professor, Geological Institute, Swiss Federal Technical Institute, Zürich, 1980-1981

Selected Recent Publications of A. Traverse

Litwin, R. J., Traverse, A. and Ash, S. R. (1980), Abstract. Spores from compressed fern megafossils of the Chinle Formation - a preliminary report, Amer. Assoc. Strat. Palynologists, Program & Abstracts, October 14-18, 1980, p. 23.

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Traverse, A. (in the press, Alcheringa), Response of world vegetation to Neogene tectonic and climatic events.

Traverse, A. and Sullivan, H. J. (in the press, Palyn.), The background, origin and early history of the American Association of Stratigraphic Palynologists.

Robbins, E. I. and Traverse, A. (1982), Abstract. Processes of natural resource accumulation in ancient lake sediments in the Newark Rift System (eastern North America), CIMP-AASP Meeting, Dublin, Abstracts:21.

May 25, 1971

Alfeed Traverse

Peter Given

Dear Peter:

You perhaps have such a good enough memory that you can still recall the small chips of wood that you gave me bearing the designation III C. We decided to demineralize and bleach and simply make a strew slide of the small particles. It is not possible in such a slide to pick up cross sections, but one can see all of the other major features of the wood on the slide enclosed. There is no doubt that the wood is coniferous, and I would take a wild guess at Taxodiaceae, but Araucariaceaeais a possibility. Ron Williams could grind oriented sections by embedding the fragments in hard plastic before sectioning. The fragments of wood in the strew slides show that even after demineralization and bleaching there is plenty of pyrite present, and I am reluctant to have Mrs. Traverse attempt sectioning with a microtome because it would ruin her blade.

Yours truly,

Alfred Traverse

AT/mdw

March 24, 1970

Alfred Traverse

Peter Given

Dear Peter:

I assigned a sample of the coal and a sample of the shale which you gave me from your collections in the Jet Basin, as an unknown to one of our palynology students this past term. As you can see from the enclosed, he got the rather surprising result that the coal is devoid of palynomorphs, apparently an exclusively woody coal, while the shale sample was only moderately productive of palynomorphs. However, the flora which was obtained is just what you would expect from the Tununk member.

Alfred Traverse

AT:kc

Enclosure

November 13, 1969

Dr. Alfred Traverse

Dr. Peter Given

Dear Peter:

Thanks very much for the report on your and Cooper's collecting and other work in South Florida. At the present it would seem that about all I can do is to read these things with interest, but I do appreciate your letting me have them for the purpose of keeping me abreast of developments.

Alfred Traverse

file as correspondence

Report on

Field Trip to Jet Basin, Wayne County, Utah

by P. H. Given

My guide was Dr. H. H. Doelling, an economic geologist of the Utah Geological Survey, and he was accompanied by Martin _____, an assistant or graduate student, who rendered substantial assistance.

Jet Basin is roughly circular, about 1 mile across, its rim being approximately at the 6000 feet contour line. It lies at the northern end of the Henry Mountains, right under Table Mountain (8500 feet) and not far from Mount Ellen (11,500 feet). Table Mountain is flat topped and steep-sided, and largely composed of diorite. Nevertheless the surrounding rocks show no sign of alteration by heat from magmatic bodies.

Jet Basin is about 25 miles south of Hanksville, a small village on State Route 24 about 60 miles south of Greenriver. It is approached by a dirt road which initially has an excellent surface, but which later deteriorates into a very rough track with sharp ascents and descents. It is not easy to find, and could not be reached in an ordinary car.

The basin has steep walls, which are in part vertical columnar cliffs of sandstone or shale, and in part steep banks with a surface cover of material eroded from higher up. The center of the basin has a large number of smooth contoured hills separated by deep gullies through which water flows. A cascade of water could be seen entering the basin from the mountain side, and water leaves the basin by the one breach in the walls, to the northwest. The basin is evidently an erosional feature, the softer rocks being removed partly by the continuous run-off of water from the mountains and partly by the occasional flash floods, which can be pretty catastrophic in magnitude.

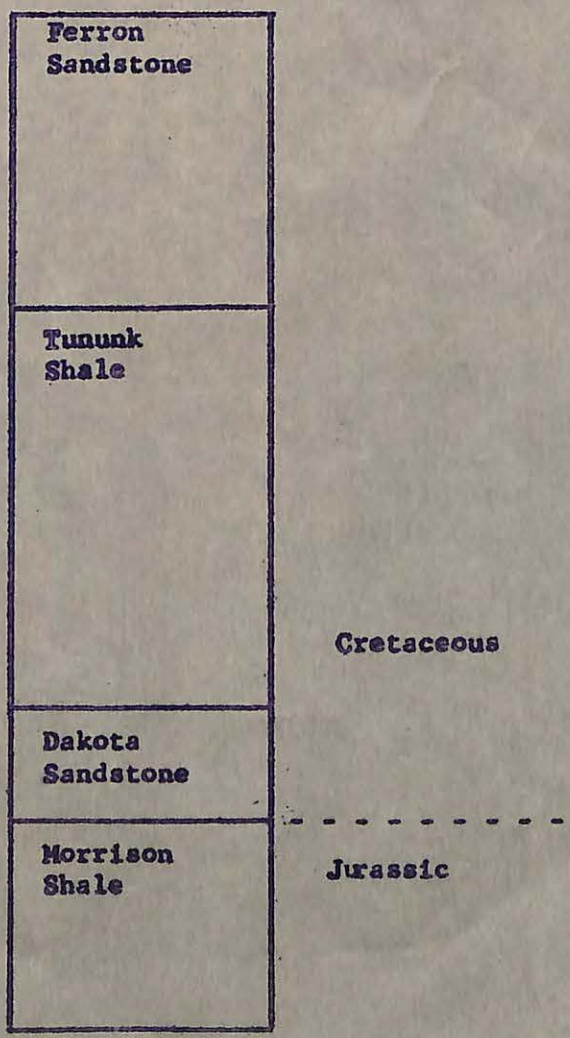
Most of the hills are covered by a layer of what looks like coarse soil, and in fact contains much bentonite formed by the erosion of granite exposed in the mountains.

The relevant section of the geologic column is shown in the Figure. The Ferron sandstone is seen only in the upper parts of the walls of the basin. The Tununk shale is several hundred feet in thickness. Where it occurs in the vertical cliffs around the perimeter, it is hard and grey. In the sloping lower parts of the walls it occurs under a layer of granular detrital material in horizontal flakes 2-10mm. in thickness. In the hills in the center of the basin, it is soft and muddy, easily broken in the hand. It is this shale that contains the jet, and it also contains a coal seam.

Figure

Geologic Column in Jet Basin

(not to scale)



Under the Tununk lies a thin stratum of sandstone, the Dakota, and under this a hard light colored shale, the Morrison shale. Dr. Doelling told me that the Morrison most probably represents the top unit of the Jurassic, though some people maintain that it is the bottom of the Cretaceous. The Dakota sandstone is most often seen as horizontal ridges in the sides of the hills, less easily eroded, but in some of the hills the Tununk has been completely removed, and the Dakota is exposed at the top surface. Vegetation only appears on this sandstone, not on the Tununk.

The coal seam can be seen in many parts of the basin in the walls and in the sides of the hills as a dark band not covered with detritus. From observations of this, and the Dakota sandstone outcrops, one would judge that the complete strata before erosion of the basin were not folded, but were slightly tilted from the horizontal. Moreover, slumping has apparently not occurred.

Observation at three or four sites within two hundred yards of each other in hills in the center of the basin, and at two or three sites around the walls, suggested that there is a fairly continuous layer of jet, 2-8 cm. thick all over the basin, and that this lies consistently 15-30 cm. below the coal seam. The jet is not, of course, continuous in the sense that one homogeneous stratum has been formed. The layer looked as if a large number of stems or branches of trees had been deposited on a single plane, in a single episode, and metamorphosed. Many of the pieces found had the external morphology of a tree stem; one piece found was still roughly circular. Another was elliptical, with horizontal axis about 15 cm. and vertical 3-4 cm., oriented diagonally into the side of a hill; it had broken into a number of sections, but it was followed some 50-60 cm. into the side of the hill.

The coal seam is 20-30 cm. thick, and is badly weathered. It is dull (durainic ?) in appearance. It is easily broken into cubic fragments, there being copious brown deposits on the surfaces and cleavage planes.

Present ideas of jet as representing logs of wood floating out to sea, sinking, and undergoing diagenesis and metamorphism in an oil shale, are difficult to reconcile with the presence of a coal seam if the coal is vitrinitic and autochthonous. Perhaps the coal is of the cannel type and allochthonous.

It should be added that the surface of some of the central hills were covered with spoil heaps accumulated when jet was mined 40-50 years ago. No samples were collected near the spoil heaps.

It was noticed that when the jet samples were taken out of the stratum they emitted distinct crackling noises. When the plastic bags in which the samples were placed were opened, after return to the laboratory, some crackling was resumed. Perhaps the noise represents relaxation of the physical structure of the solid as adsorbed water evaporates from the surface layers.

The Utah jet occurs in much softer rock than the jet in the cliffs along the seashore near Whitby, in England, and it can be found in much thicker and more continuous layers than can now be found in England. Consequently, it is much more obvious in Utah that the jet is derived from tree stems; in no English sample that I have seen is there the slightest appearance of the external morphology of tree stems. Admittedly the English occurrences have been much more extensively worked and the resources depleted; and there is now nothing to indicate whether the jet formation occurred as a single episode of deposition, as appears definitely to have been the case in Utah.

Samples Collected

The letters attached to the various samples represent code designations by which I purpose in future work to identify the samples.

Site 1 was one of the central hills some 250 m. from the old workings. The coal outcropped some 1.5 m. below the summit of the hill. The jet collected (D) was from two parallel-lying jetified logs running diagonally into the hill, starting some 20 cm. below the surface. A sample of the coal (C) and the shale (L) interbedded with the jet were collected. Some surface samples of weathered jet and of concretions containing coalified or jetified twigs were collected in the same general area, as also were two separated samples of petrified wood.

Site 2. Lower down the same hill (30-40 m. lower ?), discrete pebbles of the Morrison shale (M) were found some 20-30 cm. under the bentonitic "soil".

Site 3, at the foot of the southwestern wall of the basin, a second sample of jet was taken (E), and about 3-5 m. higher, a sample of the flaky shale (N) from 20-30 cm. below the surface.

Site 4. From the hard exposed ridges at the base of vertical cliffs of Tununk shale further around the perimeter to the east, Dr. Doelling collected a further sample (shale P).

For this profitable and informative field trip, I am deeply indebted to Dr. Doelling, without whom I could not possibly have achieved anything.

Dr. Traverse

Please note & return in due course

P. H. G.

UNIVERSITY OF UTAH

SALT LAKE CITY 84112

UTAH GEOLOGICAL
AND MINERALOGICAL SURVEY
103 Utah Geological Survey Building

June 24, 1969

Fuels

Dr. P. H. Given
Fuel Science Section
Penn State University
University Park, Pennsylvania 16802

Dear Dr. Given:

Enclosed is a small map of the jet basin area and a brief description of the stratigraphy. I hope you arrived safely back in Pennsylvania, and that your specimens of the jet proved adequate. We enjoyed very much meeting you, and wish you every success in your endeavors.

Cordially yours,

H. H. Doelling

H. H. Doelling
Economic Geologist

HHD:mb

Enclosures (2)

Hunt C.B. PP 228 Geography & Geology of Henry Mtns. USGS. Prof. Paper 228

believed to be middle and early Paleozoic (Bass,

pre-Permian rocks could be much thicker be- the Henry Mountains structural basin than on the afael Swell, if the basin had been a negative area time during the Paleozoic. There is no evidence ar on this question although similar basins in n Colorado and the Paradox basin, that extends astern Utah, were negative areas during part of leozoic.

e Hermosa formation, of Pennsylvanian age, is the formation whose presence in the region is reason- certain. In Cataract Canyon, a short distance of the Henry Mountains region, this formation, almost 1,500 ft thick, consists of interbedded fossiliferous limestone, sandstone, shale, and conglomerate (Baker, 1947). The formation is exposed also along the San Juan River and was encountered by drilling in the San Rafael Swell, north of the Henry Mountains region, and in the Circle Cliffs to the west. Probably the formation is 1,000 to 1,500 ft thick in the Henry Mountains region.

Overlying the Hermosa formation in Cataract Canyon is the Permian(?) Rico formation, which consists of interbedded sandstone, shale, siltstone, and limestone, and aggregates more than 400 ft in thickness (Baker, 1947). The formation underlies the east part of the region, but it must thin westward and northward because it is absent in the San Rafael Swell.

EXPOSED FORMATIONS

Generalized section of sedimentary rocks exposed in the Henry Mountains region.

System	Series	Group, formation, and member	Thickness (feet)	Lithology
ernary.		Alluvium, colluvium, terrace gravel, and talus.		Sandy clay, sand and gravel in alluvium and alluvial fans; terrace gravel mostly on benches along streams; slope wash and talus.
		Unconformity		
		Mesaverde formation.	400	Cliff-forming sandstone containing thin interbeds of shale.
		Mancos shale. Masuk member. Kmm	600–800	Lenticular sandstone, shale, carbonaceous shale, and shaly limestone. Mostly continental in origin, but some is marine.
		Mancos shale. Emery sandstone member. Kme	198–257	Lower 150 ft is massive sandstone. Upper 50 ft is lenticular sandstone, shale, carbonaceous shale, and coal.
aceous.	Upper Cretaceous.	Mancos shale. Blue Gate shale member. Kmbg	1,500	Shale, blue-gray, marine.
		Mancos shale. Ferron sandstone member. KFe	150–300	Lenticular sandstone, shale, carbonaceous shale and coal, in upper 50–100 ft. Sandstone and thin beds of shale in lower 90–150 ft. Lower part grades eastward into Tununk shale member.
		Mancos shale. Tununk shale member. Kmt	525–650	Shale, blue-gray, marine; numerous thin beds of bentonite.
		Dakota sandstone. Kd	0–50	Cliff-forming conglomeratic sandstone; locally coal-bearing carbonaceous beds lie between two beds of sandstone.
		Unconformity		
e.	Upper Jurassic.	Morrison formation.	500–600	Upper part mostly clay and shale, variegated, dominantly green-gray, maroon and mauve; lower part mostly sandstone and conglomerate, gray, very lenticular, massive, crossbedded; some thin lenses of limestone; gypsum locally abundant at the base; jasper and other chart concretions common.
		Unconformity		

LOCATED IN Sci. BASIN

Coal is located along this line (jet)

October 11, 1968

Dr. Peter H. Given
University of Newcastle-Upon-Tyne
Department of Geology
Porter Building
St. Thomas Street
Newcastle-Upon-Tyne 1, England

Dear Dr. Given:

Don't worry about the Gordon Conference thing--I just was a bit confused (reminded me of trying to find Holderness School in Holderness, N.H.!) about getting a bill. I believe that I cangget it paid for from one of my budgets--though travel money is getting very tight with the new NSF restrictions (most recent edict--all PSU budgets cut by 30% across the board for the year--the money will probably be available later, but we must cut expenditures now). I was really asking for advice about what to do because the scuttlebut around here was that speakers didn't have to pay. I kept saying that that wasn't what I heard being announced at Plymouth, but kept getting the same answer.

All hectic here with new palynological data program. I am now supposed to be 15 places at once instead of just 10.

My wife says to say that you are missed in the S.C. Choral Society, or whatever it's called.

Best wishes.

Yours very truly,

AlfredfTraverse
Associate Professor of Geology

AT:kwc

THE UNIVERSITY OF NEWCASTLE UPON TYNE

DEPARTMENT OF GEOLOGY

Head of Department:
Professor T. S. Westoll, F.R.S.

Professor of Geology:
J. E. Hemingway

ORGANIC GEOCHEMISTRY UNIT
PORTER BUILDING
ST. THOMAS STREET
NEWCASTLE UPON TYNE 1
TELEPHONE: NEWCASTLE 28511

4th October, 1968.

Dear Al,

I am afraid I was rather remiss in not discussing the Gordon Conference attendance fee with you when I first mentioned the Conference to you. The point is that the Conference organisers do have funds from which the attendance fee of University staff members can be paid if they have no other sources. If I had known that you would have difficulty I could have mentioned the problem to Dr. Silverman some months ago and he could probably have put $120 at your disposal. I am afraid that now it may be too late. However, I suggest you write to Silverman at the address below, since there is a small possibility that some funds might still be available. If this does not work, and you find difficulty locating any other funds, I suggest you talk to Jane about putting it on the new Everglades budget. I am very sorry about the confusion.

Yours sincerely,

Peter

P. H. Given.

Dr. A. Traverse,
Deike Building,
The University,
University Park,
Pennsylvania 16802,
United States of America.

Dr. S.R. Silverman,
Chevron Research Co.
576 Standard Avenue,
Richmond,
Calif. 94802

September 26, 1968

Dr. P.H. Given
The University of Newcastle-Upon-Tyne
Department of Geology
Organic Geochemistry Unit
Porter Building, St. Thomas Street
Newcastle-Upon-Tyne 1, England

Dear Peter:

I enclose a copy of a bill I received from the Gordon Research Conferences. Jane Dolsen suggested that I ask you whether I really am suppose to pay this or not before I try to find some way of doing so. Will you let me know?

I do hope that your work with the jets fs progressing satisfactorily. I confess that with the beginning of the new term and several new research projects getting underway, there is not much chance that I will be able to do anything constructive about jet for awhile!

Best wishes as ever.

Yours very truly,

Alfred Traverse
Associate Professor of Geology

AT:kwc

Enclosure: copy of bill

THE UNIVERSITY OF NEWCASTLE UPON TYNE

DEPARTMENT OF GEOLOGY

Head of Department:
Professor T. S. Westoll, F.R.S.

Professor of Geology:
J. E. Hemingway

ORGANIC GEOCHEMISTRY UNIT
PORTER BUILDING
ST. THOMAS STREET
NEWCASTLE UPON TYNE 1
TELEPHONE: NEWCASTLE 28511

5th August, 1968.

Dr. Alfred Traverse,
Pennsylvania State University,
Deike Building,
University Park,
Pa. 16802,
U.S.A.

Dear Al:

I was glad to get your letter of july 26th, telling me how you are getting on.

I never supposed that you could go to Utah and collect samples; I was thinking of the colleague on the spot whom you mentioned before I left State College - but he appears to be the one who does not answer your letters. So I'll have to wait. I've got enough to carry on with for a while.

I agree that it might be difficult now to concert a joint presentation at the Gordon. Perhaps what I meant was not quite that, but two consecutive presentations in which there would be different points of view and different data, even if some of the samples reported on were the same.

I think that in presenting your results you should mention the extraction conditions. I wonder whether you extracted at room temperature or for a relatively short time? I boiled the jet with about 100 ml solvent (10% ethanol in chloroform) for each 10 gms of jet, under reflux for 48 hours, filtered, and re-extracted with fresh solvent for 24 hours. An alternative is Soxhlet extraction; the men here prefer that for shales and extract for a week or two (though I admit shales are slower). Anyway, my three samples of jet gave totals of 10.1%, 10.4% and 9.9% in EtOH/$CHCl_3$, some 60% of which was soluble in pet. ether. Whereas the first extract was a semi-solid tarry mess, the petroleum ether insolubles were were granular solids, and the solubles were brown oils.

You say in your letter that "the extractives appear not to be hydrocarbons that have migrated in". I am not sure what this means. That there were no hydrocarbons at all? That there were hydrocarbons, but their composition was different from what you'd expect to come from a marine shale? Was it the petroleum ether eluate from the silica gel column that was put on the G.L.C.? This is the fraction that should contain the aliphatic hydrocarbons. I get plenty, 30-50% of the petroleum ether extract, or 20-35% of the original EtOH/$CHCl_3$ extract, confirmed by infra-red spectra. I've had little G.L.C. done yet, but hope to get a lot done ~~next~~ this week. I propose to compare G.L.C. analysis of the alkane fraction of the jets with that of the shale they occur in and the underlying shale, and I hope to present this at the Gordon. Later I hope to compare the fatty acids and porphyrins. I have, incidentally, evidence of the presence of alkanes, some aromatic hydrocarbons, fatty acids, fatty esters and ketones, and some indications of the presence of porphyrins.

The most interesting of the woody samples I sent you are the wood itself (IIIc), which has well-preserved cellular structure, IIIa (red structurless, like jet or vitrinite?) and II (which has a cellular structure much lithified and with lumina filled, looks to me different to IIIc). I have sections and hope to photograph them soon - I'll send you the pictures. Sample I seems to be largely pyrite, and we find no cellular structure. Do any of the structures resemble those in jets? What kind of wood?

I'll be in Florida late on August 13th, and I will telephone you from there.

Yours sincerely,

Peter Given

July 26, 1968

Dr. P.H. Given
The University of Newcastle-Upon-Tyne
Department of Geology
Organic Geochemistry Unit
Porter Bldg., St. Thomas Street
Newcastle-Upon-Tyne 1, England

Dear Peter:

Thank you for your letter of 17 July. Regarding the fresh samples of Utah material: This is a difficult matter on two scores--There is no possibleity of my making a trip to Utah within the foreseeable future to collect fresh samples, and my source of Utah jet (RiW. Kolvoord) persists in not answering my letters lately.

I am not sure that I agree with you about the undesirability of duplicating effort--I have often found it very illuminating for someone else and me to pursue study along the same line. I have made extractions of both Whitby and Utah jet in a mixture of benzene, methanol and carbon tetrachloride. The amount of extractive was much less than the 10% you mention--something on the order of 2% was the highest which I obtained. We fractionated the extractive on silica gel columns and did gas chromatography on some of the fractions. The results seem to show that extracted material from the jet does <u>not</u> represent hydrocarbons which migrated into the jet. This does not particulary surprise me, although the person who helped me with the extractions and gas chromatography had a hunch that such hydrocarbons would be found. I am also having carbon isotope studies made of some of the fractions which should further tie down the question of the origin of the volatile matter in the jet.

Regarding the paper for New Hampshire: I would suppose that at this distance and in the time available there is no reallpossibility of presenting a joint paper. I propose to whip up a presentation on what I have developed--what I gave at New Orleans plus the newer information from gas chromatography and carbon isotope analyses. I can see no objection at all to your having a further contribution closely associated with mine. Indeed, the idea sounds very stimulating.

I am hopeful that I can get some thin sections of your materials made and studied in time for inclusion in the paper. The problem is that things are very hectic around here for reasons quite unrelated to jet! I won't bother you with the details, but among other things my family and I are moving to a different house in about a week. I will do what I can!

Looking forward to seeing you again and to future exchanges of notions about jet, I am

Yours very truly,

Alfred Traverse
Associate Professor of Geology

AT:kwc

3 June, 1968

AIRMAIL

Dr. P. H. Given
Organic Geochemistry Unit
Porter Building
University of Newcastle
Newcastle-upon-Tyne
England

Dear Peter:

Under separate cover, I am sending you, air parcel post, the little jet pieces--I am getting pretty near the bottom of the barrel, so please excuse the small size of the samples!

Have a good summer!

Yours very truly,

Alfred Traverse