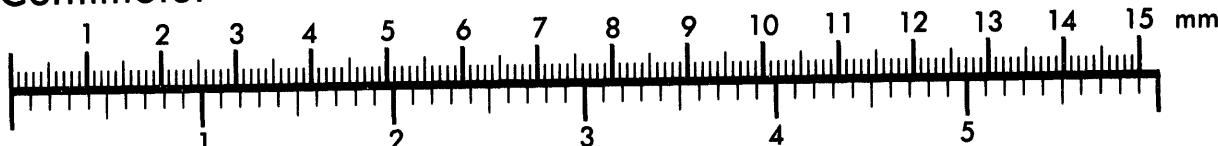




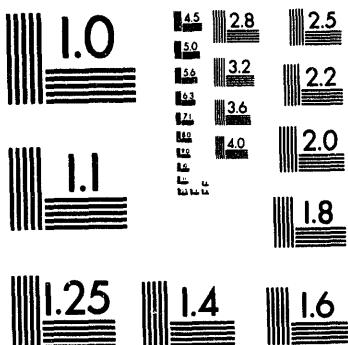
**Association for Information and Image Management**

1100 Wayne Avenue, Suite 1100  
Silver Spring, Maryland 20910  
301/587-8202

**Centimeter**



**Inches**



MANUFACTURED TO AIIM STANDARDS  
BY APPLIED IMAGE, INC.

1 of 2

## **Coal Liquefaction Process Streams Characterization and Evaluation**

### **Analysis of Coal-Derived Synthetic Crude from HRI CTSL Run CC-15 and HRI Run CMSL-2**

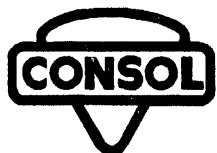
#### **Topical Report**

**Prepared by:**

**IIT Research Institute  
National Institute for Petroleum and Energy Research  
P.O. Box 2128  
Bartlesville, OK 74005**

**Gene P. Sturm, Jr.  
Je Kim  
Johanna Shay**

**Prepared for:**



**CONSOL Inc.  
Research & Development  
4000 Brownsville Road  
Library, PA 15129**

**F. P. Burke  
R. A. Winschel  
S. D. Brandes**

**January 1994**

**Under Contract to:**

**United States Department of Energy  
Contract No. DE-AC22-89PC89883**

**U.S. DOE Patent Clearance was provided by  
Chicago Operations Office on 2/17/94.**

## PROJECT ASSESSMENT

### Introduction

Under subcontract from CONSOL Inc. (U.S. DOE Contract No. DE-AC22-89PC89883), IIT Research Institute, National Institute for Petroleum and Energy Research applied a suite of petroleum inspection tests to two direct coal liquefaction, net product oils produced in two direct coal liquefaction processing runs. Two technical reports, authored by NIPER, are presented here. The following assessment briefly describes the two coal liquefaction runs and highlights the major findings of the project. It generally is concluded that the methods used in these studies can help define the value of liquefaction products and the requirements for further processing. The application of these methods adds substantially to our understanding of the coal liquefaction process and the chemistry of coal-derived materials. These results will be incorporated by CONSOL into a general overview of the application of novel analytical techniques to coal-derived materials at the conclusion of this contract.

### Background

Regardless of the specific technology used to produce transportation fuels from coal, at least some portion of the net product of the liquefaction process will have to undergo additional refining to make finished products. The presence of an on-line hydrotreater will minimize further refining requirements of the total products. However, there is a need to characterize that portion of the material leaving the liquefaction plant as net product and going to the refinery as feed. In addition, correlations drawn between operating variables of the liquefaction and finishing processes and net product characteristics will be extremely useful in directing future production efforts. It also is necessary to obtain accurate estimations of upgrading costs to produce specification fuels. Although it is acknowledged that the standard petroleum feedstock tests are not tailored for the analysis of coal liquids, it is believed that they are the best starting point for this analysis currently available.

It was recommended in CONSOL's Analytical Needs Assessment<sup>1</sup> that standard petroleum tests be performed on coal liquefaction syncrudes to assess the

applicability of those tests. Therefore, in a directed attempt to meet this particular analytical need, standard petroleum refinery feed analyses were performed on products of the Wilsonville pilot plant<sup>2,3</sup> and, as described herein, on products of the HRI Inc. bench unit.

#### Processing Runs and Samples

Two separate studies were conducted by NIPER, both are included in this volume. The first study was performed on the net product oil of HRI bench unit Run CC-15. The second study was performed with HRI bench unit CMSL-2 net product oil. The net product oil from HRI Run CMSL-2 was chosen for study because this run is considered to be representative of state-of-the-art direct coal liquefaction technology. It should be noted that, in both bench unit runs, some low-boiling material was lost during product collection and sampling. Thus, the lowest boiling components are artificially depleted somewhat in the samples analyzed here.

#### Run CC-15

The objective of HRI's CTSL Run CC-15, also called Run 227-75, was to test a predispersed (impregnated) hydrated iron oxide catalyst. The feed coal was Wyodak and Anderson seam, Black Thunder Mine, subbituminous coal. Start-up and make-up oil for Run CC-15 was filtered process-derived liquid, produced in HRI Run 260-03, which also used Black Thunder Mine coal. Throughout Run CC-15 the first stage reactor was operated thermally; Shell S-317 Ni/Mo on alumina catalyst was present in the second-stage reactor. No on-line hydrotreater was used in the run. The net product sample analyzed in this subcontract was produced by compositing a total of 26 sample aliquots obtained during the run from the separator overhead (SOH) process stream and the atmospheric still overhead (ASOH) process stream.

#### Run CMSL-2

The main objective of HRI's Run CMSL-2, also called Run 227-78, was to investigate the effect of a high coal concentration on process performance. The higher coal concentration in the coal-solvent slurries was accomplished by lowering the solvent-to-coal ratio from 1.2 (to as high as 1.6) used in previous bench-scale runs, to a value of 0.9 in Run CMSL-2. The feed coal was Illinois No. 6, Burning Star 2, bituminous

coal. Throughout Run CMSL-2, the first- and second-stage reactors were operated catalytically; Shell S-317 Ni/Mo on alumina catalyst was present in both reactors. No on-line hydrotreater was used in the run. The net product sample analyzed in this subcontract was produced by compositing a total of 10, one-half gallon sample aliquots obtained during periods 8 through 12 of the run from the separator overhead (SOH) process stream and the atmospheric still overhead (ASOH) process stream.

### Overview of Results

#### Run CC-15

The methodology employed was to analyze the whole net product sample, which in Run CC-15 was a blend of the SOH and ASOH from Conditions 2, 3, and 4. The whole sample was fractionated into four distillation cuts; naphtha (IBP-380 °F), kerosene (380-510 °F), diesel (510-650 °F), and resid (650 °F<sup>+</sup>). Each of the straight-run fractions was inspected using an appropriate suite of methods. The naphtha and kerosene fractions then were caustic washed for the removal of phenolic compounds. The washed fractions were then re-tested.

The coal liquid product quality was assessed by comparison of the physical and chemical property test data for the distillation fractions (IBP-380 °F, 380-510 °F, and 510-638 °F) to the corresponding specifications for gasolines, aviation turbine fuels, diesel fuels or fuel oils, respectively. The properties of the net product oil and its distillate fractions show that the coal-derived material has many desirable qualities. The whole crude has low sulfur, metals, ash and resid contents and boils below the maximum temperature allowed for the production of transportation fuels. The naphtha fraction (IBP-380 °F), which represents 40% of the net product, is highly naphthenic and has a low benzene content. The naphtha fraction appears to be amenable to mild hydrotreating to produce a good gasoline blendstock or reformer feedstock. The kerosene (380-510 °F) fraction, which represents 33% of the net product, is too cyclic for use as aviation fuel and it is recommended that this fraction be distributed into the two cuts on either end of it (diesel and gasoline feedstocks). The 510-680 °F fraction, which represents 22% of the net product, met most specifications as a diesel fuel and heating fuel, although its cetane index would need to be boosted

for premium diesel fuel use. Caustic washing removed 2% and 4% phenolics from the naphtha and jet fuel fraction, respectively, and provided minor improvements in the qualities of the washed fractions.

#### Run CMSL-2

The methodology used was to analyze the whole sample from Run CMSL-2 and then to fractionate it into four distillation cuts; naphtha (IBP-350 °F), kerosene (350-400 °F), diesel (400-550 °F), and resid (>550 °F). Each of the straight-run fractions was inspected using an appropriate suite of methods. A portion of the kerosene fraction was caustic washed for the removal of phenolic compounds and the washed fraction was then re-tested.

As in the previous case, the coal liquid product quality was assessed by comparison of the physical and chemical property test data for the distillation fractions to the corresponding specifications for gasolines, aviation turbine fuels, diesel fuels or fuel oils. This syncrude has many desirable properties. It is a low-sulfur crude that is nearly free of metals, ash and resid. The naphtha fraction (IBP-350 °F), which represents 25% of the crude, met a number of the specifications for gasoline; however, this material would best be mildly hydrotreated to achieve a specification vapor pressure. This material would be an acceptable feedstock for a catalytic reformer if the olefin content were reduced by mild hydrotreating. The biggest deficiency with the kerosene fraction (350-400 °F), which represents 6% of the crude, for use as an aviation turbine fuel is its high aromatic content; aromaticity affects combustion performance. Hydrogenation should improve its properties. However, the severity of hydrotreating necessary to make acceptable aviation jet fuel may not be economically favorable. It is recommended that this low-sulfur kerosene fraction, instead, be distributed into the cuts on either end of it (diesel and gasoline feedstocks). The 400-550 °F fraction, which represents 35% of the crude, meets most of the specifications for diesel fuel and heating fuel. The cetane number would need to be boosted for use as a premium diesel fuel. The >550 °F fraction, which represents 34% of the crude, met most specifications for No. 4 heating oils, and many specifications for lighter grade heating fuels.

### CONSOL Evaluation and Recommendations

Although it is acknowledged that the petroleum inspection tests were not designed for analysis of coal liquids, these tests provide the best available method for evaluation of the quality and value of the direct coal liquefaction product oils. The properties of the net product oils and the distillation fractions were shown in this work to have many desirable qualities. Verification of the suitability of these tests for coal liquids would be advantageous. It is our recommendation that test programs such as these be applied more frequently to the products of ongoing process development programs. This would provide guidance for process improvement efforts.

### References

1. Brandes, S. D.; Robbins, G. A.; Winschel, R. A.; Burke, F. P. "Coal Liquefaction Process Streams Characterization and Evaluation - Analytical Needs Assessment, Topical Report"; DOE Contract No. DE-AC22-89PC89883, March 1991.
2. Kramer, R. L. "Modified Light Oil, Southern Clean Fuels Inc. - Coal Liquefaction Material, Sample Number C9034, Research Report" in "Coal Liquefaction Process Stream Characterization and Evaluation, Technical Progress Report, October 1, 1990, through December 31, 1990", DOE/PC 89883-24, June 1991.
3. Kramer, R. L. "Modified Light Oil, Southern Clean Fuels Inc. - Coal Liquefaction Material, Sample Number C90116, Research Report" in "Coal Liquefaction Process Stream Characterization and Evaluation, Technical Progress Report, July 1, 1991, through September 30, 1991", DOE/PC 89883-24, November 1991.

**COAL LIQUEFACTION PROCESS STREAM CHARACTERIZATION AND EVALUATION**

**Analysis of Coal-Derived Synthetic Crude from HRI CTSI Run CC-15**

**Topical Report**

**Prepared by:**

**IIT RESEARCH INSTITUTE**  
National Institute for Petroleum and Energy Research  
P.O. Box 2128  
Bartlesville, OK 74005

**Gene P. Sturm, Jr.  
Je Kim  
Johanna Shay**

**Prepared for:**

**CONSOL Inc.  
Research and Development  
4000 Brownsville Road  
Library, PA 16129**

**F. P. Burke  
R. A. Winschel  
S. D. Brandes**

**June 1993**

## TABLE OF CONTENTS

	<u>Page</u>
LIST OF TABLES .....	viii
1. EXECUTIVE SUMMARY.....	1
2. EXPERIMENTAL .....	2
3. EXPERIMENTAL RESULTS.....	9
4. ASSESSMENT OF DATA QUALITY AND APPLICABILITY OF METHODS.....	9
5. ASSESSMENT OF PRODUCT QUALITY .....	11
6. REFERENCES .....	14
APPENDIX A DISTILLATION DATA.....	19
APPENDIX B DETAILED GAS CHROMATOGRAPHIC ANALYSIS DATA (PIANO).....	26
APPENDIX C HC22 MASS SPECTROMETRIC DATA.....	42
APPENDIX D JFTOT THERMAL STABILITY DATA.....	49

## TABLES

<u>Table</u>	<u>Page</u>
I. Chemical and Physical Property Data.....	15
II. Chemical and Physical Property Data for Caustic Washed Distillate Fractions.....	16
III. ASTM D 86 and Simulated Distillation Results, Temperature Readings Corrected to 101.3 kPa (760 mm Hg Pressure).....	17
IV. ASTM D 2382 Heat of Combustion Results.....	18

## 1. EXECUTIVE SUMMARY

CONSOL Inc. is conducting a program to aid in the advancement of direct coal liquefaction process development under contract from the U.S. Department of Energy (Contract DE-AC22-89PC89883). In this program, a number of research laboratories, including the IIT Research Institute, National Institute for Petroleum and Energy Research (NIPER), are analyzing direct coal liquefaction-derived materials under subcontract from CONSOL. NIPER recently investigated the properties of a synthetic crude oil produced by HRI, Inc. in Catalytic Two-Stage Liquefaction (CTSL) Run CC-15. The results of that investigation are presented in this report. The objective of HRI's CTSL Run CC-15, also called Run 227-75, was to test a predispersed (impregnated) hydrated iron oxide catalyst. The feed coal was Wyodak and Anderson seam, Black Thunder Mine, subbituminous coal. Start-up and make-up oil for Run CC-15 was filtered process-derived liquid, produced in HRI Run 260-03, which also used Black Thunder Mine coal. Throughout Run CC-15, the first stage reactor was operated without a catalyst bed at ca. 427° C. Criterion 317 Ni/Mo on alumina catalyst was present in the second-stage reactor, which was operated at about 413° C. The impregnated catalyst was activated with H<sub>2</sub>S at 275-300° C in a pretreater vessel. The on-line hydrotreater was not used in the run. The net product sample analyzed in this subcontract was produced by compositing a total of 26 sample aliquots obtained during the run from the Separator Overhead process stream and the Atmospheric Still Overhead process stream.

The composite coal-derived synthetic crude was distilled by ASTM Method D 2892 to produce an IBP-380° F distillate (40.2 weight percent), a 380-510° F distillate (33.4 weight percent), a 510-638° F distillate (22.5 weight percent), and a >638° F residue (2.7 weight percent). Portions of the IBP-380° F and 380-510° F distillate cuts were subjected to a caustic wash procedure to remove phenolic compounds (2.4 and 4.0 weight percent, respectively) and produce two additional fractions. The total sample, the three distillate fractions, the resid, and the two caustic-washed fractions were characterized by a total of approximately 175 chemical and physical property tests using ASTM, UOP, and other standard and published methods developed for petroleum and petroleum products.

The coal liquid product quality was briefly assessed by comparison of the physical and chemical property test data for the appropriate fraction against the specifications for gasolines, aviation turbine fuels, diesel fuels or fuel oils. However, it should be noted that these specifications apply to finished fuels that are normally comprised of blends of various refinery streams along with additives and thus do not even apply strictly to straight-run petroleum distillates, let alone coal liquid distillates.

The IBP-380° F distillate fraction failed the corrosion, gum, oxidation stability, octane and distillation specification tests. However, the 190-380° F portion of a petroleum crude is normally processed by catalytic reforming before blending into gasoline. This coal liquid distillate may need further processing to remove olefins before becoming suitable for reforming. Caustic washing of this fraction gave an improved product, although most of the specification tests were still not met. The greatest improvements were in oxidation stability and acidity.

The 380-510° F distillate fraction passed many of the specification tests for aviation turbine fuels although some important specification tests including aromatic content, smoke point, freezing point, and thermal stability were not met. The caustic-washed 380-510° F distillate fraction showed a significant improvement in mercaptan content and some other minor improvements. However, both of these fractions should benefit from hydrogenation or hydrocracking for blending into finished fuel.

The 510-638° F distillate fraction met most of the specifications for diesel fuel and heating fuel oils although the cetane index calculated met the specification only for Grade No. 4-D diesel fuel oil.

Overall, the coal liquid should benefit from further hydroprocessing. In particular, conversion of aromatics to naphthenes would be necessary to produce an acceptable blending product for aviation turbine fuels.

## 2. EXPERIMENTAL

Following instructions from CONSOL, the coal liquid sample was prepared by blending the entire contents of individual containers received from CONSOL and designated by HRI as Atmospheric Still Overheads 227-75- PD.6C; PD.7A, B, C; PD.8A, B, C; PD.10A, B, C; and PD.11A, B and labeled LO-6184 through LO-6195 and Separator Overheads 227-75 PD.7A, B, C; PD.8A, B, C; PD.10A, B, C; PD.11A, B, C; and PD.12A, B and labeled LO-6196 through LO-6209, respectively. The net weight of the Atmospheric Still Overheads and the Separator Overheads were reported as 6.919 Kg and 16.534 Kg, respectively. A 19.6 Kg portion of the blended coal-derived synthetic crude was distilled by ASTM D 2892 to produce a C4 fraction from debutanization, an IBP-380° F distillate, a 380-510° F distillate, a 510-638° F distillate, and a >638° F resid. The C4 fraction, amounting to only 1.0 weight percent, was discarded. Portions of the IBP-380° F and 380-510° F distillates were subjected to a caustic wash procedure to remove phenolic compounds and produce two caustic-washed fractions. Yields are listed in table I.

Experimental methods used in the analysis of this coal-derived synthetic crude and its fractions were standard ASTM or UOP methods, as noted along with the experimental results in tables I and II, with some minor exceptions as discussed later in this section. A brief description of the methods follows:

## 2.1 Gravity

Specific gravities were measured by a Mettler/Paar DMA45 at 60° F according to ASTM D 4052, Density and Relative Density of Liquids by Digital Density Meter. API gravities were calculated from the specific gravities.

## 2.2 Elemental Analysis

Carbon and Hydrogen were determined with a Perkin Elmer Model 240C. The procedure used is that described in ASTM D 5291, Standard Test Method for the Instrumental Determination of Carbon, Hydrogen, and Nitrogen in Petroleum Products and Lubricants.

Sulfur contents were measured according to method ASTM D 3120, Trace Quantities of Sulfur in Light Liquid Petroleum Hydrocarbons by Oxidative Microcoulometry, using a Mitsubishi TOX-10 microcoulometer.

Nitrogen values were measured by an Antek 730C according to ASTM D 4629, Trace Nitrogen in Liquid Petroleum Hydrocarbons by Oxidative Combustion and Chemiluminescence Detection.

Oxygen values were determined by difference by subtraction of the C, H, N, and S elemental analyses data from 100.0 percent.

Basic nitrogen values were determined by UOP 269, Nitrogen Bases in Hydrocarbons by Potentiometric Titration, using a Brinkmann 636 Titroprocessor.

Mercaptan Sulfur contents were measured by ASTM 3227, Mercaptan Sulfur in Gasoline, Kerosine, Aviation Turbine, and Distillate Fuels (Potentiometric Method).

## 2.3 Trace Metals

V, Ni, Fe, and Cu were determined by ASTM D 5185 by Inductive Coupled Plasma Atomic Emission Spectroscopy (ICP-AES), using an ARL 3560. Scandium (5ppm, Conostan) was used as an internal standard.

## 2.4 Ash

Ash contents were determined by ASTM D 482, Ash from Petroleum Products.

## 2.5 Viscosity

Kinematic Viscosities were measured according to ASTM D 445, Kinematic Viscosity of Transparent and Opaque Liquids. Cannon Certified Viscosity Standard (S-3) was used for confirmatory checks.

## 2.6 Refractive Index

All measurements for the total distillate and fractions distilling below 510° F were made using the Sodium D line at 20° C according to ASTM D 1218, Refractive Index and Refractive Dispersion of Hydrocarbon Liquids. The fractions distilling above 510° F were too dark to measure.

## 2.7 Freezing Point

Freezing points were measured by ASTM D 2386, Freezing Point of Aviation Fuels.

## 2.8 Cloud Point

Cloud point determination by ASTM D 2500 was not successful as the 510-638° F distillate was too dark to measure.

## 2.9 Pour Point

Pour points were measured according to ASTM D97, Pour Points of Petroleum Products.

## 2.10 Reid Vapor Pressure

Vapor Pressures of two fractions, IBP-380 and 380-150° F, were measured by ASTM D 5191, Vapor Pressure of Petroleum Products (Mini Method). The measured total pressures were converted to a Reid Vapor Pressure Equivalent (RVPE) by use of a correlation equation. A Grabner Instruments Model CCA-VPS was used for the measurements.

## **2.11 Micro Carbon Residue**

Carbon residues were determined on the total distillate and the fractions distilling above 510° F by ASTM D 4530, Micro Carbon Residue of Petroleum Products. This test provides results equivalent to the Conradson Carbon Residue (D189), while offering advantages such as better control of test conditions and small sample size.

## **2.12 Flash Point**

Flash points were measured by ASTM D 56, Flash Point by Tag Closed Tester (for the 380-510° F distillate), and ASTM D 93, Flash Point by Pensky-Martens Closed Tester (for the 510-638° F distillate).

## **2.13 Heptane Insolubles**

Asphaltene content in the total distillate was measured by ASTM D 3279, n-Heptane Insolubles.

## **2.14 Bromine Number and Olefin Content**

Bromine numbers were measured with a Brinkmann 636 Titroprocessor according to ASTM D 1159, Bromine Numbers of Petroleum Distillates and Commercial Aliphatic Olefins by Electrometric Titration. Olefin contents of the 380-510° F and 510-638° F distillate fractions were calculated according to Annex A4 of ASTM D 1159.

## **2.15 Aniline Point**

Aniline points were run by Method A, ASTM D 611, Aniline Point and Mixed Aniline Point of Petroleum Products and Hydrocarbon Solvents.

## **2.16 Smoke Point**

Smoke point was measured by ASTM D 1322, Smoke Point of Aviation Turbine Fuels.

## **2.17 Acidity**

Acidities were run by ASTM D 3242, Acidity in Aviation Turbine Fuel.

## 2.18 Copper Corrosion

Copper corosions were determined according to ASTM D 130, Detection of Copper Corrosion from Petroleum Products by the Copper Strip Tarnish Test.

## 2.19 Existent Gum

Existent gum was measured and reported as washed existent gum for the IBP-380° F distillate, according to ASTM D 381, existent gum in Fuels by Jet Evaporation. The upper boiling point for the 380-510° F distillate was too high for determination of existent gum on this fraction since our equipment is not equipped with superheated steam.

## 2.20 Oxidation Stability

Oxidation stability on the IBP-380° F distillate was determined by ASTM D 525, Oxidation Stability of Gasoline (Induction Period Method). Oxidation stability of the 510-638° F distillate was determined by ASTM D 2274, Oxidation Stability of Distillate Fuel Oil (Accelerated Method).

## 2.21 Thermal Stability

Thermal stability of the 380-510° F distillate was determined by ASTM D 3241, Thermal Oxidation Stability of Aviation Turbine Fuels by Jet Fuel Thermal Oxidation Tester (JFTOT).

## 2.22 Distillation, D 86 and Gas Chromatographic Simulated Distillation, D 5307 and D 2887

Simple atmospheric pressure distillation, ASTM D 86, Distillation of Petroleum Products, was used for the total distillate and three distillation fractions boiling below 638° F. The D 86 distillation data is summarized in table III. Due to thermal decomposition problems with the total distillate and the 510-638° F distillate fraction, simulated distillation data by ASTM D 5307, Determination of Boiling Range Distribution of Crude Petroleum by Gas Chromatography and by ASTM D 2887, Determination of Boiling Range Distribution of Hydrocarbon Distillates by Gas Chromatography, were acquired for the two samples, respectively.

## 2.23 Distillation, D 2892

Distillation fractions corresponding to IBP-380° F, 380-510° F, and 510-638° F and a >638° F resid were prepared by ASTM D 2892. Data from the distillation are summarized in table I with the detailed data given in Appendix A.

## 2.24 Octane Number

Octane numbers were obtained by ASTM D 2700 (Motor Method) and D 2699 (Research Method) on the IBP-380° F distillate before and after caustic washing.

## 2.25 Cetane Index

The Cetane Index for the 510-638° F distillate fraction was calculated according to method ASTM D 976.

## 2.26 Heat of Combustion

Heat of combustion was determined for the three distillate fractions by ASTM D 2832, Heat of Combustion of Hydrocarbon Fuels by Bomb Calorimeter (High-Precision Method). The values obtained are summarized in table IV.

## 2.27 Group Analysis

### A. Gas Chromatography

Detailed Hydrocarbon Analysis according to modified method ASTM D 5134 was performed on the IBP-380° F fraction. In this analysis, (sometimes termed PIANO for paraffins, isoparaffins, aromatics, naphthenes, and olefins) individual components up to tridecane are quantified. Benzene was determined by this method also. A Siemens Sichromat 2 GC with Chrom Perfect and DHA software was used. The results from the PIANO analyses are provided in Appendix B and summarized in tables I and II.

## B. Mass Spectrometry

Group type analyses of the 380-510° F and 510-638° F distillate fractions was performed by the high resolution mass spectrometric method, HC22, published by Richard Teeter (1). Naphthene content was corrected for olefin content determined by ASTM D 1159 as the HC22 method does not distinguish between olefins and naphthenes. Detailed results are given in Appendix C and are summarized in tables I and II.

## C. Naphthalenes by UV Spectroscopy

Naphthalenes were determined in the 380-510° F distillate by ASTM D 1840, Naphthalene Hydrocarbons in Aviation Turbine Fuels by Ultraviolet Spectrophotometry. Data are given in tables I and II.

### 2.28 Caustic Washing and Phenol Recovery

The caustic wash and phenol recovery procedure is described below:

The following procedure is written for the caustic wash of a single 300 g aliquot of sample. The procedure can be linearly scaled to accomplish caustic washing of larger samples.

Equipment: Separatory funnel (1 L or larger) or mixing vessel (tank)

Vacuum rotary evaporator

Supplies: 20 weight-percent NaOH solution

Concentrated HCl

Dichloromethane ( $\text{CH}_2\text{Cl}_2$ )

### Caustic Wash

Each 300 g aliquot of sample to be washed is contacted twice with equal weight (300 g) aliquots of NaOH solution. This is followed by three washes with an equal weight (300 g) of distilled water. The water mixture is allowed to settle and the water layer is drawn off.<sup>1</sup>

## Phenol Recovery

The collected aqueous phases are combined and acidified with concentrated HCl to a pH of 5.0-5.5 and transferred to a separatory funnel or mixing tank. The phenols are recovered from the acidified water by washing with three or more (300 g) aliquots of dichloromethane. The dichloromethane is removed from the separatory funnel and evaporated to obtain the phenolic extract.

<sup>1</sup>Note: If a stable emulsion forms it can be recovered separately from the oil and water phases and broken by gentle heating.

## 3. EXPERIMENTAL RESULTS

Chemical and physical property test data are listed in table I for the total distillate, IBP-380° F distillate, 380-510° F distillate, 510-638° F distillate and the >638° F resid. Similar data for the caustic-washed IBP-380° F and 380-510° F distillate fractions are listed in table II. Results from D 86 distillations and simulated distillations are given in table III. Summary D 2892 distillation data are listed in table I. Complete simulated distillation and D 2892 data are given in Appendix A.

Heat of combustion data are listed in table IV. Group type analysis data by gas chromatography (ASTM 5134) are summarized in tables I and II with the complete data included as Appendix B. Similarly, the group type analysis data determined by mass spectrometry are summarized in tables I and II with the complete data included as Appendix C. Details of the thermal stability (JFTOT) tests are given in Appendix D.

## 4. ASSESSMENT OF DATA QUALITY AND APPLICABILITY OF METHODS

Application of ASTM and other standard methods along with a quality assurance program that includes analysis of primary standards where available, secondary standards, and regular participation in interlaboratory round robin test studies should assure data quality falls within the statistical parameters associated with the particular tests employed, except for those tests that do not apply well to nonpetroleum-derived materials. Duplicate determinations are usually made for most tests and the results routinely fall within the published error limits.

An exception to the use of standard methods was the determination of oxygen by difference by subtraction of the C, H, N and S elemental analysis data from 100.0 percent. This usually results in reasonable values for oxygen content, but can lead to misleading results. For example, the value of 0.00 obtained for the oxygen content of the <380° F distillate cut is clearly in error as the phenol separation indicated 2.4 percent phenols in this fraction. The standard errors in the measurement of C, H, N and S (cumulative error is  $\pm 1\%$ ) can lead to such a result.

Almost all of the tests employed in this study were developed for application to petroleum and petroleum products. The applicability of some of the tests to coal-derived liquids is not a simple issue. The physical property tests should apply equally well to coal liquids as to petroleum products in respect to determination of the property. However, in some cases correlation of that property to performance of the material for its intended use may be somewhat different for coal-derived liquid products than for petroleum products. The potential for inaccuracy is more serious for most of the chemical tests. For example, the methods employed for the group type analyses of the <380° F, 380-510° F, and 510-638° F fractions do not determine oxygenates, nitrogen compound types or all possible sulfur compound types even for petroleum-derived fractions. This is usually not a serious omission for the lighter fractions except for the presence of phenols in the coal-derived light fractions. These limitations can be very important for fractions containing significant quantities of oxygen-, sulfur-, or nitrogen-containing compounds as indicated in the methods. Also, the HC22 mass spectrometric method employed for the 380-510° F and 510-650° F fractions were developed for petroleum-derived materials. The different distributions of isomers and alkyl-substituted homologs within the various compound types between coal liquids (and even atypical petroleum crudes) and conventional petroleum crudes can affect the accuracy of compositional data produced by the HC22 method, the corresponding ASTM methods, and other similar methods.

Some of the ASTM methods, such as D 2274, state they are "not applicable to fuels containing any significant component derived from a nonpetroleum source". For others, such as ASTM D 5134, Detailed Analysis of Petroleum Naphthas Through n-Nonane by Capillary GC, significantly different composition can be a problem for correct peak identification. For example, an oxygenate co-eluting with a hydrocarbon compound would cause an erroneously high result for that compound. In spite of the problems of applicability, the methods employed in this study are the best (or among the best) available; and in most cases they are the tests required in the specifications for the end use products for which these distillate fractions would ultimately be used, after further processing.

## 5. ASSESSMENT OF PRODUCT QUALITY

Product quality for the <380° F, 380-510° F, and 510-638° F distillate fractions will be assessed by comparison of the physical and chemical property test data against the specifications for gasolines (ASTM D 4814), aviation turbine fuels (ASTM D 1655), and diesel fuels (ASTM D 975)/fuel oils (ASTM D 396), respectively. It should be noted up front that these specifications apply to finished fuels that are normally comprised of blends of various refining streams along with additives and thus do not even apply directly to straight-run petroleum distillates, let alone coal liquid distillates.

### 5.1 Assessment of the IBP-380° F Distillate Fraction

The quality of the IBP-380° F distillate fraction is probably best assessed in terms of specifications for gasoline. The vapor pressure for this distillate fraction falls well below the maximum allowed for all of the vapor pressure/distillation classes of gasolines. In fact, this fraction would need to be blended with some lighter material to meet the minimum requirements for distillation boiling range in terms of the 10 percent evaporated maximum temperature, which ranges from 122-158° F for classes AA-E. Similarly, the 50 percent off-temperature falls outside the range of maximum temperatures for the classes (253° F compared to specifications of 230° F for class E to 250° F for classes AA and A). Finally, the maximum temperature specifications for the 90 percent off and end points are met by the IBP-380° F distillate fraction. Also, the maximum residue allowed (2 percent, volume) was met easily, as no residue was observed.

Other specification tests that were performed include copper strip corrosion, existent gum, sulfur content, and oxidation stability. The distillate fraction failed the copper strip corrosion test (3b versus 1, maximum), the washed existent gum test (11.2 versus 5, maximum), and the oxidation stability test (105 minutes versus 240 minutes, minimum). Sulfur content met the specifications (0.03 weight percent versus 0.10, maximum) in spite of the presence of some hydrogen sulfide and failure in the copper strip corrosion test.

The octane number tests gave results considerably below that required for a finished gasoline as would be expected. The octane numbers for petroleum distillates in this boiling range are usually on the order of 60-70. Typically, light straight-run gasoline, catalytic reformate, catalytically cracked gasoline, hydrocracked gasoline, polymer gasoline, alkylate, and  $\eta$ -butane are blended along with additives to produce a finished gasoline. Generally, the heavy straight-run gasoline fraction (boiling range approximately 190-380° F) is used as feed to the catalytic reformer to produce a 90-100 research octane product (2). Such a process would be necessary for the coal

liquid <380° F fraction (or at least the 190-380° F portion) to improve its qualities for gasoline blending, although removal of olefins would be required to make it acceptable as a catalytic reformer feedstock.

### 5.2 Assessment of the Caustic-Washed IBP-380° F Distillate Fraction

Results for several of the physical and chemical property tests showed improvement in the caustic-washed <380° F distillate fraction. The specific gravity, Reid Vapor pressure, and 4.76 percent losses experienced in the caustic washing are consistent with loss of some lower boiling material in the caustic wash procedure. Results that showed improvement include acidity (from 0.05 to <0.01 mg KOH/g), copper strip corrosion (from 3b to 2d, but still failed), washed existent gum (from 11.2 to 9.0 mg/100 mL, still failed), and oxidation stability (D 525) (from 105 to 1440 minutes, pass). Octane numbers showed a slight decrease after washing and heat of combustion showed a slight increase. Mercaptan sulfur showed a significant decrease after washing (from 52 to 10 ppm). Most of the changes observed are those expected from a caustic wash or are consistent with the loss of some light ends. The quality of the fraction in terms of its suitability for gasoline is somewhat, but not drastically, improved as compared to the distillate before caustic washing.

### 5.3 Assessment of the 380-510° F Distillate Fraction

The 380-510° F distillate fraction is assessed in terms of specifications for aviation turbine fuels although finished jet fuels are sometimes blended from a variety of refinery streams with the addition of various additives also. Nevertheless, this distillate fraction passed the specification tests for total sulfur content, acidity, copper strip corrosion, flash point, density and distillation final boiling point, residue and loss. Failed tests include aromatic content (41 versus 20 volume percent maximum), mercaptan sulfur (45 versus 30 ppm maximum), 10 percent distillation temperature (220 versus 205° C maximum), freezing point (-12 versus -40° F maximum), viscosity (10.8 cSt versus 8 cSt at -20° C), net heat of combustion (41.7 versus 42.8 MJ/kg minimum), smoke point (10.9 versus 20 or 25 mm minimum), naphthalenes (4.2 versus 3.0 volume percent, maximum), and thermal stability (tube deposit rating >4 versus 3 maximum). The high aromatic content of this distillate fraction is probably the most serious deficiency in its potential use as a blending stock for aviation fuel. Hydrogenation or hydrocracking should improve its properties significantly.

#### 5.4 Assessment of Caustic-Washed 380-510° F Distillate Fraction

The test result that showed the most significant improvement after caustic washing of the 380-510° F distillate fraction was the mercaptan sulfur value, which decreased from 45 ppm to less than 0.1 ppm. Most other properties showed some improvement. Overall, the caustic-washed fraction, although slightly improved for use in blending for jet fuels, is limited by the high aromatic content and related low smoke point.

#### 5.5 Assessment of the 510-638° F Distillate Fraction

The quality of the 510-638° F distillate fraction is probably best assessed using the specifications for diesel fuel oils and heating fuel oils. In terms of the diesel fuel oil specifications, the distillate meets the flash point, distillation, ash, sulfur, and copper strip corrosion tests for all grades and the cetane number for Grade No. 4-D diesel fuel oil. The viscosity was only slightly under the minimum requirement of 5.5 cSt at 104° F. The cloud point could not be determined because the fraction was too dark in color.

In terms of heating oil or fuel oil specifications, the 510-638° F distillate fraction meets the requirements in terms of flash point (except for No. 6 fuel oil), viscosity (for Grade No. 4 light, only), ash, sulfur, and copper strip corrosion. Pour point was somewhat high (35° F compared to 28° F, maximum for Grades No. 2, 4 light, and 4).

#### 5.6 Assessment of the >638° F Resid

The quality of the >638° F resid fraction is probably best assessed using the specifications for heavy heating oils, although a corresponding petroleum fraction would probably be sent to a catalytic cracking or hydrocracking unit in most refineries. The high nitrogen and metals in this fraction (based on the whole distillate values) would probably exclude it from consideration for catalytic cracking. In any case, the low ash content, low sulfur content, and copper strip corrosion value all meet the specifications for even lighter heating oil grades, indicating good quality in that respect.

## 6. REFERENCES

1. Teeter, R. M., Mass Spec. Rev., 4, 123 (1985).
2. Gary, J. H. and Handwerk, G. E., PETROLEUM REFINING: Technology and Economics, Marcel Dekker, Inc., New York, NY, 1975, Chapter 2.

Table I. - Chemical and Physical Property Data

Date Started

Date Completed 5-26-93

Property	Sample				
	Total Dist.	<380° F	380 - 510° F	510 - 638° F	>638° F
Specific Gravity @ 60° F (D4502)	0.8522	0.7798	0.8899	0.9223	0.9773
API Gravity (calculated)	34.5	50.0	27.5	21.9	13.3
Elemental Analysis, wt. %					
Carbon (D5291)	86.77	85.93	87.12	87.63	87.93
Hydrogen (D5291)	12.52	13.98	11.77	11.37	10.28
Sulfur (D3120)	0.05	0.03	0.03	0.01	0.12
Nitrogen (D4629)	0.25	0.09	0.33	0.22	0.81
Oxygen (by diff)	0.41	0.00	0.75	0.77	0.86
Basic Nitrogen (UOP269)	0.184	0.082	0.274	0.180	
Mercaptan Sulfur (D3227), ppm		51.5	45.2		
Trace Metals (D5185), Vanadium, ppm	12.2				
Nickel, ppm	15.0				
Iron, ppm	13.4				
Copper, ppm	14.6				
Ash (D482), wt. %	0.004			<0.001	0.020
Viscosity (D445), cSt					
@ 70° F	1.899			9.879	
@ 100° F	1.475			5.338	
@ -20° C			10.80		
Refractive Index, (D1218) 20° C	1.46877	1.42882	1.49198	Too Dark	Too Dark
Freezing Point (D2386), °F	-24		-12		
Cloud Point (D2500), °F				Too Dark	
Pour Point (D97), °F	<60			35	
Reid Vapor Pressure (D5191), psi		2.54	<0.01		
MicroCarbon Residue (D4530), wt. %	0.06			0.00	1.95
Flash Point (D56, D93), °C			83	136	
Heptane Insolubles (D3279), wt. %	0.39				
Group Analysis (ASTM D5134 and HC22)					
Paraffins, vol. %		38.0 <sup>1</sup>	9.6	10.1	
Naphthenes, vol. %		45.7	43.1	34.5	
Aromatics, vol. %		8.7	41.4	52.1	
Olefins, vol. %		4.6	5.8	3.3	
Benzene (PIANO, mod D5134)		0.089			
Naphthalenes (D1840), vol. %			4.23		
Bromine Number (D1159)		3.62	5.08	2.70	
Aniline Point (D611), °F		103.8	71.5	88.3	
Smoke Point (D1322), mm			10.9		
Acidity (D3242), mg KOH/g	0.07	0.05	0.04	0.22	
Copper Corrosion (D130)		3b (dark)	1a (slight)	1a (slight)	1a (slight)
Existent Gum (D381), mg/100mL		11.2 <sup>2</sup>	B.P. too high <sup>3</sup>		
Oxidation Stability (D525), min		105			0.9
Oxidation Stability (D2274), mg/100mL					
Thermal Stability (JFTOT) (D3341)			Fall		
Distillation, ASTM D86			Refer to Table III		
Distillation, ASTM D2892 Yield, wt. %		40.2	33.4	22.5	2.7
Octane Number: Motor Method (D2700)		60.7			
Research Method (D2699)		61.6			34.2
Cetane Index (D976)					
Heat of Combustion (D2382)			Refer to Table IV		
Caustic Wash & Phenol Recovery, wt. % <sup>4</sup>		W:92.86 P:2.38	W:92.08 P:4.01		

<sup>1</sup> Unknowns = 3.0 volume %.

<sup>2</sup> Washed existent gum.

<sup>3</sup> Requires superheated steam which is not available to our instrument.

<sup>4</sup> W = washed distillate, P = phenols recovered, 100-W-P = percent lost in the procedure.

Supervisor \_\_\_\_\_

**Table II. - Chemical and Physical Property Data for Caustic Washed Distillate Fractions**

Date Started	Date Completed	5-26-93
Property	After Washing Sample	
	<380° F	380 - 510° F
Specific Gravity @ 60° F (D4502)	0.7775	0.8882
API Gravity (calculated)	50.5	27.8
Elemental Analysis, wt. %		
Carbon (D5291)	86.12	87.75
Hydrogen (D5291)	13.77	11.68
Sulfur (D3120)	0.03	<0.01
Nitrogen (D4629)	0.07	0.33
Oxygen (by diff)	0.01	0.23
Basic Nitrogen (UOP269)	0.058	0.264
Mercaptan Sulfur (D3227), ppm	9.7	<0.1
Trace Metals (D5185), Vanadium, ppm		
Nickel, ppm		
Iron, ppm		
Copper, ppm		
Ash (D482), wt. %		
Viscosity (D445), cSt		
@ 70° F		
@ 100° F		
@ -20° C		9.665
Refractive Index, (D1218) 20° C	1.42836	1.49072
Freezing Point (D2386), °F		-13
Cloud Point (D2500), °F		
Pour Point (D97), °F		
Reid Vapor Pressure (D5191), psi	2.09	<0.01
MicroCarbon Residue (D4530), wt. %		
Flash Point (D56), °C		82
Heptane Insolubles (D3279), wt. %		
Group Analysis (ASTM D5134 and HC22)		
Paraffins, vol. %	34.7 <sup>1</sup>	9.1
Naphthenes, vol. %	48.8	46.0
Aromatics, vol. %	9.2	41.9
Olefins, vol. %	4.2	3.0
Benzene (PIANO, mod D5134), vol. %	0.078	
Naphthalenes (D1840), vol. %		3.74
Bromine Number (D1159)	2.37	2.69
Aniline Point (D611), °F	106.0	75.2
Smoke Point (D1322), mm		11.6
Acidity (D3242), mg KOH/g	<0.01	0.01
Copper Corrosion (D130)	2d (moderate)	1a (slight)
Existent Gum (D381), mg/100mL	9.0 <sup>2</sup>	B.P. too high <sup>3</sup>
Oxidation Stability (D525), min	1440	
Oxidation Stability (D2274), mg/100 mL		
Thermal Stability (JFTOT) (D3241)		Fall
Distillation, ASTM D86		
Distillation, ASTM D2892		
Octane Number: Motor Method (D2700)	58.1	
Research Method (D2699)	60.2	
Cetane Index (D976)		
Heat of Combustion (D2382)		Refer to Table IV

<sup>1</sup> Unknowns = 3.1 volume %.

<sup>2</sup> Washed existent gum.

<sup>3</sup> Requires superheated steam which is not available to our instrument.

**Supervisor**

Table III. - ASTM D 86 and Simulated Distillation Results, Temperature <sup>1</sup> /  
Readings Corrected to 101.3 kPa (760 mm Hg) Pressure

Sample	Total Distillate <sup>1</sup>		IBP-380° F <sup>2</sup>		380 - 510° F <sup>3</sup>		510 - 638° F <sup>3</sup>	
Barometric Pressure (mm Hg)	779		777		773		768	
	°F	°C	°F	°C	°F	°C	°F	°C
Initial Boiling Point	97	36	135.5	57.5	408.2	209.0	474	248
5% recovered	172	78	177.8	81.0	425.6	218.7	507	264
10% recovered	200	93	190.7	88.2	428.1	220.1	518	270
20% recovered	268	131	205.8	96.6	433.0	222.8	532	278
30% recovered	333	167	220.4	104.7	437.7	225.4	541	283
40% recovered	388	198	235.7	113.2	442.7	228.2	549	287
50% recovered	430	221	253.4	123.0	448.1	231.2	561	294
60% recovered	469	243	275.3	135.2	454.4	234.7	573	301
70% recovered	507	264	297.8	147.7	461.6	238.7	586	308
80% recovered	539	282	317.4	158.6	470.4	243.6	603	317
90% recovered	589	309	336.0	168.9	478.9	248.3	624	329
95% recovered	633	334	344.8	173.8	486.8	252.7	637	336
End Point	803	428	359.2	181.8	507.9	264.4	666	352
Recovery, %	100.0		100.0		99.5		—	
Residue, %	0.0		0.0		0.0		—	
Loss, %	0.0		0.0		0.4		—	

<sup>1</sup> Simulated distillation results by ASTM D 5307 since the D 86 distillation was terminated at 32 mL due to smoking.

<sup>2</sup> D 86 distillation results.

<sup>3</sup> Simulated distillation results by ASTM D 2887 since the D 86 distillation was terminated at IBP (533° F) due to smoking.

**Table IV. - ASTM D 2382 Heat of Combustion Results**

Sample	Gross Heat of Combustion at 25° C		Net Heat of Combustion at 25° C	
	MJ/kg	Btu/lb	MJ/kg	Btu/lb
IBP - 380° F	46.014	19,782	43.052	18,509
380 - 510° F	44.174	18,991	41.676	17,918
510 - 650° F	44.004	18,918	41.591	17,881
IBP - 380° F After washing	46.304	19,907	43.382	18,651
380 - 510° F After washing	44.446	19,108	41.968	18,043

**APPENDIX A**  
**DISTILLATION DATA**

## ASTM D 2892 Distillation

## **Crude Oil Properties:**

**API Gravity @ 60° F = 35.2**  
**Expected IBP = 66° F**

**Density @ 60° F = 0.8486 g/cc**

**Sarnia Charge Weight= 42.02 lbs Amt. Recovered= 41.52 lbs**

<u>Fraction</u>	<u>Weight (lbs)</u>	<u>Weight %</u>	<u>API @ 60F</u>	<u>Density (g/cc)</u>
C4	0.41	1.0	n.d.*	n.d.*
IBP-380 F	16.71	40.2	n.d.*	n.d.*
380-510 F	13.86	33.4	27.5	0.8899
510-638 F	9.35	22.5	21.9	0.9223
638+	1.10	2.7	13.3	0.9773
Trap	0.09	0.2	n.d.**	n.d.**

\* n. d. = not determined. Drager 190 H2S monitor gave readings of 50 ppm for the C4 fraction and 200+ ppm for the IBP-380 F cut.

\*\* The trap contained water/oil, and the liquid was discarded.

### Distillation Conditions:

<u>Fraction</u>	<u>Temperature (F)</u>	<u>Reflux Ratio</u>	<u>Pressure (mm Hg)</u>
	<u>Head</u>	<u>Pot</u>	
IPB-380 F	380	480	5:1
380-510 F	362	417	2:1
510-638 F	440	577	2:1

## ASTM D 5307 Simulated Distillation Crude Method

Sample Name : CONSOL COAL LIQUID 227-75 Page 1  
 Instrument : HP5880\_8  
 Analysis Date : Tue Mar 23, 1993 3:48:50 pm  
 LAS Run Status : RunStatusOK  
 EndOffBaseline  
 SIMDIS Status : CurveExtended  
 SIMDISStatusOK  
 Result File : /RESULT/D94E/CRUDE '5880 '805.RES  
 Compensated File : /RESULT/D94E/CRUDE '5880 'C '805.RES  
 Parameter File : /SD/PARAMETER/D94E/CRUDE '5880.SPAR  
 Data File : /SD/DATA/D94E/CRUDE '5880805.SDAT  
 Report Format : /FORMAT/D94E/CRUDE '5880.FMT  
 Calibration Data : /SD/DATA/D94E/CRUDE '5880800.SDAT  
 Blank Result File: /RESULT/D94E/CRUDE '5880 '801.RES  
 -----

Standard Start Time	16.56	Standard End Time	20.98
Standard Weight	.1172	Sample Weight	.7004
Weight Fraction of Internal Standard		1433	
Total Theoretical Area		57474704	

IBP: 66 Deg F      19 Deg C

%OFF	DegF	DegC									
1	97	36	26	308	153	51	433	223	76	527	275
2	130	55	27	313	156	52	437	225	77	530	277
3	152	66	28	320	160	53	441	227	78	533	278
4	163	73	29	329	165	54	446	230	79	536	280
5	172	78	30	333	167	55	450	232	80	539	282
6	181	83	31	338	170	56	453	234	81	543	284
7	182	84	32	343	173	57	456	236	82	546	286
8	184	84	33	349	176	58	461	238	83	550	288
9	194	90	34	354	179	59	466	241	84	555	2914
10	200	94	35	359	182	60	469	243	85	561	297
11	210	99	36	364	185	61	474	245	86	566	299
12	212	100	37	371	189	62	478	248	87	571	300
13	213	100	38	378	192	63	482	250	88	576	302
14	214	101	39	383	195	64	485	252	89	581	309
15	216	102	40	388	198	65	488	254	90	586	313
16	232	111	41	395	200	66	491	256	91	596	317
17	244	113	42	398	202	67	495	257	92	603	322
18	251	122	43	408	203	68	499	260	93	612	324
19	259	126	44	403	206	69	503	262	94	621	334
20	268	131	45	408	209	70	507	264	95	631	342
21	270	132	46	412	211	71	510	266	96	640	351
22	274	134	47	416	213	72	514	268	97	651	364
23	288	142	48	418	215	73	517	270	98	661	374
24	295	146	49	425	218	74	520	271	99	673	390
25	302	150	50	430	221	75	524	273			

FBP: 803 Deg F      428 Deg C  
 Percent Residue : 0.000%

ASTM D 5307 Simulated Distillation Crude Method

Page 2

Sample Name CONSOL COAL LIQUID 227-75  
Instrument HP5880\_8

IBP = 650 F 96.20 %OFF  
650 = FBP 93.80 %OFF

Cut point results

Temperature %OFF  
Start End

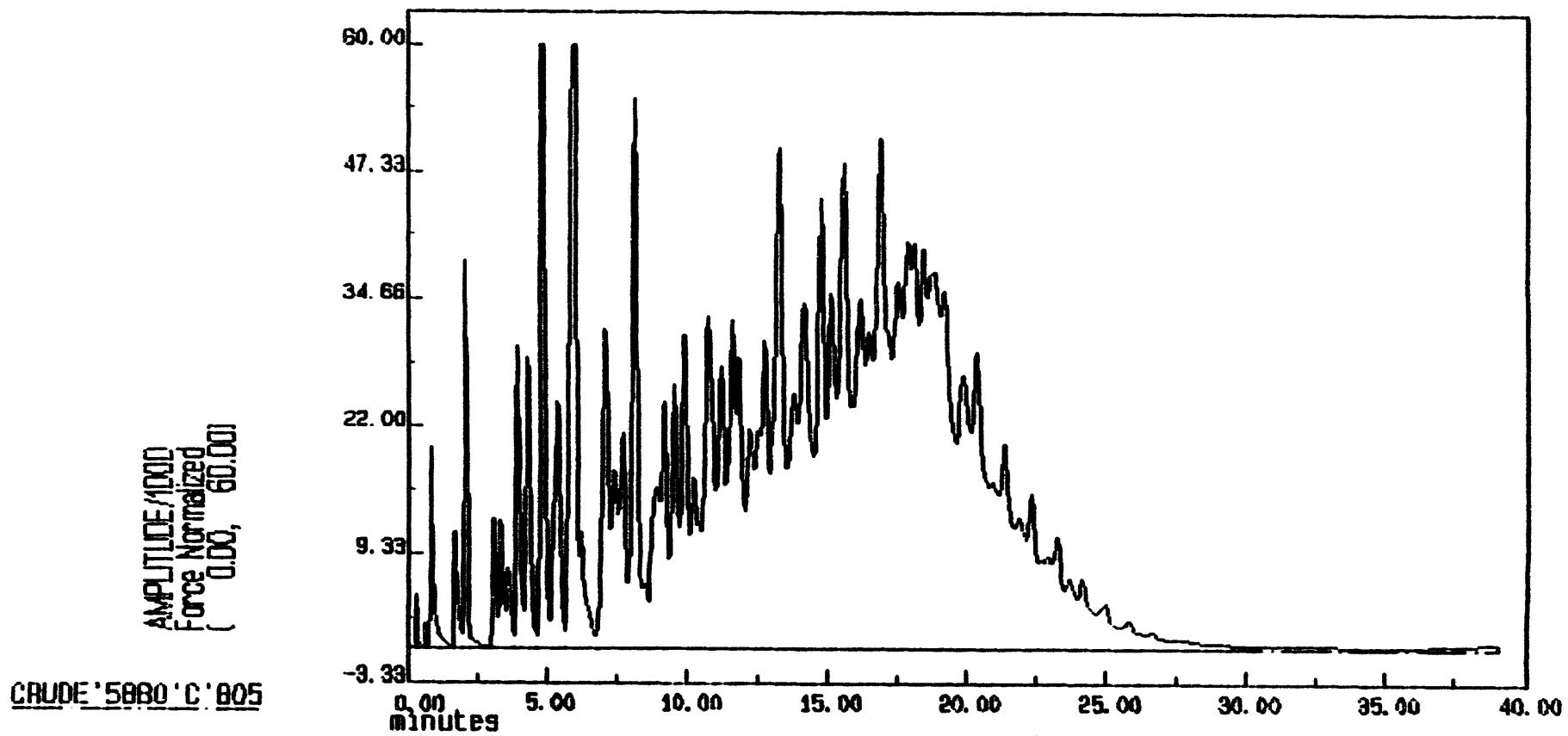
IBP	- 200	9.95
200	- 300	14.79
300	- 3400	18.81
400	- 500	24.66
500	- 6500	27.98
IBP	- 4000	43.55
400	- 650	52.65

Hempel Distribution

Fraction, DegF Yield, %

IBP	122	1.97
122	167	3.31
167	212	8.01
212	267	10.30
267	322	10.79
322	377	10.79
377	432	10.79
432	487	10.79
487	542	10.79
542	597	10.79
597	652	10.79
652	707	10.79
707	762	10.79
762	817	10.79
817	872	10.79
872	927	10.79
927	982	10.79
982	1037	10.79
1037	1092	10.79
1092	1147	10.79
1147	1202	10.79
1202	1257	10.79
1257	1312	10.79
1312	1367	10.79
1367	1422	10.79
1422	1477	10.79
1477	1532	10.79
1532	1587	10.79
1587	1642	10.79
1642	1697	10.79
1697	1752	10.79
1752	1807	10.79
1807	1862	10.79
1862	1917	10.79
1917	1972	10.79
1972	2027	10.79
2027	2082	10.79
2082	2137	10.79
2137	2192	10.79
2192	2247	10.79
2247	2292	10.79
2292	2347	10.79
2347	2392	10.79
2392	2447	10.79
2447	2492	10.79
2492	2547	10.79
2547	2592	10.79
2592	2647	10.79
2647	2692	10.79
2692	2747	10.79
2747	2792	10.79
2792	2847	10.79
2847	2892	10.79
2892	2947	10.79
2947	2992	10.79
2992	3047	10.79
3047	3092	10.79
3092	3147	10.79
3147	3192	10.79
3192	3247	10.79
3247	3292	10.79
3292	3347	10.79
3347	3392	10.79
3392	3447	10.79
3447	3492	10.79
3492	3547	10.79
3547	3592	10.79
3592	3647	10.79
3647	3692	10.79
3692	3747	10.79
3747	3792	10.79
3792	3847	10.79
3847	3892	10.79
3892	3947	10.79
3947	3992	10.79
3992	4047	10.79
4047	4092	10.79
4092	4147	10.79
4147	4192	10.79
4192	4247	10.79
4247	4292	10.79
4292	4347	10.79
4347	4392	10.79
4392	4447	10.79
4447	4492	10.79
4492	4547	10.79
4547	4592	10.79
4592	4647	10.79
4647	4692	10.79
4692	4747	10.79
4747	4792	10.79
4792	4847	10.79
4847	4892	10.79
4892	4947	10.79
4947	4992	10.79
4992	5047	10.79
5047	5092	10.79
5092	5147	10.79
5147	5192	10.79
5192	5247	10.79
5247	5292	10.79
5292	5347	10.79
5347	5392	10.79
5392	5447	10.79
5447	5492	10.79
5492	5547	10.79
5547	5592	10.79
5592	5647	10.79
5647	5692	10.79
5692	5747	10.79
5747	5792	10.79
5792	5847	10.79
5847	5892	10.79
5892	5947	10.79
5947	5992	10.79
5992	6047	10.79
6047	6092	10.79
6092	6147	10.79
6147	6192	10.79
6192	6247	10.79
6247	6292	10.79
6292	6347	10.79
6347	6392	10.79
6392	6447	10.79
6447	6492	10.79
6492	6547	10.79
6547	6592	10.79
6592	6647	10.79
6647	6692	10.79
6692	6747	10.79
6747	6792	10.79
6792	6847	10.79
6847	6892	10.79
6892	6947	10.79
6947	6992	10.79
6992	7047	10.79
7047	7092	10.79
7092	7147	10.79
7147	7192	10.79
7192	7247	10.79
7247	7292	10.79
7292	7347	10.79
7347	7392	10.79
7392	7447	10.79
7447	7492	10.79
7492	7547	10.79
7547	7592	10.79
7592	7647	10.79
7647	7692	10.79
7692	7747	10.79
7747	7792	10.79
7792	7847	10.79
7847	7892	10.79
7892	7947	10.79
7947	7992	10.79
7992	8047	10.79
8047	8092	10.79
8092	8147	10.79
8147	8192	10.79
8192	8247	10.79
8247	8292	10.79
8292	8347	10.79
8347	8392	10.79
8392	8447	10.79
8447	8492	10.79
8492	8547	10.79
8547	8592	10.79
8592	8647	10.79
8647	8692	10.79
8692	8747	10.79
8747	8792	10.79
8792	8847	10.79
8847	8892	10.79
8892	8947	10.79
8947	8992	10.79
8992	9047	10.79
9047	9092	10.79
9092	9147	10.79
9147	9192	10.79
9192	9247	10.79
9247	9292	10.79
9292	9347	10.79
9347	9392	10.79
9392	9447	10.79
9447	9492	10.79
9492	9547	10.79
9547	9592	10.79
9592	9647	10.79
9647	9692	10.79
9692	9747	10.79
9747	9792	10.79
9792	9847	10.79
9847	9892	10.79
9892	9947	10.79
9947	9992	10.79
9992	10047	10.79
10047	10092	10.79
10092	10147	10.79
10147	10192	10.79
10192	10247	10.79
10247	10292	10.79
10292	10347	10.79
10347	10392	10.79
10392	10447	10.79
10447	10492	10.79
10492	10547	10.79
10547	10592	10.79
10592	10647	10.79
10647	10692	10.79
10692	10747	10.79
10747	10792	10.79
10792	10847	10.79
10847	10892	10.79
10892	10947	10.79
10947	10992	10.79
10992	11047	10.79
11047	11092	10.79
11092	11147	10.79
11147	11192	10.79
11192	11247	10.79
11247	11292	10.79
11292	11347	10.79
11347	11392	10.79
11392	11447	10.79
11447	11492	10.79
11492	11547	10.79
11547	11592	10.79
11592	11647	10.79
11647	11692	10.79
11692	11747	10.79
11747	11792	10.79
11792	11847	10.79
11847	11892	10.79
11892	11947	10.79
11947	11992	10.79
11992	12047	10.79
12047	12092	10.79
12092	12147	10.79
12147	12192	10.79
12192	12247	10.79
12247	12292	10.79
12292	12347	10.79
12347	12392	10.79
12392	12447	10.79
12447	12492	10.79
12492	12547	10.79
12547	12592	10.79
12592	12647	10.79
12647	12692	10.79
12692	12747	10.79
12747	12792	10.79
12792	12847	10.79
12847	12892	10.79
12892	12947	10.79
12947	12992	10.79
12992	13047	10.79
13047	13092	10.79
13092	13147	10.79
13147	13192	10.79
13192	13247	10.79
13247	13292	10.79
13292	13347	10.79
13347	13392	10.79
13392	13447	10.79
13447	13492	10.79
13492	13547	10.79
13547	13592	10.79
13592	13647	10.79
13647	13692	10.79
13692	13747	10.79
13747	13792	10.79
13792	13847	10.79
13847	13892	10.79
13892	13947	10.79
13947	13992	10.79
13992	14047	10.79
14047	14092	10.79
14092	14147	10.79
14147	14192	10.79
14192	14247	10.79
14247	14292	10.79
14292	14347	10.79
14347	14392	10.79
14392	14447	10.79
14447	14492	10.79
14492	14547	10.79
14547	14592	10.79
14592	14647	10.79
14647	14692	10.79
14692	14747	10.79
14747	14792	10.79
14792	14847	10.79
14847	14892	10.79
14892	14947	10.79
14947	14992	10.79
14992	15047	10.79
15047	15092	10.79
15092	15147	10.79
15147	15192	10.79
15192	15247	10.79
15247	15292	10.79
15292	15347	10.79
15347	15392	10.79
15392	15447	10.79
15447	15492	10.79
15492	15547	10.79
15547	15592	10.79
15592	15647	10.79
15647	15692	10.79
15692	15747	10.79
15747	15792	10.79
15792	15847	10.79
15847	15892	10.79
15892	15947	10.79
15947	15992	10.79
15992	1	

23



CRUDE '5880 'C '805

SAMPLE: CONSOL COAL LIQUID 227-75

ANALYZED: Tue Mar 23, 1993 3:48:50 pm

RESULT: /RESULT/D94E/CRUDE '5880 'C '805.RES      METHOD: NCRUDE '5880

ASTM D 2887 Report 510-638° F Distillate

SAMPLE: 93GL342-3

BOTTLE #: 3

SAMPLER INJECTION @ 14:39 APR 19, 1993

% OFF	DEG F	% OFF	DEG F
IBP	474		
1	414	51	562
2	492	52	564
3	498	53	565
4	503	54	566
5	507	55	567
6	510	56	569
7	512	57	570
8	514	58	571
9	517	59	572
10	518	60	573
11	520	61	575
12	521	62	576
13	523	63	577
14	524	64	578
15	526	65	579
16	527	66	580
17	528	67	581
18	529	68	583
19	531	69	584
20	532	70	586
21	533	71	587
22	534	72	589
23	535	73	590
24	536	74	592
25	536	75	594
26	537	76	596
27	538	77	598
28	539	78	599
29	540	79	601
30	541	80	603
31	542	81	604
32	542	82	606
33	543	83	608
34	544	84	610
35	545	85	612
36	546	86	614
37	546	87	616
38	547	88	619
39	548	89	621
40	549	90	624
41	550	91	626
42	551	92	628
43	552	93	631
44	553	94	633
45	554	95	637
46	555	96	641
47	557	97	646
48	558	98	651
49	560	99	658
50	561	FBP	666

OVEN TEMP NOT READY

RT: SLICES 0.20



OVEN AT LIMIT

ASTM D 2887 CHROMATOGRAM

Sample: 93GL342-3

CONSOL COAL LIQUID 227-75, 510-638°F Distillate

RT: STOP RUN

**APPENDIX B**

**DETAILED GAS CHROMATOGRAPHIC ANALYSIS DATA (PIANO)**

National Institute for Petroleum and Energy Research  
 Detailed Hydrocarbon Analysis ( P.I.A.N.O. )

File: C:\CP\DATA1\041593CO.02R  
 Sample: Consol  
 Method: !CUT3PIAN  
 Processed 244 Peaks  
 93GL342  
 IBP-380°F

Analyzed: 04-15-1993 13:14:07  
 Reported: 04-28-1993 10:18:55  
 DHA DBase File: RI-NIPER.DBF  
 Normalized to 100.00%

Composite Report  
 Totals by Group Type & Carbon Number  
 (in Weight Percent)

	Paraffins:	I-paraffins:	Aromatics:	Naphthenes:	Olefins:	Total:
C1:	0.000	0.000	0.000	0.000	0.000	0.000
C2:	0.000	0.000	0.000	0.000	0.000	0.000
C3:	0.001	0.000	0.000	0.000	0.000	0.001
C4:	0.219	0.010	0.000	0.000	0.002	0.231
C5:	2.235	0.634	0.000	1.189	0.056	4.114
C6:	3.160	0.973	0.104	11.815	1.459	17.511
C7:	2.474	2.379	0.492	13.542	0.224	19.112
C8:	3.048	3.895	1.176	9.092	0.551	17.763
C9:	1.567	2.111	3.219	4.578	0.764	12.239
C10:	1.726	6.352	3.919	4.252	1.100	17.350
C11:	1.224	2.146	1.059	1.993	0.157	6.579
C12:	0.056	0.146	0.133	0.559	0.022	0.916
C13:	0.000	0.000	0.000	0.000	0.000	0.000
Total:	15.712	18.647	10.101	47.021	4.334	95.815

Oxygenates: 0.000      Total C14+: 0.000      Total Unknowns: 4.185  
 Grand Total: 100.000

Molecular Weight and Specific Gravity Data

Group:	Ave. Mw.:	Ave. Rel. Density:
C1:	0.000	0.000
C2:	0.000	0.000
C3:	44.097	0.501
C4:	58.110	0.578
C5:	71.526	0.656
C6:	84.576	0.734
C7:	98.525	0.745
C8:	112.504	0.752
C9:	125.082	0.780
C10:	139.500	0.774
C11:	154.181	0.778
C12:	165.812	0.800
C13:	0.000	0.000
Total Sample:	104.161	0.722

National Institute for Petroleum and Energy Research  
 Detailed Hydrocarbon Analysis ( P.I.A.N.O. )

File: C:\CP\DATA1\041593CO.02R  
 Sample: Consol  
 Method: !CUT3PIAN  
 Processed 244 Peaks  
 93GL342  
 IBP-380°F

Analyzed: 04-15-1993 13:14:07  
 Reported: 04-28-1993 10:18:55  
 DHA DBase File: RI-NIPER.DBF  
 Normalized to 100.00%

Composite Report

Totals by Group Type & Carbon Number  
 (in Volume Percent)

	Paraffins:	I-paraffins:	Aromatics:	Naphthenes:	Olefins:	Total:
C1:	0.000	0.000	0.000	0.000	0.000	0.000
C2:	0.000	0.000	0.000	0.000	0.000	0.000
C3:	0.001	0.000	0.000	0.000	0.000	0.001
C4:	0.286	0.013	0.000	0.000	0.002	0.301
C5:	2.690	0.771	0.000	1.202	0.063	4.727
C6:	3.612	1.105	0.089	11.553	1.610	17.968
C7:	2.727	2.616	0.428	13.315	0.234	19.321
C8:	3.270	4.143	1.019	8.831	0.543	17.806
C9:	1.646	2.208	2.781	4.400	0.788	11.823
C10:	1.782	6.543	3.402	3.991	1.182	16.900
C11:	1.240	2.185	0.915	1.878	0.157	6.375
C12:	0.056	0.146	0.112	0.527	0.022	0.863
C13:	0.000	0.000	0.000	0.000	0.000	0.000
Total:	17.310	19.731	8.746	45.697	4.601	96.085
Oxygenates:	0.000	Total C14+:	0.000	Total Unknowns:	3.915	
				Grand Total:	100.000	

(in Mole Percent)

	Paraffins:	I-paraffins:	Aromatics:	Naphthenes:	Olefins:	Total:
C1:	0.000	0.000	0.000	0.000	0.000	0.000
C2:	0.000	0.000	0.000	0.000	0.000	0.000
C3:	0.002	0.000	0.000	0.000	0.000	0.002
C4:	0.410	0.018	0.000	0.000	0.003	0.431
C5:	3.367	0.956	0.000	1.843	0.087	6.253
C6:	3.986	1.228	0.145	15.261	1.888	22.508
C7:	2.684	2.581	0.581	14.993	0.248	21.087
C8:	2.901	3.707	1.204	8.808	0.544	17.164
C9:	1.328	1.789	2.911	3.942	0.666	10.637
C10:	1.319	4.853	3.175	3.296	0.878	13.520
C11:	0.851	1.492	0.780	1.405	0.110	4.639
C12:	0.036	0.093	0.089	0.369	0.014	0.601
C13:	0.000	0.000	0.000	0.000	0.000	0.000
Total:	16.886	16.718	8.884	49.915	4.438	96.843
Oxygenates:	0.000	Total C14+:	0.000	Total Unknowns:	3.157	
				Grand Total:	100.000	

National Institute for Petroleum and Energy Research  
 Detailed Hydrocarbon Analysis ( P.I.A.N.O. )

File: C:\CP\DATA1\041593CO.02R  
 Sample: Consol  
 Method: !CUT3PLAN  
 Processed 244 Peaks  
 93GL342  
 IBP-380°F

Analyzed: 04-15-1993 13:14:07  
 Reported: 04-28-1993 10:18:55  
 DHA DBase File: RI-NIPER.DBF  
 Normalized to 100.00%

Boiling Point Distribution Data

	Wt. Percent Off: deg.C.:	Percent Off: deg.F.:	Vol. Percent Off: deg.C.:	Percent Off: deg.F.:
IBP (0.5%)	27.84	82.11	27.84	82.11
5.0%	58.60	137.48	49.25	120.65
10.0%	71.80	161.24	68.73	155.71
15.0%	80.72	177.30	80.72	177.30
20.0%	80.72	177.30	80.72	177.30
25.0%	91.85	197.33	91.72	197.10
30.0%	100.93	213.67	98.42	209.16
35.0%	100.93	213.67	100.93	213.67
40.0%	103.47	218.25	100.93	213.67
45.0%	118.93	246.07	118.54	245.37
50.0%	125.68	258.22	125.68	258.22
55.0%	130.96	267.73	130.96	267.73
60.0%	140.50	284.90	136.20	277.16
65.0%	150.82	303.48	144.43	291.97
70.0%	160.41	320.74	154.79	310.62
75.0%	162.01	323.62	161.20	322.16
80.0%	171.30	340.34	171.30	340.34
85.0%	174.15	345.47	174.15	345.47
90.0%	182.01	359.62	181.14	358.05
95.0%	189.52	373.14	189.52	373.14
FBP (99.5%) >	216.30	421.34	213.40	416.12

Research Octane Number = 74.81  
 (Calculated from Individual Component Values)

Contribution to Total by:

Paraffins: 5.65  
 Iso-paraffins: 14.01  
 Aromatics: 9.75  
 Naphthenes: 38.14  
 Olefins: 3.77  
 Oxygenates: 0.00

National Institute for Petroleum and Energy Research

Detailed Hydrocarbon Analysis ( P.I.A.N.O. )

File: C:\CP\DATA1\041593CO.02R  
 Sample: Consol  
 Method: !CUT3PIAN  
 Processed 244 Peaks  
 93GL342  
 IBP-380°F

Analyzed: 04-15-1993 13:14:07  
 Reported: 04-28-1993 10:18:55  
 DHA DBase File: RI-NIPER.DBF  
 Normalized to 100.00%  
 COMPONENT KEY:  
 ? = Unknown, I = Isoparaffin  
 N = Naphthene, O = Olefin  
 A = Aromatic

Components Listed in Chromatographic Order

Min.	INDEX	Component	Wt%	Vol%	Mol%
6.493	300.5	Propane	0.001	0.001	0.002
6.940	360.2	i-Butane	0.010	0.013	0.018
7.220	389.4	Butene-1	0.002	0.002	0.003
7.333	400.0	n-Butane	0.219	0.286	0.410
8.793	472.7	i-Pentane	0.634	0.771	0.956
9.213	487.9	Pentene-1	0.008	0.009	0.012
9.427	494.9	2-Methylbutene-1	0.006	0.007	0.009
9.587	500.0	n-Pentane	2.235	2.690	3.367
9.867	507.3	t-Pentene-2	0.019	0.022	0.029
10.187	515.1	c-Pentene-2	0.009	0.010	0.014
10.373	519.4	2-Methylbutene-2	0.008	0.010	0.013
12.080	552.8	Cyclopentene	0.006	0.005	0.009
12.247	555.6	4-Methylpentene-1	0.004	0.004	0.005
12.340	557.2	3-Methylpentene-1	0.006	0.007	0.008
12.720	563.2	Cyclopentane	1.189	1.202	1.843
12.800	564.4	2,3-Dimethylbutane	0.119	0.136	0.150
13.060	568.3	4-Methyl-t-pentene-2	1.255	1.404	1.621
14.087	582.6	3-Methylpentane	0.854	0.969	1.078
14.473	587.5	2-Methylpentene-1	0.006	0.007	0.008
14.560	588.6	Hexene-1	0.009	0.010	0.011
15.527	600.0	n-Hexane	3.160	3.612	3.986
15.980	605.2	t-Hexene-2	0.025	0.028	0.033
16.200	607.6	2-Methylpentene-2	0.015	0.016	0.019
16.393	609.7	3-Methylcyclopentene	0.008	0.008	0.011
16.507	610.9	3-Methyl-c-pentene-2	0.005	0.005	0.006
16.927	615.3	c-Hexene-2	0.005	0.005	0.006
17.567	621.7	3-Methyl-t-pentene-2	0.013	0.014	0.017
18.273	628.4	Methylcyclopentane	2.998	3.018	3.872
18.720	632.4	2,4-Dimethylpentane	0.052	0.058	0.056
20.273	645.4	3,4-Dimethylpentene-1	0.007	0.008	0.008
21.107	651.9	1-Methylcyclopentene	0.014	0.013	0.018
21.287	653.2	Benzene	0.104	0.089	0.145
21.740	656.6	2-Methyl-c-hexene-3	0.009	0.010	0.010
21.907	657.8	3,3-Dimethylpentane	0.015	0.016	0.016
22.380	661.1	Cyclohexane	8.817	8.535	11.388
23.780	670.5	2-Methylhexane	0.776	0.862	0.842
23.987	671.8	2,3-Dimethylpentane	0.226	0.245	0.245
24.360	674.2	1,1-Dimethylcyclopentane	0.056	0.056	0.062
24.713	676.3	Cyclohexene	0.095	0.088	0.125
25.067	678.5	3-Methylhexane	1.162	1.274	1.260
25.973	683.8	1c,3-Dimethylcyclopentane	0.464	0.469	0.513
26.400	686.3	1t,3-Dimethylcyclopentane	0.446	0.451	0.494
26.647	687.6	3-Ethylpentane	0.149	0.161	0.161
26.827	688.6	1t,2-Dimethylcyclopentane	0.724	0.726	0.801
28.433	697.2	t-Heptene-3	0.013	0.014	0.015
28.673	698.4	c-Heptene-3	0.027	0.029	0.030

28.987	700.0	n-Heptane	2.474	2.727	2.684
29.840	705.9	t-Heptene-2	0.033	0.035	0.037
30.580	710.9	O13	0.012	0.013	0.013
31.187	714.9	c-Heptene-2	0.008	0.009	0.009
31.327	715.8	2,3-Dimethylpentene-2	0.009	0.009	0.010
31.600	717.6	3-Ethylcyclopentene	0.007	0.007	0.008
32.160	721.1	Methylcyclohexane	10.837	10.615	11.998
32.753	724.8	2,2-Dimethylhexane	0.057	0.062	0.055
34.273	733.8	Ethylcyclopentane	1.015	0.998	1.124
34.600	735.7	2,2,3-Trimethylpentane	0.059	0.063	0.057
34.913	737.5	2,4-Dimethylhexane	0.152	0.164	0.145
35.153	738.9	O17	0.014	0.015	0.016
35.853	742.7	1c,2t,4-Trimethylcyclopentane	0.214	0.211	0.207
37.160	749.8	1t,2c,3-Trimethylcyclopentane	0.183	0.179	0.177
37.873	753.5	2,3,4-Trimethylpentane	0.016	0.017	0.015
38.540	756.9	Toluene	0.492	0.428	0.581
39.720	762.8	2,3-Dimethylhexane	0.146	0.154	0.139
39.927	763.8	1,1,2-Trimethylcyclopentane	0.067	0.065	0.065
40.353	765.8	O25	0.083	0.085	0.092
40.913	768.5	2-Methylheptane	0.644	0.695	0.613
41.187	769.8	4-Methylheptane	0.303	0.324	0.289
41.460	771.0	3-Methyl-3-ethylpentane	0.036	0.038	0.035
41.927	773.2	1c,2c,4-Trimethylcyclopentane	0.093	0.092	0.090
42.373	775.2	3-Methylheptane	0.482	0.514	0.458
42.553	776.0	3-Ethylhexane	1.999	2.111	1.903
42.920	777.7	1t,4-Dimethylcyclohexane	0.484	0.478	0.469
44.027	782.5	1,1-Dimethylcyclohexane	0.051	0.049	0.049
44.860	786.1	2,2,5-Trimethylhexane	0.359	0.382	0.304
45.327	788.1	1c,3-Ethylmethylcyclopentane	0.332	0.326	0.321
45.587	789.2	Octene-1	0.551	0.543	0.544
46.020	791.0	1,1-Methylethylcyclopentane	0.029	0.028	0.028
46.647	793.5	1t,2-Dimethylcyclohexane	0.817	0.793	0.791
47.940	798.7	1c,2c,3-Trimethylcyclopentane	0.036	0.035	0.035
48.273	800.0	n-Octane	3.048	3.270	2.901
49.600	807.2	I1	0.020	0.021	0.017
49.967	809.2	i-Propylcyclopentane	0.131	0.127	0.126
51.553	817.5	N1	0.011	0.011	0.011
52.667	823.2	2,3,4-Trimethylhexane	0.185	0.189	0.157
53.147	825.6	N2	0.021	0.020	0.020
54.227	830.9	1c,2-Dimethylcyclohexane	0.547	0.518	0.530
55.013	834.7	2,4-Dimethylheptane	0.011	0.012	0.009
55.647	837.7	n-Propylcyclopentane	5.901	5.728	5.716
56.147	840.1	1c,3c,5-Trimethylcyclohexane	0.240	0.235	0.206
56.480	841.7	2-Methyl-4-ethylhexane	0.052	0.054	0.044
56.973	843.9	1,1,3-Trimethylcyclohexane	0.238	0.233	0.205
57.560	846.6	1,1,4-Trimethylcyclohexane	0.023	0.023	0.020
57.747	847.5	3,3-Dimethylheptane	0.087	0.090	0.073
58.260	849.8	2,5-Dimethylheptane	0.065	0.068	0.055
58.567	851.2	N5	0.072	0.070	0.070
58.953	852.9	N6	0.064	0.061	0.062
59.873	857.0	N8	0.043	0.042	0.042
60.200	858.4	Ethylbenzene	0.282	0.245	0.289
60.540	859.8	1c,2t,4t-Trimethylcyclohexane	0.294	0.284	0.254
60.953	861.6	2-Methyloctene-1	0.106	0.117	0.094
61.387	863.5	N8	0.060	0.058	0.052
62.120	866.6	m-Xylene	0.231	0.201	0.236
62.347	867.5	p-Xylene	0.235	0.206	0.241
62.960	870.1	2,3-Dimethylheptane	0.166	0.173	0.141
63.267	871.3	N10	0.054	0.052	0.046
63.387	871.8	4-Ethylheptane	0.119	0.125	0.101
63.507	872.3	?	0.066	0.069	0.056

64.013	874.4	4-Methyloctane	0.232	0.243	0.197
64.240	875.3	2-Methyloctane	0.261	0.275	0.221
64.680	877.1	3-Ethylheptane	0.074	0.076	0.062
65.227	879.3	?	0.221	0.229	0.187
65.520	880.4	3-Methyloctane	0.441	0.461	0.374
65.807	881.5	3,3-Diethylpentane	0.039	0.039	0.033
66.073	882.6	1,1,2-Trimethylcyclohexane	0.056	0.053	0.048
66.500	884.3	o-Xylene	0.428	0.367	0.439
67.513	888.2	N12	0.363	0.351	0.312
67.693	888.9	N13	1.329	1.284	1.145
68.113	890.5	t-2-Methyloctene-3	0.375	0.362	0.323
68.620	892.4	Nonene-1	0.102	0.112	0.088
68.893	893.4	i-Butylcyclopentane	0.175	0.169	0.151
69.960	897.4	c-Nonene-3	0.037	0.041	0.033
70.327	898.7	2,3-Dimethylheptene-2	0.089	0.099	0.080
70.680	900.0	n-Nonane	1.567	1.646	1.328
71.087	903.2	3,7-Dimethyloctene-1	1.100	1.182	0.878
71.600	907.2	N18	0.217	0.207	0.187
72.460	913.8	c-Nonene-2	0.055	0.057	0.049
72.867	916.9	N20	0.321	0.306	0.276
73.247	919.8	i-Propylcyclohexane	0.526	0.494	0.453
73.667	923.0	I11	0.103	0.107	0.079
73.933	925.0	2,2-Dimethyloctane	0.084	0.088	0.064
74.193	926.9	N21	0.050	0.048	0.043
74.667	930.4	N22	0.267	0.254	0.230
75.013	933.0	2,6-Dimethyloctane	3.075	3.185	2.349
75.680	937.9	n-Butylcyclopentane	0.365	0.350	0.314
75.907	939.5	I13	0.082	0.084	0.062
76.240	942.0	I14	0.039	0.041	0.030
76.407	943.2	3,3-Dimethyloctane	0.375	0.382	0.286
76.773	945.8	N24	0.037	0.035	0.029
76.887	946.6	?	0.068	0.064	0.053
77.173	948.7	n-Propylbenzene	0.164	0.143	0.148
77.300	949.6	3,6-Dimethyloctane	0.139	0.143	0.107
77.473	950.8	3-Methyl-5-ethylheptane	0.145	0.150	0.111
77.647	952.1	?	0.071	0.074	0.054
77.887	953.8	?	0.090	0.093	0.069
78.407	957.4	1-Methyl-3-ethylbenzene	1.280	1.116	1.158
78.653	959.2	1-Methyl-4-ethylbenzene	0.228	0.199	0.206
79.073	962.1	2,3-Dimethyloctane	0.190	0.194	0.145
79.340	963.9	1,3,5-Trimethylbenzene	0.028	0.024	0.025
79.467	964.8	I15	0.278	0.284	0.213
79.727	966.6	N27	0.080	0.075	0.062
79.933	968.0	I16	0.063	0.064	0.048
80.033	968.7	I17	0.116	0.118	0.089
80.247	970.2	5-Methylnonane	0.221	0.227	0.169
80.567	972.4	2-Methylnonane	0.206	0.214	0.157
80.667	973.1	1-Methyl-2-ethylbenzene	0.148	0.127	0.134
80.953	975.0	3-Ethyloctane	0.074	0.076	0.057
81.067	975.8	N28	0.030	0.028	0.023
81.353	977.7	3-Methylnonane	0.467	0.480	0.357
81.733	980.3	N29	0.131	0.123	0.101
82.093	982.7	I18	0.055	0.056	0.042
82.613	986.2	1,2,4-Trimethylbenzene	0.905	0.778	0.818
82.720	986.9	t-Butylcyclohexane	2.640	2.477	2.046
82.960	988.5	i-Butylcyclohexane	0.602	0.570	0.467
83.200	990.1	I21	0.166	0.169	0.127
83.507	992.1	I22	0.227	0.231	0.173
84.020	995.4	I24/2,3-Dimethyloctene-2	0.247	0.251	0.189
84.213	996.7	1t-Methyl-2-n-propylcyclohexan	0.250	0.236	0.194
84.480	998.4	i-Butylbenzene	0.049	0.043	0.040

84.607	999.3	sec-Butylbenzene	0.262	0.229	0.212
84.720	1000.0	n-Decane	1.726	1.782	1.319
85.147	1004.3	I26	0.171	0.174	0.119
85.240	1005.2	?	0.227	0.231	0.158
85.440	1007.2	N31	0.630	0.594	0.444
85.800	1010.8	1,2,3-Trimethylbenzene	0.466	0.393	0.422
86.267	1015.5	1-Methyl-4-i-propylbenzene	0.496	0.436	0.402
86.953	1022.2	I28	0.080	0.082	0.056
87.053	1023.2	I29	0.383	0.390	0.267
87.393	1026.5	sec-Butylcyclohexane	0.483	0.447	0.374
87.673	1029.3	?	0.029	0.027	0.023
87.967	1032.1	3-Ethylnonane	0.082	0.083	0.057
88.167	1034.1	?/33	1.104	1.118	0.768
88.573	1038.0	I31	0.242	0.247	0.168
88.887	1041.0	1,3-Diethylbenzene	1.000	0.872	0.810
89.067	1042.7	1-Methyl-3-n-propylbenzene	0.242	0.212	0.196
89.187	1043.9	?	0.475	0.416	0.385
89.513	1047.0	1,4-Diethylbenzene	0.258	0.225	0.209
89.713	1048.9	?	0.251	0.219	0.203
89.907	1050.7	n-Butylbenzene	0.226	0.198	0.183
90.187	1053.4	1,2-Diethylbenzene	0.072	0.062	0.058
90.433	1055.7	N34	0.457	0.431	0.322
90.600	1057.3	N35	0.906	0.853	0.638
90.853	1059.7	1-Methyl-2-n-propylbenzene	0.400	0.345	0.324
91.067	1061.7	I35	0.139	0.142	0.097
91.293	1063.8	I36	0.074	0.076	0.052
91.393	1064.7	I37	0.105	0.107	0.073
91.760	1068.1	I38	0.519	0.529	0.361
91.907	1069.5	1,4-Dimethyl-2-ethylbenzene	0.139	0.119	0.112
92.107	1071.3	s-C5Bz / 1,3-DM-4-EtBz	0.125	0.110	0.092
92.200	1072.2	?	0.193	0.169	0.141
92.413	1074.1	?	0.142	0.125	0.104
92.713	1076.9	1,2-Dimethyl-4-ethylbenzene	0.554	0.477	0.448
93.020	1079.7	I41	0.058	0.059	0.040
93.347	1082.7	1,3-Dimethyl-2-ethylbenzene	0.015	0.012	0.012
93.520	1084.3	?	0.009	0.007	0.007
93.660	1085.5	I42	0.026	0.026	0.018
93.813	1086.9	I43	0.266	0.271	0.185
94.220	1090.6	Undecene-1	0.157	0.157	0.110
94.427	1092.5	1-Methyl-4-t-butylbenzene	0.363	0.322	0.266
94.813	1095.9	1,2-Dimethyl-3-ethylbenzene	0.136	0.115	0.110
95.113	1098.6	?	0.247	0.209	0.200
95.267	1100.0	n-Undecane	1.224	1.240	0.851
95.640	1104.3	?	0.065	0.066	0.045
95.900	1107.2	1,2,4,5-Tetramethylbenzene	0.006	0.005	0.005
96.327	1112.0	1,2,3,5-Tetramethylbenzene	0.022	0.018	0.018
96.560	1114.7	?	0.202	0.171	0.163
96.887	1118.3	?	0.108	0.092	0.088
97.027	1119.9	?	0.122	0.104	0.099
97.373	1123.8	1-t-Butyl-2-methylbenzene	0.020	0.017	0.015
97.893	1129.6	?	0.028	0.023	0.020
98.053	1131.3	?	0.240	0.203	0.176
98.167	1132.6	?	0.118	0.100	0.086
98.360	1134.7	I43	0.044	0.044	0.028
98.713	1138.6	1-Ethyl-2-n-propylbenzene	0.245	0.207	0.179
98.893	1140.6	2-Methylindan	0.040	0.034	0.033
99.020	1142.0	1-Methyl-3-n-butylbenzene	0.230	0.194	0.168
99.393	1146.1	1,3-Di-i-propylbenzene	0.122	0.103	0.082
99.600	1148.3	s-Pentylbenzene	0.012	0.010	0.009
99.873	1151.3	n-Pentylbenzene	0.024	0.020	0.018
100.027	1153.0	1t-M-2-(4-MP)cyclopentane	0.559	0.527	0.369

100.487	1158.0	?	0.016	0.015	0.010
100.767	1161.0	?	0.026	0.025	0.017
100.953	1163.0	?	0.023	0.022	0.015
101.333	1167.1	1,2,3,4-Tetrahydronaphthalene	0.031	0.024	0.025
101.780	1171.8	Naphthalene	0.012	0.009	0.010
101.953	1173.7	I44	0.019	0.019	0.012
102.247	1176.8	I45	0.017	0.017	0.011
102.613	1180.7	I46	0.043	0.043	0.027
102.793	1182.6	?	0.013	0.013	0.008
103.200	1186.9	I48	0.023	0.023	0.015
103.533	1190.3	Dodecene-1	0.022	0.022	0.014
103.960	1194.8	?	0.014	0.014	0.009
104.460	1200.0	n-Dodecane	0.056	0.056	0.036
105.140	1208.5	?	0.018	0.018	0.012
105.853	1217.3	1t-Butyl-4-ethylbenzene	0.011	0.009	0.007

National Institute for Petroleum and Energy Research

Detailed Hydrocarbon Analysis ( P.I.A.N.O. )

File: C:\CP\DATA1\042893CO.02R  
 Sample: 93GL342  
 Method: !CUT3PLAN  
 Processed 216 Peaks  
 CONSOL  
 IBP-380°F after Washing

Analyzed: 04-28-1993 13:02:42  
 Reported: 04-29-1993 10:56:59  
 DHA DBase File: RI-NIPER.DBF  
 Normalized to 100.00%

Composite Report  
 Totals by Group Type & Carbon Number  
 (in Weight Percent)

	Paraffins:	I-paraffins:	Aromatics:	Naphthenes:	Olefins:	Total:
C1:	0.000	0.000	0.000	0.000	0.000	0.000
C2:	0.000	0.000	0.000	0.000	0.000	0.000
C3:	0.000	0.000	0.000	0.000	0.000	0.000
C4:	0.027	0.000	0.000	0.000	0.002	0.029
C5:	1.068	0.237	0.000	0.771	0.000	2.077
C6:	2.505	0.732	0.090	11.730	1.035	16.092
C7:	2.396	2.244	0.442	14.764	0.286	20.133
C8:	3.079	3.869	1.445	9.368	0.568	18.330
C9:	1.666	2.175	3.431	4.749	0.737	12.758
C10:	1.858	6.823	4.045	4.563	1.165	18.454
C11:	1.300	2.107	0.979	3.275	0.164	7.825
C12:	0.065	0.091	0.114	0.633	0.030	0.932
C13:	0.000	0.000	0.000	0.000	0.000	0.000
Total:	13.964	18.279	10.546	49.853	3.988	96.629
Oxygenates:	0.000		Total C14+:	0.000	Total Unknowns:	3.371
					Grand Total:	100.000

Molecular Weight and Specific Gravity Data

Group:	Ave. Mw.:	Ave. Rel. Density:
C1:	0.000	0.000
C2:	0.000	0.000
C3:	0.000	0.000
C4:	57.996	0.580
C5:	71.389	0.665
C6:	84.510	0.741
C7:	98.498	0.747
C8:	112.399	0.754
C9:	125.058	0.781
C10:	139.555	0.773
C11:	154.333	0.780
C12:	165.627	0.800
C13:	0.000	0.000
Total Sample:	107.088	0.734

National Institute for Petroleum and Energy Research

Detailed Hydrocarbon Analysis ( P.I.A.N.O. )

File: C:\CP\DATA1\042893CO.02R  
 Sample: 93GL342  
 Method: !CUT3PLAN  
 Processed 216 Peaks  
 CONSOL  
 IBP-380°F after Washing

Analyzed: 04-28-1993 13:02:42  
 Reported: 04-29-1993 10:56:59  
 DHA DBase File: RI-NIPER.DBF  
 Normalized to 100.00%

Composite Report

Totals by Group Type & Carbon Number  
 (in Volume Percent)

	Paraffins:	I-paraffins:	Aromatics:	Naphthenes:	Olefins:	Total:
C1:	0.000	0.000	0.000	0.000	0.000	0.000
C2:	0.000	0.000	0.000	0.000	0.000	0.000
C3:	0.000	0.000	0.000	0.000	0.000	0.000
C4:	0.036	0.000	0.000	0.000	0.002	0.038
C5:	1.296	0.291	0.000	0.786	0.000	2.373
C6:	2.886	0.837	0.078	11.546	1.148	16.496
C7:	2.663	2.488	0.388	14.630	0.299	20.468
C8:	3.330	4.149	1.264	9.174	0.565	18.481
C9:	1.764	2.295	2.988	4.602	0.760	12.409
C10:	1.934	7.083	3.543	4.317	1.263	18.140
C11:	1.328	2.163	0.856	3.110	0.166	7.623
C12:	0.065	0.092	0.097	0.601	0.030	0.885
C13:	0.000	0.000	0.000	0.000	0.000	0.000
Total:	15.302	19.398	9.213	48.768	4.233	96.914

Oxygenates: 0.000      Total C14+: 0.000      Total Unknowns: 3.086  
 Grand Total: 100.000

(in Mole Percent)

	Paraffins:	I-paraffins:	Aromatics:	Naphthenes:	Olefins:	Total:
C1:	0.000	0.000	0.000	0.000	0.000	0.000
C2:	0.000	0.000	0.000	0.000	0.000	0.000
C3:	0.000	0.000	0.000	0.000	0.000	0.000
C4:	0.052	0.000	0.000	0.000	0.004	0.056
C5:	1.641	0.365	0.000	1.218	0.000	3.224
C6:	3.221	0.941	0.128	15.446	1.366	21.103
C7:	2.650	2.482	0.532	16.663	0.324	22.652
C8:	2.987	3.754	1.509	9.252	0.572	18.073
C9:	1.439	1.880	3.163	4.169	0.654	11.306
C10:	1.447	5.314	3.341	3.605	0.948	14.655
C11:	0.922	1.494	0.733	2.352	0.118	5.619
C12:	0.042	0.059	0.078	0.425	0.020	0.624
C13:	0.000	0.000	0.000	0.000	0.000	0.000
Total:	14.402	16.288	9.483	53.132	4.006	97.310

Oxygenates: 0.000      Total C14+: 0.000      Total Unknowns: 2.690  
 Grand Total: 100.000

National Institute for Petroleum and Energy Research  
 Detailed Hydrocarbon Analysis ( P.I.A.N.O. )

File: C:\CP\DATA1\042893CO.02R  
 Sample: 93GL342  
 Method: !CUT3PIAN  
 Processed 216 Peaks  
 CONSOL  
 IBP-380°F after Washing

Analyzed: 04-28-1993 13:02:42  
 Reported: 04-29-1993 10:56:59  
 DHA DBase File: RI-NIPER.DBF  
 Normalized to 100.00%

Boiling Point Distribution Data

	Wt. Percent Off: deg.C.:	Vol. Percent Off: deg.C.:
	deg.F.:	deg.F.:
IBP (0.5%)	36.06	36.06
5.0%	68.73	68.73
10.0%	80.72	80.72
15.0%	80.72	80.72
20.0%	91.72	90.05
25.0%	100.93	98.42
30.0%	100.93	100.93
35.0%	100.93	100.93
40.0%	117.65	113.73
45.0%	124.09	121.53
50.0%	130.96	125.68
55.0%	130.96	130.96
60.0%	144.43	143.00
65.0%	150.82	150.82
70.0%	160.41	160.41
75.0%	166.50	164.34
80.0%	171.30	171.30
85.0%	176.12	174.15
90.0%	182.01	181.14
95.0%	189.52	189.52
FBP (99.5%)	205.40	205.40
	401.72	401.72

Research Octane Number = 75.21  
 (Calculated from Individual Component Values)

Contribution to Total by:  
 Paraffins: 4.85  
 Iso-paraffins: 13.69  
 Aromatics: 10.27  
 Naphthenes: 40.21  
 Olefins: 3.49  
 Oxygenates: 0.00

National Institute for Petroleum and Energy Research

Detailed Hydrocarbon Analysis ( P.I.A.N.O. )

File: C:\CP\DATA1\042893CO.02R  
 Sample: 93GL342  
 Method: !CUT3PLAN  
 Processed 216 Peaks  
 CONSOL  
 IBP-380°F after Washing

Analyzed: 04-28-1993 13:02:42  
 Reported: 04-29-1993 10:56:59  
 DHA DBase File: RI-NIPER.DBF  
 Normalized to 100.00%  
 COMPONENT KEY:  
 ? = Unknown, I = Isoparaffin  
 N = Naphthalene, O = Olefin  
 A = Aromatic

Components Listed in Chromatographic Order

Min.	INDEX	Component	Wt%	Vol%	Mol%
7.247	392.0	Butene-1	0.002	0.002	0.004
7.333	400.0	n-Butane	0.027	0.036	0.052
8.780	472.5	i-Pentane	0.237	0.291	0.365
9.573	500.0	n-Pentane	1.068	1.296	1.641
12.687	563.2	Cyclopentane	0.771	0.786	1.218
12.767	564.4	2,3-Dimethylbutane	0.077	0.088	0.099
13.033	568.4	4-Methyl-t-pentane-2	0.910	1.026	1.198
14.053	582.7	3-Methylpentane	0.655	0.749	0.842
14.547	589.0	Hexene-1	0.022	0.024	0.029
15.480	600.0	n-Hexane	2.505	2.886	3.221
17.940	625.8	2,2-Dimethylpentane	0.008	0.009	0.009
18.220	628.4	Methylcyclopentane	2.497	2.534	3.288
18.660	632.4	2,4-Dimethylpentane	0.054	0.060	0.059
21.033	651.8	1-Methylcyclopentene	0.013	0.013	0.018
21.233	653.3	Benzene	0.090	0.078	0.128
22.333	661.2	Cyclohexane	9.233	9.012	12.158
23.707	670.5	2-Methylhexane	0.735	0.823	0.813
23.913	671.8	2,3-Dimethylpentane	0.213	0.233	0.236
24.293	674.2	1,1-Dimethylcyclopentane	0.060	0.060	0.067
24.640	676.3	Cyclohexene	0.090	0.085	0.122
24.993	678.5	3-Methylhexane	1.094	1.210	1.210
25.900	683.8	1c,3-Dimethylcyclopentane	0.448	0.457	0.506
26.327	686.3	1t,3-Dimethylcyclopentane	0.436	0.445	0.492
26.573	687.6	3-Ethylpentane	0.140	0.152	0.155
26.753	688.6	1t,2-Dimethylcyclopentane	0.708	0.716	0.799
27.227	691.2	?	0.019	0.020	0.022
27.440	692.4	1,5-Heptadiene	0.021	0.022	0.025
27.640	693.5	O12	0.026	0.029	0.030
27.840	694.5	?	0.017	0.018	0.019
28.020	695.5	3-Methyl-c-hexene-3	0.019	0.020	0.021
28.907	700.0	n-Heptane	2.396	2.663	2.650
31.020	714.4	c-Heptene-2	0.023	0.025	0.026
31.233	715.7	2,3-Dimethylpentene-2	0.021	0.021	0.023
32.107	721.3	Methylcyclohexane	12.082	11.932	13.637
32.673	724.8	2,2-Dimethylhexane	0.047	0.051	0.045
33.127	727.5	O14	0.023	0.024	0.026
33.340	728.8	O15	0.017	0.017	0.019
34.213	733.9	Ethylcyclopentane	1.030	1.021	1.162
34.520	735.7	2,2,3-Trimethylpentane	0.102	0.109	0.099
34.847	737.6	2,4-Dimethylhexane	0.158	0.171	0.153
35.060	738.8	O17	0.012	0.013	0.014
35.780	742.8	1c,2t,4-Trimethylcyclopentane	0.206	0.205	0.203
37.107	749.9	1t,2c,3-Trimethylcyclopentane	0.193	0.191	0.191
38.473	756.9	Toluene	0.442	0.388	0.532
39.660	762.8	2,3-Dimethylhexane	0.144	0.153	0.139
39.873	763.9	1,1,2-Trimethylcyclopentane	0.072	0.071	0.071

40.300	765.9	025	0.124	0.128	0.140
40.847	768.5	2-Methylheptane	0.640	0.697	0.621
41.127	769.8	4-Methylheptane	0.256	0.276	0.248
41.840	773.1	1c,2c,4-Trimethylcyclopentane	0.093	0.092	0.091
42.300	775.2	3-Methylheptane	0.515	0.554	0.499
42.460	775.9	3-Ethylhexane	2.008	2.138	1.948
42.847	777.7	1t,4-Dimethylcyclohexane	0.492	0.490	0.486
43.967	782.6	1,1-Dimethylcyclohexane	0.054	0.052	0.053
44.780	786.1	2,2,5-Trimethylhexane	0.370	0.397	0.320
45.247	788.0	1c,3-Ethylmethylcyclopentane	0.339	0.336	0.335
45.513	789.1	Octene-1	0.568	0.565	0.572
45.940	790.9	1,1-Methylethylcyclopentane	0.034	0.033	0.034
46.560	793.4	1t,2-Dimethylcyclohexane	0.892	0.874	0.881
47.880	798.7	1c,2c,3-Trimethylcyclopentane	0.026	0.026	0.026
48.213	800.0	n-Octane	3.079	3.330	2.987
49.893	809.1	i-Propylcyclopentane	0.135	0.132	0.134
51.487	817.5	N1	0.008	0.008	0.008
52.593	823.1	2,3,4-Trimethylhexane	0.169	0.173	0.146
53.073	825.5	N2	0.017	0.016	0.017
54.147	830.8	1c,2-Dimethylcyclohexane	0.576	0.549	0.569
54.960	834.7	2,4-Dimethylheptane	0.023	0.024	0.019
55.567	837.6	n-Propylcyclopentane	6.097	5.967	6.021
56.073	840.0	1c,3c,5-Trimethylcyclohexane	0.217	0.214	0.191
56.447	841.7	2-Methyl-4-ethylhexane	0.031	0.032	0.027
56.913	843.9	1,1,3-Trimethylcyclohexane	0.235	0.231	0.206
57.700	847.5	3,3-Dimethylheptane	0.065	0.068	0.056
58.220	849.8	2,5-Dimethylheptane	0.055	0.059	0.048
58.493	851.0	N5	0.089	0.087	0.088
58.827	852.5	N6	0.008	0.008	0.008
58.893	852.8	?	0.058	0.056	0.057
59.807	856.8	N8	0.038	0.037	0.038
60.167	858.4	Ethylbenzene	0.291	0.255	0.304
60.513	859.9	1c,2t,4t-Trimethylcyclohexane	0.293	0.285	0.257
60.913	861.6	2-Methyloctene-1	0.108	0.120	0.098
61.367	863.5	N8	0.072	0.070	0.063
62.087	866.6	m-Xylene	0.268	0.235	0.279
62.320	867.5	p-Xylene	0.409	0.361	0.427
62.940	870.1	2,3-Dimethylheptane	0.279	0.292	0.241
63.360	871.8	N10	0.252	0.246	0.222
63.493	872.4	?	0.111	0.108	0.097
63.987	874.4	4-Methyloctane	0.273	0.288	0.236
64.213	875.3	2-Methyloctane	0.298	0.317	0.258
64.653	877.1	3-Ethylheptane	0.092	0.097	0.080
65.207	879.3	?	0.244	0.255	0.211
65.500	880.4	3-Methyloctane	0.476	0.502	0.411
65.767	881.5	3,3-Diethylpentane	0.044	0.045	0.038
66.053	882.6	1,1,2-Trimethylcyclohexane	0.061	0.058	0.053
66.493	884.3	o-Xylene	0.477	0.412	0.498
67.507	888.2	N12	0.399	0.389	0.350
67.680	888.9	N13	1.373	1.337	1.205
68.093	890.5	t-2-Methyloctene-3	0.392	0.381	0.344
68.600	892.4	Nonene-1	0.062	0.091	0.072
68.867	893.4	i-Butylcyclopentane	0.060	0.058	0.052
70.307	898.7	c-Nonene-3	0.090	0.100	0.082
70.667	900.0	n-Nonane	1.666	1.764	1.439
71.080	903.2	3,7-Dimethyloctene-1	1.165	1.263	0.948
71.593	907.2	N18	0.230	0.222	0.202
72.447	913.8	c-Nonene-2	0.065	0.067	0.059
72.847	916.9	N20	0.337	0.324	0.296
73.227	919.7	i-Propylcyclohexane	0.551	0.522	0.484
73.653	923.0	I11	0.094	0.098	0.073

73.927	925.0	2,2-Dimethyloctane	0.068	0.071	0.053
74.660	930.5	N22	0.281	0.270	0.246
74.993	932.9	2,6-Dimethyloctane	3.218	3.360	2.506
75.667	937.9	n-Butylcyclopentane	0.388	0.376	0.341
75.893	939.5	I13	0.071	0.073	0.055
76.220	941.9	I14	0.041	0.043	0.032
76.407	943.2	3,3-Dimethyloctane	0.398	0.409	0.310
76.767	945.8	N24	0.037	0.036	0.030
76.867	946.6	?	0.072	0.068	0.057
77.167	948.7	n-Propylbenzene	0.203	0.179	0.188
77.467	950.8	3-Methyl-5-ethylheptane	0.139	0.145	0.108
77.653	952.2	?	0.055	0.058	0.043
77.893	953.9	?	0.035	0.036	0.027
78.393	957.4	1-Methyl-3-ethylbenzene	1.348	1.185	1.243
78.647	959.2	1-Methyl-4-ethylbenzene	0.243	0.214	0.224
79.067	962.1	2,3-Dimethyloctane	0.202	0.209	0.198
79.460	964.8	I15	0.332	0.341	0.258
79.713	966.6	N27	0.087	0.083	0.069
79.933	968.1	I16	0.072	0.074	0.056
80.027	968.8	I17	0.125	0.128	0.097
80.240	970.2	5-Methylnonane	0.247	0.256	0.192
80.567	972.5	2-Methylnonane	0.254	0.265	0.198
80.653	973.0	1-Methyl-2-ethylbenzene	0.212	0.183	0.196
80.953	975.1	3-Ethyloctane	0.224	0.230	0.174
81.207	976.8	N28	0.031	0.029	0.025
81.353	977.8	3-Methylnonane	0.580	0.601	0.452
81.733	980.4	N29	0.166	0.158	0.131
82.093	982.8	I18	0.054	0.056	0.042
82.613	986.2	1,2,4-Trimethylbenzene	0.926	0.804	0.854
82.713	986.9	t-Butylcyclohexane	2.830	2.677	2.236
82.953	988.5	i-Butylcyclohexane	0.641	0.612	0.506
83.193	990.1	I21	0.190	0.195	0.148
83.507	992.1	I22	0.259	0.266	0.202
84.013	995.5	I24/2,3-Dimethyloctene-2	0.255	0.262	0.198
84.213	996.8	1t-Methyl-2-n-propylcyclohexan	0.252	0.239	0.199
84.473	998.4	i-Butylbenzene	0.046	0.041	0.038
84.607	999.3	sec-Butylbenzene	0.242	0.213	0.200
84.713	1000.0	n-Decane	1.858	1.934	1.447
85.147	1004.4	I26	0.185	0.190	0.131
85.233	1005.2	?	0.247	0.253	0.175
85.447	1007.4	N31	0.685	0.650	0.492
85.813	1011.0	1,2,3-Trimethylbenzene	0.498	0.423	0.459
86.267	1015.5	1-Methyl-4-i-propylbenzene	0.528	0.468	0.436
87.053	1023.3	I29	0.351	0.360	0.249
87.407	1026.7	sec-Butylcyclohexane	0.518	0.484	0.409
87.680	1029.4	?	0.027	0.025	0.021
87.967	1032.2	3-Ethylnonane	0.094	0.096	0.067
88.167	1034.1	N33	1.185	1.126	0.851
88.580	1038.1	I31	0.262	0.269	0.186
88.887	1041.1	1,3-Diethylbenzene	1.069	0.940	0.882
89.067	1042.8	1-Methyl-3-n-propylbenzene	0.259	0.229	0.214
89.187	1043.9	?	0.516	0.455	0.426
89.513	1047.0	1,4-Diethylbenzene	0.269	0.237	0.222
89.713	1048.9	?	0.252	0.222	0.208
89.900	1050.7	n-Butylbenzene	0.210	0.185	0.173
90.207	1053.6	1,2-Diethylbenzene	0.066	0.057	0.054
90.433	1055.7	N34	0.473	0.449	0.340
90.607	1057.4	N35	0.932	0.885	0.670
90.853	1059.7	1-Methyl-2-n-propylbenzene	0.411	0.358	0.339
91.073	1061.7	I35	0.135	0.139	0.096
91.293	1063.8	I36	0.077	0.079	0.054

91.393	1064.7	I37	0.106	0.109	0.075
91.753	1068.1	I38	0.349	0.564	0.389
91.907	1069.5	1,4-Dimethyl-2-ethylbenzene	0.152	0.132	0.126
92.100	1071.3	s-C5Bz / 1,3-DM-4-EtBz	0.150	0.133	0.112
92.200	1072.2	?	0.190	0.168	0.142
92.427	1074.3	?	0.158	0.139	0.118
92.720	1077.0	1,2-Dimethyl-4-ethylbenzene	0.591	0.514	0.488
93.033	1079.8	I41	0.071	0.073	0.051
93.213	1081.5	?	0.016	0.017	0.011
93.527	1084.3	?	0.012	0.012	0.008
93.660	1085.6	I42	0.026	0.027	0.018
93.820	1087.0	I43	0.250	0.256	0.177
94.227	1090.7	Undecene-1	0.164	0.166	0.118
94.433	1092.5	1-Methyl-4-t-butylbenzene	0.386	0.345	0.288
94.827	1096.1	1,2-Dimethyl-3-ethylbenzene	0.143	0.122	0.118
95.120	1098.7	?	0.267	0.227	0.220
95.267	1100.0	n-Undecane	1.300	1.328	0.922
95.633	1104.2	?	0.073	0.075	0.052
95.907	1107.3	1,2,4,5-Tetramethylbenzene	0.009	0.008	0.007
96.327	1112.0	1,2,3,5-Tetramethylbenzene	0.024	0.021	0.020
96.560	1114.6	?	0.213	0.182	0.176
96.913	1118.6	?	0.116	0.099	0.096
97.027	1119.9	?	0.144	0.123	0.119
97.367	1123.7	1-t-Butyl-2-methylbenzene	0.038	0.033	0.029
97.893	1129.5	?	0.035	0.030	0.026
98.053	1131.3	?	0.252	0.215	0.189
98.167	1132.6	?	0.102	0.087	0.076
98.373	1134.8	I43	0.021	0.021	0.014
98.707	1138.5	1-Ethyl-2-n-propylbenzene	0.162	0.138	0.121
98.900	1140.6	2-Methylindan	0.016	0.013	0.013
99.027	1142.0	1-Methyl-3-n-butylbenzene	0.191	0.163	0.143
99.387	1146.0	1,3-Di-1-propylbenzene	0.097	0.083	0.066
99.607	1148.4	s-Pentylbenzene	0.009	0.008	0.007
99.900	1151.5	n-Pentylbenzene	0.026	0.022	0.020
100.033	1153.0	1t-M-2-(4-MP)cyclopentane	0.633	0.601	0.425
100.480	1157.8	?	0.036	0.034	0.024
100.767	1160.9	?	0.036	0.034	0.024
100.953	1162.9	?	0.022	0.021	0.015
101.340	1167.1	1,2,3,4-Tetrahydronaphthalene	0.017	0.013	0.014
101.800	1172.0	Naphthalene	0.009	0.007	0.008
101.960	1173.7	I44	0.013	0.014	0.009
102.633	1180.8	I45	0.039	0.039	0.025
103.207	1186.8	I48	0.018	0.018	0.012
103.533	1190.2	Dodecene-1	0.030	0.030	0.020
103.960	1194.7	?	0.017	0.017	0.011
104.473	1200.0	n-Dodecane	0.065	0.065	0.042
105.147	1208.4	?	0.030	0.030	0.019
105.887	1217.6	1t-Butyl-4-ethylbenzene	0.017	0.014	0.011

**APPENDIX C**  
**HC22 MASS SPECTROMETRIC DATA**

IIT RESEARCH INSTITUTE  
NATIONAL INSTITUTE FOR PETROLEUM AND ENERGY RESEARCH  
P.O. BOX 2128, BARTLESVILLE, OK 74008

MASS SPECTROMETRY LABORATORY

22-COMPONENT HYDROCARBON TYPE ANALYSIS

CLIENT: CONSOL  
P.O. NO.

NIPER ACCT. NO: B06761

SAMPLE: 04263B. 4/26/93. HC22 ANALYSIS OF CONSOL 380-510 DEG F DIST  
AVERAGE RESULTS FROM SCANS 18, 19, 20

		AVE	LV %	SDEV	AVE	WT %	SDEV
SATURATES							
C(N)H(2N+2)	PARAFFINS		9.6	0.4		8.2	0.3
C(N)H(2N)	MONOCYCLOPARAFFINS		19.4	0.2		17.8	0.2
C(N)H(2N-2)	DICYCLOPARAFFINS		20.8	0.5		20.7	0.5
C(N)H(2N-4)	TRICYCLOPARAFFINS		8.7	0.2		9.2	0.2
C(N)H(2N-6)	TETRACYCLOPARAFFINS		0.0	0.0		0.0	0.0
C(N)H(2N-8)	PENTACYCLOPARAFFINS		0.0	0.0		0.0	0.0
C(N)H(2N-10)	HEXACYCLOPARAFFINS		0.0	0.0		0.0	0.0
C(N)H(2N-12)	HEPTACYCLOPARAFFINS		0.0	0.0		0.0	0.0
	TOTAL SATURATES		58.5	0.7		55.9	0.8
MONOAROMATICS							
C(N)H(2N-6)	ALKYLBENZENES		10.2	0.2		10.0	0.2
C(N)H(2N-8)	BENZOCYCLOPARAFFINS		19.4	0.8		20.9	0.8
C(N)H(2N-10)	BENZODICYCLOPARAFFINS		4.9	0.3		5.2	0.3
DIAROMATICS							
C(N)H(2N-12)	NAPHTHALENES		7.0	0.2		8.0	0.2
C(N)H(2N-14)			0.0	0.0		0.0	0.0
C(N)H(2N-16)			0.0	0.0		0.0	0.0
TRIAROMATICS							
C(N)H(2N-18)			0.0	0.0		0.0	0.0
C(N)H(2N-22)			0.0	0.0		0.0	0.0
TETRAAROMATICS							
C(N)H(2N-24)			0.0	0.0		0.0	0.0
C(N)H(2N-28)			0.0	0.0		0.0	0.0
	TOTAL AROMATICS		41.4	0.7		44.0	0.7
SULFUR COMPOUNDS							
C(N)H(2N-4)S	THIOPHENES		0.0	0.0		0.0	0.0
C(N)H(2N-10)S	BENZOTHIOPHENES		0.0	0.0		0.0	0.0
C(N)H(2N-16)S	DIBENZOTHIOPHENES		0.0	0.0		0.0	0.0
C(N)H(2N-22)S	NAPHTHOBENZOTHIOPHENES		0.0	0.0		0.0	0.0
	TOTAL THIOPHENIC COMPOUNDS		0.0	0.0		0.0	0.0

CONTINUED ON PAGE 2

CLIENT: CONSOL  
P.O. NO.

NIPER ACCT. NO: B06761

SAMPLE: 04263B. 4/26/93. HC22 ANALYSIS OF CONSOL 380-510 DEG F DIST  
AVERAGE RESULTS FROM SCANS 18, 19, 20

CONTINUATION FROM PAGE 1:

	AVG	SDEV
CARBON NUMBER	12.9	----
MOLECULAR WEIGHT	177.2	----
<b>ELEMENTAL ANALYSIS:</b>		
	WT %	SDEV
C	87.6	0.0
H	12.4	0.0
THIOPHENIC S	0.0	0.0
<b>N-D-M CARBON TYPE:</b>		
	PCT	SDEV
AROMATIC	21.4	0.4
NAPHTHENIC	43.6	0.1
PARAFFINIC	35.0	0.3
<b>N-D-M RING TYPE:</b>		
	NO.	SDEV
AROMATIC	0.5	0.0
NAPHTHENIC	1.2	0.0

NOTE: THIS METHOD DETERMINES LISTED COMPOUND TYPES IN NONOLEFINIC HYDROCARBON FRACTIONS WITH AVERAGE CARBON NUMBERS BETWEEN 12 AND 36 (BOILING RANGE FROM 350 TO 1050 DEG F) AND HAVING LESS THAN 5 MOLE % TOTAL OF COMPOUNDS CONTAINING OXYGEN, NITROGEN, AND SULFUR.

<sup>1</sup> Data calculated from the average molecular weight and HC22 results for comparison with n-d-M analysis results. The true n-d-M method (ASTM D 3238) calculates the values based on refractive index (n), density (d), and average molecular weight data.

IIT RESEARCH INSTITUTE  
 NATIONAL INSTITUTE FOR PETROLEUM AND ENERGY RESEARCH  
 P.O. BOX 2128, BARTLESVILLE, OK 74005

## MASS SPECTROMETRY LABORATORY

## 22-COMPONENT HYDROCARBON TYPE ANALYSIS

CLIENT: CONSOL  
 P.O. NO.

NIPER ACCT. NO: B06761

SAMPLE: 04303C. 4/30/93. HC22 ANAL. OF CONSOL 380-510 CAUSTIC WASHED  
 AVERAGE RESULTS FROM SCANS 16, 17, 18

		AVE	LV %	SDEV	AVE	WT %	SDEV
SATURATES							
C(N)H(2N+2)	PARAFFINS		9.1	0.7		7.8	0.6
C(N)H(2N)	MONOCYCLOPARAFFINS		19.6	0.5		18.0	0.5
C(N)H(2N-2)	DICYCLOPARAFFINS		20.3	0.3		20.2	0.3
C(N)H(2N-4)	TRICYCLOPARAFFINS		9.1	0.4		9.5	0.4
C(N)H(2N-6)	TETRACYCLOPARAFFINS		0.0	0.0		0.0	0.0
C(N)H(2N-8)	PENTACYCLOPARAFFINS		0.0	0.0		0.0	0.0
C(N)H(2N-10)	HEXACYCLOPARAFFINS		0.0	0.0		0.0	0.0
C(N)H(2N-12)	HEPTACYCLOPARAFFINS		0.0	0.0		0.0	0.0
	TOTAL SATURATES		58.1	0.8		55.4	0.8
MONOAROMATICS							
C(N)H(2N-6)	ALKYLBENZENES		9.8	0.2		9.6	0.2
C(N)H(2N-8)	BENZOCYCLOPARAFFINS		20.2	0.5		21.8	0.6
C(N)H(2N-10)	BENZODICYCLOPARAFFINS		4.7	0.4		5.1	0.4
DIAROMATICS							
C(N)H(2N-12)	NAPHTHALENES		7.1	0.4		8.0	0.4
C(N)H(2N-14)			0.0	0.0		0.0	0.0
C(N)H(2N-16)			0.0	0.0		0.0	0.0
TRIAROMATICS							
C(N)H(2N-18)			0.0	0.0		0.0	0.0
C(N)H(2N-22)			0.0	0.0		0.0	0.0
TETRAAROMATICS							
C(N)H(2N-24)			0.0	0.0		0.0	0.0
C(N)H(2N-28)			0.0	0.0		0.0	0.0
	TOTAL AROMATICS		41.9	0.7		44.5	0.8
SULFUR COMPOUNDS							
C(N)H(2N-4)S	THIOPHENES		0.0	0.0		0.0	0.0
C(N)H(2N-10)S	BENZOTHIOPHENES		0.0	0.0		0.0	0.0
C(N)H(2N-16)S	DIBENZOTHIOPHENES		0.0	0.0		0.0	0.0
C(N)H(2N-22)S	NAPHTHOBENZOTHIOPHENES		0.0	0.0		0.0	0.0
	TOTAL THIOPHENIC COMPOUNDS		0.0	0.0		0.0	0.0

CONTINUED ON PAGE 2

CLIENT: CONSOL  
P.O. NO.

NIPER ACCT. NO: B06761

SAMPLE: 04303C. 4/30/93. HC22 ANAL. OF CONSOL 380-510 CAUSTIC WASHED  
AVERAGE RESULTS FROM SCANS 16, 17, 18

CONTINUATION FROM PAGE 1:

	AVG	SDEV
CARBON NUMBER	12.9	---
MOLECULAR WEIGHT	177.2	---
<b>ELEMENTAL ANALYSIS:</b>		
	WT %	SDEV
C	87.7	0.1
H	12.3	0.1
THIOPHENIC S	0.0	0.0
<b>N-D-M CARBON TYPE:</b>		
	PCT	SDEV
AROMATIC	21.7	0.5
NAPHTHENIC	43.9	0.5
PARAFFINIC	34.5	0.5
<b>N-D-M RING TYPE:</b>		
	NO.	SDEV
AROMATIC	0.5	0.0
NAPHTHENIC	1.2	0.0

NOTE: THIS METHOD DETERMINES LISTED COMPOUND TYPES IN NONOLEFINIC HYDROCARBON FRACTIONS WITH AVERAGE CARBON NUMBERS BETWEEN 12 AND 36 (BOILING RANGE FROM 350 TO 1050 DEG F) AND HAVING LESS THAN 5 MOLE % TOTAL OF COMPOUNDS CONTAINING OXYGEN, NITROGEN, AND SULFUR.

<sup>1</sup> Data calculated from the average molecular weight and HC22 results for comparison with n-d-M analysis results. The true n-d-M method (ASTM D 3238) calculates the values based on refractive index (n), density (d), and average molecular weight data.

IIT RESEARCH INSTITUTE  
NATIONAL INSTITUTE FOR PETROLEUM AND ENERGY RESEARCH  
P.O. BOX 2128, BARTLESVILLE, OK 74005

## MASS SPECTROMETRY LABORATORY

## 22-COMPONENT HYDROCARBON TYPE ANALYSIS

CLIENT: CONSOL  
P.O. NO.

NIPER ACCT. NO: B06761

SAMPLE: 04263C. 4/26/93. HC22 ANALYSIS OF CONSOL 510-638 DEG F DIST  
AVERAGE RESULTS FROM SCANS 19, 20, 21

		AVE	LV %	SDEV	AVE	WT %	SDEV
<b>SATURATES</b>							
C(N)H(2N+2)	PARAFFINS	10.1	0.2	8.4	0.2		
C(N)H(2N)	MONOCYCLOPARAFFINS	11.2	0.5	9.9	0.4		
C(N)H(2N-2)	DICYCLOPARAFFINS	9.9	0.4	9.3	0.4		
C(N)H(2N-4)	TRICYCLOPARAFFINS	9.6	0.1	9.6	0.1		
C(N)H(2N-6)	TETRACYCLOPARAFFINS	7.2	0.5	7.2	0.5		
C(N)H(2N-8)	PENTACYCLOPARAFFINS	0.0	0.0	0.0	0.0		
C(N)H(2N-10)	HEXACYCLOPARAFFINS	0.0	0.0	0.0	0.0		
C(N)H(2N-12)	HEPTACYCLOPARAFFINS	0.0	0.0	0.0	0.0		
	<b>TOTAL SATURATES</b>	47.9	0.2	44.4	0.2		
<b>MONOAROMATICS</b>							
C(N)H(2N-6)	ALKYLBENZENES	3.5	0.2	3.2	0.2		
C(N)H(2N-8)	BENZOCYCLOPARAFFINS	10.6	0.1	10.7	0.1		
C(N)H(2N-10)	BENZODICYCLOPARAFFINS	12.7	0.2	12.9	0.2		
<b>DIAROMATICS</b>							
C(N)H(2N-12)	NAPHTHALENES	9.3	0.2	9.9	0.2		
C(N)H(2N-14)		8.3	0.2	9.5	0.2		
C(N)H(2N-16)		7.4	0.0	8.8	0.1		
<b>TRIAROMATICS</b>							
C(N)H(2N-18)		0.0	0.0	0.0	0.1		
C(N)H(2N-22)		0.0	0.0	0.0	0.0		
<b>TETRAAROMATICS</b>							
C(N)H(2N-24)		0.0	0.0	0.0	0.0		
C(N)H(2N-28)		0.0	0.0	0.0	0.0		
	<b>TOTAL AROMATICS</b>	51.8	0.2	55.1	0.2		
<b>SULFUR COMPOUNDS</b>							
C(N)H(2N-4)S	THIOPHENES	0.0	0.0	0.0	0.0		
C(N)H(2N-10)S	BENZOTHIOPHENES	0.3	0.1	0.4	0.1		
C(N)H(2N-16)S	DIBENZOTHIOPHENES	0.0	0.0	0.0	0.0		
C(N)H(2N-22)S	NAPHTHOBENZOTHIOPHENES	0.0	0.0	0.0	0.0		
	<b>TOTAL THIOPHENIC COMPOUNDS</b>	0.3	0.1	0.4	0.1		

CONTINUED ON PAGE 2

CLIENT: CONSOL  
P.O. NO.

NIPER ACCT. NO: B06761

SAMPLE: 04263C. 4/26/93. HC22 ANALYSIS OF CONSOL 510-638 DEG F DIST  
AVERAGE RESULTS FROM SCANS 19, 20, 21

CONTINUATION FROM PAGE 1:

	AVG	SDEV
CARBON NUMBER	15.3	----
MOLECULAR WEIGHT	210.6	----
<b>ELEMENTAL ANALYSIS:</b>		
	WT %	SDEV
C	88.3	0.0
H	11.6	0.0
THIOPHENIC S	0.1	0.0
<b>N-D-M CARBON TYPE:</b>		
	PCT	SDEV
AROMATIC	26.7	0.2
NAPHTHENIC	41.3	0.3
PARAFFINIC	31.9	0.2
<b>N-D-M RING TYPE:</b>		
	NO.	SDEV
AROMATIC	0.8	0.0
NAPHTHENIC	1.2	0.0

NOTE: THIS METHOD DETERMINES LISTED COMPOUND TYPES IN NONOLEFINIC HYDROCARBON FRACTIONS WITH AVERAGE CARBON NUMBERS BETWEEN 12 AND 36 (BOILING RANGE FROM 350 TO 1050 DEG F) AND HAVING LESS THAN 5 MOLE % TOTAL OF COMPOUNDS CONTAINING OXYGEN, NITROGEN, AND SULFUR.

<sup>1</sup> Data calculated from the average molecular weight and HC22 results for comparison with n-d-M analysis results. The true n-d-M method (ASTM D 3238) calculates the values based on refractive index (n), density (d), and average molecular weight data.

**APPENDIX D**  
**JFTOT THERMAL STABILITY DATA**

JFTOT test of samples: 93GL342, 380-510F and 93GL342-5

Test procedure: ASTM D3241, "Standard Test Method for Thermal Stability of Aviation Turbine Fuels (JFTOT Procedure)"

The test conditions were those listed in Paragraph 4.5.2.1.1 of MIL-T-5624P, "Military Specification, Turbine Fuel, Aviation, Grades JP-4, JP-5, and JP-5/JP-8ST".

Test Conditions: Heater tube temperature: 260°C (500°F)  
Fuel system pressure: 3.45 MPa (500 psig)  
Fuel flow rate: 3.0 mL/minute  
Test duration: 150 minutes

The requirements for jet fuel are:

Maximum heater tube rating is less than code 3 (faint brown stain).  
Heater tube shows neither peacock nor abnormal deposit.  
Maximum pressure drop across test filter is 25 mm mercury.

Test results:

Both samples failed the JFTOT thermal stability test by a wide margin.

Sample: 93GL342, 380-510°F:

Heater tube rating: > > 4 (heavy black deposit)  
Filter pressure drop: 0.0 mm

Sample: 93GL342-5

Heater tube rating: 4P (P = peacock colors)  
Filter pressure drop: > 125 mm

(Filter pressure drop reached 25 mm at about 100 minutes. The pressure drop reached 125 mm at 136 minutes; bypass valve was opened and test was continued to 150 minutes.)

**COAL LIQUEFACTION PROCESS STREAM CHARACTERIZATION AND EVALUATION**

**Analysis of Coal-Derived Synthetic Crude from HRI Run CMSL-2**

**Final Report**

**Prepared by:**

**IIT RESEARCH INSTITUTE  
National Institute for Petroleum and Energy Research  
P.O. Box 2128  
Bartlesville, OK 74005**

**Gene P. Sturm, Jr.  
Je Kim  
Johanna Shay**

**Prepared for:**

**CONSOL Inc.  
Research and Development  
4000 Brownsville Road  
Library, PA 16129**

**F. P. Burke  
R. A. Winschel  
S. D. Brandes**

**December 1993**

## TABLE OF CONTENTS

	Page
<b>LIST OF TABLES</b>	ii
1. EXECUTIVE SUMMARY	1
2. EXPERIMENTAL	3
3. EXPERIMENTAL RESULTS	11
4. ASSESSMENT OF DATA QUALITY AND APPLICABILITY OF METHODS	12
5. ASSESSMENT OF PRODUCT QUALITY	14
6. REFERENCES	18
APPENDIX A CHROMATOGRAM from	
APPENDIX B ASTM D 2887 SIMULATED DISTILLATION DETAILED GAS CHROMATOGRAPHIC	23
APPENDIX C ANALYSIS DATA (PIANO)	27
APPENDIX D HC22 MASS SPECTROMETRIC DATA	35
APPENDIX E ASTM D 86 DISTILLATION CURVES	42

## TABLES

<u>Table</u>	<u>Page</u>
I. Chemical and Physical Property Data	19
II. ASTM D 86 Distillation Results, Temperature Readings Corrected to 101.3 kPa (760 mm Hg Pressure)	20
III. ASTM D 2887 Simulated Distillation Data	21
IV. ASTM D 2892 Distillation	22

## 1. EXECUTIVE SUMMARY

CONSOL Inc. is conducting a program to aid in the advancement of direct coal liquefaction process development under contract from the U.S. Department of Energy (Contract DE-AC22-89PC89883). In this program, a number of research laboratories, including the IIT Research Institute, National Institute for Petroleum and Energy Research (NIPER), are analyzing direct coal liquefaction-derived materials under subcontract from CONSOL. NIPER recently investigated the properties of a synthetic crude oil produced by HRI, Inc. in Catalytic Multi-Stage Liquefaction (CMSL) Run-2. The results of that investigation are presented in this report.

The main objective of HRI's Run CMSL-2, also called Run 227-78, was to investigate the effect of a high coal concentration on process performance. In this continuous two-stage liquefaction run the higher coal concentration in the coal-solvent slurries was accomplished by lowering the solvent-to-coal ratio from 1.2 (to as high as 1.6) used in previous bench-scale runs, to a value of 0.9 in CMSL-2. The feed coal was Illinois No. 6, Burning Star 2, bituminous coal. Throughout Run CMSL-2 the first- and second-stage reactors were operated catalytically; Shell S-317 Ni/Mo on alumina catalyst was present in both reactors. No on-line hydrotreater was used in the run. The net product sample analyzed in this subcontract was produced by compositing a total of 10, one-half gallon sample aliquots obtained during periods 8 through 12 of the run from the Separator Overhead process stream and the Atmospheric Still Overhead process stream.

The composite coal-derived synthetic crude was distilled by ASTM Method D 2892 in a preliminary run to produce an IBP-180° F distillate (2.8 weight percent), a 180-350° F distillate (19.6 weight percent), and a 350-400° F distillate (7.9 weight percent). A subsequent large scale distillation by a slightly modified ASTM D 2892 procedure was made in an attempt to produce a sufficient quantity of the 350-400° F distillate for testing. This distillation produced an IBP-350° F distillate (25.1 weight percent), a 350-400° F distillate (5.6 weight percent), a 400-550° F distillate (35.2 weight percent), and a > 550° F residue

(34.1 weight percent). Losses amounted to only 0.62 weight percent. A portion of the 350-400° F distillate cut was subjected to a caustic wash procedure to remove phenolic compounds (1.1 weight percent) and produce an additional fraction. The total sample, the three distillate fractions, the resid, and the caustic washed fraction were characterized by a total of approximately 130 chemical and physical property tests using ASTM, UOP, and other standard and published methods developed for petroleum and petroleum products.

The coal liquid product quality was briefly assessed by comparison of the physical and chemical property test data for the appropriate fraction against the specifications for gasolines, aviation turbine fuels, diesel fuels or fuel oils. However, it should be noted that these specifications apply to finished fuels which are normally comprised of blends of various refinery streams along with additives and thus do not even apply strictly to straight run petroleum distillates, let alone coal liquid distillates.

The IBP-180° F and 180-350° F fractions from the preliminary distillation were tested for specific gravity (API gravity was calculated). Unless otherwise noted, all subsequent tests were run on the distillate fractions from the large scale modified D 2892 distillation.

The IBP-350° F distillate fraction failed the corrosion and octane tests, and exceeded the maximum temperature for the 50% point in the distillation specification test. However, the 190-380° F portion of a petroleum crude is normally processed by catalytic reforming before blending into gasoline. This coal liquid distillate may need further processing to remove olefins before becoming suitable for reforming.

The 350-400° F distillate fraction passed many of the specification tests for aviation turbine fuels although some important specification tests including aromatic content, smoke point, density, and luminometer number were not met. The caustic washed 350-400° F distillate fraction showed a significant improvement in mercaptan content and some other minor improvements.

The 400-550° F distillate fraction met most of the specifications for diesel fuel and heating fuel oils although the cetane index calculated met the specification only for Grade No. 4-D diesel fuel oil and the 90% off distillation temperature was slightly below the minimum specified for grade 2-D diesel fuel. The >550° F resid met the specifications for a number 4 fuel oil.

Overall, the coal liquid might benefit from further hydroprocessing. In particular, conversion of aromatics to naphthenes or blending with a suitable low-aromatic blending stock would be necessary to produce an acceptable product for aviation turbine fuel.

## 2. EXPERIMENTAL

Following instructions from CONSOL, the coal liquid sample was prepared by blending the entire contents of two individual containers received from CONSOL and designated by HRI as Atmospheric Still Overheads (ASOH) 227-78- 8, 9, 11, 12 (LO#6251) and Separator Overheads (SOH) 227-78- 8, 9, 11, 12 (LO#6250). The net weight of the Atmospheric Still Overheads and the Separator Overheads were reported as 10.66 Kg and 10.87 Kg, respectively. A 3.259 Kg portion of the blended coal-derived synthetic crude was distilled by ASTM D 2892 to produce an IBP-180° F distillate (2.8 weight percent), a 180-350° F distillate (19.6 weight percent), a 350-400° F distillate (7.9 weight percent), and a resid. Specific gravity determinations were made on the IBP-180° F and 180-350° F distillate fractions. In order to maximize the quantity of the 350-400° F distillate fraction for testing, a subsequent large scale distillation was made using the bulk of the remaining coal liquid. In this distillation, a 16.7 Kg portion of the blended synthetic crude was distilled by a slightly modified ASTM D 2892 procedure to produce an IBP-350° F distillate, a 350-400° F distillate, a 400-550° F distillate, and a >550° F resid. Unless otherwise specified, all subsequent tests were performed on the fractions produced in this large scale distillation. Also, a portion of the 350-400° F distillate was subjected to a caustic wash procedure to remove phenolic compounds and produce a caustic-washed fraction, with yields listed in table

## I.

Experimental methods used in the analysis of this coal-derived synthetic crude and its fractions were standard ASTM or UOP methods, as noted along with the experimental results in table I, with some minor exceptions as discussed later in this section. Brief descriptions of the methods follow:

### 2.1 Gravity

Specific gravities were measured by a Mettler/Paar DMA45 at 60° F according to ASTM D 4052, Density and Relative Density of Liquids by Digital Density Meter. API gravities were calculated from the specific gravities.

### 2.2 Elemental Analysis

Carbon and Hydrogen were determined with a Perkin Elmer Model 240C. The procedure used is that described in ASTM D 5291, Standard Test Method for the Instrumental Determination of Carbon, Hydrogen, and Nitrogen in Petroleum Products and Lubricants.

Sulfur contents were measured according to method ASTM D 3120, Trace Quantities of Sulfur in Light Liquid Petroleum Hydrocarbons by Oxidative Microcoulometry, using a Mitsubishi TOX-10 microcoulometer.

Nitrogen values for fractions up to 550° F were measured by an Antek 730C according to ASTM D 4629, Trace Nitrogen in Liquid Petroleum Hydrocarbons by Oxidative Combustion and Chemiluminescence Detection. A modified ASTM D 4629 procedure (1) was used for the >550° F resid.

Basic nitrogen values were determined by UOP 269, Nitrogen Bases in Hydrocarbons by Potentiometric Titration, using a Brinkmann 636 Titroprocessor.

Mercaptan Sulfur contents were measured by UOP 163, Hydrogen Sulfide and Mercaptan

## **Sulfur in Liquid Hydrocarbons by Potentiometric Titration.**

### **2.3 Trace Metals**

**V, Ni, Fe, and Cu were determined by ASTM D 5185 by Inductive Coupled Plasma Atomic Emission Spectroscopy (ICP-AES), usng an AR<sup>1</sup>, Maxim I instrument. Scandium (5 ppm, Conostan) was used as an internal standard.**

### **2.4 Ash**

**Ash contents were determined by ASTM D 482, Ash from Petroleum Products.**

### **2.5 Viscosity**

**Kinematic Viscosities were measured according to ASTM D 445, Kinematic Viscosity of Transparent and Opaque Liquids.**

### **2.6 Freezing Point**

**Freezing points were measured by ASTM D 2386, Freezing Point of Aviation Fuels.**

### **2.7 Cloud Point**

**Cloud points were determined by ASTM D 2500, Cloud Point of Petroleum Products.**

### **2.8 Pour Point**

**Pour points were measured according to ASTM D97, Pour Points of Petroleum Products.**

## **2.9 Reid Vapor Pressure**

Vapor Pressures were measured by ASTM D 5191, Vapor Pressure of Petroleum Products (Mini Method). The measured total pressures were converted to a Reid Vapor Pressure Equivalent (RVPE) by use of a correlation equation. A Grabner Instruments Model CCA-VPS was used for the measurements.

## **2.10 Micro Carbon Residue**

Carbon residues were determined on the total distillate and the fractions distilling above 400° F by ASTM D 4530, Micro Carbon Residue of Petroleum Products. This test provides results equivalent to the Conradson Carbon Residue (D189), while offering advantages such as better control of test conditions and small sample size.

## **2.11 Flash Point**

Flash points were measured by ASTM D 56, Flash Point by Tag Closed Tester (350-400° F fraction) and ASTM D 93, Flash Point by Pensky-Martens Closed Tester (400-550° F fraction).

## **2.12 Heptane Insolubles**

Asphaltene content in the total distillate was measured by ASTM D 3279, n-Heptane Insolubles.

## **2.13 Bromine Number and Olefin Content**

Bromine numbers were measured with a Brinkmann 636 Titroprocessor according to ASTM D 1159, Bromine Numbers of Petroleum Distillates and Commercial Aliphatic Olefins by Electrometric Titration. Olefin contents of the 350-400° F and 400-550° F distillate

**fractions were calculated according to Annex A4 of ASTM D 1159.**

#### **2.14 Aniline Point**

**Aniline point was run by Method A, ASTM D 611, Aniline Point and Mixed Aniline Point of Petroleum Products and Hydrocarbon Solvents.**

#### **2.15 Smoke Point**

**Smoke points were measured by ASTM D 1322, Smoke Point of Aviation Turbine Fuels.**

#### **2.16 Acidity**

**Acidities were run by ASTM D 3242, Acidity in Aviation Turbine Fuel.**

#### **2.17 Copper Corrosion**

**Copper corrossions were determined according to ASTM D 130, Detection of Copper Corrosion from Petroleum Products by the Copper Strip Tarnish Test.**

#### **2.18 Existnt Gum**

**Existnt gum was measured and reported as washed existnt gum according to ASTM D 381, Existnt Gum in Fuels by Jet Evaporation. The procedure was modified slightly for the 400-550° F fraction as it was allowed to evaporate for 60 minutes instead of 30 minutes.**

#### **2.19 Oxidation Stability**

**Oxidation stability on the IBP-350° F distillate and the 350-400° F distillate samples were determined by ASTM D 525, Oxidation Stability of Gasoline (Induction Period Method).**

Oxidation stability of the 400-550° F distillate was determined by ASTM D 2274, Oxidation Stability of Distillate Fuel Oil (Accelerated Method).

## 2.20 Thermal Stability

Thermal stability of the 350-400° F distillate sample was not determined due to insufficient sample from the distillation.

## 2.21 Distillation, D 86 and Gas Chromatographic Simulated Distillation and D 2887

Simple atmospheric pressure distillation, ASTM D 86, Distillation of Petroleum Products, was used for the three distillation fractions boiling below 550° F and the >550° F resid. The D 86 distillation data are summarized in table II. The total distillate was analyzed by ASTM D 2887, Determination of Boiling Range Distribution of Hydrocarbon Distillates by Gas Chromatography. The D 2887 simulated distillation data are summarized in table III. The chromatogram is shown in Appendix A.

## 2.22 Distillation, D 2892

Distillation fractions corresponding to IBP-180° F, 180-350° F, 350-400° F, and a resid were prepared by ASTM D 2892. Large scale distillation fractions corresponding to IBP-350° F, 350-400° F, and 400-550° F and a >550° F resid were prepared by a slightly modified ASTM D 2892 procedure. Data from the large scale distillation are summarized in table IV.

## 2.23 Octane Number

Octane numbers were obtained by modified ASTM D 2700 (Motor Method) and D 2699 (Research Method) on the IBP-350° F distillate.

## **2.24 Cetane Index**

**The Cetane Index for the 350-400° F and 400-550° F distillate fractions and the >550° F resid were calculated according to method ASTM D 976.**

## **2.25 Heat of Combustion**

**Heat of combustion was determined by ASTM D 240, Heat of Combustion of Hydrocarbon Fuels by Bomb Calorimeter.**

## **2.26 Luminometer Number**

**Luminometer numbers were determined by ASTM D 740, Luminometer Numbers of Aviation Turbine Fuels.**

## **2.27 Group Analysis**

### **A. Gas Chromatography**

**Detailed Hydrocarbon Analysis according to modified method ASTM D 5134 was performed on the IBP-350° F fraction. In this analysis, (sometimes termed PIANO for paraffins, isoparaffins, aromatics, naphthenes, and olefins) individual components up to tridecane are quantified. Benzene was determined by this method also. A Siemens Sichromat 2 GC with Chrom Perfect and DHA software was used. The results from the PIANO analyses are provided in Appendix B and summarized in table I.**

### **B. Mass Spectrometry**

**Group type analyses of the 350-400° F and 400-550° F distillate fractions was performed by the high resolution mass spectrometric method, HC22, published by Richard Teeter (2). Naphthene content was corrected for olefin content determined by ASTM D 1159 as the**

HC22 method does not distinguish between olefins and naphthenes. Detailed results are given in Appendix C and are summarized in table I.

### C. Naphthalenes by UV Spectroscopy

Naphthalenes were determined in the 350-400° F distillate by ASTM D 1840, Naphthalene Hydrocarbons in Aviation Turbine Fuels by Ultraviolet Spectrophotometry. Data are given in table I.

#### 2.28 Caustic Washing and Phenol Recovery

The caustic wash and phenol recovery procedure is described below:

The following procedure is written for the caustic wash of a single 1,700 g aliquot of sample. The procedure can be linearly scaled to accomplish caustic washing of smaller or larger samples.

Changes were made in the caustic wash procedure used in the analysis of the Run CMSL-2 samples from that which was used for the Run CC-15 sample analyzed in a previous project. This was done to decrease the large volume of acid solution needed for neutralization and to decrease the heat generated and the time required for the procedure. Any loss in extraction efficiency should be more than compensated by the extra extraction which was added.

Equipment: Separatory funnel (4 L bottle for mixing vessel)

Vacuum rotary evaporator

Supplies: 6 wt% NaOH solution

Concentrated HCl

Dichloromethane ( $\text{CH}_2\text{Cl}_2$ )

Each 1,700 g aliquot of sample to be washed is contacted three times with about 300 mL of NaOH solution. A mechanical shaker or magnetic stirrer should be used for mixing; a separatory funnel is used to separate the two phases. This is followed by two washes with about 200 mL of distilled water. The water-oil mixture is allowed to settle and the water layer is drawn off. (Note: If a stable emulsion forms it can be recovered separately from the oil and water phases and broken by gentle heating.)

#### Phenol Recovery

The collected aqueous phases are combined and acidified with concentrated HCl to a pH of < 5 (about 115 mL is required). This step should be done slowly (to allow for heat dissipation) in an unstoppered container stirred with a magnetic stirrer. The phenols are recovered from the acidified water by washing with three (300 g) aliquots of dichloromethane. If significant color or odor persists after washing, add 100 g NaCl and wash two more times wth dichloromethane. The dichloromethane is evaporated to obtain the phenolic extract.

### 3. EXPERIMENTAL RESULTS

Chemical and physical property test data are listed in table I for the total distillate, IBP-180° F distillate, 180-350° F distillate, IBP-350° F distillate, 350-400° F distillate, 400-550° F distillate and the > 550° F resid. Data for the caustic washed 350-400° F distillate fraction are listed in table I also. Results from D 86 distillations of distillate fractions and simulated distillation of the total distillate are given in tables II and III. D 2892 distillation data are listed in table IV. The chromatogram from the simulated distillation is given in Appendix A.

Group type analysis data by gas chromatography (modified ASTM 5134) are summarized in table I with the complete data included as Appendix B. Similarly, the group type analysis

data determined by mass spectrometry are summarized in table I with the complete data included as Appendix C.

#### 4. ASSESSMENT OF DATA QUALITY AND APPLICABILITY OF METHODS

Application of ASTM and other standard methods along with a quality assurance program which includes analysis of primary standards where available, secondary standards, and regular participation in interlaboratory round robin test studies should assure data quality falls within the statistical parameters associated with the particular tests employed, except for those tests which do not apply well to non-petroleum derived materials. Duplicate determinations are usually made for most tests and the results routinely fall within the published error limits.

A comparison of yields from the small scale standard ASTM D 2892 distillation with those from the large scale modified procedure shows some differences.

D 2892	IBP-350° F: 22.4 wt pct	350-400° F: 7.9 wt pct	Total: 30.3 wt pct
Mod. D 2892	IBP-350° F: 25.0 wt pct	350-400° F: 5.6 wt pct	Total: 30.7 wt pct

The modified procedure involves use of reflux ratios of 1/1, 3/1, and 5/1 as the cut point is approached. This is designed to speed up the distillation while minimizing deviation from the standard D 2892 results. Although the total yield of the IBP-350° F and 350-400° F distillates from the two distillations were nearly equal, the two individual yields differed by more than the reproducibility expected for the standard D 2892 method (1.2 mass percent). The differences could be due to the use of different reflux ratios or differences in pot temperatures and residence times from the different scale of the two distillations. The latter could result in differences in decomposition of the sample. Such decomposition was noted in

the D 86 distillation performed on the 350-400° F fraction.

Almost all of the tests employed in this study were developed for application to petroleum and petroleum products. The applicability of some of the tests to coal-derived liquids is not a simple issue. The physical property tests should apply equally well to coal liquids as to petroleum products in respect to determination of the property. However, in some cases correlation of that property to performance of the material for its intended use may be somewhat different for coal-derived liquid products than for petroleum products. Also, coal liquid samples sometimes present problems in some tests which are not typical for petroleum samples. For example, the initial boiling point detected in the D86 test for the 350-400° F distillate fraction was most likely low due to smoking of the sample which probably resulted from formation of water by decomposition. The potential for inaccuracy is more serious for most of the chemical tests. For example, the methods employed for the group type analyses of the <350° F, 350-400° F, and 400-550° F fractions do not determine oxygenates, nitrogen compound types or all possible sulfur compound types even for petroleum-derived fractions. This is usually not a serious omission for the lighter fractions except for the presence of phenols in the coal-derived light fractions. These limitations can be very important for fractions containing significant quantities of oxygen-, sulfur-, or nitrogen-containing compounds as indicated in the methods. Also, the HC22 mass spectrometric method employed for the 350-400° F and 400-550° F fractions were developed for petroleum-derived materials. The different distributions of isomers and alkyl-substituted homologs within the various compound types between coal liquids (and even atypical petroleum crudes) and conventional petroleum crudes can affect the accuracy of compositional data produced by the HC22 method, the corresponding ASTM methods, and other similar methods.

Some of the ASTM methods, such as D 2274, state they are "not applicable to fuels containing any significant component derived from a nonpetroleum source". For others, such as ASTM D 5134, Detailed Analysis of Petroleum Naphthas Through n-Nonane by Capillary GC, significantly different composition can be a problem for correct peak

identification. For example, an oxygenate co-eluting with a hydrocarbon compound would cause an erroneously high result for that compound. In spite of the problems of applicability, the methods employed in this study are the best (or among the best) available; and in most cases they are the tests required in the specifications for the end use products for which these distillate fractions would ultimately be used, after further processing.

## 5. ASSESSMENT OF PRODUCT QUALITY

Product quality for the <350° F, 350-400° F, and 400-550° F distillate fractions and the >550° F resid will be assessed by comparison of the physical and chemical property test data against the specifications for gasolines (ASTM D 4814), aviation turbine fuels (ASTM D 1655), diesel fuels (ASTM D 975) and fuel oils (ASTM D 396) respectively. It should be noted up front that these specifications apply to finished fuels which are normally comprised of blends of various refining streams along with additives and thus do not even apply directly to straight run petroleum distillates, let alone coal liquid distillates.

### 5.1 Assessment of the IBP-350° F Distillate Fraction

The quality of the IBP-350° F distillate fraction is probably best assessed in terms of specifications for gasoline. The vapor pressure for this distillate fraction falls well below the maximum allowed for all of the vapor pressure/distillation classes of gasolines. In fact, this fraction would need to be blended with some lighter material to meet the minimum requirements for distillation boiling range in terms of the 10% evaporated maximum temperature which ranges from 122-158° F for classes AA-E. Similarly, the 50% off temperature falls outside the range of maximum temperatures for the classes (261° F compared to specifications of 230° F for class E to 250° F for classes AA and A). Finally, the maximum temperature specifications for the 90% off and end points are met by the IBP-350° F distillate fraction. Also, the maximum residue allowed (2%, vol) was met easily, as only 0.7% residue was observed.

Other specification tests which were performed include copper strip corrosion, existent gum, sulfur content, and oxidation stability. The distillate fraction failed the copper strip corrosion test (3b versus 1, maximum). Sulfur content met the specifications (0.01 weight percent versus 0.10, maximum) in spite of the presence of some hydrogen sulfide and failure in the copper strip corrosion test.

The octane number tests gave results considerably below that required for a finished gasoline as would be expected. The octane numbers for petroleum distillates in this boiling range are usually on the order of 60-70. (The close values for the research and motor octane numbers is not at all unusual for straight run distillates from petroleum crudes or coal liquids in our experience.) Typically, light straight-run gasoline, catalytic reformat, catalytically cracked gasoline, hydrocracked gasoline, polymer gasoline, alkylate, and  $\eta$ -butane are blended along with additives to produce a finished gasoline. Generally, the heavy straight-run gasoline fraction (boiling range approximately 190-380° F) is used as feed to the catalytic reformer to produce a 90-100 research octane product (3). Such a process would be necessary for the coal liquid <350° F fraction (or at least the 190-350° F portion) to improve its qualities for gasoline blending, although removal of olefins would be required to make it acceptable as a catalytic reformer feedstock.

## 5.2 Assessment of the 350-400° F Distillate Fraction

The 350-400° F distillate fraction is assessed in terms of specifications for aviation turbine fuels although finished jet fuels are sometimes blended from a variety of refinery streams with the addition of various additives also. Nevertheless, this distillate fraction passed the specification tests for total sulfur content, freezing point, acidity, copper strip corrosion, flash point, density, heat of combustion and distillation final boiling point, residue and loss. Failed tests include aromatic content (28 versus 20 volume percent maximum), smoke point (15.6 versus 20 or 25 mm minimum), and luminometer number (27.3 versus 45 minimum). The high aromatic content of this distillate fraction is probably the most serious deficiency in its potential use as a blending stock for aviation fuel. Hydrogenation or hydrocracking

should improve its properties significantly. Alternatively, blending with a suitable low-aromatic blending stock might be feasible.

### 5.3 Assessment of Caustic Washed 350-400° F Distillate Fraction

The test which showed the most significant improvement after caustic washing of the 380-510° F distillate fraction was the mercaptan sulfur value which decreased from 19 ppm to 6 ppm. Some other properties showed improvement also. The decrease in oxidation stability most likely resulted from removal of hindered phenols, which are known antioxidants, in the caustic washing procedure. Overall, the caustic-washed fraction, although slightly improved for use in blending for jet fuels, is limited by the high aromatic content and related low smoke point.

### 5.4 Assessment of the 400-550° F Distillate Fraction

The quality of the 400-550° distillate fraction is probably best assessed using the specifications for diesel fuel oils and heating fuel oils. In terms of the diesel fuel oil specifications, the distillate meets the flash point, cloud point, distillation, ash, sulfur, and copper strip corrosion tests for all grades and the cetane number for Grade No. 4-D diesel fuel oil, except the 90% off distillation temperature was slightly below the minimum specified for grade 2-D diesel fuel.

In terms of heating oil or fuel oil specifications, the 400-550° F distillate fraction meets the requirements in terms of flash point, pour point, viscosity (for Grade No. 4 light, only), ash, sulfur, and copper strip corrosion.

### 5.5 Assessment of the >550° F Resid

The quality of the >550° F resid fraction is probably best assessed using the specifications for heavy heating oils, although a corresponding petroleum fraction would probably be sent

to a catalytic cracking or hydrocracking unit in most refineries. This fraction meets the specifications for a number 4 fuel oil. The low ash content, low sulfur content, and copper strip corrosion value all meet the specifications for even lighter heating oil grades, indicating good quality in that respect.

## 6. REFERENCES

1. Shay, J. Y., and P. W. Woodward. A Chemiluminescent Method for Determination of Nitrogen Content of Petroleum of Petroleum Residua. American Laboratory, October, 1986 pp 114-123.
2. Teeter, R. M., Mass Spec. Rev., 4, 123 (1985).
3. Gary, J. H. and Handwerk, G. E., PETROLEUM REFINING: Technology and Economics, Marcel Dekker, Inc., New York, N. Y., 1975, Chapter 2.

Table I. - Chemical and Physical Property Data

Date Started \_\_\_\_\_

Date Completed \_\_\_\_\_

Property	Total Dist.	Sample					
		<350° F		350 - 400° F		400 - 550° F	
		<180	>180	before	after washing		
Specific Gravity @ 60° F (D4052) <sup>1</sup>	0.8687	0.7202	0.7654	0.8492	0.8484	0.8892	0.9262
API Gravity (calculated)	31.4	64.9	48.7	35.1	35.3	27.6	21.3
Elemental Analysis, wt. %							
Carbon (D5291)	07.33	65.69	60.76	66.80	67.46	67.80	
Hydrogen (D5291)	12.66	14.24	12.72	13.08	12.27	11.84	
Sulfur (D3120)	0.02	0.01	0.01	0.01	0.01	0.01	
Nitrogen (D4629)	0.03	0.01	0.03	0.02	0.03	0.06	
Basic Nitrogen (UOP289)			0.006	0.023	0.023	0.029	0.031
Mercaptan Sulfur (UOP163), ppm				19.0	6.0		
Trace Metals (D5185), Vanadium, ppm	0.18						0.19
Nickel, ppm	0.14						0.56
Iron, ppm	0.30						2.00
Copper, ppm	0.20						0.18
Ash (D482), wt. %	<0.001					0.001	0.003
Viscosity (D445), cSt							
@ 104° F	2.104					2.503	8.774
@ 210° F	0.9679			0.6653	0.6741	1.056	2.239
@ -20° C			1.764	4.683	4.359		
Freezing Point (D2386), °F	-7			-55	-55		
Cloud Point (D2500), °F				<-60	<-60	-60	
Pour Point (D97), °F	-50			<-60	<-60	-55	10
Reid Vapor Pressure (D5191), psi		2.74	0.02		<0.01		
MicroCarbon Residue (D4530), wt. %	<0.01					<0.01	<0.01
Flash Point (D56, D93), °C				50	57	94.5	
Heptane Insolubles (D3279), wt. %	0.06						
Group Analysis (ASTM D5134 and HC22)							
Paraffins, vol. %		36.9 <sup>2</sup>	7.5	8.0	7.5		
Naphthenes, vol. %		53.9	61.3	61.5	53.0		
Aromatics, vol. %		5.3	28.4	27.8	37.5		
Olefins, vol. %		3.2	2.8	2.5	2.0		
Benzene (PIANO, mod D5134), vol. %		0.198					
Naphthalenes (D1840), vol. %			0.48	0.32			
Bromine Number (D1159)		3.20	3.00	2.71	1.94		
Aniline Point (D611), °F							118.2
Smoke Point (D1322), mm				15.6	15.4		
Acidity (D3242), mg KOH/g	<0.01	<0.01	0.01	<0.01	0.01		
Copper Corrosion (D130)		3b (dark)	1a (slight)	1a (slight)	1a (slight)	1a (slight)	
Existent Gum (D381), mg/100mL <sup>3</sup>		1.0	6.4	6.2	52.6		
Oxidation Stability (D525), min		1440	1440	720			
Oxidation Stability (D2274), mg/100mL						1.0±0.1	
Thermal Stability (JFTOT) (D3341)							
Distillation, ASTM D 2887 and D86							
Distillation, ASTM D2892 Yield, wt. %		Table IV					
Octane Number: Motor Method (D2700)			58.7				
Research Method (D2699)			60.1				
Cetane Index (D976)				20.8		32.7	35.3
Heat of Combustion (D240), Net Btu/lb (MJ/kg)		18,806 (43.3)	18,401 (42.8)	18,411 (42.8)			
Luminometer Number (D1740)		62.9	27.3	27.0			
Caustic Wash & Phenol Recovery, wt. % <sup>4</sup>				W:95.4/P:1.1			

Table II

<sup>1</sup> Specific and API gravities of IBP - 180° F and 180 - 350° F fractions from the standard ASTM D2892 fractions. All other tests run on modified D2892 fractions.

<sup>2</sup> Unknowns from the D5134 analysis of the <350° F distillate = 0.7 volume %.

<sup>3</sup> Washed existent gum.

<sup>4</sup> W = washed distillate, P = phenols recovered, 100 - W - P = percent lost in the procedure (3.5 wt. %).

**Table II. - ASTM D 86 Distillation Results, Temperature Readings  
Corrected to 101.3 kPa (760 mm Hg) Pressure**

Sample	<350° F		350 - 400° F		400 - 550° F		>550° F	
	Barometric Pressure (mm Hg)		748		743		739	
	°F	°C	°F	°C	°F	°C	°F	°C
Initial Boiling Point	158.9	70.5	322.7	161.5	434.8	223.8	580.4	304.7
5% recovered	188.6	87.0	362.1	183.4	457.7	236.5	592.3	311.3
10% recovered	204.2	95.7	365.9	185.5	461.6	238.7	595.4	313.0
20% recovered	221.1	105.1	368.2	186.8	466.3	241.3	596.3	313.5
30% recovered	234.3	112.4	370.0	187.8	473.5	245.3	600.2	315.7
40% recovered	246.2	119.0	372.5	189.2	480.5	249.2	603.8	317.7
50% recovered	261.1	127.3	375.2	190.7	486.6	252.6	609.6	320.9
60% recovered	276.9	136.1	378.1	192.3	494.9	257.2	615.5	324.2
70% recovered	295.5	146.4	381.3	194.1	504.5	262.5	623.4	328.6
80% recovered	312.9	156.1	385.3	196.3	513.3	267.4	634.2	334.2
90% recovered	329.9	165.5	391.8	199.9	526.1	274.5	651.9	344.4
95% recovered	339.6	170.9	397.2	202.9	535.2	279.6	669.7	354.3
End Point	350.4	176.9	401.5	205.3	540.5	282.5	678.7	359.3
Recovery, %	98.3		97.1		97.7		97.4	
Residue, %	0.7		0.9		1.3		0.9	
Loss, %	1.0		2.0		1.0		1.7	

**Table III. - ASTM D 2887 Simulated Distillation Data**

<b>SAMPLE: CONSOL CMSL-2 Total Distillate</b>		<b>BOTTLE#3</b>	
<b>SAMPLER INJECTION @ 15:17 SEP 8, 1993</b>			
<b>% OFF</b>	<b>DEG F</b>	<b>% OFF</b>	<b>DEG F</b>
IBP	98		
1	146	51	501
2	174	52	505
3	180	53	509
4	183	54	513
5	202	55	517
6	211	56	520
7	212	57	524
8	214	58	527
9	229	59	530
10	243	60	533
11	252	61	536
12	264	62	540
13	268	63	543
14	282	64	546
15	293	65	549
16	303	66	553
17	310	67	557
18	316	68	561
19	327	69	564
20	333	70	568
21	340	71	571
22	348	72	575
23	354	73	578
24	360	74	580
25	368	75	584
26	376	76	588
27	382	77	591
28	388	78	595
29	393	79	598
30	398	80	602
31	404	81	605
32	410	82	608
33	415	83	612
34	420	84	616
35	427	85	619
36	432	86	623
37	438	87	627
38	443	88	631
39	449	89	636
40	453	90	640
41	458	91	645
42	463	92	650
43	468	93	655
44	472	94	662
45	477	95	669
46	482	96	677
47	485	97	687
48	489	98	700
49	493	99	723
50	497	FBP	745

### Table IV. - ASTM D 2892 Distillation

Sample: CONSOL CMSL-2 Total Distillate

Crude Oil Properties:

API Gravity @ 60° F = 31.4

Expected IBP\* = 98° F

Density @ 60° F = 0.8687 g/cc

Measured IBP = 53° F

Sarnia Charge Weight = 36.82 lbs.

Amt. Recovered = 36.59 lbs.

<u>Fraction</u>	<u>Weight (lbs.)</u>	<u>Weight %</u>	<u>API @ 60° F</u>	<u>Density (g/cc)</u>
IBP-350° F	9.17	25.1	50.5	0.7771
350-400° F	2.05	5.6	35.4	0.8474
400-550° F	12.90	35.2	28.3	0.8850
550 +° F	12.47	34.1	21.7	0.9231

\* Initial boiling point from D 2887 Simulated Distillation.

Distillate Conditions:

<u>Fraction</u>	<u>Temperature (°F)</u>		<u>Reflux Ratio</u>	<u>Pressure (mm Hg)</u>
	<u>Head</u>	<u>Pot</u>		
IBP-350° F	350	491	5:1	754
350-400° F	400	521	5:1	754
400-550° F	361	436	2:1	40

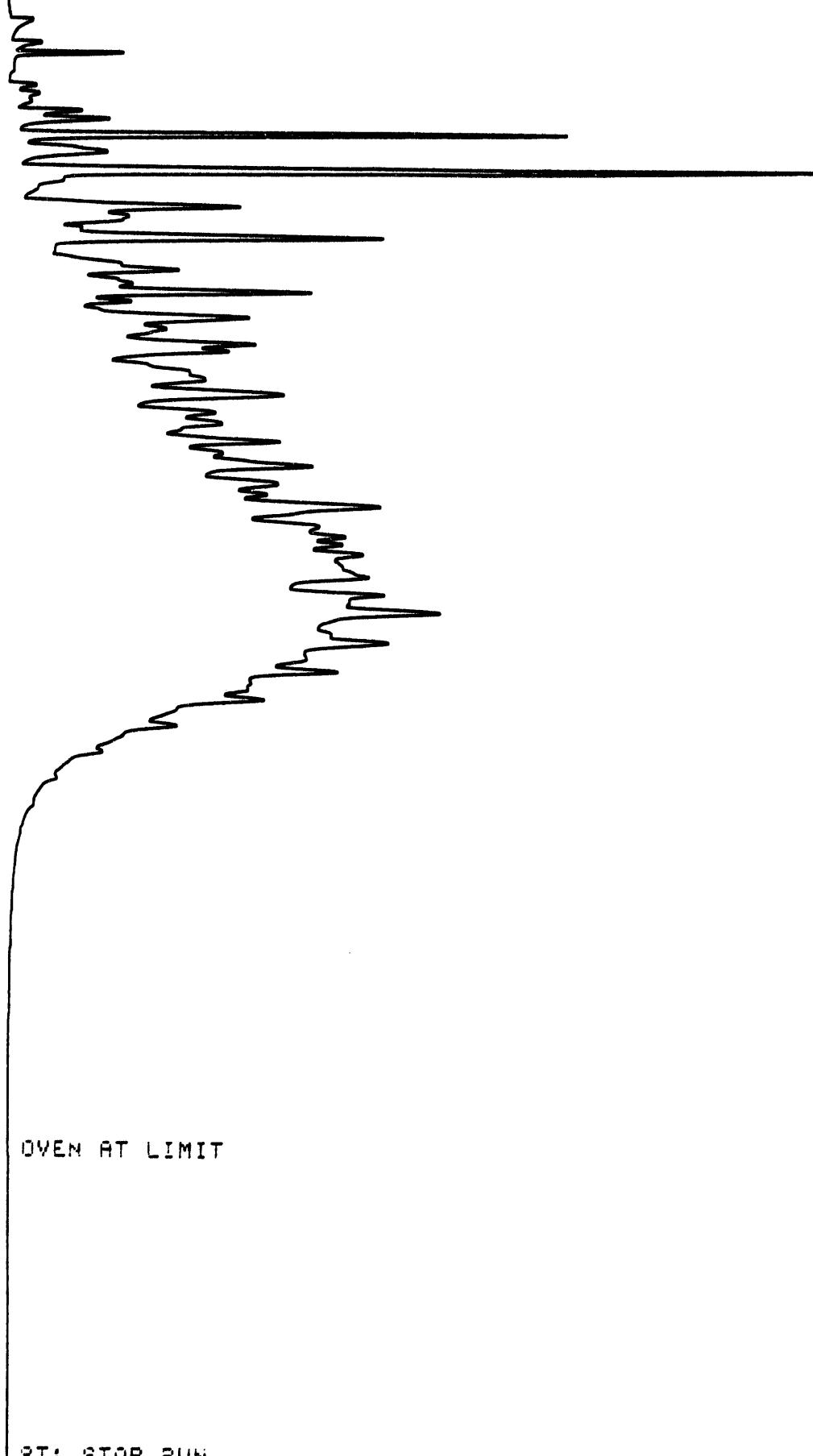
## **APPENDIX A**

### **CHROMATOGRAM From ASTM D 2887 SIMULATED DISTILLATION**

**ASTM D 2887 CHROMATOGRAM**  
**Sample: 93GL613**  
**CONSOL COAL LIQUID CMSL-2 Total Distillate**

OVEN TEMP NOT READY

RT: SLICES 0.20



D-86 CORRELATION

%OFF	DEG F
IBP	222
10	300
20	361
30	411
50	490
70	543
80	572
90	605
FBP	659

END OF PROGRAM

## **APPENDIX B**

### **DETAILED GAS CHROMATOGRAPHIC ANALYSIS DATA**

National Institute for Petroleum and Energy Research

Detailed Hydrocarbon Analysis ( P.I.A.N.O. )

File: C:\CP\DATA1\111093CO.02R  
 Sample: 93GL613  
 Method: !PIANO  
 Processed 189 Peaks  
 CONSOL  
 IBP-350'F

Analyzed: 11-10-1993 12:32:51  
 Reported: 12-02-1993 15:58:38  
 DHA DBase File: PI-NIPER.DBF  
 Normalized to 100.00%

Composite Report  
 Totals by Group Type & Carbon Number  
 (in Weight Percent)

	Paraffins:	I-paraffins:	Aromatics:	Naphthenes:	Olefins:	Total:
C1:	0.000	0.000	0.000	0.000	0.000	0.000
C2:	0.000	0.000	0.000	0.000	0.000	0.000
C3:	0.076	0.000	0.000	0.000	0.000	0.076
C4:	1.700	0.150	0.000	0.000	0.029	1.880
C5:	3.056	1.563	0.000	1.027	0.225	5.870
C6:	3.179	2.646	0.234	17.371	0.418	23.849
C7:	1.868	2.691	1.193	18.863	0.296	24.911
C8:	2.491	4.204	1.025	9.310	0.383	17.412
C9:	0.764	1.567	1.514	3.956	0.653	8.454
C10:	0.626	5.843	2.058	3.867	1.055	13.450
C11:	0.052	1.198	0.112	1.766	0.029	3.157
C12:	0.000	0.000	0.000	0.023	0.008	0.031
C13:	0.000	0.000	0.000	0.000	0.000	0.000
Total:	13.813	19.863	6.135	56.181	3.098	99.090
Oxygenates:	0.000	Total C14+:	0.000	Total Unknowns:	0.910	
				Grand Total:	100.000	

Molecular Weight and Specific Gravity Data

Group:	Ave. Mw.:	Ave. Rel. Density:
C1:	0.000	0.000
C2:	0.000	0.000
C3:	44.097	0.501
C4:	52.304	0.577
C5:	71.699	0.644
C6:	84.561	0.742
C7:	98.242	0.754
C8:	112.557	0.751
C9:	125.547	0.775
C10:	139.934	0.766
C11:	154.860	0.777
C12:	165.843	0.789
C13:	0.000	0.000
Total Sample:	99.041	0.736

National Institute for Petroleum and Energy Research

Detailed Hydrocarbon Analysis ( P.I.A.N.O. )

File: C:\CP\DATA1\111093CO.02R  
 Sample: 93GL613  
 Method: !PIANO  
 Processed 189 Peaks  
 CONSOL  
 IBP-350'F

Analyzed: 11-10-1993 12:32:51  
 Reported: 12-02-1993 15:58:38  
 DHA DBase File: RI-NIPER.DBF  
 Normalized to 100.00%

Composite Report

Totals by Group Type & Carbon Number  
 (in Volume Percent)

	Paraffins:	I-paraffins:	Aromatics:	Naphthenes:	Olefins:	Total:
C1:	0.000	0.000	0.000	0.000	0.000	0.000
C2:	0.000	0.000	0.000	0.000	0.000	0.000
C3:	0.112	0.000	0.000	0.000	0.000	0.112
C4:	2.183	0.200	0.000	0.000	0.036	2.420
C5:	3.627	1.874	0.000	1.023	0.251	6.776
C6:	3.583	2.990	0.198	16.693	0.420	23.884
C7:	2.031	2.920	1.022	18.265	0.304	24.543
C8:	2.635	4.411	0.881	8.924	0.372	17.224
C9:	0.791	1.614	1.302	3.748	0.655	8.111
C10:	0.637	5.945	1.770	3.578	1.118	13.049
C11:	0.052	1.203	0.095	1.641	0.029	3.020
C12:	0.000	0.000	0.000	0.022	0.008	0.029
C13:	0.000	0.000	0.000	0.000	0.000	0.000
Total:	15.652	21.157	5.270	53.894	3.195	99.167

Oxygenates: 0.000      Total C14+: 0.000      Total Unknowns: 0.833  
 Grand Total: 100.000

(in Mole Percent)

	Paraffins:	I-paraffins:	Aromatics:	Naphthenes:	Olefins:	Total:
C1:	0.000	0.000	0.000	0.000	0.000	0.000
C2:	0.000	0.000	0.000	0.000	0.000	0.000
C3:	0.172	0.000	0.000	0.000	0.000	0.172
C4:	2.924	0.258	0.000	0.000	0.410	3.592
C5:	4.234	2.165	0.000	1.463	0.322	8.183
C6:	3.687	3.069	0.300	20.629	0.503	28.189
C7:	1.864	2.684	1.294	19.201	0.301	25.344
C8:	2.179	3.679	0.965	8.292	0.348	15.462
C9:	0.595	1.221	1.259	3.132	0.523	6.730
C10:	0.440	4.105	1.533	2.755	0.774	9.607
C11:	0.033	0.766	0.075	1.144	0.019	2.038
C12:	0.000	0.000	0.000	0.014	0.005	0.019
C13:	0.000	0.000	0.000	0.000	0.000	0.000
Total:	16.128	17.947	5.425	56.631	3.205	99.336

Oxygenates: 0.000      Total C14+: 0.000      Total Unknowns: 0.664  
 Grand Total: 100.000

National Institute for Petroleum and Energy Research

Detailed Hydrocarbon Analysis ( P.I.A.N.O. )

File: C:\CP\DATA1\111093CO.02R  
 Sample: 93GL613  
 Method: !PIANO  
 Processed 189 Peaks  
 CONSOL  
 IBP-350°F

Analyzed: 11-10-1993 12:32:51  
 Reported: 12-02-1993 15:58:38  
 DHA DBase File: RI-NIPER.DBF  
 Normalized to 100.00%

Boiling Point Distribution Data

	Wt. Percent Off: deg.C.:	Vol. Percent Off: deg.C.:
	deg.F.:	deg.F.:
IBP (0.5%)	-0.50	31.10
5.0%	36.06	96.91
10.0%	63.27	145.89
15.0%	71.80	161.24
20.0%	80.72	177.30
25.0%	80.72	177.30
30.0%	80.72	177.30
35.0%	91.85	197.33
40.0%	100.93	213.67
45.0%	100.93	213.67
50.0%	100.93	213.67
55.0%	103.47	218.25
60.0%	118.54	245.37
65.0%	125.68	258.22
70.0%	130.96	267.73
75.0%	139.12	282.42
80.0%	150.82	303.48
85.0%	160.41	320.74
90.0%	171.30	340.34
95.0%	177.13	350.83
FBP (99.5%)	189.52	373.14
		188.24
		370.83

Research Octane Number = 75.25  
 (Calculated from Individual Component Values)

Contribution to Total by:

Paraffins: 5.29  
 Iso-paraffins: 15.14  
 Aromatics: 6.45  
 Naphthenes: 44.88  
 Olefins: 2.80  
 Oxygenates: 0.00

National Institute for Petroleum and Energy Research

Detailed Hydrocarbon Analysis ( P.I.A.N.O. )

File: C:\CP\DATA1\111093CO.02R  
 Sample: 93GL613  
 Method: !PIANO  
 Processed 189 Peaks  
 CONSOL  
 IBP-350°F

Analyzed: 11-10-1993 12:32:51  
 Reported: 12-02-1993 15:58:38  
 DHA DBase File: RI-NIPER.DBF  
 Normalized to 100.00%

Components Listed in Chromatographic Order

Min.	INDEX	Component	Wt%	Vol%	Mol%
6.393	300.0	Propane	0.076	0.112	0.172
6.847	360.9	i-Butane	0.150	0.200	0.258
7.113	388.3	Butene-1	0.025	0.031	0.402
7.240	400.0	n-Butane	1.700	2.183	2.924
7.607	422.8	c-Butene-2	0.005	0.006	0.008
8.240	454.4	?	0.009	0.011	0.016
8.687	472.8	i-Pentane	1.563	1.874	2.165
9.107	487.9	Pentene-1	0.060	0.070	0.086
9.327	495.2	2-Methylbutene-1	0.038	0.043	0.053
9.480	500.0	n-Pentane	3.056	3.627	4.234
9.760	507.4	t-Pentene-2	0.044	0.050	0.062
10.053	514.6	c-Pentene-2	0.014	0.016	0.020
10.273	519.8	2-Methylbutene-2	0.036	0.041	0.051
11.940	552.6	Cyclopentene	0.033	0.032	0.049
12.100	555.3	4-Methylpentene-1	0.025	0.028	0.029
12.200	557.0	3-Methylpentene-1	0.012	0.014	0.015
12.580	563.0	Cyclopentane	1.027	1.023	1.463
12.667	564.4	2,3-Dimethylbutane	0.161	0.181	0.187
12.927	568.3	2-Methylpentane	1.480	1.684	1.716
13.960	582.7	3-Methylpentane	1.005	1.125	1.166
14.333	587.5	2-Methylpentene-1	0.029	0.032	0.035
14.427	588.6	Hexene-1	0.065	0.071	0.077
15.393	600.0	n-Hexane	3.179	3.583	3.687
16.053	607.5	2-Methylpentene-2	0.039	0.042	0.046
16.267	609.8	3-Methylcyclopentene	0.027	0.027	0.033
16.387	611.1	3-Methyl-c-pentene-2	0.013	0.014	0.016
16.753	614.9	c-Hexene-2	0.012	0.013	0.014
17.680	624.1	4,4-Dimethyl-t-pentene-2	0.009	0.010	0.009
17.847	625.7	2,2-Dimethylpentane	0.010	0.011	0.010
18.140	628.4	Methylcyclopentane	2.911	2.890	3.457
18.600	632.6	2,4-Dimethylpentane	0.091	0.100	0.090
20.967	651.9	1-Methylcyclopentene	0.038	0.037	0.047
21.153	653.3	Benzene	0.234	0.198	0.300
21.780	657.8	3,3-Dimethylpentane	0.024	0.026	0.024
22.267	661.3	Cyclohexane	14.460	13.803	17.172
23.640	670.4	2-Methylhexane	0.940	1.029	0.938
23.853	671.8	2,3-Dimethylpentane	0.298	0.318	0.297
24.213	674.1	1,1-Dimethylcyclopentane	0.069	0.068	0.071
24.567	676.3	Cyclohexene	0.158	0.145	0.192
24.933	678.5	3-Methylhexane	1.212	1.310	1.209
25.833	683.7	1c,3-Dimethylcyclopentane	0.467	0.466	0.476
26.267	686.2	1t,3-Dimethylcyclopentane	0.425	0.424	0.432
26.520	687.6	3-Ethylpentane	0.117	0.124	0.116
26.687	688.5	1t,2-Dimethylcyclopentane	0.565	0.559	0.575
26.980	690.1	2,2,4-Trimethylpentane/Heptene-1	0.040	0.043	0.041
28.313	697.2	t-Heptene-3	0.008	0.009	0.008

28.573	698.5	c-Heptene-3	0.019	0.020	0.019
28.873	700.0	n-Heptane	1.868	2.031	1.864
29.973	707.7	3-Ethylpentene-2	0.014	0.014	0.014
32.067	721.3	Methylcyclohexane	16.458	15.896	16.753
32.613	724.7	2,2-Dimethylhexane	0.056	0.060	0.049
34.160	733.9	Ethylcyclopentane	0.878	0.852	0.894
34.473	735.8	2,5-Dimethylhexane	0.125	0.134	0.110
34.793	737.6	2,4-Dimethylhexane	0.188	0.200	0.165
35.000	738.8	O17	0.030	0.031	0.031
35.740	742.9	1c,2t,4-Trimethylcyclopentane	0.157	0.153	0.140
37.047	749.9	1t,2c,3-Trimethylcyclopentane	0.131	0.127	0.117
37.747	753.6	2,3,4-Trimethylpentane	0.009	0.009	0.008
38.407	757.0	Toluene	1.193	1.022	1.294
39.600	762.9	2,3-Dimethylhexane	0.220	0.230	0.193
39.800	763.9	1,1,2-Trimethylcyclopentane	0.100	0.097	0.089
40.233	766.0	O25	0.176	0.179	0.179
40.800	768.7	2-Methylheptane	0.618	0.658	0.541
41.060	769.9	4-Methylheptane	0.200	0.211	0.175
41.707	772.9	1c,2c,4-Trimethylcyclopentane	0.078	0.076	0.070
42.247	775.4	3-Methylheptane	0.532	0.561	0.466
42.393	776.0	3-Ethylhexane	2.255	2.348	1.973
42.773	777.7	1t,4-Dimethylcyclohexane	0.643	0.626	0.572
44.453	785.1	2,2,5-Trimethylhexane	0.018	0.019	0.014
44.687	786.1	1t,3-Ethylmethylcyclopentane	0.296	0.287	0.264
45.153	788.0	1c,3-Ethylmethylcyclopentane	0.239	0.232	0.213
45.420	789.2	Octene-1	0.383	0.372	0.348
46.440	793.4	1t,2-Dimethylcyclohexane	0.988	0.946	0.880
48.100	800.0	n-Octane	2.491	2.635	2.179
49.740	808.9	i-Propylcyclopentane	0.106	0.101	0.094
52.460	823.0	2,3,4-Trimethylhexane	0.085	0.086	0.067
53.993	830.6	1c,2-Dimethylcyclohexane	0.437	0.408	0.389
55.460	837.7	n-Propylcyclopentane	6.081	5.822	5.417
55.973	840.1	1c,3c,5-Trimethylcyclohexane	0.204	0.197	0.162
56.273	841.5	2-Methyl-4-Ethylhexane	0.034	0.035	0.026
56.807	844.0	1,1,3-Trimethylcyclohexane	0.136	0.131	0.107
57.233	845.9	1,1,4-Trimethylcyclohexane	0.021	0.021	0.017
57.593	847.6	3,3-Dimethylheptane	0.144	0.147	0.112
58.127	850.0	2,5-Dimethylheptane	0.046	0.048	0.036
58.440	851.4	N5	0.053	0.051	0.048
58.833	853.1	2,4-Dimethylheptene-1	0.048	0.053	0.040
60.047	858.4	Ethylbenzene	0.278	0.238	0.262
60.387	859.9	1c,2t,4t-Trimethylcyclohexane	0.325	0.310	0.258
60.800	861.7	2-Methyloctene-1	0.045	0.048	0.036
61.260	863.6	N8	0.070	0.066	0.055
61.960	866.6	m-Xylene	0.267	0.229	0.251
62.227	867.7	p-Xylene	0.436	0.377	0.411
62.813	870.1	2,3-Dimethylheptane	0.183	0.187	0.142
63.273	872.0	4-Ethylheptane	0.209	0.215	0.162
63.907	874.6	4-Methyloctane	0.239	0.247	0.186
64.120	875.5	2-Methyloctane	0.218	0.227	0.170
64.533	877.1	N11	0.041	0.039	0.032
65.107	879.4	?	0.129	0.123	0.102
65.393	880.5	3-Methylocane	0.391	0.403	0.305
65.940	882.7	1,1,2-Trimethylcyclohexane	0.095	0.088	0.075
66.380	884.4	o-Xylene	0.044	0.037	0.041
67.387	888.3	N12	0.222	0.212	0.176
67.560	889.0	N13/t-Nonene-2	1.309	1.247	1.036
67.967	890.5	t-2-Methyloctene-3	0.383	0.364	0.303
68.473	892.4	Nonene-1	0.049	0.054	0.039
68.733	893.4	i-Butylcyclopentane	0.112	0.107	0.089
69.473	896.1	t-Nonene-3	0.006	0.007	0.005

70.007	898.1	N17/c-Nonene-2	0.018	0.017	0.014
70.160	898.7	c-Nonene-3	0.067	0.073	0.055
70.527	900.0	n-Nonane	0.764	0.791	0.595
70.920	903.1	3,7-Dimethyloctene-1	0.995	1.054	0.730
71.420	907.0	N18	0.217	0.204	0.172
72.280	913.6	c-Nonene-2	0.056	0.056	0.046
72.680	916.6	N20	0.201	0.189	0.159
73.060	919.5	i-Propylcyclohexane	0.518	0.480	0.410
73.487	922.7	I11	0.069	0.070	0.048
73.753	924.7	2,2-Dimethyloctane	0.042	0.043	0.029
74.360	929.3	?	0.009	0.009	0.006
74.493	930.2	N22	0.232	0.218	0.184
74.833	932.8	2,6-Dimethyloctane	3.712	3.791	2.608
75.327	936.4	I12	0.011	0.011	0.008
75.507	937.7	n-Butylcyclopentane	0.234	0.222	0.185
75.687	939.0	I13	0.033	0.033	0.023
76.067	941.8	I14	0.010	0.010	0.007
76.253	943.1	3,3-Dimethyloctane	0.226	0.228	0.159
76.607	945.7	N24	0.066	0.062	0.047
77.020	948.6	n-Propylbenzene	0.210	0.181	0.175
77.313	950.7	3-Methyl-5-ethylheptane	0.080	0.082	0.056
77.707	953.5	?	0.014	0.014	0.010
78.233	957.2	1-Methyl-3-ethylbenzene	1.119	0.962	0.931
78.480	958.9	1-Methyl-4-ethylbenzene	0.184	0.159	0.153
78.887	961.8	2,3-Dimethyloctane	0.087	0.088	0.061
79.053	962.9	?	0.015	0.015	0.011
79.340	964.9	I15	0.274	0.275	0.193
79.773	967.9	I16	0.062	0.062	0.044
79.913	968.9	I17	0.080	0.080	0.056
80.127	970.3	5-Methylnonane	0.165	0.167	0.116
80.460	972.6	2-Methylnonane	0.225	0.230	0.158
81.233	977.9	3-Methylnonane	0.303	0.307	0.213
81.420	979.1	3-Ethyl-2-methylheptene-2	0.060	0.064	0.044
81.593	980.3	N29	0.099	0.092	0.071
81.947	982.7	I18	0.039	0.039	0.028
82.580	986.9	t-Butylcyclohexane	2.543	2.353	1.812
82.827	988.5	i-Butylcyclohexane	0.495	0.462	0.353
83.067	990.1	I21	0.119	0.120	0.084
83.373	992.1	I22	0.139	0.140	0.098
83.880	995.4	I24/2,3-Dimethyloctene-2	0.165	0.166	0.116
84.080	996.7	1t-Methyl-2-n-propylcyclohexan	0.225	0.209	0.160
84.473	999.3	sec-Butylbenzene	0.252	0.218	0.188
84.587	1000.0	n-Decane	0.626	0.637	0.440
85.000	1004.2	I26	0.120	0.121	0.077
85.087	1005.0	?	0.121	0.121	0.077
85.300	1007.2	N31	0.372	0.345	0.241
85.667	1010.9	1-Methyl-3-i-propylbenzene	0.258	0.223	0.192
86.127	1015.5	1-Methyl-4-i-propylbenzene	0.314	0.273	0.234
86.907	1023.2	I29	0.602	0.604	0.385
87.233	1026.4	sec-Butylcyclohexane	0.438	0.400	0.312
87.827	1032.2	3-Ethynonane	0.060	0.060	0.038
88.020	1034.0	N33	0.688	0.639	0.446
88.433	1038.0	I31	0.123	0.123	0.079
88.727	1040.9	1,3-Diethylbenzene	0.434	0.374	0.323
88.900	1042.5	1-Methyl-3-n-propylbenzene	0.131	0.113	0.097
89.033	1043.8	?	0.297	0.256	0.221
89.367	1047.0	1,4-Diethylbenzene	0.152	0.131	0.113
89.560	1048.9	?	0.146	0.126	0.109
89.760	1050.8	n-Butylbenzene	0.113	0.098	0.084
90.000	1053.0	1,2-Diethylbenzene	0.031	0.026	0.023
90.273	1055.6	N34	0.187	0.173	0.121

90.440	1057.2	N35		0.520	0.483	0.337
90.607	1059.5	1-Methyl-2-n-propylbenzene		0.166	0.142	0.124
90.933	1061.8	I35		0.061	0.061	0.039
91.253	1064.8	I37		0.042	0.042	0.027
91.593	1068.0	I38		0.137	0.137	0.087
91.940	1071.2	s-C5Bz / 1,3-DM-4-EtBz		0.024	0.021	0.016
92.033	1072.1	?		0.061	0.053	0.041
92.253	1074.1	?		0.040	0.034	0.027
92.547	1076.8	1,2-Dimethyl-4-ethylbenzene		0.190	0.161	0.141
93.653	1087.0	I43		0.054	0.054	0.034
94.067	1090.7	Undecene-1		0.029	0.029	0.019
94.273	1092.6	1-Methyl-4-t-butylbenzene		0.032	0.028	0.022
94.653	1096.0	1,2-Dimethyl-3-ethylbenzene		0.016	0.013	0.012
94.947	1098.6	1-Ethyl-2-1-propylbenzene		0.040	0.034	0.027
95.100	1100.0	n-Undecane		0.052	0.052	0.033
96.387	1114.6	?		0.038	0.038	0.024
97.860	1131.1	?		0.014	0.014	0.009
98.527	1138.5	?		0.019	0.019	0.012
98.840	1142.0	1-Methyl-3-n-butylbenzene		0.015	0.013	0.010
99.820	1152.7	1t-M-2-(4-MP)cyclopentane		0.023	0.022	0.014
103.307	1189.9	Dodecene-1		0.008	0.008	0.005

## **APPENDIX C**

### **HC22 MASS SPECTROMETRIC DATA**

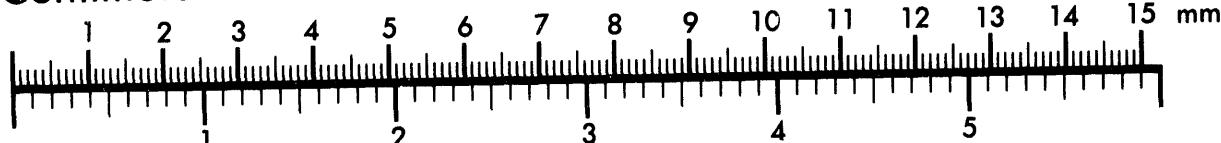


**AIIM**

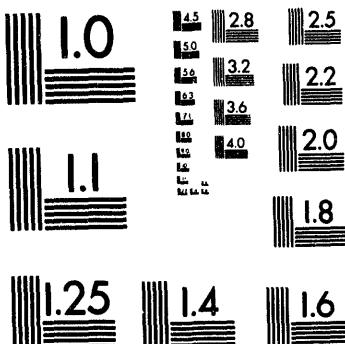
**Association for Information and Image Management**

1100 Wayne Avenue, Suite 1100  
Silver Spring, Maryland 20910  
301/587-8202

**Centimeter**



**Inches**



MANUFACTURED TO AIIM STANDARDS  
BY APPLIED IMAGE, INC.

2 of 2

IIT RESEARCH INSTITUTE  
NATIONAL INSTITUTE FOR PETROLEUM AND ENERGY RESEARCH  
P.O. BOX 2128, BARTLESVILLE, OK 74005

MASS SPECTROMETRY LABORATORY

22-COMPONENT HYDROCARBON TYPE ANALYSIS

CLIENT: CONSOL  
P.O. NO.

NIPER ACCT. NO: B06761

SAMPLE: 12133B. 12/13/93. HC22 ANAL. OF CONSOL 93 GL 613-3  
AVERAGE RESULTS FROM SCANS 14, 15, 16

		AVE	LV %	SDEV	AVE	WT %	SDEV
SATURATES							
C(N)H(2N+2)	PARAFFINS		7.5	0.8		6.6	0.8
C(N)H(2N)	MONOCYCLOPARAFFINS		38.8	0.6		36.6	0.4
C(N)H(2N-2)	DICYCLOPARAFFINS		21.0	0.8		21.8	0.9
C(N)H(2N-4)	TRICYCLOPARAFFINS		4.3	0.2		4.7	0.2
C(N)H(2N-6)	TETRACYCLOPARAFFINS		0.0	0.0		0.0	0.0
C(N)H(2N-8)	PENTACYCLOPARAFFINS		0.0	0.0		0.0	0.0
C(N)H(2N-10)	HEXACYCLOPARAFFINS		0.0	0.0		0.0	0.0
C(N)H(2N-12)	HEPTACYCLOPARAFFINS		0.0	0.0		0.0	0.0
	TOTAL SATURATES		71.6	0.5		69.7	0.6
MONOAROMATICS							
C(N)H(2N-6)	ALKYLBENZENES		14.8	0.3		15.0	0.3
C(N)H(2N-8)	BENZOCYCLOPARAFFINS		11.8	0.2		13.2	0.3
C(N)H(2N-10)	BENZODICYCLOPARAFFINS		0.0	0.0		0.0	0.0
DIAROMATICS							
C(N)H(2N-12)	NAPHTHALENES		1.8	0.1		2.1	0.1
C(N)H(2N-14)			0.0	0.0		0.0	0.0
C(N)H(2N-16)			0.0	0.0		0.0	0.0
TRIAROMATICS							
C(N)H(2N-18)			0.0	0.0		0.0	0.1
C(N)H(2N-22)			0.0	0.0		0.0	0.0
TETRAAROMATICS							
C(N)H(2N-24)			0.0	0.0		0.0	0.0
C(N)H(2N-28)			0.0	0.0		0.0	0.0
	TOTAL AROMATICS		28.4	0.6		30.3	0.7
SULFUR COMPOUNDS							
C(N)H(2N-4)S	THIOPHENES		0.0	0.0		0.0	0.0
C(N)H(2N-10)S	BENZOTHIOPHENES		0.0	0.0		0.0	0.0
C(N)H(2N-16)S	DIBENZOTHIOPHENES		0.0	0.0		0.0	0.0
C(N)H(2N-22)S	NAPHTHOBENZOTHIOPHENES		0.0	0.0		0.0	0.0
	TOTAL THIOPHENIC COMPOUNDS		0.0	0.0		0.0	0.0

CONTINUED ON PAGE 2

CLIENT: CONSOL  
P.O. NO.

NIPER ACCT. NO: B06761

SAMPLE: 12133B. 12/13/93. HC22 ANAL. OF CONSOL 93 GL 613-3  
AVERAGE RESULTS FROM SCANS 14, 15, 16

CONTINUATION FROM PAGE 1:

	AVG	SDEV
CARBON NUMBER	12.0	---
MOLECULAR WEIGHT	164.0	---
<b>ELEMENTAL ANALYSIS:</b>		
	WT %	SDEV
C	86.9	0.0
H	13.1	0.0
THIOPHENIC S	0.0	0.0
<b>N-D-M CARBON TYPE:</b>		
	PCT	SDEV
AROMATIC	15.0	0.3
NAPHTHENIC	46.4	0.4
PARAFFINIC	38.6	0.4
<b>N-D-M RING TYPE:</b>		
	NO.	SDEV
AROMATIC	0.3	0.0
NAPHTHENIC	1.1	0.1

NOTE: THIS METHOD DETERMINES LISTED COMPOUND TYPES IN NONOLEFINIC HYDROCARBON FRACTIONS WITH AVERAGE CARBON NUMBERS BETWEEN 12 AND 36 (BOILING RANGE FROM 350 TO 1050 DEG F) AND HAVING LESS THAN 5 MOL % TOTAL OF COMPOUNDS CONTAINING OXYGEN, NITROGEN, AND SULFUR.

IIT RESEARCH INSTITUTE  
NATIONAL INSTITUTE FOR PETROLEUM AND ENERGY RESEARCH  
P.O. BOX 2128, BARTLESVILLE, OK 74005

MASS SPECTROMETRY LABORATORY

22-COMPONENT HYDROCARBON TYPE ANALYSIS

CLIENT: CONSOL  
P.O. NO.

NIPER ACCT. NO: B06761

SAMPLE: 12143A. 12/14/93. HC22 ANAL. OF CONSOL 93 GL 613-6  
AVERAGE RESULTS FROM SCANS 15, 16, 17

		AVE	LV %	SDEV	AVE	WT %	SDEV
SATURATES							
C(N)H(2N+2)	PARAFFINS		8.0	0.5		7.1	0.5
C(N)H(2N)	MONOCYCLOPARAFFINS		39.4	0.6		37.2	0.6
C(N)H(2N-2)	DICYCLOPARAFFINS		20.4	0.2		21.2	0.2
C(N)H(2N-4)	TRICYCLOPARAFFINS		4.2	0.2		4.6	0.2
C(N)H(2N-6)	TETRACYCLOPARAFFINS		0.0	0.0		0.0	0.0
C(N)H(2N-8)	PENTACYCLOPARAFFINS		0.0	0.0		0.0	0.0
C(N)H(2N-10)	HEXACYCLOPARAFFINS		0.0	0.0		0.0	0.0
C(N)H(2N-12)	HEPTACYCLOPARAFFINS		0.0	0.0		0.0	0.0
	TOTAL SATURATES		72.1	0.4		70.1	0.5
MONOAROMATICS							
C(N)H(2N-6)	ALKYLBENZENES		14.5	0.1		14.7	0.1
C(N)H(2N-8)	BENZOCYCLOPARAFFINS		11.6	0.5		13.0	0.5
C(N)H(2N-10)	BENZODICYCLOPARAFFINS		0.0	0.0		0.0	0.0
DIAROMATICS							
C(N)H(2N-12)	NAPHTHALENES		1.6	0.1		2.0	0.1
C(N)H(2N-14)			0.0	0.0		0.0	0.0
C(N)H(2N-16)			0.0	0.0		0.0	0.0
TRIAROMATICS							
C(N)H(2N-18)			0.0	0.0		0.0	0.1
C(N)H(2N-22)			0.0	0.0		0.0	0.0
TETRAAROMATICS							
C(N)H(2N-24)			0.0	0.0		0.0	0.0
C(N)H(2N-28)			0.0	0.0		0.0	0.0
	TOTAL AROMATICS		27.8	0.5		29.8	0.5
SULFUR COMPOUNDS							
C(N)H(2N-4)S	THIOPHENES		0.0	0.0		0.0	0.0
C(N)H(2N-10)S	BENZOTHIOPHENES		0.0	0.0		0.0	0.0
C(N)H(2N-16)S	DIBENZOTHIOPHENES		0.0	0.0		0.0	0.0
C(N)H(2N-22)S	NAPHTOBENZOTHIOPHENES		0.0	0.0		0.0	0.0
	TOTAL THIOPHENIC COMPOUNDS		0.0	0.0		0.0	0.0

CONTINUED ON PAGE 2

CLIENT: CONSOL  
P.O. NO.

NIPER ACCT. NO: B06761

SAMPLE: 12143A. 12/14/93. HC22 ANAL. OF CONSOL 93 GL 613-6  
AVERAGE RESULTS FROM SCANS 15, 16, 17

CONTINUATION FROM PAGE 1:

	AVG	SDEV
CARBON NUMBER	12.0	---
MOLECULAR WEIGHT	164.0	---
<b>ELEMENTAL ANALYSIS:</b>		
	WT %	SDEV
C	86.9	0.0
H	13.1	0.0
THIOPHENIC S	0.0	0.0
<b>N-D-M CARBON TYPE:</b>		
	PCT	SDEV
AROMATIC	14.7	0.2
NAPHTHENIC	46.1	0.3
PARAFFINIC	39.3	0.5
<b>N-D-M RING TYPE:</b>		
	NO.	SDEV
AROMATIC	0.3	0.0
NAPHTHENIC	1.0	0.1

NOTE: THIS METHOD DETERMINES LISTED COMPOUND TYPES IN NONOLEFINIC HYDROCARBON FRACTIONS WITH AVERAGE CARBON NUMBERS BETWEEN 12 AND 36 (BOILING RANGE FROM 350 TO 1050 DEG F) AND HAVING LESS THAN 5 MOL % TOTAL OF COMPOUNDS CONTAINING OXYGEN, NITROGEN, AND SULFUR.

IIT RESEARCH INSTITUTE  
NATIONAL INSTITUTE FOR PETROLEUM AND ENERGY RESEARCH  
P.O. BOX 2128, BARTLESVILLE, OK 74005

## MASS SPECTROMETRY LABORATORY

## 22-COMPONENT HYDROCARBON TYPE ANALYSIS

CLIENT: CONSOL  
P.O. NO.

NIPER ACCT. NO: B06761

SAMPLE: 12133C. 12/13/93. HC22 ANAL. OF CONSOL 93 GL 613-4  
AVERAGE RESULTS FROM SCANS 14, 15, 16

		AVE	LV %	SDEV	AVE	WT %	SDEV
C(N)H(2N+2)	PARAFFINS		7.5	0.5		6.5	0.4
C(N)H(2N)	MONOCYCLOPARAFFINS		21.5	0.6		19.8	0.5
C(N)H(2N-2)	DICYCLOPARAFFINS		20.4	0.1		20.1	0.1
C(N)H(2N-4)	TRICYCLOPARAFFINS		13.1	0.3		13.6	0.3
C(N)H(2N-6)	TETRACYCLOPARAFFINS		0.0	0.0		0.0	0.0
C(N)H(2N-8)	PENTACYCLOPARAFFINS		0.0	0.0		0.0	0.0
C(N)H(2N-10)	HEXACYCLOPARAFFINS		0.0	0.0		0.0	0.0
C(N)H(2N-12)	HEPTACYCLOPARAFFINS		0.0	0.0		0.0	0.0
TOTAL SATURATES			62.5	0.3		60.1	0.2
<b>MONOAROMATICS</b>							
C(N)H(2N-6)	ALKYLBENZENES		7.1	0.2		7.0	0.2
C(N)H(2N-8)	BENZOCYCLOPARAFFINS		16.5	0.2		17.5	0.2
C(N)H(2N-10)	BENZODICYCLOPARAFFINS		6.6	0.2		7.1	0.2
<b>DIAROMATICS</b>							
C(N)H(2N-12)	NAPHTHALENES		5.7	0.2		6.5	0.2
C(N)H(2N-14)			1.1	0.1		1.3	0.1
C(N)H(2N-16)			0.5	0.0		0.7	0.0
<b>TRIAROMATICS</b>							
C(N)H(2N-18)			0.0	0.0		0.0	0.0
C(N)H(2N-22)			0.0	0.0		0.0	0.0
<b>TETRAAROMATICS</b>							
C(N)H(2N-24)			0.0	0.0		0.0	0.0
C(N)H(2N-28)			0.0	0.0		0.0	0.0
TOTAL AROMATICS			37.5	0.3		40.1	0.3
<b>SULFUR COMPOUNDS</b>							
C(N)H(2N-4)S	THIOPHENES		0.0	0.0		0.0	0.0
C(N)H(2N-10)S	BENZOTHIOPHENES		0.0	0.0		0.0	0.0
C(N)H(2N-16)S	DIBENZOTHIOPHENES		0.0	0.0		0.0	0.0
C(N)H(2N-22)S	NAPHTHOBENZOTHIOPHENES		0.0	0.0		0.0	0.0
TOTAL THIOPHENIC COMPOUNDS			0.0	0.0		0.0	0.0

CONTINUED ON PAGE 2

CLIENT: CONSOL  
P.O. NO.

NIPER ACCT. NO: B06761

SAMPLE: 12133C. 12/13/93. HC22 ANAL. OF CONSOL 93 GL 613-4  
AVERAGE RESULTS FROM SCANS 14, 15, 16

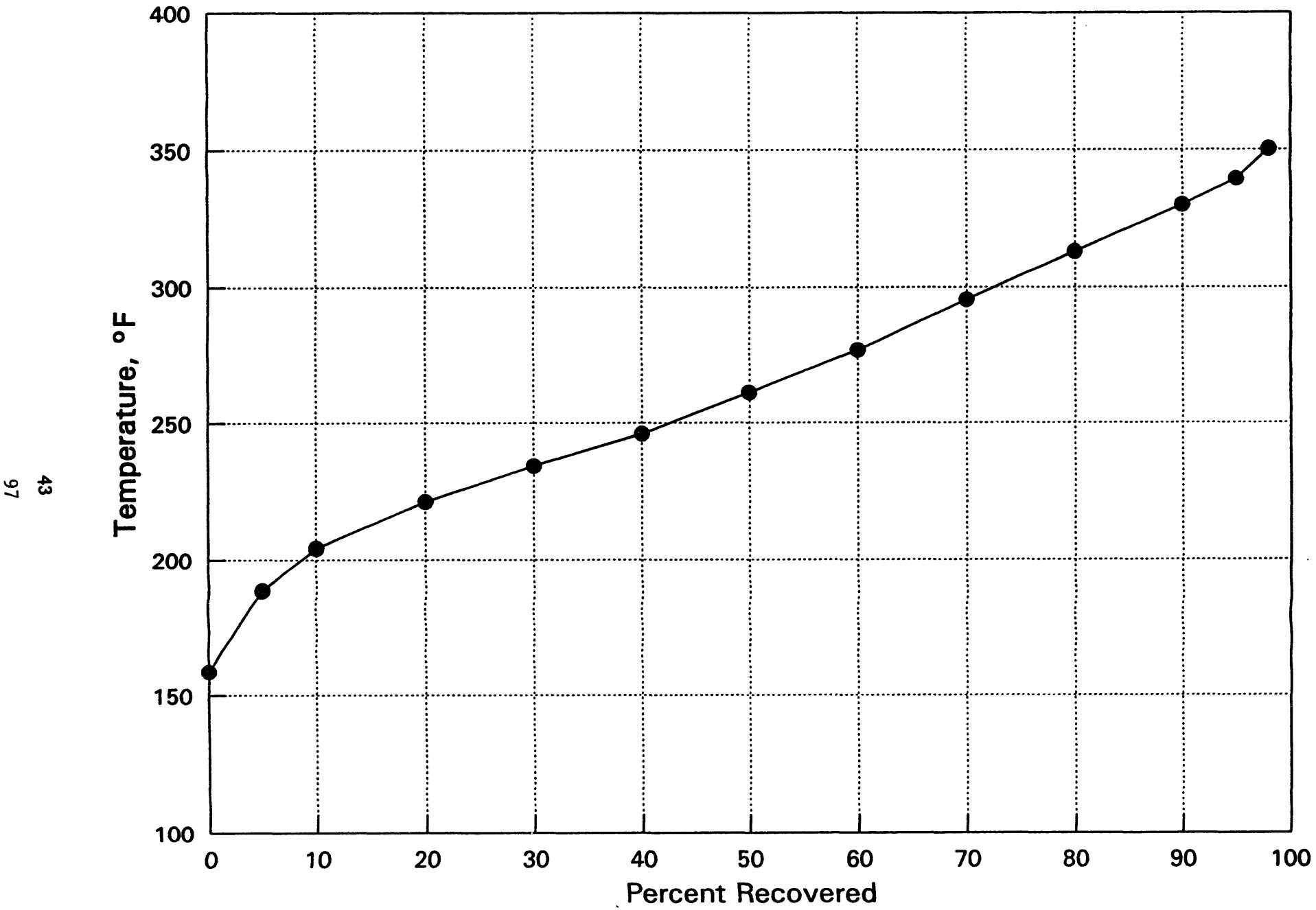
CONTINUATION FROM PAGE 1:

	AVG	SDEV
CARBON NUMBER	13.9	---
MOLECULAR WEIGHT	191.1	---
<b>ELEMENTAL ANALYSIS:</b>		
	WT %	SDEV
C	87.5	0.0
H	12.5	0.0
THIOPHENIC S	0.0	0.0
<b>N-D-M CARBON TYPE:</b>		
	PCT	SDEV
AROMATIC	18.3	0.1
NAPHTHENIC	46.1	0.4
PARAFFINIC	35.6	0.3
<b>N-D-M RING TYPE:</b>		
	NO.	SDEV
AROMATIC	0.4	0.1
NAPHTHENIC	1.3	0.0

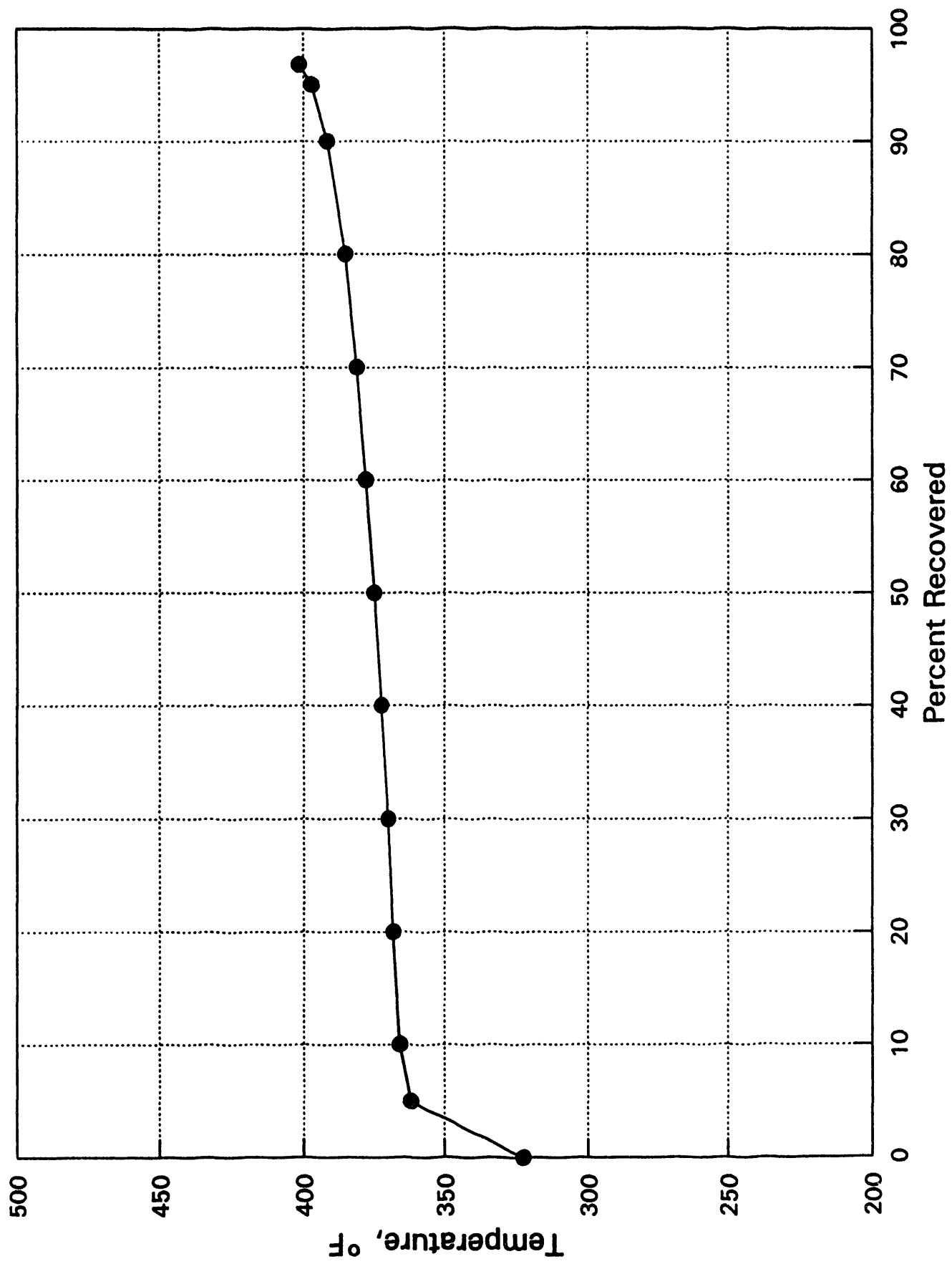
NOTE: THIS METHOD DETERMINES LISTED COMPOUND TYPES IN NONOLEFINIC HYDROCARBON FRACTIONS WITH AVERAGE CARBON NUMBERS BETWEEN 12 AND 36 (BOILING RANGE FROM 350 TO 1050 DEG F) AND HAVING LESS THAN 5 MOL % TOTAL OF COMPOUNDS CONTAINING OXYGEN, NITROGEN, AND SULFUR.

## **APPENDIX D**

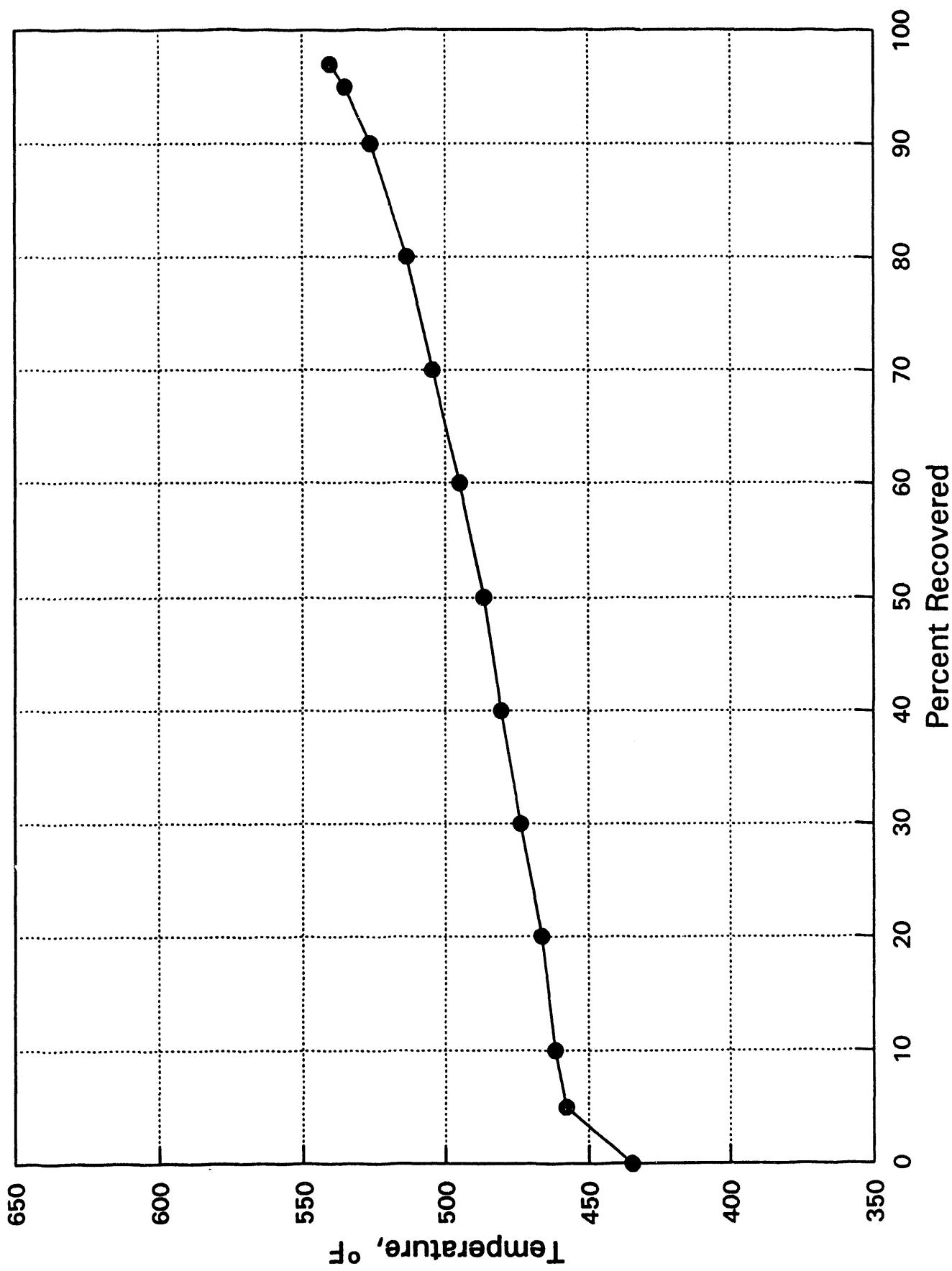
### **ASTM D 86 DISTILLATION CURVES**



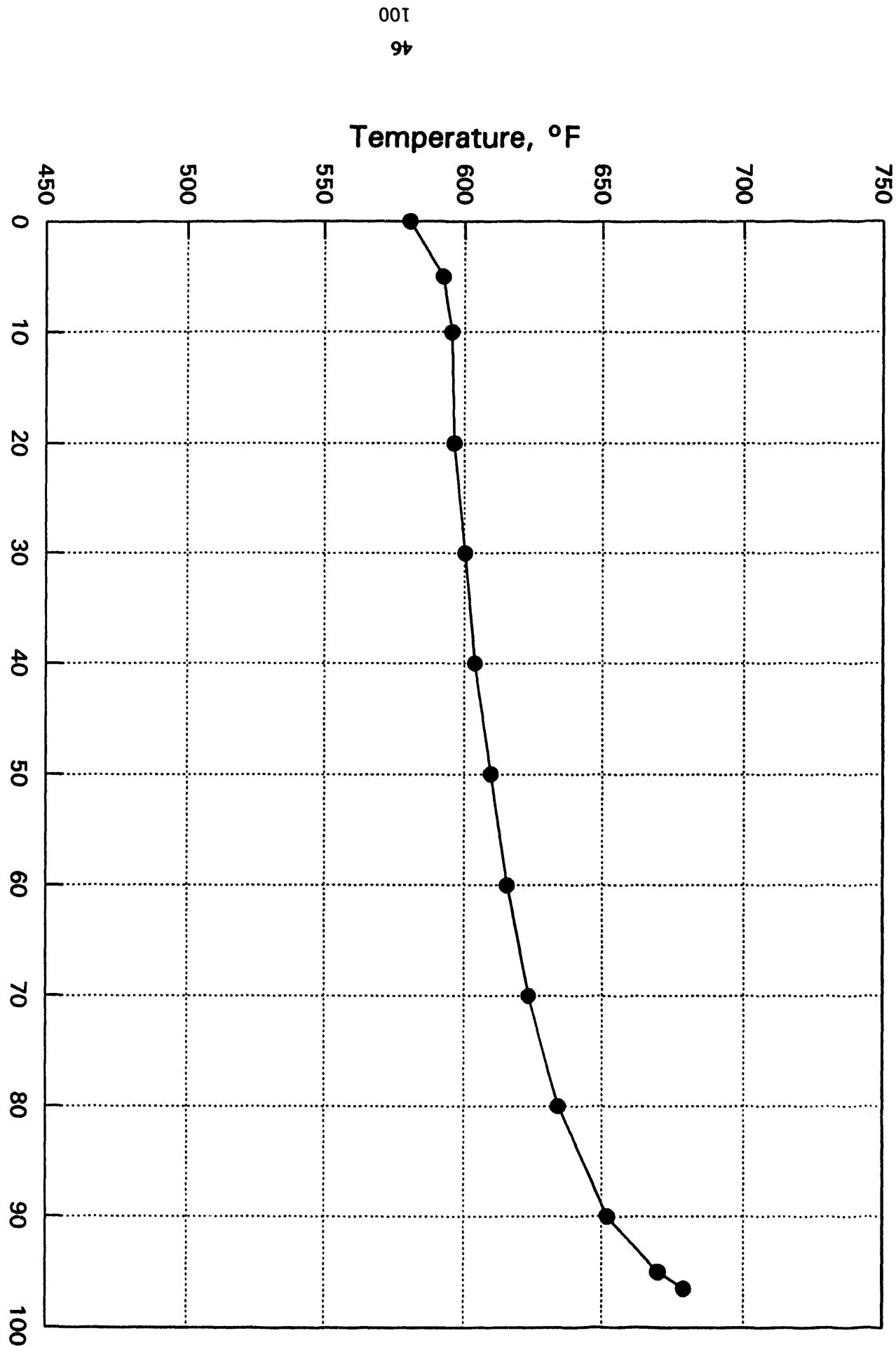
D86, CMSL-2 <350° F DISTILLATE



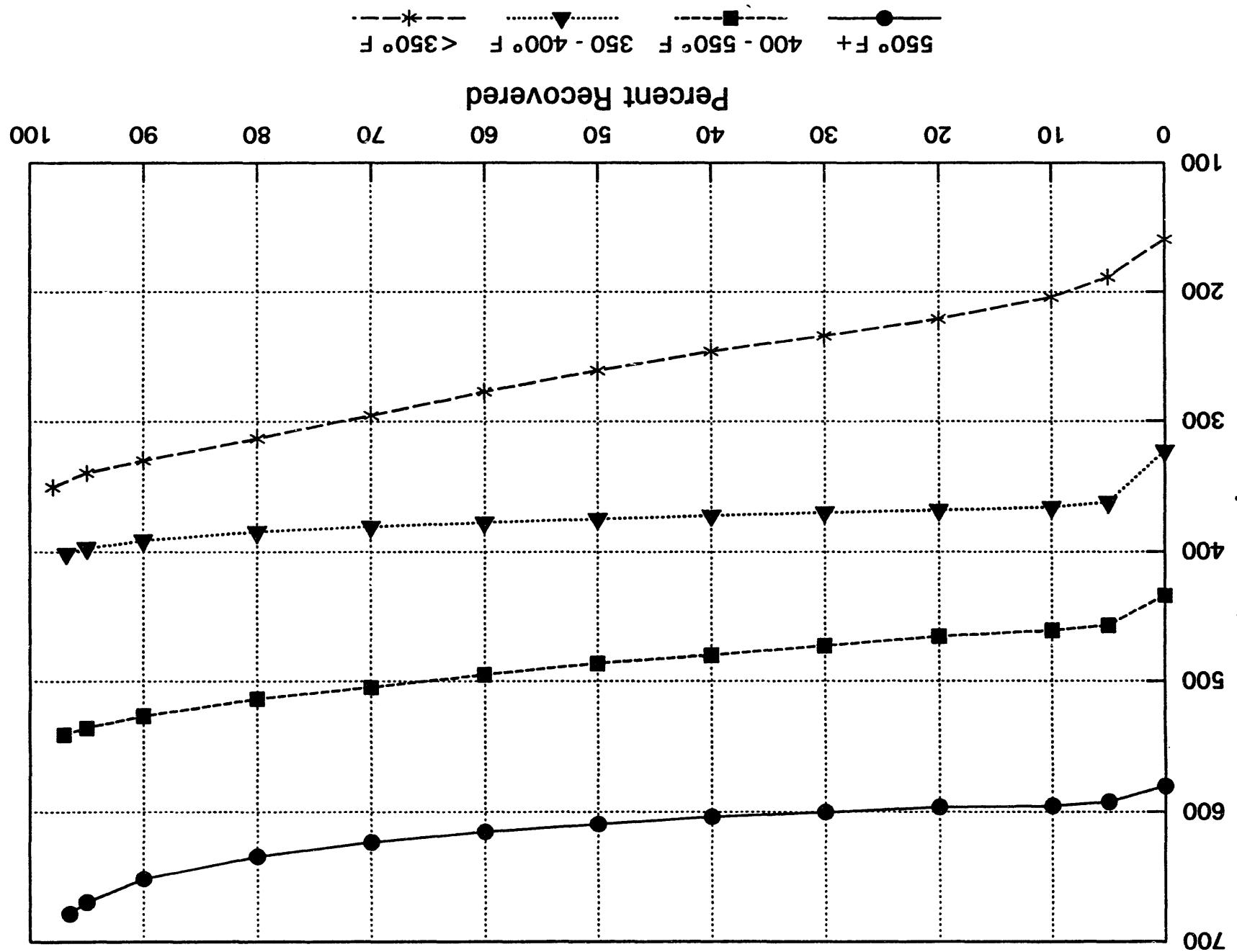
D86, CMSL-2 400 - 550° F DISTILLATE



D86, CMSL-2 550° F + RESID



# D86, CML-2 FRACTIONS



U.S. GOVERNMENT PRINTING OFFICE: 1964-550-1668-00018

100-1000

DATA  
FILED  
HARRIS  
JULY 12 1988

