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HYDROCARBON TYPE ANALYSIS OF JET FUELS BY ^1H AND ^{13}C NMR

By
D. A. Netzel
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Date Published: May 1981

Laramie Energy Technology Center
Laramie, Wyoming

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Foreward

The work described in this report was performed under a research program (Cooperative Hydrocarbon Analysis Evaluation, Contract No. MIPR FY1455-80-00621) administered by the Fuels Branch AFWAL/POSF, Fuels and Lubrication Division, Aero Propulsion Laboratory, Air Force Wright Aeronautical Laboratories, Wright Patterson Air Force Base, Ohio. The Air Force Project engineer was Major Donald D. Potter and the principal investigator for LETC was Dr. Daniel A. Netzel. The authors gratefully acknowledge the special technical assistance of Dr. John Duvall (LETC), Mr. Bob Mendoza (University of Wyoming) and AWU Fellowship recipients: Dr. David Barnhart (Eastern Montana College) and Dr. Dale McKay (Colorado State University). The authors are indebted to Dr. Jeffery Solash (Naval Air Propulsion Test Center) for a copy of the computer program for determining average molecular parameters from proton NMR data of aromatic fractions developed by Dr. Clutter et al at the Gulf Research and Development Company, Pittsburgh, PA.

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HYDROCARBON TYPE ANALYSIS OF JET FUELS BY ^1H AND ^{13}C NMR

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ABSTRACT

This report describes the application of NMR spectroscopy to the chemical characterization without prior chromatographic separation of jet fuels and various fuel blends containing varying amounts of paraffinic and aromatic constituents. Equations are derived by which the total percent paraffins and aromatics as well as percent monoaromatics and diaromatics can be calculated. Computer programs for the various calculations are included. The results obtained by NMR are compared to those obtained by MS.

INTRODUCTION

For several years the Department of Defense has had research programs aimed at characterizing and evaluating liquid hydrocarbon fuels obtained from various fossil sources because the chemical composition of a jet fuel affects jet engine performance, power output, engine life and operation cost. The results of these programs have shown that the combustion properties of fuels are directly related to the hydrogen content of a fuel which, in turn, is governed by the amount and types of aromatics in its composition. Heat of combustion, smoke point and luminometer number also has been shown to correlate with the hydrogen content of the fuel. In particular, the smoke point of a fuel depends on a large number of chemical factors: (1) the smoke point varies according to the general trend; paraffins > naphthenes > aromatics, (2) branching and/or branched substituents effectively decreases the smoke point, (3) the smoke point increases as the size of the alkyl substituent increases, (4) mixtures containing naphthalene have lower smoke point than blends of alkyl benzenes at the same concentration and (5) the smoke point correlates better with the percent aromatic carbon as defined by chromatographic procedures than it does with the total aromatic content.

Fuels are complex mixtures of hydrocarbons. However, it is not necessary to perform a complete analysis to determine every component within a fuel to establish correlations between the combustion properties and the fuel composition. A fuel can be characterized in terms of the various compound types or classes because hydrocarbons within a class behave similarly. A number of instrumental methods of analysis have been applied to fuel characterization.

Mass Spectrometry (MS) has often been used as a means of establishing not only compound types but also individual components in fuels. However, it is necessary to separate the fuels into paraffinic, olefinic and aromatic fractions. The separation procedure in conjunction with mass spectrometry is time consuming when many jet fuels and jet fuel blends must be evaluated to establish if specification criteria have been met.

Nuclear magnetic resonance spectroscopy (NMR) has been used extensively to characterize various fossil fuels in terms of average molecular structural parameters. As in previous studies of hydrocarbon mixtures, it was almost always necessary to separate the mixture into paraffinic, olefinic and aromatic fractions. NMR spectroscopy in principle can provide rapid hydrocarbon type analysis without prior sample separation if equations can be derived with a minimum number of assumptions which relate spectral parameters to composition. Myers et al.¹ have determined the hydrocarbon-type distribution in gasoline by NMR without prior separation. Their procedure was modified by Hodgson and Tobias² for aircraft fuels. However, the disadvantage of using these methods are (1) percent total aromatics and diaromatics could not be obtained for fuels having relatively high amounts of diaromatics, and (2) gas chromatographic simulated distillation is needed to obtain the average carbon number of the fuel. Diaromatic content of fuels is necessary for correlations of chemical properties of the fuels with their combustion properties.

This report describes the application of NMR spectroscopy to the chemical characterization without prior chromatographic separation of jet fuels and various fuel blends containing varying amounts of paraffinics and aromatics. Equations are derived by which the total percent paraffins and aromatics as well as percent monoaromatics and diaromatics can be calculated. The results obtained by NMR are compared to those obtained by MS.

EXPERIMENTAL PROCEDURE

- A. Source of Samples: Syncrude JP-4 (DDP-79-263-01), shale JP-4 (Fuel 15B-WPAFB) and 30 blends (VN-80-39 to VN-80-69) were received from Wright-Patterson Air Force Base (WPAFB). A description of the source for each sample is given below:

Sample Designation	Source Description
Syncrude JP-4	JP-4 Jet Fuel Refined from Paraho Shale Oil Crude by Gary Western Refinery in 1975.
Shale JP-4-15B	JP-4 Jet Fuel Refined from Geokinetics Shale Oil Crude by Hydrocarbon Research, Inc. in 1980.
VN-80-61	Same as JP-4-15B above (Second Shipment, Lot 1).
VN-80-67	Same as JP-4-15B above (First Shipment, Lot 2).
VN-80-62	JP-8 Jet Fuel Refined from Paraho Shale Oil Crude by Sohio (Navy Project, 1978-79).
VN-80-41 VN-80-55 VN-80-68	Petroleum Stock JP-4 (Jet Fuel Refined by Different Companies. Military Specification MIL-T-5624K).
VN-80-69	Petroleum Stock JP-5 (Military Specification MIL-T-5624K).

VN-80-42	Petroleum Stock JP-8 (Jet Fuel Refined by Different
VN-80-56	Companies. Military Specification MIL-T-83133).
VN-80-63	Blends of Petroleum Refining Streams (Properties
VN-80-64	Equivalent to Jet Fuels).
VN-80-65	
VN-80-66	
VN-80-53	Petroleum Stock #2 Diesel Fuel (Refined by Different
VN-80-59	Companies).
VN-80-39	A xylene bottom consisting mostly of C-3 alkyl-
	benzenes
VN-80-40	2040 solvent consisting mostly of alkylnaphthalenes
VN-80-54	Gulf mineral seal oil consisting mostly of paraf-
	finic hydrocarbons
VN-80-43	Blend of VN-80-42 and VN-80-54
VN-80-44	Blend of VN-80-42 and VN-80-40
VN-80-45	Blend of VN-80-42 and VN-80-39
VN-80-46	Blend of VN-80-42 and VN-80-39
VN-80-47	Blend of VN-80-42 and VN-80-40
VN-80-48	Blend of VN-80-41 and VN-80-40
VN-80-49	Blend of VN-80-41 and VN-80-40
VN-80-50	Blend of VN-80-41 and VN-80-39
VN-80-51	Blend of VN-80-41 and VN-80-39
VN-80-52	Blend of VN-80-41, VN-80-39 and VN-80-54
VN-80-57	Nearly same as VN-80-48
VN-80-58	Nearly same as VN-80-49
VN-80-60	Blend of VN-80-53 and VN-80-40

The syncrude JP-4 and shale JP-4-15B jet fuels were fractionated into paraffin and aromatic fractions using displacement and elution chromatographic methods. Samples VN-80-42, VN-80-53 and VN-80-62 were also fractionated using only elution chromatography.

B. Chromatographic Separation

1. Displacement Chromatography: Details of this method are given in references 3 and 4. This method used 2-propanol as the eluant,

silica gel as the absorbant and the refractive index to monitor the cut points. The amount of paraffins and aromatics is reported as volume percent.

2. Elution Chromatography: The method uses n-pentane, methyl acetate and/or acetone as the eluants to selectively desorb the paraffins and aromatics from a silica gel column. The amount of hydrocarbon type is reported as weight percent.

C. Elemental Analysis

Carbon and hydrogen elemental analyses using the combustion technique were performed by the General Analysis Section of the Research Support Division at LETC and by Huffman Laboratories of Denver, Colorado, which also reported amounts of nitrogen, sulfur and oxygen. The hydrogen content of the samples was also measured by personnel at WPAFB using low resolution nuclear magnetic resonance spectrometry⁵.

D. Mass Spectrometry

The volume percent of paraffins, monocycloparaffins, dicycloparaffins, alkylbenzenes, indanes and tetralins, indenenes and dihydronaphthalenes and naphthalenes were determined by mass spectrometry for WPAFB (by Monsanto Research Corporation, Dayton Laboratory, Contract No. F33615-78-C-2004), using a modified version of the ASTM procedure D2789-71.

E. Nuclear Magnetic Resonance Spectroscopy

1. Proton NMR: All ^1H NMR data were obtained on a Varian HA-100 CW spectrometer* located at the University of Wyoming. Samples were dissolved in CDCl_3 (~75/25 sample to solvent volume ratio) and 3-12% tetramethylsilane (TMS) was added as an internal reference and signal lock. In some cases, because of spectral artifacts due to the TMS lock signal, it was necessary to dissolve the sample in CHCl_3 and use the proton signal as the lock signal. Ethanol used as an inhibitor in CHCl_3 is evident in these spectra. The observed methylene signal from the fuel samples was corrected for the CH_3 resonance due to the alcohol.
2. Carbon-13 NMR: The ^{13}C spectra were obtained on a Varian CFT-20 FT spectrometer* at LETC. The samples prepared for ^1H NMR studies (5 mm NMR tube) were also used initially to obtain carbon-13 survey spectra, using gated decoupling and with a 5 sec pulse delay. From conclusions based on this study, a second series of samples was prepared, placed in 10 mm NMR tubes and spectra obtained using gated decoupling and a 20 sec pulse delay. These spectra were used for the quantitative results listed in this report.

*Reference to specific brand names does not imply endorsement by the U.S. Department of Energy or the Laramie Energy Technology Center.

RESULTS AND DISCUSSION

The carbon aromaticity (f^C) versus the pulsed delay time were measured for several samples. Figure 1^a is a plot of the fraction of aromatic carbons as a function of the pulse delay time for blend VN-80-61. As can be seen in the Figure, a pulse delay time of 20 sec will still give a low value for the fraction of aromatic carbons in a sample. However, the maximum percent error may be only 6% which is about the best which can be achieved without increasing the experimental time per sample considerably. Superconducting, widebore spectrometers could undoubtedly increase the accuracy, since the sensitivity and sample size would be increased, thus, reducing the total time of the experiment even though long delay times are employed. Relaxation agents though not used in this investigation can also be used to shorten the experimental time and increase the accuracy of the carbon aromaticity value.

A. Investigation of Total Jet Fuels and Blends

The complete set of ^{13}C and ^1H NMR spectra of the jet fuels and blends are too numerous to be included in this report. For illustrative purposes the ^{13}C and ^1H spectra of syncrude JP-4 are shown in Figures 2 and 3, respectively. Figures 4 and 5 are the ^{13}C and ^1H spectra, respectively, of the sample VN-80-64 which is typical of a blended fuel.

For the computation of the various average molecular parameters derived from the NMR data all area measurements have been normalized. The normalized proton and carbon-13 NMR data for all samples studied in this investigation are given in Tables I and II, respectively. Elemental analysis data are given in Table III. The hydrogen analysis data in the table are those received from Wright Patterson Air Force Base except those pertaining to the samples which were fractionated. Definitions of the symbols used in Tables I, II and III and the chemical shift range over which the area integration were performed are given in Table IV.

It was necessary to develop a set of equations for determining mono- and diaromatics applicable to jet fuels and blends prior to any separation. Even though the equations derived are for the special case of jet fuels, they should be applicable to other fossil fuel with slight modifications for triaromatics and olefinic content provided the assumptions made remain valid. Table V list the set of equations for calculating the average molecular structure parameters of hydrocarbon mixtures. The definitions of the symbols are listed in Table VI. A listing of the Computer Program for calculating the parameters of hydrocarbon mixtures is given in Appendix A.

Equation 2 in Table V gives the fraction of monoaromatic molecules to the total number of aromatic molecules in the sample and is identical to the equation given by Clutter et al.⁶. Several assumptions are necessary for this relationship to be valid: (1) The sample contains only mono- and diaromatics which in most cases is valid since triaromatics in jet fuels are almost nonexistent, (2) the unsubstituted non-bridge aromatic ring carbon protons are sufficiently separated in the ^1H spectrum such that the ratio mono-to diaromatic protons can be determined, and (3) the number of substituents in the mono- and diaromatic components is the same. The factor $(6-\text{RS})/(8-\text{RS})$ is necessary to give the proper ratio

since the number of non-bridge aromatic ring carbons is not the same in mono- and diaromatic ring systems. The number of alpha-alkyl substituents (RS) is not known initially and is obtained by an iterative process⁶ using Equations 2 and 3 (Table V).

To obtain the total mole percent of aromatics in the mixture (Equation 5, Table V) it is necessary again to use the factor $(6-RS)/(8-RS)$. The terms $(H_{\beta} - 1.5H_{\alpha-1})/2 + H_{\beta-N}/2 + H_{\gamma}/3$ represent the paraffinic content of the mixture. The H_{β} term (methylene hydrogens) must be corrected for the β -methyl hydrogens of alkyl substituted aromatic ring systems ($1.5 H_{\alpha-1}$) since the chemical shift is in the same region of the n-alkane methylene hydrogens.

From Equation 12, Table V, the fraction of long chain n-alkane can be estimated if the individual n-alkane carbon resonances can be observed with baseline resolution. This is not often the case. Some branch alkane carbons and alkyl carbons of alkylaromatics will give rise to carbon-13 chemical shifts similar to n-alkanes. However, the contribution of these components to the resonance signal of any n-alkane can be assumed to be small⁷. Equation 13, Table V, represents the fraction of α and β alkane carbons of alkylaromatics as well as carbons of the cyclo and branched alkanes.

The set of equations listed in Table V were tested using a hypothetical mixture of 10 mole percent of 2,6-dimethylnaphthalene, 25 mole percent of 1-methyl-2-ethylbenzene and 65 mole percent of n-hexane. Table VII lists the theoretical ¹H and ¹³C NMR and elemental analysis data for this mixture. Table VIII gives the results using the equations in Table V (calculated) and the results obtained by counting carbon and hydrogen atoms (theoretical).

The average molecular structure parameters calculated for the unseparated hydrocarbon mixtures; Syncrude JP-4, shale JP-4-15B and the blends VN-80-39 to VN-80-69, are given in Table IX. Table X lists the paraffinic and aromatic composition of the jet fuels and blends as determined by chromatography, NMR and MS techniques. As may be seen in Table X, the results of paraffinic and aromatic composition by elution chromatography for syncrude JP-4 and shale JP-4-15B is questionable when compared to the NMR and MS techniques. It is also evident from the NMR data that solvent peaks are present in the samples derived from elution chromatography.

The NMR data plotted against the mass spectral data obtained from WPAFB are shown in Figures 6 to 8 for the paraffins/aromatics, monoaromatics and diaromatics, respectively. The solid lines in the figures represent a 1:1 correlation of the two techniques and the dash lines represents an error of $\pm 10\%$. The mole percent as determined by NMR and the volume percent as determined by MS can be correlated since the volume percent as determined by MS is directly related to mole percent as expressed by the equation-of-state of an ideal gas.

As shown in Figure 6 both the aromatic and paraffinic data obtained from NMR and MS, for most part, correlate well with an error of $\pm 10\%$. Only if the aromatic content of a sample is below 20% is the correlation between techniques outside the 10% error limit. It is not possible to conclude

whether the NMR or MS data is in error or both. It is probable that the inherent error of either technique is much greater than $\pm 10\%$ at small absolute values.

The correlation of NMR and MS data for monoaromatics (Figure 7) is quite good even for absolute values less than 20%. The data, however, for diaromatics (Figure 8) does not appear to be as good. This may be due to the fact that the samples contain only very small amounts of diaromatics and estimating the diaromatic content from the NMR spectra proved to be difficult.

B. Investigation of the Fractions Separated from Jet Fuels and Blends

Figures 9 and 10 are the carbon-13 NMR spectra of the paraffin and aromatic fractions, respectively, obtained from syncrude JP-4 by displacement chromatography. The corresponding proton NMR spectra are shown in Figures 11 and 12. The NMR spectra of the paraffinic and aromatic fractions for shale JP-4-15B, VN-80-42, VN-80-53 and VN-80-62 are similar and, thus, not included in this report.

Several sets of equations have been derived by other investigators to determine the average molecular structure parameters of aromatic fractions. Two sets of equations were selected and applied to the aromatic fractions. One set of equations uses only ^1H NMR data while the other set uses both ^1H and ^{13}C NMR data. Using these sets of equations one can compare the results of the different NMR methods and/or the different chromatographic separation schemes.

The average molecular parameters were calculated using the equations of Clutter et al.⁶. This set of equations has the advantage that only proton NMR data is necessary for the computation of the parameters. In addition to the standard average molecular parameters which may be calculated, the number of carbons and hydrogens, molecular weight, carbon aromaticity and weight fraction of carbon and hydrogen can also be determined. Table XI list the parameters calculated for the aromatic fractions of the five samples which have been separated by either displacement or elution chromatography or both. Definitions of the terms used in Table XI are listed in Table XII. For completeness, the equations⁶ used to calculate the parameters are given in Table XIII and the computer program in Appendix B.

Cantor⁸ has derived a similar set of equations for determining average molecular parameters of aromatic fractions using ^1H and ^{13}C NMR data as well as elemental analysis and molecular weight data. Table XIV list the parameters calculated for fuel samples using the set of equations derived by Cantor and the molecular weight calculated by the method of Clutter et al.⁶ (listed in Table XI). Definitions and equations of the terms listed in Table XIV are given in Table XV and XVI, respectively. A listing of the computer program is also given in Appendix B. A survey of similar parameters for the same fuel samples listed in Tables XI and XIV indicate some large discrepancies between the procedures used.

To investigate the source of these discrepancies and the effects of aromaticity and the weight fraction of carbon and hydrogen on the set of

parameters derived by Cantor, the values for the weight fraction of carbon and hydrogen, molecular weight and aromaticity listed in Table XI were used in the set of equations by Cantor⁸. Table XVII list the new set of parameters calculated. The most noticeable change occurred in the number of aromatic carbons per molecule.

Little information can be obtained from the ¹H and ¹³C NMR spectra of the paraffinic fractions of the separated fuels samples. Table XVIII lists the methylene to methyl ration (R^H); the fraction of n-alkane (f^C); the fraction of α - β alkyl carbons of alkylaromatics, branch and/or cyclo alkane carbons ($f^C_{\alpha\beta cb}$) and the average carbon chain length (C_L).

C. Average Molecular Structure Parameters for Samples VN-80-39 and VN-80-40

Samples VN-80-39 and VN-80-40 were chosen to check the validity of the average molecular structure parameter calculations. Sample VN-80-39 is composed mostly of xylenes and other short chain alkyl substituted benzenes (98.7%) while VN-80-40 is composed mostly of alkylbenzenes and alkyl naphthalenes (95.6%). Thus these two samples are essentially aromatic. Average molecular parameters were calculated using the method of Clutter et al.⁶, (Table XIX) and the method of Cantor⁸ (Table XX). Again using the method of Cantor, the parameters were calculated two ways: (A) Using the experimental values for the weight fraction of carbon and hydrogen, the carbon aromaticity and the derived value of the molecular weight from Table XI; and (B) using the derived values for the weight fraction of carbon and hydrogen, the aromaticity and the molecular weight as listed in Table XI. A comparison of the NMR results to the mass spectral results indicate some serious discrepancy.

CONCLUSIONS

It has been determined that the total aromatic and paraffinic content of the jet fuels and blends obtained by NMR and MS correlate well with an error of $\pm 10\%$. If, however, the aromatic content of a sample is below 20%, the correlation between the techniques lie outside the 10% error limit. It was also observed that, if the sample is highly diaromatic such as VN-80-40 (predominantly alkyl naphthalenes), the calculations from NMR data do not agree with mass spectral data.

The correlation of NMR and MS data for monoaromatics is quite good even for absolute values less than 20%. However, the data for diaromatics does not appear to be good possibly because of the relatively small amounts of diaromatics in most samples.

The average molecular structure parameters for the aromatic fractions of syncrude JP-4, shale JP-4-15B, VN-80-42, VN-80-53 and VN-80-62 were calculated using two different methods of calculations. A survey of similar parameters for the same fuel samples indicates some discrepancies between the procedures used. The most noticeable discrepancy occurs in the number of aromatic carbons per molecule.

The two computational procedures applicable to aromatic fractions were applied to samples VN-80-39 and VN-80-40 which are mostly alkylbenzenes and

alkylnaphthalenes, respectively. The NMR results compare favorably with the mass spectral results for VN-80-39 (95.4% for the monoaromatic content versus 98.7%, respectively). However, NMR results for VN-80-40 gives 50.3% monoaromatics, whereas, the MS result was found to be 29.2%. Similar discrepancies were found for the diaromatic content (49.7% and 66.4% from NMR and MS data, respectively).

For the most part, a good correlation exist between NMR and MS data for essentially all of the samples investigated. Additional work will be necessary to improve the correlation of NMR and MS data for samples containing relatively low diaromatic content.

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Figure 1. Carbon Aromaticity as a Function of the Instrument Pulse Delay Time for Blend VN-80-61.

Figure 2. Carbon-13 NMR Spectrum of Syncrude JP-4 Jet Fuel.

Figure 3. Proton NMR Spectrum of Syncrude JP-4 Jet Fuel.

Figure 4. Carbon-13 NMR Spectrum of Blend VN-80-64.

Figure 5. Proton NMR Spectrum of Blend VW-80-64.

Figure 6. Correlation of NMR and MS Data for the Total Aromatics and Paraffinics in Jet Fuels and Blends.

Figure 7. Correlation of NMR and MS Data for Monoaromatics in Jet Fuels and Blends.

Figure 8. Correlation of NMR and MS Data for Diaromatics in Jet Fuels and Blends.

Figure 9. Carbon-13 NMR Spectrum of the Syncrude JP-4 Jet Fuel Paraffinic Fraction Obtained from Displacement Chromatography.

Figure 10. Carbon-13 NMR Spectrum of the Syncrude JP-4 Jet Fuel Aromatic Fraction Obtained from Displacement Chromatography.

Figure 11. Proton NMR Spectrum of the Syncrude JP-4 Jet Fuel Paraffinic Fraction Obtained from Displacement Chromatography.

Figure 12. Proton NMR Spectrum of the Syncrude JP-4 Jet Fuel Aromatic Fraction Obtained from Displacement Chromatography.

TABLE I. NORMALIZED PROTON NMR INTEGRATION DATA

SAMPLE	H _{Mo}	H _{Di}	H _{Tri}	H _{α-1}	H _{α-2}	H _{β-N}	H _β	H _γ	H _{Ar}	H _{α-T}	H _{β-γ}
Synchrude JP-4	.0370	0.0		.0093	.0401	.0833	.4691	.3611	.0370	.0494	.9135
Paraffin Fraction ¹						.1676	.4341	.3984			
Paraffin Fraction ²						.0906	.5227	.3867			
Aromatic Fraction ¹	.2360	.0354		.1563	.3776	.0619	.0973	.0354	.2714	.5339	.1946
Aromatic Fraction ²	.2453	.0161		.1197	.3036	.0876	.1401	.0876	.2613	.4233	.3153
Shale JP-4-15B	.0270	0.0		.0150	.0330	.1231	.4204	.3814	.0270	.0480	.9249
Paraffin Fraction ¹						.1118	.4474	.4408			
Paraffin Fraction ²						.1111	.4798	.4091			
Aromatic Fraction ¹	.2196	.0119		.1543	.2611	.1068	.1365	.1098	.2315	.4154	.3531
Aromatic Fraction ²	.1732	.0056	(.0056) ³	.0335	.2067	.1006	.2458	.2291	.1788	.2400	.5755
VN-80-39	.2986	.0217		.1116	.3159	.0551	.1507	.0464	.3203	.4275	.2522
VN-80-40	.1818	.2696		.2508	.1753	.0408	.0533	.0282	.4514	.4263	.1223
VN-80-41	.0286	0.0		.0086	.0286	.1257	.3886	.4200	.0286	.0372	.9343
VN-80-42	.0259	.0052		.0231	.0288	.1326	.4383	.3460	.0311	.0519	.9169
23 Paraffin Fraction ²						.0952	.4762	.4286			
Aromatic Fraction ²	.1547	.0387		.1436	.2155	.1713	.1657	.1105	.1934	.3591	.4475
VN-80-43	.0248	.0031		.0186	.0248	.0991	.4706	.3591	.0279	.0434	.9288
VN-80-44	.0516	.0804		.0789	.0607	.1032	.3581	.2671	.1321	.1396	.7289
VN-80-45	.0741	.0090		.0327	.0846	.1037	.3930	.3029	.0830	.0119	.7996
VN-80-46	.1449	.0063		.0504	.1575	.0882	.3213	.2315	.1512	.2079	.6410
VN-80-47	.0428	.0494		.0512	.0448	.1279	.3645	.3261	.0921	.0960	.8120
VN-80-48	.0633	.1022		.0806	.0691	.0748	.3165	.2935	.1654	.1497	.6848
VN-80-49	.0463	.0585		.0503	.0531	.1129	.3333	.3456	.1048	.1034	.7918
VN-80-50	.1606	.0061		.0561	.1636	.0924	.2848	.2364	.1667	.2197	.6136
VN-80-51	.1054	.0027		.0403	.1065	.1094	.3235	.3109	.1071	.1468	.7438
VN-80-52	.0449	.0056		.0169	.0449	.1236	.3961	.3680	.0505	.0618	.8877
VN-80-53	.0349	.0349		.0640	.0349	.1047	.4360	.2907	.0698	.0989	.8314
Paraffin Fraction ²						.1460	.5189	.3351			
Aromatic Fraction ²	.1622	.0919	.0054	.2378	.1405	.1459	.1189	.0973	.2595	.3783	.3621
VN-80-54	.0168	.0011		.0095	.0112	.0838	.5869	.2907	.0179	.0207	.9614
VN-80-55	.0409	.0031		.0131	.0367	.0944	.3763	.4354	.0440	.0498	.9061
VN-80-56	.0275	.0041		.0146	.0293	.1024	.4535	.3686	.0316	.0439	.9245

TABLE I. NORMALIZED PROTON NMR INTEGRATION DATA (Continued)

SAMPLE	H _{Mo}	H _{Di}	H _{Tri}	H _{α-1}	H _{α-2}	H _{β-N}	H _{β}	H _{γ}	H _{Ar}	H _{α-T}	H _{β-γ}
VN-80-57	.0676	.0865		.0757	.0784	.0892	.2973	.3054	.1540	.1541	.6919
VN-80-58	.0368	.0613		.0553	.0583	.1288	.3129	.3466	.0982	.1132	.7883
VN-80-59	.0315	.0252		.0505	.0315	.1104	.4543	.2965	.0568	.0820	.8612
VN-80-60	.0480	.0819		.0932	.0593	.1017	.3729	.2429	.1299	.1525	.7175
VN-80-61	.0248	.0031		.0217	.0341	.1672	.3839	.3653	.0279	.0558	.9164
VN-80-62	.0417	.0026		.0339	.0469	.1068	.4427	.3255	.0443	.0808	.8750
Paraffin Fraction ²						.1348	.5605	.3057			
Aromatic Fraction ²	.1936	.0202		.1629	.2640	.0955	.1517	.1180	.2018	.4269	.3652
VN-80-63	.0194	.0129		.0275	.0244	.1068	.4396	.3694	.0323	.0519	.9158
VN-80-64	.0629	.0029		.0229	.1029	.1086	.3714	.3286	.0658	.1258	.8086
VN-80-65	.0279	.0011		.0112	.0391	.1060	.4464	.3683	.0290	.0503	.9207
VN-80-66	.1371	0.0		.0414	.1921	.0650	.1743	.3901	.1371	.2335	.6294
VN-80-67	.0243	.0032		.0162	.0270	.1621	.3782	.3890	.0275	.0432	.9293
VN-80-68	.0320	.0058		.0217	.0352	.1003	.3877	.4176	.0374	.0569	.9056
VN-80-69	.0242	.0097		.0217	.0314	.1111	.4155	.3865	.0338	.0531	.9131

1. Fraction obtained from Displacement Chromatography.
2. Fraction obtained from Elution Chromatography.
3. Olefinic Hydrogens instead of Triaromatic Hydrogens.

TABLE II. NORMALIZED CARBON-13 NMR INTEGRATION DATA

Sample	C _{Ar}	C _{A1}	C ₁	C ₂	C ₃	C _{4, 5, n}
Syncrude JP-4	.1078	.8922	.0987	.1367	.0987	.1443
Paraffin Fraction ¹		1.0	.0969	.1378	.0765	.1327
Paraffin Fraction ²		1.0	.1493	.1306	.1045	.1940
Aromatic Fraction ¹	.6545	.3455				
Aromatic Fraction ²	.5460	.4540				
Shale JP-4-15B	.0680	.9320	.0670	.1088	.0670	.1228
Paraffin Fraction ¹		1.0	.0811	.1216	.0777	.1520
Paraffin Fraction ²		1.0	.1132	.1509	.0503	.1321
Aromatic Fraction ¹	.4930	.5070				
Aromatic Fraction ²	.4255	.5745				
VN-80-39	.6212	.3788				
VN-80-40	.7425	.2575				
VN-80-41	.0817	.9183	.0926	.1253	.0899	.1063
VN-80-42	.0781	.9219	.0677	.0938	.0573	.1432
Paraffin Fraction ²		1.0	.0821	.1194	.0597	.1567
Aromatic Fraction ²	.4724	.5276				
VN-80-43	.0694	.9306	.0566	.0771	.0720	.1594
VN-80-44	.3037	.6963	.0491	.0602	.0524	.1099
VN-80-45	.1979	.8021	.0508	.0615	.0508	.1069
VN-80-46	.3324	.6676	.0423	.0507	.0338	.0676
VN-80-47	.1867	.8133	.0560	.0640	.0720	.1216
VN-80-48	.3609	.6391	.0592	.0799	.0592	.0710
VN-80-49	.2337	.7663	.0761	.0978	.0679	.0978
VN-80-50	.3691	.6309				
VN-80-51	.2485	.7515	.0710	.0947	.0680	.0858
VN-80-52	.1282	.8718	.0846	.1179	.0923	.1282
VN-80-53	.1891	.8109	.0486	.0729	.0820	.1519
Paraffin Fraction ²		1.0	.0916	.1127	.0634	.2078
Aromatic Fraction ²	.6043	.3957				
VN-80-54	.0410	.9590	.0665	.0915	.0942	.2938
VN-80-55	.0982	.9018	.1043	.1288	.0828	.1288
VN-80-56	.0757	.9243	.0730	.0973	.0865	.1378
VN-80-57	.3478	.6522	.0683	.0870	.0621	.0807
VN-80-58	.2241	.7759	.0805	.1035	.0747	.0891
VN-80-59	.1471	.8529	.0559	.0794	.0706	.1588
VN-80-60	.3019	.6981	.0472	.0566	.0629	.1415
VN-80-61	.0733	.9267	.1200	.1067	.1000	.1333
VN-80-62	.1320	.8680	.0755	.1016	.0755	.1625
Paraffin Fraction ²		1.0	.1111	.1389	.0635	.1825
Aromatic Fraction ²	.4679	.5321				
VN-80-63	.0761	.9239	.0831	.1107	.0831	.1730
VN-80-64	.1726	.8274	.0717	.0977	.0782	.1303
VN-80-65	.0757	.9243	.0757	.0973	.0892	.1676
VN-80-66	.3784	.6216				
VN-80-67	.0541	.9459	.0781	.1141	.0961	.1321
VN-80-68	.0769	.9231	.0962	.1282	.0865	.1378
VN-80-69	.0939	.9061	.0718	.0912	.0774	.1381

¹Fraction obtained by Displacement Chromatography²Fraction obtained by Elution Chromatography

TABLE III. ELEMENTAL ANALYSIS DATA
WEIGHT PERCENT

SAMPLE	CARBON (C _f X100)	HYDROGEN (H _f X100)	NITROGEN	SULFUR	OXYGEN
Syncrude JP-4	85.57	14.49	0.195	0.085	0.042
Paraffin Fraction ¹	81.97	15.41			
Paraffin Fraction ²	83.95	15.88			
Aromatic Fraction ¹	89.87	9.77			
Aromatic Fraction ²	87.40	10.08			
Shale JP-4-15B	84.54	14.33			
Paraffin Fraction ¹	84.24	15.63			
Paraffin Fraction ²	84.28	15.66			
Aromatic Fraction ¹	87.80	10.65			
Aromatic Fraction ²	87.38	10.54			
VN-80-39	89.34	10.11			
VN-80-40	91.37	8.27	0.135	0.05	0.265
VN-80-41	84.81	14.48			
VN-80-42	86.50	13.94	0.07	0.12	0.23
Paraffin Fraction ²	85.36	14.74			
Aromatic Fraction ²	88.42	9.77			
VN-80-43	86.73	13.93	0.055	0.155	0.26
VN-80-44	88.36	11.93	0.07	0.075	0.295
VN-80-45	86.30	13.02			
VN-80-46	87.13	12.04			
VN-80-47	86.97	12.93			
VN-80-48	87.60	11.94			
VN-80-49	86.25	12.95			
VN-80-50	88.00	12.08			
VN-80-51	85.81	12.96			
VN-80-52	85.18	14.02			
VN-80-53	86.71	12.89	0.065	0.305	0.26
Paraffin Fraction ²	85.52	15.19			
Aromatic Fraction ²	90.56	8.49			
VN-80-54	85.59	14.18	0.07	0.035	0.51
VN-80-55	85.11	14.47	0.045	0.03	0.10
VN-80-56	86.17	13.92			
VN-80-57	87.76	12.11			
VN-80-58	86.56	13.16			
VN-80-59	87.79	13.16			
VN-80-60	88.95	11.92			
VN-80-61	85.98	14.34			
VN-80-62	85.21	13.81			
Paraffin Fraction ²	87.25	14.89			
Aromatic Fraction ²	90.49	9.89			
VN-80-63	86.34	14.24			
VN-80-64	85.65	13.44			
VN-80-65	85.79	14.04			
VN-80-66	84.98	12.27			
VN-80-67	81.57	14.54	0.22		
VN-80-68	83.83	14.39			
VN-80-69	84.94	13.78			

¹Fraction obtained from Displacement Chromatography

²Fraction obtained from Elution Chromatography

TABLE IV. ELEMENTAL ANALYSIS AND ^1H AND ^{13}C NMR NORMALIZED AREA INPUT PARAMETERS: DEFINITIONS AND EQUATIONS

Symbol	Definitions and/or Equations	Chemical Shift Range (ppm from TMS)
C_f	= Weight Fraction of Carbon (Experimental)	
H_f	= Weight Fraction of Hydrogen (Experimental)	
H_{Mo}	= Monoaromatic Hydrogens	6.6-7.2
H_{Di}	= Diaromatic Hydrogens	7.2-7.8
H_{Tri}	= Triaromatic Hydrogens	7.8-8.3
H_{Ol}	= Olefinic Hydrogens	4.0-6.0
$H_{\alpha-1}$	= Methylene Hydrogens Alpha to Aromatic Ring	2.3-4.0
$H_{\alpha-2}$	= Methyl Hydrogens Alpha to Aromatic Ring	1.9-2.3
$H_{\beta-N}$	= Naphthene Hydrogens Beta to Aromatic Ring	1.6-1.9
H_{β}	= $\beta\text{-CH}_2\text{-}$ and $\beta\text{-CH}_3$ to aromatic Ring and Normal Alkane $\text{-CH}_2\text{-}$ Hydrogens	1.0-1.6
H_{γ}	= $\gamma\text{-CH}_3$ to Aromatic Ring and Normal or Branch Alkane -CH_3 Hydrogens	0.5-1.0
H_{Ar}	= Total Aromatic Hydrogens	6.6-8.3
$H_{\alpha-T}$	= Total Alpha Alkylaromatic Hydrogens	1.9-4.0
$H_{\beta-\gamma}$	= Total Beta-Gamma Alkyl and Alkane Hydrogens	0.5-1.9
C_{Ar}	= Total Aromatic Carbons	100-150
C_{Al}	= Total Aliphatic Carbons	5-50
C_1	= Methyl Carbons of n-Alkanes	13.8-14.2
C_2	= $C_2\text{-Methylene}$ Carbons of n-Alkanes	22.7-23.0
C_3	= $C_3\text{-Methylene}$ Carbons of n-Alkanes	31.8-32.0
$C_{4,5,n}$	= $C_{4,5,n}\text{-Methylene}$ Carbons of n-Alkanes	29-30
H_{Ar}	= $H_{Mo} + H_{Di} + H_{Tri}$	(1)
$H_{\alpha-T}$	= $H_{\alpha-1} + H_{\alpha-2}$	(2)
$H_{\beta-\gamma}$	= $H_{\beta-N} + H_{\beta} + H_{\gamma}$	(3)

TABLE V. EQUATIONS FOR CALCULATING THE AVERAGE MOLECULAR
STRUCTURE PARAMETERS OF HYDROCARBON MIXTURES

$$f_a^H = \frac{H_{Ar}}{H_T}, \text{ where } H_T = H_{Ar} + H_{\alpha-T} + H_{\beta-\gamma} \quad (1)$$

$$f_{Mo} = \frac{H_{Mo}}{H_{Mo} + [(6-RS)/(8-RS)]H_{Di}} \quad (2)$$

$$RS = \frac{(8-2f_{Mo})(H_{\alpha-1})/2 + (H_{\alpha-2})/3}{H_{Mo} + H_{Di} + (H_{\alpha-1})/2 + (H_{\alpha-2})/3} \quad (3)$$

$$f_{Di} = 1 - f_{Mo} \quad (4)$$

$$\%Ar = \frac{[(6-RS)/(8-RS)]H_{Di} + H_{Mo} + (H_{\alpha-1})/2 + (H_{\alpha-2})/3}{[(6-RS)/(8-RS)]H_{Di} + H_{Mo} + (H_{\alpha-1})/2 + (H_{\alpha-2})/3 + H_p} \cdot 100 \quad (5)$$

$$\text{where } H_p = (H_{\beta} - 1.5H_{\alpha-1})/2 + (H_{\beta-N})/2 + (H_{\gamma})/3$$

$$\%Ar^{Mo} = \%Ar(f_{Mo}) \quad (6)$$

$$\%Ar^{Di} = \%Ar(f_{Di}) \quad (7)$$

$$\%Par = 100 - \%Ar \quad (8)$$

$$R^H = \frac{3(H_{\beta} - 1.5H_{\alpha-1})}{2H_{\gamma}} \quad (9)$$

$$f_a^C = \frac{C_{Ar}}{C_{Ar} + C_{Al}} \quad (10)$$

$$C_L = \frac{2(C_{4,5,n})}{C_1} + 6 \quad (11)$$

$$f_n^C = \frac{C_1 + C_2 + C_3 + C_{4,5,n}}{C_{Al}} \quad (12)$$

$$f_{\alpha\beta cb}^C = 1 - f_n^C \quad (13)$$

$$(H/C)_T = (12.01)H_f / (1.008)C_f \quad (14)$$

$$(H/C)_{Ar} = (12.01)H_f \cdot f_a^H / (1.008)C_f \cdot f_a^C \quad (15)$$

$$(H/C)_{Al} = (12.01)H_f \cdot (1 - f_a^H) / (1.008)C_f \cdot (1 - f_a^C) \quad (16)$$

$$f_{s+b}^C = f_a^C - (H/C)_T \cdot f_a^H \quad (17)^9$$

$$f_u^C = (H/C)_T \cdot f_a^H \quad (18)^9$$

TABLE VI. DEFINITIONS OF SYMBOLS USED IN CALCULATING THE AVERAGE MOLECULAR STRUCTURE PARAMETERS OF HYDROCARBON MIXTURES

f_a^H	=	Aromaticity-Hydrogen (Fraction of Aromatic Hydrogens)
f_{Mo}	=	Fraction of Monoaromatic Rings
f_{Di}	=	Fraction of Diaromatic Rings
f_a^C	=	Aromaticity-Carbon (Fraction of Aromatic Carbons)
f_{s+b}^C	=	Fraction of Bridged and Substituted Aromatic Carbons
f_u^C	=	Fraction of Unsubstituted Aromatic Carbons
RS	=	Number of Alpha Alkyl Carbons per Aromatic Molecule
R^H	=	Methylene to Methyl Ratio (CH_2/CH_3) of Normal and/or Branched Alkanes
f_n^C	=	Fraction of n-Alkane Carbons
$f_{\alpha\beta cb}^C$	=	Fraction of α and β Alkane Carbons of Alkylaromatic and Cyclo and Branched Alkane Carbons
C_L	=	Average Carbon Chain-length
$(H/C)_T$	=	Total Hydrogen to Carbon Ratio
$(H/C)_{Ar}$	=	Aromatic Hydrogen to Carbon Ratio
$(H/C)_{Al}$	=	Aliphatic Hydrogen to Carbon Ratio
%Ar	=	Total Mole Percent Aromatics
%Ar ^{Mo}	=	Mole Percent Monoaromatics
%Ar ^{Di}	=	Mole Percent Diaromatics
%Par	=	Mole Percent Paraffins

TABLE VII. HYPOTHETICAL HYDROCARBON MIXTURE: INPUT DATA

<u>Compounds</u>	<u>Mole Percent</u>
2,6-Dimethylnaphthalene	10
1-Methyl-2-Ethylbenzene	25
n-Hexane	65
<u>Theoretical Proton NMR Data</u>	<u>Normalized Area</u>
H _{Mo} , Monoaromatic Hydrogens	.0752
H _{Di} , Diaromatic Hydrogens	.0451
H _{α-1} , Methylene Hydrogens Alpha to Aromatic Ring	.0376
H _{α-2} , Methyl Hydrogens Alpha to Aromatic Ring	.1015
H _β , β-CH ₂ and β-CH ₃ to Aromatic Ring and Normal Alkane -CH ₂ Hydrogens	.4474
H _γ , γ-CH ₃ to Aromatic Ring and Normal Alkane -CH ₃ Hydrogens	.2932
<u>Theoretical Carbon-13 NMR Data</u>	
C _{Ar} , Total Aromatic Carbons	.3401
C _{Al} , Total Aliphatic Carbons	.6599
C ₁ , Methyl Carbons of n-Hexane	.1769
C ₂ , C ₂ -Methylene Carbons of n-Hexane	.1769
C ₃ , C ₃ -Methylene Carbons of n-Hexane	.1769
<u>Elemental Analysis</u>	<u>Weight Fraction</u>
C _f , Weight fraction of carbon	.8607
H _f , Weight fraction of Hydrogen	.1393

TABLE VIII. AVERAGE MOLECULAR STRUCTURE PARAMETERS CALCULATED FOR THE
HYPOTHETICAL HYDROCARBON MIXTURE

<u>Parameter</u>	<u>Theoretical</u>	<u>Calculated</u>
f_a^H , Hydrogen Aromaticity	.1203	.12
f_a^C , Carbon Aromaticity	.3401	.34
%Ar, Total Mole Percent Aromatics	35.0	35.0
%Mo, Mole Percent Monoaromatic	25.0	25.0
%Di, Mole Percent Diaromatic	10.0	10.0
f_{Mo} , Fraction of Monoaromatic Molecules	.7142	.71
f_{Di} , Fraction of Diaromatic Molecules	.2858	.29
f_{s+b}^C , Fraction of Bridged and Substituted Aromatic Carbons	.1224	.11
f_u^C , Fraction of Unsubstituted Aromatic Carbons	.2177	.23
RS, Number of Alpha Carbons per Aromatic Molecule	2.0	2.0
%Par, Total Mole Percent of Paraffins	65.0	65.0
f_n^C , Fraction of n-Alkane Carbons	.8041	.80
$f_{\alpha\beta cb}^C$, Fraction of α and β Alkane Carbons of Alkylaromatics and Cyclo and Branched Alkanes	.1959	.20
C_L , Average Carbon Chain-Length of n-Alkanes	6	6
R^H , Methylene to Methyl Ratio of Normal and/or Branched Alkanes	2	2
$(H/C)_T$, Total Hydrogen to Carbon Ratio	1.8095	1.93
$(H/C)_{Ar}$, Aromatic Hydrogen to Carbon Ratio	.64	.68
$(H/C)_{Al}$, Alkane Hydrogen to Carbon Ratio	2.55	2.57

TABLE IX. CALCULATED AVERAGE MOLECULAR STRUCTURE PARAMETERS FOR JET FUELS AND BLENDS

SAMPLE	f_a^H	f_{Mo}	f_{Di}	f_a^C	f_{s+b}^C	f_u^C	RS	R^H	f_n^C	$f_{\alpha\beta cb}^C$	C_L	$(H/C)_T$	$(H/C)_{Ar}$	$(H/C)_{Al}$
Syncrude														
JP-4	.04	1.00	.00	.11	.03	.07	1.96	1.89	.54	.46	9.0	2.02	.69	2.18
Shale														
JP-4-15B	.03	1.00	.00	.07	.01	.05	2.44	1.57	.39	.61	9.7	2.02	.80	2.11
VN-80-39	.32	.95	.05	.62	.19	.43	2.04	----	.00	1.00	0.0	1.35	.70	2.42
40	.45	.50	.50	.74	.26	.49	2.02	----	.00	1.00	0.0	1.08	.66	2.30
41	.03	1.00	.00	.08	.02	.06	1.96	1.34	.45	.55	8.3	2.03	.71	2.15
42	.03	.89	.11	.08	.02	.06	2.52	1.75	.39	.61	10.2	1.92	.76	2.02
43	.03	.93	.07	.07	.02	.05	2.38	1.85	.39	.61	11.6	1.91	.77	2.00
44	.13	.49	.51	.30	.09	.21	2.18	1.35	.39	.61	10.7	1.61	.70	2.01
45	.08	.93	.07	.20	.05	.15	2.15	1.70	.34	.66	10.2	1.80	.75	2.05
46	.15	.97	.03	.33	.08	.25	2.06	1.59	.29	.71	9.2	1.65	.75	2.09
47	.09	.57	.43	.19	.02	.16	2.10	1.32	.39	.61	10.3	1.77	.87	1.98
48	.17	.48	.52	.36	.09	.27	1.93	1.00	.42	.58	8.4	1.62	.75	2.12
49	.10	.54	.46	.23	.05	.19	2.01	1.12	.44	.56	8.6	1.79	.80	2.09
50	.17	.98	.02	.37	.10	.27	2.00	1.27	.00	1.00	0.0	1.64	.74	2.16
51	.11	.98	.02	.25	.05	.19	2.05	1.27	.43	.57	8.4	1.80	.78	2.14
52	.05	.92	.08	.13	.03	.10	1.95	1.51	.49	.51	9.0	1.96	.77	2.14
53	.07	.61	.39	.19	.07	.12	2.61	1.75	.44	.56	12.3	1.77	.65	2.03
54	.02	.96	.04	.04	.01	.04	1.96	2.96	.57	.43	14.8	1.97	.86	2.02
55	.04	.95	.05	.10	.01	.09	1.82	1.23	.49	.51	8.5	2.02	.91	2.15
56	.03	.91	.09	.08	.01	.06	2.17	1.76	.43	.57	9.8	1.92	.80	2.02
57	.15	.54	.46	.35	.09	.25	2.03	.90	.46	.54	8.4	1.64	.73	2.13
58	.10	.48	.52	.22	.05	.18	2.28	1.00	.45	.55	8.2	1.81	.79	2.11
59	.06	.66	.34	.15	.05	.10	2.58	1.92	.43	.57	11.7	1.79	.69	1.98
60	.13	.48	.52	.30	.09	.21	2.38	1.44	.44	.56	12.0	1.60	.69	1.99
61	.03	.93	.07	.07	.01	.06	2.72	1.44	.49	.51	8.2	1.99	.84	2.07
62	.04	.96	.04	.13	.05	.09	2.57	1.81	.48	.52	10.3	1.93	.65	2.13
63	.03	.71	.29	.08	.01	.06	2.66	1.62	.49	.51	10.3	1.97	.83	2.06
64	.07	.97	.03	.17	.05	.12	2.48	1.54	.40	.60	9.6	1.87	.71	2.11
65	.03	.98	.02	.08	.02	.06	2.37	1.75	.47	.53	10.4	1.95	.75	2.05
66	.14	1.00	.00	.38	.14	.24	2.29	.43	.00	1.00	0.0	1.72	.63	2.38
67	.03	.92	.08	.05	.00	.06	2.36	1.37	.44	.56	9.4	2.12	1.08	2.18
68	.04	.89	.11	.08	.00	.08	2.32	1.28	.49	.51	8.9	2.00	.98	2.08
VN-80-69	.03	.80	.20	.09	.03	.07	2.47	1.49	.42	.58	9.9	1.93	.70	2.06

TABLE X. PARAFFINIC AND AROMATIC COMPOSITION OF JET FUELS AND BLENDS BY CHROMATOGRAPHY,
NUCLEAR MAGNETIC RESONANCE AND MASS SPECTRAL TECHNIQUES

SAMPLE	CHROMATOGRAPHY				NMR				MS			
	ELUTION		DISPLACEMENT		MOLE PERCENT				VOLUME PERCENT			
	WEIGHT PERCENT		VOLUME PERCENT		PARAFFINS (%Par)	TOTAL AROMATICS (%Ar)	MONO- AROMATICS (%Ar ^{MO})	DI- AROMATICS (%Ar ^{DI})	PARAFFINS	TOTAL AROMATICS	MONO- AROMATICS	DI- AROMATICS
	PARAFFINS	AROMATICS	PARAFFINS	AROMATICS								
Syncrude												
JP-4	73	31	87	13	87.6	12.4	12.4	0.0	88.6	11.4	11.4	0.0
Shale												
JP-4-15B	75	21			89.5	10.5	10.5	0.0	89.0	11.0	11.0	0.0
VN-80-39					6.8	93.2	88.9	4.3	1.3	98.7	98.7	0.0
40					---	---	---	---	4.4	95.6	29.2	66.4
41					90.2	9.8	9.8	0.0	90.0	10.0	9.5	0.5
42	87	19			88.4	11.6	10.3	1.3	86.8	13.2	11.3	1.9
43					89.8	10.2	9.4	0.8	87.2	12.8	11.0	1.8
44					61.4	38.6	19.1	19.5	61.1	38.9	16.9	22.0
45					72.3	27.7	25.7	2.0	68.7	31.3	29.7	1.6
46					51.8	48.2	46.8	1.4	47.8	52.2	51.4	0.8
47					73.2	26.8	15.2	11.6	74.0	26.0	14.1	11.9
48					54.5	45.5	21.9	23.6	58.3	41.7	17.2	24.5
49					70.1	29.9	16.2	13.7	72.3	27.7	14.0	13.7
50					47.7	52.3	51.0	1.3	46.5	53.5	53.1	0.4
51					64.0	36.0	35.4	0.6	64.7	35.3	34.9	0.4
52					83.7	16.3	15.0	1.3	84.6	15.4	14.9	0.5
53	73	32			76.1	23.9	14.7	9.2	78.4	21.6	14.1	7.5
54					94.2	5.8	5.5	0.3	93.2	6.8	6.0	0.8
55					85.7	14.3	13.6	0.7	86.5	13.5	13.5	0.0
56					89.2	10.8	9.8	1.0	86.4	13.6	11.7	1.9
57					55.8	44.2	23.9	20.3	58.7	41.3	19.2	22.1
58					70.4	29.6	14.2	15.4	73.1	26.9	15.0	11.9
59					80.5	19.5	13.0	6.5	81.9	19.1	13.7	5.4
60					59.8	40.2	19.2	21.0	61.5	38.5	17.6	20.9
61					88.6	11.4	10.6	0.8	89.0	11.0	11.0	0.0
62	87	19			82.5	17.5	16.8	0.7	79.5	20.5	19.7	0.8
63					88.4	11.6	8.2	3.4	89.5	10.5	8.4	2.1
64					75.1	24.9	24.2	0.7	72.5	27.5	26.8	0.7
65					89.2	10.8	10.5	0.3	86.2	13.8	13.1	0.7
66					49.6	50.4	50.4	0.0	44.6	55.4	55.0	0.4
67					89.9	10.1	9.3	0.8	89.9	10.1	10.1	0.0
68					86.3	13.7	12.3	1.4	88.9	11.1	10.9	0.2
VN-80-69					87.9	12.1	9.6	2.5	82.6	17.4	14.6	2.8

TABLE XI. AVERAGE MOLECULAR STRUCTURE PARAMETERS CALCULATED FROM ^1H NMR DATA
FOR THE AROMATIC FRACTION OF JET FUELS AND BLENDS

PARAMETER	SYNCRUDE JP-4 CHROMATOGRAPHY		SHALE JP-4-15B CHROMATOGRAPHY		VN-80-42	VN-80-53 CHROMATOGRAPHY	VN-80-62
	DISPLACEMENT	ELUTION	DISPLACEMENT	ELUTION	ELUTION	ELUTION	ELUTION
%Ar	91.41	95.9	96.67	97.88	86.49	76.66	93.90
%DAr	8.59	4.08	3.33	2.12	13.5	22.15	6.10
%TAr	0.00	0.00	0.00	0.00	0.00	4.19	0.00
f_a^{CH}	.6112	.5677	.5340	.4249	.4729	.5586	.5232
R_A	1.09	1.04	1.03	1.02	1.14	1.31	1.06
#C _A	6.34	6.16	6.13	6.08	6.54	7.22	6.24
#C ₁	6.17	6.08	6.07	6.04	6.27	6.61	6.12
%AS	43.2	38.2	41.6	32.4	43.0	39.8	44.4
R_N	.40	.63	.82	1.15	1.58	1.12	.76
%C _N	13.5	20.3	24.9	28.1	40.0	30.27	22.3
%C _S	38.9	43.2	46.6	57.5	52.7	44.1	47.7
R_S	2.64	2.32	2.52	1.96	2.67	2.58	2.71
n	1.52	2.02	2.13	4.21	2.73	2.21	2.10
#C	10.38	10.86	11.49	14.32	13.83	12.93	11.93
#H	12.92	14.37	15.30	22.70	18.47	15.32	16.01
MW	137.69	144.88	153.38	194.87	184.72	170.72	159.48
C_f	.9054	.9000	.8994	.8826	.8992	.9095	.8988
H_f	.0946	.1000	.1006	.1174	.1008	.0905	.1012

TABLE XII. AVERAGE MOLECULAR STRUCTURE PARAMETERS FROM
PROTON NMR DATA: DEFINITIONS

%MAr	=	Percent of Monoaromatics
%DAr	=	Percent of Diaromatics
%TAr	=	Percent of Triaromatics
f_a^{CH}	=	Carbon Aromaticity (Calculated from Proton NMR)
R_A	=	Average Number of Aromatic Rings per Average Alkylaromatic Molecule
$\#C_A$	=	Average Number of Aromatic Ring Carbon Atoms per Average Alkylaromatic Molecule
$\#C_1$	=	Average Number of Non-bridge Aromatic Ring Carbon Atoms per Average Alkylaromatic Molecule
%AS	=	Percent Substitution of Alkyl Groups on Non-bridged Alkylaromatic Ring Carbons
R_N	=	Average Number of Naphthenic Rings per Average Alkylaromatic Molecule
%C _N	=	Percent Naphthenic Carbons
%C _S	=	Percent Saturate Carbons
R_S	=	Average Number of Alkyl Substituents per Average Alkylaromatic Molecule
n	=	Average Number of Carbon Atoms per Alkyl Substituent
$\#C$	=	Number of Carbon Atoms per Average Alkylaromatic Molecule
$\#H$	=	Number of Hydrogen Atoms per Average Alkylaromatic Molecule
MW	=	Average Molecular Weight (Calculated)
C_f	=	Weight Fraction of Carbon (Calculated)
H_f	=	Weight Fraction of Hydrogen (Calculated)

TABLE XIII. AVERAGE MOLECULAR STRUCTURE PARAMETERS FROM
PROTON NMR DATA: EQUATIONS⁶

%Ar	=	$100f_{Mo}$	(1)
%DAr	=	$100(f_{Di} - f_{Tri})$	(2)
%TAr	=	$100f_{Tri}$	(3)
f_a^{CH}	=	$\#C_A/\#C$	(4)
R_A	=	$1 + f_{Di} + 2f_{Tri}$	(5)
$\#C_A$	=	$6f_{Mo} + 10f_{Di} + 14f_{Tri}$	(6)
$\#C_1$	=	$6f_{Mo} + 8f_{Di} + 10f_{Tri}$	(7)
%AS	=	$100(RS)(f_{Mo}/6 + f_{Di}/8 + f_{Tri}/10)$	(8)
R_N	=	$[H_{\beta-N}(1-AS)\#C_1]/2H_{Ar}$	(9)
%C _N	=	$100(3.5R_N/\#C)$	(10)
%C _S	=	$100(1 - \#C_A/\#C)$	(11)
RS	=	$\frac{(8-2f_{Mo})[(H_{\alpha-1})/2 + (H_{\alpha-2})/3]}{H_{Mo} + H_{Di} + (H_{\alpha-1})/2 + (H_{\alpha-2})/3}$	(12)
n	=	$\frac{(H_{\alpha-1})/2 + (H_{\alpha-2})/3 + 3(H_{\beta-N})/4 + (H_{\beta})/2 + (H_{\gamma})/3}{(H_{\alpha-1})/2 + (H_{\alpha-2})/3}$	(13)
#C	=	$\#C_A + \frac{(H_{\alpha-1})/2 + (H_{\alpha-2})/3 + 3(H_{\beta-N})/4 + (H_{\beta})/2 + (H_{\gamma})/3}{H_{Ar} + (H_{\alpha-1})/2 + (H_{\alpha-2})/3} \#C_1$	(14)
#H	=	$1 + \frac{H_{\alpha-1} + H_{\alpha-2} + H_{\beta} + H_{\beta-N} + H_{\gamma}}{H_{Ar}} (1 - AS)\#C_1$	(15)
MW ⁻	=	$12.01(\#C) + 1.008(\#H)$	(16)
C _f ⁻	=	$\frac{12.011(\#C)}{MW^-}$	(17)
H _f ⁻	=	$\frac{1.008(\#H)}{MW^-}$	(18)
f _{Mo}	=	$\frac{H_{Mo}}{H_{Mo} + H_{Di} \frac{(6 - RS)}{(8 - RS)}}$	(19)

TABLE XIII. AVERAGE MOLECULAR STRUCTURE PARAMETERS FROM
PROTON NMR DATA: EQUATIONS⁶ (Continued)

f_{Di}	=	$1 - f_{Mo}$	(20)
f_{Tri}	=	$f_{Di}(8 - RS)H_{Tri} / 2H_{Di}$	(21)
f_{Di}	=	$f'_{Di} - f_{Tri}$	(22)
$\#C_{Mo}$	=	$6f_{Mo}$	(23)
$\#C_{Di}$	=	$10f_{Di}$	(24)
$\#C_{Tri}$	=	$14f_{Tri}$	(25)
$\#C_{Br}$	=	$2f_{Di} + 4f_{Tri}$	(26)
AS	=	$\%AS/100$	(27)

TABLE XIV. AVERAGE MOLECULAR STRUCTURE PARAMETERS CALCULATED FROM ELEMENTAL ANALYSIS,
¹H AND ¹³C NMR DATA FOR THE AROMATIC FRACTION OF JET FUELS AND BLENDS¹

PARAMETERS	SYNCRUDE JP-4 CHROMATOGRAPHY		SHALE JP-4-15B CHROMATOGRAPHY		VN-80-42	VN-80-53 CHROMATOGRAPHY	VN-80-62
	DISPLACEMENT	ELUTION	DISPLACEMENT	ELUTION	ELUTION	ELUTION	ELUTION
f _a ^C	.6545	.5460	.4930	.4255	.4724	.6043	.4679
R _A	1.24	.60	.34	.98	.87	1.71	.40
#C _A	6.74	5.75	5.52	6.03	6.42	7.78	5.62
#C _S	3.56	4.79	5.68	8.14	7.17	5.09	6.39
#C ₁	6.26	6.56	6.85	6.07	6.68	6.36	6.82
%AS	41.7	41.8	44.8	39.5	47.8	40.9	50.5
R _N	-0.03	.77	.95	.97	.50	1.03	1.88
R _S	2.61	2.74	3.07	2.40	3.19	2.60	3.45
n	1.36	1.74	1.85	3.40	2.25	1.96	1.86
r	-0.01	.28	.31	.41	.47	.40	.54
C _A	.588	.477	.433	.372	.418	.547	.423
C ₁	.546	.544	.537	.374	.435	.448	.514
C ₁ ^S	.228	.227	.241	.148	.208	.183	.260
C ₁ ^U	.319	.317	.296	.226	.227	.265	.254
f	4.36	5.33	5.44	5.84	5.92	5.70	6.15
f ₁	22.18	18.11	17.56	19.73	22.11	24.84	20.02
f _{s+b} ^C	.303	.187	.158	.167	.218	.314	.191

¹Molecular Weight Data from Table XI

TABLE XV. AVERAGE MOLECULAR STRUCTURE PARAMETERS FROM
¹H AND ¹³C NMR DATA: DEFINITIONS

C_f	=	Weight Fraction of Carbon (Experimental)
H_f	=	Weight Fraction of Hydrogen (Experimental)
MW	=	Average Molecular Weight (Experimental)
f_a^C	=	Fraction of Carbons Which Are Aromatic (Carbon Aromaticity)
R_A	=	Number of Fused Aromatic Rings per Alkylaromatic Molecule
$\#C_A$	=	Average Number of Aromatic Carbons per Alkylaromatic Molecule
$\#C_S$	=	Number of Saturate Carbons per Alkylaromatic Molecule
$\#C_1$	=	Number of Non-bridged Aromatic Carbons per Alkylaromatic molecule
%AS	=	Percent Substitution of Non-bridged Aromatic Carbon Atoms
R_N	=	Number of Saturate Rings per Alkylaromatic Molecule
n	=	Number of Carbon Atoms per Substituent
r	=	Number of Saturate Rings per Substituent
C_A	=	Weight Fraction of Sample Which is Aromatic Carbon
C_1	=	Weight Fraction of Sample Which is Non-bridge Aromatic Carbon
C_1^S	=	Fraction of C_1 Aromatic Carbons Which are Alkyl Substituted
C_1^U	=	Fraction of C_1 Aromatic Carbons Which Are Unsubstituted
f	=	C/H Weight Ratio in Alkyl Groups
f_1	=	C/H Weight Ratio in Aromatic Groups
f_{s+b}^C	=	Fraction of Bridged and Substituted Aromatic Carbons

TABLE XVI. AVERAGE MOLECULAR STRUCTURE PARAMETERS FROM
¹H AND ¹³C NMR DATA: EQUATIONS⁸

f_a^c	=	$C_{Ar}/(C_{Ar} + C_{Al})$	(1)
R_A	=	$1 + (\#C_A - \#C_1)/2$	(2)
$\#C_A$	=	$C_A MW/12.011$	(3)
$\#C_s$	=	$C_{Al} C_f MW/12.011$	(4)
$\#C_1$	=	$C_1 MW/12.011$	(5)
%AS	=	$100 C_1^S / C_1$	(6)
R_N	=	$r R_S$	(7)
R_S	=	$\%AS \#C_1 / 100$	(8)
n	=	$(H_{\alpha-T} + H_{\beta-\gamma}) / H_{\alpha-T}$	(9)
r	=	$n + 0.5 - 6n/f$	(10)
C_A	=	$f_a^c C_f$	(11)
C_1	=	$C_1^S + C_1^U$	(12)
C_1^S	=	$C_{Al} C_f / n$	(13)
C_1^U	=	$12.011 H_{Ar} H_f$	(14)
f	=	$C_{Al} C_f / (H_{\alpha-T} + H_{\beta-\gamma}) H_f$	(15)
f_1	=	$C_{Ar} C_f / H_{Ar} H_f$	(16)
f_{s+b}^c	=	$f_a^c - \frac{(12.011) H_f \cdot H_{Ar}}{(1.008) C_f \cdot H_T}$	(17) ⁹

TABLE XVII. AVERAGE MOLECULAR STRUCTURE PARAMETERS CALCULATED FROM ^1H AND ^{13}C NMR DATA FOR THE AROMATIC FRACTION OF JET FUELS AND BLENDS¹

PARAMETERS	SYNCRUDE JP-4 CHROMATOGRAPHY		SHALE JP-4-15B CHROMATOGRAPHY		VN-80-42	VN-80-53 CHROMATOGRAPHY	VN-80-62
	DISPLACEMENT	ELUTION	DISPLACEMENT	ELUTION	ELUTION	ELUTION	ELUTION
f_a^{CH}	.6112	.5677	.5340	.4249	.4729	.5586	.5232
R_A	.93	.84	.83	.78	.85	1.15	.86
$\#C_A$	6.34	6.16	6.13	6.08	6.54	7.22	6.24
$\#C_S$	4.04	4.69	5.35	8.23	7.29	5.71	5.69
$\#C_1$	6.49	6.48	6.46	6.52	6.85	6.92	6.52
%AS	45.6	41.5	44.8	37.2	47.4	42.1	47.1
R_N	.78	.69	.88	.12	1.41	1.45	.84
R_S	2.96	2.69	2.89	2.42	3.25	2.92	3.07
n	1.36	1.74	1.85	3.40	2.25	1.96	1.86
r	.26	.25	.30	.05	.43	.50	.27
C_A	.553	.511	.480	.375	.425	.508	.470
C_1	.566	.537	.506	.402	.445	.487	.491
C_1^S	.258	.223	.227	.149	.211	.205	.231
C_1^U	.308	.314	.280	.252	.234	.282	.260
f	5.11	5.27	5.42	5.30	5.83	5.99	5.34
f_1	21.56	19.55	20.63	17.86	21.82	21.64	21.74
f_{s+b}^C	.273	.222	.226	.140	.215	.251	.238

¹Input data for carbon aromaticity, weight fractions of carbon and hydrogen, and molecular weight from Table XI.

TABLE XVIII. AVERAGE MOLECULAR STRUCTURE PARAMETERS CALCULATED FROM ^1H AND ^{13}C NMR DATA FOR THE PARAFFIN FRACTION OF JET FUELS AND BLENDS

PARAMETERS	SYNCRUDE JP-4 CHROMATOGRAPHY		SHALE JP-4-15B CHROMATOGRAPHY		VN-80-42	VN-80-53 CHROMATOGRAPHY	VN-80-62
	DISPLACEMENT	ELUTION	DISPLACEMENT	ELUTION	ELUTION	ELUTION	ELUTION
R^H	1.63	2.05	1.52	1.76	1.67	2.32	2.72
f_n^C	.44	.58	.43	.45	.42	.48	.50
$f_{\alpha\beta cb}^C$	.56	.42	.57	.55	.58	.52	.50
C_L	8.74	8.60	9.75	8.33	9.82	10.54	9.29

TABLE XIX. AVERAGE MOLECULAR PARAMETERS FROM ^1H NMR
DATA FOR BLENDS VN-80-39 AND VN-80-40

PARAMETERS	VN-80-39	VN-80-40
%MAr	95.39	50.34
%DAr	4.61	49.66
%TAr	0.0	0.0
f_a^{CH}	.6250	.7433
R_A	1.05	1.50
$\#C_A$	6.18	7.99
$\#C_1$	6.09	6.99
%AS	33.6	29.5
R_N	.34	.22
%C _N	12.31	7.25
%C _S	37.5	25.7
RS	2.04	2.02
n	1.82	1.36
#C	9.90	10.74
#H	12.63	10.91
MW	131.58	140.05
C_f'	.9032	.9215
H_f'	.0968	.0785

TABLE XX. AVERAGE MOLECULAR PARAMETERS FROM ^1H AND ^{13}C
NMR DATA FOR BLENDS VN-80-39 AND VN-80-40

PARAMETERS	VN-80-39		VN-80-40	
	A ¹	B ²	A	B
$f_a^C; f_a^{CH}$	.6212	.6250	.7425	.7433
R_A	.74	.89	1.28	1.44
$\#C_A$	6.08	6.18	7.91	7.99
$\#C_S$	3.71	3.71	2.74	2.76
$\#C_1$	6.59	6.41	7.36	7.11
%AS	35.4	36.4	29.0	30.1
R_N	.35	.55	.64	.82
R_S	2.33	2.33	2.13	2.14
n	1.59	1.59	1.29	1.29
r	.15	.24	.30	.38
C_A	.555	.565	.678	.685
C_1	.601	.585	.631	.610
C_1^S	.213	.213	.183	.184
C_1^U	.389	.372	.448	.426
f	4.92	5.15	5.19	5.49
f_1	17.14	18.21	18.17	19.32
f_{s+b}^C	.189	.216	.256	.285

1. Method A calculations based on experimental data for carbon aromaticity, weight fractions of carbon and hydrogen. Molecular weight from Table XIX.
2. Method B calculations based on carbon aromaticity, weight fractions of carbon and hydrogen and molecular weight data from Table XIX.

APPENDIX A

Computer Program to Determine Average Molecular Structure Parameters for Hydrocarbon Mixtures

```

PROGRAM MIXPRAM (MXDATA,PRAM,OUTPUT,MXLBL,TAPE16=MXLBL,
1    TAPE6=OUTPUT,TAPE10=PRAM,TAPE15=MXDATA)
C *****
C PROGRAM TO DETERMINE AVERAGE MOLECULAR PARAMETERS USING JUST
C PROTON NMR DATA, CARBON 13 NMR DATA, AND CHEMICAL ANALYSIS
C OF CARBON AND HYDROGEN WEIGHT FRACTIONS.
C *****
C
C SUBROUTINES,FILES ,AND FUNCTIONS USED
C
C *****
C
C 1)FUNCTION DIVZERO
C     THIS FUNCTION CHECKS FOR ZERO VALUES WHICH
C     WILL RESULT IN DIVISION BY ZERO THUS TERMINATING
C     THE PROGRAM RUN.
C
C 2) MXDATA
C     THIS LOCAL FILE PROVIDES THE DATA FOR THE
C     INPUT OF DATA TO MXPRAM. THE DATA SHOULD BE 0
C     ENTERED IN THE ORDER BELOW:
C
C     A) PERSON OR GROUP WHO SUBMITTED THE WORK.(LIMIT 20 CHAR.)
C     B) CONTRACT NUMBER OF THE WORK. (LIMIT: 20 CHARACTERS)
C     C) DATE SUBMITTED. (YR/MO/DA)
C     D) SERIES NAME. (LIMIT: 10 CHARACTERS)
C     E) SERIES DISCRIPTION. (LIMIT: 40 CHARACTERS)
C     F) SPECTROSCOPIST. LIMIT: 20 CHARACTERS)
C     G) NUMBER OF SAMPLES. (INTEGER VALUE)
C     H) DATA FOR EACH SAMPLE IN THE FOLLOWING ORDER:
C         1) SAMPLE NAME
C         2) H MONOAROMATIC
C         3) H DIAROMATIC
C         4) H TRIAROMATIC
C         4) H OLEFINIC
C         6) H ALPHA 1
C         7) H ALPHA 2
C         8) H BETA N
C         9) H BETA
C         10) H GAMMA
C         11) 1.0 SINCE CARBON DATA IS TO BE ENTERED
C             ENTER C13 DATA AS FOLLOWS:
C                 A) CARBON SUBSTITUTED (0 IF UNKNOWN)
C                 B) CARBON BRIDGED (0 IF UNKNOWN)
C                 C) CARBON UNSUBSTITUTED ( 0 IF UNKNOWN)
C                 D) AROMATIC CARBON
C                 E) ALIPHATIC CARBON
C                 F) C1-METHYL CARBON PEAK (.000001 IF UNKNOWN)
C                 G) 2-METHYLENE PEAK (0 IF UNKNOWN)
C                 H) 3-METHYLENE PEAK (0 IF UNKNOWN)
C                 I) 4-METHYLENE PEAK ( 0 IF UNKNOWN)
C                 J) 5-METHYLENE PEAK ( 0 IF UNKNOWN OR IF
C                     CAN NOT DISTINGUISH FROM 4-METHYLENE PEAK)

```

INTERNAL FUNCTION. RETURNS THE CURRENT TIME.

C P	PARAMETER NAME	Q) SYMBOL
C 1)	NORMALIZED AREA UNDER H MONOAROMATIC 6.6-7.3 PPM	1) HMO
C 2)"	" H DIAROMATIC 7.3-7.8 PPM	2) HDI
C 3)"	" H TRIAROMATIC 7.8-8.3 PPM	3) HTRI
C -)"	" H OLEFINIC 4.0-6.0 PPM	4) HOL
C 4)"	" H ALIPHATIC1 2.3-4.0 PPM	5) HALP1
C 5)"	" H ALIPHATIC2 1.9-2.3 PPM	6) HALP2
C 6)"	" H BETA 1.0-1.9 PPM	8) HBETA
C 7)"	" H BETA NAPHTHENE 1.65-1.9 PPM	7) HBETN
C 8)"	" H GAMMA .05-1.0 PPM	9) HGAMA
C -)"	" H AROMATIC 6.6-8.3 PPM	10) HAR
C -)"	" H OLEFINIC 4.0-6.0 PPM	11) HOL
C -)"	" H ALIPHATIC TOTAL 1.9-4.0	12) HAL-T
C -)"	" H BETA-GAMMA .05-1.9	13) HBET-GAM
C -)	ENTRY OF CARBON 13 DATA (1.0=YES,0.0=NO)	14) C13 ENTER
C -)	NORMALIZED AREA UNDER CARBON SUBSTITUTED	15) CS
C -)"	" CARBON BRIDGED	16) CB
C -)"	" CARBON UNSUBSTITUTED	17) CU
C 9)"	" C AROMATIC 100-150 PPM	18) CAR
C 10)"	" C ALIPHATIC 5-50 PPM	19) CAL
C 11)"	" C ALKANE 1 PEAK AT 14.2 PPM	20) C1
C 12)"	" C ALKANE 2 PEAK AT 23.0 PPM	21) C2
C 13)"	" C ALKANE 3 PEAK AT 31.8 PPM	22) C3
C 14)"	" C ALKANE 4 PEAK AT 29.7 PPM	23) C4
C 15)"	" C ALKANE 5 PEAK AT 30.0 PPM	24) C5
C --)	ENTRY OF CHEMICAL ANALYSIS DATA (1.0=YES,0.0=NO)	25) CHEM ENTER

C 16) HYDROGEN WEIGHT FRACTION	27) HYDROGEN
C 17) CARBON WEIGHT FRACTION	26) CARBON
C --) AVERAGE MOLECULAR WEIGHT	28) MW
C 18) FRACTION OF AROMATIC HYDROGEN	29) FA SUP H
C 19) FRACTION OF AROMATIC THAT IS MONOAROMATIC	30) FMO
C 20) FRACTION OF AROMATIC THAT IS DIAROMATIC	31) FDI
C 21) NUMBER OF ALKYL SUBSTITUENTS/MOLECULE	32) RS
C 22) PERCENT OF AROMATIC IN THE MIXTURE	33) %AR
C 23) PERCENT OF MONOAROMATIC IN THE MIXTURE	34) % MOAR
C 24) PERCENT OF DIAROMATIC IN THE MIXTURE	35) % DIAR
C --) PERCENT OF OLEFINIC IN THE MIXTURE	36) % OL
C 25) PERCENT OF PARAFFINIC MATERIAL IN THE MIXTURE	37) % PAR
C 26) NUMBER OF METHYLENE TO NUMBER OF METHYL	38) R SUPER H
C 27) TOTAL HYDROGEN TO CARBON IN THE MIXTURE	39) (H/C)T
C 28) AROMATIC HYDROGEN CARBON RATIO	40) (H/C)AR
C 29) PARAFFINIC HYDROGEN CARBON RATIO	41) (H/C)PAR
C 30) FRACTION OF SUBSTITUTED AROMATICS	42) F S+B SUPC
C 31) FRACTION OF UNSUBSTITUTED AROMATICS	43) F U SUP C
C 32) FRACTION OF AROMATIC CARBONS	44) F A SUP C
C 33) CARBON CHAIN LENGTH	45) CL
C 34) FRACTION OF NORMAL ALKANES	46) F N SUP C
C 35) FRACTION OF BRANCHED ALKANES	47) F B SUP C

C *****

C
C PROGRAMER: PATRICK M. HUNTER
C UNDER ASSOCIATED WESTERN UNIVERSITIES FELLOWSHIP
C LARAMIE ENERGY TECHNOLOGY CENTER
C OFFICE OF RESEARCH AND DEVELOPMENT
C DIVISION OF RESEARCH SUPPORT
C SPECTROSCOPIC METHODS
C NMR GROUP
C

C *****

DIMENSION A(2),BI(3),P(35,100),ID(100),Q(47,100),EI(4),FI(2),
1 HOL(100),CS(100),CU(100),CB(100),PEROL(100),MW(100),
2 CARB(100),LBL(47),LBLA(47),LBLB(47),CHEM(100)
REAL HAR,HAL,HB,TS,RS,FMONO,AINT,TEST,COR,T,B,WRC,TOTL,IDUM,
1 PEROL,P,Q,HOL,CS,CB,CU,MW,CHEM,CARB
INTEGER J,N,I,DIVZERO,I1,K
DATA BLANK/"XXXXXXXXXX"/

C *****

C INPUT OF SAMPLE INFORMATION

C *****

DO 999 I=1,100
ID(I)=BLANK
999 CONTINUE
1000 READ (15,15)(A(I),I=1,2)
READ (15,15)(BI(I),I=1,2)
READ (15,25) C
READ (15,25) D
READ (15,20) (EI(I),I=1,4)
READ (15,15) (FI(I),I=1,2)
CALL DATE(MDATE)

```

      CALL CLOCK(MTIME)
      READ (15,*) N
      DO 1040 J=1,N
1015  READ (15,25) ID(J)
C*****
C  INPUT OF PROTON NMR DATA
C*****
      1001  READ (15,*) P(1,J)
      1002  READ (15,*) P(2,J)
      1003  READ (15,*) P(3,J)
            TOTL=P(1,J)+P(2,J)+P(3,J)
            READ (15,*) HOL(J)
      1004  READ (15,*) P(4,J)
            TOTL=TOTL+P(4,J)
      1005  READ (15,*) P(5,J)
            TOTL=TOTL+P(5,J)
      1007  READ (15,*) P(7,J)
            TOTL=TOTL+P(7,J)
      1006  READ (15,*) P(6,J)
      1008  READ (15,*) P(8,J)
            IF (DIVZERO(P(8,J),ID(J),6) .EQ. 0) GOTO 1090
C*****
C
C  INPUT OF CARBON 13 NMR DATA
C
C*****
      TOTL=0
      READ (15,*) CARB(J)
      READ (15,*) CS(J)
      READ (15,*) CB(J)
      READ (15,*) CU(J)
      1011  READ (15,*) P(9,J)
            TOTL=P(9,J)
      1012  READ (15,*) P(10,J)
            IF (DIVZERO(P(10,J),ID(J),6) .EQ. 0) GOTO 1090
      1016  READ (15,*) P(11,J)
            IF (DIVZERO(P(11,J),ID(J),6) .EQ. 0) GOTO 1090
            READ (15,*) P(12,J)
            READ (15,*) P(13,J)
            READ (15,*) P(14,J)
            READ (15,*) P(15,J)
C*****
C
C  INPUT CHEMICAL ANALYSIS DATA
C
C*****
      READ (15,*) CHEM(J)
      TOTL=P(11,J)+P(12,J)+P(13,J)+P(14,J)+P(15,J)
      1017  READ (15,*) P(17,J)
      1018  READ (15,*) P(16,J)
            READ (15,*) MW(J)
            IF (DIVZERO(P(17,J),ID(J),6) .EQ. 0 ) GOTO 1090
C*****

```

C CALCULATION OF PARAMETERS

C*****

```

1019   HAR=P(1,J)+P(2,J)+P(3,J)
      IF(DIVZERO(HAR,ID(J),6) .EQ. 0) GOTO 1001
      HAL=P(4,J)+P(5,J)
      IF (DIVZERO(HAL,ID(J),6) .EQ. 0)GOTO 1001
      HB=P(6,J)+P(7,J)+P(8,J)

```

C*****

C CALCULATION OF % MONO AND DIAROMATIC MOLECULES

C*****

```

      TS=0
      RS=0
      DO 1025 IN=1,10
        FMONO=P(1,J)/(P(1,J)+P(2,J)*(6.0-RS)/(8.0-RS))
        AINT=(8.0-2.0*FMONO)/(P(1,J)+P(2,J)+P(4,J)/2.0+P(5,J)/3.0)
        RS=AINT*(P(4,J)/2.0+P(5,J)/3.0)
        TEST= ABS(RS-TS)
        IF (TEST-0.005) 1030,1020,1020
1020     TS=RS
1025     CONTINUE
        WRITE (6,260)
        GOTO 1015
1030     CONTINUE

```

C*****

C CALCULATION OF ALL PARAMETERS

C*****

```

      P(19,J)=FMONO
      P(20,J)=1.0-FMONO
      P(18,J)= HAR
      P(21,J)= RS
      COR=(6.0-RS)/(8.0-RS)
      T=COR*P(2,J)+P(1,J)+1.0/2.0*P(4,J)+1.0/3.0*P(5,J)
      TEMP=1.0/3.0*P(8,J)+HOL(J)
      B=T+1.0/2.0*(P(6,J)-1.5*P(4,J))+1.0/2.0*P(7,J)+TEMP
      P(22,J)=(T/B)*100.0
      P(23,J)= P(22,J)*P(19,J)
      P(24,J)= P(22,J)*P(20,J)
      PEROL(J)=100.0*(HOL(J)/B)
      P(25,J)= 100.0-P(22,J)-PEROL(J)
      P(26,J)=3.0*(P(6,J)-1.5*P(4,J))/(2.0*P(8,J))
      WRC= 12.01/1.008
      P(27,J)= WRC*(P(16,J)/P(17,J))
      P(32,J)= P(9,J)/(P(9,J)+P(10,J))
      P(33,J)= 2.0*(P(14,J)+P(15,J))/P(11,J) +6.0
      P(34,J)= (P(11,J)+P(12,J)+P(13,J)+P(14,J)+P(15,J))/P(10,J)
      P(35,J)= 1.0-P(34,J)
      P(28,J)= WRC*(P(16,J)*P(18,J))/(P(17,J)*P(32,J))
      P(29,J)= WRC*( P(16,J)*(1.0-P(18,J)))/
1      (P(17,J)*(1.0-P(32,J)))
      P(31,J)= WRC*P(16,J)*P(18,J)/P(17,J)
1040   P(30,J)= P(32,J)-P(31,J)

```

C*****

C PRINT ROUTINE FOR OUTPUT

C*****

```

DO 1050 J=1,N
  Q(1,J)=P(1,J)
  Q(2,J)=P(2,J)
  Q(3,J)=P(3,J)
  Q(4,J)=HOL(J)
  Q(5,J)=P(4,J)
  Q(6,J)=P(5,J)
  Q(8,J)=P(6,J)
  Q(7,J)=P(7,J)
  Q(9,J)=P(8,J)
  Q(10,J)=Q(1,J)+Q(2,J)+Q(3,J)
  Q(11,J)=Q(4,J)
  Q(12,J)=Q(5,J)+Q(6,J)
  Q(13,J)=Q(7,J)+Q(8,J)+Q(9,J)
  Q(14,J)=CARB(J)
  Q(15,J)=CS(J)
  Q(16,J)=CB(J)
  Q(17,J)=CU(J)
DO 1041 I=18,24
  I1=I-9
  Q(I,J)=P(I1,J)
1041 CONTINUE
  Q(25,J)=CHEM(J)
  Q(26,J)=P(17,J)
  Q(27,J)=P(16,J)
  Q(28,J)=MW(J)
DO 1042 I=29,35
  I1=I-11
  Q(I,J)=P(I1,J)
1042 CONTINUE
  Q(36,J)=PEROL(J)
DO 1043 I=37,47
  I1=I-12
  Q(I,J)=P(I1,J)
1043 CONTINUE
1050 CONTINUE
  CALL MYLABEL (LBL,LBLA,LBLB,16,47)
  WRITE (10,180)
  WRITE (10,190) D,N
  WRITE (10,200) (A(I),I=1,2),(BI(I),I=1,2)
  WRITE (10,210) (EI(I),I=1,4)
  WRITE (10,220) C,MDATE
  WRITE (10,230) (FI(I),I=1,2),MTIME
  WRITE (10,240)
DO 1089 I1=1,N,5
  K=I1+4
  WRITE (10,245)
  WRITE (10,110) (ID(J),J=I1,K)
DO 1060 I=1,28
  WRITE (10,120) LBL(I),(Q(I,J),J=I1,K)
1060 CONTINUE
  WRITE (10,130)
DO 1070 I=29,38
  WRITE (10,120) LBL(I),(Q(I,J),J=I1,K)

```



```

1070      CONTINUE
        WRITE (10,250)
        DO 1080 I=39,47
            WRITE (10,120) LBL(I),(Q(I,J),J=I1,K)
1080      CONTINUE
1089      CONTINUE
        WRITE (6,410) D
C*****
C                      FORMATS
C*****
15  FORMAT(2(A10))
20  FORMAT (4A10)
25  FORMAT(A10)
260  FORMAT(" ITERATION FOR FRACTION OF HMONO DID NOT CONVERGE IN",/,
1      " TEN PASSES, ENTER DATA AGAIN ")
110  FORMAT (1X,"*****",5(2X,A10),/)
120  FORMAT (1X,A10,2X,F8.4,4(4X,F8.4))
130  FORMAT (/ ,17X,"PARAMETERS CALCULATED FROM PROTON NMR",/)
180  FORMAT (///,20X,"LARAMIE ENERGY TECHNOLOGY CENTER",/,22X,"DIVI",
1      "SION OF REASEARCH SUPPORT",/,25X," SPECTROSCOPY SECTION",/,
2      /,13X,"AVERAGE MOLECULAR STRUCTURE PARAMETERS OBTAINED",/,
3      18X,"FROM NUCLEAR MAGNETIC RESONANCE TO",/,18X,
4      "CHARACTERIZE HYDROCARBON MIXTURES",/)
190  FORMAT (5X,"SERIES NAME: ",A10," SERIES",5X,"NUMBER OF SAMPLES",
1      " ": ",I3,/)
200  FORMAT (5X,"SUBMITTED BY: ",2A10,4X,"CONTRACT #: ",2A10,/)
210  FORMAT (5X,"SERIES DISCRIPTION: ",4A10,/)
220  FORMAT (5X,"DATE OF SUBMISSION: ",A10,5X,"DATE OF COMPUTATION: "
1      ,A10,/)
230  FORMAT (5X,"SPECTROSCOPIST: ",2A10,5X,"COMPUTATION TIME: ",A10)
240  FORMAT (/ ,72(" "),/,25X,"REPORT OF ANALYSIS",/,72(" "))
245  FORMAT(//,26X"MEASURED PARAMETERS",///,1X,"PARAMETER \" ,25X,"S",
1      "AMPLE NAME")
250  FORMAT (/ ,9X,"PARAMETERS CALCULATED FROM H,C NMR AND ELEMENTAL"
1      " ANALYSIS",/)
410  FORMAT (////////,"NOTE* THE PARAMETER LIST FOR THE ",A10,
1      " SERIES IS STORED ",/, " IN LOCAL FILE PRAM. TO SEE THIS "
2      "FILE USE THE FOLLOWING COMMANDS:",/,10X,"/REWIND,*",/,
3      ,10X,"/COPY,PRAM",///)
1090 STOP
      END
C*****
C      SUBROUTINE TO PROVIDE DATA LABELS
C*****
C
      SUBROUTINE MYLABEL (LBL1,LBL2,LBL3,DA,N)
C
C*****
C
C      FORMAL PARAMETERS
C      LBL1= THE FIRST 10 CHARACTERS OF DATA LABEL I
C      LBL2(I)= THE SECOND 10 CHARCTERS OF DATA LABEL I
C      LBL3(I)= THE THIRD 10 CHARACTERS OF DATA LABEL I
C      DA= TAPE NUMBER OF THE DATA LABEL FILE

```

```

C      N= NUMBER OF DATA LABELS IN THE FILE
C
C*****
C
C      PROGRAMER: PATRICK M. HUNTER
C
C*****
C
C      INTEGER N,DA
C      DIMENSION LBL1(N),LBL2(N),LBL3(N)
C      DO 20 I=1,N
C          READ (DA,10) LBL1(I),LBL2(I),LBL3(I)
10      FORMAT (3A10)
20      CONTINUE
C      RETURN
C      END
C*****
C      FUNCTION DIVZERO(VAL,NAME,O)
C*****
C
C      FORMAL PARAMETERS
C          VAL=VALUE TO BE CHECKED FOR ZERO VALUE
C          NAME=SAMPLE NAME WHOSE PARAMETER IS BEING CHECKED
C          O=OUTPUT FILE NUMBER
C
C*****
C
C      PROGRAMER: PATRICK M. HUNTER
C
C*****
C
C      THIS FUNCTION CHECKS FOR A ZERO VALUE AND IF THE INPUT
C          HAS A ZERO VALUE THE FUNCTION WILL PRINT A
C          MESSAGE THAT THE PROGRAM WILL ABORT WITH
C          THE DATA ENTERED AND TO REENTER THE DATA.
C          IF VAL =0 THEN DIVZERO=0
C
C*****
C
C      REAL VAL
C      INTEGER O
C      DIVZERO=1
C      IF (VAL .NE. 0)RETURN
C      WRITE (O,10) NAME
10  FORMAT ("THE PARAMETERS ENTERED FOR SAMPLE ",A10," WILL",
1      " ABORT",/," THE PROGRAM SINCE IT RESULTS IN DIVISION",
2      " BY ZERO!!! ",/," CHECK DATA IN MXDATA!!!!")
C      DIVZERO=0
C      RETURN
C      END
C      EOI ENCOUNTERED.
/

```

HMO
HDI
HTRI
HOL
HALP1
HALP2
HBETN
HBETA
HGAMA
HAR
HOL
HAL-T
HBET-GAM
C13 ENTER
CS
CB
CU
CAR
CAL
C1
C2
C3
C4
C5
CHEM ENTER
CARBON
HYDROGEN
MW
FA SUP H
FMO
FDI
RS.
% AR
% MOAR
% DIAR
% OL
% PAR
R SUPER H
(H/C)T
(H/C)AR
(H/C)PAR
F S+B SUPC
F U SUP C
F A SUP C
CL
F N SUP C
F B SUP C
EOI ENCOUNTERED.

DATA LABELS FOR MXPRAM
FILE NAME: MXLBL

EXAMPLE OF DATA FILES FOR
MXPRAM AND AROFIL

PATRICK HUNTER/LETC
IN HOUSE
80/09/??
SAMPLE OF
SAMPLE OF DATA FILE
NETZEL/HUNTER

5

SAMPLE I

.0595

.0108

0

.0216

.0811

.0486

.1243

.4378

.2162

1.0

0

0

0

.2790

.7210

.0381

.0469

.0469

.1694

0

1.0

.8457

.1140

0

SAMPLE II

.0488

.0054

0

.0271

.0921

.0461

.1491

.4282

.2033

1.0

0

0

0

.2453

.7547

.0287

.0476

.0287

.1800

0

1.0

.8508
.1144
0
SAMPLE III
.0497
.0062
0
.0311
.0870
.0497
.1429
.4348
.1988
1.0
0
0
0
.2809
.7191
.0328
.0512
.0478
.1940
0
1.0
.8431
.1142
0
SAMPLE IV
.1371
.0229
.0114
.0171
.1314
.0857
.1314
.2857
.1771
1.0
0
0
0
.5014
.4986
.0248
.0269
.0269
.0496
0
1.0
.8546
.0942
0
SAMPLE V

.0843

.0181

0

.0181

.1265

.0964

.1506

.3193

.1867

1.0

0

0

0

.3342

.6658

.0242

.0281

.0230

.0561

0

1.0

.8491

.0983

0

EOI ENCOUNTERED.

/

OUTPUT OF MXPRAM

LARAMIE ENERGY TECHNOLOGY CENTER
DIVISION OF RESEARCH SUPPORT
SPECTROSCOPY SECTION

AVERAGE MOLECULAR STRUCTURE PARAMETERS OBTAINED
FROM NUCLEAR MAGNETIC RESONANCE TO
CHARACTERIZE HYDROCARBON MIXTURES

SERIES NAME: SAMPLE OF SERIES NUMBER OF SAMPLES: 5

SUBMITTED BY: PATRICK HUNTER/LETC CONTRACT #: IN HOUSE

SERIES DISCRIPTION: SAMPLE OF DATA FILE

DATE OF SUBMISSION: 80/09/?? DATE OF COMPUTATION: 81/05/19.

SPECTROSCOPIST: NETZEL/HUNTER COMPUTATION TIME: 10.42.26.

REPORT OF ANALYSIS

MEASURED PARAMETERS

PARAMETER \	SAMPLE NAME				
*****	SAMPLE I	SAMPLE II	SAMPLE III	SAMPLE IV	SAMPLE V
HMO	.0595	.0488	.0497	.1371	.0843
HDI	.0108	.0054	.0062	.0229	.0181
HTRI	0.0000	0.0000	0.0000	.0114	0.0000
HOL	.0216	.0271	.0311	.0171	.0181
HALP1	.0811	.0921	.0870	.1314	.1265
HALP2	.0486	.0461	.0497	.0857	.0964
HBETN	.1243	.1491	.1429	.1314	.1506
HBETA	.4378	.4282	.4348	.2857	.3193
HGAMA	.2162	.2033	.1988	.1771	.1867
HAR	.0703	.0542	.0559	.1714	.1024
HOL	.0216	.0271	.0311	.0171	.0181
HAL-T	.1297	.1382	.1367	.2171	.2229
HBET-GAM	.7783	.7806	.7765	.5942	.6566
C13 ENTER	1.0000	1.0000	1.0000	1.0000	1.0000
CS	0.0000	0.0000	0.0000	0.0000	0.0000
CB	0.0000	0.0000	0.0000	0.0000	0.0000
CU	0.0000	0.0000	0.0000	0.0000	0.0000
CAR	.2790	.2453	.2809	.5014	.3342
CAL	.7210	.7547	.7191	.4986	.6658
C1	.0381	.0287	.0328	.0248	.0242
C2	.0469	.0476	.0512	.0269	.0281
C3	.0469	.0287	.0478	.0269	.0230
C4	.1694	.1800	.1940	.0496	.0561
C5	0.0000	0.0000	0.0000	0.0000	0.0000

CHEM ENTER	1.0000	1.0000	1.0000	1.0000	1.0000
CARBON	.8457	.8508	.8431	.8546	.8491
HYDROGEN	.1140	.1144	.1142	.0942	.0983
MW	0.0000	0.0000	0.0000	0.0000	0.0000

PARAMETERS CALCULATED FROM PROTON NMR

FA SUP H	.0703	.0542	.0559	.1714	.1024
FMO	.8992	.9398	.9320	.9022	.8859
FDI	.1008	.0602	.0680	.0978	.1141
RS	2.7701	3.2512	3.1783	2.2970	3.0036
% AR	28.1403	26.4952	26.1061	56.9504	46.3657
% MOAR	25.3037	24.9003	24.3299	51.3781	41.0763
% DIAR	2.8366	1.5950	1.7762	5.5722	5.2894
% OL	4.9449	6.3350	7.1599	3.9550	4.4045
% PAR	66.9148	67.1698	66.7339	39.0947	49.2299
R SUPER H	2.1935	2.1401	2.2960	.7504	1.0408

PARAMETERS CALCULATED FROM H,C NMR AND ELEMENTAL ANALYSIS

(H/C)T	1.6061	1.6021	1.6139	1.3133	1.3794
(H/C)AR	.4047	.3540	.3212	.4489	.4226
(H/C)PAR	2.0710	2.0077	2.1188	2.1825	1.8596
F S+B SUPC	.1661	.1585	.1907	.2763	.1930
F U SUP C	.1129	.0868	.0902	.2251	.1412
F A SUP C	.2790	.2453	.2809	.5014	.3342
CL	14.8924	18.5436	17.8293	10.0000	10.6364
F N SUP C	.4179	.3776	.4531	.2571	.1974
F B SUP C	.5821	.6224	.5469	.7429	.8026

EOI ENCOUNTERED.

APPENDIX B

Computer Program to Determine Average Molecular Structure Parameters for Aromatic Hydrocarbon Fractions

PROGRAM AROFIL (ARODAT,ARPRAM,AROLBL,TAPE5=ARODAT,TAPE6=ARPRAM,
1 TAPE20=AROLBL)

C
C
C THIS PROGRAM WAS WRITTEN FOR FOSSIL FUEL STUDIES AT:

C
C THE DEPARTMENT OF ENERGY
C LARAMIE ENERGY TECHNOLOGY CENTER
C OFFICE OF REASEARCH AND DEVELOPMENT
C DIVISION OF RESEARCH SUPPORT
C SPECTROSCOPIC METHODS SECTION
C NMR GROUP
C

C *****
C
C PROGRAMER: PATRICK M. HUNTER
C UNDER ASSOCIATED WESTERN UNIVERSITIES FELLOWSHIP
C DANIEL A. NETZEL - SUPERVISOR
C

C *****
C
C CREDITS GO TO:

C
C D.M. CANTOR: "NUCLEAR MAGNETIC RESONANCE SPECTROMIC
C DETERMINATION OF AVERAGE MOLECULAR
C STRUCTURE PARAMETERS FOR COAL DER-
C IVED LIQUIDS."
C ANAL. CHEM. VOL. 50 ,NO.8,JULY 1978.
C

C
C D.R. CLUTTER: "NUCLEAR MAGNETIC RESONANCE SPECTROMETRY
C OF PETROLEUM FRACTIONS - C13 AND PROTON
C CHARACTERIZATION IN TERMS OF AVERAGE MOL-
C ECULAR PARAMETERS."
C ANAL. CHEM. VOL. 44,NO. 8,JULY 1972
C

C
C H.C. DORN: "PROTON AND C13 FORIER TRANSFORM NMR CHAR-
C ACTERIZATION OF JET FUELS DERIVED FROM
C ALTERNATIVE ENERGY SOURCES."
C FINAL PROGRESS REPORT FOR PERIOD:
C 3/23/79 - 8/30/79
C FOR THE NAVEL RESEARCH LABORATORY.
C

C *****
C
C PROGRAM TO DETERMINE AVERAGE MOLECULAR PARAMETERS FOR
C AROMATIC HYDOCARBON FUEL FRACTIONS USING
C PROTON NMR SPECTRA AND/OR C13 NMR SPECTRA
C AND/OR ELEMENTAL ANALYSIS DATA INCLUDING
C CARBON WEIGHT FRACTION, HYDROGEN WEIGHT
C FRACTION AND AVERAGE MOLECULAR WEIGHT.
C

C PROGRAM IS WRITTEN IN FORTRAN IV FOR A CYBER 730/760
C

```

C *****
C
C SUBROUTINES, FUNCTIONS AND EXTERNAL FILES USED WITH AROFIL
C
C SUBROUTINES:
C
C 1) MYLABEL
C     SUBROUTINE TO PROVIDE DATA LABELS FOR THE PRAMETER
C     OUTPUT. THIS SUBROUTINE NEEDS THE
C     EXTERNAL FILE AROLBL TO RUN. THE
C     SUBROUTINE WILL PROVIDE DATA LABELS
C     UP TO 30 CHARACTERS.
C
C FUNCTIONS:
C
C 1) DATE
C     A CYBER 760 INTERNAL FUNCTION. RETURNS THE DATE.
C
C 2) CLOCK
C     A CYBER 760 INTERNAL FUNCTION. RETURNS THE TIME.
C
C EXTERNAL FILES
C
C 1) ARODAT
C     DATA FILE FOR AROFIL. SEE THE INSTRUCTIONS
C     FOR FORMING THIS FILE IN THE NEXT SECTION.
C
C 2) AROLBL
C     FILE CONTAINING THE PARAMETER LABELS FOR THE
C     OUTPUT. FOR THE DEFINITIONS FOR THESE
C     PARAMETERS SEE THE SECOND SECTION AFTER
C     THIS ONE.
C
C 3) ARPRAM
C     OUTPUT FILE ON WHICH THE THE OUTPUT DATA IS STORED.
C
C *****
C
C INSTRUCTIONS FOR FORMING THE DATA FILE ARODAT
C
C 1) ENTER XEDIT BY TYPING /XEDIT,ARODAT
C 2) THE CYBER WILL RESPOND: ?? .TYPE: I#
C 3) THE COMPUTER WILL RESPOND: ?
C 4) ENTER THE FOLLOWING INFORMATION IN THIS ORDER:
C     A) PERSON OR GROUP SUBMITTING THE WORK. 20 CHARACTERS
C     B) CONTRACT NUMBER SUBMITTED UNDER. 20 CHARACTERS
C     C) DATE SUBMITTED. YR/MO/DA
C     D) SERIES NAME. 10 CHARACTERS
C     E) SERIES DISCRIPTION. 40 CHARACTERS
C     F) SPECTROSCOPIST. 20 CHARACTERS
C     G) NUMBER OF SAMPLES IN SERIES. INTEGER VALUE
C     H) DATA FOR EACH SAMPLE AS FOLLOWS

```

- 1) SAMPLE NAME
- 2) NORMALIZED AREAS UNDER PROTON NMR SPECTRA
 - A) HMONO
 - B) HDI
 - C) HTRI
 - D) HOL
 - E) H ALPHA 1
 - F) H ALPHA 2
 - G) H BETA N
 - H) H BETA
 - I) H GAMMA
- 3) 1.0 IF C13 DATA IS TO BE ENTERED 0.0 IF NOT
 IF C13 DATA IS ENTERED ENTER NORMALIZED AREAS FOR
 - A) C SUBSTITUTED. (MAY BE 0 IF UNKNOWN)
 - B) C BRIDGED. (MAY BE 0 IF UNKNOWN)
 - C) C UNSUBSTITUTED. (MAY BE 0 IF UNKNOWN)
 - D) C AROMATIC
 - E) C ALIPHATIC
 - F) C ALKANE PEAK 1 (MAY BE .0000001 IF UNKNOWN)
 - G) " 2 (MAY BE 0 IF UNKNOWN)
 - H) " 3 (MAY BE 0 IF UNKNOWN)
 - I) " 4 (ENTER TOTAL OF 4,5 IF CAN NOT
MEASURE BOTH. ENTER 0 IF UNKNOWN)
 - J) " 5 (ENTER 0 IF UNKNOWN OR CAN NOT
DISTINGUISH BETWEEN 4 AND 5)
- 4) 1.0 IF CHEMICAL DATA IS TO BE ENTERED 0.0 IF NOT
 - A) CARBON WEIGHT FRACTION
 - B) HYDROGEN WEIGHT FRACTION
 - C) AVERAGE MOLECULAR WEIGHT, 0.0 IF YOU DON'T
HAVE IT.

DEFINITIONS OF PARAMETER SYMBOLS

MEASURED PARAMETERS

P/Q) SYMBOL= PARAMETER NAME

- 1/1) HMO= HMONO 6.6-7.2 PPM
- 2/2) HDI= DIAROMATIC HYDROGEN 7.2-7.8 PPM
- 3/3) HTRI= TRIAROMATIC HYDROGEN 7.8-8.3 PPM
- 3/-) HOL = OLEFINIC HYDROGEN 4.0-6.0 PPM
- 5/4) HALP1= ALPHA1-ALKYL HYDROGEN 2.3-4.0 PPM
- 6/5) HALP2= ALPHA2-ALKYL HYDROGEN 1.9-2.3 PPM
- 7/6) HBETN= BETA-NAPHTHENE HYDROGEN 1.6-1.9 PPM
- 8/7) HBETA= BETA-ALKYL HYDROGEN 1.0-1.6 PPM
- 9/8) HGAMA= GAMMA-ALKYL HYDROGEN 0.5-1.0 PPM
- 10/9) HAR = AROMATIC HYDROGEN 6.6-8.3 PPM
- 11/-) HOL = OLEFINIC HYDROGEN 4.0-6.0 PPM
- 12/10) HAL-T = ALPHA-ALKYL HYDROGEN 1.9-4.0 PPM

C 13/11) HBET-GAM = BETA-GAMMA ALKYL HYDROGEN 0.5-1.9 PPM
 C 14/12) C13 ENTER = C13 NMR DATA ENTERED 1.0=YES, 0.0=NO
 C 15/-) CS = SUBSTITUTED CARBON
 C 16/-) CB = BRIDGED CARBON
 C 17/-) CU = UNSUBSTITUTED CARBON
 C 18/13) CAR = AROMATIC CARBON 100-150 PPM
 C 19/14) CAL = ALIPHATIC CARBON 5-50 PPM
 C 20/-) C1 = METHYL CARBONS OF N-ALKANES 13.8-14.2 PPM
 C 21/-) C2 = 2-METHYLENE CARBONS OF N-ALKANES 22.7-23.0 PPM
 C 22/-) C3 = 3-METHYLENE CARBONS OF N-ALKANES 31.8-32.0
 C 23/-) C4 = 4-METHYLENE CARBONS OF N-ALKANES 29-28 PPM
 C 24/-) C5 = 5-METHYLENE CARBONS OF N-ALKANES 28.0-30.0 PPM
 C 25/15) CHEM ENTER= CHEM. ANALYSIS DATA ENTERED, 1=YES,0=NO
 C 26/16) CARBON= CARBON WEIGHT FRACTION
 C 27/17) HYDROGEN= HYDROGEN WEIGHT FRACTION
 C 28/18) MW= MOLECULAR WEIGHT

PARAMETERS CALCULATED FROM PROTON NMR DATA ONLY

P/Q) SYMBOL=PARAMETER NAME

C 29/19) %MAR= PERCENT OF MONOAROMATIC
 C 30/20) %DAR= PERCENT OF DIAROMATICS
 C 31/21) %TAR= PERCENT OF TRIAROMATICS
 C 32/22) FA SUP CH= CARBON AROMATICITY (FROM PROTON NMR DATA)
 C 33/23) RA= AVERAGE OF AROMATIC RINGS PER AVERAGE MOLECULE
 C 34/24) #CA= AVERAGE NUMBER OF AROMATIC CARBON RING ATOMS/MOL.
 C 35/25) #C= AVERAGE NUMBER OF CARBONS PER MOLECULE
 C 36/26) #H= AVERAGE NUMBER OF HYDROGEN ATOMS PER MOL.
 C 37/27) MW= AVERAGE MOLECULAR CALCULATED FROM PROTON NMR DATA
 C 38/28) %CS= PERCENT SATURATE CARBONS
 C 39/29) RS= AVE. NUMBER ALKYL SUBSTITUENTS PER MOLECULE
 C 40/30) N= AVE. NUMBER CARBON ATOMS PER ALKYL SUBSTITUENT
 C 41/31) #C1= AVE. NUMBER NON-BRIDGE AROMATIC RING CARBONS/MOL.
 C 42/32) %AS= PERCENT SUBSTITUTION ALKYL GROUPS ON NON-BRIDGE
 C AROMATIC RING CARBONS
 C 43/33) RN= AVE. NUMBER NAPHTHENIC RINGS/ AVE. MOLECULE
 C 44/34) %CN= PERCENT NAPHTHENIC CARBONS
 C CF1/CF1) CF SUP H= CARBON WEIGHT FRACTION (FROM PROTON NMR DATA)
 C HF1/HF1) HF SUP H= HYDROGEN WEIGHT FRACTION (FROM PROTON NMR DATA)

PARAMETERS CALCULATED FROM PROTON NMR, C13 NMR
AND CHEMICAL ANALYSIS DATA

C 45/35) #CA= SEE 34/24)
 C 46/36) #CS= NUMBER OF SATURATE CARBONS / MOLECULE
 C 47/37) RS= SEE 39/29)
 C 48/38) N= SEE 40/30)
 C 49/39) RA= SEE 34/24)
 C 50/40) #C1= SEE 41/31)
 C 51/41) RN= SEE 43/33)
 C 52/42) R=NUMBER OF SATURATE RINGS/SUBSTITUENT
 C 53/43) F= C/H WEIGHT RATIO IN ALKYL GROUPS
 C 54/44) F1= C/H WEIGHT RATIO IN AROMATIC GROUPS

```

C      55/45) FA SUP C= CARBON AROMATICITY
C      56/46) CA= WEIGHT FRACTION OF AROMATIC CARBON
C      57/47) C1= " " NON-BRIDGE AROMATIC CARBON
C      58/48) C1 SUP S= FRACTION OF C1 CARBONS THAT ARE ALKYL SUB.
C      59/49) C1 SUP U= FRACTION OF C1 CARBONS THAT ARE NON-SUB
C      60/50) %AS= SEE 42/32)
C      61/51) FS+B SUPC= FRACTION OF BRIDGED AND SUB AROMATIC CARBONS
C
C
C*****
C
C
C      PROGRAM BODY
C
C*****
C
C      DIMENSION, INTERGER AND REAL DECLARATIONS
C
C:*****
C*****
C
C
C      DIMENSION ID(100),Q(51,100),LBL(61),LBL1(61),LBL2(61),
1      CF1(100),HF1(100),BI(2),EI(4),P(61,100),AI(2),FI(2)
REAL P,FMO,FDI,FTRI,A,RS,TS,TEST,B,HF,CF,AB,CAR,CAL,MW,
1      CF1,HF1,B1,Q
INTEGER ID,LBL,J,I,N,IN,K,AI,BI,DI,EI,FI,TEMP1
DATA BLANK/" "/
C*****
C      SET ALL SAMPLE NAMES TO BLANK
C*****
C      DO 5 I=1,51
5      ID(I)=BLANK
C*****
C      READ DATA FROM ARODAT FILE - TAPE 5
C:!*%&*&#*!#$%***&#*!***&#*!#$%$%$?]]][[[&&&&*&#*!%$*&XXXXEEEEEEEEEEEEEEEE
      READ (5,160) (AI(J),J=1,2)
      READ (5,160) (BI(J),J=1,2)
      READ (5,100) CI
      READ (5,100) DI
      READ (5,170) (EI(J),J=1,4)
      READ (5,160) (FI(J),J=1,2)
      READ (5,*) N
      CALL DATE(MDATE)
      CALL CLOCK(MTIME)
      DO 20 J=1,N
          READ (5,100) ID(J)
          DO 10 I=1,9
              READ (5,*) P(I,J)
10      CONTINUE
          READ (5,*) P(14,J)
          IF ( P(14,J) .NE. 1.0) GOTO 15
          DO 14 I=15,24
              READ (5,*) P(I,J)

```

```

14  CONTINUE
15  READ (5,*) P(25,J)
    IF (P(25,J) .NE. 1.0) GOTO 16
    READ (5,*) P(26,J)
    READ (5,*) P(27,J)
    READ (5,*) P(28,J)
C*****
C  DEFINE PARAMETERS FOR CALCULATIONS. NOT REALLY NECESSARY.
C      JUST CONVEINENT WHEN THIS PROGRAM WAS REVISED
C      NOTE THAT SOME INPUT PARAMETERS ARE NEVER USED
C      OTHER PROGRAMS DO USE THIS DATA. THE DATA FILES
C      ARE SET UP TO WORK IN ALL PROGRAMS.
C*****
16  Q(1,J)=P(1,J)
    Q(2,J)=P(2,J)
    Q(3,J)=P(3,J)
    Q(4,J)=P(5,J)
    Q(5,J)=P(6,J)
    Q(6,J)=P(7,J)
    Q(7,J)=P(8,J)
    Q(8,J)=P(9,J)
    Q(9,J)=P(10,J)
    Q(10,J)=P(12,J)
    Q(11,J)=P(13,J)
    Q(12,J)=P(14,J)
    Q(13,J)=P(18,J)
    Q(14,J)=P(19,J)
    Q(15,J)=P(25,J)
    Q(16,J)=P(26,J)
    Q(17,J)=P(27,J)
    Q(18,J)=P(28,J)
20  CONTINUE
C*****
C  CALL DATA LABEL SUBROUTINE
C*****
    CALL MYLABEL (LBL,LBL1,LBL2,20,61)
C*****
C  BEGIN CALCULATIONS
C*****
    DO 30 J=1,N
        Q(9,J)= Q(1,J)+ Q(2,J) + Q(3,J)
        Q(10,J) = Q(4,J) + Q(5,J)
        Q(11,J) = Q(6,J) + Q(7,J)+Q(8,J)
        P(10,J)=Q(9,J)
        P(11,J)=P(4,J)
        P(12,J)=Q(10,J)
        P(13,J)=Q(11,J)
C*****
C*****
C  BEGIN CLUTTER'S CALCULATIONS
C*****
C*****
C  ITERATION TO DETERMINE THE FRACTION OF MONOAROMATIC

```

```

C*****
C INITIALIZE RS=0
C ASSUME NO TRIAROMATICS
C CALCULATE PMONO
C CALCULATE RS
C TEST CHANGE IN RS
C REPEAT IF NECESSARY IF NOT CONTINUE
C*****
      TS=0
      RS=0
      DO 25 I=1,10
        FMO= Q(1,J)/( Q(1,J)+Q(2,J)*((6.0-RS)/(8.0-RS)))
        A= (8.0-2.0*FMO)*(Q(4,J)/2.0+Q(5,J)/3.0)
        RS=A/(Q(1,J)+Q(2,J)+Q(4,J)/2.0+Q(5,J)/3.0)
        TEST=ABS(RS-TS)
        IF (TEST-0.005) 26,24,24
24      TS=RS
25      CONTINUE
26      CONTINUE
C*****
C CONTINUE CALCULATIONS (NOTE TO EXTRACT CALCULATIONS SEE DEF.S
C ABOVE)
C*****
      Q(19,J)=100.0*FMO
      FDI=1.0-FMO
      FTRI= FDI*(8.0-RS)*Q(3,J)/(2.0*Q(2,J))
      FDI=FDI-FTRI
      Q(20,J)= 100.0*FDI
      Q(21,J)= 100.0* FTRI
      Q(24,J)=6.0*FMO+10.0*FDI+14.0*FTRI
      Q(31,J)= Q(24,J)-2.0*FDI-4.0*FTRI
      AB=Q(4,J)/2.0+Q(5,J)/3.0
      B=AB+3.0*Q(6,J)/4.0+Q(7,J)/2.0+Q(8,J)/3.0
      Q(25,J)=Q(24,J)+Q(31,J)*B/(Q(9,J)+AB)
      Q(22,J)=Q(24,J)/Q(25,J)
      Q(32,J)=100.0*RS*(FMO/6.0+FDI/8.0+FTRI/10.0)
      B1=(Q(9,J)+Q(10,J)+Q(11,J))/Q(9,J)
      Q(26,J)=Q(31,J)*(1.0-Q(32,J)/100.0)* B1
      Q(27,J)= 12.011*Q(25,J)+1.008*Q(26,J)
      CF=12.011*Q(25,J)/Q(27,J)
      CF1(J)=CF
      HF=1.008*Q(26,J)/Q(27,J)
      HF1(J)=HF
      Q(23,J)=1.0+FDI+2.0*FTRI
      Q(28,J)=100.0*(1.0-Q(22,J))
      Q(30,J)=B/AB
      Q(33,J)=Q(6,J)*(1.0-Q(32,J)/100.0)*Q(31,J)/2.0/Q(9,J)
      Q(34,J)=100.0*3.5*Q(33,J)/Q(25,J)
      Q(29,J)=RS
      CAR=Q(22,J)
      CAL=1.0-Q(22,J)
      MW=Q(27,J)
C*****
C CHECK FOR C13 INPUT. IF SO USE IT IF NOT USE CALCULATED VALUES.

```



```

C*****
IF (Q(12,J) .NE. 1.0 ) GOTO 27
CAR=Q(13,J)
CAL=Q(14,J)
C*****
C CHECK FOR CHEMICAL DATA INPUT. IF SO USE IT, IF NOT USE CALCULATED
C VALUES.
C*****
27 IF (Q(15,J) .NE. 1.0 ) GOTO 28
MW= Q(18,J)
CF= Q(16,J)
HF= Q(17,J)
C*****
C*****
C BEGIN CANTOR'S CALCULATIONS
C*****
28 Q(38,J)=(Q(10,J)+Q(11,J))/Q(10,J)
C*****
C NOTE: HERE THE PROGRAM CHECKS FOR THE CIRCUMSTANCE THAT CARBON AND
C HYDROGEN WEIGHT FRACTIONS HAVE BEEN ENTERED
C BUT THE MOLECULAR WEIGHT WAS UNKNOWN AND
C THUS ENTERED AS 0. THE PROGRAM WILL USE
C CALCULATED MOLECULAR WEIGHT IF THIS IS
C THE CASE.
C*****
IF (MW .EQ. 0.0) MW=Q(27,J)
Q(45,J)= CAR/(CAR+CAL)
Q(46,J)= Q(45,J)*CF
Q(48,J)= CAL*CF/Q(38,J)
Q(49,J)= 12.011*Q(9,J)*HF
Q(47,J)= Q(48,J)+Q(49,J)
Q(50,J)=100.0*Q(48,J)/Q(47,J)
Q(43,J)=CAL*CF/(Q(10,J)+Q(11,J))/HF
Q(42,J)= Q(38,J)+.5-6.0*Q(38,J)/Q(43,J)
Q(35,J)=Q(46,J)/12.011*MW
Q(40,J)= Q(47,J)/12.011*MW
Q(36,J)= CAL*CF/12.011*MW
Q(39,J)= 1.0+(Q(35,J)-Q(40,J))/2.0
Q(37,J)=Q(50,J)*Q(40,J)/100.0
Q(41,J)=Q(42,J)*Q(37,J)
Q(44,J)= CAR*CF/Q(9,J)/HF
Q(51,J)= Q(45,J)-HF*12.011/(CF*1.008*B1)
C*****
C
C
C THIS ROUTINE WRITES THE DATA ON THE FILE ARPRAM.
C
C*****
C
DO 29 I=19,51
TEMP1=I+10
P(TEMP1,J)=Q(I,J)
29 CONTINUE

```

```

30      CONTINUE
      WRITE (6,180)
      WRITE (6,190) DI,N
      WRITE (6,200) (AI(J),J=1,2),(BI(J),J=1,2)
      WRITE (6,210) (EI(J),J=1,4)
      WRITE (6,220) CI,MDATE
      WRITE (6,230) (FI(J),J=1,2),MTIME
      WRITE (6,240)
      DO 90 IN=1,N,5
        K=IN+4
        WRITE (6,245)
        WRITE (6,110) (ID(J),J=IN,K)
        DO 50 I=1,28
          WRITE (6,120) LBL(I),(P(I,J),J=IN,K)
50      CONTINUE
        WRITE (6,130)
        DO 60 I=29,44
          WRITE (6,120) LBL(I),(P(I,J),J=IN,K)
60      CONTINUE
        WRITE (6,140) (CF1(J),J=IN,K)
        WRITE (6,150) (HF1(J),J=IN,K)
        WRITE (6,250)
        DO 70 I=45,61
          WRITE (6,120) LBL(I),(P(I,J),J=IN,K)
70      CONTINUE
90      CONTINUE
C*****
C      FORMATS
C*****
100     FORMAT (A10)
110     FORMAT (1X,"*****",5(2X,A10),/)
120     FORMAT (1X,A10,2X,F8.4,4(4X,F8.4))
130     FORMAT (/ ,17X,"PARAMETERS CALCULATED FROM PROTON NMR",/)
140     FORMAT (1X,"CF SUP H  ",2X,F8.4,4(4X,F8.4) )
150     FORMAT (1X,"HF SUP H  ",2X,F8.4,4(4X,F8.4) )
160     FORMAT (2A10)
170     FORMAT (4A10)
180     FORMAT (///,20X,"LARAMIE ENERGY TECHNOLOGY CENTER",/,22X,"DIVI",
1"SION OF REASEARCH SUPPORT",/,25X," SPECTROSCOPY SECTION",/,
2/,13X,"AVERAGE MOLECULAR STRUCTURE PARAMETERS OBTAINED",/
3      18X,"FROM NUCLEAR MAGNETIC RESONANCE TO",/,14X,
4      "CHARACTERIZE AROMATIC HYDROCARBON FRACTIONS",/)
190     FORMAT (5X,"SERIES NAME: ",A10," SERIES",5X,"NUMBER OF SAMPLES",
1      " : ",I3,/)
200     FORMAT (5X,"SUBMITTED BY: ",2A10,4X,"CONTRACT #: ",2A10,/)
210     FORMAT (5X,"SERIES DISCRIPTION: ",4A10,/)
220     FORMAT (5X,"DATE OF SUBMISSION: ",A10,5X,"DATE OF COMPUTATION: "
2      ,A10,/)
230     FORMAT (5X,"SPECTROSCOPIST: ",2A10,5X,"COMPUTATION TIME: ",A10)
240     FORMAT (/ ,72(" "),/,25X,"REPORT OF ANALYSIS",/,72(" "))
245     FORMAT (///,26X,"MEASURED PARAMETERS",//,1X,"PARAMETER /",25X,
1      " SAMPLE NAME")
250     FORMAT (/ ,9X,"PARAMETERS CALCULATED FROM H,C NMR AND ",
1      "ELEMENTAL ANALYSIS",/)

```

[illegible]

DATA LABELS FOR AROFIL
FILE NAME: AROLBL

HMO
HDI
HTRI
HOL
HALP1
HALP2
HBETN
HBETA
HGAMA
HAR
HOL
HAL-T
HBET-GAM
C13 ENTER
CS
CB
CU
CAR
CAL
C1
C2
C3
C4
C5
CHEM ENTER
CARBON
HYDROGEN
MW
%MAR
%DAR
%TAR
FA SUP CH
RA
#CA
#C
#H
MW
%CS
RS
N
#C1
%AS
RN
%CN
#CA
#CS
RS
N
RA
#C1
RN
R
F
F1

FA SUP C

CA

C1

C1 SUP S

C1 SUP U

%AS

FS+B SUPC

EOI ENCOUNTERED.

EXAMPLE OF DATA FILES FOR
MXPRAM AND AROFIL

PATRICK HUNTER/LETC
IN HOUSE
80/09/??
SAMPLE OF
SAMPLE OF DATA FILE
NETZEL/HUNTER

5

SAMPLE I

.0595

.0108

0

.0216

.0811

.0486

.1243

.4378

.2162

1.0

0

0

0

.2790

.7210

.0381

.0469

.0469

.1694

0

1.0

.8457

.1140

0

SAMPLE II

.0488

.0054

0

.0271

.0921

.0461

.1491

.4282

.2033

1.0

0

0

0

.2453

.7547

.0287

.0476

.0287

.1800

0

1.0

.8508
.1144
0
SAMPLE III

.0497
.0062
0

.0311
.0870
.0497
.1429
.4348
.1988
1.0

0
0
0

.2809
.7191
.0328
.0512
.0478
.1940

0
1.0
.8431
.1142

0
SAMPLE IV

.1371
.0229
.0114
.0171
.1314
.0857
.1314
.2857
.1771

1.0
0
0
0

.5014
.4986
.0248
.0269
.0269
.0496

0
1.0
.8546
.0942

0
SAMPLE V

.0843

.0181

0

.0181

.1265

.0964

.1506

.3193

.1867

1.0

0

0

0

.3342

.6658

.0242

.0281

.0230

.0561

0

1.0

.8491

.0983

0

EOI ENCOUNTERED.

/

SAMPLE OF OUTPUT OF AROFIL
LARAMIE ENERGY TECHNOLOGY CENTER
DIVISION OF RESEARCH SUPPORT
SPECTROSCOPY SECTION

AVERAGE MOLECULAR STRUCTURE PARAMETERS OBTAINED
FROM NUCLEAR MAGNETIC RESONANCE TO
CHARACTERIZE AROMATIC HYDROCARBON FRACTIONS

SERIES NAME: SAMPLE OF SERIES NUMBER OF SAMPLES: 5
SUBMITTED BY: PATRICK HUNTER/LETC CONTRACT #: IN HOUSE
SERIES DISCRIPTION: SAMPLE OF DATA FILE
DATE OF SUBMISSION: 80/09/?? DATE OF COMPUTATION: 81/05/19.
SPECTROSCOPIST: NETZEL/HUNTER COMPUTATION TIME: 10.48.20.

REPORT OF ANALYSIS

MEASURED PARAMETERS

PARAMETER / *****	SAMPLE I	SAMPLE II	SAMPLE NAME SAMPLE III	SAMPLE IV	SAMPLE V
HMO	.0595	.0488	.0497	.1371	.0843
HDI	.0108	.0054	.0062	.0229	.0181
HTRI	0.0000	0.0000	0.0000	.0114	0.0000
HOL	.0216	.0271	.0311	.0171	.0181
HALP1	.0811	.0921	.0870	.1314	.1265
HALP2	.0486	.0461	.0497	.0857	.0964
HBETN	.1243	.1491	.1429	.1314	.1506
HBETA	.4378	.4282	.4348	.2857	.3193
HGAMA	.2162	.2033	.1988	.1771	.1867
HAR	.0703	.0542	.0559	.1714	.1024
HOL	.0216	.0271	.0311	.0171	.0181
HAL-T	.1297	.1382	.1367	.2171	.2229
HBET-GAM	.7783	.7806	.7765	.5942	.6566
C13 ENTER	1.0000	1.0000	1.0000	1.0000	1.0000
CS	0.0000	0.0000	0.0000	0.0000	0.0000
CB	0.0000	0.0000	0.0000	0.0000	0.0000
CU	0.0000	0.0000	0.0000	0.0000	0.0000
CAR	.2790	.2453	.2809	.5014	.3342
CAL	.7210	.7547	.7191	.4986	.6658
C1	.0381	.0287	.0328	.0248	.0242
C2	.0469	.0476	.0512	.0269	.0281
C3	.0469	.0287	.0478	.0269	.0230
C4	.1694	.1800	.1940	.0496	.0561
C5	0.0000	0.0000	0.0000	0.0000	0.0000
CHEM ENTER	1.0000	1.0000	1.0000	1.0000	1.0000

CARBON	.8457	.8508	.8431	.8546	.8491
HYDROGEN	.1140	.1144	.1142	.0942	.0983
MW	0.0000	0.0000	0.0000	0.0000	0.0000

PARAMETERS CALCULATED FROM PROTON NMR

%MAR	89.9199	93.9802	93.1961	90.2156	88.5921
%DAR	10.0801	6.0198	6.8039	-4.1048	11.4079
%TAR	0.0000	0.0000	0.0000	13.8892	0.0000
FA SUP CH	.2293	.2057	.2082	.4194	.3228
RA	1.1008	1.0602	1.0680	1.2367	1.1141
#CA	6.4032	6.2408	6.2722	6.9469	6.4563
#C	27.9266	30.3328	30.1308	16.5646	20.0038
#H	47.4619	51.2325	50.9863	23.5497	30.6773
MW	383.2678	415.9702	413.2953	222.6950	271.1878
%CS	77.0713	79.4256	79.1836	58.0614	67.7245
RS	2.7701	3.2512	3.1783	2.2970	3.0036
N	7.7699	7.4102	7.5068	4.1871	4.5104
#C1	6.2016	6.1204	6.1361	6.4735	6.2282
%AS	45.0048	53.3714	52.0702	36.5491	48.6323
RN	3.0152	3.9254	3.7591	1.5745	2.3526
%CN	37.7889	45.2934	43.6661	33.2673	41.1624
CF SUP H	.8752	.8759	.8756	.8934	.8860
HF SUP H	.1248	.1241	.1244	.1066	.1140

PARAMETERS CALCULATED FROM H,C NMR AND ELEMENTAL ANALYSIS

#CA	7.5291	7.2278	8.1491	7.9447	6.4070
#CS	19.4569	22.2374	20.8617	7.9004	12.7642
RS	2.7793	3.3448	3.1229	2.1141	3.2350
N	7.0008	6.6483	6.6803	3.7370	3.9457
RA	1.8391	1.6519	2.1940	2.1175	1.2212
#C1	5.8508	5.9240	5.7612	5.7097	5.9647
RN	1.0283	2.0684	.8921	.4555	2.6697
R	.3700	.6184	.2857	.2155	.8253
F	5.8906	6.1088	5.8135	5.5755	6.5390
F1	29.4415	33.6589	37.0982	26.5391	28.1911
FA SUP C	.2790	.2453	.2809	.5014	.3342
CA	.2360	.2087	.2368	.4285	.2838
C1	.1834	.1711	.1674	.3080	.2642
C1 SUP S	.0871	.0966	.0908	.1140	.1433
C1 SUP U	.0963	.0745	.0767	.1939	.1209
%AS	47.5018	56.4618	54.2046	37.0264	54.2349
FS+B SUPC	.1636	.1561	.1878	.2723	.1903

EOI ENCOUNTERED.