

A Method for the Rapid, Accurate Prediction of the Physical Properties
of Middle Distillate Fuels from LC-¹H NMR Derived Data

by

Allen Caswell

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Approved:

Dr. H.C. Dorn, Chairman

Dr. L.T. Taylor

Dr. R.E. Dessy

Dr. J.F. Wolfe

Dr. J.M. Tanko

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Dr. H.C. Dorn, Committee Chairman

Department of Chemistry

(ABSTRACT)

A method has been developed whereby various physical properties of middle distillate fuels may be rapidly and accurately calculated by a group property approach from data obtained from a directly coupled Liquid Chromatograph - ¹H Nuclear Magnetic Resonance Spectrometer (LC-¹H NMR). The physical properties include cetane number, cetane index, density, specific gravity, pour point, flash point, viscosity, filterability, heat of combustion, cloud point, volume percent aromatics, residual carbon content, and initial, 10%, 50%, 90%, and end boiling points. These property predictions have accuracies approaching the error for measurement of the experimental physical property and require less than two hours analysis time per fuel. An interface was developed between the NMR spectrometer and a personal computer to aid in automation of the LC-¹H NMR data collection and to perform off-line analysis of the LC-¹H NMR data. This interface and all associated software is described.

Also presented is a series of model compound studies in which the physical properties of pure hydrocarbons (i.e., alkanes, monocyclic and dicyclic aromatics) were predicted by a similar group property approach.

This dissertation is dedicated to my family,
for their love, support, and faith that
I would someday finish school.

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It is true that research projects are not conducted in a vacuum. Several coworkers have made significant contributions to this project and their contributions should not be overlooked. Foremost among these is Dr. H.C. Dorn. Not only has his advice and insight proven indispensable, but his ability to envision experiments has proven invaluable in giving direction to the project. I would especially like to thank _____, without whose assistance the operation of the LC-¹H NMR apparatus would have been much more difficult. Also, the assistance of Dr. Lee Allen is appreciated.

Finally, I would like to point out _____ and _____ of the US Army, for providing both the middle distillate fuel samples and the physical property data for the fuel samples which form the basis of this work. I also wish to thank the US Army for providing partial financial support for this research.

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Foreword

Over the past 30 years, the tools available to the analytical chemist have become both much more complex and much more powerful, opening ever increasing avenues of investigation. The increasing pressures of technology have forced the analytical chemist to wear many hats. In addition to the traditional chemist's role, these new skills include computer programmer, machinist, plumber, electrical engineer, and mechanical engineer. At the same time, however, the constantly growing number of disciplines included under the umbrella of analytical chemistry have opened unprecedented areas of research for the analytical chemist. One of the most rapidly expanding areas of analytical chemistry is the computerization and optimization of routine analyses. The advent of the low cost, yet very powerful, personal computer has allowed multifold improvements in analytical techniques, while providing a plethora of information which was unobtainable just 10 years ago.

One such area of research by many workers has been the area of fuel analysis. With the growing demand for high quality, affordable, and clean energy sources, the need for precise analytical measurements of fuels has become paramount. However, fuels are notoriously complex mixtures which provide quite a challenge to the analytical chemist. During the past few years, however, the development of separation techniques, such as gas (GC), liquid (LC), and supercritical fluid chromatography (SFC), and instrumental techniques such as nuclear magnetic resonance (NMR), infrared spectrometry (IR), mass spectrometry (MS), etc., have considerably eased the chemist's burden.

The primary goal of the project reported in this dissertation was to utilize instrumental and computer techniques such as these to develop a rapid, precise method of predicting a wide variety of the physical properties of middle distillate (i.e, jet and diesel) fuels. In particular, we were interested in utilizing the large information content of a directly coupled liquid chromatograph - proton nuclear magnetic resonance spectrometer (LC-¹H

NMR) as a predictive tool for a range of the physical properties of the middle distillate fuels. If one assumes that the physical properties of a fuel are primarily determined by chemical structures of the individual fuel components, then a measurement of the number and type of chemical structures present in the fuel will allow the calculation of the physical properties for that fuel. We felt that analysis of the ^1H NMR data would provide sufficient chemical structural information on the fuel constituents to allow accurate predictions of the physical properties of the fuel.

The project to predict the physical properties of the fuels involved essentially three distinct phases. The first phase was the development of a system of computer hardware and software to aid in the collection and analysis of the LC- ^1H NMR data. This computer software system would also be responsible for the development of correlations between the chemical structure which are present in the fuel and the physical properties of the fuel. The hardware and software for this system is described in Chapter 2. The second phase of the project was very much a learning step. In order to test the validity of the chosen methods and the software to be utilized in the prediction of the fuel properties, a series of model compound tests were conducted. These tests proved that it is indeed possible to accurately predict a wide variety of the physical properties of hydrocarbons (the primary components of middle distillate fuels) from their chemical structure. The results of these model studies are presented in Chapter 3. The final phase of the research involved the development of correlations between the chemical structures and the physical properties of a large number of middle distillate fuels. These correlations rely heavily on both the hardware and software developed in phase one of the research and the experience and insight gained from the model studies. The results of the fuel physical property predictions are discussed in Chapter 4.

As previously stated, this project involved the development of a large amount of computer software. The software developed to assist in the collection and analysis of the LC- ^1H NMR data is listed in Appendix I. Likewise, the software used to perform the physical

property - chemical structure correlations, as well as the analysis of these correlations is listed in Appendix II. The development of these correlations led directly to the development of the "second generation" software which is listed in Appendix III. The collection of programs listed in Appendix III is the actual implementation of the techniques learned in the correlations phase of the research. These programs apply the correlations in short, easy-to-use, packages designed to calculate the physical properties of hydrocarbons, fuel mixtures, or fuel blends.

Chapter 1

A HISTORY OF COUPLED CHROMATOGRAPHY-NMR, PETROLEUM SAMPLE ANALYSIS, AND PHYSICAL PROPERTY PREDICTION METHODS

Coupled Chromatography-NMR

Since the inception of nuclear magnetic resonance (NMR), chemists have investigated NMR of flowing systems. The non-invasive nature of NMR has made it the analytical technique of choice for many applications. The first report of the effect of a flowing system on the NMR signal was by Suryan (1) in 1951. In the years since this original work, numerous authors have published practical applications of the NMR of flowing systems. Many of these investigations have been reviewed by Jones and Child (2). In 1965, Zhernovoi and Latyshev (3) produced a comprehensive mathematical treatment of the theory related to signal intensity and linewidth for NMR of flowing systems.

A logical extension of the development of flow NMR is the direct coupling of a chromatographic eluent stream to the NMR system. This was first reported by Watanabe and Nicki (4) in 1978. However, the inherent insensitivity of the NMR experiment forced Watanabe and Niki to operate their chromatograph in a stopped-flow manner. The first continuous flow HPLC-¹H NMR experiments were reported in 1979 by Bayer *et al.* (5) and by Buddrus and Herzog (6) in 1980. Both of these groups utilized carbon tetrachloride (CCl₄) as the chromatographic solvent to provide a proton-free background for the NMR signal. These groups demonstrated static (i.e., nonflowing) NMR linewidths of 2.5 and 1.5 Hz, respectively, and were able to observe spin-spin couplings.

Also in 1980, Haw *et al.* demonstrated the direct coupling of a liquid chromatograph to a 100 MHz ^1H NMR spectrometer for the analysis of model as well as actual jet fuels. The chromatographic solvent used in this study was Freon 113 (1,1,2-trichlorotrifluoroethane) and nonflowing linewidths to approximately 5 Hz were observed (7). Haw also demonstrated the reconstruction of the chromatogram via the total proton count in the ^1H NMR, a process which is similar to the Gram-Schmidt reconstruction commonly employed in GC-FTIR. In 1981, Haw and coworkers demonstrated the use of a high-field (200 MHz ^1H) superconducting NMR spectrometer for the analysis of fuel samples (8). The use of the high field magnet provided ^1H NMR linewidths of 2 - 4 Hz with limits of detection of approximately 10 μg . The quantitative considerations of flow NMR were also considered by Haw (9). Subsequently, Haw *et al.* (10) utilized the large information content of the spectra obtained in the LC- ^1H NMR experiment to quantitate the hydrocarbon structures which are found in the fuel samples.

Several chromatographic solvent systems have been utilized for directly coupled LC- ^1H NMR. As previously pointed out, the first applications of NMR for a chromatographic detector employed either CCl_4 or freon as a solvent system. In 1981, Buddrus and Herzog demonstrated the use of the protonated solvent CHCl_3 (11). Although CHCl_3 produces a large solvent background signal in the ^1H NMR, linewidths were found to be approximately 2 Hz. Portions of the background signal were reduced by selective presaturation methods and the overall sensitivity was increased through the use of an expanded range analog-to-digital converter (ADC). These experiments lead directly to the application of NMR as a detector for reverse phase HPLC. Typically, reverse phase HPLC utilizes a water/methanol or water/acetonitrile mixture as the chromatographic solvent. These protonated solvents produce large ^1H NMR backgrounds and render large portions of the ^1H NMR spectrum unusable. Bayer *et al.* were the first to report reverse phase LC- ^1H NMR (12). Bayer also points out that when using gradient elution, the solvent background in the ^1H NMR changes over time,

making solvent suppression techniques very difficult.

In order to reduce the dynamic range of the solvent line in the ^1H NMR spectrum, several solvent suppression techniques have been proposed. Bayer (12) utilized homo-decoupling and homo-gated decoupling to reduce the solvent background when using acetonitrile as a solvent in reverse phase LC- ^1H NMR. In order to implement the homo-gated decoupling, however, long time periods were required which forced the liquid chromatograph to operate in a stopped flow mode. Laude *et al.* (13) have demonstrated the use of reverse phase LC- ^1H NMR for the separation of biomolecules. This separation utilized 98% D_2O and CH_3CN as the solvent system and Clore's 1-1 hard pulse technique for solvent suppression (14). Hore has demonstrated the use of the 3-3-1 hard pulse sequence (15) for a 1% diethylether solution in a 50:50 $\text{CH}_3\text{CH}/\text{H}_2\text{O}$ solvent system. This pulse technique was very effective and a suppression ration of 200:1 was obtained.

Liquid chromatography is not the only chromatography technique which has been coupled with NMR. In 1981, Buddrus and Herzog demonstrated the direct coupling of a gas chromatograph with a NMR spectrometer (16). This interface was limited to volatile samples which could be eluted from the GC column at $<50^\circ\text{C}$. With the addition of a heated interface (17), samples eluting up to 200°C could be analyzed in the NMR magnet. The inherent insensitivity of the NMR experiment, however, has limited the practicality of directly coupled GC-NMR. Although the NMR linewidths remain acceptable, the decrease in the instrumental signal to noise ratio with increasing temperature requires sample volumes too large to be easily managed by gas chromatography. Recently, Allen and Dorn (18,19) have demonstrated the direct coupling of a supercritical fluid chromatograph (SFC) to a superconducting NMR spectrometer. This technique has the advantage of nonprotonated CO_2 as the mobile phase, thus offering reverse phase type chromatographic separations without the solvent background of traditional reverse phase LC solvents. Also, Allen *et al.* (20) have demonstrated ^{19}F detection for LC-NMR for the analysis of derivatized alcohols. The ^{19}F

detection was accomplished via a specially constructed NMR probe and MLEV-16 phase cycle ^1H decoupling.

Analysis of Petroleum Samples

The analysis of petroleum fractions has traditionally been a very tedious proposition due to the complexities of petroleum mixtures. Although most petroleum samples are predominately composed of mid-boiling (i.e., $\text{C}_5\text{-C}_{25}$) hydrocarbons, various petroleum fractions may contain much larger ($\geq\text{C}_{25}$) polynuclear aromatic hydrocarbons (PAH's), heterocyclics, and/or trace metals. The wide variety of petroleum constituents and the considerable number of physical properties of the petroleum mixtures which are commonly measured have presented the analytical chemist with a considerable challenge. Various analytical techniques have been applied to petroleum analyses, with mixed results. Most of the methodologies developed for fuel analysis have involved some form of chromatographic separation, either LC, GC, or SFC, with some form of spectroscopic detection (i.e., IR, NMR, MS, UV, etc.). These methods have utilized both directly coupled and off-line chromatographic separation of the petroleum samples. An attempt will be made to briefly discuss several of these techniques, with an emphasis on analytical techniques utilizing chromatography and/or NMR spectroscopy as applied to middle distillate (i.e., jet and diesel) fuel samples.

The current standard methodology for the analytical testing of the physical properties of fuel samples are methods published annually by the American Society for Testing and Materials (ASTM) (21). Recently, these techniques have come under close scrutiny due to relatively poor reproducibility (22). Also the economics of fuel production have pushed the petroleum refiner into producing fuels with smaller performance margins (23), thus increasing the need for accurate physical property analysis. These trends in the composition and performance of JP-4 type fuels have been reviewed by Harrison (24).

One of the most widely studied properties of the middle distillate fuels is the cetane number. In its most simple form, the cetane number of a diesel fuel can be thought of as the analog of the octane number of a gasoline sample. In fact, the octane and cetane numbers can be related (25). Recently, Indritz (26) has described the cetane number, the ASTM test method for establishment of cetane (27), and the structural influences of various carbon types on the cetane number. Various other studies have been performed to determine the optimum cetane number for diesel fuels (28).

As was previously mentioned, several analytical techniques have been applied to the analysis of petroleum based samples. In 1980, Buchar (29) reported a method for the determination of hydrocarbon types in jet fuels by infrared spectroscopy. This process analyzes the total amount of aromatics and olefins, then determines the amount of saturates present in the fuel by difference. More recently, methods have been reported for the determination of various physical properties of petroleum samples by differential scanning calorimetry (DSC) (30). In 1982, Moynihan and coworkers (31) applied DSC to the analysis of melting and freezing points of jet and diesel fuels. Melting point analysis in this manner was found to be much quicker than the ASTM melting point methods. It was also found that the area of the DSC melting endotherms correlated well with the *n*-alkane content of the fuels, suggesting that the *n*-alkanes are one of the first petroleum constituents to freeze out of solution. In 1981, Bothe (32) reported the use of energy-dispersive x-ray fluorescence spectrometry for multielement trace analysis of diesel fuels. Recently, Bello and Hurtubise (33) have reported the use of solid-surface room temperature luminescence for the characterization of mixtures in PAH's. Various other analytical methods and apparatus for the determination of flash point (34,35), cloud and pour points (36,37), initial boiling point and saturated vapor pressure (38), cetane number (39), hydrogen content (40), API gravity (41), and boiling point (42) have been proposed as modifications of, or alternatives to, the current ASTM standard methods.

Table 1.1
Significant developments in petroleum characterization
by magnetic resonance techniques.

<u>Year</u>	<u>Event</u>	<u>Lit. Cited</u>
1957	First reports of petroleum characterization by high resolution ^1H NMR	(45,46,47)
1958	ESR detection of carbonaceous free radicals and vanadium porphyrins in petroleum	(48,49)
1959	Early patent for ^1H NMR as process control device	(51)
1959	First use of ^1H NMR for elemental hydrogen content measurement on petroleum materials	(50)
1960	First report on nuclear magnetism logging as a drilling control technique	(148)
1967	First quantitative ^{13}C NMR spectrum of a petroleum fraction by time-averaged slow passage technique	(57)
1976	Detailed investigation of crude oils and petroleum products by quantitative ^{13}C FTNMR	(53)
1978	First ASTM standard method using ^1H NMR	(149)

Almost since its inception, NMR has been utilized for the analysis of petroleum samples. Much of the early work in this area has been reviewed by Retcofsky, Rose, and Miknis (43). Table 1.1 has been reproduced from Retcofsky's review. The earliest application of NMR to fuel analysis was in 1955 by Williams (44). The first actual ESR and NMR spectra of petroleum samples were published in 1957 (45 - 47) and 1958 (48,49) and were obtained at 30 MHz. The first use of NMR to measure the elemental hydrogen content of fuel samples was by Williams in 1957 (50). A patent (51) was issued in 1959 for process control based on NMR determination of the degree of branching in alkyl substituted aromatic hydrocarbons. In 1967, petroleum analysis by NMR took a giant step forward with the introduction of high resolution ^{13}C NMR (52) for fuel samples. These techniques were further refined with the introduction of high resolution fourier transform ^{13}C NMR (53) in 1976.

The large amount of chemical structural information available from NMR spectra has allowed many diverse applications in petroleum analysis. NMR has even been utilized in the analysis of petroleum products found in fire debris (54) to aid in arson investigation. One of the first uses of NMR for structure elucidation of fuels was by Brown, Ladner, and Sheppard (55,56) in 1959. Similar studies have also been performed by Knight (57), and Clutter *et al.* (58). In particular, Clutter was able to integrate the ^1H and ^{13}C NMR spectra of fuel samples to determine average structural parameters such as the ^1H and ^{13}C aromaticities, molecular weight, and a "branchiness index" which were representative of the compounds found in the fuels. In 1981, this work was expanded by Netzel and Hunter (59) who demonstrated a computer program to calculate the total content of paraffins, monocyclic aromatics, and dicyclic aromatics for ^1H and ^{13}C NMR data, without the necessity of chromatographic separation prior to NMR analysis. Ohi and coworkers (60) reported work similar to that of Netzel and Hunter in 1981, although Ohi's calculations were based not only on whole fuel samples, but also subfractions of the fuels which had been collected via off-line HPLC. In 1983, Cookson and Smith (61) reported the use of the spin echo broad band

off-resonance decoupling (SEBBORD) technique to improve quantitation of quaternary carbon resonances in the ^{13}C NMR spectra of unseparated petroleum samples. Likewise, Laude and Wilkins (62) have reported application of quantitative ^{13}C NMR and ^{13}C NMR spectral editing techniques for the identification of organic mixture components without prior chromatographic separation. Cookson and Smith (63) have also applied ^{13}C NMR techniques to determine structural characteristics of saturates in kerosine (i.e., jet) and diesel fuels.

NMR spectrometry has also been applied to various other forms of petroleum products. In 1984, Dalling, Baily, and Pugmire (64) reported the use of ^1H and ^{13}C NMR data for compositional analysis of both jet fuels and shale-derived refinery products. In this study, Dalling *et al.* developed average structural compositions of these petroleum products in a manner similar to Haw (10), as well as reporting the separation of petroleum products by supercritical fluids chromatography (SFC). With the rise of alternate energy sources came the need for new analytical methods to address the specialized analytical requirements of the new fuels. In 1985, Renzoni and coworkers (65) reported the use of NMR to determine the alcohol content in gasoline/alcohol blends. Shofstahl and Hardy have reported the determination of C_1 - C_4 alcohols in gasoline by multiple ion detection (66).

As previously mentioned, the use of all forms of chromatography for fuel analysis has been widely reported. In 1979, Warner and Kenan (67) reported the use of a UV detector for the GC separation of jet fuels. A glass capillary GC column was utilized which allowed direct UV detection of the aromatic components of the chromatographic eluent. This technique produced a detection limit of approximately 0.05% for the aromatics. Bradley (68) has reported the use of coupled GC-microwave induced plasma (GC-MIP) as an oxygen selective detector for petroleum products. The heavy constituents of coal liquids have been analyzed by means of combined GC-vacuum thermogravimetric analysis by Southern and coworkers (69).

HPLC has also been widely used for the determination of fuel composition (70 - 73). In particular, silver nitrate (AgNO_3) columns with backflush systems have been applied to HPLC in an attempt to quantitate the olefin content of diesel and jet fuels (74,75). Most of these analysis methods employ dual detection schemes. A refractive index detector is utilized for saturate concentration analysis and UV detection is employed for quantitation of the aromatics. Electrochemical detection in LC has been demonstrated by MacChehan and coworkers for the determination of phenols in petroleum (76) and nitrated polyaromatic hydrocarbons in air and diesel particulates (77). Mass spectrometry has been utilized as a LC detector for the hydrocarbon composition of coal liquid samples by Allen, Hurtubise, and Silver (78). A modified flame ionization detector was utilized with LC by Pearson and Gharfeh (79) for the rapid analysis of petroleum fractions which boil above 350°F. Column chromatography has been applied by Zrelav *et al.* (80) for the determination of hydrogen content. Column chromatography has also been compared to HPLC and GC for quantitative analysis of hydrocarbon group content by Cookson and Smith (81). The larger PAH constituents of heavy petroleum fractions have been separated by means of size exclusion chromatography by Laflue and Wornat (82) and by Larsen *et al.* (83) utilizing gel permeation chromatography coupled with field desorption mass spectrometry.

In 1983, McNair and Apffel (84) reported the use of multidimensional gas and liquid chromatography for hydrocarbon group analysis. This system utilized a HPLC silica gel column to separate petroleum samples into saturates, unsaturates, aromatics, and polar compounds. These fractions were then subsequently characterized by capillary GC-FID. Multidimensional microbore LC/capillary GC analysis of petroleum samples has recently been reported by Davies and coworkers (85,86).

The recent emergence of SFC as a separation technique has also had an impact on fuel analysis. Lee *et al.* have utilized SFC for the fractionation of petroleum and coal-derived mixtures (87), fractionation and characterization of sulfur heterocyclics (88), and hydrocarbon

group analysis in gasolines and middle distillate fuels (89).

Physical Property Prediction Methods

The past fifty years has seen an increase in both the number of physical properties which are commonly measured and the accuracy with which these measurements are taken. This proliferation has placed an increased burden on the analytical chemist. However, the advent of the computer, and in particular the personal computer, has placed new worlds of affordable computational power at the disposal of the chemist. As early as 1981, personal computers were used to store and manipulate data bases of physical properties (90). These computers have allowed the development of both data base management systems of physical properties (91,92) and computational techniques to calculate the physical properties of compounds (93,94).

PURE COMPOUND PROPERTY PREDICTION TECHNIQUES: The calculation of the physical properties of pure compounds has received much attention in the chemical literature. For many years, chemical engineers utilized simple equations to predict the physical properties of a compound or simple hydrocarbon mixtures. A summary of the some of the physical properties of pure compounds for which equations have been derived is shown in Table 1.2. This table lists the physical property and the references given for the calculation of that property. Many of these physical property prediction schemes have relied on a group property approach. In a group property approach, one assumes that, to a first level of approximation, the physical property of the compound is determined solely by the chemical groups (i.e., chemical structures) which are present in compound. A prime example of this approach is the work by Fisher (95,96) in which physical properties such as density, critical temperature, boiling point, etc. are calculated for linear alkanes. Fisher's approach utilizes simple linear equations to calculate the physical property from the carbon chain length of the

Table 1.2
References for the calculation of the indicated physical property
for pure compounds.

<u>Property</u>	<u>References</u>
Boiling Point	103, 99, 100, 95, 102
Critical Pressure	113, 99, 109, 96, 102
Critical Temperature	113, 99, 109, 96, 102
Critical Volume	113, 99, 109, 96,
Density	98, 99, 114, 109, 104, 111, 95, 96, 112, 110, 116
Dielectric Constant	95, 102
Enthalpy	97, 99
Flash Point	106, 107
Freezing Point	103, 95, 102
Heat Capacity	103, 113, 109, 104
Heat of Combustion	100
Heat of Formation	104, 100
Heat of Vaporization	103, 113, 109, 104, 100, 102
Magnetic Susceptibility	102, 116
Molar Volume	109, 100
Molecular Weight	109, 102
Refractive Index	95, 110
Surface Tension	113, 104, 95, 102
Thermal Conductivity	113, 104, 112, 102
Vapor Pressure	108, 95
Viscosity	103, 113, 104, 105, 101, 112

n-alkane. An example of this is Equation 1.1, the equation for calculation of *n*-alkane density

$$[1.1] \quad (x-0.528)/d_4^{20} = 1.27119 + 1.17085x$$

where *x* is the number of carbons in the chain, and d_4^{20} is the density of a liquid at 20°C relative to the density of water at 4°C. Equation 1.1 yields a correlation between predicted and observed density of 0.99999992 for *n*-alkanes C₅-C₄₀. Through a group property approach which assumes that the physical properties of the *n*-alkanes are determined solely by the length of the carbon chain, Fisher was able to obtain correlation coefficients of better than 0.9998 over a range of at least 10 carbons for each property. Although very accurate, Fisher's approach is limited in that it is applicable only to linear alkanes. Cardozo (97) has developed an equation based on the number of carbon and halogen atoms to predict the enthalpy of formation for a variety of organic compounds. On a rather limited basis set, this equation has predicted the enthalpy of formation of organic liquids with an error of less than 5%. Further examples of group property approaches are available in the work of Eckart *et al.* (98), Adams and So (99), Mekenyan *et al.* (100), Daymond and Young (101), and Cramer (102). Also Bungler and coworkers (103) have reported a model for the determination of a nine of physical properties of hydrocarbons in the C₆ to C₂₀ range with correlation coefficients ranging from 0.954 to 0.999. Many of these approaches have been implemented into calculator programs for use by engineers (104 - 107).

A second very popular approach to the prediction of the physical properties of pure compounds is the calculation of one physical property from another physical property. Several of the physical properties have been shown to be interrelated and therefore it is possible to calculate several physical properties based on a knowledge of only one or two physical properties. The work by Dutt (108) is a good example of this technique. Based on

a study of 218 compounds in a homologous series, Dutt was able to determine the relationship between the vapor pressure and the boiling point of hydrocarbons. The error in this relationship is given as less than 5% for paraffins, olefins, and aromatics. Likewise, Riazi and Daubert (109) have used an equation of the form

$$[1.2] \quad \phi = aT_b^b S^c$$

to predicted nine physical properties for hydrocarbons boiling in the range of 100 to 850°F. In Equation 1.2, $a, b,$ and c are constants, ϕ is the property being calculated, T_b is the boiling point, and S is the specific gravity. Based on a basis set of 90 to 198 compounds, Equation 1.2 yields predicted physical properties of with errors of approximately 5 - 10%. In this work, Riazi states that the terms T_b and S need only be parameters capable of characterizing molecular forces. Therefore, any physical properties which describe molecular forces or molecular size may be utilized for the development of physical property correlations. Further examples of this type of correlations can be found in the work by Roy (110) in which the refractive index of n -alkyl derivatives of organic compounds was found to be inversely proportional to their density. Chen and Vedam have (111) also reported the relationship between density and refractive index as a function of temperature. Also, Ely (112), Wooley (113), Singh and Singa (114), Fainerman (115), and Rudkevich *et al.* (116) have reported correlations studies of this type.

FUEL PHYSICAL PROPERTY PREDICTION TECHNIQUES: The same methodologies which have been applied to the prediction of the physical properties of pure compounds have also been applied to the prediction of the physical properties of petroleum based mixtures. Both group property predictions (117) and property-correlation (118) methods have been successfully applied to the fuel property prediction. A large body of literature exists for detailed explanations of these prediction schemes (119 - 143). The fuel physical properties

Table 1.3
References for the calculation of the indicated physical property
for fuels and mixtures.

<u>Property</u>	<u>References</u>
Aniline Point	126, 133
Boiling Point	124, 125, 126, 128, 146, 91, 133, 134, 137, 138
Cetane Number	144, 117, 126, 146, 133, 139, 140, 142
Cloud Point	126
Density	123, 125, 146, 91, 134, 141
Flash Point	128
Freezing Point	121, 145
Gravity	119, 118, 124, 125, 126, 146, 145, 133
Heat Capacity	120
Heat of Combustion	119, 145
Heat of Formation	147
Molecular Weight	118, 147, 124, 134, 141
Octane Number	137
Pour Point	124
Refractive Index	118, 146, 136
Smoke Point	119, 145
Surface Tension	119
Vapor Pressure	128, 137
Viscosity	119, 118, 122, 127, 128, 146, 145, 134
Volatility	119

which have been predicted by these various techniques and the references where they may be found are summarized in Table 1.3.

Of particular interest is the work by Gülder and Glavincevski (144). Published in 1986, this work provides a method for the calculation of the cetane number of a diesel fuel based on the ^1H NMR spectrum of the fuel sample. Through integration of various regions in the ^1H spectrum taken at 60 MHz, the authors were able to develop a equation of the form

$$[1.3] \quad \text{GCN} = B_{\sigma} + [B_1/C_A + B_2/C_A^2] + (B_3C_{\alpha} + B_4 \ln C_{\alpha}) + (B_5C_2 + B_6C_6^2) + (B_7C_3 + B_8C_3^2)$$

where GCN is the calculated cetane number, B_{σ} are constants, C_{α} is the integration of the ^1H region directly adjacent to aromatic rings, C_2 and C_3 are the integration areas of the methylene and methyl regions respectively, and C_A is a calculated integration area, based on aromatic ^1H regions. For a total of 67 fuel samples which had cetane numbers of 20 - 75, Equation 1.2 yielded a correlation coefficient (r) between predicted and observed cetane of 0.992, with an error (σ_r) of ± 1.11 cetane. This is indeed a very good correlation and points to the applicability of NMR analysis for physical property prediction, although this particular application is limited only to the prediction of cetane number.

In 1987, Cookson, Lloyd and Smith (145) also reported the use of ^1H NMR data for the prediction of petroleum product physical properties. Utilizing off-line chromatographic separation (GC or HPLC), the fuels were separated into hydrocarbon classes and the ^1H NMR spectra of these fractions were measured. A three parameter equation was then developed

$$[1.2] \quad P = a_1[n] + a_2[BC] + a_3[Ar]$$

to predict various physical properties (P) of a fuel, based on the weight fraction of n -alkanes, [n], branched plus cyclic saturates, [BC], and aromatics [Ar] present in the fuel sample. The

terms $a_{1,3}$ are constants. Equation 1.2 has been utilized to predict the smoke point, aromatics content, ^{13}C and ^1H aromaticities, heat of combustion, H content, freezing point, and inverse specific gravity of a range of kerosene (i.e., jet) fuel samples. The data base for this work consisted of approximately 40 fuels and the properties were predicted with correlation coefficients of 0.76 to 0.95, and errors of approximately 5 - 10%. Again, this technique has proven successful although the off-line chromatographic separation of fuel samples is very time consuming. Also, some of the properties which are correlated (i.e., ^1H and ^{13}C aromaticity) are directly measurable by NMR and do not need to be correlated.

Also of interest is the work of Riazi and Daubert (146). Essentially, this work operates in reverse of the work by Cookson. Instead of predicting the physical properties of petroleum fractions from the chemical composition of the fractions, Riazi has developed a method whereby the fractional composition of saturates, naphthalenes, and aromatics is calculated from the viscosity, specific gravity, and refractive index of a fuel sample. Based on a data set of approximately 80 fuels, Riazi found that this approach can predict the hydrocarbon class composition of the fuels with an error of 5 - 15%, depending on the hydrocarbon class.

Honigs, Hirschfeld, and Hieftje (147) have taken a slightly different approach to the prediction of the physical properties of hydrocarbons through the use of near-infrared spectroscopy. This technique utilizes equations based on the absorbance of the sample at four wavelengths to predict the heat of formation, molecular weight, and number of methyl groups per molecule. An example would be the equation for the calculation of the heat of formation:

$$[1.3] \quad \text{Heat of Formation} = -3.8 \text{ Abs}_{(2181)} + 9.4 \text{ Abs}_{(2150)} - 2.7 \text{ Abs}_{(1958)} - 2.9 \text{ Abs}_{(1701)}$$

The weighting constants and the absorbance wavelengths for each property are tabulated by the authors. On a basis set of 90 hydrocarbon mixtures, this technique provided correlation

coefficients of 0.993, 0.986, and 0.997 for the heat of formation, molecular weight, and number of methyl group predictions, respectively. Correlation coefficients in this range correspond to prediction errors of $\leq 4\%$. As with the techniques based on NMR, this method provides good correlations for the indicated physical properties. However, the use of near-IR data dictates that physical properties such as molecular weight and number of methyl groups per molecule must be correlated whereas the use of NMR analysis allows for the direct measurement of properties such as these.

Chapter 2

A PERSONAL COMPUTER-BASED HARDWARE AND SOFTWARE SYSTEM FOR THE ANALYSIS OF LC-¹H NMR DATA

Introduction

For several years our laboratory has been involved in the development of directly coupled Liquid Chromatography - Proton Nuclear Magnetic Resonance (LC-¹H NMR) for the analysis of middle distillate fuels (e.g., jet and diesel fuels) (7,8). This analysis, however, has proven to be quite tedious due to the large volume of data produced by the LC-¹H NMR and the limitations of the software available for our JEOL FX-200 NMR instrumentation. To overcome this, the system which is described in this chapter has been developed to better handle the data produced by the LC-¹H NMR. This system consists of two distinct sections, the first to aid in the collection of the LC-¹H NMR data and the second to reduce the raw NMR data to a form which yields usable chemical information.

The initial phase of the development of this system principally consisted of the development of the hardware necessary to collect the LC-¹H NMR data for the middle distillate fuels. Although the actual development of the liquid chromatograph - NMR interface has been previously published (10), substantial effort was expended to update the LC-¹H NMR system to require less operator intervention. This involved interfacing the refractive index detector on the liquid chromatograph to the IBM CS/9000 microcomputer to provide automated collection of the refractive index traces. Also, a Tandy TRS-80 microcomputer was interfaced to the JEOL FX-200 NMR spectrometer to provide automatic changing of the NMR receiver gain as well as advancement of the LC fraction collector.

The second phase of the project was the development of a variety of software which was designed to run on an IBM Personal Computer. First in the series of software packages is a transfer program, developed with the assistance of Larry Jackson of the VPI&SU Chemistry Department Electronics Shop, which will transfer data serially between the FX-200 NMR and the Personal Computer. Once stored in the PC, the second software package, LCNMR, is utilized to integrate the NMR spectra and calculate average structural parameters which quantitate the chemical functionalities present in the middle distillate fuels. After the average structural parameters are calculated, correlations between these parameters and the physical properties of the fuels were determined by a series of programs which are listed in Appendix II. The integration and structure calculation software is listed in Appendix I.

Experimental

EQUIPMENT: At the core of the system which we have developed is a JEOL FX-200 NMR spectrometer. (Figure 2.1) The liquid chromatography system used for the separation of the middle distillate fuels consists of a Waters M-45 pump, Whatman Magnum-9 PAC-10 semi-preparative scale column, and a Chromatronix refractive index detector. To aid in the collection and analysis of the data produced by the LC-¹H NMR technique, three separate computer systems were employed. The first computer was an IBM CS/9000 laboratory computer system which includes four 30 Hz analog-to-digital converters. This system is utilized to collect the refractive index chromatographic data. Once the refractive index trace is digitalized, specialized software on the CS/9000 calculates the parameters necessary for accurate LC-NMR data collection of the fuel samples. The ¹H NMR data was collected on a JEOL FX-200 NMR spectrometer which is controlled by a Texas Instruments 980B computer. The NMR instrument is interfaced to the second computer utilized in the system, a TRS-80 Model I microcomputer. The TRS-80 is interfaced to the JEOL FX-200 NMR spectrometer to automate changing of the receiver gain and to advance the

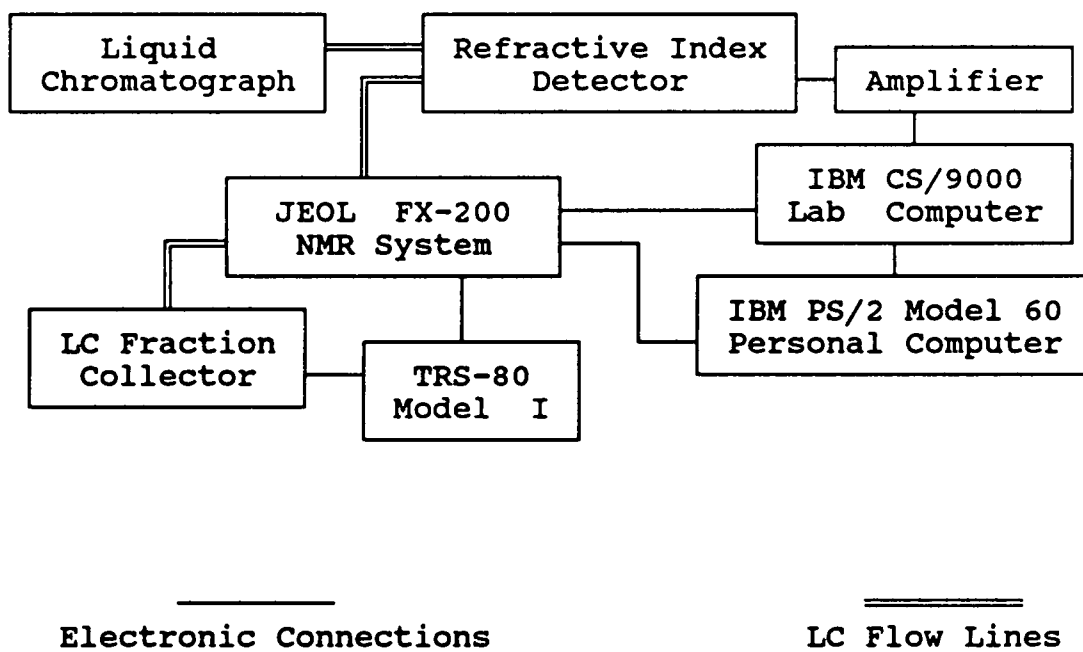


Figure 2.1 Block diagram of the LC-¹H NMR hardware system.

chromatographic fraction collector. This interface to the JEOL FX-200 NMR and the chromatographic fraction collector was accomplished via a Tychon Programmable Peripheral Interface Adapter which was modified with the additional circuitry depicted in Figure 2.2.

After the ^1H NMR data has been collected and stored on the JEOL NMR, it is transferred to the third computer, an IBM Personal System 2 Model 60-071 microcomputer. The PS/2 then integrates and analyzes the NMR data to calculate the molecular composition of the fuel, *vide infra*.

SOFTWARE: The software on the IBM CS/9000 lab computer has been specifically written in IBM Instrument's interpretative BASIC to collect the refractive index traces for the separation of the middle distillate fuels. The Chromatronix refractive index detector produces a response of 10 mV full scale which was found to suffer from superimposed 60 Hz noise. In order to adequately digitalize this signal, an amplifier was constructed to boost the signal to 10 V full scale, as well as filter the signal to remove any 60 Hz noise. This signal can then be transmitted to the CS/9000 for digitalization by the analog-to-digital converter. Once digitalized, the chromatographic software developed for the CS/9000 stores, displays, and analyzes the chromatogram. This chromatographic software is controlled via a Tandy Corporation joystick which was modified to operate in concert with the internal analog-to-digital converters on the CS/9000. This joystick controls a cursor on the chromatogram which will calculate the number of NMR scans which may be obtained in each chromatographic peak. During the collection of the LC- ^1H NMR data, it is desirable to instruct the NMR spectrometer to scan average (i.e., coadd successive Free Induction Decays) over the elution of an entire chromatographic peak. That is, the NMR is instructed to scan average across the entire chromatographic elution volume of alkane constituents of the middle distillate fuels, then scan average over the monocyclic aromatic constituents, then the dicyclic aromatic constituents, etc. Through a knowledge of the NMR cell volume, the chromatographic flow rate, and the time required to acquire a NMR scan, the software on the CS/9000 is able to

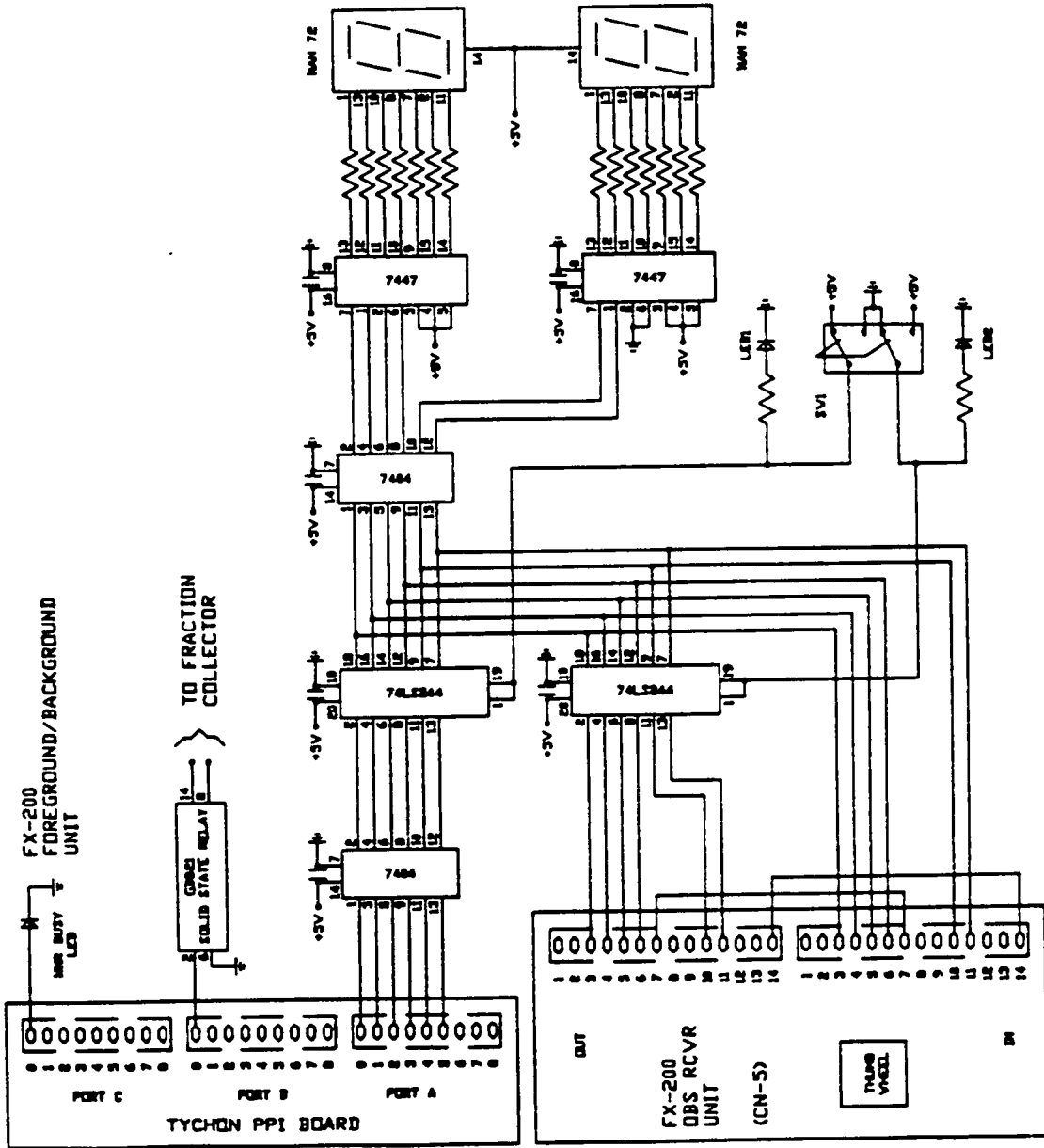


Figure 2.2 Schematic diagram of TRS-80 Model I/ JEOL FX-200 NMR spectrometer interface.

calculate the number of NMR scans which could be acquired during the elution of a given chromatographic peak. For example, if the chromatographic flow rate is 4.0 ml/min, and the NMR flow cell has a volume of 50 μ L, the delay between NMR pulses would be adjusted so that the cell volume would be flushed between NMR scans, i.e. 0.75 seconds total acquisition time for each scan. Since the chromatographic peak was 1.0 min wide, a total of 80 NMR scans would be required to scan average across that particular peak. This calculation assumes plug flow of the chromatographic eluent through the NMR flow cell.

Since the middle distillate fuels are predominately composed of aliphatic compounds, it is necessary to increase the receiver gain on the NMR spectrometer after the elution of the aliphatic chromatographic fraction to adequately acquire the ^1H NMR spectra of the aromatic chromatographic fractions. It is possible to monitor the elution of these fractions by monitoring the BUSY light on the foreground/background unit of the JEOL FX-200. Since this indicator light turns off briefly while the NMR spectrometer stores each file on the floppy disk, the TRS-80 Model I may determine the number of NMR spectra which have been stored by counting the number of blinks of the BUSY indicator light. After the collection of the NMR spectra of the alkane chromatographic fraction, (12 spectra in the case of the middle distillate fuels), the TRS-80 Model I will automatically change the receiver gain on the JEOL FX-200 and advance the chromatographic fraction collector. The fraction collector is advanced by providing a switch closure at the relay depicted in Figure 2.2. The software for this microcomputer was written in Radio Shack interpreter BASIC and is listed in Appendix I.

A NMR data analysis package was developed for the IBM PS/2 which consists of several individual programs (see Appendix I), all of which run under Borland Corporation's *TurboBASIC*. The most important of these programs are the data transfer software, FX200.BAS, and the LC-NMR data analysis software, LCNMR.BAS. The data transfer software facilitates the transfer of the NMR data from the JEOL FX-200 to the PS/2 via a

9600 baud RS-232 serial communications line. Although this transfer software will transfer either a FID or a transformed and phased NMR spectrum, it was found that the JEOL NMR can Fourier transform and phase the NMR data faster than the PS/2. Therefore, in an effort to save analysis time and disk storage space, the NMR spectra are transformed and phased with the JEOL NMR with only the acquisition parameters and real data points of the NMR spectra being transferred to the PS/2. The transfer software described here will transfer the acquisition parameters and real points of 2k point NMR spectrum to the PS/2 in approximately 10 seconds. The acquisition parameters and both real and imaginary points of a 2k point spectrum requires approximately 17 seconds to transfer.

The second major piece of NMR data analysis software is the LCNMR program. This software is essentially a NMR workstation which was specifically designed to manipulate LC-NMR data. This software integrates the NMR spectra of the chromatographic fractions and calculates the average structural parameters for each chemical class present in the fuels, according to equations previously published (10).

Also running on the PS/2 are a series of programs designed to correlate the average structural parameters as calculated by the LC-NMR data analysis software with the physical properties of the middle distillate fuel samples. Each of the programs in this package is listed in Appendix II. Essentially this software package consists of a data base management program to service the files containing the physical properties of the fuels, a multiple regression analysis program to find correlations between the physical properties and the average structural parameters, and graphical and statistical software to analyze the quality of the correlations determined by the multiple regression analysis.

Results and Discussion

Perhaps the most remarkable feature of the system presented here is the speed at which it operates. The chromatographic separation of the middle distillate fuels requires

approximately 1 - 1.5 hours and has now become the limiting factor in the overall analysis of the fuel samples. Before the implementation of this system, the reduction and analysis of the LC-¹H NMR data required more time than the collection of the LC-¹H NMR data. The software package developed for the PS/2 allows interactive integration of the NMR spectra of each chromatographic fraction and the calculation of the average structural parameters in a drastically reduced amount of time. Before implementation of this system, integration of a complete set of chromatographic files on the FX-200 required approximately one hour of operator time. With the LC-NMR software on the PS/2, the same set of files can be integrated in $\approx 3 - 5$ minutes.

The main reason for this speed is demonstrated in Figures 2.3 and 2.4, which portray screens taken directly from the LC-NMR software. Figure 2.3 is the integration screen for the alkane chromatographic fraction of a fuel and Figure 2.4 is the integration screen for the monocyclic aromatic chromatographic fraction. The rightmost peak in these figures is the quantitative shift and integration reference hexamethyldisiloxane (HMDS) which is added to the LC solvent. The LC-NMR software automatically finds the HMDS peak and sets it as the reference peak. Since NMR spectra do not always possess a perfectly flat baseline, the LC-NMR software will subtract a background spectrum to correct for any impurities in the LC solvent or background from the flow NMR probe. After the background subtraction, the spectrum is then displayed to the screen and baselines are drawn across the integration areas. Once the baselines have been drawn, the spectrum is integrated between the integration divisions, normalized against HMDS, and the average structural parameters for the chromatographic fraction are calculated. (Please note that in the alkane chromatographic fraction of the fuels, mole fraction data is obtained on the fuel composition, not average structural data similar to that which is obtained in the aromatic chromatographic fractions.) These average structures are shown across the top of the screen depicted in Figure 2.4. Note that each integration screen also shows the NMR shifts (relative to HMDS at 0.07 ppm) and

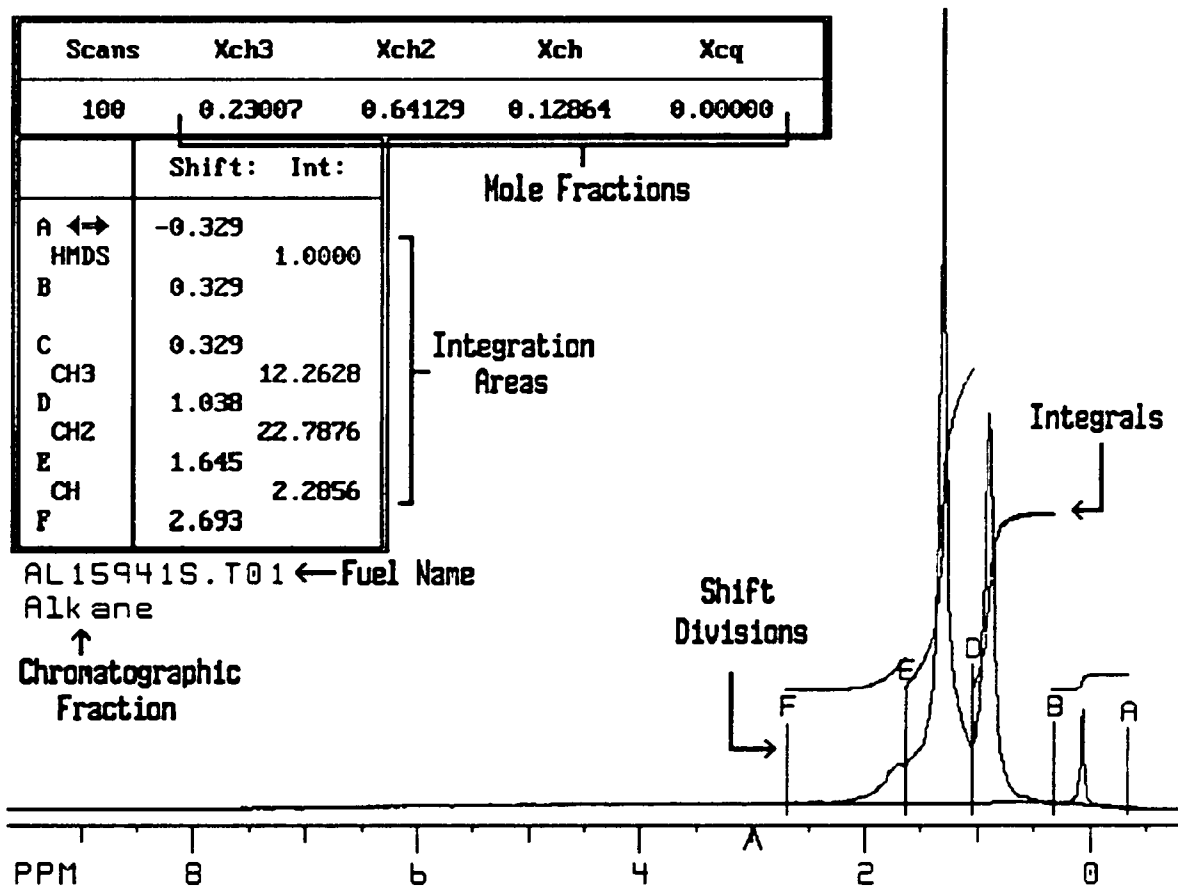


Figure 2.3 Integration screen from Program I.3 (LCNMR.BAS) depicting the integration of the alkane chromatographic fraction.

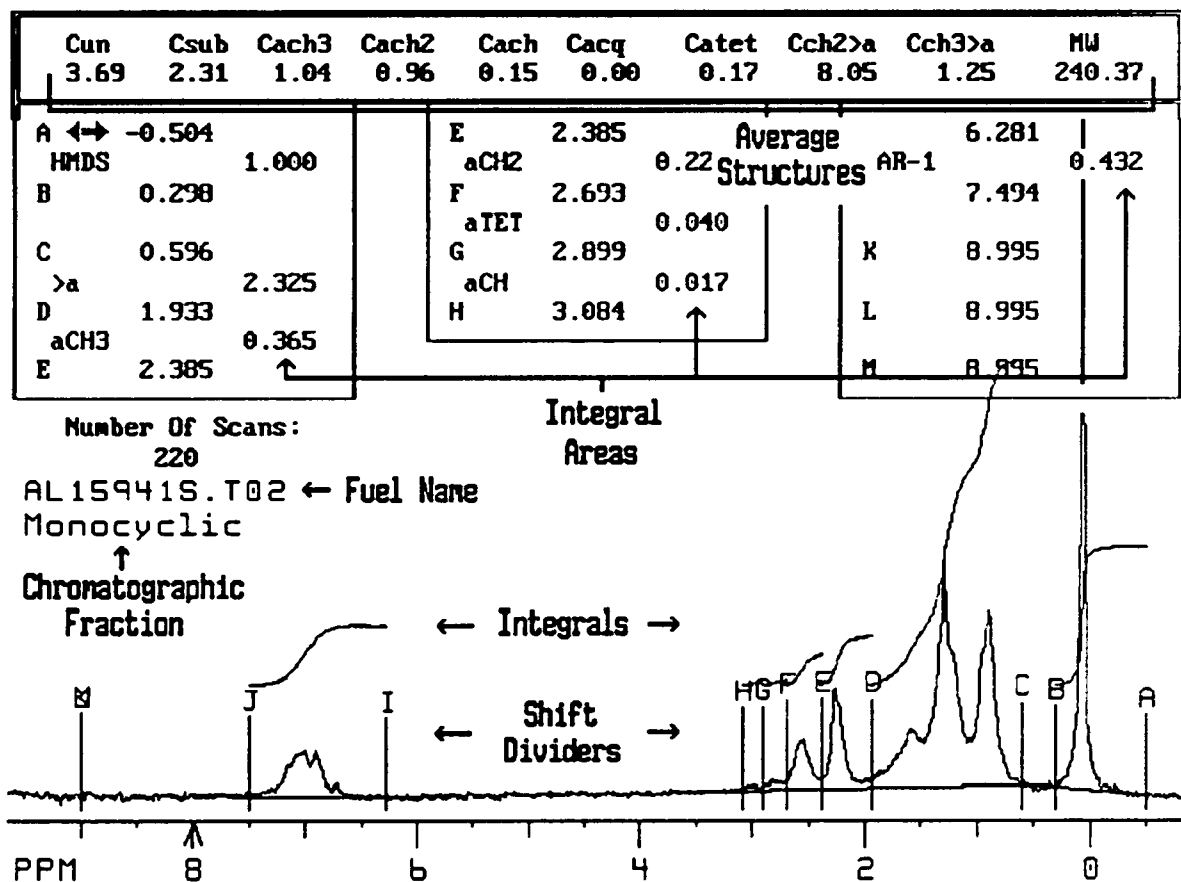


Figure 2.4 Integration screen from Program I.3 (LCNMR.BAS) depicting the integration of the monocyclic aromatic chromatographic fraction.

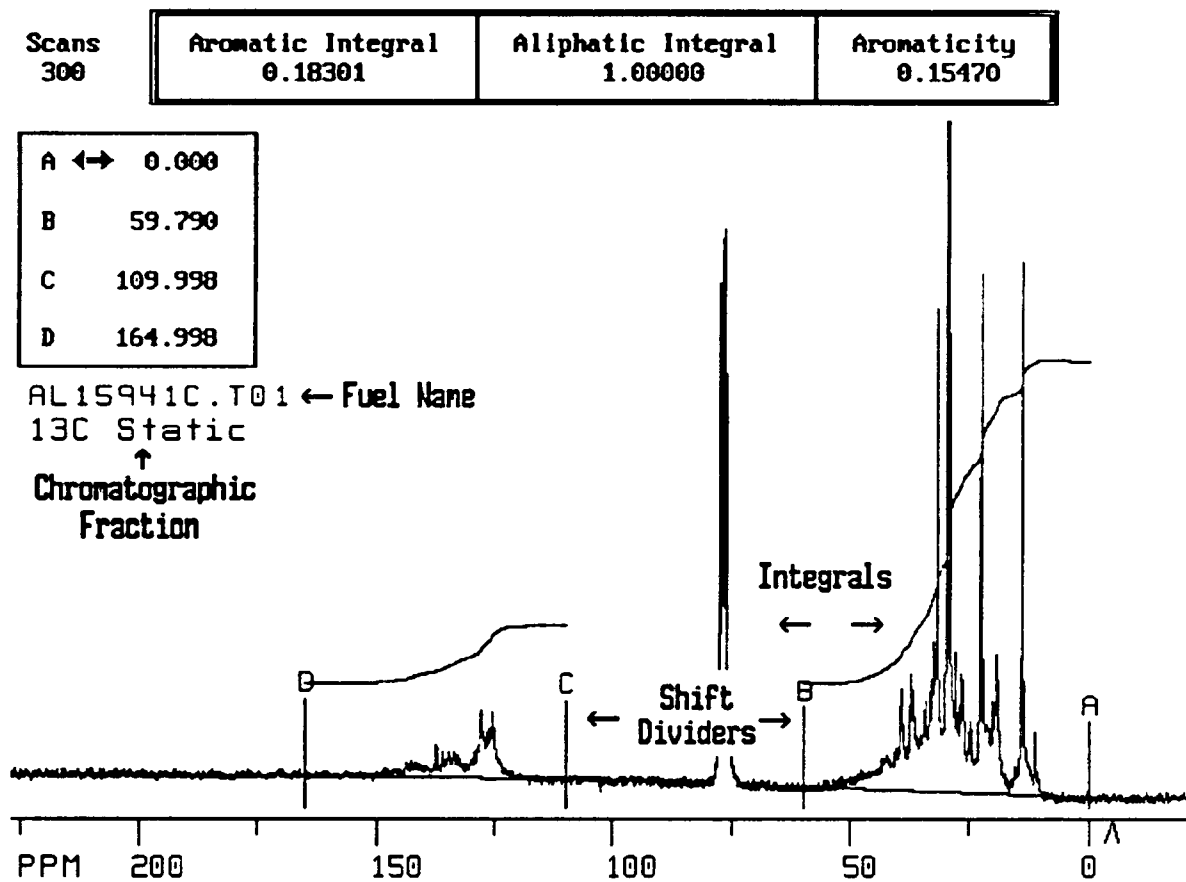


Figure 2.5 Integration screen from Program I.3 (LCNMR.BAS) depicting the integration of a static ^{13}C NMR spectrum.

the normalized integrations areas.

Perhaps the most useful feature of the LC-NMR software is the ability to interactively adjust the baselines and the integration endpoints of the NMR integrals. Whenever either an integration endpoint or a baseline is changed, the NMR spectrum is automatically reintegrated, the average structural parameters recalculated for the new integration areas, and the new integration areas and average structural information are displayed on the screen. Although the time required for perform this recalculation and display is dependant on then number of spectra points and the exact computer configuration, the analysis time for the 2k ^1H NMR files which are analyzed on the PS/2 is usually less than one second and many times is nearly imperceptible.

This system, however, is not limited only to LC- ^1H NMR data. The NMR workstation features represented in the software may be equally applied to conventional NMR experiments on nearly any NMR active nucleus. Shown in Figure 2.5 is the integration of a traditional ^{13}C NMR spectrum of a middle distillate fuel. As with the LC- ^1H NMR data, this software package performs the baseline correction and integration as well as calculation of the ^{13}C aromaticity for the fuel samples. The use of the LC-NMR software in this manner provides a direct measurement the ^{13}C aromaticity of the fuel sample, usually in less than 5 seconds.

Once the fuel has been integrated and the average structures calculated, both the integrals and the average structural information are filed. This file may be later recalled and edited using a full screen editor which has been written into the LC-NMR software. The average structural parameters may also be recalculated from this file, if so desired. The ability to recalculate the average structural information without the need of reintegrating the NMR spectra has proven to be extremely useful and extraordinarily fast, usually requiring less than 30 seconds per fuel. The files containing the LC-NMR average structures for the fuels also form the basis of a data set used to predict the physical properties of middle

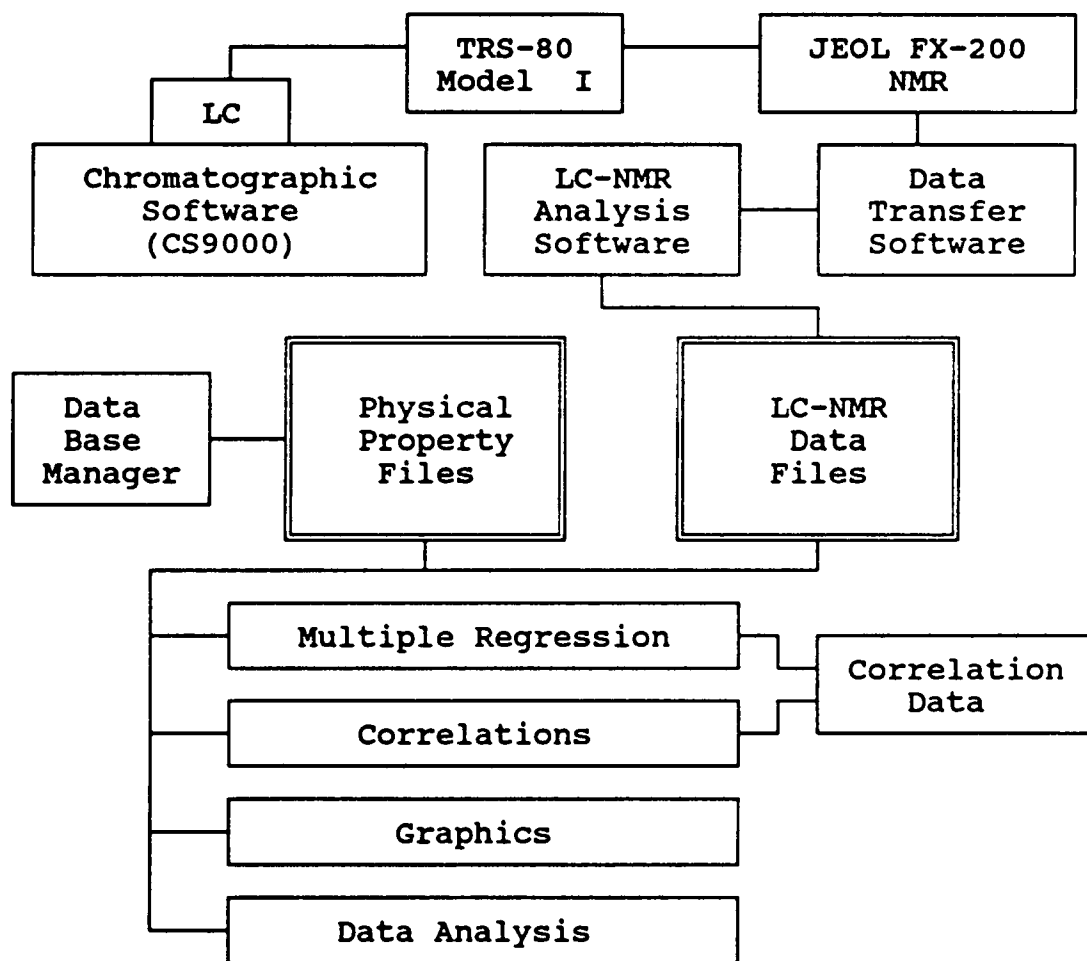


Figure 2.6 Block diagram of the LC-¹H NMR software system.

distillate fuels (150). The overall block diagram for the LC-¹H NMR software system, including the physical property prediction software, is shown in Figure 2.6. Thus far, seventeen physical properties of middle distillate fuels have been predicted in this manner. These predictions have proven to be quite accurate, and have been incorporated into the LC-NMR software, allowing the prediction of the physical properties of a fuel as the LC-NMR average structural parameters are calculated.

Conclusion

With the system presented here, it is possible to collect the NMR spectra of a fuel as it is being separated chromatographically, integrate these NMR spectra, calculate the average chemical composition of the fuel, and accurately predict 17 of the physical properties of the fuel. Generally, the complete analysis time is less than 2 hours. As previously mentioned, this is in sharp contrast to the time required for manual integration of the LC-¹H NMR spectra and calculation of the average structural parameters. In addition, the automatic integration of the NMR data has proven to be more consistent than manual integration of the same data due to the elimination of operator bias in the adjustment of the baselines and integral phasing.

The off-line approach to data analysis which is described here through the use of the PS/2 for the analysis of the LC-NMR spectra also allows more efficient utilization of the NMR instrument time. The entire instrument may now be devoted directly to the collection of data, rather than to the analysis of the data once that data has been collected.

It should also be stressed that although the software described here was developed specifically for the analysis of LC-¹H NMR data of middle distillate fuels, the software and the concepts which it represents are by no means limited to this one application. With the ability to transfer the NMR data to a personal computer where it can later be manipulated, this system represents an economical and practical alternative to costly NMR workstations.

Chapter 3

A RAPID METHOD FOR THE CALCULATION OF PHYSICAL PROPERTIES OF HYDROCARBONS

Introduction

Over the past several years, numerous methods have been developed to predict the physical properties of various classes of organic compounds (103,113). Many of these methods have utilized group property approaches (97,98) which assume that the physical properties of a compound are predominately determined by the number and type of chemical functional groups present in the compound (99,151,152). This group property approach is not limited only to pure compounds, but has also been applied to mixtures as well (114, 144, 153, 120). In a group property approach, one assumes, to a first level of approximation, that the physical properties of a given compound are controlled by the functional groups present in the compound. In hydrocarbons, for example, the carbon groups (e.g., methyl, methylene, methine, and quaternary carbon) are the controlling factors in the physical properties of a given molecule. The physical property, then, is simply a linear combination of these intrinsic intramolecular carbon groups, with each group weighted by a mixing coefficient, *vide infra*. For example, a group property approach used to calculate the density for a given hydrocarbon would proceed as follows. In the hydrocarbon, a methyl group may contribute x amount to the density of the compound, a methylene group may contribute x' , a methine group may contribute x'' , and a quaternary carbon group may contribute x''' to the density of the hydrocarbon. The overall density of the hydrocarbon can then be calculated by multiplying the total number of chemical groups (e.g., methyl, methylene, methine, or quaternary) present in the molecule by the group contribution factor (i.e., mixing coefficient). The overall

density of the hydrocarbon is then found by summing these individual products. If the mixing coefficients for this example were of the form $a_0 - a_4$, the equation for the density of the hydrocarbon would have the form:

$$[3.1] \quad \text{Density} = a_0 + a_1x + a_2x' + a_3x'' + a_4x'''$$

Through a knowledge of the mixing coefficients for each physical property, a wide range of physical properties of various hydrocarbons may be calculated in a similar manner.

As previously mentioned, group property approaches have been applied to physical property prediction of pure compounds by several workers. For a more complete review of these approaches, see the PHYSICAL PROPERTY PREDICTION METHODS section of Chapter 1. Of particular interest is the work of Fisher (95,96) on the prediction of the physical properties of *n*-alkanes. Although limited to only linear alkanes, Fisher has been able to accurately predict eleven physical properties with errors of less than 1%. Cardozo (97) has applied a group property approach to the prediction of the enthalpy of formation for a wide range of organic compounds. This approach has yielded errors of approximately 5%. Likewise, several of the other property prediction schemes utilizing a group property approach have reported property prediction errors of approximately 5 - 10%. Note, however, that the exact error in the property predictions depends on the property being predicted as well as the prediction method. For example, Fisher obtained a correlation coefficient (*r*) of 0.99999992 over *n*-alkanes C₅-C₄₀ for the prediction of density, but only a correlation coefficient of 0.999872 for the C₁₅-C₂₇ *n*-alkanes in the boiling point prediction. This differential in the correlation coefficients is readily explained. Boiling points and various other physical properties are well known to be somewhat dependent on inter- as well as intra-molecular forces. However, a group property approach such as Fisher's models only intra-molecular bonding forces, yielding larger errors for such properties as boiling point.

For the last several years, our laboratory has been interested in the development of directly coupled liquid chromatography - proton nuclear magnetic resonance (LC- ^1H NMR) for the analysis of middle distillate (i.e., jet and diesel) fuels (8,10). One goal of this research has been to develop the capability to predict the physical properties of these complex mixtures (e.g., fuels) from the group property information obtainable in the LC- ^1H NMR approach. The predictive capabilities of the LC- ^1H NMR technique for a wide range of physical properties of middle distillate fuels have proven very successful (150). Prior to the development of these LC- ^1H NMR techniques, however, a study of model compounds was also undertaken in an effort to determine the predictive capability of the group property information obtainable by ^1H NMR. The present study represents the development of a series of equations which can be utilized to calculate various physical properties of pure hydrocarbons. The results of this work for acyclic alkane, monocyclic aromatic, and dicyclic aromatic hydrocarbons are presented here. The group property approach for the prediction of the physical properties of these hydrocarbon classes provides an easy to use computer algorithm which allows the rapid and precise estimation of a wide range of physical properties of hydrocarbons from a knowledge of the carbon structure of the compound.

Experimental

To determine possible correlations between the chemical groups and the physical properties of the hydrocarbons, a computer data base was assembled from literature reference tables (154 - 158). This data base contains both the carbon structural information and a wide range of physical properties for acyclic alkane, monocyclic aromatic, and dicyclic aromatic hydrocarbons. The data base contains this information on 189 acyclic alkane compounds, 107 monocyclic aromatic compounds, and 73 dicyclic aromatic compounds. Figure 3.1 depicts the distribution of acyclic alkane compounds used in the data base. Each bar indicates the total number of structural isomers of the corresponding carbon number

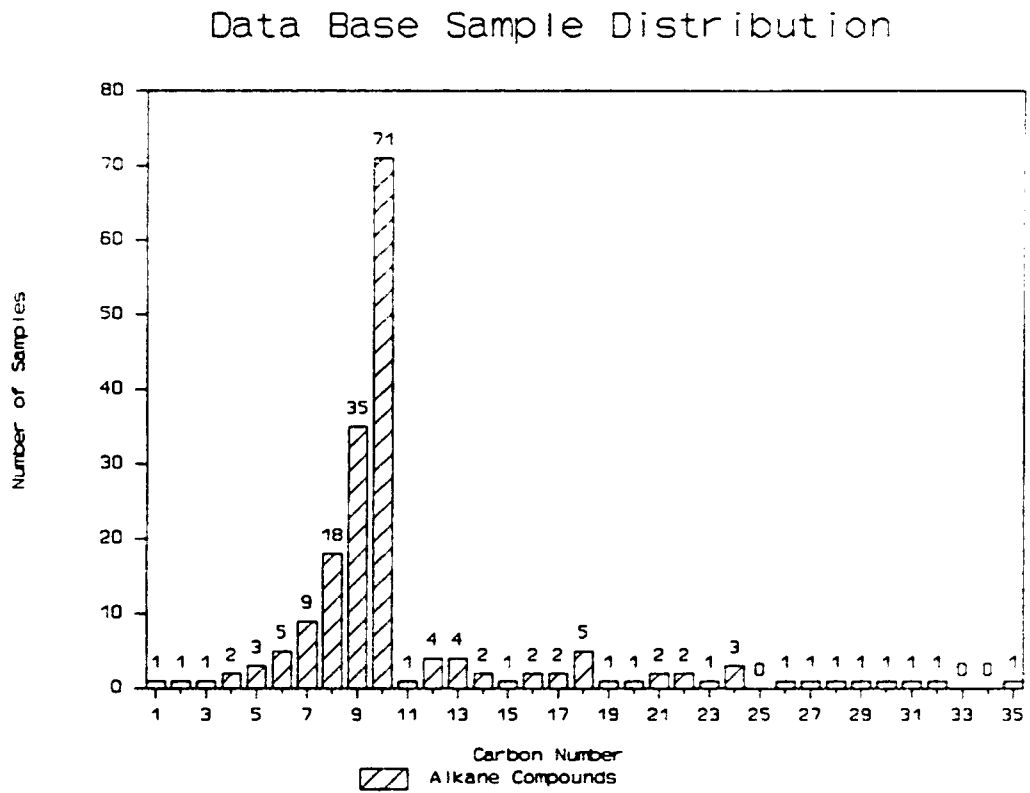


Figure 3.1 Distribution of alkane compounds in the model compound data base.

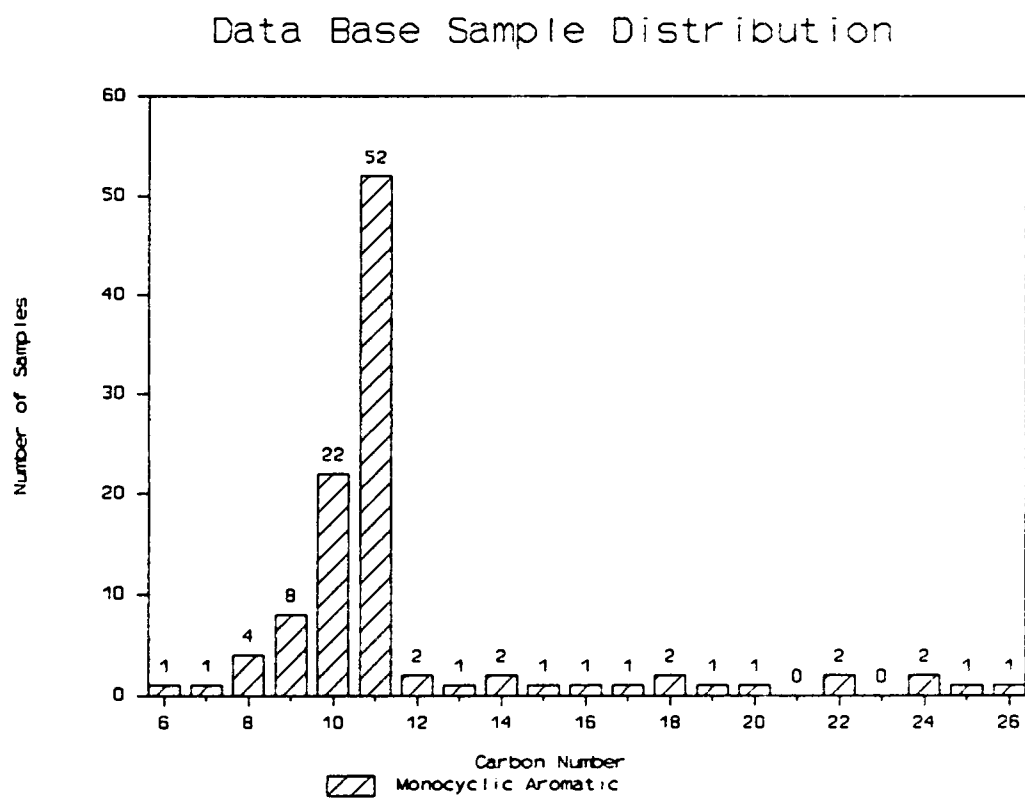


Figure 3.2 Distribution of monocyclic aromatic compounds in the model compound data base.

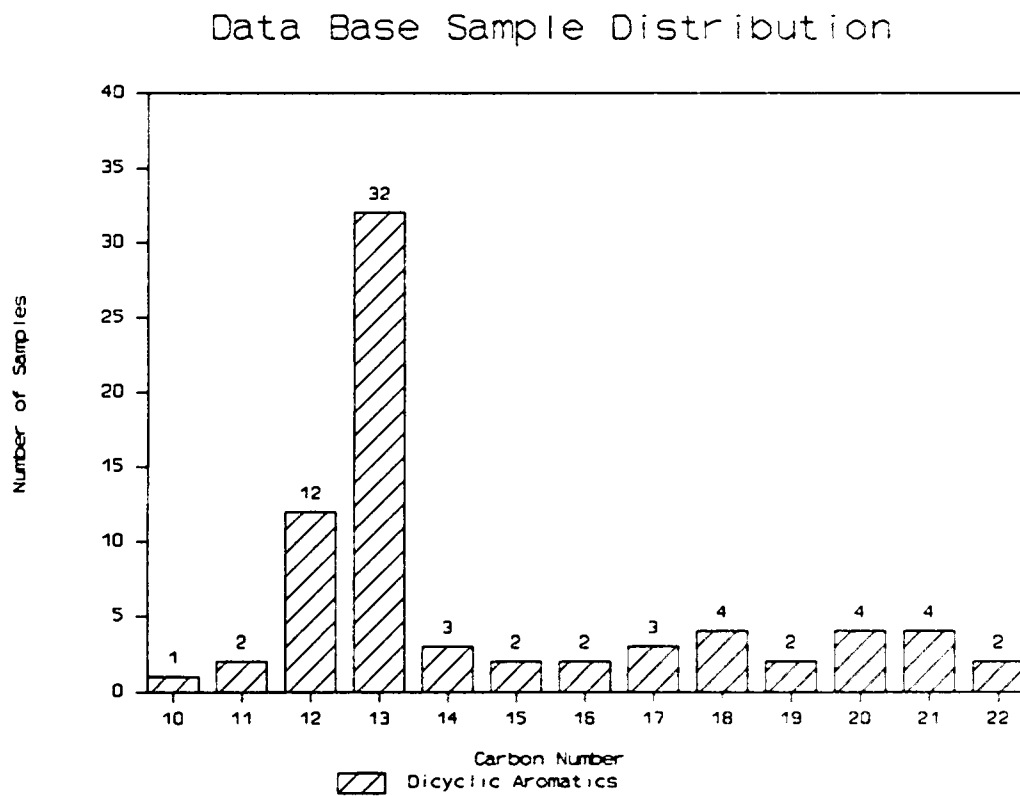


Figure 3.3 Distribution of dicyclic aromatic compounds in the model compound data base.

which were present in the data base. As seen in Figure 3.1, the acyclic alkane compounds utilized in the data base ranged for methane (C_1) to n-pentatricontane (C_{33}) and include all structural isomers for methane (C_1) through nonane (C_9). In addition, 71 of the possible 75 structural isomers for decane (C_{10}) were employed in the data base. Likewise, Figures 3.2 and 3.3 depict the data base sample distribution for monocyclic aromatic and dicyclic aromatic compounds, respectively.

The development of the chemical structure - physical property correlations consists of three primary processes. First, an equation is chosen which contains the chemical structures believed to be important in determining the physical property to be correlated. This equation also specifies the number of mixing coefficients variables which provide the weighting functions necessary to calculate a given physical property from the chemical structure of a given compound. The mixing coefficients are then determined by the second step in the development of the correlation, the multiple regression analysis. In this second step, the data base of sample compounds is scanned by a computer and a multiple regression analysis is performed to calculate the best fit for the mixing coefficients variables in the equation chosen in step one. The third stage of the correlation process then utilizes these mixing coefficients in the correlation equation to determine overall validity of the correlation. In the third stage, a complete equation is available for the calculation of the physical property from the chemical structure of a given compound. Using this equation, the entire data base of compound structures is again scanned, and the physical property being correlated is calculated for each compound in the data base. The predicted (i.e., calculated) physical property value is then compared against the true (i.e., literature) physical property value for each compound in the data base to determine the quality of the predictions. This comparison is accomplished via the generation of a correlation plot of the predicted versus observed physical property for each compound in the data base. A linear regression analysis of the correlation plot provides the correlation coefficient (r) as well as the standard deviation of

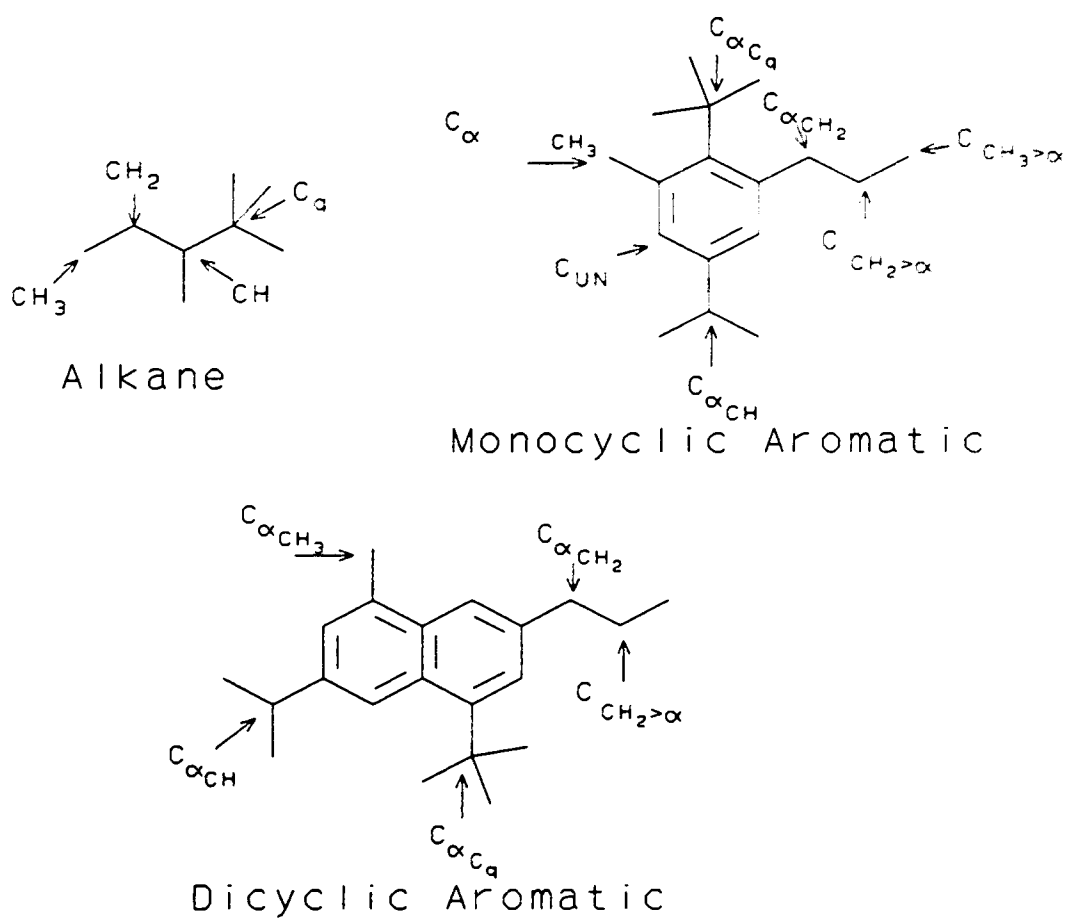


Figure 3.4 Nomenclature utilized in the model compound correlation studies.

residuals (σ_r) for each chemical structure - physical property correlation.

The computer software necessary to perform these correlations consists of several sections: a data base manager to administer the files containing the physical properties and chemical structures, multiple regression analysis software to calculate the mixing coefficients, and graphical and statistical software to display and analyze the correlation plots. Each section of this software was specifically developed for the specialized needs of the physical property predictions. Each program is described and is listed in Appendix II.

For the acyclic alkane compounds, the equations to correlate the physical properties and the chemical structure information were all based on the mole fractions of the different carbon types present in the compounds. The acyclic alkane properties were found to be either linear, reciprocal, or square root functions of the carbon mole fractions present in the compounds. The general form of these equations is presented in Equation 3.2:

$$[3.2] \quad \text{Physical Property} = m [b_0 + b_1(x_{\text{CH}_3}) + b_2(x_{\text{CH}_2}) + b_3(x_{\text{CH}}) + b_4(x_{\text{C}_q})]^n + B$$

The exact function type is specified by selecting $n = 1, -1, \text{ or } 0.5$ to produce either linear, reciprocal, or square root function types. The specific form of each equation (i.e., linear, reciprocal, or square root) which was ultimately utilized for the calculation of a physical property was determined empirically by performing the physical property - chemical structure correlation for each of the three function types. The function type which yielded the highest correlation coefficient was then utilized for the calculation of the physical properties. For a complete description of the model compound nomenclature used in all correlation equations, see Figure 3.4. A complete glossary of the terms used in all correlation equations may be found in Table 3.1.

Correlations between the chemical structures and various physical properties of monocyclic and dicyclic aromatic compounds were performed in a similar manner. In these

Table 3.1
Glossary of terms used in model compound correlation study.

<u>Term:</u>	<u>Definition:</u>
m	slope factor
B	intercept factor
b_{1-6}	mixing coefficients from regression analysis
x_{CH_3}	mole fraction of alkane methyl carbon
x_{CH_2}	mole fraction of alkane methylene carbon
x_{CH}	mole fraction of alkane methine carbon
x_{C_4}	mole fraction of alkane quaternary carbon
$C_{\alpha CH_3}$	number of methyl carbons α to aromatic rings
$C_{\alpha CH_2}$	number of methylene carbons α to aromatic rings
$C_{\alpha CH}$	number of methine carbons α to aromatic rings
$C_{\alpha C_4}$	number of quaternary carbons α to aromatic rings
$C_{CH_2 > \alpha}$	number of methylene carbons not bonded to aromatic rings
$C_{CH_3 > \alpha}$	number of methyl carbons not bonded to aromatic rings

correlations, the monocyclic aromatic compounds were found to follow either carbon type:

$$[3.3] \quad \text{Property} = m [b_0 + b_1(C_{\alpha\text{CH}_3}) + b_2(C_{\alpha\text{CH}_2}) + b_3(C_{\alpha\text{CH}}) + b_4(C_{\alpha\text{C}_q}) + b_5(C_{\text{CH}_2>\alpha})] + B$$

or total carbon number:

$$[3.4] \quad \text{Property} = m [b_0 + b_1(6 + C_{\alpha\text{CH}_3} + C_{\alpha\text{CH}_2} + C_{\alpha\text{CH}} + C_{\alpha\text{C}_q} + C_{\text{CH}_2>\alpha} + C_{\text{CH}_3>\alpha}) + b_2(\text{ADS})] + B$$

functions. The carbon type functions are equations which contain independent parameters for each type of carbon present in the compounds. That is, the number of methyl groups adjacent to the aromatic rings (i.e., $C_{\alpha\text{CH}_3}$), the number of methylene groups adjacent to the aromatic ring (i.e., $C_{\alpha\text{CH}_2}$), etc., are each independent parameters which influence the given physical property of the monocyclic aromatic compound. In contrast, the total carbon function is an equation type in which the physical property is predominately dependent on only two variables, the total number of carbons present in the compound and the number of aromatic carbons which contain alkyl substituents (i.e., the average degree of substitution of the aromatic ring, ADS). All of the physical properties which were correlated for the dicyclic aromatic compounds were found to follow total carbon functions of the type depicted in Equation 3.4.

Although the physical properties were found to follow several function types, all of the equations utilized in this study consist of two primary sets of parameters. The first set of parameters is the b_i terms which are the mixing coefficients as determined by the multiple regression analysis previously described. These b_i terms are unique to each physical property and chemical class. It is these mixing coefficients which are the weighting factors that determine the relative importance of each carbon structural group type which is present in the molecule. The second set of terms is carbon chemical structure group terms. As

previously mentioned, mole fraction terms (i.e., χ_i) are used to represent the chemical structures found in acyclic alkane compounds, and normalized carbon number (i.e., C_n) terms are utilized to represent the structural components present in aromatic hydrocarbon compounds. It is this second set of terms which identifies the chemical structure (i.e., groups) which are unique to an individual molecule by quantifying the number of each chemical group type present in an individual molecule. Each equation also includes m and B terms. These terms are determined by via a linear regression analysis of the correlation plot of a predicted versus observed physical property. The slope and intercept of this plot then determine the m and B factors which are used to correct the slope and intercept of the correlation plot to 1 and 0.

Results and Discussion

Table 3.2 summarizes the function types which were found to provide the best physical property - chemical structure correlation for each physical property in each chemical class. The function types listed in Table 3.2 refer to the functions listed in Equations 3.2 - 3.4. For example, consider the freezing point correlations. For the freezing point of acyclic alkanes, a reciprocal function was utilized, therefore, $n=-1$ in Equation 3.2. Likewise, the freezing point was found to follow carbon type functions in the aromatic compounds. Therefore, Equation 3.3 should be utilized for the calculation of the freezing points of both monocyclic and dicyclic aromatic compounds. The constants for each physical property equation for each chemical class are given in Tables 3.3, 3.4, and 3.5. Table 3.3 lists the constants for the acyclic alkane physical properties, Table 3.4 the monocyclic aromatic physical property equations, and Table 3.5 the dicyclic aromatic physical property equations. Also included are the m and B factors. The correlation plots for each of physical properties which have been correlated are presented in Figures 3.5 - 3.20. By plotting the predicted (i.e., calculated) value against the observed (i.e., literature) value for each physical property,

Table 3.2
 Summary of function types utilized for physical property - chemical structure correlations.

Physical Property	Function Type:		
	Alkane	Monocyclic	Dicyclic
Cetane Number	Linear	Carbon Type	Carbon Type
Boiling Point	Reciprocal	Carbon Type	Carbon Type
Freezing Point	Reciprocal	Carbon Type	Carbon Type
Flash Point	Linear	Total Carbon	
Density	Linear	Carbon Type	Carbon Type
Refractive Index	Linear	Carbon Type	Carbon Type
Surface Tension	Linear	Carbon Type	
Critical Pressure	Square Root	Carbon Type	
Critical Temperature	Linear	Carbon Type	
Critical Volume	Reciprocal	Carbon Type	
Heat Capacity	Reciprocal	Total Carbon	
Heat of Vaporization	Reciprocal	Total Carbon	
Heat of Formation	Reciprocal	Total Carbon	
Free Energy of Formation	Reciprocal	Total Carbon	
Heat of Combustion	Reciprocal	Total Carbon	
Molecular Volume	Reciprocal	Total Carbon	Carbon Type

Table 3.3
Mixing coefficients for alkane physical property calculations.

$$\text{Property} = m [b_0 + b_1(X_{\text{CH}_3}) + b_2(X_{\text{CH}_2}) + b_3(X_{\text{CH}}) + b_4(X_{\text{C}_q})]^n + B$$

	m	Linear Functions ($n=1$)				B
		b_0	b_1	b_2	b_3	
Cetane	1.41	+2.58566x10 ⁷	-2.58566x10 ⁷	-2.58565x10 ⁷	-2.58566x10 ⁷	-32.8
Flash Point	1.07	+210	-744	-8	+1488	+0
Density	1.04	-1686.5001	+1686.7285	+1687.3565	+1688.0271	+1688.7404
Refractive Index	1.09	-1277.53	+1278.69	+1279.00	+1279.33	+1279.68
Surface Tension	1.23	+19592.3	-19603.1	-19560.6	-19520.2	-1948.1
Critical Temp	1.04	-1.34064x10 ⁶	+1.34034x10 ⁶	+1.34114x10 ⁶	+1.34191x10 ⁶	+1.34266x10 ⁶

	Reciprocal Functions ($n=-1$)						
Boiling Point	1.17	+18.8689	-18.8622	-18.8677	-18.8726	-18.8778	-24.9491
Freezing Point	1.28	+43.6760	+43.68048	+43.6777	+43.6763	+43.6726	-608.633
Critical Volume	1.08	-14359.3	+14366.4	+14359.6	+14353.0	+14346.7	-0.0446
Heat Capacity	1.11	+151.38	-151.322	-151.377	-151.431	-151.484	-5.587
Ht Vaporization	0.99	+309.486	-309.069	-309.491	-309.882	-310.252	-0.00677
Ht of Formation	1.10	-69.5276	+69.4799	+69.5217	+69.5646	+69.6077	+6.778
Free Energy Form	1.34	-5671.32	+5671.71	+4671.31	+4670.91	+5670.50	-11.17
Ht of Combustion	1.02	+1.07229	-1.06909	-1.07225	-1.07541	-1.07857	-15.5
Molecular Volume	1.11	+29.5695	-29.5493	-29.5682	-29.5866	-29.6049	-18.809

	Square Root Function ($n=0.5$)					
Critical Pressure	1.15	-4.77345x10 ⁶	+4.77601x10 ⁶	+4.77344x10 ⁶	+4.76854x10 ⁶	-4.35

Table 3.4
Mixing coefficients for monocyclic aromatic physical property calculations.

Carbon Type Functions:

$$m [b_0 + b_1(C_{\alpha}CH_3) + b_2(C_{\alpha}CH_2) + b_3(C_{\alpha}CH) + b_4(C_{\alpha}C) + b_5(C_{CH_2 > \alpha})] + B$$

	m	b_0	b_1	b_2	b_3	b_4	b_5	B
Cetane Number	1.12	+5.41407	-10.6485	-0.08139	-8.75867	-36.3951	+5.32162	-3.87011
Boil Point	1.03	+88.3291	+26.9481	+45.9035	+59.5801	+80.1192	+20.8839	-5.81442
Freezing Point	2.43	-69.6631	+16.0080	-6.76148	-4.78162	-12.8200	+3.29933	+67.6255
Density	1.85	+0.85649	+8.73778x10 ⁻³	+4.49975x10 ⁻³	+3.49110x10 ⁻³	+1.62951x10 ⁻²	-4.18860x10 ⁻⁴	-0.74023
Refractive Index	1.20	+1.48634	+6.90782x10 ⁻³	+4.43701x10 ⁻³	+2.19348x10 ⁻³	+7.52145x10 ⁻³	-7.35995x10 ⁻⁴	-0.30429
Surface Tension	3.12	+27.7420	+0.48400	+0.6300	-0.06200	+0	+0.07800	-60.5514
Critical Press	1.07	+45.6034	-4.66159	-9.79832	-12.9361	-16.3435	-3.07235	-2.34544
Critical Temp	1.09	+293.631	+27.8109	+50.8221	+77.4144	+93.3687	+22.9388	-35.1693
Critical Volume	1.02	+0.26700	+5.83743x10 ⁻²	+0.11540	+0.16285	+0.19900	+5.26144x10 ⁻²	-0.00667
Molecular Volume	1.01	+92.3659	+14.7968	+31.2141	+47.9291	+63.0310	+16.7311	-1.22483

Total Carbon Functions:

$$m [b_0 + b_1(6 + C_{\alpha}CH_3 + C_{\alpha}CH_2 + C_{\alpha}CH + C_{\alpha}C + C_{CH_2 > \alpha} + C_{CH_3 > \alpha}) - b_2(ADS)] + B$$

	m	b_0	b_1	b_2	B
Flash Point	1.01	-134.610	+19.9731	+1.49346	-1.07934
Heat Capacity	1.01	-3.58220	+5.97422	+0.27893	-0.50899
Heat of Vaporization	1.04	+1.82060	+0.96428	+0.42899	-0.42434
Heat of Formation	1.00	+48.0728	-6.07026	-2.66568	-0.01958
Free Energy of Form	1.06	+23.4941	+0.95517	-2.41353	-1.67917
Heat of Combustion	1.00	-127.579	+146.085	-2.75543	-0.03731

Table 3.5
Mixing coefficients for dicyclic aromatic physical property calculations.

Carbon Type Functions:

$$m [b_0 + b_1(C_{\alpha}CH_3) + b_2(C_{\alpha}CH_2) + b_3(C_{\alpha}CH) + b_4(C_{\alpha}C_q) + b_5(C_{\alpha}CH_2>_d)] + B$$

	m	b_0	b_1	b_2	b_3	b_4	b_5	B
Boil Point	1.01	+226.242	+18.3062	+29.2193	+41.7533	-149.280	+16.3238	-2.16541
Freezing Point	2.51	+30.5489	+4.85880	-38.2106	-30.7689	-65.7594	+1.95242	-22.2000
Density	1.07	+0.99718	+3.87330x10 ⁻³	-9.83778x10 ⁻³	-1.48817x10 ⁻³	-1.19222x10 ⁻²	-7.84452x10 ⁻⁴	-0.00690
Refractive Index	1.05	+1.60694	-1.76429x10 ⁻⁴	-1.35066x10 ⁻²	-1.84910x10 ⁻²	-2.01570x10 ⁻²	-6.76352x10 ⁻³	-0.00846
Molecular Vol.	1.00	+128.755	+13.4959	+28.2471	+44.5698	+0	-16.6543	-0.00826

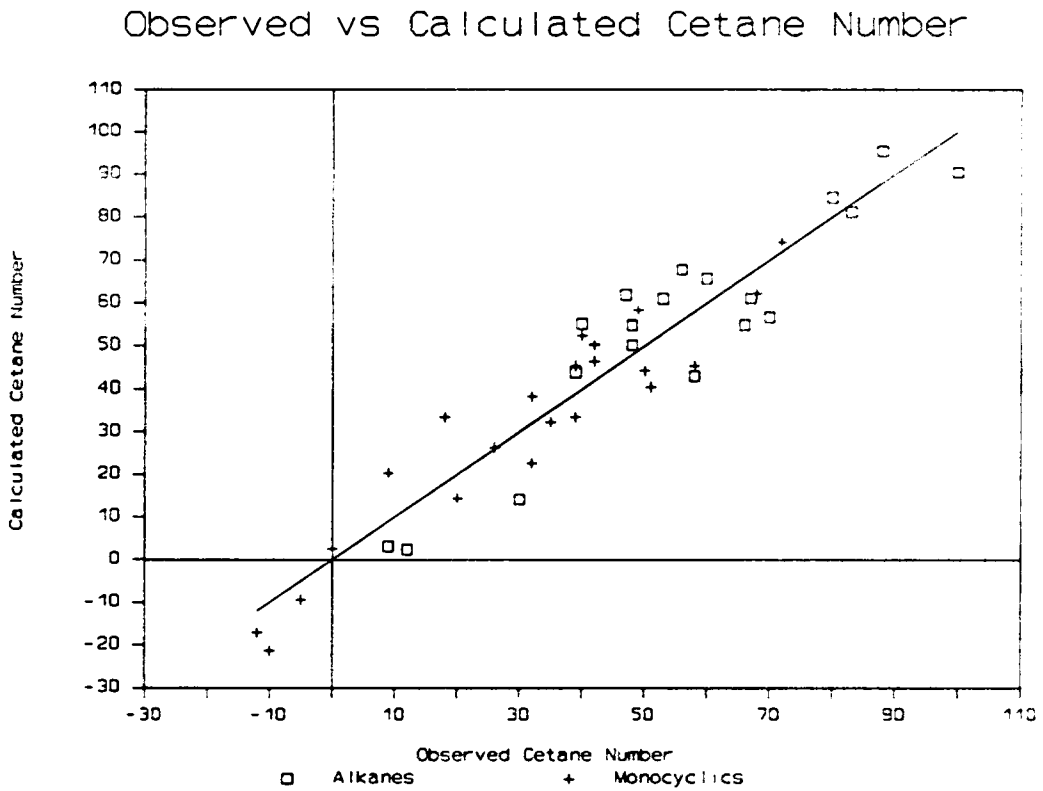


Figure 3.5 Correlation plot for model compound cetane number predictions. Alkane $r=0.918$, Monocyclic $r=0.944$.

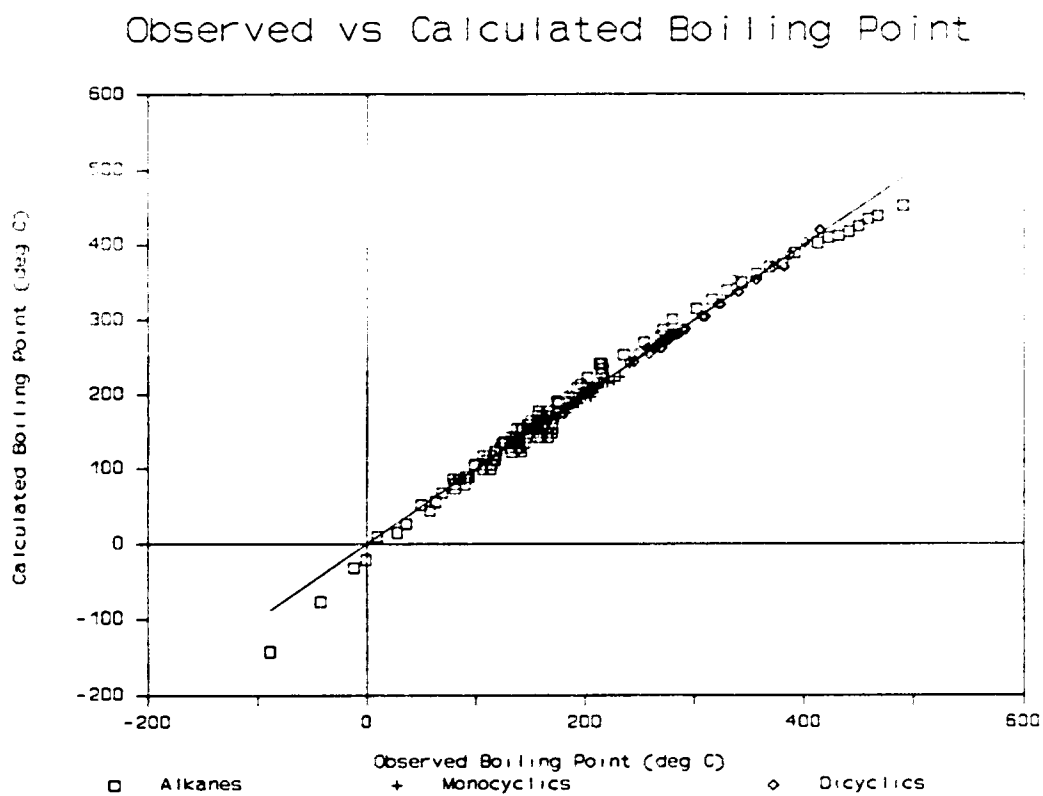


Figure 3.6 Correlation plot for model compound boiling point predictions. Alkane $r=0.991$, Monocyclic $r=0.985$, Dicyclic $r=0.996$.

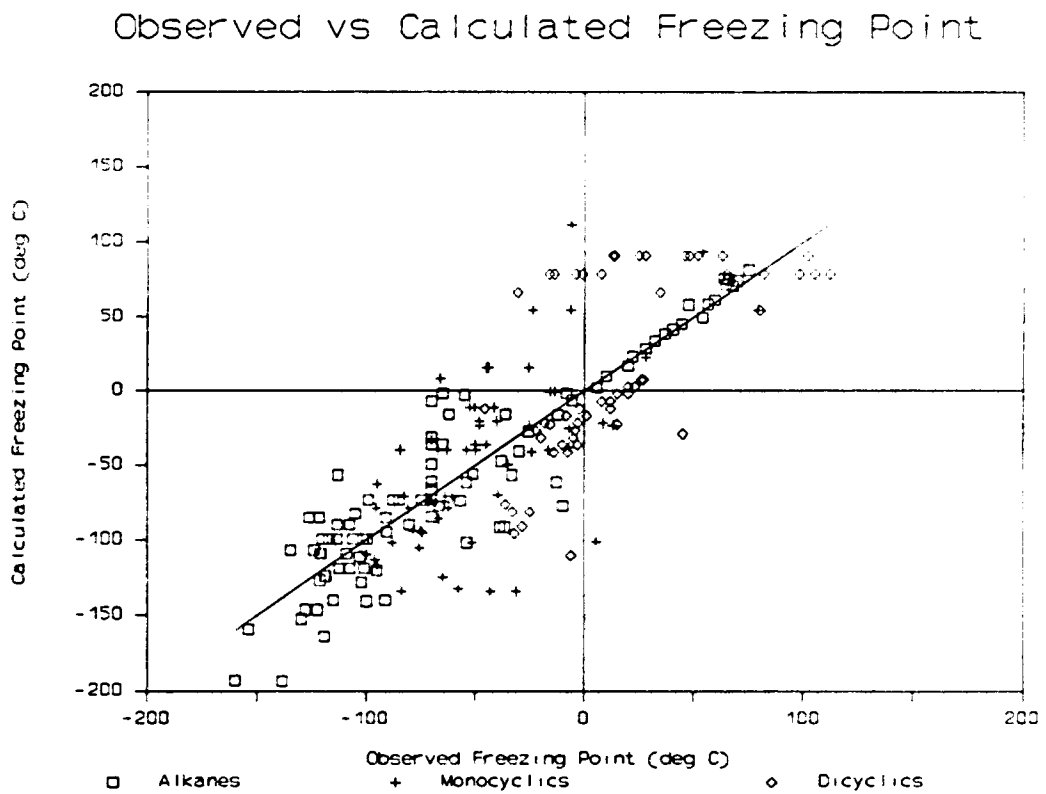


Figure 3.7 Correlation plot for model compound freezing point predictions. Alkane $r=0.928$, Monocyclic $r=0.642$, Dicyclic $r=0.632$.

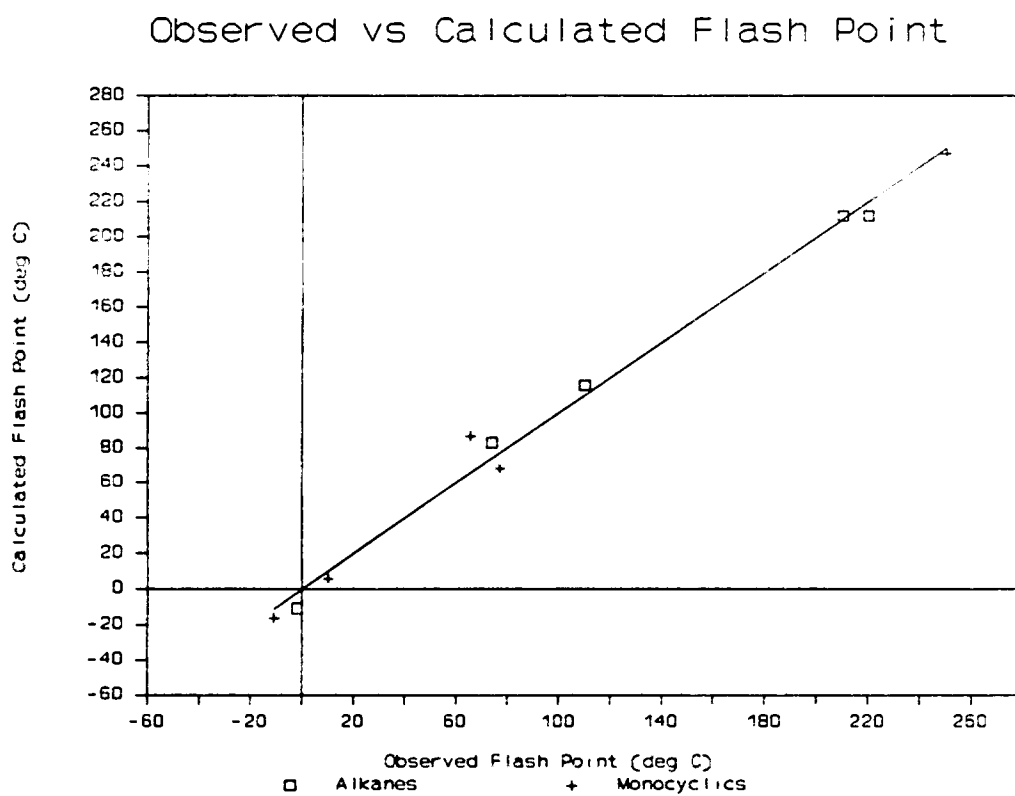


Figure 3.8 Correlation plot for model compound flash point predictions. Alkane $r=0.996$, Monocyclic $r=0.994$.

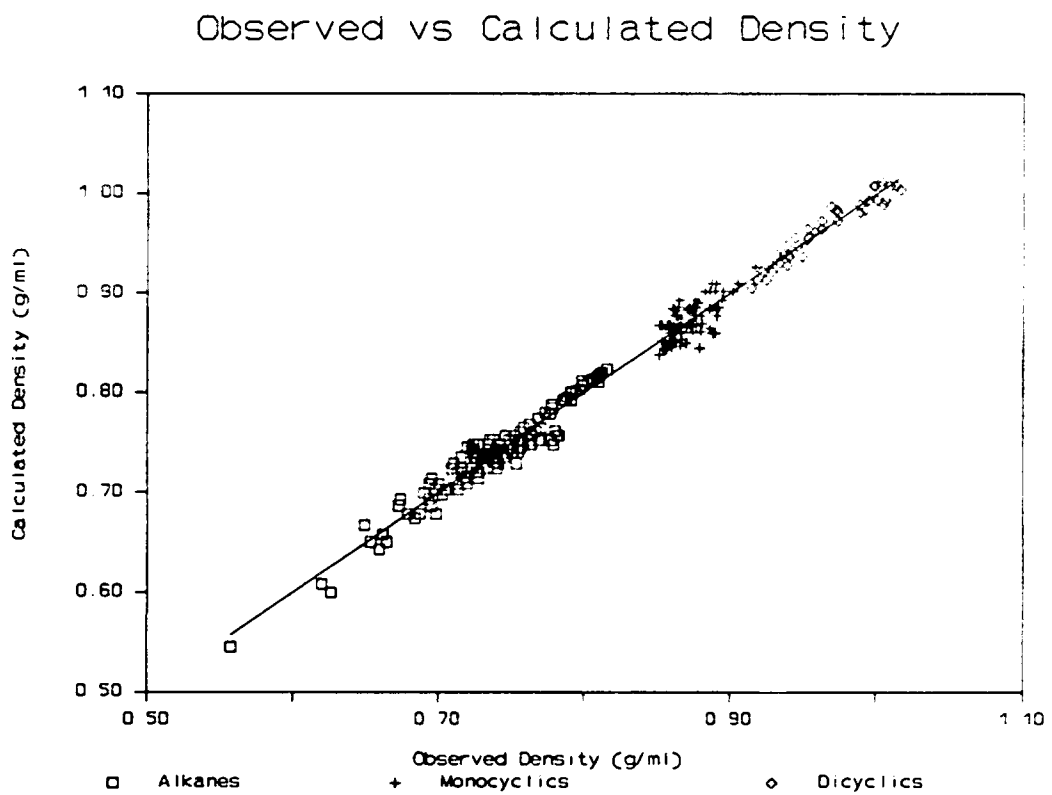


Figure 3.9 Correlation plot for model compound density predictions. Alkane $r=0.963$, Monocyclic $r=0.735$, Dicyclic $r=0.966$.

Observed vs Calculated Refractive Index

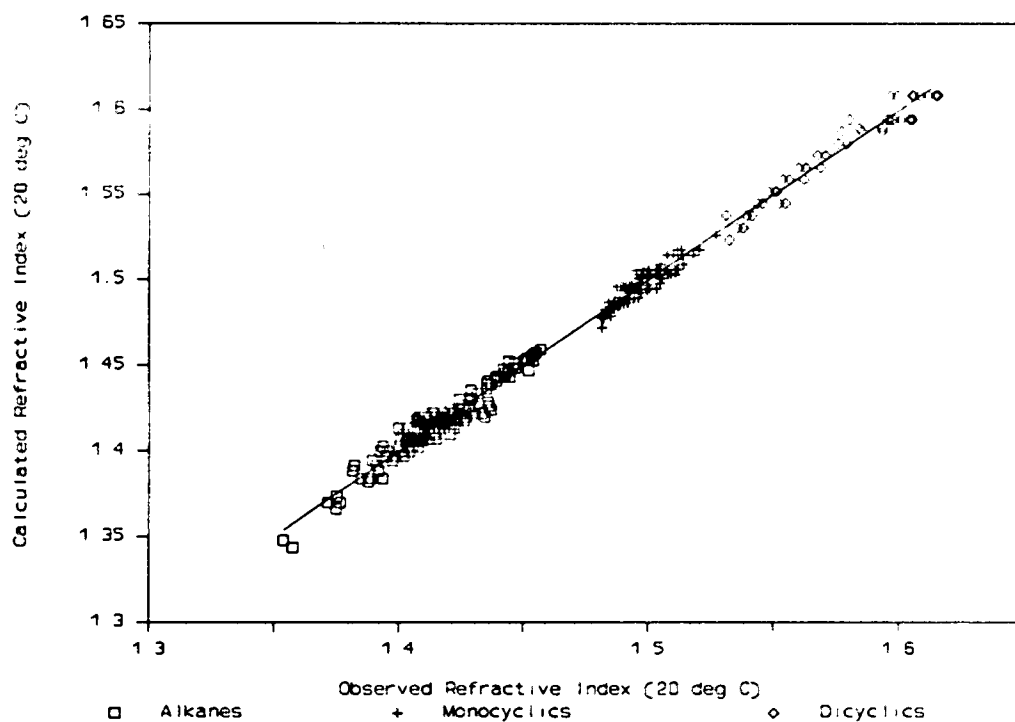


Figure 3.10 Correlation plot for model compound refractive index predictions. Alkane $r=0.962$, Monocyclic $r=0.912$, Dicyclic $r=0.974$.

Observed vs Calculated Surface Tension

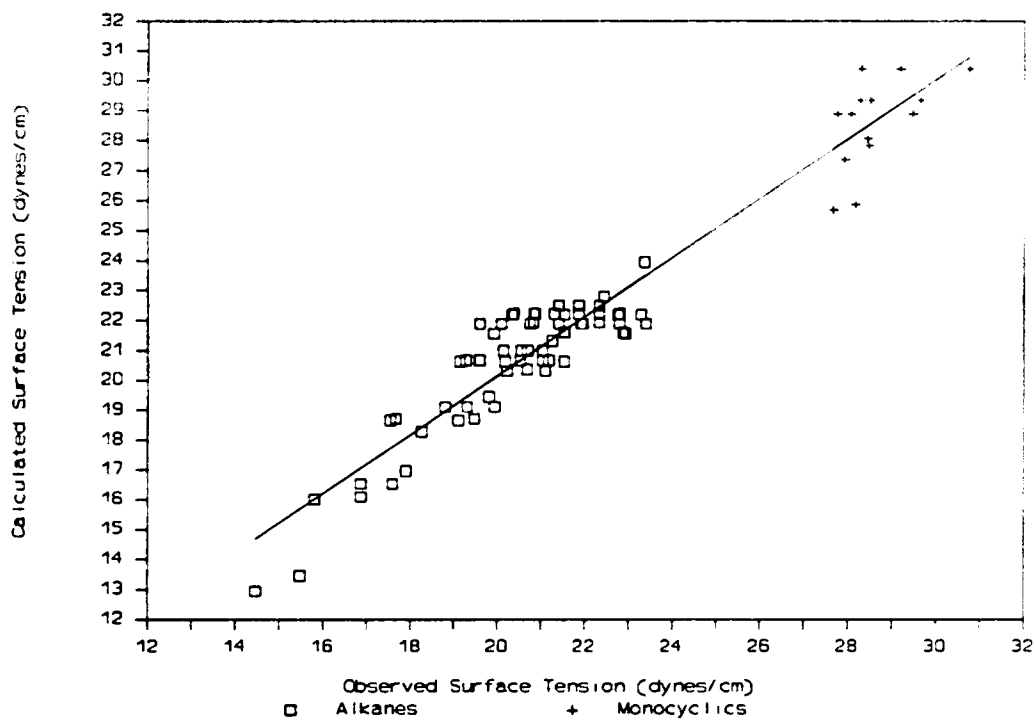


Figure 3.11 Correlation plot for model compound surface tension predictions. Alkane $r=0.903$, Monocyclic $r=0.567$.

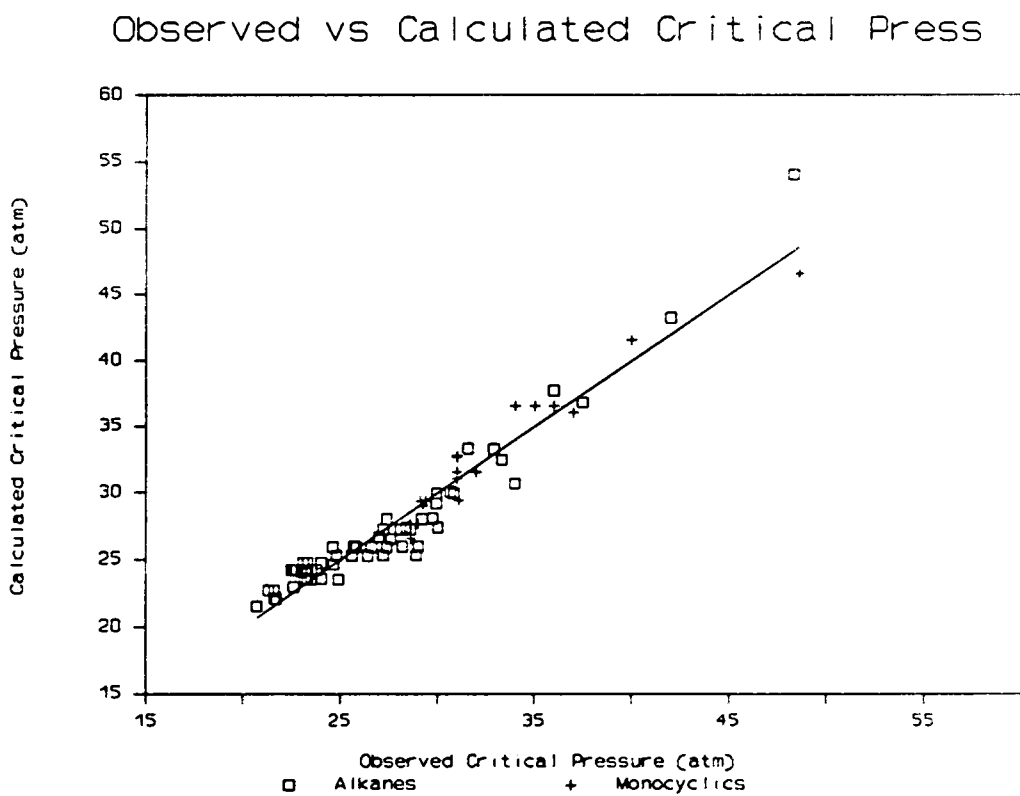


Figure 3.12 Correlation plot for model compound critical pressure predictions. Alkane $r=0.961$, Monocyclic $r=0.965$.

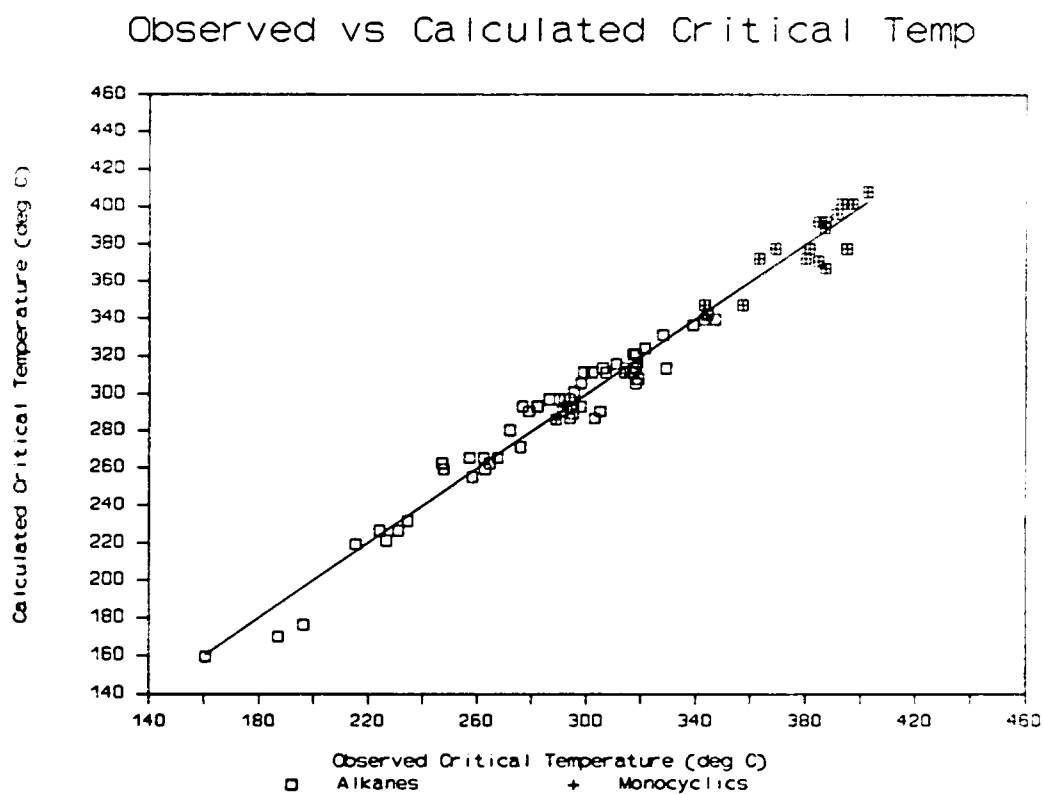


Figure 3.13 Correlation plot for model compound critical temperature predictions. Alkane $r=0.981$, Monocyclic $r=0.956$.

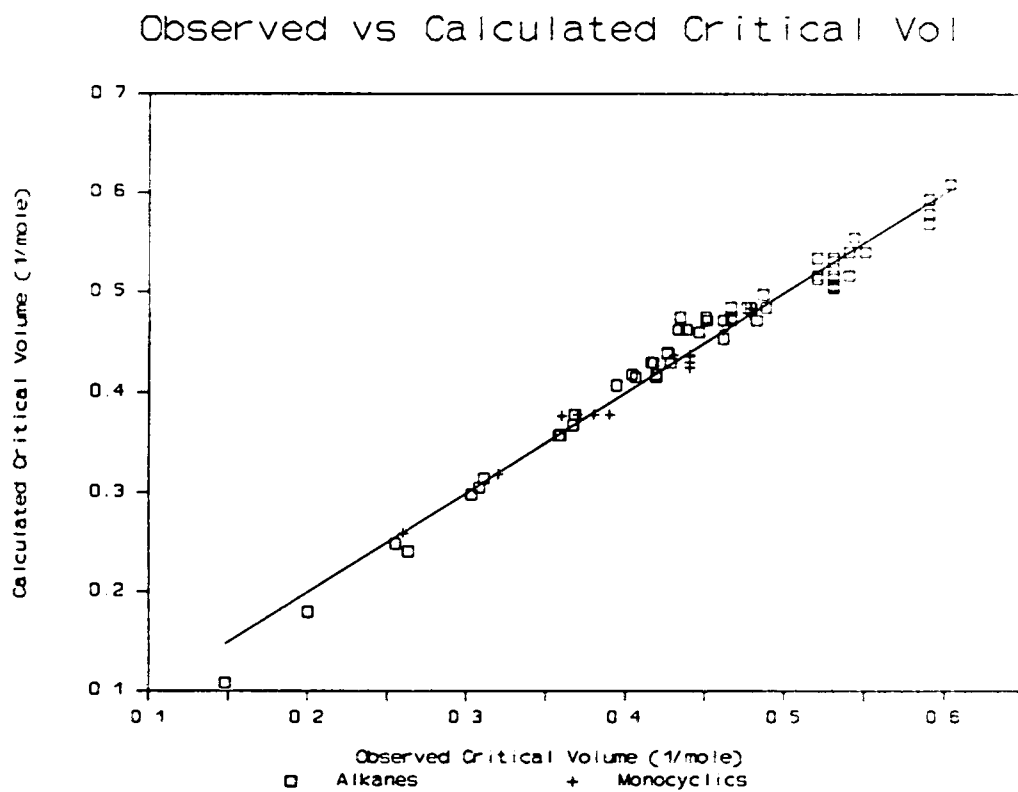


Figure 3.14 Correlation plot for model compound critical volume predictions. Alkane $r=0.988$, Monocyclic $r=0.992$.

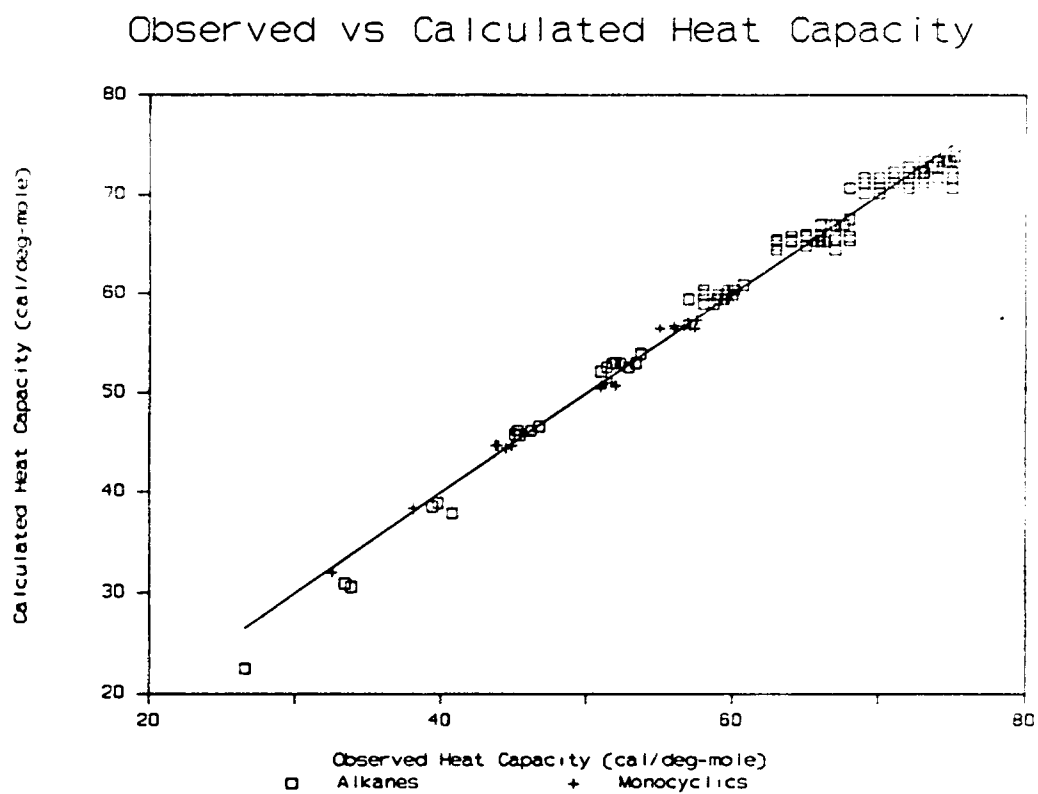


Figure 3.15 Correlation plot for model compound heat capacity predictions. Alkane $r=0.990$, Monocyclic $r=0.995$.

Observed vs Calc Ht of Vaporization

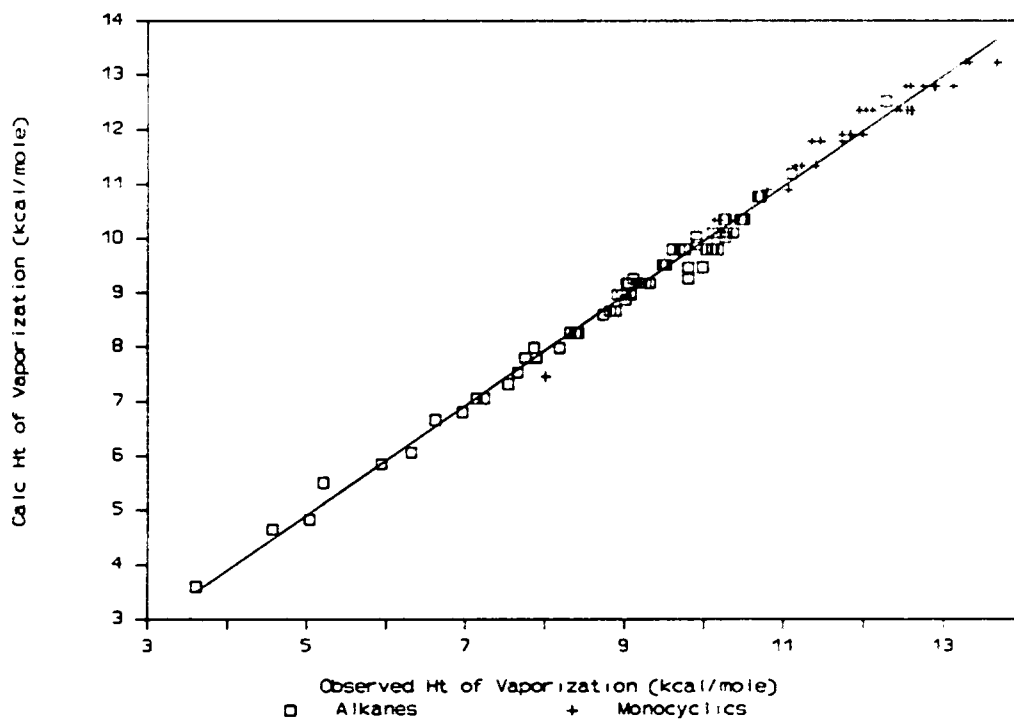


Figure 3.16 Correlation plot for model compound heat of vaporization predictions. Alkane $r=0.995$, Monocyclic $r=0.982$.

Observed vs Calculated Ht of Formation

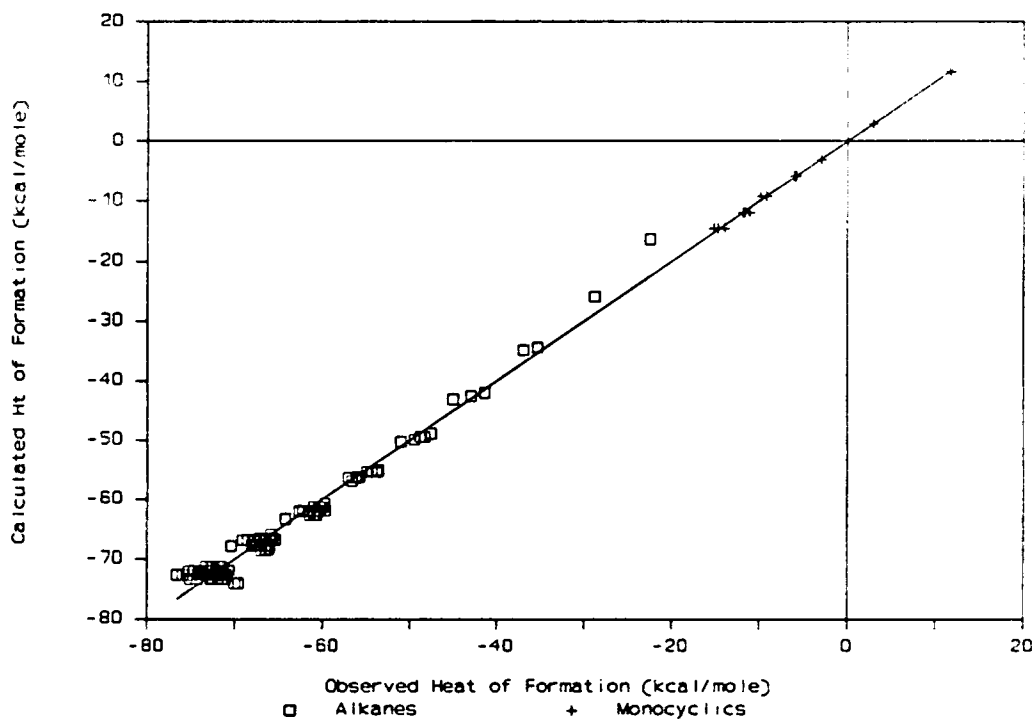


Figure 3.17 Correlation plot for model compound heat of formation predictions. Alkane $r=0.988$, Monocyclic $r=0.999$.

Observed vs Calculated Free Energy Form

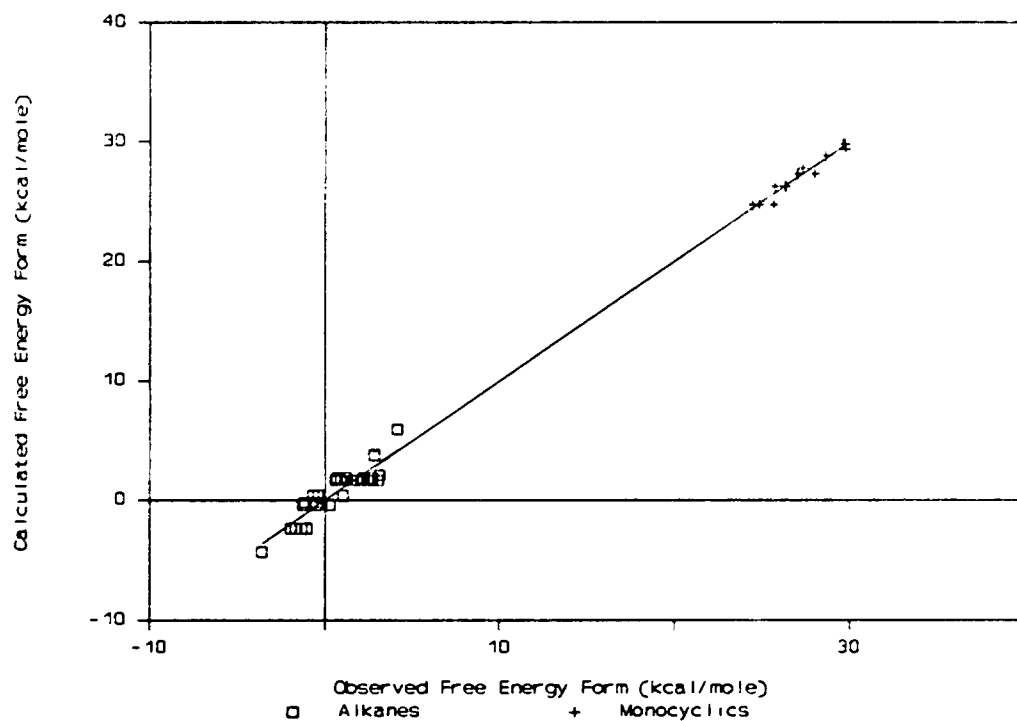


Figure 3.18 Correlation plot for model compound free energy of formation predictions. Alkane $r=0.906$, Monocyclic $r=0.970$.

Observed vs Calculated Ht of Combustion

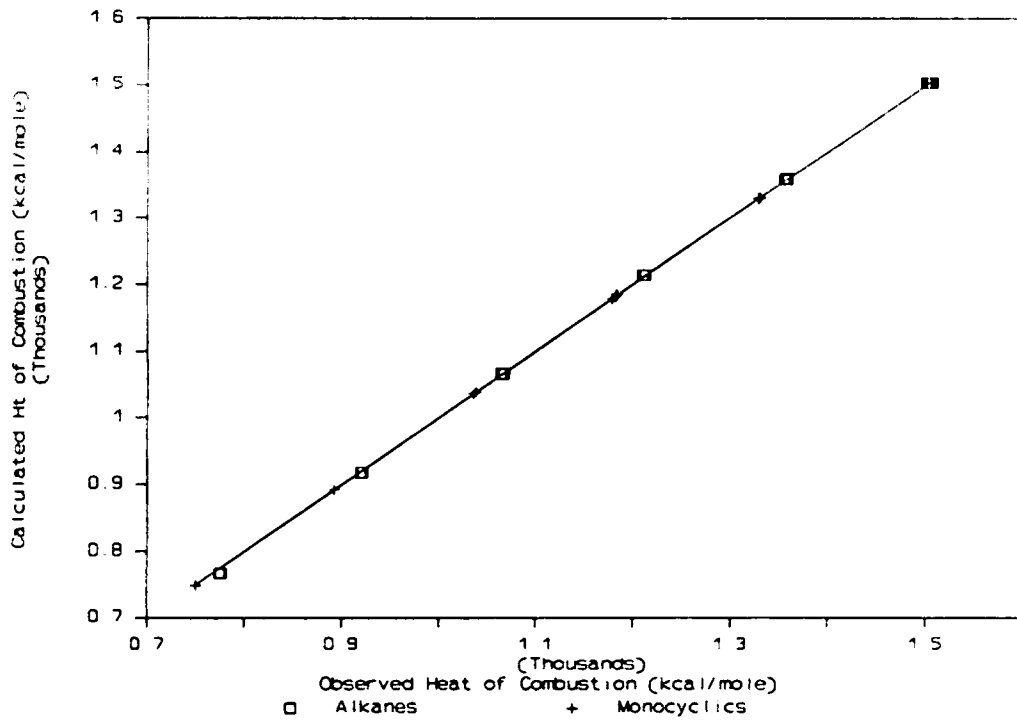


Figure 3.19 Correlation plot for model compound heat of combustion predictions. Alkane $r=1.000$, Monocyclic $r=1.000$.

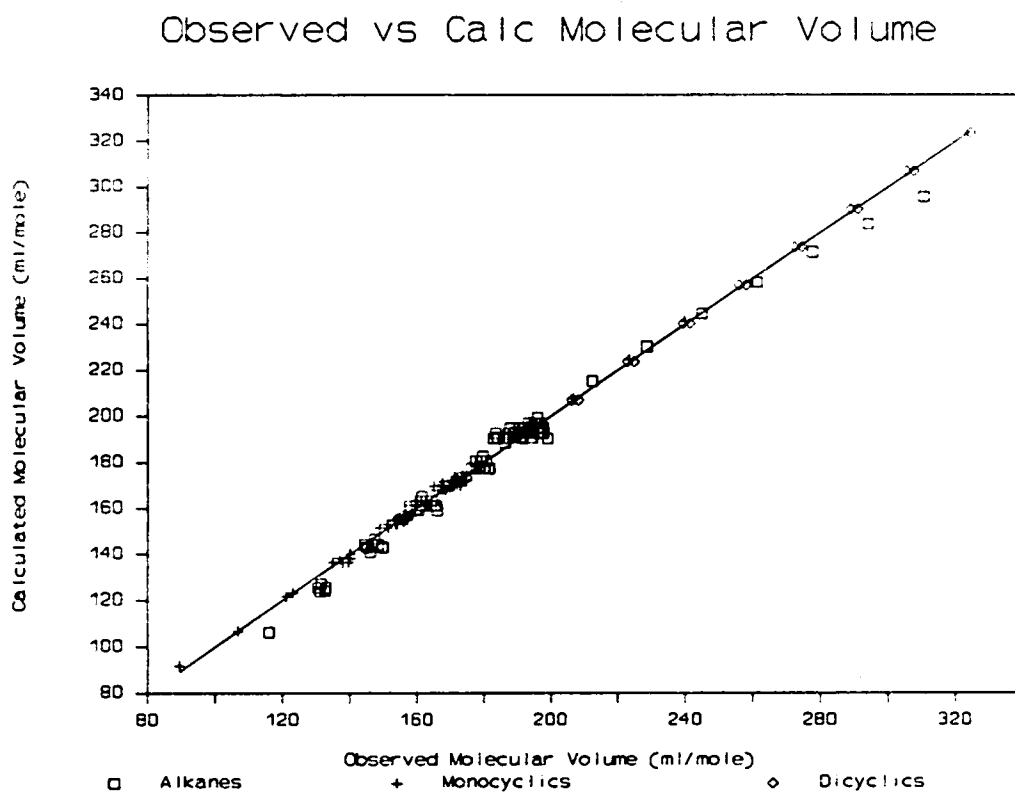


Figure 3.20 Correlation plot for model compound molecular volume predictions. Alkane $r=0.989$, Monocyclic $r=0.996$, Dicyclic $r=1.000$.

the quality of the correlations becomes evident.

A summary of the results of the physical property predictions for the acyclic alkane compounds is presented in Table 3.6. A similar summary for the results of the physical property predictions for the monocyclic aromatic compounds is presented in Table 3.7, and the dicyclic aromatic physical property predictions are summarized in Table 3.8. These tables clearly demonstrate that a group property approach allows the prediction of a wide range of the physical properties for the acyclic alkane and monocyclic aromatic hydrocarbon classes. Although only a limited data set of dicyclic aromatic compounds and their physical properties were utilized in this study, it is reasonable to assume that the same variety of physical properties of dicyclic aromatic compounds may be predicted by this methodology if a larger dicyclic aromatic basis set were used which contains a greater variety of chemical structures and physical properties. Each summary table includes the correlation coefficient, as determined from the correlation plot, the number of points (i.e., compounds) used in the physical property calculations, the standard deviation of residuals, the range of physical property values over which the correlation was performed, and the units for each of the physical properties which were predicted. For example, Table 3.6 reveals that the heat of combustion was predicted for a total of 136 different acyclic alkane compounds possessing heat of combustion values ranging from 775 to 1507 kcal/mole. From the correlation plot (i.e., the plot of calculated vs. observed heat of combustion), the correlation coefficient was found to be 1.00 and the standard deviation of the residuals was found to be 1.90 kcal/mole. The standard deviation of the residuals is generally considered to be the error in the prediction, and therefore, the heat of combustion for acyclic alkane compounds may be calculated to ± 1.90 kcal/mole over a range of 775 to 1507 kcal/mole.

It should be noted that not every physical property correlation was based on the same number of compounds. For example, 106 monocyclic aromatic compounds were utilized for the density correlation whereas only 22 monocyclic aromatic compounds were utilized in the

Table 3.6
Summary of alkane physical property - chemical structure correlations.

Property	r	N	σ_r	Range of Values	Units
Cetane Number	0.918	20	10.3	9 → 100	Cetane Number
Boiling Point	0.991	177	12.0	-89 → 490	°C
Freezing Point	0.928	92	25.7	-160 → 75	°C
Flash Point	0.996	5	9.25	-2 → 220	°C
Density	0.963	173	0.011	0.557 → 0.816	g/ml
Refractive Index	0.962	175	0.005	1.35 → 1.46	n_D^{20}
Surface Tension	0.903	68	0.94	14.5 → 23.4	dynes/cm (25°C)
Critical Pressure	0.961	64	1.47	21 → 48	atm
Critical Temperature	0.981	60	8.14	161 → 347	°C
Critical Volume	0.988	65	0.015	0.148 → 0.603	mole ⁻¹
Heat Capacity	0.990	145	1.36	26.5 → 75.2	cal/deg-mole
Heat of Vaporization	0.995	72	0.168	3.6 → 12.3	kcal/mole (25°C)
Heat of Formation	0.988	145	1.51	-79.6 → -22.5	kcal/mole (25°C)
Free Energy of Formation	0.906	33	0.846	-3.6 → 4.13	kcal/mole (25°C)
Heat of Combustion	1.000	136	1.90	775 → 1507	kcal/mole (25°C)
Molecular Volume	0.989	128	4.01	116 → 311	ml/mole

Legend:

r = correlation coefficient

N = number of points (compounds)

 σ_r = standard deviation of residuals

Table 3.7
 Summary of monocyclic aromatic physical property - chemical structure correlations.

Property	r	N	σ_r	Range of Values	Units
Cetane Number	0.944	22	8.54	-12 → 72	Cetane Number
Boiling Point	0.985	91	4.69	80 → 280	°C
Freezing Point	0.642	61	17.6	-99.5 → 79.2	°C
Flash Point	0.994	5	13.9	-11 → 250	°C
Density	0.735	106	0.012	0.851 → 0.917	g/ml
Refractive Index	0.912	175	0.004	1.48 → 1.53	n_D^{20}
Surface Tension	0.567	14	1.30	27.7 → 30.8	dynes/cm (25°C)
Critical Pressure	0.965	22	1.30	28.6 → 48.6	atm
Critical Temperature	0.956	22	9.03	289 → 403	°C
Critical Volume	0.992	21	0.008	0.26 → 0.48	mole ⁻¹
Heat Capacity	0.995	21	0.716	32.5 → 57.5	cal/deg-mole
Heat of Vaporization	0.982	36	0.235	8.0 → 13.7	kcal/mole (25°C)
Heat of Formation	0.999	14	0.400	-15.2 → 11.7	kcal/mole (25°C)
Free Energy of Formation	0.970	14	0.456	24.5 → 29.8	kcal/mole (25°C)
Heat of Combustion	1.000	21	0.718	750 → 1331	kcal/mole (25°C)
Molecular Volume	0.996	87	1.72	89 → 280	ml/mole

Legend:

r = correlation coefficient

N = number of points (compounds)

 σ_r = standard deviation of residuals

Table 3.8
Summary of dicyclic aromatic physical property - chemical structure correlations.

Property	r	N	σ_r	Range of Values	Units
Boiling Point	0.996	70	4.82	137 → 415	°C
Freezing Point	0.632	54	47.9	-46 → 112	°C
Density	0.966	41	0.008	0.915 → 1.016	g/ml
Refractive Index	0.974	44	0.006	1.53 → 1.62	n_D^{20}
Molecular Volume	1.000	32	1.10	154 → 324	ml/mole

Legend:

r = correlation coefficient

N = number of points (compounds)

σ_r = standard deviation of residuals

critical pressure correlations. This was due to the limited availability of literature values for all physical properties. For each property correlated in each chemical class, the maximum number of compounds possible was utilized in each correlation. A specific data point (i.e., compound) was subject to rejection from the data set by an examination of a plot of residuals for a correlation. The plot of residuals for the acyclic alkane density predictions is representative of the residual plots obtained in this manner and is shown in Figure 3.21. If the residual of any individual compound was found to be more than 20% larger than the residual of the remaining compounds, this was taken to be an indication of one of two possible alternatives: either the literature value for the physical property of that compound was in error, or a group property approach for that particular structural isomer was not feasible. Therefore, a physical property calculation whose residual met this criteria was subject to removal from the data base. Of the over 2,500 predicted physical properties reported in the three chemical classes, less than 5% of all calculated values fell into this category and were rejected due to poor correlation fits.

As described above, a multiple regression analysis algorithm was employed to calculate the mixing coefficients for each chemical class-physical property correlation. These mixing coefficients are labeled b_i in Equations 3.2 - 3.4. Within one physical property prediction, the mixing coefficients are constant for each chemical class, and the physical property of each compound is determined by the carbon functional groups present in the compound. As previously stated, the chemical groups present in a given compound are represented by the χ_x and C_x terms in Equations 3.2 - 3.4. Therefore, to calculate the different physical properties for each compound, only the mixing coefficients in the equations change. The same physical property for a different compound may be calculated by simply changing the χ_x or C_x terms to represent the new compound.

Consider the example of 4,4-dimethylheptane as an illustration of the technique used to calculate the physical property of a given compound. The compound 4,4-dimethylheptane

Distirbution of Errors: Alkane Density

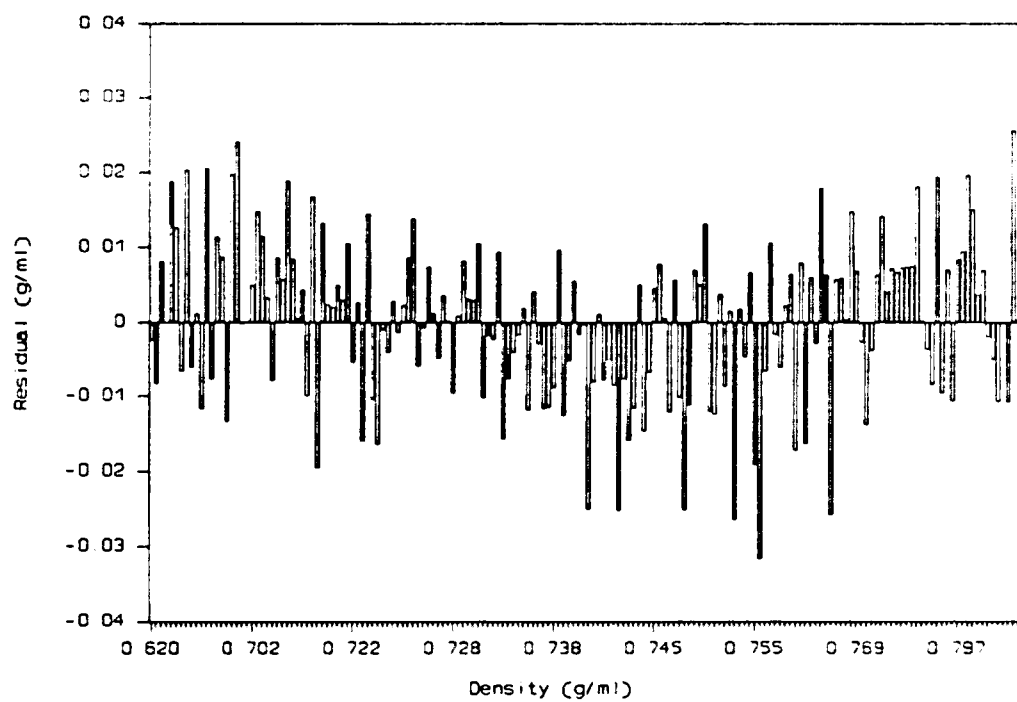


Figure 3.21 Distribution of errors plot for the alkane density correlation.

has chemical group values of $\chi_{\text{CH}_3}=0.444$, $\chi_{\text{CH}_2}=0.444$, $\chi_{\text{CH}}=0$, and $\chi_{\text{C}_q}=0.111$. From Table 3.3, the mixing coefficients for the heat of combustion for the acyclic alkanes are $m=1.0203915$, $b_0=1.07229$, $b_1=-1.06909$, $b_2=-1.07225$, $b_3=-1.07541$, $b_4=-1.07857$, and $B=-15.497781$. Table 3.2 indicates that the heat of combustion for acyclic alkane compounds follows an inverse function. Therefore, substitution of the mixing coefficient and chemical group values into Equation 3.2 with $n=-1$, yields a heat of combustion value of 1357 ± 1.90 kcal/mole. This compares very favorably with the literature value of 1356.61 kcal/mole (156) for the heat of combustion of 4,4-dimethylheptane. The density of 4,4-dimethylheptane is calculated in an analogous manner with the chemical group terms remaining constant and only the mixing coefficients changing. Again, from Table 3.3, the mixing coefficients for the density of an acyclic alkane are $m=1.0379129$, $b_0=-1686.5001$, $b_1=1686.7285$, $b_2=1687.3565$, $b_3=1688.0271$, $b_4=1688.7404$, and $B=-0.0284012$. For the density of an acyclic alkane, Table 3.3 indicates a linear function. Substitution of these mixing coefficient and chemical group values into Equation 3.2 with $n=1$ yields a calculated density of 0.729 ± 0.011 g/ml for 4,4-dimethylheptane. Again, this value compares very favorably with the literature value 0.7256 g/ml. The correlation plot for the acyclic alkane compound heat of combustion is depicted in Figure 3.19 and the correlation plot for the acyclic alkane density is depicted in Figure 3.9.

Please note that while manual manipulation of Equations 3.2 - 3.4 with the mixing coefficients in Tables 3.3 - 3.5 proves to be quite cumbersome, calculations of this type are quite easily handled by a personal computer. The software which is listed in Appendix II is capable of accessing both the chemical structural information and mixing coefficients to perform calculations such as these is less than two seconds. In addition to the correlation software described above, specialized software has been developed to calculate the physical properties of acyclic alkane, monocyclic aromatic, and dicyclic aromatic compounds in an interactive manner. This physical property calculation program is called PHYSPROP.BAS and is listed in Appendix III. By simply entering the number of each type of carbon structural

unit of a compound, this software will calculate sixteen of the physical properties for acyclic alkane and monocyclic aromatic compounds (five properties for dicyclic aromatic compounds) in less than one second.

Similar results were obtained for each of the physical properties for each chemical class listed in Tables 3.6 - 3.8. It should be noted, however, that the error associated with each physical property calculation is dependent on both the chemical class for which the property is being calculated and the physical property which is being calculated. Care should be taken when interpreting the data contained in Tables 3.6- 3.8. As an example, consider the density predictions for each chemical class. The correlation coefficient for the 173 acyclic alkane compound density predictions is much higher than the correlation coefficient for the monocyclic aromatic compounds although the error (σ_r) for each chemical class is approximately the same. This apparent discrepancy may be traced to the range of density values used in each data set. The acyclic alkane compounds utilized in the basis set possessed densities which span a range of 0.259 g/ml whereas the monocyclic aromatic compounds utilized in the basis set span only 0.066 g/ml. Therefore, the actual error in the calculation of the monocyclic aromatic density is approximately the same as the error in the calculation of the acyclic alkane density, although the alkane density calculation has a much higher correlation coefficient. This effect is especially noticeable in the calculation of the freezing point for the dicyclic aromatic compounds. This correlation contains both the smallest number of data points and the smallest range of values of any of the freezing point correlations. It is reasonable, therefore, that the dicyclic freezing point calculations would have the largest error. It is also necessary to point out that all of the dicyclic aromatic physical property predictions were performed on a data set which was limited in both the number of compounds available and the physical properties available for those compounds. The main objective of the correlations on the dicyclic aromatic data set was to confirm the ability of the predictive process on another chemical class. Therefore, this data set contains

fewer compounds and fewer physical properties in contrast to the data sets for the acyclic alkane and monocyclic aromatic compounds.

It is also interesting to contrast those physical properties which have good correlations against those which do not correlate as well. Since a group property approach assumes only intramolecular bonding interactions, one would not expect physical properties which are largely dependent on intermolecular forces to correlate as well. This point is illustrated by comparing Figures 3.19 and 3.7, the correlation plots for heat of combustion and freezing point, respectively. In Figure 3.19, the heat of combustion exhibits an excellent correlation between the observed and calculated values. This is consistent with the observation that the heat of combustion is predominately dependent on the number of carbon groups present in a compound (i.e., the heat of combustion is predominately dependent on intramolecular bonding forces). Such a property is easily modeled in a group property approach such as the one presented here. Conversely, the correlation plot for freezing point is depicted in Figure 3.7 and demonstrates a significantly less satisfactory correlation. The freezing point is well known to be largely dependent on other factors such as molecular symmetry and intermolecular bonding interactions. Physical properties such as freezing point are more difficult to model by a group property approach and will therefore exhibit larger errors in the calculated values of the physical property.

Care should also be taken when examining the flash point data. Due to a very limited literature values, only 5 acyclic alkane and 5 monocyclic aromatic compounds were available for use in the model compound data set. Although the correlation coefficients of these correlations are very high, they are based on an incomplete basis set. Therefore, any flash points predicted with the mixing coefficients presented in Tables 3.3 and 3.4 should be considered only as approximate values.

It is interesting to contrast the physical property predictions made by this method against physical property predictions found in the literature. Previously mentioned was the

work by Fisher (95,96). Utilizing only *n*-alkanes, Fisher was obtained a correlation coefficient of 0.99999992 for the density prediction of C₅-C₄₀ alkanes. The methodology presented here results in a correlation coefficient of 0.963 for 173 alkane isomer density predictions for alkanes C₅-C₃₅. Likewise, Fisher was able to predict the boiling point of *n*-alkanes C₁₅-C₂₇ with a correlation coefficient of 0.999872. Our methodology predicted the boiling point of 177 acyclic alkane isomers from C₅-C₃₅ with a correlation coefficient of 0.991. Although the actual predicted properties may not be quite as accurate as those by Fisher, but the larger range in isomer structures allows much more freedom in the property predictions. In a similar manner, many of the physical property prediction schemes for pure compounds which are described in Chapter 1 quote correlation coefficients of approximately 0.85 or higher, and prediction errors that average between 5 - 15%, depending on the physical property that was predicted. This compares very favorably with the results summarized in Tables 3.6 - 3.8 of this work. With few exception, nearly all of the predictions presented in these tables possess correlation coefficients of 0.90 or better with prediction errors of less than 10%.

Conclusion

A group property approach may be employed to calculate various physical properties of hydrocarbons. This approach is easily incorporated into a computer program which allows very rapid and precise prediction of these physical properties from a knowledge of the carbon structure of the compound. This group property approach allows the calculation of sixteen physical properties of a given acyclic alkane or monocyclic aromatic compound, as well as a limited number of physical properties of dicyclic aromatic compounds.

The physical properties of the hydrocarbons may be divided into two general groups: physical properties which are chiefly dependent upon intramolecular bonding forces (i.e., density, heat of combustion, etc.) and physical properties which are more dependent on

intermolecular bonding forces (i.e., boiling point, freezing point). Most of the physical properties which may be calculated by the methodology presented here are physical properties which are dependent on intramolecular forces. Employing a group property approach for the calculation of these physical properties yields very accurate information, usually with an error of less than 5 to 10% of the standard value. Nevertheless, the group property approach was also employed for the calculation of the physical properties which are chiefly dependent on intermolecular forces. Since the group property approach can not directly include factors for the intermolecular forces, the error associated with the calculation of these physical properties is somewhat higher, approximately 10 to 15% of the standard value.

The equations presented lend themselves well to incorporation into a computer program to calculate these physical properties. This program is easily written for a personal computer or a programmable calculator. Such a program will determine the physical properties of a given acyclic alkane or monocyclic aromatic compound in a matter of seconds. The only data necessary for the determination of these physical properties is a knowledge of the chemical groups which are present in the molecule. Such a program has been written for the IBM Personal Computer and is listed in Appendix III under the name `PHYSPROP.BAS`.

The methodology presented here is presumably not limited only to acyclic alkane, monocyclic aromatic and dicyclic aromatic compounds. Similar equations could be developed for nearly all classes of organic hydrocarbons. This methodology should also prove useful in the prediction of the physical properties of other hydrocarbon classes, and perhaps heteroatom-containing organics as well. The only requirement for such correlations is the development of a data base of compounds whose chemical group information and physical properties are known which will sufficiently represent the overall range of compounds and physical properties in the new chemical classes being correlated. In particular, the number of physical properties of dicyclic aromatic compound which may be calculated in this manner could be greatly increased if a more complete data base were employed.

Chapter 4

THE RAPID PREDICTION OF VARIOUS PHYSICAL PROPERTIES FOR MIDDLE DISTILLATE FUELS FROM LC-¹H NMR DATA

Introduction

For many years, chemists have wrestled with the difficulties involved in the measurement of numerous physical properties for both pure compounds and complex mixtures. The wide variety of physical properties which are commonly measured for petroleum samples generally dictates a wide range of testing procedures, many of which can be quite tedious. This situation has spawned several attempts to calculate or predict various physical properties through a variety of less complex methods. One of the most common approaches to physical property prediction has been a group property approach (151, 159, 109, 104) in which one assumes that the physical properties of a molecule are determined by the number and types of chemical groups (eg, methyl, methylene, methine) present. Although synergistic effects between the chemical compounds present in a complex mixture such as a fuel could be important for certain physical properties, it has been shown that a group property approach is useful for calculation of several physical properties of both pure compounds and fuel mixtures (144,117). In addition, the availability of analytical methodology for the prediction of the physical properties of simple component mixtures could have important industrial utility. In particular, Honigs *et al.* (147), have described an approach utilizing near infrared spectrometry to predict the heat of formation, molecular weight, and number of methyl groups per molecule for mixtures of benzene, cyclohexane, isooctane, and *n*-heptane. Also, Cookson and coworkers (145) have utilized the NMR spectra

of GC and LC separated kerosene samples to either predict or calculate a limited set of physical properties. However, these approaches, like many of the fuel predictive approaches, have been limited in scope because of their ability to predict only a limited number of fuel properties and the relatively long analysis time required.

Concurrent with the development of these predictive approaches, several advances have been made in analytical techniques for the analysis of fuel samples. Predominant among these approaches are the chromatographic techniques (89,85,73). Spectroscopic techniques such as NMR, IR, and MS have also been employed in fuel analysis (160,62,78). Fuel analysis is periodically reviewed (161). It has also been noted that fuel property analysis by ASTM methods, while usually quite accurate, may become quite tedious and may consume considerable quantities of each fuel sample. Therefore, several alternatives to ASTM methods have been proposed in an effort to provide predicted fuel properties in a more timely fashion. Among these alternatives are the measurement of cloud point by Differential Scanning Calorimetry (30), and an alternative to the ASTM engine test for determination of cetane number (39). There have also been attempts to measure only a few of the fuel properties (e.g., specific gravity) and from these select properties, predict several other physical properties for the fuel (119). A more complete review of petroleum product analysis techniques may be found in Chapter 1.

For several years, our laboratory has been involved in the development of nuclear magnetic chemical fingerprinting of middle distillate fuel samples by LC-¹H NMR analysis (7,8). In the LC-¹H NMR approach, a 100 μ L sample of the neat fuel is injected on a semi-prep scale normal phase chromatographic column where the fuel is separated into alkane, monocyclic, and dicyclic chemical classes. The chromatographic eluent then flows directly into the superconducting NMR magnet where ¹H NMR spectra are obtained on the flowing eluent stream. These ¹H NMR spectra are then integrated and an average chemical structure which is representative of the average of all chemical structures found in each

chromatographic fraction is calculated according to methods previously published (10).

In this chapter, we report the prediction of various physical properties of middle distillate fuels based on average molecular structures obtained by LC-¹H NMR analysis of the fuel samples. This technique has allowed us to predict seventeen physical properties of these middle distillate fuels much faster and with a much smaller sample size than the corresponding ASTM method for fuel property measurement. The errors encountered in the LC-¹H NMR technique are generally less than or equal to the measurement error in the ASTM methods.

EXPERIMENTAL

The fuels and their corresponding ASTM physical property data which form the data set were provided by the U.S. Army (U.S.A. Belvoir Research, Development, and Engineering Center, Ft. Belvoir, Virginia and Belvoir Fuels and Lubricants Research Facility (SwRI), San Antonio, Texas). Included in this basis set of fuels were 77 DF-2, 18 JP-8, and 14 JP-5 fuel samples which comprise a total of 109 fuels. This distribution of samples is shown graphically in Figure 4.1. The LC-¹H NMR data for these fuels was obtained using a JEOL FX-200 NMR spectrometer and later transferred via a RS-232 serial transfer line to an IBM PS/2 Model 60 personal computer, where the average structural composition data for the fuels was calculated. The personal computer interface and software which was developed in our laboratory provided us with what is essentially a complete system for the off-line integration and analysis of NMR data. This computer data collection and analysis system has been described in Chapter 2. Once the off-line ¹H NMR data was integrated, files containing average structural information were generated and stored. To establish possible correlations with the physical properties, these average molecular structure files were then compared to a second set of files which contain the physical properties of each fuel as determined by ASTM methods. Since the average molecular structure data furnished by the LC-¹H NMR

Distribution of Fuel Classes

109 Total Fuels

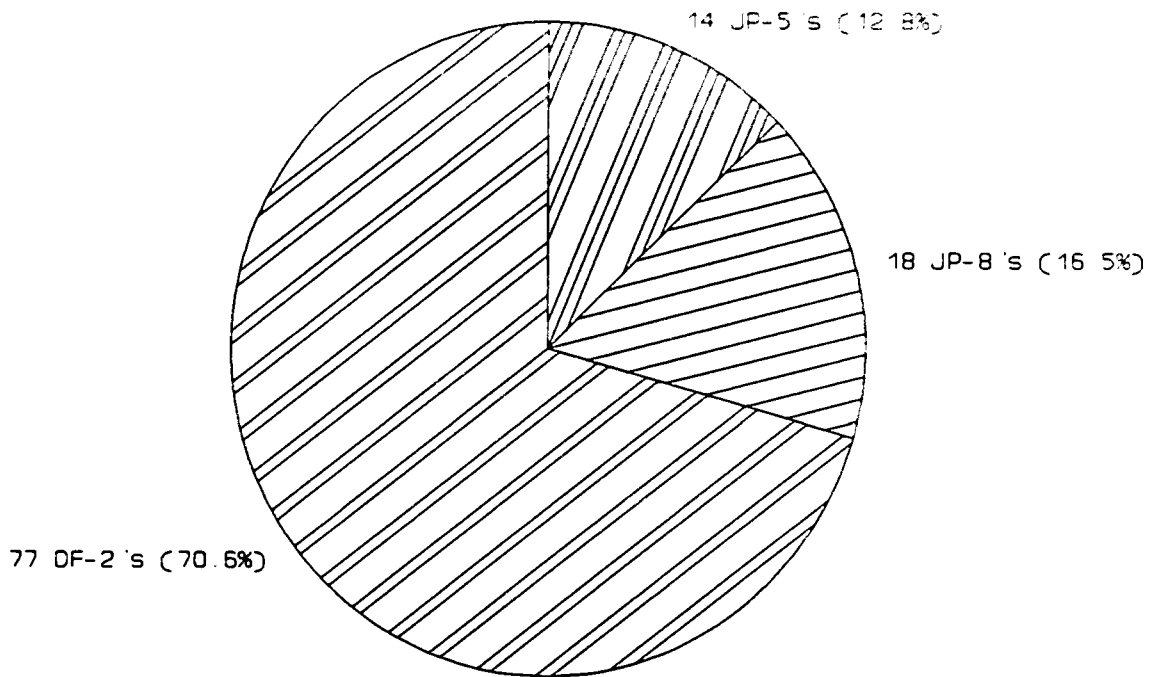


Figure 4.1 Distribution of fuel classes utilized for fuel physical property/chemical structure correlations.

is a quantitative representation of the chemical groups present in the fuels, correlations obtained between the average molecular structure data and the physical properties of the fuel are analogous to the group property predictions mentioned earlier. The actual correlations which are presented here were accomplished by a multiple regression analysis of thirteen LC-¹H NMR derived parameters and the physical properties of the fuel. These thirteen LC-¹H NMR derived parameters characterize the chemical structure groups present in the alkane, monocyclic, and dicyclic chromatographic fractions of the fuel. The nomenclature used for identification of these structural groups is depicted in Figure 4.2. Although it is recognized that not all of these 13 structural parameters are truly independent for all cases, the thirteen parameters were chosen for a variety of reasons: to be consistent with a series of model compound studies conducted in our laboratory and reported in Chapter 3, to model the maximum number of different chemical structures present in a middle distillate fuel which may be measured by LC-¹H NMR, and to provide sufficient structural information for the development of correlations for a wide range of physical properties.

For each physical property studied, the multiple regression analysis provides the 14 mixing coefficients which are labeled b₀-b₁₃ in Equation 4.1.

$$\begin{aligned}
 [4.1] \quad \text{Physical Property} = m * (& b_0 \\
 & + \\
 & {}^1f_c (b_1 \chi_{\text{CH}_3} + b_2 \chi_{\text{CH}_2} + b_3 \chi_{\text{CH}}) \\
 & \quad \text{Alkane} \\
 & + \\
 & {}^m f_c (b_4 {}^m C_{\text{UN}} + b_5 {}^m C_{\alpha} \text{CH}_3 + b_6 {}^m C_{\alpha} \text{CH}_2 + b_7 {}^m C_{\alpha} \text{CH} + b_8 {}^m C_{\alpha} C_{\alpha} + b_9 {}^m C_{\text{CH}_2 > \alpha}) \\
 & \quad \text{Monocyclic} \\
 & + \\
 & {}^d f_c (b_{10} {}^d C_{\text{UN}} + b_{11} {}^d C_{\alpha} \text{CH}_3 + b_{12} {}^d C_{\alpha} \text{CH}_2 + b_{13} {}^d C_{\text{CH}_2 > \alpha})) + B \\
 & \quad \text{Dicyclic}
 \end{aligned}$$

This equation depicts the overall form for the equation chosen to calculate the physical properties of the fuels and is labeled to show the terms for each of the three chromatographic

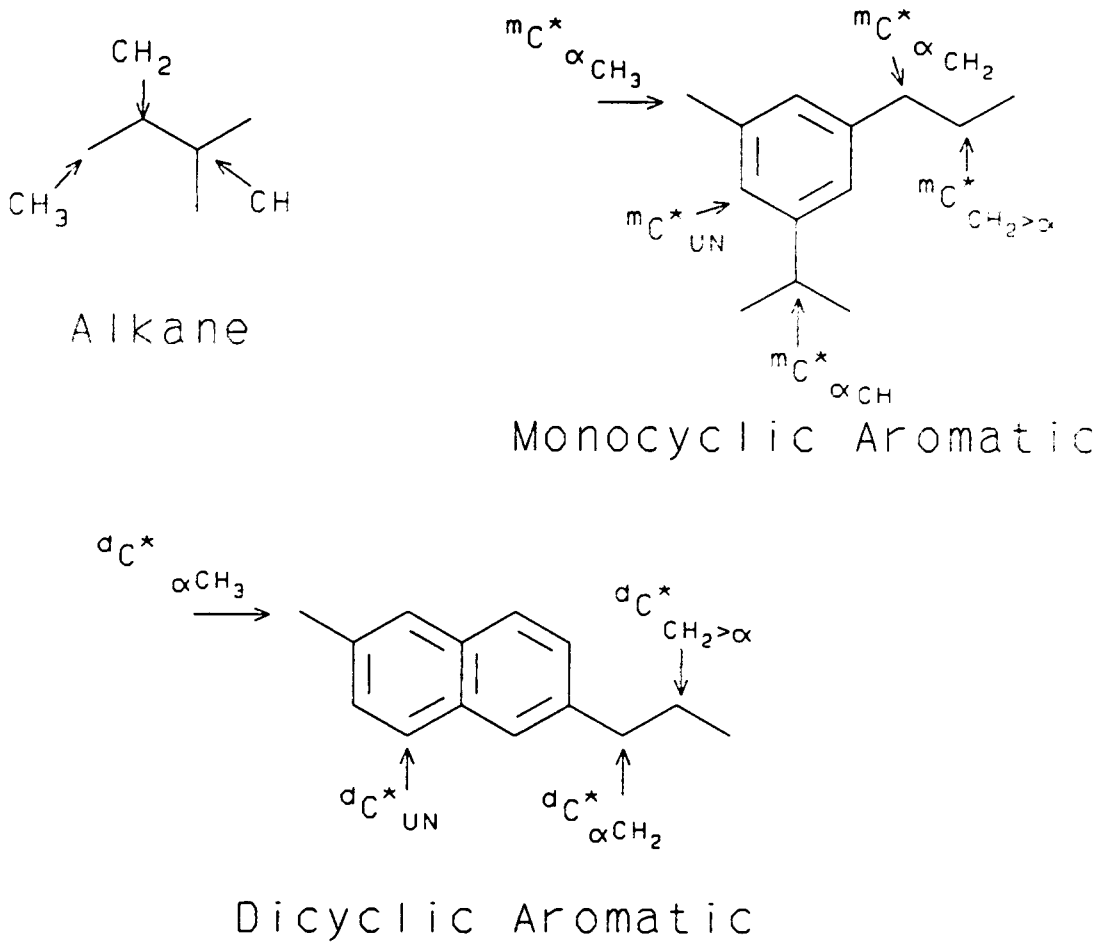


Figure 4.2 Nomenclature used to describe the chemical structures quantitated for fuel physical property/chemical structure correlations.

fractions. Once the regression coefficients have been calculated, the result is an equation for the prediction of the fuel property which consists of the thirteen terms derived from LC-¹H NMR data and the b_0 term. Each of these thirteen LC-¹H NMR terms is actually a product of three individual terms: the average molecular structure group (e.g., ${}^mC_{UN}^*$) contribution, the mixing coefficient obtained in the multiple regression analysis (e.g., b_i), and the fraction of total carbon contained in the respective chemical class (e.g., mf_c). For example, if 30% of the total carbon in the fuel is contained the monocyclic aromatic class (${}^mf_c=0.3$) and, on average, each monocyclic aromatic ring is mono substituted (${}^mC_{UN}^*=5$), the product for the ${}^mC_{UN}^*$ term would be $(0.3 \times 5 \times b_i)$. In essence, it is possible to think of the this approach as the following: the b_0 term defines a base value from which the individual molecular structures of a given fuel either increase or decrease the value for the physical property of the fuel. These molecular structure parameters, combined with the fraction of total carbon present in each class, define the unique differences between individual fuels and therefore dictate the physical properties of the individual fuel.

The value of the exponent n in Equation 4.1 is software selectable for a given physical property and allows the prediction of either the true fuel property or the reciprocal of the fuel property. For example, in the prediction of the initial boiling point, a value of $n=-1$ is selected and the inverse of the initial boiling point is actually predicted. The correlation is then performed and the predicted initial boiling point is inverted to give the true predicted initial boiling point, in °C. Table 4.1 summarizes those properties which were predicted as an inverse function ($n=-1$) and those which were predicted as a linear function ($n=1$). The value of n was suggested by the model studies performed in our lab and was determined empirically for each fuel property. This empirical determination was made by comparing the correlation coefficients obtained from the predicted verses observed physical property plots (i.e., correlation plots) for both the linear and inverse function types.

Table 4.1
Summary of results for the prediction of the fuel properties.

Property	r^a	N^a	n^b	Range of Property Values	Units
Cetane Number	0.9672	30	1	38 → 48	Cetane
Cetane Index	0.9789	65	1	37 → 57	Cetane
Density	0.9653	64	1	0.791 → 0.891	kg/L
Specific Gravity	0.9731	37	1	0.825 → 0.870	60/60°F
Initial Boiling Point	0.8995	64	-1	151 → 220	°C
Boiling Point: 10%	0.9393	67	-1	170 → 252	°C
Boiling Point: 50%	0.9532	104	-1	193 → 301	°C
Boiling Point: 90%	0.9185	105	-1	224 → 373	°C
End Boiling Point	0.9142	102	-1	244 → 406	°C
Pour Point	0.9080	72	1	-43 → 10	°C
Flash Point	0.7129	103	1	36 → 83	°C
Cloud Point	0.9284	70	1	-29 → 14	°C
Viscosity	0.9517	104	1	1.1 → 4.3	cSt
Filterability	0.7970	38	1	9 → 78	
Heat of Combustion	0.9298	29	1	42.7 → 43.2	MJ/kg
Percent Aromatics	0.9733	70	1	14.8 → 42.1	vol %
Residual Carbon	0.8137	83	1	0.09 → 2	vol %

^a The r values are correlation coefficients calculated from the data set consisting of N data points (fuels).

^b The value of n represents the exponent for the function in Equation 4.1.

Table 4.2
Comparison of ASTM physical property measurement errors and calculated standard deviation of residuals.

Property	ASTM Method	ASTM ^a Repeatability	ASTM ^a Reproducibility	Calculated ^b σ	Units
Cetane Number	D613	0.7	2.9	0.85	Cetane
Cetane Index ^c	D976	2.0		1.10	Cetane
Density	D1298	0.0005	0.0012	0.005	kg/L
Specific Gravity	D1298	0.0005	0.0012	0.002	60/60°F
Initial Boiling Point	D86	2	5	5.88	°C
Boiling Point: 10%	D86	2	5	6.25	°C
Boiling Point: 50%	D86	2	5	9.91	°C
Boiling Point: 90%	D86	2	5	18.8	°C
End Boiling Point	D86	2	5	20.6	°C
Pour Point	D97	3	6	5.18	°C
Flash Point	D93	5	10	9.47	°C
Cloud Point	D2500	2	4	3.77	°C
Viscosity	D445	0.05	0.24	0.27	cSt
Filterability ^d				19.1	
Heat of Combustion	D240	0.13	0.40	0.06	MJ/kg
Percent Aromatics	D1319	1.4	3.0	1.85	vol %
Residual Carbon	D524	0.16	0.26	0.29	vol %

^a The exact reproducibility and repeatability for the ASTM tests are dependent on the fuel class being tested and the exact conditions of the test. The values presented here are representative for the fuels utilized in this study.

^b The calculated σ , values represent the error in the predicted values of the physical properties obtained in the present study.

^c The cetane index is a correlation with the cetane number. Therefore, the error in cetane index is dependent on the error in the cetane number. ASTM D976 quotes only the error shown here.

^d The filterability data utilized for this study was a filterability index, and not the filterability measured by ASTM D4539.

RESULTS AND DISCUSSION

The correlation plots for the 17 different physical properties which were predicted by the methodology presented here are shown in Figures 4.3a - 4.19a. Table 4.1 summarizes the results of these 17 different fuel physical properties predicted from LC-¹H NMR data. Table 4.2 compares the errors of each physical property prediction and the reproducibility of the ASTM methods for determining each fuel property. The error of the physical property prediction is given as the standard deviation of the residuals (σ_r) from the prediction. As can be seen in Table 4.2, most of these predictions are either within or are approximately equal to the experimental error of the ASTM measurement for that property. Tables 4.3 - 4.6 list the individual b_i terms utilized in Equation 4.1. It should be noted that although there are a total of 109 fuels in the data base, values for all measured physical properties for each of the 109 fuels were not available. Wherever possible, the maximum number of fuels for which the ASTM physical property data was available were included in each correlation. Within the data sets available for each physical property, it was rarely necessary to reject any fuel average molecular structure or physical property data due to a poor regression fit for an individual fuel. Of the over 1200 predictions fuel physical property predictions presented, less than 3% of the predictions were rejected due to poor regression fits. In performing the prediction correlations, a data point (i.e., fuel) was subject to rejection if the residual for that particular fuel was greater than 20% higher than the next largest residual from the regression analysis. The distribution of errors for the predicted versus observed cetane number is representative of the residual plots for the fuel physical properties and is presented in Figure 4.20.

One feature of the data base compiled for the correlation of the fuel properties is that the data base includes three classes of fuels. Figure 4.5a illustrates the density predictions with the individual fuels labeled so as to indicate which predicted density value corresponds to a fuel contained in a specific fuel class. This distribution of predicted points is consistent

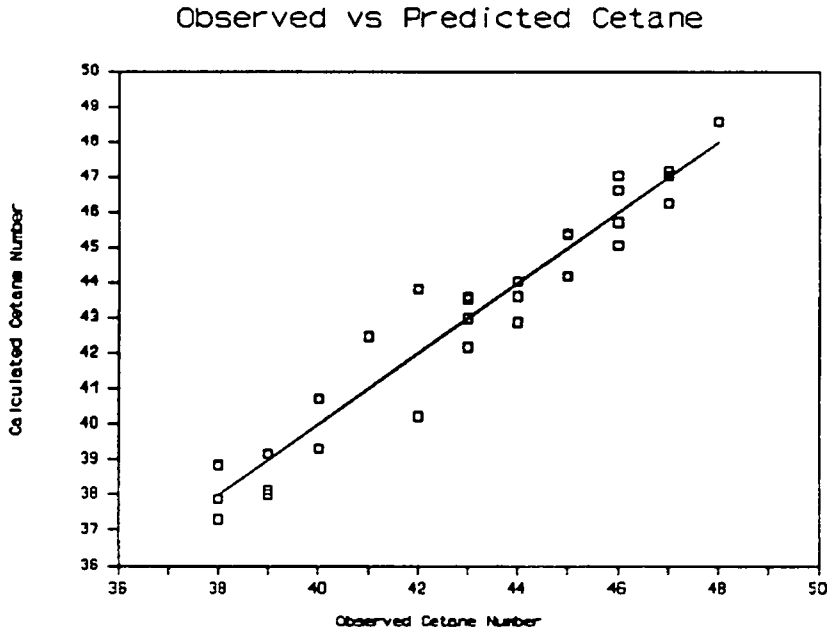


Figure 4.3a Correlation plot for fuel cetane number predictions. $r=0.9672$

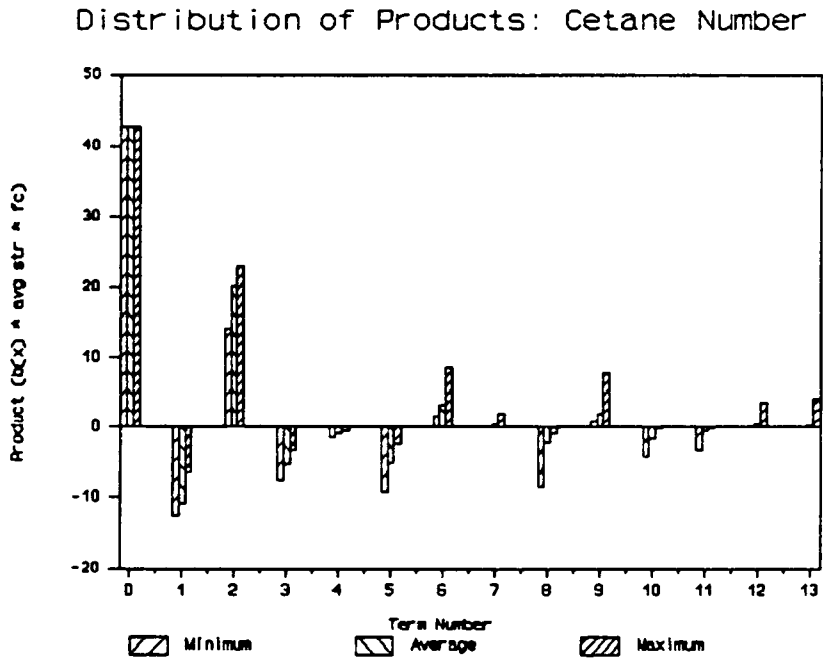


Figure 4.3b Distribution of products plot for fuel cetane number predictions.

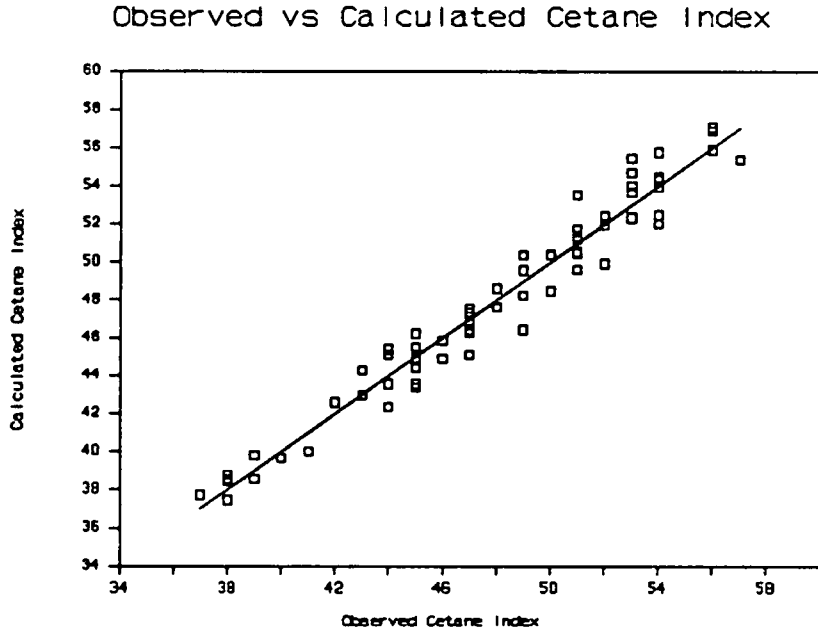


Figure 4.4a Correlation plot for fuel cetane index predictions. $r=0.9789$

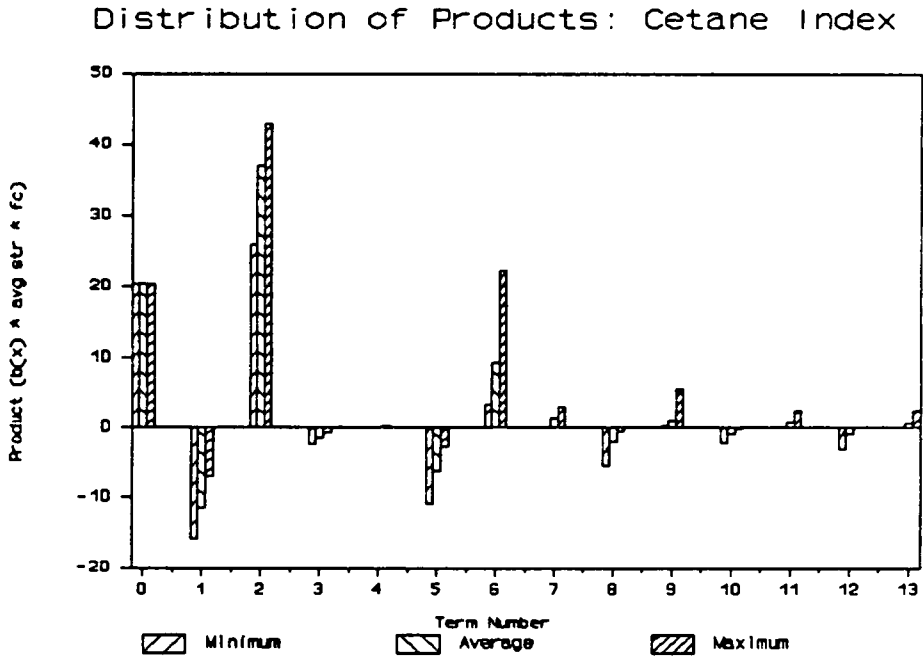


Figure 4.4b Distribution of products plot for fuel cetane index predictions.

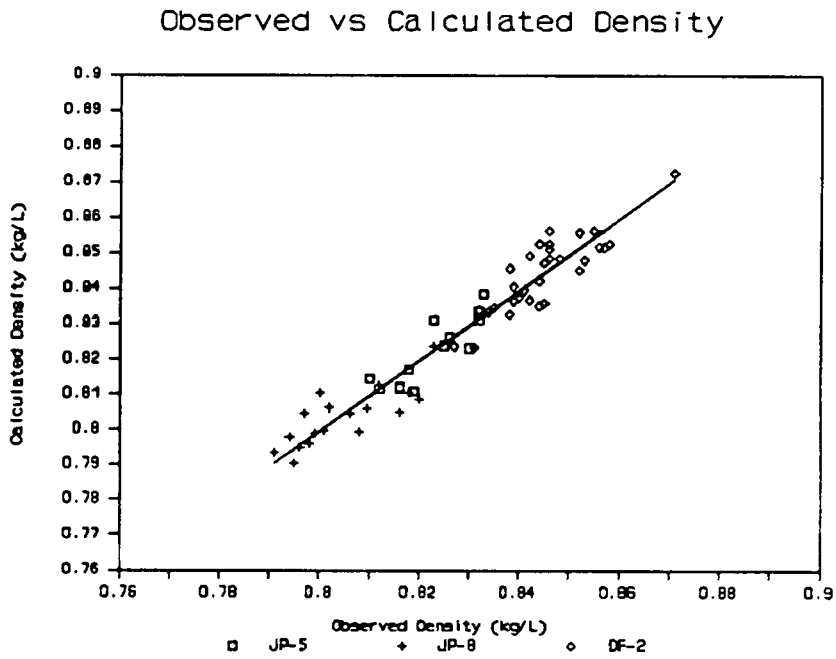


Figure 4.5a Correlation plot for fuel density predictions. $r=0.9653$

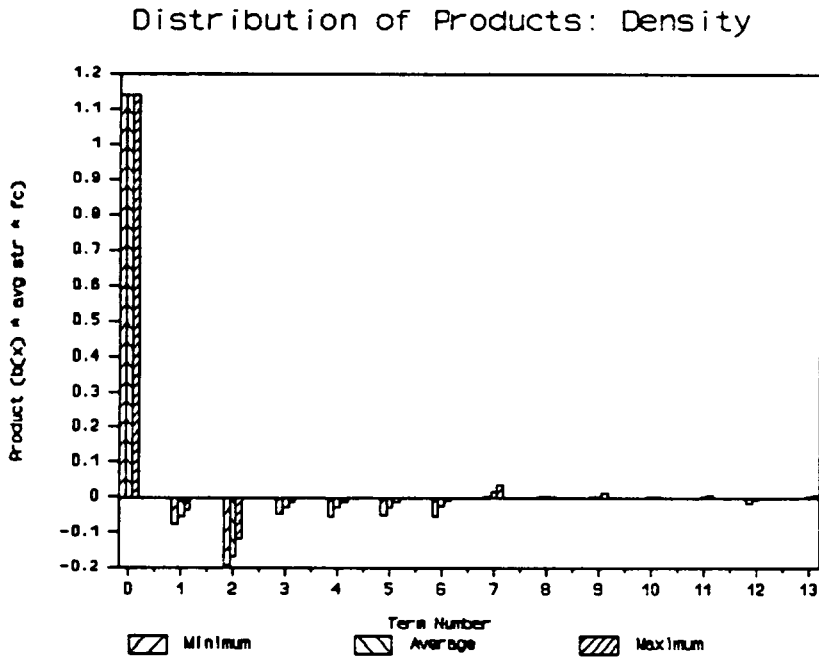


Figure 4.5b Distribution of products plot for fuel density.

Observed vs Calculated Specific Gravity

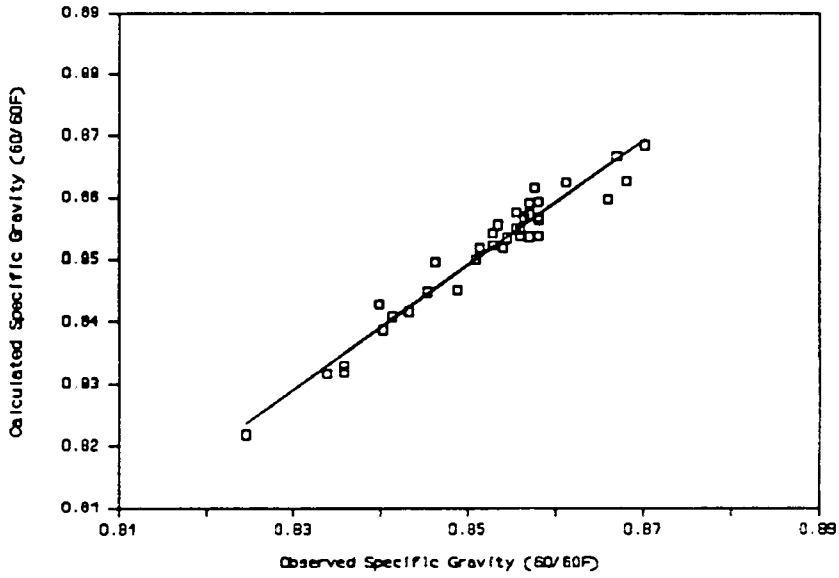


Figure 4.6a Correlation plot for fuel specific gravity predictions. $r=0.9731$

Distribution of Products: Sp. Gravity

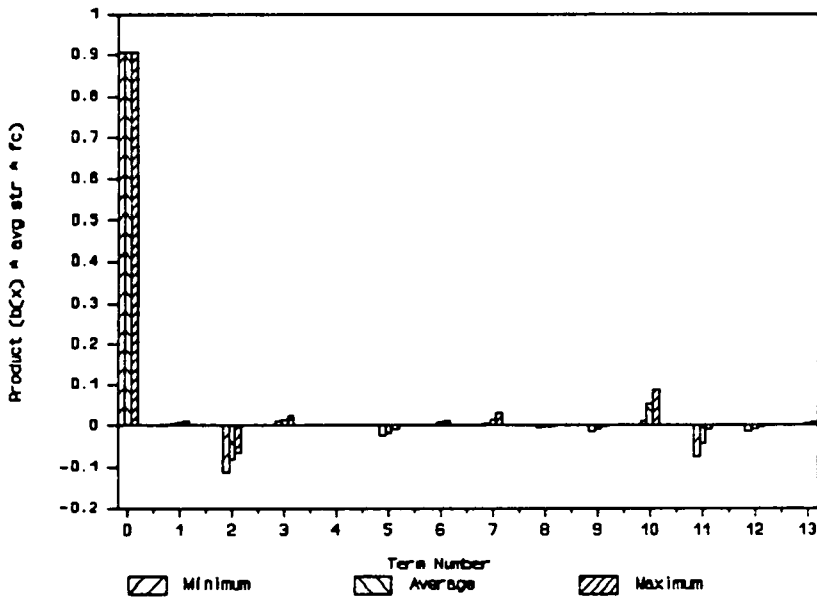


Figure 4.6b Distribution of products plot for fuel specific gravity.

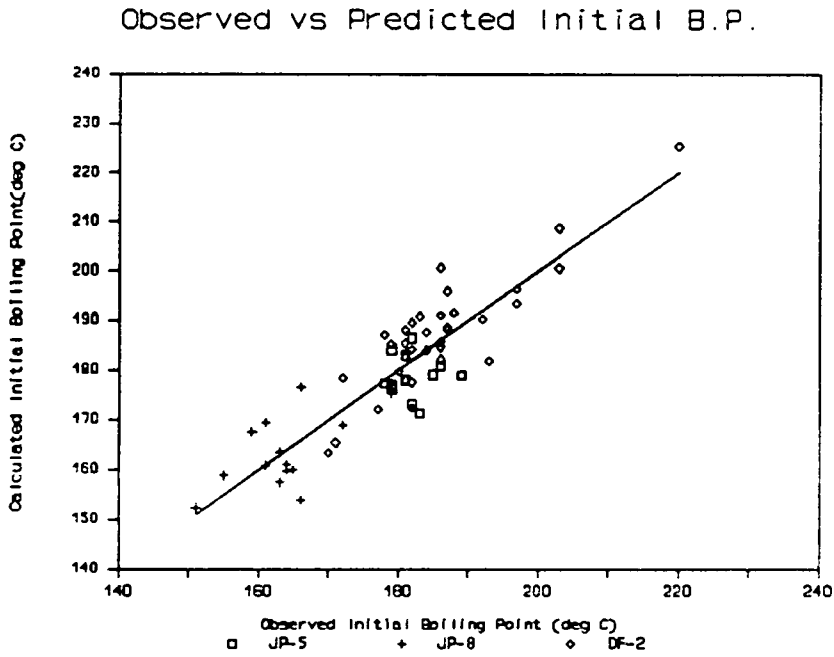


Figure 4.7a Correlation plot for fuel initial boiling point predictions. $r=0.8995$

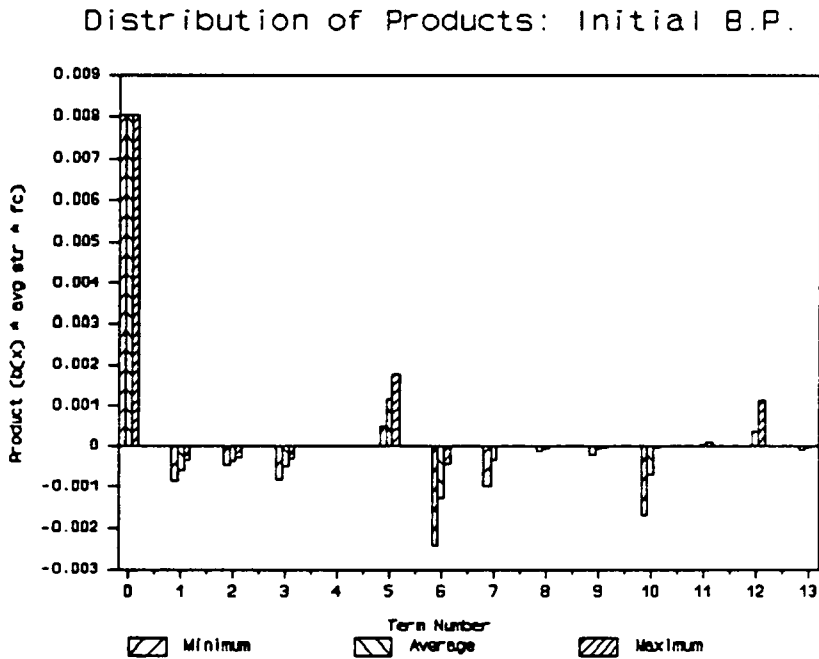


Figure 4.7b Distribution of products plot for fuel initial boiling point.

Observed vs Calculated 10% Boil Point

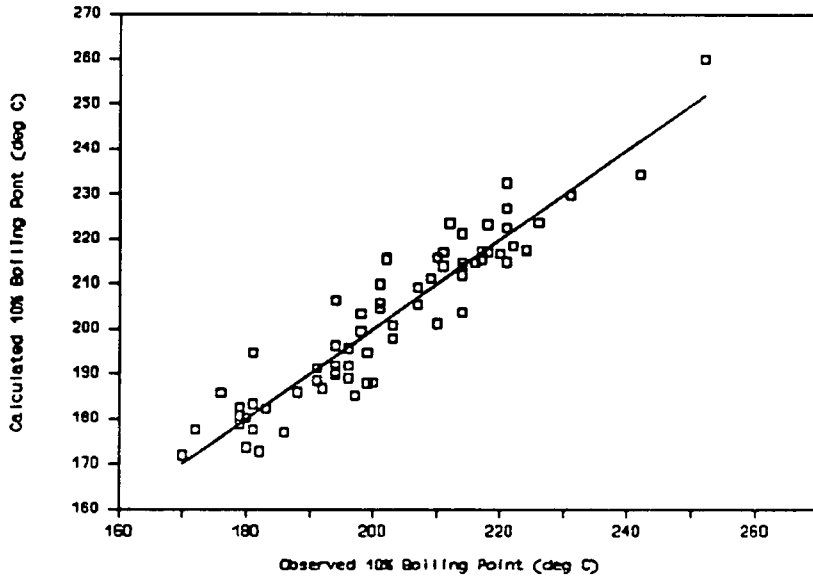


Figure 4.8a Correlation plot for fuel 10% boiling point predictions. $r=0.9393$

Distribution of Products: 10% B.P.

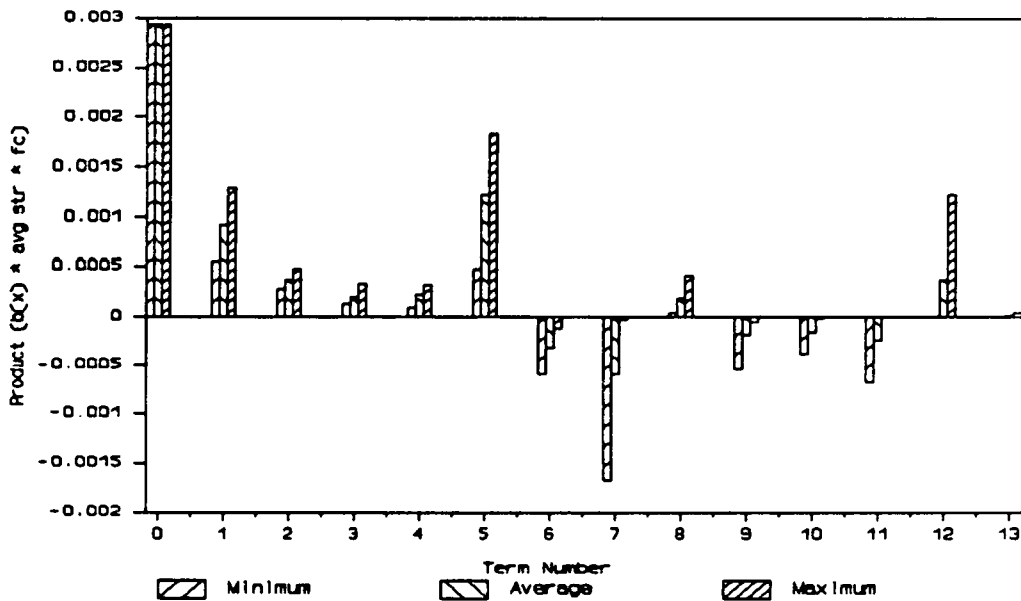


Figure 4.8b Distribution of products plot for fuel 10% boiling point.

Observed vs Calculated 50% Boil Point

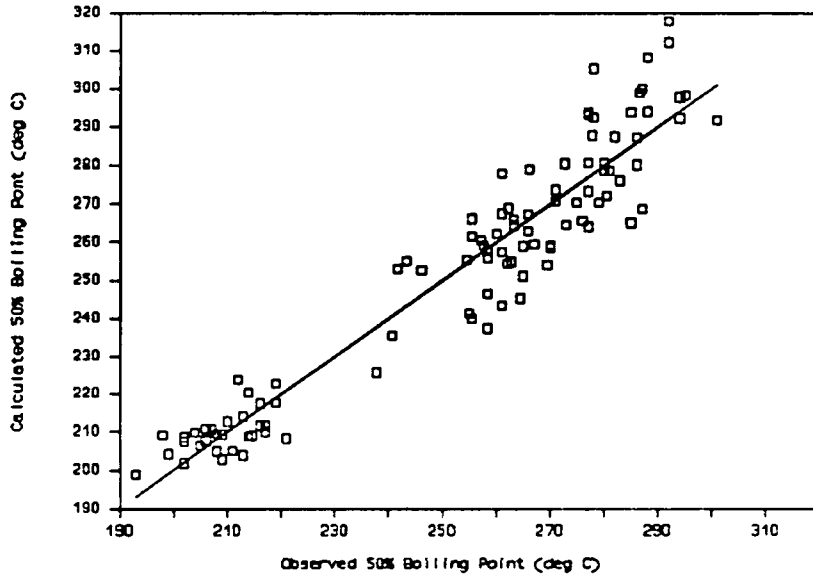


Figure 4.9a Correlation plot for fuel 50% boiling point predictions. $r=0.9532$

Distribution of Products: 50% Boil Pt

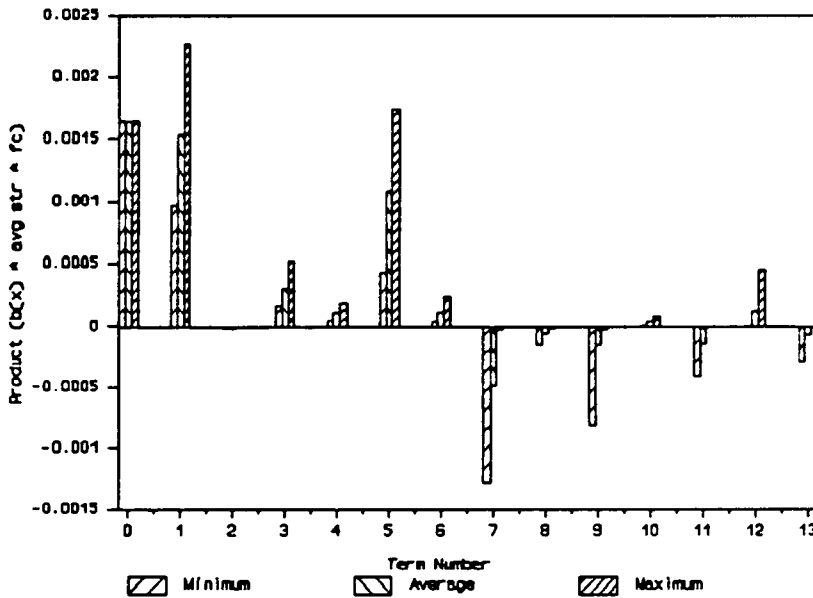


Figure 4.9b Distribution of products plot for fuel 50% boiling point.

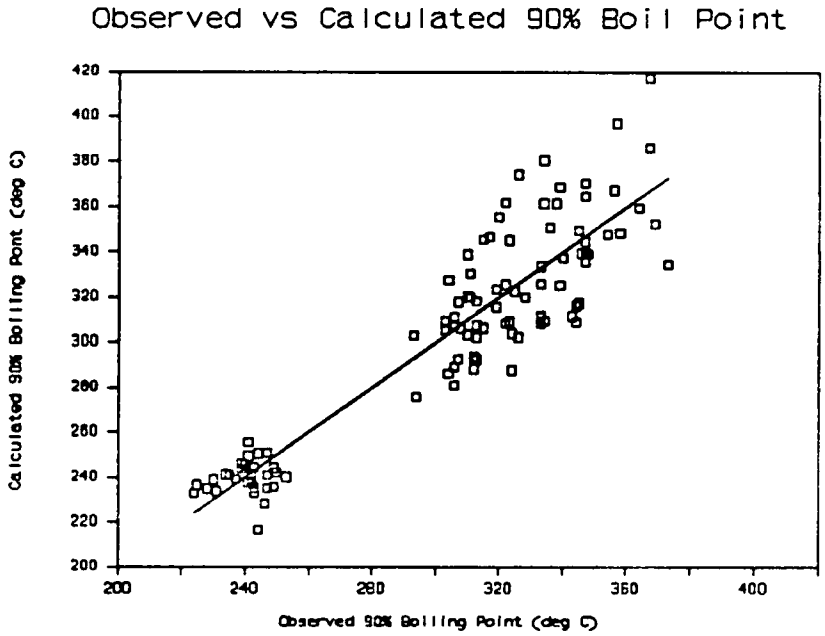


Figure 4.10a Correlation plot for fuel 90% boiling point predictions. $r=0.9185$

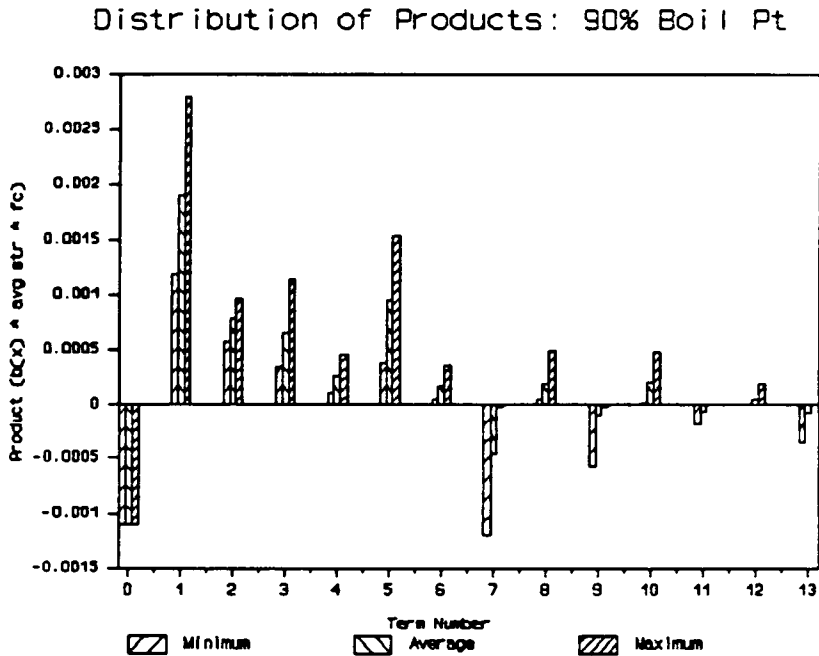


Figure 4.10b Distribution of products plot for fuel 90% boiling point.

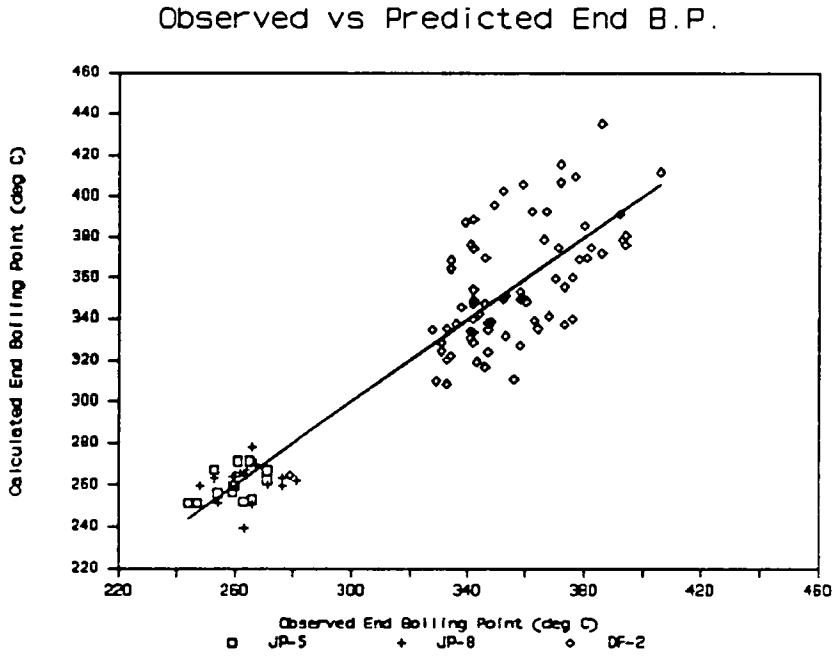


Figure 4.11a Correlation plot for fuel end boiling point predictions. $r=0.9142$

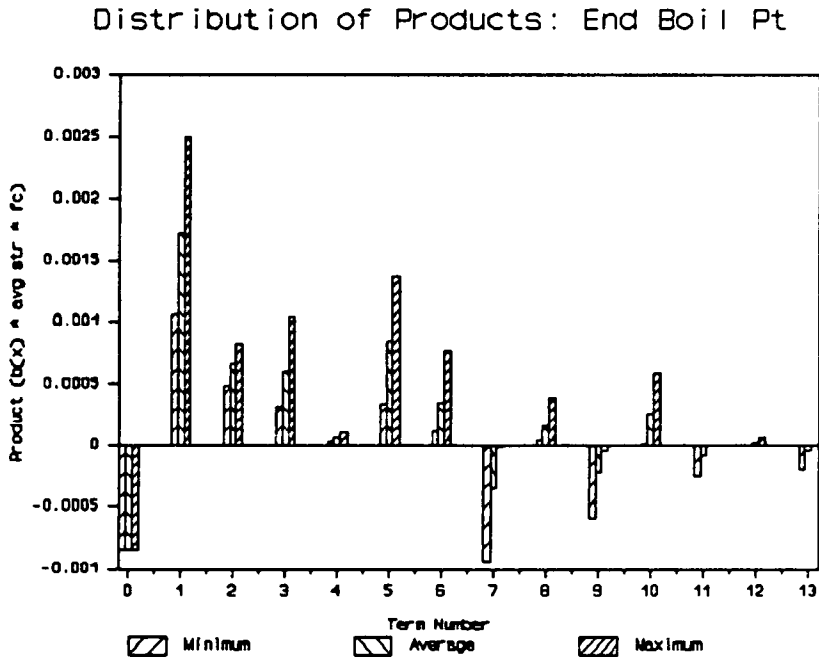


Figure 4.11b Distribution of products plot for fuel end boiling point.

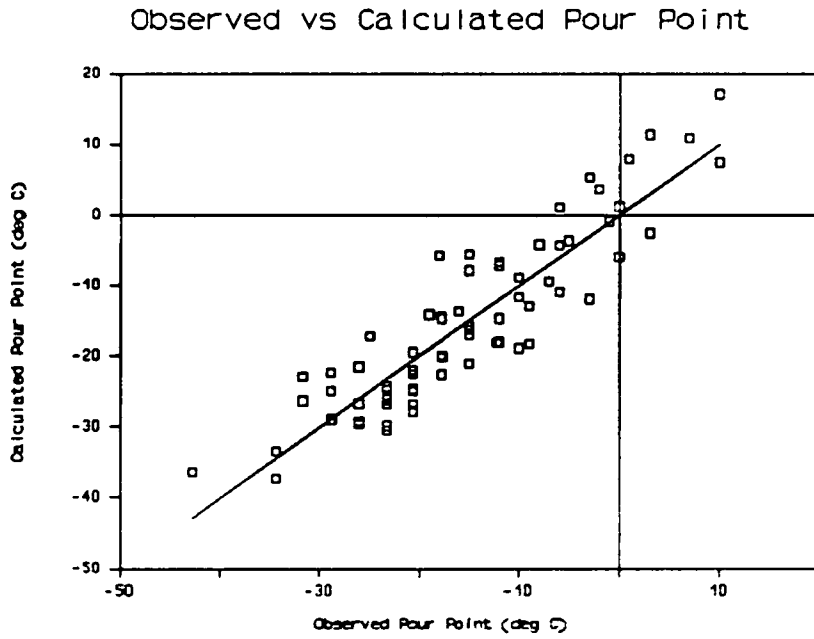


Figure 4.12a Correlation plot for fuel pour point predictions. $r=0.9080$

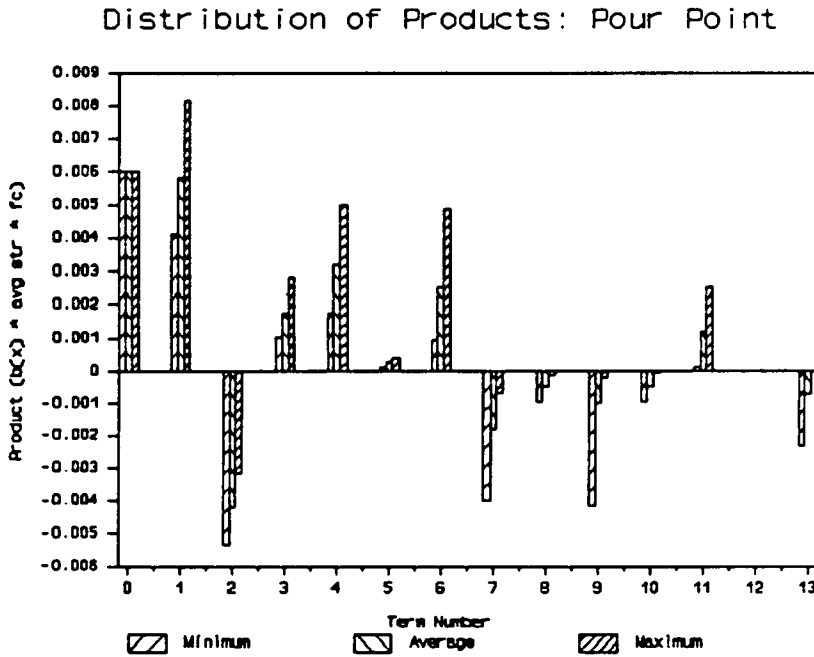


Figure 4.12b Distribution of products plot for fuel pour point.

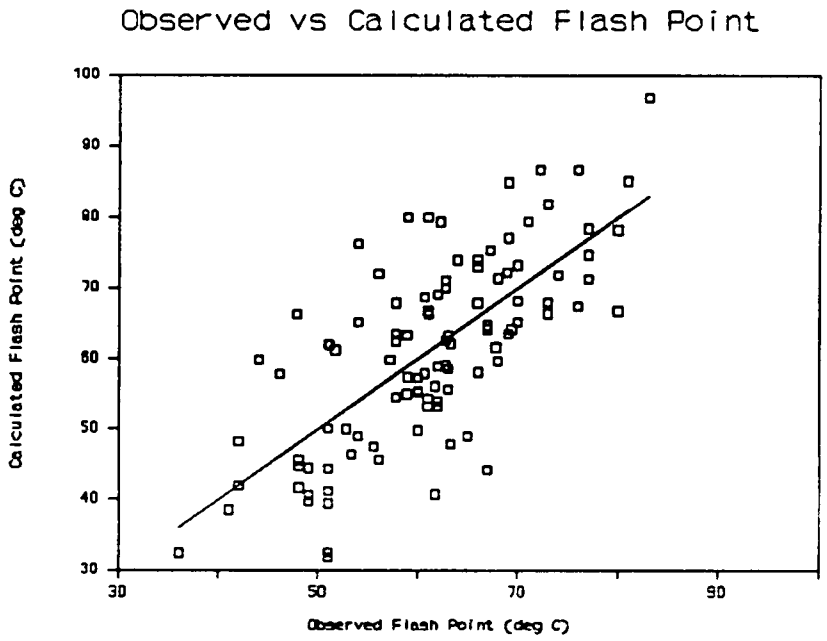


Figure 4.13a Correlation plot for fuel flash point predictions. $r=0.7129$

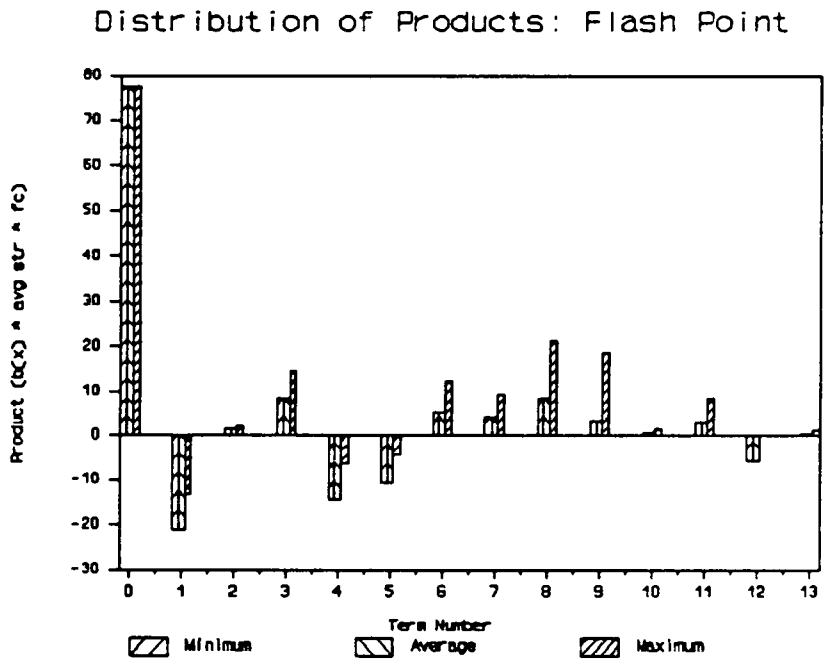


Figure 4.13b Distribution of products for fuel flash point.

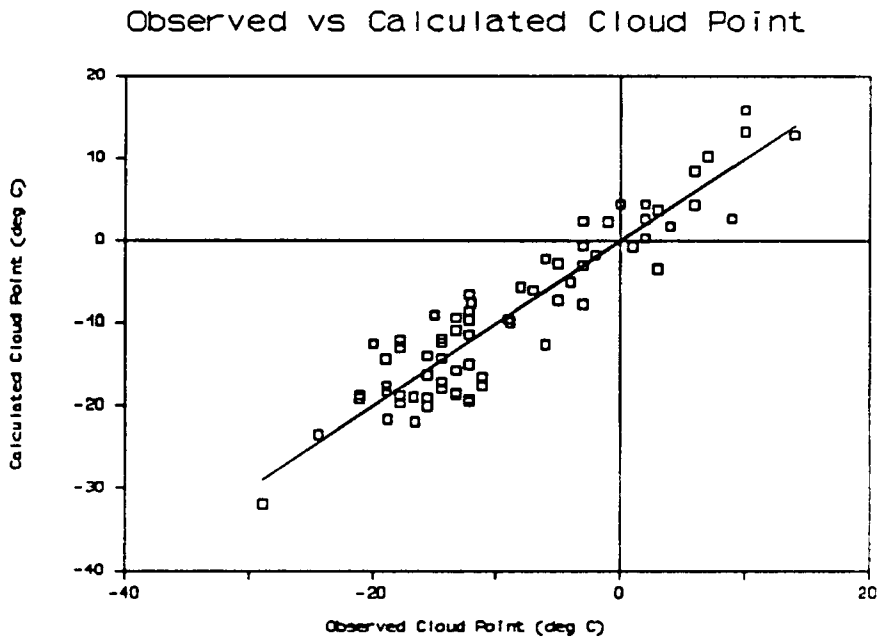


Figure 5.14a Correlation plot for fuel cloud point predictions. $r=0.9284$

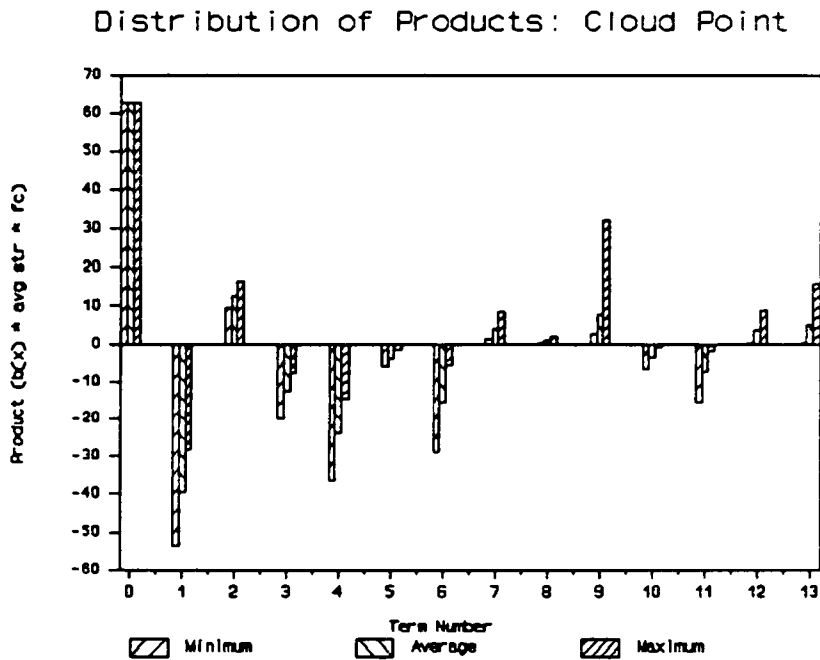


Figure 4.14b Distribution of products plot for fuel cloud point.

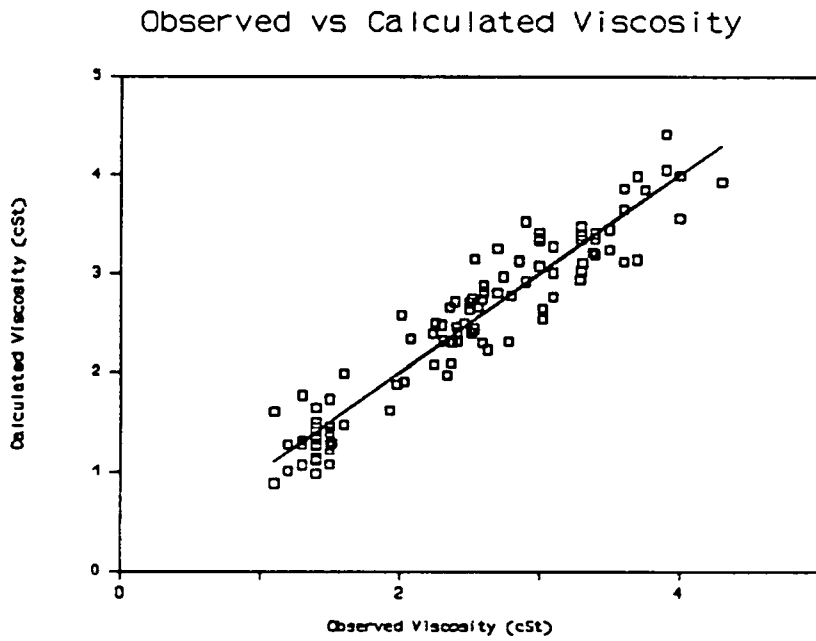


Figure 4.15a Correlation plot for fuel viscosity predictions. $r=0.9517$

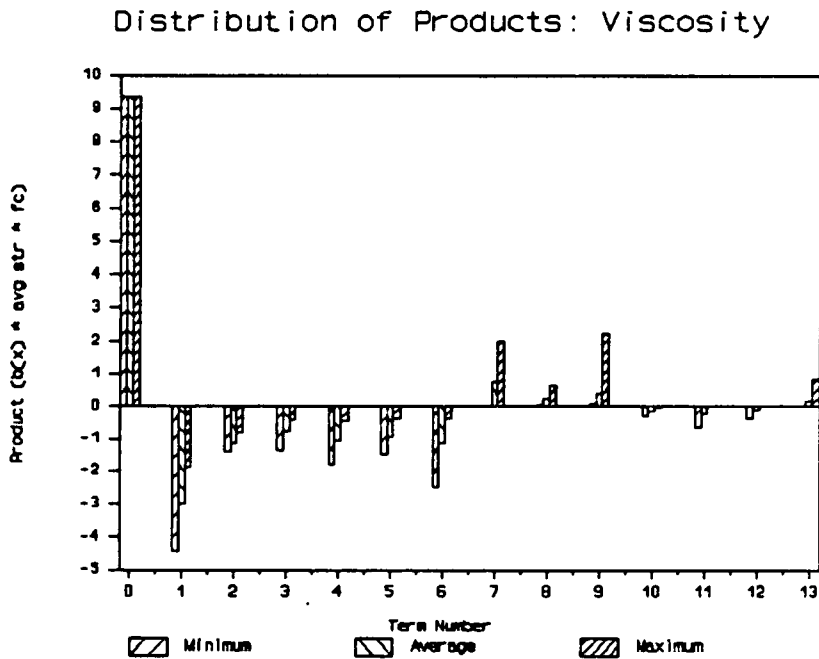


Figure 4.15b Distribution of products plot for fuel viscosity.

Observed vs Calculated Filterability

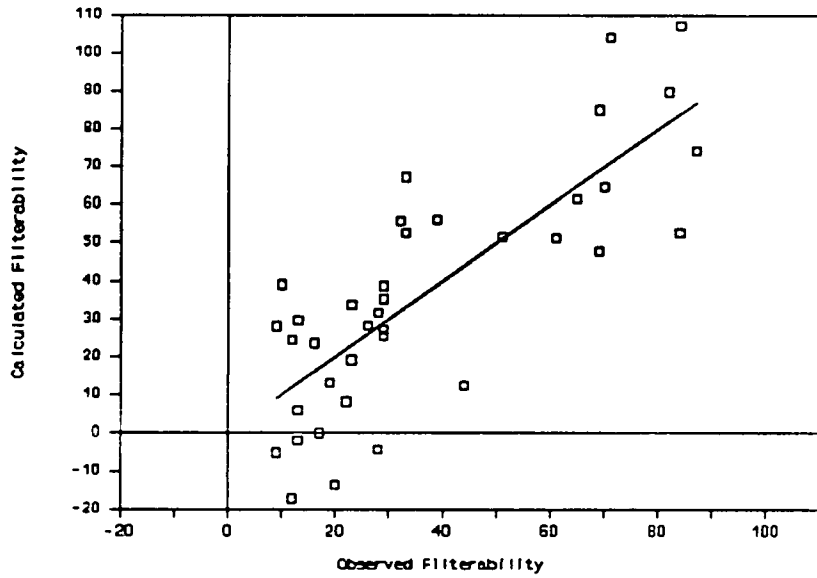


Figure 4.16a Correlation plot for fuel filterability predictions. $r=0.7970$

Distribution of Products: Filterability

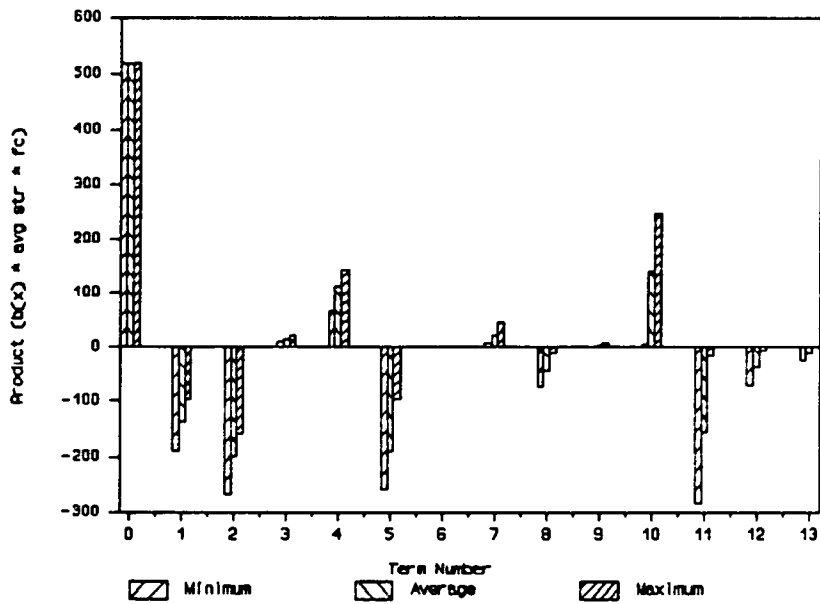


Figure 4.16b Distribution of products plot for fuel filterability.

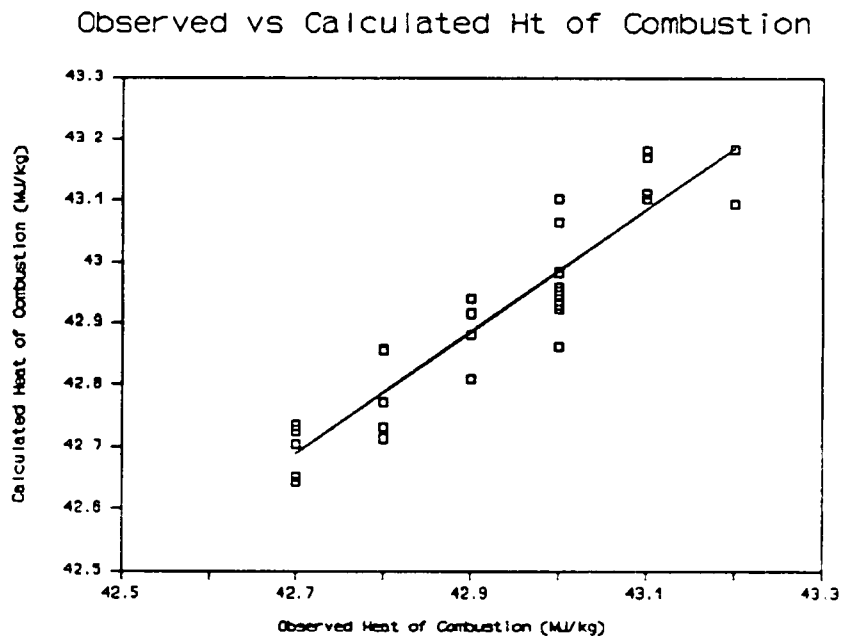


Figure 4.17a Correlation plot for fuel heat of combustion predictions. $r=0.9298$

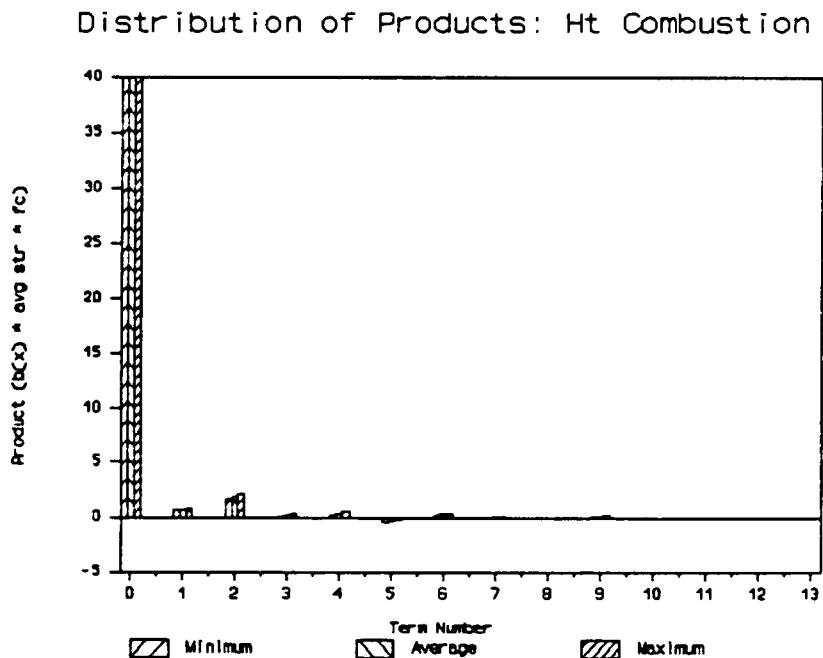


Figure 4.17b Distribution of products plot for fuel heat of combustion.

Observed vs Calculated Percent Aromatic

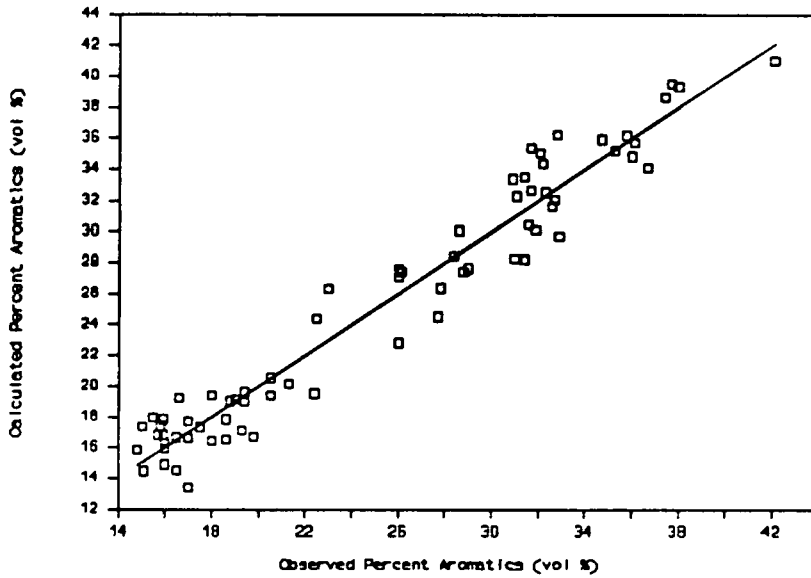


Figure 4.18a Correlation plot for fuel volume percent aromatics predictions. $r=0.9733$

Distribution of Products: % Aromatics

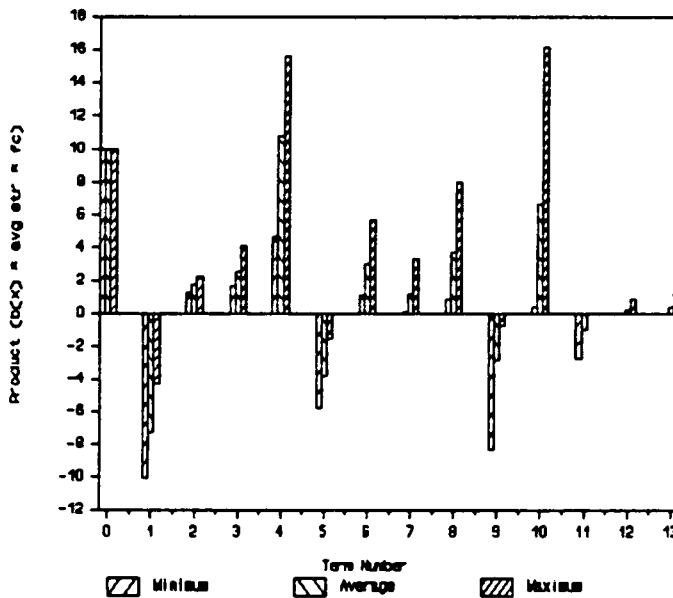


Figure 4.18b Distribution of products plot for fuel volume percent aromatics.

Observed vs Calculated Residual Carbon

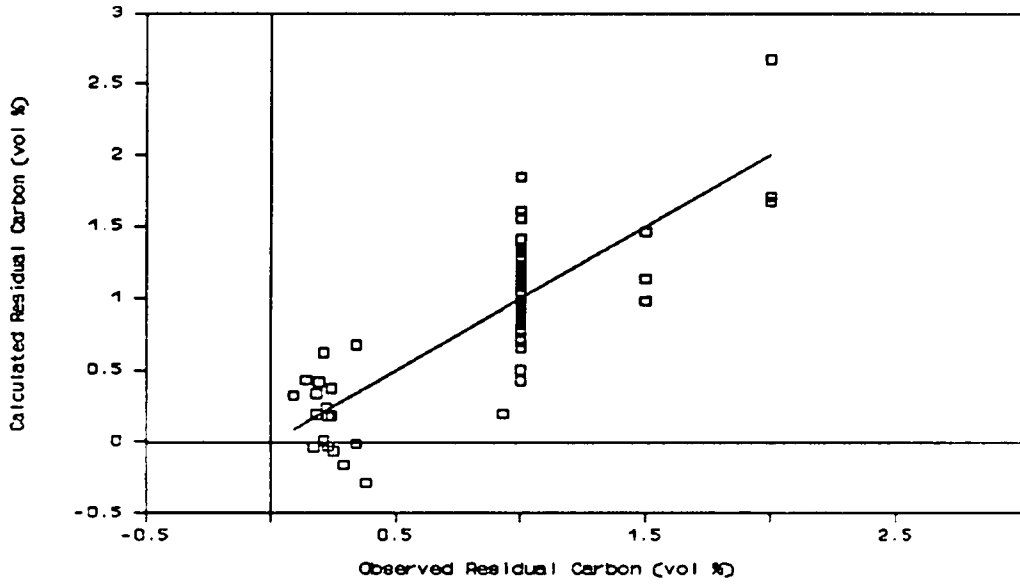


Figure 4.19a Correlation plot for fuel residual carbon predictions. $r=0.8137$

Distribution of Products: C Residual

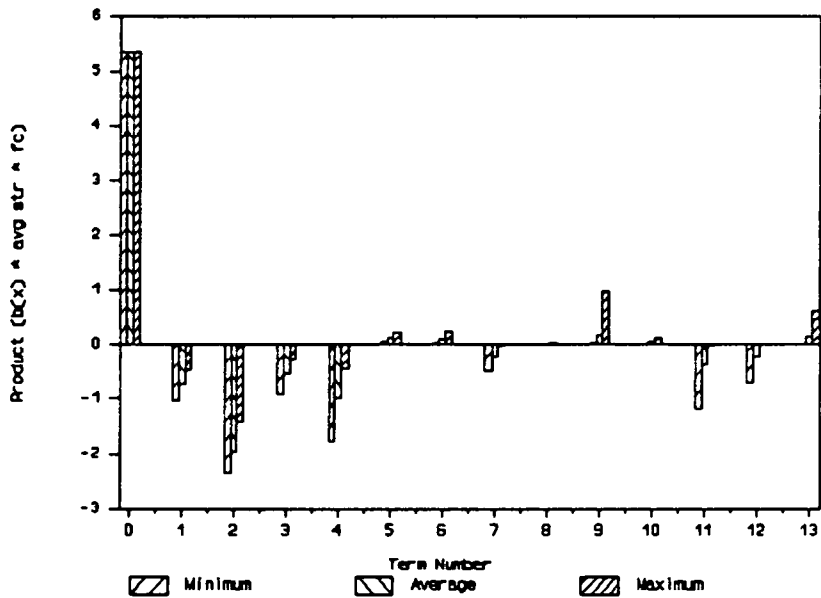


Figure 4.19b Distribution of products plot for fuel residual carbon.

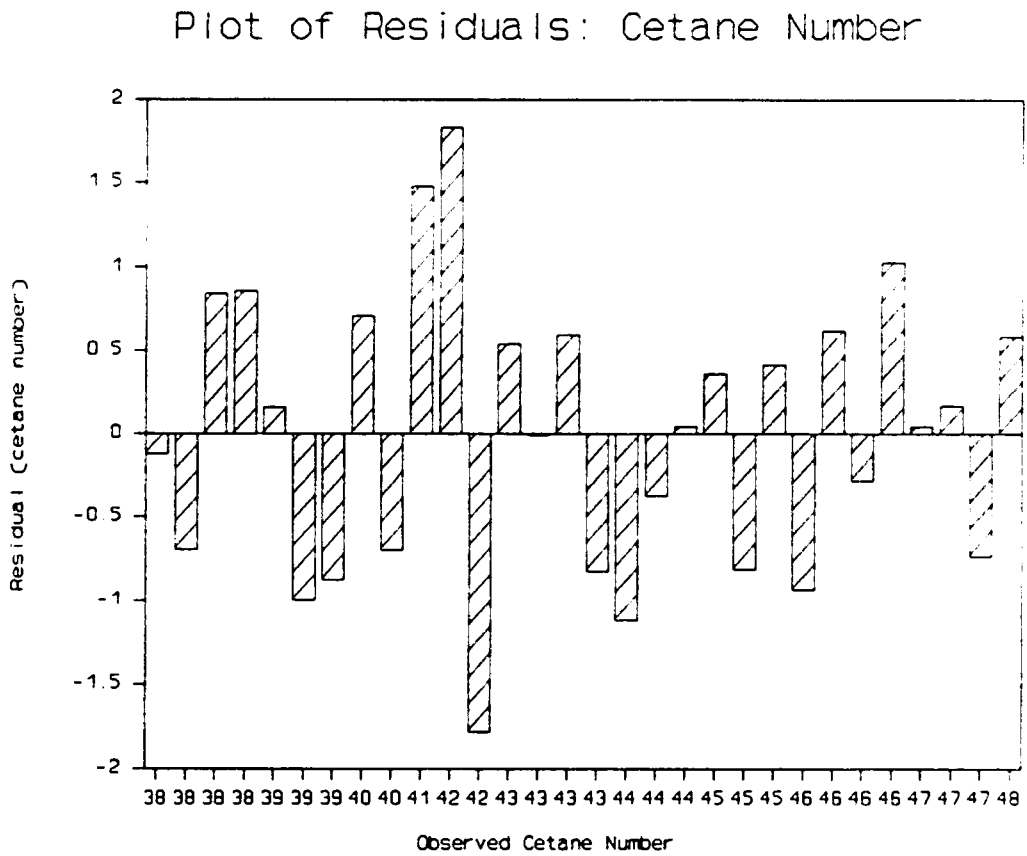


Figure 4.20 Distribution of errors between predicted and observed fuel cetane numbers.

Table 4.3
 Mixing coefficients (b.) for fuel physical property predictions.

Property	Cetane Number	Cetane Index	Density	Sp. Grav
Function Type	X	X	X	X
m	1.068743	1.043563	1.072568	1.058877
B	-2.987988	-2.080621	-0.059619	-0.051083
b ₀	42.790615	20.391577	1.141245	0.907092
b ₁	-53.159149	-67.289856	-0.322357	0.055655
b ₂	45.101429	83.158203	-0.376671	-0.214524
b ₃	-43.480862	-13.164763	-0.276214	0.159126
b ₄	-1.280107	0.140966	-0.042166	0.002301
b ₅	-16.859465	-19.420818	-0.093124	-0.044868
b ₆	20.115643	43.675358	-0.105747	0.029108
b ₇	17.004040	27.506891	0.314635	0.189619
b ₈	-39.308002	-25.552015	0.010995	-0.026140
b ₉	4.193141	0.968525	0.002593	-0.006462
b ₁₀	-7.788609	-2.352672	0.002202	0.085869
b ₁₁	-20.838055	11.871347	0.022225	-0.239383
b ₁₂	236.523727	-88.255753	-0.433496	-0.196373
b ₁₃	32.650623	11.214881	0.031183	0.093534

Table 4.4
Mixing coefficients (b_i) for fuel physical property predictions.

Property	BP - IBP	BP - 10%	BP - 50%	BP - 90%	BP - End
Function Type	1/X	1/X	1/X	1/X	1/X
m	1.227041	1.128774	1.048720	1.104677	1.114051
B	-40.281322	-26.102655	-12.446733	-30.591337	-36.780582
b_0	0.008039	0.002935	0.001638	-0.001097	-0.000850
b_1	-0.003587	0.005496	0.009649	0.011893	0.010673
b_2	-0.000938	0.000916	-0.000036	0.001863	0.001587
b_3	-0.004793	0.001929	0.003065	0.006681	0.006052
b_4	-0.000011	0.000295	0.000151	0.000365	0.000084
b_5	0.003362	0.003501	0.003133	0.002762	0.002463
b_6	-0.005824	-0.001434	0.000463	0.000716	0.001525
b_7	-0.006302	-0.010744	-0.008263	-0.007695	-0.006045
b_8	-0.000699	0.002195	-0.000695	0.002247	0.001808
b_9	-0.000090	-0.000234	-0.000140	-0.000100	-0.000215
b_{10}	-0.001629	-0.000375	0.000083	0.000468	0.000576
b_{11}	0.000267	-0.002200	-0.001349	-0.000619	-0.000830
b_{12}	0.016833	0.017790	0.006498	0.002879	0.000967
b_{13}	-0.001068	0.000485	-0.001405	-0.001637	-0.000967

Table 4.5
Mixing coefficients (b_i) for fuel physical property predictions.

Property	Pour Point	Flash Point	Cloud Point	Viscosity
Function Type	1/X	X	X	X
m	1.163718	1.967969	1.160160	1.103905
B	2.841140	-59.081909	1.396656	-0.249182
b ₀	0.006004	77.723267	62.696518	9.349231
b ₁	0.041327	-131.375778	-280.605286	-18.815029
b ₂	-0.010335	3.944968	31.564106	-2.726321
b ₃	0.019989	85.070053	-142.456543	-7.971931
b ₄	0.003983	-19.824430	-29.133873	-1.444859
b ₅	0.000743	-30.838520	-10.544805	-2.686664
b ₆	0.009625	23.928070	-57.107380	-4.893856
b ₇	-0.025848	71.303154	55.578785	12.896148
b ₈	-0.004391	98.134903	8.884830	2.902785
b ₉	-0.000720	3.222337	5.539066	0.381784
b ₁₀	-0.000908	1.550857	-6.479242	-0.286348
b ₁₁	0.008347	28.180758	-50.705273	-2.177922
b ₁₂	-0.000227	-293.710083	129.058411	-5.685808
b ₁₃	-0.010994	5.497871	73.635612	3.978954

Table 4.6
Mixing coefficients (b_i) for fuel physical property predictions.

Property	Filterability	Ht. Comb	% Arom	Carbon Resid
Function Type	X	X	X	X
m	1.574714	1.164666	1.055420	1.509954
B	-21.814034	-7.131920	-1.360885	-0.452864
b ₀	517.848450	39.948025	9.941298	5.348406
b ₁	-958.528748	3.456096	-42.934433	-4.419346
b ₂	-517.385376	4.031006	4.238798	-4.530634
b ₃	151.743408	1.496271	23.822035	-5.294518
b ₄	133.850601	0.615067	14.603270	-1.422858
b ₅	-489.167603	-1.105226	-10.989076	0.386922
b ₆	4.735073	1.819155	13.827999	0.482771
b ₇	295.034729	1.148136	21.362810	-4.466881
b ₈	-394.079163	-1.257226	42.959312	0.127976
b ₉	3.713158	0.263971	-3.602182	0.169352
b ₁₀	240.419113	-0.108686	15.721320	0.135997
b ₁₁	-930.338135	-2.168218	-9.075648	-4.236497
b ₁₂	-1041.752319	-16.221022	12.355459	-15.711843
b ₁₃	-267.429016	-2.526381	13.840097	2.964007

with the boiling points of the different fuel classes. That is, a JP-8 is generally a lower boiling fraction fuel than a JP-5, which is usually a lower boiling fraction than a DF-2 fuel. In addition, densities of these fuel classes usually follow a similar trend. This trend is confirmed in Figure 4.5a which clearly establishes that the JP-5's exhibit lower densities than the JP-8's, which in turn have lower densities than the DF-2's. The ability to make such distinctions based solely on the predicted density allows prediction of fuel classes (e.g., DF-2, JP-5, or JP-8) on middle distillate fuels of unknown origin.

Perhaps more important than the ability to distinguish fuel classes is the ability of the method presented here to directly determine the influence of each chemical group type on an individual physical property. A comparison between the values for the product of the average molecular structure parameter, fraction carbon parameter, and mixing coefficient, reveals the relative importance of each chemical group type on the property under study. These comparisons between the individual product terms of Equation 4.1 are demonstrated by the bar graphs in Figures 4.3b - 4.19b. These bar graphs consist of fourteen clusters of three bars each, with each three bar cluster representing one b_i term in Equation 4.1. The center bar in each cluster on the chart represents the average of the three term products for each chemical group type over the entire range of fuels used in the prediction. The outermost bars in each cluster represent the minimum and maximum values of the product encountered across all fuels used in the correlation. A typical comparison is illustrated in Figures 4.7b and 4.11b which show the distribution of these three term products in the prediction of the initial and end boiling points for the fuels. From these bar graphs, it is apparent that the initial boiling point for the fuels is relatively insensitive to the chemical composition of the fuel and is instead dominated by the b_0 (i.e., base) value. The end boiling point prediction, however, clearly exhibits a much greater dependence on the chemical structure of the fuel. Not only are the products more important in the end boiling point, but the broad range of product values (as shown by the range between the minimum and maximum bars in each three bar

cluster on the graph) indicate that the end boiling point is much more sensitive to variations in the chemical structures of the fuels. This trend is further established in Figures 4.7a and 4.11a, the correlation plots of predicted vs observed initial boiling point and end boiling point. The initial boiling point graph demonstrates very little distinction between the fuel classes present in the data base. In contrast, the end boiling point graph shows a large distinction between the DF-2 fuels and the JP-5 and JP-8 fuels. This is also consistent with the results for the distribution of products bar graphs. If the bar graph for the distribution of products indicates that the initial boiling point is relatively independent of the chemical structures present in the fuel, then the correlation plot of predicted vs observed initial boiling point should exhibit no distinction between the different fuel classes (i.e., DF-2, JP-5, and JP-8). Likewise, the strong structural dependence of the end boiling point upon chemical structure shown in Figure 4.11b would result in the separation of the fuel classes as seen in Figure 4.11a. Also, note that the end boiling point and 90% boiling point correlations contain a greater error than the initial and 10% boiling points. This is due to the fact that the higher boiling point distributions are more dependent on the larger aromatic ring systems which are present in the fuel. In the current study, only monocyclic and dicyclic aromatic ring parameters were utilized. If Equation 4.1 were expanded to include parameters for larger ring systems, it is likely that the higher boiling point correlations would improve.

One of the most common measurements of the combustion properties of a fuel is the cetane number. Both cetane number and cetane index have been predicted by the methods presented in this work. Based on thirty fuels ranging in cetane number from 38 to 48, we are able to predict the cetane number to within ± 0.85 cetane units. ASTM method D613 cites a repeatability of approximately ± 0.7 cetane units and a reproducibility of approximately ± 2.9 cetane units for direct cetane measurement in a standard reference engine (21). Likewise, for 65 fuels which range in cetane index from 37 to 57, we are able to predict the cetane index to ± 1.10 cetane. By ASTM standards, the cetane index will only correlate to within ± 2.0

cetane of the measured cetane number. Currently, however, the LC-¹H NMR technique is limited to fuels which do not contain a cetane improver. The cetane of a fuel is usually adjusted by the addition of a small amount (less than 1 percent by volume) of a variety of compounds (162,163). These compounds are not normally detected by ¹H NMR, and therefore, their effects cannot be predicted by the methods presented here.

In a manner analogous to that demonstrated for the boiling points, we are able to obtain the influences of the fuel molecular structure on the cetane of the fuel. This is illustrated in Figures 4.3b and 4.4b which depict the distribution of products for cetane number and cetane index. For either cetane number or cetane index, an increase in the chain length of any of the aliphatic or aromatic fractions will increase the cetane while an increase in the branching of the molecules will decrease the cetane. An example of this may be found in the alkane parameters for the fuel. Figures 4.3b and 4.4b reveal that the b_2 (i.e., ${}^3\chi_{CH_2}$) term will increase the cetane number of the fuel mixture whereas the b_1 and b_3 (i.e., ${}^2\chi_{CH}$ and ${}^0\chi_{CH_3}$) terms, which are indicators of molecular branching, both decrease the cetane of the mixture. Likewise, an examination of the terms in the aromatic fractions reveals that the b_7 and b_9 terms, which indicate the chain length of the branching, increase the cetane while the b_4 , b_5 , and b_8 terms, which indicate the number of branches on the aromatic ring, decrease the cetane of the fuel mixture.

Although the correlation coefficient of the heat of combustion is relatively low at only 0.9298, this was anticipated. As noted in Table 4.1, the overall range of the heat of combustion for the fuels in the data base is only 0.50 MJ/kg and, in Table 4.2, the ASTM reproducibility of the heat of combustion measurements is 0.40 MJ/kg. Thus, the distribution of products bar graph in Figure 4.17b indicates that the heat of combustion of the fuels is nearly independent of the chemical structures present in the fuel and is instead dominated by the b_0 value, determined by the multiple regression analysis. However, it is well known that the heat of combustion is indeed dependent on the chemical structure of the molecule

(159). In the data base established for this work, heat of combustion data was not available for the DF-2 fuel samples, thus reducing the range of observed values. The JP-5 and JP-8 fuels are structurally very similar, and moreover, have a very narrow range of heat of combustion values. This limited basis set provides a cursory impression that the heat of combustion of the fuels is independent of the molecular structure of the fuel, as indicated in Figure 4.17a. A larger data set which spans a larger range of fuel classes would very likely exhibit a larger dependence on chemical structure for the determination of heat of combustion.

The above data clearly demonstrates that it is indeed possible to utilize LC-¹H NMR data to predict the physical properties of middle distillate fuels. Table 4.2 is a side-by-side comparison of the standard deviation of the residuals from the LC-¹H NMR prediction of the fuel properties and the quoted errors of the ASTM measurements of these properties (164). From this table, it is clearly evident that the LC-¹H NMR approach is indeed viable for a large range of fuel properties. In many cases, it is possible to predict the physical properties of the fuel by LC-¹H NMR analysis as accurately as by measuring the physical properties by ASTM methods. The LC-¹H NMR analysis also has the added advantage of requiring only 1 - 2 hours total analysis time and 3 - 5 ml of sample. In contrast, measurement of all 17 of these properties by the ASTM methods would require nearly 50 hours of analysis time and approximately 1 - 3 L of the fuel sample.

The correlations developed in this manner have also allowed the development of "second generation" software which takes the correlations derived here and apply them to the analysis of mixtures. These programs are listed in Appendix III. For example, the program FUELCALC.BAS allows the operator to ask "what-if" questions. This program reads the thirteen chemical structural parameters and three fraction of carbon parameters from a file from the files written by the NMR software described in Chapter 1, and allows the operator to selectively manipulate the individual parameters. After any parameter is altered, the

physical properties for new set of parameters are quickly and automatically calculated. The second fuel program listed in Appendix III is FUELMIX.BAS. This program will calculate the physical properties of a mixture of two fuels. The structural parameters for each fuel are read from the LC-NMR files, and the operator is able to selectively mix the fuels on a volume percent basis. After any change is made to the percent composition of either fuel or any structural parameter is changed, the new physical properties for the mixture are automatically calculated. In this manner, the physical properties of fuel blends may be calculated before the fuels are ever mixed. Of course, both of these programs will not operate correctly if the parameters of the fuel are altered in a way to make them not representative of the parameters found in middle distillate fuels. For example, if the program FUELCALC.BAS were used to change the fraction of alkane carbon (i.e., $^{\circ}f_c$) parameter to 1 (i.e., 100%), the resulting theoretical mixture would be outside of the range of the basis set upon which the calculations are based. Although the software will calculate values for the physical properties of such a theoretical mixture, these values would be unverified (and therefore unreliable) given the current basis set of middle distillate fuels.

CONCLUSION

As demonstrated in this chapter, a LC- ^1H NMR approach is indeed a viable alternative to the ASTM methods of fuel property measurement for many middle distillate fuel properties. In particular, this technique is readily amenable in situations where a large number of physical properties of a limited amount of fuel sample are required in a very short period of time. This methodology is particularly adept at the prediction of physical properties which are primarily dependent on intramolecular bonding forces. This is demonstrated in the correlation of such physical properties as the heat of combustion and cetane number. Likewise, the group property approach presented here tends to break down in the calculation of physical properties which are dependent on intermolecular bonding

forces as evidenced by the larger errors in the prediction of the end and 90% boiling points.

The technique presented here is not limited only to the fuel classes used in this study. It could also prove acceptable for the prediction of physical properties of fuels such as coal derived liquids and fuels boiling in the gasoline range. Of course, extension of the predictions to other fuel classes assumes that a sufficient number of these fuels, along with their physical properties, can be added to the current basis set of 109 fuels to accurately represent the chemical structures present in the new fuel classes. In building such a basis set, one has the opportunity to determine the interrelationship between the different fuel properties. For example, the basis set for the fuel property determination allows one to observe the changes in density with changes in the cetane number of the fuels. By plotting the values of one physical property against another physical property for a series of fuels, the relationships between all of the independent physical properties may be explored. This leads directly to the types of physical property correlations as were developed by Kydd (119) whereby one or more physical properties of a fuel may be predicted from the measurement of only one or two other physical properties.

The insight gained by examining the chemical factors which determine each property should also prove invaluable in future studies. With the insight gained from present predictive abilities, it should be possible to not only analyze a fuel to determine the physical properties, but to calculate the chemical structures necessary to give a desired set of physical properties. These techniques could also allow determination of the physical properties of a fuel blend even before the two fuels have been mixed. By simply calculating the structures present in a theoretical mixture of two or more fuel samples, the physical properties of the mixture may then be calculated. Of course, this blending is not limited only to mixing fuel samples. A fuel may be blended with either a feed stock or a pure compound, allowing specific tailoring of the physical properties of the resultant mixture. By utilizing the basis set of fuels developed in this correlation study, it should be possible to build a library of

available mixing feedstocks. Through a process of a simple search through this library, it should be possible to choose the proper feedstock to achieve the desired physical properties of a given blend.

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Appendix I

Introduction

This appendix contains the program listings for the LC-NMR software package. This package consists of four separate programs with the option of adding in fifth program. The first program is NMR with is simply an opening screen and menu. From this opening menu, the following programs may be called:

Program I.1: NMR.BAS This program is designed as a "front end" program for the LC-NMR software. It is the common entry and exit point for the LC-NMR transfer, analysis, and disk read software. It also contains the opening and closing screens for the system.

Program I.2: FX200.BAS This program allows the transfer of NMR data from a JEOL FX series NMR to an IBM Personal Computer via a RS-232 serial connection.

Program I.3: LCNMR.BAS This program is the main program for the analysis of the LC-NMR data. It integrates the NMR spectra, calculates the average structures and physical properties, as well as reads and writes the average structure files.

Program I.4: DISK.BAS Although not complete at this time, this program may be called from the menu contained in the NMR program. When complete, this software should allow an eight inch diskette which has been written by any NMR to be read by an IBM Personal Computer.

Program I.5: NMR This is a program written to run on the TRS-80 Model I. It provides the software support for the interface of the TRS-80 to the JEOL FX-200 NMR spectrometer. It changes the receiver gain on the FX-200 and advances the chromatographic fraction collector.

Additionally, there is another program, LCNMRCFG.BAS which services the configuration file for the LCNMR.BAS program. LCNMRCFG.BAS is called from within

the LCNMR program main menu. Finally, there are three data files which must be either in the default directory or in the path for operation of the LC-NMR software. These data files are FUELPARAM.DAT which contains the constants utilized for the calculation of the physical properties of the fuels, LCNMRCFG.DAT which contains the configuration information (chemical shifts, screen colors, constants, etc.) for the LCNMR program, and CHARACTER.DAT which contains a character set for use in displaying alphanumeric information on graphics (e.g. VGA) screens. This character set is read by both the NMR and LCNMR programs and was originally generated by the program CHARACTER.BAS.

Listing for Program 1.1: NMR.BAS

Program Name: NMR Ver 1.00 Date Written: 07/22/1988
 Author: Allen Carwell Date Modified: 07/22/1988

This is the NMR program. It is designed as a front end to the LC-NMR program. That is, it contains the first menu of the LC-NMR system. From this program, the LC-NMR, FX-200 transfer, and disk read programs may be called. This allows one integrated package through which all programs in the NMR series are accessed.

First must set up the variables.

ON ERROR GOTO ErrorMessage
 COMMON TEMPS

DIM OPTN\$(1), OPTN\$(4)

Next are the options of the menus.
 OPTN\$(1)=1
 VERSNS =Ver 1.00

Next will draw the opening screen.
 AS=INKEY\$
 IF AS=CHRS(27) THEN TEMPS="OFF"
 IF TEMPS<>"OFF" THEN GOSUB DrawOpeningScreen

MainMenu:

This is the section to do the MAIN MENU

OPTN\$(1)="LC-NMR Program"
 OPTN\$(2)="Transfer FX-200 Data"
 OPTN\$(3)="Read 8" Disk"
 OPTN\$(4)="Quit to DOS"

Will draw the screen.
 SCREEN 0 : WIDTH 80
 COLOR 15, 0 : CLS
 COLOR 15, 4

LOCATE 1, 5 : PRINT CHR\$(201),STRING\$(88,205),CHR\$(187) ' top line
 LOCATE 2, 5 : PRINT CHR\$(186),STRING\$(89, 32),CHR\$(186) ' ends
 LOCATE 3, 5 : PRINT CHR\$(200),STRING\$(88,205),CHR\$(188) ' bottom line
 LOCATE 1,31 : PRINT CHR\$(209); ' top junct
 LOCATE 2,31 : PRINT CHR\$(179); ' middle line
 LOCATE 3,31 : PRINT CHR\$(207); ' bottom junct

LOCATE 2,10 : PRINT " NMR "; ' no key
 LOCATE 2,19 : PRINT VERSNS; ' return
 LOCATE 2,35 : PRINT " NMR Data Analysis Package "; ' LC-NMR pgm

Main Menu box

COLOR 10,1
 LOCATE 8,15 : PRINT CHR\$(219);STRING\$(49,186),CHR\$(181); ' top line
 FOR %=9 TO 19
 LOCATE %,15 : PRINT CHR\$(179);TAB(65),CHR\$(179); ' middle
 NEXT %
 LOCATE 20,15 : PRINT CHR\$(192);STRING\$(49,186),CHR\$(217); ' bottom line
 COLOR 10,1
 LOCATE 10,20 : PRINT TIMES; ' transfer
 LOCATE 10,51 : PRINT DATES; ' read disk
 COLOR 15,1
 LOCATE 10,35 : PRINT "NMR MENU"; ' quit
 COLOR 14,1
 FOR %=1 TO 4
 LOCATE (%-1)*2+12,40-(0.5*LEN(OPTN\$(%)))
 COLOR 11,1 : PRINT LEFT\$(OPTN\$(%),1); ' up-down
 COLOR 14,1 : PRINT RIGHT\$(OPTN\$(%),LEN(OPTN\$(%))-1);
 NEXT %

Next are commands.
 COLOR 3,0 ' no key
 LOCATE 24,18 : PRINT " To select the desired function, ' ;
 LOCATE 25,18 : PRINT "Press the highlighted letter or <ENTER> to select";

Next see what to do.
 COLOR 14,0
 LOCATE (OPTN\$(1)-1)*2+12,38-(0.5*LEN(OPTN\$(OPTN\$(1))))
 PRINT " *OPTN\$(OPTN\$(1)):" ;

Startup!
 AS=INKEY\$
 SELECT CASE AS
 CASE =
 COLOR 10, 1
 LOCATE 10,20 : PRINT TIMES;
 CASE CHR\$(13)
 GOTO DoOption1
 CASE "1",7
 OPTN\$(1)=1 : GOTO DoOption1
 CASE "1",7
 OPTN\$(1)=2 : GOTO DoOption1
 CASE "R",7
 OPTN\$(1)=3 : GOTO DoOption1
 CASE "2",7,CHR\$(27)
 OPTN\$(1)=4 : GOTO DoOption1
 CASE CHR\$(0)+CHR\$(72), CHR\$(0)+CHR\$(80)
 LOCATE (OPTN\$(1)-1)*2+12,38-(0.5*LEN(OPTN\$(OPTN\$(1))))
 COLOR 11,1
 PRINT " *LEFT\$(OPTN\$(OPTN\$(1)),1);
 COLOR 14,1
 PRINT RIGHT\$(OPTN\$(OPTN\$(1)),LEN(OPTN\$(OPTN\$(1)))-1) ;
 IF AS=CHR\$(0)+CHR\$(72) THEN DECR OPTN\$(1) ELSE INCR OPTN\$(1)
 IF OPTN\$(1)<1 THEN OPTN\$(1)=4
 IF OPTN\$(1)>4 THEN OPTN\$(1)=1
 COLOR 14,0
 LOCATE (OPTN\$(1)-1)*2+12,38-(0.5*LEN(OPTN\$(OPTN\$(1))))
 PRINT " *OPTN\$(OPTN\$(1)):" ;

```

FOR I%=51 TO 186
  UM%=0.77*I% - 105 : LM%=0.77*I% - 65
  LINE (I%+X,LM%+Y)-(I%+X,UM%+Y),C%,BF
NEXT I%
C%=14
LINE (X-1, Y-55)-(X+1,Y+125),C%,BF
LINE (X-1, Y-66)-(X+1,Y-125),C%,BF
LINE (X-125,Y-1)-(X+122,Y+1),C%,BF
FOR I%=1 TO 2: LINE (X-71+I%,Y-56)-(X+71+I%,Y+56),C%: NEXT I%: Y Axis
OPEN "CHARACTR.DAT" FOR RANDOM AS #1
FIELD #1, 40 AS CHARS
DRAW "S12"
TEMP%=1:CNMR : C2%=11
DRAW "C"+STR$(C2%)
TEMP%=375
FOR I%=1 TO LEN(TEMP%)
  IF ASC(MID$(TEMP%,I,1)) >= 33 AND ASC(MID$(TEMP%,I,1)) <= 122 THEN
    GET #1,ASC(MID$(TEMP%,I,1))
    DRAW "B1"+STR$(TEMP%)+",125 TAO "+CHARS
  END IF
  INCR TEMP%,38
NEXT I%
DRAW "S4"
TEMP%=VERSNS
TEMP%=435 : C2%=10: draw versn
DRAW "C"+STR$(C2%)
FOR I%=1 TO LEN(TEMP%)
  IF ASC(MID$(TEMP%,I,1)) >= 33 AND ASC(MID$(TEMP%,I,1)) <= 122 THEN
    GET #1,ASC(MID$(TEMP%,I,1))
    DRAW "B1"+STR$(TEMP%)+",150 TAO "+CHARS
  END IF
  INCR TEMP%,12
NEXT I%
TEMP%="Developed By:"
TEMP%=360 : C2%=10
DRAW "C"+STR$(C2%)
DRAW "S4"
FOR I%=1 TO LEN(TEMP%)
  IF ASC(MID$(TEMP%,I,1)) >= 33 AND ASC(MID$(TEMP%,I,1)) <= 122 THEN
    GET #1,ASC(MID$(TEMP%,I,1))
    DRAW "B1"+STR$(TEMP%)+",350 TAO "+CHARS
  END IF
  INCR TEMP%,12
NEXT I%
TEMP%="AC Software"
TEMP%=280 : C2%=12
DRAW "C"+STR$(C2%)
DRAW "S8"
FOR I%=1 TO LEN(TEMP%)
  IF ASC(MID$(TEMP%,I,1)) >= 33 AND ASC(MID$(TEMP%,I,1)) <= 122 THEN
    GET #1,ASC(MID$(TEMP%,I,1))
    DRAW "B1"+STR$(TEMP%)+",385 TAO "+CHARS
  END IF
  INCR TEMP%,24
NEXT I%
CLOSE
C%=10 : I%=1
AS=INKEY$
WHILE AS=""
  XX=-SIN(I%*1.7453293E-02)*100+X : YY=0.55*COS(I%*1.7453293E-02)*100+Y

```

```

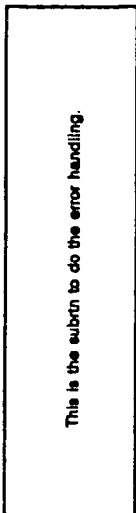
' left-right
' oopel
CASE CHR$(0)+CHR$(75),CHR$(0)+CHR$(77)
CASE ELSE
  SOUND 1000,3 : SOUND 800,1,5
END SELECT
GOTO Startloop
DoOption1:
SELECT CASE OPTN%(1)
CASE 1,2
  COLOR 10, 0
  FOR I%=6 TO 20
    LOCATE I%,1 : PRINT SPACES(79);
  NEXT I%
  LOCATE 21, 30 : PRINT "One moment please...";
  TEMP%="OFF"
  IF OPTN%(1)=1 THEN CHAIN "LCNMR.EXE"
  IF OPTN%(1)=2 THEN CHAIN "FX200.EXE"
  ' IF OPTN%(1)=3 THEN CHAIN "DISK.EXE"
CASE 3
  COLOR 12, 0 : CLS
  LOCATE 11,18 : PRINT "Eight Inch Disk Read Option Not Yet Available";
  LOCATE 12,18 : PRINT "==== Coming soon to a theatre near you! ===";
  COLOR 31, 3
  LOCATE 24,25 : PRINT " Press any key to continue ";
  AS=INPUT$(1)
CASE 4
  CLOSE : COLOR 12,0 : CLS
  GOSUB Logo
  LOCATE 1,1
  PRINT "There is something happening here,"
  PRINT "And what it is ain't exactly clear..."
  AS=INPUT$(1)
END
END SELECT
GOTO MainMenu
DrawingOpeningScreen:
'
'
'
'
' This is the subroutine to draw the opening screen.
'
'
'
'
SCREEN 12 : COLOR 11,0 : WINDOW (0,0)-(770,480)
CLS : X=250 : Y=240
LM%=50 : UM%=430 : C%=12
FOR I%=384 TO 767 STEP 10
  LINE (I%,UM%)-(I%+5,480),C%,BF : LINE (763-I%,UM%)-(758-I%,480),C%,BF
  LINE (I%, 0)-(I%+5,LM%),C%,BF : LINE (763-I%,0)-(758-I%,LM%),C%,BF
  IF I%>717 THEN LM%=240 : UM%=241
NEXT I%
'
' Next is rest of ellipse and plane.
C%=11
CIRCLE (X,Y),100,C%,,0,68
LINE (X-185,Y-56)-(X+50,Y-56),C% : LINE (X+51,Y-56)-(X+186,Y+56),C%
LINE (X+185,Y+56)-(X-50,Y+56),C% : LINE (X-51,Y+56)-(X-186,Y-56),C%
LINE (X-186,Y-56)-(X+50,Y-65),C%,BF

```

```

IF COS(I%) > 1 THEN M = .75 ELSE M = -0.75
LINE (X,Y)-(XX,YY),0 : DELAY 0.052 : LINE (X,Y)-(XX,YY),C%
INCR I%,5 : IF I% > 360 THEN I% = 1
A$ = INKEY$
WEND
RETURN
    
```

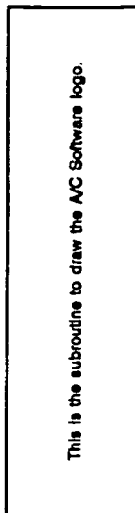
ErrorMessage:



```

SCREEN 0 : COLOR 15,0 : CLS
COLOR 0,4
LOCATE 8,5 : PRINT CHR$(201);STRINGS(80,200);CHR$(187);
FOR I%=9 TO 15
    LOCATE I%,5 : PRINT CHR$(186);TAB(75);CHR$(186);
NEXT I%
LOCATE 16,5 : PRINT CHR$(200);STRINGS(80,200);CHR$(186);
COLOR 31,4
LOCATE 11,26 : PRINT USING ">>> Error ### encountered <<<";ERR;
COLOR 14,4
TEMP$ = "See Appendix E, p. 412, in Turbo Basic Manual for full message."
LOCATE 13,9 : PRINT TEMP$;
COLOR 0,3
LOCATE 24,19 : PRINT " Press any key to return to the NMR Menu ";
TEMP$ = INPUT$(1)
CLOSE
GOTO MainMenu
    
```

Logo:



```

SCREEN 12
COLOR 11,0
WINDOW (-100,-100)-(100,100)
C1=15 : C2=12 : C3=15 : C4=1 : C5=1 : C6=1 : C8=186
    
```

```

* First are boxes
LINE (-41,-43)-(-41,43),C1,B
LINE (-41,-31)-(-41,31),C1
LINE (-41,31)-(-41,31),C1
LINE (-28,-43)-(-28,43),C1
LINE (-28,-43)-(-28,43),C1
PAINT (-38,-40),CHR$(C8)
PAINT (-38,40),CHR$(C8)
PAINT (-38,-40),CHR$(C8)
PAINT (-38,40),CHR$(C8)
    
```

```

* Next are web lines
TEMP=30
FOR I%=27 TO 27 STEP 6
    LINE (-27,TEMP)-(I%,-30),C2
    LINE (I%,-30)-(-27,TEMP),C2
    DECR TEMP,(60/54)*6
NEXT I%

* Next is AC in center.
PI# = 4*ATN(1)
CIRCLE (-13,0),15,C3,,,1,25
CIRCLE (-13,0),22,C3,,,1,25
PAINT ( 0,0),CHR$(8HFF)
LINE (-3.5,-23)-( 1.22),C3,B
LINE (-3.25,-21)-(0.75,21),C4,BF
CIRCLE ( 17,0),15,C3,PI#/4,7*PI#/4,1,25
CIRCLE ( 17,0),22,C3,PI#/4,7*PI#/4,1,25
LINE ( 28.7, 15.5)-(23.5, 10.2)
LINE ( 28.7,-15.5)-(23.5,-10.2)
PAINT (5,0),CHR$(8HFF)

* Next is software labie.
LOCATE 10,31 : PRINT "Software - Software";
LOCATE 21,31 : PRINT "Software - Software";
TEMP$ = "Software"
FOR I%=1 TO LEN(TEMP$)
    LOCATE 11+I%,27 : PRINT MID$(TEMP$,I%,1);
    LOCATE 11+I%,54 : PRINT MID$(TEMP$,I%,1);
NEXT I%
RETURN
    
```

* calc PI
* draws A

* draws C

* outer box
* inner lines

* corner boxes

```
* RAW DATA
* 52=PARAM & REAL
* 50=PARAM & FULL
* RECEIVE MODE
* TRANSMIT MODE
* CONVERSAT MODE
* TRAN MAIN MENU
* PARAM - FULL DATA
* PARAMETER ONLY
* PARAM - REAL DATA
* START TRANSFER
* START HEADING
* END TRANSFER
* TRAN SUCC
* TRAN UNSUC
* ESCAPE TRAN
* CR RETURN
* BLOCK COUNT
```

```
DIM RDATA%(2 56E2)
TODATA%=&H52
```

```
TODATA%="PARAMETERS AND REAL DATA"
```

```
REC%=&H60
TRANS%=&H81
CONVER%=&H62
MENU%=&H1B
PARDATA%=&H50
PARA%=&H51
PARAMDATA%=&H52
START%=&H41
SOH%=&H01
EOT%=&H04
ACK%=&H06
NAK%=&H15
ESC%=&H1B
CR%=&H0D
BL%=&0
```

```
REM **** MAIN PROGRAM ****
```

```
MainProgram:
```

```
GOSUB FindInitialDirectory
```

```
GOSUB 6700
```

```
GOSUB 1000
```

```
K1%=1 : GOSUB 6100
```

```
GOSUB 5100
```

```
GOSUB 3000
```

```
CO%=&CR% : GOSUB 4000 : TIM=0.5 : GOSUB 6000
```

```
CO%=&ESC% : GOSUB 4000 : TIM=0.5 : GOSUB 6000
```

```
CO%=&TRANS% : GOSUB 4000 : TIM=0.5 : GOSUB 6000
```

```
CO%=&TODATA% : GOSUB 4000 : TIM=0.5 : GOSUB 6000
```

```
GOSUB 3000 : C1%=&CO% : GOSUB 6000
```

```
GOSUB 7000
```

```
IF TODATA%<>&H51 THEN GOSUB 7400
```

```
CLOSE
```

```
GOTO 1
```

```
1000 REM **** SETUP PORT
```

```
COM(1) OFF
```

```
PORT%=&1016
```

```
OUT PORT%+3 (128 OR 27)
```

```
OUT PORT%.12 : OUT PORT%+1.0
```

```
REM OUT PORT%.24 : OUT PORT%+1.0
```

```
REM OUT PORT%.48 : OUT PORT%+1.0
```

```
REM OUT PORT%.96 : OUT PORT%+1.0
```

```
OUT PORT%.192 : OUT PORT%+1.1
```

```
RETURN
```

```
1100 REM **** CLEAR PART OF ERRORS AND DATA
```

```
1110 IF (INP(PORT%+5) AND 15)=1 THEN C%=INP(PORT%)
```

```
STATUS%=INP(PORT%+5)
```

```
IF STATUS%=0 OR STATUS%=32 OR STATUS%=&H61 THEN 1110
```

```
IF STATUS%=&H60 THEN RETURN
```

```
BEEP
```

```
INCR CURSOR% : IF CURSOR%>17 THEN GOSUB ClearDisplayArea
```

Listing for Program 1.2: FX200.BAS

```
* Program Name: FX200.BAS Date Written: Fall 1987
* Author: Larry Jackson Date Modified: 07/21/1988
* Modification Author: Allen Caswell
```

```
* This program is written to facilitate the serial transfer of data from a
* JEOL FX-200 NMR to an IBM Personal Computer. The program is menu-driven
* and operates in conjunction with the "conversation" mode on the FX-200.
* The program was originally written by Larry Jackson of the VPI&SU Chem
* Dept Electronics Shop to run under Microsoft's QuickBASIC. It was modified
* by Allen Caswell to run under Borland's TurboBASIC so that it may be
* chained to run with the LG-NMR software, also written in TurboBASIC.
```

```
ON ERROR GOTO ErrorReset
```

```
COMMON TEMP%
```

```
SCREEN ,,2,2
```

```
COLOR 4,0
```

```
CLS
```

```
SCREEN ,,1,1
```

```
COLOR 4,0 : CLS
```

```
LOCATE 1,28 : PRINT CHR$(201);STRING$(24,CHR$(205));CHR$(187);
```

```
LOCATE 2,2 : PRINT CHR$(201);STRING$(25,CHR$(205));CHR$(185);
```

```
LOCATE 2,50 : PRINT CHR$(204);STRING$(25,CHR$(205));CHR$(187);
```

```
LOCATE 3,2 : PRINT CHR$(186);
```

```
LOCATE 3,26 : PRINT CHR$(200);STRING$(24,CHR$(205));CHR$(188);
```

```
LOCATE 3,76 : PRINT CHR$(186);
```

```
FOR I%=4 TO 10
```

```
LOCATE I%,2 : PRINT CHR$(186);TAB(79);CHR$(186);
```

```
NEXT I%
```

```
LOCATE 11,2 : PRINT CHR$(200);STRING$(76,205);CHR$(188);
```

```
LOCATE 22,2 : PRINT CHR$(201);STRING$(76,205);CHR$(187);
```

```
FOR I%=23 TO 24
```

```
LOCATE I%,2 : PRINT CHR$(186);TAB(79);CHR$(186);
```

```
NEXT I%
```

```
LOCATE 25,2 : PRINT CHR$(200);STRING$(76,205);CHR$(188);
```

```
LOCATE 2,26 : PRINT * FX-200 TO IBM TRANSFER *;
```

```
CURSORM%=&12
```

```
ON KEY(1) GOSUB 6600
```

```
ON KEY(2) GOSUB 6800
```

```
ON KEY(3) GOSUB 8300
```

```
ON KEY(4) GOSUB 6950
```

```
ON KEY(5) GOSUB 6500
```

```
ON KEY(6) GOSUB 6200
```

```
ON KEY(7) GOSUB 6400
```

```
KEY(1) ON
```

```
KEY(2) ON
```

```
KEY(3) ON
```

```
KEY(4) ON
```

```
KEY(5) ON
```

```
KEY(6) ON
```

```
KEY(7) ON
```

```
: REM SELECT DISK DRIVE
: REM SELECT DIRECTORY
: REM LIST FILES
: REM DELETE A FILE
: REM TRANSFER DATA TYPE
: REM END TRANSFER
: REM END PROGRAM
```

```
* RAW DATA
```

```
* 52=PARAM & REAL
```

```
* 50=PARAM & FULL
```

```
* RECEIVE MODE
```

```
* TRANSMIT MODE
```

```
* CONVERSAT MODE
```

```
* TRAN MAIN MENU
```

```
* PARAM - FULL DATA
```

```
* PARAMETER ONLY
```

```
* PARAM - REAL DATA
```

```
* START TRANSFER
```

```
* START HEADING
```

```
* END TRANSFER
```

```
* TRAN SUCC
```

```
* TRAN UNSUC
```

```
* ESCAPE TRAN
```

```
* CR RETURN
```

```
* BLOCK COUNT
```

```
* FIND DIR NAME
```

```
* SETUP PORT
```

```
* CLEAR ERRORS
```

```
* PRINT HELP MENU
```

```
* LOOK CONV CH
```

```
* GET NAME, OPEN
```

```
* SENT CR RET
```

```
* ESC:TRAN MENU
```

```
* TRANS OPTION
```

```
* PARAM, DATA
```

```
* OBTAIN PARAM
```

```
* OBTAIN DATA
```

```
* COM1
```

```
* DLAB = 1
```

```
* BAUD = 9600
```

```
* BAUD = 4800
```

```
* BAUD = 2400
```

```
* BAUD = 1200
```

```
* BAUD = 300
```

```
* 8 BITS, EVEN PARITY,
```

```
* 1 END BIT, DLAB = 0
```

```

LOCATE CURSOR%4 : PRINT "ERROR ON CLEARING COM1: UART" : INCR CURSOR%
LOCATE CURSOR%4 : PRINT "  UART STATUS: "HEX$(STATUS%) : INCR CURSOR%
IF (STATUS% AND 1)=1 THEN
  LOCATE CURSOR%4
  PRINT "    CHARACTER: "HEX$(INP(PORT%)): WAS UNEXPECTED "; : INCR CURSOR%
END IF
IF (STATUS% AND 2)=2 THEN
  LOCATE CURSOR%4 : PRINT "    OVERRUN ERROR "; : INCR CURSOR%
END IF
IF (STATUS% AND 4)=4 THEN
  LOCATE CURSOR%4 : PRINT "    PARITY ERROR "; : INCR CURSOR%
END IF
IF (STATUS% AND 8)=8 THEN
  LOCATE CURSOR%4 : PRINT "    FRAMING ERROR "; : INCR CURSOR%
END IF
OUT PORT%:ESC% : TIM=0.5 : GOSUB 8000 : STATUS%=INP(PORT%)
OUT PORT%:MENU%
GOTO ErrorReset

3000 REM ***** ROUTINE TO OBTAIN FILE NAME
3010 L$=CHR$(8+H2)+ENTER FILE NAME: "+CHR$(8+H2)
GOSUB 3100
GOSUB 3200 : F$=L$
RESPONSE
ERR%=0 : GOSUB 3300
IF ERR%=1 THEN GOSUB 3400 : ERR%=0 : GOTO 3010
$HELL "DIR "+F$+" > FDIR ZZZ
INCR CURSOR% : IF CURSOR%>21 THEN GOSUB ClearDisplayArea
LOCATE CURSOR%4 : PRINT
OPEN "FDIR ZZZ" FOR INPUT AS #1
FOR A%=1 TO 4
  LINE INPUT #1,L$
NEXT A%
IF EOF(1) THEN L$="FILE NOT FOUND" ELSE LINE INPUT #1,L$
CLOSE #1
KILL "FDIR ZZZ"
IF L$="FILE NOT FOUND" THEN 3040
3030 L$=CHR$(8+H2)+CHR$(13)+F$+" HAS BEEN USED "+CHR$(13) : GOSUB 3100
L$="DO YOU WISH TO USE IT? (Y/N) "+CHR$(8+H2) : GOSUB 3100
GOSUB 3200 : REM OBTAIN OPERATOR RESPONSE
IF LEFT$(L$,1)="Y" THEN 3010
IF LEFT$(L$,1)<>"Y" THEN 3030
3040 OPEN F$ FOR OUTPUT AS #1
GOSUB 6150
INCR CURSOR% : IF CURSOR%>21 THEN GOSUB ClearDisplayArea
LOCATE CURSOR%4 : PRINT "FILE NAME: "
PRINT #1,F$
RETURN

3100 REM ***** ROUTINE TO SENT A LINE OF TEXT
FOR A1%=1 TO LEN(L$)
  CO%=(ASC(MID$(L$,A1%,1)) : GOSUB 4000 : TIM=0.01 : GOSUB 8000
NEXT A1%
RETURN

3200 REM ***** OBTAIN OPERATOR RESPONSE
L$="" : C%=0
WHILE C%<>8+H0
  GOSUB 5000 : REM OBTAIN A CHARACTER

```

```

IF C%=8 AND LEN(L$)=1 THEN L$="" : GOTO 3210
IF C%=8 AND LEN(L$)=2 THEN L$=LEFT$(L$,LEN(L$)-1) : GOTO 3210
L$=L$+CHR$(C%)
3210 WEND
L$=LEFT$(L$,LEN(L$)-1)
RETURN

```

```

3300 REM ***** CHECK FILE NAME
IF LEN(F$)=0 OR LEN(F$)>12 THEN ERR%=1 : RETURN
FOR A1%=1 TO LEN(F$)
  A$=MID$(F$,A1%,1)
  IF NOT((A$="A" AND A$<="Z") OR (A$="0" OR (A$>"0" AND A$<="9"))) THEN ERR%=1
  NEXT A1%
IF ERR%=1 THEN RETURN ELSE A$=LEFT$(F$,P%-1)
IF LEN(A$)>8 THEN ERR%=1
RETURN

```

```

3400 REM ***** ROUTINE TO PRINT FILE NAME BS
L$="NAMES CANNOT BE MORE THAN 8 CHARACTERS "+CHR$(13) : GOSUB 3100
L$="EXTENSIONS NOT MORE THAN 3 CHARACTERS "+CHR$(13) : GOSUB 3100
L$="NAMES AND EXTENSIONS MUST CONTAIN ONLY "+CHR$(13) : GOSUB 3100
L$=" LETTERS AND NUMBERS "+CHR$(13) : GOSUB 3100
RETURN

```

```

4000 REM ***** TRANSMIT A CHARACTER
STATUS%=INP(PORT%+5)
4010 IF STATUS%=&H80 THEN OUT PORT%,CO% : RETURN
IF STATUS%=0 OR STATUS%=&32 THEN 4010
4020 BEEP

```

```

INCR CURSOR% : IF CURSOR%>17 THEN GOSUB ClearDisplayArea
LOCATE CURSOR%4 : PRINT "COMMUNICATION ERROR" : INCR CURSOR%
LOCATE CURSOR%4 : PRINT "  UART STATUS: "HEX$(STATUS%) : INCR CURSOR%
IF (STATUS% AND 1)=1 THEN
  LOCATE CURSOR%4 : PRINT "CHARACTER: "HEX$(INP(PORT%)): INCR CURSOR%
END IF
IF (STATUS% AND 2)=2 THEN
  LOCATE CURSOR%4 : PRINT "    OVERRUN ERROR "; : INCR CURSOR%
END IF
IF (STATUS% AND 4)=4 THEN
  LOCATE CURSOR%4 : PRINT "    PARITY ERROR "; : INCR CURSOR%
END IF
IF (STATUS% AND 8)=8 THEN
  LOCATE CURSOR%4 : PRINT "    FRAMING ERROR "; : INCR CURSOR%
END IF
OUT PORT%:ESC% : TIM=0.5 : GOSUB 8000 : STATUS%=INP(PORT%)
OUT PORT%:MENU%
GOTO ErrorReset

```

```

5000 REM ***** RECEIVE A CHARACTER
5010 STATUS%=INP(1021) AND 15) : IF STATUS%=1 THEN C%=(INP(1016)) : RETURN
IF STATUS%=0 THEN 5010
5020 BEEP
INCR CURSOR% : IF CURSOR%>17 THEN GOSUB ClearDisplayArea
LOCATE CURSOR%4 : PRINT "COMMUNICATION ERROR" : INCR CURSOR%
LOCATE CURSOR%4 : PRINT "  COM1 STATUS: "HEX$(STATUS%) : INCR CURSOR%
IF 1%=>30000 THEN
  LOCATE CURSOR%4 : PRINT "    RECEIVE TIME OUT ERROR" : INCR CURSOR%
END IF
IF (STATUS% AND 1)=1 THEN

```

```

LOCATE CURSOR%,4 : PRINT *
END IF
IF (STATUS% AND 2)=2 THEN
  LOCATE CURSOR%,4 : PRINT *
END IF
IF (STATUS% AND 4)=4 THEN
  LOCATE CURSOR%,4 : PRINT *
END IF
IF (STATUS% AND 8)=8 THEN
  LOCATE CURSOR%,4 : PRINT *
END IF
LOCATE CURSOR%,4 : PRINT *
OUT PORT%,ESC% : TIM=0.5 : GOSUB 8000 : STATUS%=INP(PORT%)
GOTO ErrorReset

5100 REM **** ROUTINE TO LOOK FOR CONVERSATION CHARACTER
5110 STATUS%=(INP(1021) AND 19) : IF STATUS%=1 THEN C%=(INP(1016) : GOTO 5120
IF STATUS%=0 THEN
  LOCATE CURSOR%,4 : PRINT *
  GOTO 5110
END IF
BEEP
INCR CURSOR% : IF CURSOR%>21 THEN GOSUB ClearDisplayArea
PRINT "COMMUNICATION ERROR - LOOKING FOR CONVERSATION CHARACTER"
LOCATE CURSOR%,4 : PRINT * COM1 STATUS: *HEX$(C%): INCR CURSOR%
IF (STATUS% AND 1)=1 THEN
  LOCATE CURSOR%,4 : PRINT * CHARACTER: *HEX$(INP(PORT%)) : INCR CURSOR%
END IF
IF (STATUS% AND 2)=2 THEN
  LOCATE CURSOR%,4 : PRINT * OVERRRUN ERROR : INCR CURSOR%
END IF
IF (STATUS% AND 4)=4 THEN
  LOCATE CURSOR%,4 : PRINT * PARITY ERROR : INCR CURSOR%
END IF
IF (STATUS% AND 8)=8 THEN
  LOCATE CURSOR%,4 : PRINT * FRAMING ERROR : INCR CURSOR%
END IF
OUT PORT%,ESC% : TIM=0.5 : GOSUB 8000 : STATUS%=INP(PORT%)
OUT PORT%,MENU%
GOTO ErrorReset

5100 REM **** ROUTINE TO DISPLAY HELP MENU
COLOR 14,0
LOCATE 4,25 : PRINT 'F1 KEY ..... SELECT DISK DRIVE
LOCATE 5,25 : PRINT 'F2 KEY ..... SELECT DIRECTORY
LOCATE 6,25 : PRINT 'F3 KEY ..... LIST FILES
LOCATE 7,25 : PRINT 'F4 KEY ..... DELETE A FILE
LOCATE 8,25 : PRINT 'F5 KEY ..... CHANGE TRANSFER DATA TYPE
LOCATE 9,25 : PRINT 'F6 KEY ..... END TRANSFER
LOCATE 10,25 : PRINT 'F7 KEY ..... RETURN TO NMR MENU
COLOR 14,0
LOCATE 23,4 : PRINT 'DRIVE: *DIRECTORY*:STRINGS$(30,* *)
PRINT 'TYPE OF TRANSFER:
COLOR 11,0
GOSUB 6800 : REM PRINT STATUS LINE
KEY(1) ON
KEY(2) ON
KEY(3) ON
KEY(4) ON
KEY(5) ON
RETURN

5150 REM **** ROUTINE TO DISPLAY HELP MENU
COLOR 14,0
LOCATE 4,25 : PRINT 'F1 KEY ..... NOT AVAILABLE
LOCATE 5,25 : PRINT 'F2 KEY ..... NOT AVAILABLE
LOCATE 6,25 : PRINT 'F3 KEY ..... NOT AVAILABLE
LOCATE 7,25 : PRINT 'F4 KEY ..... NOT AVAILABLE
LOCATE 8,25 : PRINT 'F5 KEY ..... NOT AVAILABLE
LOCATE 9,25 : PRINT 'F6 KEY ..... END TRANSFER
LOCATE 10,25 : PRINT 'F7 KEY ..... END PROGRAM
COLOR 11,0
KEY(1) OFF
KEY(2) OFF
KEY(3) OFF
KEY(4) OFF
KEY(5) OFF
RETURN

6100 REM **** ROUTINE TO END TRANSFER
BEEP
L$="TRANSFER ENDED BY OPERATOR"
INCR CURSOR% : IF CURSOR%>21 THEN GOSUB ClearDisplayArea
LOCATE CURSOR%,4 : PRINT L$
PRINT #1,L$
OUT PORT%,ESC% : TIM=0.5 : GOSUB 8000 : STATUS%=INP(PORT%)
OUT PORT%,MENU%
CLOSE
GOTO ErrorReset

6300 REM **** ROUTINE TO LIST FILE NAMES'
SCREEN ,2,2

```

```

LOCATE CURSOR%,4 : PRINT *
CHARACTER: *HEX$(INP(PORT%)) : INCR CURSOR%
END IF
OVERRRUN ERROR : INCR CURSOR%
END IF
PARITY ERROR : INCR CURSOR%
END IF
FRAMING ERROR : INCR CURSOR%
END IF
GOTO 5120

5100 REM **** ROUTINE TO LOOK FOR CONVERSATION CHARACTER
5110 STATUS%=(INP(1021) AND 19) : IF STATUS%=1 THEN C%=(INP(1016) : GOTO 5120
IF STATUS%=0 THEN
  LOCATE CURSOR%,4 : PRINT *
  GOTO 5110
END IF
BEEP
INCR CURSOR% : IF CURSOR%>21 THEN GOSUB ClearDisplayArea
PRINT "COMMUNICATION ERROR - LOOKING FOR CONVERSATION CHARACTER"
LOCATE CURSOR%,4 : PRINT * COM1 STATUS: *HEX$(STATUS%): INCR CURSOR%
IF (STATUS% AND 1)=1 THEN
  LOCATE CURSOR%,4 : PRINT * CHARACTER: *HEX$(INP(PORT%)) : INCR CURSOR%
END IF
IF (STATUS% AND 2)=2 THEN
  LOCATE CURSOR%,4 : PRINT * OVERRRUN ERROR : INCR CURSOR%
END IF
IF (STATUS% AND 4)=4 THEN
  LOCATE CURSOR%,4 : PRINT * PARITY ERROR : INCR CURSOR%
END IF
IF (STATUS% AND 8)=8 THEN
  LOCATE CURSOR%,4 : PRINT * FRAMING ERROR : INCR CURSOR%
END IF
OUT PORT%,ESC% : TIM=0.5 : GOSUB 8000 : STATUS%=INP(PORT%)
OUT PORT%,MENU%
GOTO ErrorReset

5120 IF C%=&H1B THEN 5110
IF C%=&H82 THEN
  INCR CURSOR% : IF CURSOR%>21 THEN GOSUB ClearDisplayArea
  LOCATE CURSOR%,4 : PRINT "CONVERSATION CHARACTER RECEIVED"
  RETURN
END IF
IF C%=&H16 THEN 5110
BEEP
INCR CURSOR% : IF CURSOR%>19 THEN GOSUB ClearDisplayArea
LOCATE CURSOR%,4 : PRINT "COMMUNICATION ERROR - LOOKING FOR CONVERSATION CHARACTER"
LOCATE CURSOR%,4 : PRINT * WAS LOOKING FOR AN: 62 - RECEIVED AN: *HEX$(C%)
OUT PORT%,ESC% : TIM=0.5 : GOSUB 8000 : STATUS%=INP(PORT%)
OUT PORT%,MENU%
GOTO ErrorReset

8000 REM **** ROUTINE COMPARE TWO CHARACTERS

```



```

COLOR 12,0
LOCATE 1,1
CLS
SHELL "DIR /P"
COLOR 31,3
LOCATE 1,28 : PRINT " HIT ANY KEY TO CONTINUE " ;
COLOR 11,0
8310 Z$=INKEY$: IF Z$="" THEN 8310
SCREEN ,,1,1
COLOR 11,0
RETURN

8400 REM ***** ROUTINE TO END PROGRAM
BEEP
INCR CURSOR% : IF CURSOR%>20 THEN GOSUB ClearDisplayArea
LOCATE CURSOR%,4 : PRINT "TRANSFER ENDED"
COLOR 31,3
Startloop1:
LOCATE CURSOR%,4 : PRINT " Exit to NMR Menu? (Y/N) " ;
AS=INKEY$
SELECT CASE AS
CASE " "
CASE "Y"
GOSUB ClearDisplayArea
COLOR 10,0
LOCATE 14,31 : PRINT "One moment please...";
OUT PORT%ESC% : TIM=0.5 : GOSUB 8000 : STATUS%=INP(PORT%)
OUT PORT%,MENU%
.
. Need to reset to initial dir and disk, then run NMR menu.
SHELL InitialDisk
SHELL "CD +InitialDir$
TEMP%="OFF"
CHAIN "NMR EXE"
CASE "N","n"
COLOR 11,0
LOCATE CURSOR%,4 : PRINT " Exit to NMR Menu? (Y/N) " ;
RETURN
CASE ELSE
BEEP
END SELECT
GOTO Startloop1

8500 REM ***** ROUTINE TO CHANGE TYPE OF DATA TRANSFER
IF TODATA%=&H50 THEN
TODATA%=&H51 : TODATA$="PARAMETERS ONLY"
ELSEIF TODATA%=&H51 THEN
TODATA%=&H52 : TODATA$="PARAMETERS & REAL DATA"
ELSEIF TODATA%=&H52 THEN
TODATA%=&H50 : TODATA$="PARAMETERS & FULL DATA"
ELSE
INCR CURSOR% : IF CURSOR%>21 THEN GOSUB ClearDisplayArea
LOCATE CURSOR%,4 : PRINT "PROGRAM ERROR" : GOTO ErrorReset
END IF
GOSUB 8000
RETURN

8600 REM ***** ROUTINE TO SELECT A DIRECTORY
GOSUB 8000
INCR CURSOR% : IF CURSOR%>21 THEN GOSUB ClearDisplayArea
LOCATE CURSOR%,4 : LINE INPUT "ENTER DIRECTORY: "AS
SHELL "CD "+AS
GOSUB 8700 : REM FIND OUT CURRENT DIRECTORY
GOSUB 6800 : REM PRINT STATUS LINE
INCR CURSOR% : IF CURSOR%>21 THEN GOSUB ClearDisplayArea
RETURN

8700 REM ***** ROUTINE TO FIND OUT CURRENT DIRECTORY NAME
SHELL "DIR > BS TXT"
OPEN "BS TXT" FOR INPUT AS #1
FOR A1%=1 TO 3
IF EOF(1) THEN
INCR CURSOR% : IF CURSOR%>21 THEN GOSUB ClearDisplayArea
LOCATE CURSOR%,4 : PRINT "PROGRAM ERROR" : GOTO ErrorReset
END IF
LINE INPUT #1,L$
NEXT A1%
CLOSE #1 : KILL "BS TXT"
DSK$=MID$(L$,18,2)
DSK$=DSK$+STRING$(7-LEN(DSK$)," ")
DIR$=MID$(L$,18,LEN(L$))
DIR$=DIR$+STRING$(40-LEN(DIR$)," ")
RETURN

8800 REM ***** ROUTINE TO PRINT STATUS LINE
LOCATE 24,4 : PRINT STRING$(72," ");
LOCATE 24,4 : PRINT DSK$,DIR$,TODATA$;
RETURN

8850 REM ***** ROUTINE TO SELECT DISK DRIVE
GOSUB 8000
INCR CURSOR% : IF CURSOR%>21 THEN GOSUB ClearDisplayArea
LOCATE CURSOR%,4 : LINE INPUT "ENTER DRIVE LETTER: "AS
SHELL AS+**
GOSUB 8700 : REM FIND OUT CURRENT DIRECTORY
GOSUB 6800 : REM PRINT STATUS LINE
INCR CURSOR% : IF CURSOR%>21 THEN GOSUB ClearDisplayArea
RETURN

8900 REM ***** ROUTINE TO DELETE A FILE
GOSUB 8000 : REM CLEAR KEYBOARD
INCR CURSOR% : IF CURSOR%>21 THEN GOSUB ClearDisplayArea
LOCATE CURSOR%,4 : LINE INPUT "ENTER FILE TO BE ERASED: "F$
IF F$="" THEN
INCR CURSOR% : IF CURSOR%>21 THEN GOSUB ClearDisplayArea
RETURN
END IF
ER%="0" : GOSUB 3300 : REM CHECK FILE NAME
IF ER%="0" THEN
SHELL "ERASE "+F$
INCR CURSOR% : IF CURSOR%>21 THEN GOSUB ClearDisplayArea
RETURN
ELSE
BEEP
INCR CURSOR% : IF CURSOR%>18 THEN GOSUB ClearDisplayArea
LOCATE CURSOR%,4
PRINT "NAMES CANNOT BE MORE THAN 8 CHARACTERS" : INCR CURSOR%
LOCATE CURSOR%,4
PRINT "EXTENSIONS CANNOT BE > 3 CHARACTERS" : INCR CURSOR%
LOCATE CURSOR%,4

```

```

PRINT 'NAMES AND EXTENSIONS MUST CONTAIN ' ; INCR CURSOR%
PRINT 'ONLY LETTERS AND NUMBERS.'
END IF
GOTO 6890

7000 REM **** ROUTINE TO OBTAIN PARAMETERS
BL%=0
CO%=START% ; GOSUB 4000
GOSUB 5000 ; CH=CO% ; GOSUB 6000
IF BC%=SOH% THEN
GOSUB 7100
GOSUB 7500
GOSUB 7300
CO%=ACK% ; GOSUB 4000
GOTO 7010
ELSEIF BC%=EOT% AND TODATA%=&H51 THEN
BEEP
LS=TRANSFER SUCCESSFUL'
PRINT #1,LS
INCR CURSOR% ; IF CURSOR%>21 THEN GOSUB ClearDisplayArea
COLOR 12,0 ; LOCATE CURSOR%,4 ; PRINT LS ; COLOR 11,0
CO%=ACK% ; GOSUB 4000 ; TIM=0.1 ; GOSUB 6000
CO%=ESC% ; GOSUB 4000 ; TIM=0.5 ; GOSUB 6000
GOSUB 5000 ; CH=CO% ; GOSUB 6000
CO%=MENU% ; GOSUB 4000 ; TIM=0.5 ; GOSUB 6000
INCR CURSOR% ; IF CURSOR%>21 THEN GOSUB ClearDisplayArea
RETURN
ELSEIF BC%=EOT% THEN
RETURN
ELSE
LS=TRANSFER UNSUCCESSFUL - BLOCK CODE: *+HEX$(BC%)
IF BC%=ESC% THEN LS=LS+' - TRANSFER TERMINATED BY FX:200'
BEEP
INCR CURSOR% ; IF CURSOR%>21 THEN GOSUB ClearDisplayArea
LOCATE CURSOR%,4 ; PRINT LS
OUT PORT%,ACK% ; TIM=0.1 ; GOSUB 6000
OUT PORT%,ESC% ; TIM=0.5 ; GOSUB 6000
OUT PORT%,MENU% ; TIM=0.5 ; GOSUB 6000
GOTO ErrorReset
END IF
BEEP
INCR CURSOR% ; IF CURSOR%>21 THEN GOSUB ClearDisplayArea
LOCATE CURSOR%,4 ; PRINT 'PROGRAM ERROR'
GOTO ErrorReset

7100 REM **** ROUTINE TO RECEIVE ONE BLOCK
BL%=BL%+1
REM * OBTAIN BLOCK CODE
T%=0
7104 STATUS%=(INP(1021) AND 15)
IF STATUS%=1 THEN BC%=INP(1016) ; GOTO 7108
T%=T%+1 ; IF STATUS%=0 AND T%<30000 THEN 7104 ELSE 5020
BEEP
INCR CURSOR% ; IF CURSOR%>21 THEN GOSUB ClearDisplayArea
LOCATE CURSOR%,4 ; PRINT 'PROGRAM ERROR' ; GOTO ErrorReset

7108 REM * CHECK BLOCK CODE
IF BC%=EOT% OR BC%=ESC% THEN RETURN

7110 REM * OBTAIN BLOCK SIZE
T%=0
STATUS%=(INP(1021) AND 15)
IF STATUS%=1 THEN BS%=(INP(1016))^2 ; GOTO 7120
T%=T%+1 ; IF STATUS%=0 AND T%<30000 THEN 7114 ELSE 5020
BEEP
INCR CURSOR% ; IF CURSOR%>21 THEN GOSUB ClearDisplayArea
LOCATE CURSOR%,4 ; PRINT 'PROGRAM ERROR' ; GOTO ErrorReset

7120 REM * OBTAIN STARTING ADDRESS
T%=0
STATUS%=(INP(1021) AND 15)
IF STATUS%=1 THEN SA%=(INP(1016)) ; GOTO 7126
T%=T%+1 ; IF STATUS%=0 AND T%<30000 THEN 7124 ELSE 5020
BEEP
INCR CURSOR% ; IF CURSOR%>21 THEN GOSUB ClearDisplayArea
LOCATE CURSOR%,4 ; PRINT 'PROGRAM ERROR' ; GOTO ErrorReset

7126 STATUS%=(INP(1021) AND 15) IF STATUS%=1 THEN SA0%=(INP(1016)) GOTO 7130
T%=T%+1 ; IF STATUS%=0 AND T%<30000 THEN 7128 ELSE 5020
BEEP
INCR CURSOR% ; IF CURSOR%>21 THEN GOSUB ClearDisplayArea
LOCATE CURSOR%,4 ; PRINT 'PROGRAM ERROR' ; GOTO ErrorReset

7130 REM * OBTAIN DATA
FOR A1%=1 TO BS%
T%=0
STATUS%=(INP(1021) AND 15)
IF STATUS%=1 THEN RDATA%(A1%)=(INP(1016)) ; GOTO 7138
T%=T%+1 ; IF STATUS%=0 AND T%<30000 THEN 7134 ELSE 5020
BEEP
INCR CURSOR% ; IF CURSOR%>21 THEN GOSUB ClearDisplayArea
LOCATE CURSOR%,4 ; PRINT 'PROGRAM ERROR' ; GOTO ErrorReset

7138 NEXT A1%

7140 REM * OBTAIN CHECK SUM
T%=0
7144 STATUS%=(INP(1021) AND 15)
IF STATUS%=1 THEN CS1%=(INP(1016)) ; GOTO 7148
T%=T%+1 ; IF STATUS%=0 AND T%<30000 THEN 7144 ELSE 5020
BEEP
INCR CURSOR% ; IF CURSOR%>21 THEN GOSUB ClearDisplayArea
LOCATE CURSOR%,4 ; PRINT 'PROGRAM ERROR' ; GOTO ErrorReset

7148 STATUS%=(INP(1021) AND 15)
IF STATUS%=1 THEN CS0%=(INP(1016)) ; GOTO 7150
T%=T%+1 ; IF STATUS%=0 AND T%<30000 THEN 7148 ELSE 5020
BEEP
INCR CURSOR% ; IF CURSOR%>21 THEN GOSUB ClearDisplayArea
LOCATE CURSOR%,4 ; PRINT 'PROGRAM ERROR' ; GOTO ErrorReset

7150 RETURN

7200 REM **** ROUTINE TO SAVE DATA
CS=0
N%=BL% ; GOSUB 8200 ; BL%=NS
N%=CS1% ; GOSUB 8200 ; CS1%=NS
N%=CS0% ; GOSUB 8200 ; CS0%=NS
INCR CURSOR% ; IF CURSOR%>21 THEN GOSUB ClearDisplayArea
LOCATE CURSOR%,4 ; PRINT 'DATA - BLOCK: 'BL$
FOR A1%=1 TO BS% STEP 2
CS=CS+RDATA%(A1%)+RDATA%(A1%+1)

```

```

7500 REM ***** ROUTINE TO SAVE PARAMETERS
CS=0
N%=BL% : GOSUB 8200 : BL%=N$
N%=CS1% : GOSUB 8200 : CS1=N$
N%=CS0% : GOSUB 8200 : CS0=N$
INCR CURSOR% : IF CURSOR%>21 THEN GOSUB ClearDisplayArea
LOCATE CURSOR%,4 : PRINT "PARAMETER - BLOCK: ",BL$
FOR A1%=1 TO BS% STEP 2
  CS=CS+RDATA%(A1%)+RDATA%(A1%+1)
NEXT A1%
IF BL%=1 THEN
  A1%=1 : GOSUB 7560 : PRINT #1,"SIZE OF DATA: "
  PRINT #1,D#
  A1%=5 : GOSUB 7560 : PRINT #1,"SPECTRAL WIDTH: "
  PRINT #1,D#
  A1%=9 : GOSUB 7560 : PRINT #1,"SCANS COMPLETED: "
  PRINT #1,D#
  A1%=17 : GOSUB 7560 : PRINT #1,"FILTER WIDTH: "
  PRINT #1,D#
  A1%=23 : GOSUB 7550 : PRINT #1,"SPECT FREQ: "
  PRINT #1,(D#*10^2)
  A1%=45 : GOSUB 7550
  IF D#>2^12 THEN D#=D#-(2^12) : GOTO 7510
  PRINT #1,"PULSE WIDTH: "
  PRINT #1,(D#*(10^(ASC(LEFT$(DA18,1))-48)/7))
  A1%=99 : GOSUB 7560 : PRINT #1,"SCANS REQUIRED: "
  PRINT #1,D#
  ELSEIF BL%=3 THEN
    L$=""
    FOR A1%=117 TO 124
      L$=L$+CHR$(RDATA%(A1%)-128)
    NEXT A1%
    PRINT #1,"COMMENT: "
    PRINT #1,L$
  END IF
  RETURN
7550 REM * SUB ROUTINE TO OBTAIN DEC NUMBER USING 4 HEX BYES
IF A1%>128 THEN
  INCR CURSOR% : IF CURSOR%>21 THEN GOSUB ClearDisplayArea
  LOCATE CURSOR%,4 : PRINT "PGM ERROR - BLOCK EXCESS 128 - A1%: ",A1%
  GOTO ErrorReset
END IF
D1%=RDATA%(A1%)
D0%=RDATA%(A1%+1)
N%=D1% : GOSUB 8200 : DA1$=N$
N%=D0% : GOSUB 8200 : DA0$=N$
D#=(D1%*2^8)+D0%
IF D#>2^15 THEN D#=D#-(2^16) : REM IF D=>32768 THEN D=D-65535
RETURN
7560 REM * SUB ROUTINE TO OBTAIN DEC NUMBER USING 8 HEX BYES
IF A1%>128 THEN
  INCR CURSOR% : IF CURSOR%>21 THEN GOSUB ClearDisplayArea
  LOCATE CURSOR%,4 : PRINT "PGM ERROR - BLOCK EXCESS 128 - A1%: ",A1%
  GOTO ErrorReset
END IF
D3%=RDATA%(A1%)
D2%=RDATA%(A1%+1)

```

```

D1%=RDATA%(A1%)
D0%=RDATA%(A1%+1)
N%=D1% : GOSUB 8200 : DA1$=N$
N%=D0% : GOSUB 8200 : DA0$=N$
GOSUB 7550
PRINT #1,D#
NEXT A1%
RETURN
7000 REM ***** ROUTINE TO CHECK CHECK SUM
CS=CS+SA1%+SA0%
7310 IF CS>65535 THEN CS=CS-65536 : GOTO 7310
IF CS=((CS1%*256)+CS0%) THEN RETURN
BEEP
L$="CHECK SUM ERROR - RECEIVE CK SUM: "+CS18+CS0$+" - CALCULATED: "+HEX$(CS)
INCR CURSOR% : IF CURSOR%>21 THEN GOSUB ClearDisplayArea
LOCATE CURSOR%,4 : PRINT L$
PRINT #1,L$
OUT PORT%,ACK% : TIM=0.1 : GOSUB 8000
OUT PORT%,ESC% : TIM=0.5 : GOSUB 8000
OUT PORT%,MENU% : TIM=0.5 : GOSUB 8000
GOTO ErrorReset
7400 REM ***** ROUTINE TO OBTAIN DATA
BL%=0
IF TODATA%=8160 THEN PRINT #1,"FULL DATA" ELSE PRINT #1,"HALF DATA"
: REM RECEIVE 1 BLOCK DATA
: REM SAVE DATA
: REM CHECK CHECK SUM
GOSUB 7100
IF BC%<SOH% THEN
  GOSUB 7200
  GOSUB 7300
  GOTO 7410
ELSEIF BC%<EOT% THEN
  BEEP
  L$="TRANSFER SUCCESSFUL"
  PRINT #1,L$
  INCR CURSOR% : IF CURSOR%>21 THEN GOSUB ClearDisplayArea
  COLOR 12,0 : LOCATE CURSOR%,4 : PRINT L$ : COLOR 11,0
  CO%<ACK% : GOSUB 4000 : TIM=0.1 : GOSUB 8000
  CO%<ESC% : GOSUB 4000 : TIM=0.5 : GOSUB 8000
  GOSUB 5000 : C%=CO% : GOSUB 6000
  CO%<MENU% : GOSUB 4000 : TIM=0.5 : GOSUB 8000
  INCR CURSOR% : IF CURSOR%>21 THEN GOSUB ClearDisplayArea
  COLOR 12,0 : LOCATE CURSOR%,4 : PRINT L$ : COLOR 11,0
  RETURN
ELSE
  L$="TRANSFER UNSUCCESSFUL - BLOCK CODE: "+HEX$(BC%)
  IF BC%<ESC% THEN L$=L$+" - TRANSFER TERMINATED BY FX:200"
  BEEP
  PRINT #1,L$
  INCR CURSOR% : IF CURSOR%>21 THEN GOSUB ClearDisplayArea
  LOCATE CURSOR%,4 : PRINT L$
  OUT PORT%,ACK% : TIM=0.1 : GOSUB 8000
  OUT PORT%,ESC% : TIM=0.5 : GOSUB 8000
  OUT PORT%,MENU% : TIM=0.5 : GOSUB 8000
  GOTO ErrorReset
END IF
BEEP
INCR CURSOR% : IF CURSOR%>21 THEN GOSUB ClearDisplayArea
LOCATE CURSOR%,4 : PRINT "PROGRAM ERROR" : GOTO ErrorReset

```

Listing for Program I.3: LCNMR.BAS

Program Name: LCNMR Ver 3.31 Date Written: 08/18/1988
 Author: Allen Caswell Date Modified: 07/22/1988

This is it - the LC-NMR program. This program was written to analyze the data from the LC-NMR experiments. The seven LC-NMR files are stored and read by this program. It takes the files, integrates them, and calculates the average structures. It also does the physical property calculations whenever possible. The data that the program calculates is stored in a sequential file with order contained in the file LCNMRDOC.BAS. This is version 3.0X - it was written for the PS/2 in Boreland's Turbo BASIC. In order for the program to run, there must be two files in the default directory. These are CHARACTER.DAT and LCNMRCFG.DAT. The first contains the character set which is used in drawing the file name and file type on the screen with each spectrum. The second is the configuration file for the program. This file is serviced by the program LCNMRCFG.BAS which is called as a chain file from MainMenu option number one.

Please note: as of 7/22/88, this program is called through the NMR system menu. Although this program is chained to that menu, it may still be called individually at the C:> by typing LCNMR. The NMR menu is called by typing NMR at the C:> menu.

First must set up the variables and read the config file.

```

D1%=RDATA%A1%+2
D0%=RDATA%A1%+3
N%=D3% : GOSUB 8200 : DA3$=N$
N%=D2% : GOSUB 8200 : DA2$=N$
N%=D1% : GOSUB 8200 : DA1$=N$
N%=D0% : GOSUB 8200 : DA0$=N$
D#=(D3%*2^24)+(D2%*2^16)+(D1%*2^8)+D0%
IF D#>2^31 THEN D#=D#*2^32
RETURN

9000 REM ***** ROUTINE FOR TIME DELAY
Z11=TIMER+TIM
8020 Z21=TIMER : IF Z21<Z11 THEN 8020 ELSE RETURN

9000 REM **** ROUTINE TO CONVERT DEC TO HEX
N$=HEX(N%)
8210 IF LEN(N$)<2 THEN N$="0"+N$ : GOTO 8210
RETURN

9000 REM **** ROUTINE TO CLEAR KEYBOARD BUFFER
9010 A$=INKEY$: IF A$="" THEN RETURN ELSE 9010

ClearDisplayArea:
. This is a subroutine to clear the display area.
COLOR 11,0
FOR I%=12 TO 21
LOCATE I%,1 : PRINT SPACES(70);
NEXT I%
CURSOR% = 12
RETURN

ErrorReset:
. This is a subroutine to reset the NMR and PS/2 after an error.
OUT PORT%,ESC% : TIM=0:5 : GOSUB 8000 : STATUS%=INP(PORT%)
OUT PORT%,MENU%
CLOSE
GOTO MainProgram

FindInitialDirectory:
. This is a subroutine to find the initial directory.
SHELL "DIR > BS.TXT"
OPEN "BS.TXT" FOR INPUT AS #1
FOR A1%=1 TO 3
IF EOF(1) THEN
INCR CURSOR% : IF CURSOR%>21 THEN GOSUB ClearDisplayArea
LOCATE CURSOR%,4 : PRINT "PROGRAM ERROR" : GOTO ErrorReset
END IF
LINE INPUT #1,I$
NEXT A1%
CLOSE #1 : KILL "BS.TXT"
DSK$=MID$(I$,18,2)
DSK$=DSK$+STRING$(7-LEN(DSK$),")
DIR$=DIR$+STRING$(18-LEN(I$))
InitialDisk$=DSK$
InitialDir$=DIR$
RETURN

```

ON ERROR GOTO ErrorMessage
 COMMON TEMPS

DIM DA(4100), DS(350), INTNAME\$(7,12), PPM(7,13), BASEEND(7,8), FT\$(7,13)
 DIM GAIN(7), CTRL(PTNS\$(8)), FILETYPE\$(7), FUELNAME\$(100), FILETYPE\$(8)
 DIM BEGPT\$(7,8), ENDPT\$(7,8), BEGAVG\$(7,8), ENDAVG\$(7,8), BA(4100)
 DIM ACTIVE\$(2,8), YOFFSET\$(7), SHIFTS\$(7), BASESTEP\$(7), BLANK(350)
 DIM NAMEUSE\$(100), INTXP\$(7), INTNF\$(7), MIXCOEFF(22), T\$(22)

. Next are the options of the menus

```

FOR I%=1 TO 8
OPTN%(I%) = 1
IF I%<=8 THEN ACTIVE%(1,I%) = 1
IF I%<=8 THEN ACTIVE%(2,I%) = 1
NEXT I%
OPTN%(1)=2
PAGE%=1

```

. Next will read the configuration file.
 GOSUB ReadConfigFile

MainMenu:

This is the section to do the MAIN MENU.

```

OPTN$(1)="Change Default Parameters"
OPTN$(2)="Analyze Fuel Data"
OPTN$(3)="Recalculate Fuel Data"
OPTN$(4)="Stack Plot Fuel Data"
OPTN$(5)="Work Up Blank Data"
OPTN$(6)="Print Fuel Reports"
OPTN$(7)="Edit Fuel Integrations"
OPTN$(8)="Quit to NMR Menu"

* Will draw the screen.
SCREEN 0 : WIDTH 80
COLOR 15, 0 : CLS
COLOR 15, 4
LOCATE 1, 5 : PRINT CHR$(201);STRING$(80,205);CHR$(187)
LOCATE 2, 5 : PRINT CHR$(186);STRING$(80, 32);CHR$(186)
LOCATE 3, 5 : PRINT CHR$(200);STRING$(80,205);CHR$(188)
LOCATE 1,31 : PRINT CHR$(208);
LOCATE 2,31 : PRINT CHR$(179);
LOCATE 3,31 : PRINT CHR$(207);
LOCATE 2,10 : PRINT "LC-NMR"
LOCATE 2,19 : PRINT VERS
LOCATE 2,35 : PRINT " LC-NMR Data Analysis Software ";

* Main Menu box.
COLOR 10,1
LOCATE 5,15 : PRINT CHR$(218);STRING$(49,188);CHR$(191);
FOR I%=6 TO 22
    LOCATE I%,15 : PRINT CHR$(179);TAB(95);CHR$(179);
NEXT I%
LOCATE 23,15 : PRINT CHR$(192);STRING$(49,188);CHR$(217);
COLOR 10,1
LOCATE 6,20 : PRINT TIMES;
LOCATE 6,51 : PRINT DATES;
COLOR 15,1
LOCATE 6,35 : PRINT "MAIN MENU";
COLOR 14,1
FOR I%=1 TO 8
    LOCATE (I%-1)*2+8,40:(0.5*LEN(OPTN$(I%)))
    COLOR 11,1 : PRINT LEFT$(OPTN$(I%),1);
    COLOR 14,1 : PRINT RIGHT$(OPTN$(I%),LEN(OPTN$(I%))-1);
NEXT I%

* Next are commands.
COLOR 3,0
LOCATE 25,18 : PRINT "Press the highlighted letter or <ENTER> to select.";
* Next see what to do.
COLOR 14,0
LOCATE (OPTN$(1)-1)*2+8,38:(0.5*LEN(OPTN$(OPTN$(1))))
PRINT " *",OPTN$(OPTN$(1)),";
* no key
* return
* change
* analyze
* recalc
* stack plot
* work up blk
* print
* edit
* quit
* up-down
* left-right
* oops!
* ChangeDefaultParams

```

```

Startloop1:
AS=INKEY$
SELECT CASE AS
CASE =
    COLOR 10,1
    LOCATE 8,20 : PRINT TIMES;
    CASE CHR$(13)
    GOTO DoOption1
CASE "C,"
    OPTN$(1)=1 : GOTO DoOption1
CASE "A,"
    OPTN$(1)=2 : GOTO DoOption1
CASE "R,"
    OPTN$(1)=3 : GOTO DoOption1
CASE "S,"
    OPTN$(1)=4 : GOTO DoOption1
CASE "W,"
    OPTN$(1)=5 : GOTO DoOption1
CASE "P,"
    OPTN$(1)=6 : GOTO DoOption1
CASE "E,"
    OPTN$(1)=7 : GOTO DoOption1
CASE "O,"
    OPTN$(1)=8 : GOTO DoOption1
CASE CHR$(72)
    LOCATE (OPTN$(1)-1)*2+8,38:(0.5*LEN(OPTN$(OPTN$(1))))
    COLOR 11,1
    PRINT " *LEFTS (OPTN$(OPTN$(1)),1);
    COLOR 14,1
    IF AS=CHR$(0)+CHR$(72) THEN DECOR OPTN$(1) ELSE INCR OPTN$(1)
    IF OPTN$(1)<1 THEN OPTN$(1)=8
    IF OPTN$(1)>8 THEN OPTN$(1)=1
    COLOR 14,0
    LOCATE (OPTN$(1)-1)*2+8,38:(0.5*LEN(OPTN$(OPTN$(1))))
    PRINT " *",OPTN$(OPTN$(1)),";
CASE CHR$(0)+CHR$(79);CHR$(0)+CHR$(77)
CASE ELSE
    SOUND 1000,3 : SOUND 800,1.5
END SELECT
GOTO Startloop1
DoOption1:
SELECT CASE OPTN$(1)
CASE 1 : GOTO ChangeDefaultParams
CASE 2 : GOTO AnalyzeFuelData
CASE 3 : GOTO Recalculate
CASE 4 : GOTO StackPlot
CASE 5 : GOTO WorkUpBlank
CASE 6 : GOTO PrintReports
CASE 7 : GOTO EditIntegrations
CASE 8 : TEMPS="OFF" : CHAIN "NMR.EXE"
END SELECT

```

..... This section contains the main menu options.
ChangeDefaultParams

Main menu selection to change the default parameters.

```
CHAIN 'LCNMRCFG.EXE'
```

AnalyzeFuelData:

This is the main menu selection to analyze the NMR data.

```

* Must first get the fuel names to analyze.
GOSUB GetNames
* Next start loop for 100 fuels - do only selected fuels.
FOR L%=1 TO 100
  IF FUELNAME$(L%)<>' ' AND NAMEUSE$(L%)=1 THEN
    FOR I%=1 TO 350 : D$(I%)='': NEXT I%
  First must get the file names for each fuel, background info.
  TEMP1%=10 : TEMP2%=1
  COLOR 15,0 : CLS
  GOSUB DrawFuelName
  GOSUB FileNames
  COLOR 15,0 : CLS
  TEMP1%=10 : TEMP2%=1
  GOSUB DrawFuelName
  GOSUB GetBackgroundInfo
* Must see if need to get blank
  IF D$(143)='BLANK1' OR D$(143)='BLANK2' OR D$(143)='BLANK3' THEN
    COLOR 12,0 : CLS
    LOCATE 12,27 : PRINT 'Getting the data for 'D$(143)
    GOSUB GetBlankData
  END IF
* Next start loop for 7 files, get nmr file, and display it.
  K%=1
  Startloop19:
  IF FILETYPE$(K%)<>' ' THEN
    SCREEN 0 : WIDTH 80 : COLOR 15,0 : CLS
    COLOR 14,3
    LOCATE 10,1 : PRINT CHR$(218);STRING$(78,196);CHR$(191)
    FOR I%=11 TO 14
      LOCATE I%,1 : PRINT CHR$(179);STRING$(78,32);CHR$(179);
    NEXT I%
    LOCATE 15,1 : PRINT CHR$(192);STRING$(78,196);CHR$(217)
    COLOR 0,3
    TEMP%='Reading NMR data for file '+FILENAME$(K%)
    LOCATE 12,40:(0.5*LEN(TEMP%)) : PRINT TEMP%
    PRINT TEMP%
  
```

```

LOCATE 14,28
PRINT 'Treating file as 'FILETYPE$(FILETYPE$(K%));
GOSUB ReadNMRFile
CLS
GOSUB DisplayNMRFile
GOSUB DisplayAxis
* Have got spectrum, so draw boxes and table.
GOSUB DrawAvgStScreens
* Next must integrate spectrum and draw results.
GOSUB CalculateAndDrawShift
GOSUB CalculateAndDrawBase
GOSUB CalculateIntegrals
GOSUB CalculateAverageStructures
GOSUB DrawAvgStData
IF INTEGRALS='ON' THEN
  TEMP%='ON' : GOSUB DrawIntegralRegions
END IF
* Have done everything so see if change anything
TEMP%='ON' : GOSUB MarkActiveShift
TEMP%='ON' : GOSUB MarkActiveBase
GOSUB SpectraEditMenu
ELSE
  GOSUB WipeOutRecalcData
END IF
INCR K%
IF K%<=7 THEN GOTO Startloop19
* Have got NMR files finished, so calc and display summary.
GOSUB CalculateSummaryData
GOSUB PrintSummaryScreen
GOSUB DoControlOptions
END IF
NEXT L%
GOTO MainMenu
* outta here

Recalculate:
* This is the main menu selection to recalculate the data.
* Must first get the fuel names to analyze.
GOSUB GetNames
* Next start loop for 50 fuels - do only non null fuels.
FOR L%=1 TO 100
  IF FUELNAME$(L%)<' ' AND NAMEUSE$(L%)=1 THEN
    FOR I%=1 TO 350 : D$(I%)='': NEXT I%
  First must get the file names for each fuel, background info
  COLOR 12,0 : CLS
  TEMP%='Getting data for file '+INPUTDIR$+FUELNAME$(L%)+'.DAT'
  LOCATE 12,40:(0.5*LEN(TEMP%)) : PRINT TEMP%
  
```

```

GOSUB GetAvgStrData
TEMP1%=10 : TEMP2%=1
COLOR 15,0 : CLS
GOSUB DrawFuelName
GOSUB FileNamees
    . Next start loop for 7 files, get nmr file, and display it.
FOR K%=1 TO 7
    IF FILETYPE%(K%) < >6 THEN
        SCREEN 12
        COLOR DATA COL%,BACK COL% : CLS
    . Must integrate spectrum and draw results.
    NOSC%=VAL(D$(261+FILETYPE%(K%)))
    GOSUB DrawAvgStrScreens
    GOSUB CalculateAverageStructures
    GOSUB DrawAvgStrData
    . Have done everything so see if continue.
    LOCATE 25,5
    PRINT "Press <RETURN> to continue to next fraction, ";
    PRINT " <O> to exit to Main Menu. ";
    Startloop11:
    AS=INPUT$(1)
    SELECT CASE AS
        CASE "q","Q","CHR$(27)
            GOTO MainMenu
        CASE CHR$(13)
            GOTO Continue11
        CASE ELSE
            SOUND 1000,3 : SOUND 800,1.5
    END SELECT
    GOTO Startloop11
    Continue11:
    ELSE
        GOSUB WipeOutRecalcData
    END IF
    NEXT K%
    . Have got NMR files finished, so calc and display summary.
    GOSUB CalculateSummaryData
    GOSUB PrintSummaryScreen
    GOSUB DoControlOptions
    END IF
NEXT L%
GOTO MainMenu
StackPlot:
    .
    .
    .
    .
    . This is the main menu option to do the stack plots.
    .
    .
    .
    .
    .
    .
    .
    .
    .
    .
    . Have done everything so see if change anything.
    TEMPS="ON" : GOSUB DrawIntegrRegions
    TEMPS="ON" : GOSUB MarkActiveShift
    TEMPS="ON" : GOSUB MarkActiveBase
    GOSUB SpectraEditMode
    NEXT K%

```

```

AS=INPUT$(1)
GOTO MainMenu
WorkUpBlank:
    .
    .
    . This is the main menu option to work up the blank data.
    .
    .
    .
    .
    .
    . First must get the blank name.
    GOSUB GetBlankName
    . Have got names so get data and edit it.
    L%=1
    SELECT CASE OPTM%(7)
        CASE 1 : FUELNAME$(L%)="BLANK1"
        CASE 2 : FUELNAME$(L%)="BLANK2"
        CASE 3 : FUELNAME$(L%)="BLANK3"
    END SELECT
    . Next start loop for 7 files, get nmr file, and display it.
    COLOR 15,0 : CLS
    TEMP1%=10 : TEMP2%=1
    GOSUB DrawFuelName
    TEMPS=INPUTDIRS : INPUTDIRS=BLANKDIRS
    GOSUB GetBackgroundInfo
    INPUTDIRS=TEMPS
    FOR I%=1 TO 350 : DS(I%)=" " : NEXT I%
    FOR K%=1 TO 5
        FILETYPE%(K%)=K%
        FILENAME$(K%)=BLANKDIRS+FUELNAME$(L%)+".T01"
        COLOR 12,0 : CLS
        TEMPS="Reading NMR data for blank "+FILENAME$(K%)
        LOCATE 12,40:(0.5*LEN(TEMPS))
        PRINT TEMPS,
        LOCATE 14,28
        PRINT "Treating file as "+FILETYPE$(FILETYPE%(K%)):
        GOSUB ReadNMRFile
        CLS
        GOSUB DisplayNMRFile
        GOSUB DisplayAxis
        GOSUB DrawAvgStrScreens
        GOSUB CalculateAndDrawShift
        GOSUB CalculateAndDrawBase
        GOSUB CalculateIntegrals
        GOSUB CalculateAverageStructures
        GOSUB DrawAvgStrData
    . Have done everything so see if change anything.
    TEMPS="ON" : GOSUB DrawIntegrRegions
    TEMPS="ON" : GOSUB MarkActiveShift
    TEMPS="ON" : GOSUB MarkActiveBase
    GOSUB SpectraEditMode
    NEXT K%

```

' outta here

' get blank

' outta here

StackPlot:

```

COLOR 12,0 : CLS
LOCATE 11,18 : PRINT *** Stack Plot Option Not Yet Available ***;
LOCATE 12,18 : PRINT * Coming soon to a theatre near you!! * ;

```

```

* Have integrated so divide by number of scans and file.
GOSUB DivideBlankIntegrals      : DS(2)=DATES
DS(1)=FUELNAME$(L%)           : DS(2)=DATE$
DS(205)=" " : DS(210)=" " : DS(222)=" "
DS(234)=" " : DS(249)=" "
GOSUB FileBlankDataMenu
GOTO MainMenu
PrintReports:
* outta here
This is the Main Menu section to print the reports.
*
* First must get the printer type and printer options.
GOSUB PrinterMenu
IF PRINTER%=1 THEN GOSUB PrinterFontMenu
*
* Have got the printer options, so get fuel names.
GOSUB GetNames
*
* Have got all of the preliminaries, so print the stuff.
COLOR 31, 4
LOCATE 11, 1 : PRINT SPACES(80);
LOCATE 11,17 : PRINT *** Printing the highlighted fuel data ***;
FOR L%=1 TO 100
IF L%=1 THEN PAGE%=1 : GOSUB PageOfNames
IF L%=>51 THEN PAGE%=2 : GOSUB PageOfNames
IF FUELNAME$(L%)<>" " AND NAMEUSE$(L%)=1 THEN
COLOR 14,3
TEMP%=INT((L%-(PAGE%-1)*50)/10)
LOCATE (L%-(PAGE%-1)*50)-TEMP%*10+13,TEMP%*15+7
IF NAMEUSE$(L%)=0 THEN
PRINT " " : FUELNAME$(L%); " "
ELSE
PRINT " " : CHR$(16),FUELNAME$(L%); " "
END IF
GOSUB GetAvgStrData
IF CTRL-OPTS(4)="Y" THEN GOSUB HardCopyIntegrals
IF CTRL-OPTS(3)="Y" THEN GOSUB HardCopyResults
IF CTRL-OPTS(6)="Y" THEN GOSUB HardCopyPrope
AS=INKEY$
IF AS="Q" OR AS="q" OR AS="r" OR AS="R" THEN GOTO MainMenu
END IF
NEXT L%
PAGE%=1 : GOSUB PageOfNames
GOTO MainMenu
EditIntegrations:
* outta here
This is the main menu option to edit integrations.
*
* First must get the fuel names and then draw the screen.
GOSUB GetNames
* get names
*
* Have got names so get data and edit it.
FOR L%=1 TO 100
IF FUELNAME$(L%)<>" " AND NAMEUSE$(L%)=1 THEN
FOR I%=1 TO 350 : DS(I%)=" " : NEXT I%
TEMP1%=10 : TEMP2%=1
COLOR 15,0 : CLS
GOSUB DrawFuelName
GOSUB EditIntegrationMenu
IF OPTN%(6)=1 THEN
COLOR 12,0 : CLS
LOCATE 12,28 : PRINT "Getting data for fuel " : FUELNAME$(L%);
GOSUB GetAvgStrData
* read data
ELSE
GOSUB GetBackgroundInfo
* get background
END IF
*
* Have got data so see if change number of scans.
TEMP1%=10 : TEMP2%=1
COLOR 15,0 : CLS
GOSUB DrawFuelName
GOSUB EditNumberOfScans
*
* Have got data so display and edit.
GOSUB DrawIntegrationScreen
TEMP1%=1 : TEMP2%=1
COLOR 12,0
GOSUB HighHighlightIntegral
GOSUB EditDisplayedInt
END IF
Continue:
NEXT L%
GOTO MainMenu
*
***** This section contains the main calculation subroutines *****
*****
CalculateAverageStructures:
*
This is the subroutine to calculate the average structures.
*
SELECT CASE FILETYPE$(K%)
CASE 1
HMDS=VAL(D$(205))
VOL =(MDS%*SCANTIME*FLOWRATE)/CONVERT
KV =(HMDS*CONC*VOL*18)/HMDS
CH3 =VAL(D$(207)) : CH2=VAL(D$(208)) : CH=VAL(D$(209))
* cq=val(d$(20a))
* NF =(CH3 (3*CH))/6
* AVGCCH3=CH3/(NF*3) AVGCCH2=CH2/(NF*2) AVGCCH=CHNF*AVGCQ=COJNF

```



```

* ADB =AVGCH + (2*AVGCO)
* MOLWT=12*AVGCO + 13*AVGCH + 14*AVGCH2 + 15*AVGCH3
NF=(CH3/3) + (CH2/2) + CH + CO
AVGCH3=(CH3/3)/NF : AVGCH2=(CH2/2)/NF : AVGCH=CH/NF : AVGCO=CQ/NF
ADB=0 : MOLWT=0
* Will calculate the physical properties.
* CET=2.58566E07*2.58566E07*AVGCH3-2.58566E07*AVGCH2 : Cetane #
* CET = CET - 2.58566E07*AVGCH - 2.58566E07*AVGCO
* CET = 1.4076022*CET - 32.7687
* DEN=1.688.5001+1898.7285*AVGCH3+1687.3565*AVGCH2 : Density
* DEN = DEN + 1688.0271*AVGCH + 1688.7404*AVGCO
* DEN = 1.0378128*DEN - 2.84012E-02
* QL = 11088 + 757*DEN - 2100*DEN ^ 2
* VCal=QL * DEN
* PRO4=0 : PRO5=0 : PRO6=0 : PRO7=0 : PRO8=0
* Will next calc the absolute # moles for each carbon.
NF =KV * NF
ABSCH3=AVGCH3*NF : ABSCH2=AVGCH2*NF : ABSCH=AVGCH*NF : ABSCO=AVGCO*NF
MOLC=ABSCH3 + ABSCH2 + ABSCH + ABSCO
* Must put the values back into D#
D#(108)=STRS(AVGCH3) : D#(107)=STRS(ABSCH3)
D#(108)=STRS(AVGCH2) : D#(108)=STRS(ABSCH2)
D#(110)=STRS(AVGCH) : D#(111)=STRS(ABSCH)
D#(147)=STRS(AVGCO) : D#(148)=STRS(ABSCO) : D#(262)=STRS(NOSCC%)
D#(112)=STRS(MOLWT) : D#(113)=STRS(ADB) : D#(114)=STRS(MOLC)
D#(157)=STRS(CET) : D#(158)=STRS(QL) : D#(159)=STRS(DEN)
* D#(160)=STRS(MCAL) : D#(161)=STRS(PRO2) : D#(162)=STRS(PRO3)
* D#(163)=STRS(PRO4) : D#(164)=STRS(PRO5)
CASE 2
HMDS =VAL(D#(210)) : GA =VAL(D#(212)) : ACH3 =VAL(D#(213))
ACH2 =VAL(D#(214)) : ATET =VAL(D#(215)) : ACH =VAL(D#(216))
AR1 =VAL(D#(218)) : AR2 =VAL(D#(219)) : AR3 =VAL(D#(220))
AR4 =VAL(D#(221))
VOL =NOSC% * SCANTIME * FLOWRATE) / CONVERT
KV =HMDSOONG * VOL * 18 / HMDS
TAL =GA + ACH3/3 + ACH2/2 + ATET/2 + ACH
TAR =AR1
AROM =TAR / (TAL+TAR)
NF =TAR / 4
NF =(TAR + (TAL-GA))/8
CSUN =TAR / NF
CSSUB=6 * CSUN
CSCH3=(ACH3/3) / NF
CSCH2=(ACH2/2) / NF
CSCH =ACH / 1 / NF
CSJET=(ATET/2) / NF
CSAQ =CSSUB + (CSCH3+CSCH2 + CSCH +CSJET)
NF2 =KV * NF
CUN =CSUN * NF2
CSUB =CSSUB * NF2
CCH3 =CSCH3 * NF2
CCH2 =CSCH2 * NF2
CCH =CSCH * NF2
CJET =CSJET * NF2
CAQ =CSAQ * NF2
* Protons > alpha
* # alpha branches
* *Cch2>a
* *Cch3>a
* *Cch3>a
* Cch2>a
* *Cch3>a
* *Cch3>a
* Avg Deg of Substn
* Fraction Sub Sites
* Molecular Wt
* Tot Mol Aromatic C
* Tot Mol Aliphatic C
* Total Moles Carbon
* Will next calc the physical properties.
* CET = 5.71407 - 10.8485*CSCH3 - 8.13828E-02*CSCH2
* CET = CET - 8.75887*CSCH - 38.3681*CSCO
* CET = CET + 5.32182*CSH3G
* DEN = 1.225058*CET - 3.87011
* DEN = 0.858488 + 8.73778E-03*CSCH3
* DEN = DEN + 4.48875E-03*CSCH2
* DEN = DEN + 3.49110E-03*CSCH
* DEN = DEN + 1.82851E-03*CSCO
* DEN = DEN + 4.18890E-04*CSH3G
* DEN = 1.850632*DEN - 0.740225
* QL = 11088 + 757*DEN - 2100*DEN ^ 2
* VCal=QL * DEN
* PRO5=0 : PRO6=0 : PRO7=0 : PRO8=0
D#( 3)=STRS(CSUN) : D#( 4)=STRS(CUN) : D#( 5)=STRS(CSSUB)
D#( 6)=STRS(CSUB) : D#( 7)=STRS(C) : D#( 8)=STRS(O)
D#( 9)=STRS(CSCH3) : D#( 10)=STRS(CCH3) : D#( 11)=STRS(CSCH2)
D#( 12)=STRS(CCH2) : D#( 13)=STRS(CSCH) : D#( 14)=STRS(CCH)
D#( 15)=STRS(CSCH2G) : D#( 16)=STRS(CCH2G) : D#( 17)=STRS(CSH3G)
D#( 18)=STRS(CCH3G) : D#( 19)=STRS(CSJET) : D#( 20)=STRS(CTET)
D#( 21)=STRS(MW) : D#( 22)=STRS(FSS) : D#( 23)=STRS(ADS)
D#( 24)=STRS(TMAR) : D#( 25)=STRS(MOLC) : D#( 26)=STRS(FRACA)
D#( 27)=STRS(FRACC) : D#(283)=STRS(NOSCC%)
* D#(185)=STRS(CET) : D#(186)=STRS(QL) : D#(187)=STRS(DEN)
* D#(188)=STRS(MCAL) : D#(189)=STRS(PRO5) : D#(170)=STRS(PRO6)
* D#(171)=STRS(PRO7) : D#(172)=STRS(PRO8)
CASE 3,4,5
IF FILETYPE%(K%)=3 THEN T%=0
IF FILETYPE%(K%)=4 THEN T%=12
IF FILETYPE%(K%)=5 THEN T%=24
D#(228+T%)=STRS(O)
HMDS =VAL(D#(222+T%)) : GA =VAL(D#(224+T%)) : ACH3 =VAL(D#(228+T%))
ACH2 =VAL(D#(227+T%)) : ACH =VAL(D#(228+T%)) : AR1 =VAL(D#(230+T%))
AR2 =VAL(D#(231+T%)) : AR3 =VAL(D#(232+T%)) : AR4 =VAL(D#(233+T%))
T%=FILETYPE%(K%)
IF T%=5 THEN TC%=10 ELSE TC%=8
VOL =(NOSC% * SCANTIME * FLOWRATE) / CONVERT
KV =HMDSOONG * VOL * 18 / HMDS
TAL =GA + ACH3/3 + ACH2/2 + ACH
TAR =AR1
AROM =TAR / (TAL+TAR)
NF =TAR / 4
* Gives Total Carbon
* Volume of peak
* Ref response factor
* Total aliphatic C
* Total aromatic C
* Aromaticity
* Normalization factor
* Di -> Phenan
* set Ach = 0
ACH3 =VAL(D#(228+T%))
ACH2 =VAL(D#(227+T%))
AR1 =VAL(D#(230+T%))
AR2 =VAL(D#(231+T%))
AR3 =VAL(D#(232+T%))
AR4 =VAL(D#(233+T%))
T%=FILETYPE%(K%)
IF T%=5 THEN TC%=10 ELSE TC%=8
VOL =(NOSC% * SCANTIME * FLOWRATE) / CONVERT
KV =HMDSOONG * VOL * 18 / HMDS
TAL =GA + ACH3/3 + ACH2/2 + ACH
TAR =AR1
AROM =TAR / (TAL+TAR)
NF =TAR / 4

```

```

IF T% = 5 THEN TEMP% = 10 ELSE TEMP% = 8
NF = (IAR + (IATL - GA)) / TEMP%
CSUN = IAR / NF
CSSUB = TC% - CSUN
CSCH3 = (ACH3/3) / NF
CSCH2 = (ACH2/2) / NF
CSCH = (ACH/1) / NF
CSCQ = CSSUB - (CSCH3 + CSCH2 + CSCH)
IF T% = 4 THEN CSCH2 = CSCH2 + 1

NF2 = IV * NF
CUN = CSUN * NF2
CSUB = CSSUB * NF2
CCH3 = CSCH3 * NF2
CCH2 = CSCH2 * NF2
CCH = CSCH * NF2
CTET = TS1TET * NF2
CAQ = CSAQ * NF2

PGA = GA / NF
IF T% = 4 THEN TEMP = CSCH2.1 ELSE TEMP = CSCH2
NBR = TEMP + 2 * CSCH + 3 * CSCQ
CSH2G = (PGA - NBR * 3) / 2
IF CSH2G < 0 THEN CSH2G = 0
CCH2G = CSH2G * NF2
CSH3G = NBR
CCH3G = CSH3G * NF2
ADS = CSSUB
FSS = ADS / TC%
IF T% = 3 THEN CSBH = 2 ELSE CSBH = 4
CBH = CSBH * NF2
MW = 13 * CSUN + 12 * CSSUB + 15 * CSCH3 + 14 * CSCH2
MW = MW + 13 * CSCH + 14 * CS1TET + 12 * CSCQ
MW = MW + 14 * CSH2G + 15 * CSH3G + 12 * CSBH
TMAR = CUN + CSUB
TMAL = CCH3 + CCH2 + CCH + CQ + CTET + CCH2G + CCH3G
MOLC = TMAR + TMAL

```

```

. Will next calc the physical properties
DEN = 0.7511804 + 2.3814241 * CSCH2 + 0.0794783 * NBR
CETANE = 0.967182 + 3.8733E-03 * CSCH3 + 9.83778E-03 * CSCH2
DEN = DEN + 1.48817E-02 * CSCH + 1.1922E-02 * CSCQ
QL = 11088 + 757 * DEN - 2100 * DEN ^ 2
VCAL = QL * DEN

IF T% = 3 THEN S1% = 28 : S2% = 0
IF T% = 4 THEN S1% = 54 : S2% = 6
IF T% = 5 THEN S1% = 80 : S2% = 16
D8(S1% + 0) = STRS(CSUN) : D8(S1% + 1) = STRS(CUN) : D8(S1% + 2) = STRS(CSSUB)
D8(S1% + 3) = STRS(CSUB) : D8(S1% + 4) = STRS(CSBH) : D8(S1% + 5) = STRS(CBH)
D8(S1% + 6) = STRS(CSCH3) : D8(S1% + 7) = STRS(CCH3) : D8(S1% + 8) = STRS(CSCH2)
D8(S1% + 9) = STRS(CCH2) : D8(S1% + 10) = STRS(CSCH) : D8(S1% + 11) = STRS(CCH)
D8(S1% + 12) = STRS(CSCH2G) : D8(S1% + 13) = STRS(CCH2G) : D8(S1% + 14) = STRS(CSH3G)
D8(S1% + 15) = STRS(CCH3G) : D8(S1% + 16) = STRS(CS1TET) : D8(S1% + 17) = STRS(CTET)
D8(S1% + 18) = STRS(MW) : D8(S1% + 19) = STRS(FSS) : D8(S1% + 20) = STRS(ADS)
D8(S1% + 21) = STRS(TMAR) : D8(S1% + 22) = STRS(MOLC) : D8(S1% + 23) = STRS(FRACA)
D8(S1% + 24) = STRS(FRACC) : D8(S1% + 25) = STRS(NOSCQ)
D8(S2% + 173) = STRS(CTET) : D8(S2% + 174) = STRS(QL) : D8(S2% + 175) = STRS(DEN)
D8(S2% + 176) = STRS(VCAL) : D8(S2% + 177) = STRS(PRO2) : D8(S2% + 178) = STRS(PRO3)

```

```

. Norm Factor *C->C
Cun
Caub
Cach3
Cach2
Cach
Cacet
Caq
Fluorene *CH2

. alpha branches
Cch2 > a
Cch3 > a
Cch3 > a
Avg Deg of Substn
FracSub Sites
Bridgehead C
Abe Moles BH C
Molecular Wt

. Tot Mol Aromatic C
. Tot Mol Aliph C
. Total Moles Carbon

```

```

CalculateSummaryData
Subroutine to calculate the summary data.

```

```

. Must determine if aromaticities are zero and fix if so.
IF VAL(DS(133)) <= 0 THEN
  TEMPS = "Proton" : TEMP1% = 133 : TEMP2% = 258
  GOSUB GetAromaticity
  END IF
IF VAL(DS(132)) <= 0 THEN
  TEMPS = "Carbon" : TEMP1% = 132 : TEMP2% = 260
  GOSUB GetAromaticity
  END IF

```

```

. Will print a message to the user during calculation.
SCREEN 0 : WIDTH 80 : COLOR 15,0 : CLS
COLOR 10,1
LOCATE 10,15 : PRINT CHR$(218),STRINGS(48,166),CHR$(191)
FOR I% = 11 TO 13
  LOCATE I%,15 : PRINT CHR$(179),STRINGS(48,32),CHR$(179);
NEXT I%
LOCATE 14,15 : PRINT CHR$(192),STRINGS(48,166),CHR$(217)
COLOR 90,1
LOCATE 12,28 : PRINT "Calculating Summary Data";

```

```

. Next calculate total moles carbon.
MOLAR = VAL(DS(24)) + VAL(DS(49)) + VAL(DS(75))
MOLAR = MOLAR + VAL(DS(101))
MOLCT = VAL(DS(25)) + VAL(DS(50)) + VAL(DS(76))
MOLCT = MOLCT + VAL(DS(102))
MOLAK = (MOLAR / VAL(DS(132))) - MOLCT

```

```

. If calculating the percent alkane carbon by 13C difference, must take
the value calculated immediately above (MOLAK) and place into the
output data string (DS(114)). If calculating by direct, 1H integration
simply ignore the section immediately above and accept the value
already stored in DS(114) as it was calculated in the section to
calculate the alkane average structures.
IF CTRLOPTNS(2) = "Y" THEN DS(114) = STRS(MOLAK)
. First must calculate the fraction carbon in peaks.
CalculateTotalCarbon

```

. 1H Static
. 13C Static
. find 1H arom
. find 13C arom
. Moles C Ar
. Moles C Total
. Moles Al C

```

* Total Moles C
TOTC =VAL(D8(114)) + VAL(D8(25)) + VAL(D8(50))
TOTC =TOTC + VAL(D8(76)) + VAL(D8(102))
FCALK=VAL(D8(114)) / TOTC
FCOMN=VAL(D8(25)) / TOTC
FCDC=VAL(D8(50)) / TOTC
FCFLU=VAL(D8(76)) / TOTC
FCPHE=VAL(D8(102)) / TOTC
.
.
.
* Must see if any fraction below 0.25%, if so blank out
IF FCALK<0.0025 AND FCALK>0 THEN
  T1%=106 : T2%=115 : T3%=205 : T4%=206 : T5%=262 : GOTO WipeOut
END IF
IF FCOMN<0.0025 AND FCOMN>0 THEN
  T1%=3 : T2%=27 : T3%=210 : T4%=221 : T5%=263 : GOTO WipeOut
END IF
IF FCDC<0.0025 AND FCDC<>0 THEN
  T1%=28 : T2%=52 : T3%=222 : T4%=233 : T5%=264 : GOTO WipeOut
END IF
IF FCFLU<0.0025 AND FCFLU<>0 THEN
  T1%=54 : T2%=78 : T3%=234 : T4%=245 : T5%=265 : GOTO WipeOut
END IF
IF FCPHE<0.0025 AND FCPHE<>0 THEN
  T1%=80 : T2%=104 : T3%=246 : T4%=257 : T5%=266 : GOTO WipeOut
END IF
* Must put data back into array D8
D8(116)=STR$(FCALK) : D8(27)=STR$(FCOMN) : D8(82)=STR$(FCDC)
D8(78)=STR$(FCFLU) : D8(104)=STR$(FCPHE)
.
.
* Next is fractional aromaticity.
C13AROM=VAL(D8(132))
TOTAR=VAL(D8(25)) + VAL(D8(50)) + VAL(D8(76)) + VAL(D8(102))
FAMON=(C13AROM * VAL(D8(25))) / TOTAR
FADIC=(C13AROM * VAL(D8(50))) / TOTAR
FAFLU=(C13AROM * VAL(D8(76))) / TOTAR
FAPHE=(C13AROM * VAL(D8(102))) / TOTAR
FAROM=FAMON + FADIC + FAFLU + FAPHE
.
D8(26)=STR$(FAMON) : D8(51)=STR$(FADIC)
D8(77)=STR$(FAFLU) : D8(103)=STR$(FAPHE)
D8(148)=STR$(FAROM)
.
* Next are physical properties
FILENAME$=PARAMIDIR$+"FUELPARM.DAT"
GOSUB CheckForFile
OPEN PARAMDIR$+"FUELPARM.DAT" FOR RANDOM AS #5 LEN=729
FIELD #5, 25 AS S$, 25 AS I$, 25 AS O$, 25 AS F$, 25 AS T$(1),
25 AS T$(2), 25 AS T$(3), 25 AS T$(4), 25 AS T$(5), 25 AS T$(6),
25 AS T$(7), 25 AS T$(8), 25 AS T$(9), 25 AS T$(10), 25 AS T$(11),
25 AS T$(12), 25 AS T$(13), 25 AS T$(14), 25 AS T$(15), 25 AS T$(16),
25 AS T$(17), 25 AS T$(18), 25 AS T$(19), 25 AS T$(20), 25 AS T$(21),
25 AS T$(22)
FOR I%=1 TO 42
  GET 5,I%
  SLOPEFACTOR=VAL(S$) : INTOFFACTOR=VAL(I$)
  OFFSEFACTR=VAL(O$) : FUNCTION$=F$
  FOR J%=1 TO 22
    MIXCOEFF(I%,J%)=VAL(T$(J%))
  NEXT J%
  GOSUB DoFuelPropertyCalc
  DS(158+I%)=STR$(PROF)
  . Calc Prop
  . Store data
  . set up b a
  . get param
  . prop loop
FOR I%=1 TO 42
  GET 5,I%
  SLOPEFACTOR=VAL(S$) : INTOFFACTOR=VAL(I$)
  OFFSEFACTR=VAL(O$) : FUNCTION$=F$
  FOR J%=1 TO 22
    MIXCOEFF(I%,J%)=VAL(T$(J%))
  NEXT J%
  GOSUB DoFuelPropertyCalc
  DS(158+I%)=STR$(PROF)
  . Calc Prop
  . Store data
  . set up b a
  . get param
  . prop loop

```

```

NEXT I%
CLOSE #5
RETURN
CalculateIntegrals
.
.
.
This is the subroutine to calculate the integral values.
.
.
.
T%=FILETYPE%(K%)
SELECT CASE FILETYPE%(K%)
CASE 1 : TEMP1%=5 : TEMP2%=205 : TEMP3%=1
CASE 2 : TEMP1%=12 : TEMP2%=210 : TEMP3%=1
CASE 3 : TEMP1%=12 : TEMP2%=222 : TEMP3%=1
CASE 4 : TEMP1%=12 : TEMP2%=234 : TEMP3%=1
CASE 5 : TEMP1%=12 : TEMP2%=248 : TEMP3%=1
CASE 6 : TEMP1%=3 : TEMP2%=258 : TEMP3%=2
CASE 7 : TEMP1%=3 : TEMP2%=260 : TEMP3%=2
END SELECT
FOR I%=1 TO TEMP1% STEP TEMP3%
  TEMP4%=0
  FOR J%=PT%(I%)+1 TO PT%(I%,I%)
    INCR TEMP4,DS(I%,J%)
  NEXT J%
  IF TEMP4<=0 THEN TEMP4=0.000001
  IF T%>=6 THEN TEMP4%=INT(I%/3) ELSE TEMP4%=I%-1
  DS(TEMP2%+TEMP4%)=STR$(TEMP4)
  IF TEMP4<=0 THEN DS(TEMP2%+TEMP4%)=STR$(0.000001)
NEXT I%
NEXT J%
INTNF(T%)=1/VAL(D8(TEMP2%))
FOR I%=1 TO TEMP1% STEP TEMP3%
  IF T%>=6 THEN TEMP4%=INT(I%/3) ELSE TEMP4%=I%-1
  DS(TEMP2%+TEMP4%)=STR$(INTNF(T%) * VAL(D8(TEMP2%+TEMP4%)))
  IF LEFT$(DS(143),5)="BLANK" THEN
    TEMP=VAL(D8(TEMP2%+TEMP4%))
    TEMP=TEMP - BLANK(TEMP2%+TEMP4%) * SQR(NOSC%)
    DS(TEMP2%+TEMP4%)=STR$(TEMP)
  END IF
END IF
NEXT I%
RETURN
.
.
.
***** This section contains the include calculation subroutines *****
.
.
.
CalculateAndDrawShift
$INCLUDE "LCNMR13 INC"
CalculateAndDrawBase
$INCLUDE "LCNMR14 INC"
WipeOutRecalcData
$INCLUDE "LCNMR23 INC"
WipeOut
$INCLUDE "LCNMR48 INC"
DivideBlankIntegrals
$INCLUDE "LCNMR27 INC"
DoFuelPropertyCalc

```

```

$INCLUDE 'LCNMR47.INC'
.....
..... This section contains the include screen subroutines .....
.....
GetNames:
$INCLUDE 'LCNMR04.INC'
DrawFuelName:
$INCLUDE 'LCNMR05.INC'
FileNames:
$INCLUDE 'LCNMR08.INC'
GetBackgroundInfo:
$INCLUDE 'LCNMR07.INC'
DisplayNMRFile:
$INCLUDE 'LCNMR10.INC'
DisplayAxis:
$INCLUDE 'LCNMR11.INC'
DrawAvgStrScreens:
$INCLUDE 'LCNMR12.INC'
DrawAvgStrData:
$INCLUDE 'LCNMR15.INC'
MarkActiveShift:
$INCLUDE 'LCNMR16.INC'
MarkActiveBase:
$INCLUDE 'LCNMR17.INC'
MoveActiveShift:
$INCLUDE 'LCNMR36.INC'
MoveActiveBase:
$INCLUDE 'LCNMR38.INC'
PrintSummaryScreen:
$INCLUDE 'LCNMR18.INC'
DoControlOptions:
$INCLUDE 'LCNMR19.INC'
HelpScreen:
$INCLUDE 'LCNMR22.INC'
GetBlankName:
$INCLUDE 'LCNMR25.INC'
SpectraEditMenu:
$INCLUDE 'LCNMR28.INC'
FileBlankDataMenu:
$INCLUDE 'LCNMR28.INC'
PrinterMenu:
$INCLUDE 'LCNMR28.INC'
PrinterFontMenu:
$INCLUDE 'LCNMR37.INC'
EditIntegrationMenu:
$INCLUDE 'LCNMR30.INC'
DrawIntegrationScreen:
$INCLUDE 'LCNMR31.INC'
EditDisplayedInt:
$INCLUDE 'LCNMR32.INC'
HighlightIntegral:
$INCLUDE 'LCNMR33.INC'
$SEGMENT
GetAromaticity:
$INCLUDE 'LCNMR42.INC'
ErrorMessage:

```

```

$INCLUDE 'LCNMR44.INC'
DrawIntegralRegions:
$INCLUDE 'LCNMR45.INC'
EditNumberOfYScans:
$INCLUDE 'LCNMR49.INC'
.....
..... This section contains the include filing subroutines .....
.....
ReadConfigFile:
$INCLUDE 'LCNMR03.INC'
GetBlankData:
$INCLUDE 'LCNMR08.INC'
ReadNMRFile:
$INCLUDE 'LCNMR08.INC'
GetAvgStrData:
$INCLUDE 'LCNMR20.INC'
FileAvgStrData:
$INCLUDE 'LCNMR21.INC'
HardCopyIntegrals:
$INCLUDE 'LCNMR34.INC'
HardCopyResults:
$INCLUDE 'LCNMR35.INC'
HardCopyProps:
$INCLUDE 'LCNMR38.INC'
CheckForFile:
$INCLUDE 'LCNMR43.INC'
AutoCheckForFile:
$INCLUDE 'LCNMR48.INC'
.....
..... This section contains the LC-NMR file system documentation .....
.....
FileDocumentation:
$INCLUDE 'LCNMR41.INC'

```

Code Listing for LCNMR03.INC

This is the subroutine to read the configuration file

```

.....
..... Will write message to the user.
COLOR 0,3
LOCATE 10,20 : PRINT CHR$(201),STRINGS(39,205),CHR$(187);
FOR I%=11 TO 13
LOCATE I%,20 : PRINT CHR$(186),TAB(60),CHR$(186);
NEXT I%
LOCATE 14,20 : PRINT CHR$(200),STRINGS(39,205),CHR$(186);
COLOR 4,3
LOCATE 12,29 : PRINT "Reading the "; COLOR 14,3 : PRINT "Param File";

```

```

FILENAME$=ODIR$+L\CNMRCFG.DAT
GOSUB CheckFile
OPEN ODIR$+L\CNMRCFG.DAT FOR INPUT AS #1
INPUT #1,HMDSHIFT
INPUT #1,CDOGL3$SHIFT
INPUT #1,PPMPT2KH
INPUT #1,PPMPT8KH
INPUT #1,PPMPT8KC
INPUT #1,HMDS$ONG
INPUT #1,FLOWRATE
INPUT #1,SCANTIME
INPUT #1,CONVERT

      Next are the control parameters for the LC-NMR program.
INPUT #1,Cq
INPUT #1,VER$
INPUT #1,PRINTER$
INPUT #1,FONT$
INPUT #1,SPECTCL$
INPUT #1,AXISCOL$
INPUT #1,LABLECL$
INPUT #1,SHIFTCL$
INPUT #1,BASECOL$
INPUT #1,DATACOL$
INPUT #1,INTCOL$
INPUT #1,BACKCOL$
INPUT #1,INTEGRALS
INPUT #1,NMRDIR$
INPUT #1,INPUTDIR$
INPUT #1,OUTPUTDIR$
INPUT #1,BLANKDIR$
INPUT #1,SCRDIR$
INPUT #1,PARAMDIR$
FOR I%=1 TO 8
  INPUT #1,CTRLOPT$(I%)
NEXT I%
FOR I%=1 TO 7
  INPUT #1,FILETYPE$(I%)
NEXT I%
FOR I%=1 TO 7
  INPUT #1,YOFFSET$(I%)
NEXT I%
FOR I%=1 TO 7
  INPUT #1,SHIFTSTEP$(I%)
NEXT I%
FOR I%=1 TO 7
  INPUT #1,BASESTEP$(I%)
NEXT I%

      Next are the fraction names.
FOR I%=1 TO 8 : INPUT #1, FILETYPE$(I%) : NEXT I%

      Next are the integration region names for each class
FOR I%=1 TO 5 : INPUT #1,INTNAME$(1,I%) : NEXT I%
FOR I%=1 TO 12 : INPUT #1,INTNAME$(2,I%) : NEXT I%
FOR I%=1 TO 12 : INPUT #1,INTNAME$(3,I%) : NEXT I%
FOR I%=1 TO 12 : INPUT #1,INTNAME$(4,I%) : NEXT I%
FOR I%=1 TO 12 : INPUT #1,INTNAME$(5,I%) : NEXT I%
FOR I%=1 TO 3 : INPUT #1,INTNAME$(6,I%) : NEXT I%
FOR I%=1 TO 3 : INPUT #1,INTNAME$(7,I%) : NEXT I%

```

chemical shift for HMDS
 chemical shift for CDOGL3
 PPM/pt for 2K file
 PPM/pt for 8K file- 1H
 PPM/pt for 8K file- 13C
 HMDS Concentration
 Chromato flow rate
 Time for scan
 Conversion factor

Cquant for alkanes
 Version Number
 ProPrinter
 Regular data font
 Spectrum color
 Axis color
 Label color
 Shift division color
 Baseline color
 Data foreground color
 Integral display color
 Background color
 Display integrals
 NMR spectra directory
 Input data file dir
 Output data file dir
 Blank data directory
 Scratch file directory
 Params for prop calca

Control Options
 File Types
 Spectrum vertical offset
 Step for shift movement
 Step for baseline moves
 Alkane -> 13C
 Alkane
 Monocyclic
 Dicyclic
 Fluorene
 Phenanthrene
 1H Static
 13C Static

```

      Next are the integral divisions in PPM for each class.
FOR I%=1 TO 8 : INPUT #1,PPM(1,I%) : NEXT I%
FOR I%=1 TO 13 : INPUT #1,PPM(2,I%) : NEXT I%
FOR I%=1 TO 13 : INPUT #1,PPM(3,I%) : NEXT I%
FOR I%=1 TO 13 : INPUT #1,PPM(4,I%) : NEXT I%
FOR I%=1 TO 13 : INPUT #1,PPM(5,I%) : NEXT I%
FOR I%=1 TO 4 : INPUT #1,PPM(6,I%) : NEXT I%
FOR I%=1 TO 4 : INPUT #1,PPM(7,I%) : NEXT I%

      Next are the endpoints for the baselines.
FOR I%=1 TO 4 : INPUT #1,BASEEND(1,I%) : NEXT I%
FOR I%=1 TO 8 : INPUT #1,BASEEND(2,I%) : NEXT I%
FOR I%=1 TO 8 : INPUT #1,BASEEND(3,I%) : NEXT I%
FOR I%=1 TO 8 : INPUT #1,BASEEND(4,I%) : NEXT I%
FOR I%=1 TO 8 : INPUT #1,BASEEND(5,I%) : NEXT I%
FOR I%=1 TO 4 : INPUT #1,BASEEND(6,I%) : NEXT I%
FOR I%=1 TO 4 : INPUT #1,BASEEND(7,I%) : NEXT I%

      Next are the gain settings for displaying the spectra.
FOR I%=1 TO 7 : INPUT #1,GAIN(I%) : NEXT I%

      Next are the gain settings for displaying the integrals.
FOR I%=1 TO 7 : INPUT #1,INTEP$(I%) : NEXT I%
CLOSE #1
RETURN

```

Alkane
 Monocyclic
 Dicyclic
 Fluorene
 Phenanthrene
 Static 1H
 Static 13C

Alkane - 13C Static
 Alkane - 13C Static

Code Listing for LCNMRO4.INC

This is the subroutine to get the fuel names and parameters.

```

StartOfSubroutine.
      First must draw the screen - top box for commands first
COLOR 15,0 CLS
COLOR 0,15
LOCATE 1,10 PRINT CHR$(216),STRING$(58,168);CHR$(191);
FOR I%=2 TO 9
  LOCATE I%,10 : PRINT CHR$(179);TAB(69);CHR$(179);
NEXT I%
LOCATE 10,10 PRINT CHR$(192);STRING$(58,168);CHR$(217);
COLOR 10,15
LOCATE 2,12 PRINT TIMES;
LOCATE 2,57 PRINT DATES;
COLOR 1,15
LOCATE 2,31 PRINT *Command Options*;;
COLOR 0,15
LOCATE 3,14 PRINT * NMR Spectra Directory*;;
LOCATE 4,14 PRINT * Blank Data Directory*;;
LOCATE 5,14 PRINT * Input Data File Directory*;;
LOCATE 6,14 PRINT *Output Data File Directory*;;
LOCATE 7,14 PRINT * File Results: Hard Copy Integrals*;;
LOCATE 8,14 : PRINT * 13C Difference: Hard Copy Results*;;

```

options box
 top line
 middle
 bottom line

```

LOCATE 9,14 : PRINT "Auto File Select:";
COLOR 4,15
LOCATE 3,43 : PRINT NIMRODIRS
LOCATE 4,43 : PRINT BLANKDIRS
LOCATE 5,43 : PRINT INPUTDIRS
LOCATE 6,43 : PRINT OUTPUTDIRS
FOR I%=1 TO 6
  IF I%<4 THEN LOCATE I%+9,33 ELSE LOCATE I%+3,63
  PRINT CTRLPTDIRS(I%);
NEXT I%
.
. Next is names box
COLOR 10,1
LOCATE 12,1 : PRINT CHR$(216),STRING$(78,196),CHR$(191);
FOR I%=13 TO 23
  CHR$(179);TAB(60);CHR$(179);
NEXT I%
LOCATE 24, 1 : PRINT CHR$(192);STRING$(78,196);CHR$(217);
COLOR 11, 1
LOCATE 13,31 : PRINT "Fuel Names to Use:";
LOCATE 13,65 : PRINT "Page:";
COLOR 10, 1
LOCATE 13,70 : PRINT USING "@@#";PAGE%;
GOSUB PageOfNames
.
. Next are commands.
COLOR 3,0
GOSUB Commands
LOCATE 1,71 : PRINT "<-> load";
LOCATE 2,71 : PRINT "from";
LOCATE 3,71 : PRINT "file";
LOCATE 4,71 : PRINT "<F1> dir";
LOCATE 5,71 : PRINT "<BS> def";
LOCATE 6,71 : PRINT "<SP> mark";
LOCATE 7,71 : PRINT "<PG> page";
LOCATE 8,71 : PRINT "<*> mark";
LOCATE 9,71 : PRINT "all";
LOCATE 10,71 : PRINT "<-> unmark";
LOCATE 11,71 : PRINT "all";
.
. Have drawn screen, so highlight options and get changes.
TEMP1%=12 : TEMP2%=0
GOSUB Highlight
Startloop2:
AS=INKEY$
SELECT CASE AS
CASE =
  COLOR 10,15
  LOCATE 2,12 : PRINT TIMES;
CASE CHR$(27),"Q","q"
  GOTO MainMenu;
CASE CHR$(13)
  RETURN
CASE CHR$(0)+CHR$(72), CHR$(0)+CHR$(80)
  IF OPTN%(2)=1 THEN
    TEMP1%= 4 : TEMP2%=15
  GOSUB Highlight
  IF AS=CHR$(0)+CHR$(72) THEN DECR OPTN%(3) ELSE INCR OPTN%(3)
  IF OPTN%(3)<1 THEN OPTN%(4)=PAGE%*50 : OPTN%(2)=2
.
IF OPTN%(3)>10 THEN OPTN%(4)=(PAGE%-1)*50+1 : OPTN%(2)=2
ELSE
  IF NAMEUSE%(OPTN%(4))=0 THEN
    TEMP1%=12 : TEMP2%=1
  ELSE
    TEMP1%=11 : TEMP2%=1
  END IF
  GOSUB Highlight
  IF AS=CHR$(0)+CHR$(72) THEN DECR OPTN%(4) ELSE INCR OPTN%(4)
  IF OPTN%(4)>PAGE%*50 THEN OPTN%(3)=10 : OPTN%(2)=1
  IF OPTN%(4)>PAGE%*50 THEN OPTN%(3)=1 : OPTN%(2)=1
END IF
IF OPTN%(2)=2 AND NAMEUSE%(OPTN%(4))=1 THEN
  TEMP1%=11 : TEMP2%=0
ELSE
  TEMP1%=12 : TEMP2%=0
END IF
GOSUB Highlight
CASE CHR$(0)+CHR$(75),CHR$(0)+CHR$(77)
  CASE CHR$(8)
    . left-right
    . delete name
  FUELNAME$(OPTN%(4))= : NAMEUSE%(OPTN%(4))=0
  COLOR 12,1
  TEMP%=INT((OPTN%(4)-(PAGE%-1)*50-1)/10)
  LOCATE (OPTN%(4)-(PAGE%-1)*50)-TEMP%*10+13,TEMP%*15+7
  PRINT SPACES(12);
  COLOR 12,0
  LOCATE (OPTN%(4)-(PAGE%-1)*50)-TEMP%*10+13,TEMP%*15+7
  PRINT SPACES(2);
END IF
CASE CHR$(0)+CHR$(73), CHR$(0)+CHR$(81)
  IF PAGE%=1 THEN
    PAGE%=2 : INCR OPTN%(4),50
  ELSE
    PAGE%=1 : DECR OPTN%(4),50
  END IF
  COLOR 10, 1
  LOCATE 13,70 : PRINT USING "@@#";PAGE%;
  GOSUB PageOfNames
  IF OPTN%(2)=2 THEN
    IF NAMEUSE%(OPTN%(4))=1 THEN TEMP1%=11 ELSE TEMP1%=12
    TEMP2%=0 : GOSUB Highlight
  END IF
CASE CHR$(0)+CHR$(56)
  COLOR 28,0
  TEMPS="Mask (NUL="+NIMRODIRS+"*");
  LOCATE 11,1 : PRINT TEMPS;
  COLOR 10,0
  LINE INPUT TEMPS
  IF TEMPS="" THEN TEMPS=NIMRODIRS
  COLOR 14,0 : CLS
  TEMPS="DIR "+TEMPS+" /P"
  SHELL TEMPS
  COLOR 12,0
  PRINT ">>> Press any key to return to the LC-NMR program <<<";
  TEMPS=INPUT$(1)
  GOTO StartOfSubroutine
CASE ....
  TEMP4%=OPTN%(4) : TEMPS%=OPTN%(2) : OPTN%(2)=2 : TEMP2%=1
  IF AS="" THEN TEMP1%=11 ELSE TEMP1%=12
  . mark/unmark

```

```

FOR %k=1 TO 100
  OPTN%(4)=%k
  IF AS=*** AND FUELNAME$(%k)<>= THEN NAMEUSE$(%k)=1
  IF AS=** AND FUELNAME$(%k)<>= THEN NAMEUSE$(%k)=0
  IF PAGE%=1 AND %k<=50 THEN GOSUB Highlight
  IF PAGE%=2 AND %k>=51 THEN GOSUB Highlight
NEXT %k
OPTN%(4)=TEMP% : OPTN%(2)=TEMP% : TEMP% = TEMP%+0
IF OPTN%(2)=2 THEN GOSUB Highlight
CASE CHR$(32)
  . space
  IF OPTN%(3)=1 THEN
    IF OPTN%(3)>=5 AND OPTN%(3)<=10 THEN
      IF CTRLOPTN$(OPTN%(3)-4)=Y THEN
        CTRLOPTN$(OPTN%(3)-4)=N
      ELSE
        CTRLOPTN$(OPTN%(3)-4)=Y
      END IF
    TEMP1%=12 : TEMP2%=0
    GOSUB Highlight
  END IF
  ELSE
    IF NAMEUSE$(OPTN%(4))=0 THEN
      TEMP1%=12 : TEMP2%=1
    ELSE
      TEMP1%=11 : TEMP2%=1
    END IF
  GOSUB Highlight
  IF NAMEUSE$(OPTN%(4))=0 THEN
    NAMEUSE$(OPTN%(4))=1 : TEMP1%=11 : TEMP2%=0
  ELSE
    NAMEUSE$(OPTN%(4))=0 : TEMP1%=12 : TEMP2%=0
  END IF
  GOSUB Highlight
END IF
CASE Y
  COLOR 14, 4
  TEMP% = Load directory: *+NMRODRS+*
  LOCATE 11,40-0.5*LEN(TEMP%) : PRINT TEMP%
  COLOR 30, 4
  TEMP% = Load fuel names from .<T>02 files, .<D>AT files,
  TEMP% = TEMP% +or <Q>uit?
  LOCATE 25,40-0.5*LEN(TEMP%) : PRINT TEMP%
  LOCATE 1, 1 : PRINT "
  Startloop15:
  AS=INKEY$
  SELECT CASE AS
  CASE = : GOTO Startloop 15
  CASE T, Y : TEMP% = "T02"
  CASE D, Q : TEMP% = "DAT"
  CASE O, q
    COLOR 3,0
    LOCATE 11,5 : PRINT SPACES(80);
    GOSUB Commands
    GOTO Startloop2
  CASE ELSE
    SOUND 1000,3 : SOUND 800,1.5
    GOTO Startloop 15
  END SELECT
  COLOR 18, 3
  LOCATE 25, 5 : PRINT SPACES(70);
  LOCATE 25,23 : PRINT **** Loading the requested files ****;
  SHELL "DIR *+NMRODRS+TEMP%+* > TEMP.ZZZ"
  OPEN TEMP.ZZZ FOR INPUT AS #1
  COUNT%=1
  WHILE NOT EOF(1) AND COUNT%<=100
    INPUT #1,AS
    IF MIDS(AS,28,1)=-* AND MIDS(AS,29,1)=-* THEN
      IF TEMP%=-.DAT THEN
        %k=1
        WHILE MIDS(AS,%k,1)<>* AND %k<=8
          INCR %k
        WEND
        FUELNAME$(COUNT%)=LEFT$(AS,%k-1)
      ELSE
        %k=8
        WHILE MIDS(AS,%k,1)<>8* AND %k>1
          DECR %k
        WEND
        FUELNAME$(COUNT%)=LEFT$(AS,%k-1)
      END IF
      INCR COUNT%
    WEND
    CLOSE 1
    KILL TEMP.ZZZ
    GOSUB PageOfNames
    COLOR 3,0
    LOCATE 11,5 : PRINT SPACES(70);
    GOSUB Commands
    IF OPTN%(2)=2 THEN
      IF NAMEUSE$(OPTN%(4))=1 THEN TEMP1%=11 ELSE TEMP1%=12
      TEMP2%=0 : GOSUB Highlight
    END IF
  CASE ELSE
    IF ASC(AS)<48 OR ASC(AS)>122 THEN GOTO Startloop2
    IF OPTN%(2)=1 THEN
      COLOR 4,15
      IF OPTN%(3)<5 THEN
        LOCATE OPTN%(3)+2,42 : PRINT SPACES(25);
        LOCATE OPTN%(3)+2,43 : PRINT AS : LINE INPUT TEMP%
        TEMP% = AS +TEMP% +Y : TEMP% = UCASE$(TEMP%)
        IF OPTN%(3)=1 THEN NMRODRS =TEMP%
        IF OPTN%(3)=2 THEN BLANKDRS =TEMP%
        IF OPTN%(3)=3 THEN INPUTDRS =TEMP%
        IF OPTN%(3)=4 THEN OUTPUTDRS =TEMP%
      ELSE
        IF CTRLOPTN$(OPTN%(3)-4)=Y THEN
          CTRLOPTN$(OPTN%(3)-4)=N
        ELSE
          CTRLOPTN$(OPTN%(3)-4)=Y
        END IF
      END IF
    ELSE
      COLOR 15,1
      TEMP% = INT((OPTN%(4)-(PAGE%-1)*50):1/10)
      LOCATE (OPTN%(4)-(PAGE%-1)*50):TEMP%*10+13,TEMP%*15+7
      PRINT SPACES(12);
      LOCATE (OPTN%(4)-(PAGE%-1)*50):TEMP%*10+13,TEMP%*15+8
      PRINT AS : LINE INPUT TEMP%
      TEMP% = AS +TEMP% : TEMP% = UCASE$(TEMP%)
    END IF
  END IF
END IF

```

Code Listing for LCNMRO5.INC

This is the subroutine to draw the fuel name window.

```

COLOR 0,15
LOCATE TEMP1%,TEMP2%
PRINT CHR$(218),STRING$(10,196),CHR$(191);
LOCATE TEMP1%+1,TEMP2%
PRINT CHR$(179);
LOCATE TEMP1%+2,TEMP2%
PRINT CHR$(195),STRING$(10,196),CHR$(180);
LOCATE TEMP1%+3,TEMP2%
PRINT CHR$(179);
LOCATE TEMP1%+4,TEMP2%
PRINT CHR$(192),STRING$(10,196),CHR$(217);
RETURN
    
```

Code Listing for LCNMRO6.INC

This is the subroutine to get the filenames and types.

```

FOR I%=1 TO 7
IF FILENAMES(I%)="" THEN FILENAMES(I%)=""
NEXT I%
IF CTRLOPT$(3)="Y" THEN
FOR I%=1 TO 5
FILENAMES(I%)=NMRODIRS+FUELNAME$(L%)+S TO +CHR$(48+I%)
NEXT I%
FILENAMES(6)=NMRODIRS+FUELNAME$(L%)+H.T01
FILENAMES(7)=NMRODIRS+FUELNAME$(L%)+C.T01
GOSUB AutoCheckOfFile
END IF
NEXT I%
Next must draw the screen.
COLOR 10,1
LOCATE 2,13 : PRINT CHR$(218),STRING$(55,196),CHR$(191);
FOR I%=3 TO 21
LOCATE I%,13 : PRINT CHR$(179);TAB(89);CHR$(179);
NEXT I%
LOCATE 22,13 : PRINT CHR$(192),STRING$(55,196),CHR$(217);
LOCATE 6,13 : PRINT CHR$(195),STRING$(55,196),CHR$(180);
COLOR 10,0
LOCATE 1,12 : PRINT TIMES;
    
```

```

FUELNAME$(OPTN%(4))=TEMP$
END IF
IF NAMEUSE$(OPTN%(4))=1 THEN TEMP1%=11 ELSE TEMP1%=12
TEMP2%=0 : GOSUB Highlight
END SELECT
GOTO Startloop2

Highlight:
* This is a mini-subroutine to highlight the selection.
IF OPTN%(2)=1 THEN
COLOR TEMP1%,TEMP2%
IF OPTN%(3)<5 THEN
IF OPTN%(3)=1 THEN TEMP$=NMRODIRS
IF OPTN%(3)=2 THEN TEMP$=BLANKDIRS
IF OPTN%(3)=3 THEN TEMP$=INPUTDIRS
IF OPTN%(3)=4 THEN TEMP$=OUTPUTDIRS
LOCATE OPTN%(3)+2,42 : PRINT " ";TEMP$;
ELSE
IF OPTN%(3)<8 THEN LOCATE OPTN%(3)+2,32 ELSE LOCATE OPTN%(3)-1,82
PRINT " ";CTRLOPT$(OPTN%(3)-4);
END IF
ELSE
COLOR TEMP1%,TEMP2%
TEMP%=INT(((OPTN%(4)-(PAGE%-1)*50)-1)/10)
LOCATE (OPTN%(4)-(PAGE%-1)*50)-TEMP%*10+13,TEMP%*15+7
IF NAMEUSE$(OPTN%(4))=0 THEN
PRINT " ";FUELNAME$(OPTN%(4));
ELSE
PRINT " ";CHR$(16),FUELNAME$(OPTN%(4));
END IF
END IF
RETURN
    
```

```

PageOfNames.
FOR I%=(PAGE%-1)*50+1 TO PAGE%*50
TEMP%=INT(((PAGE%-1)*50)-1)/10
LOCATE (I%-(PAGE%-1)*50)-TEMP%*10+13,TEMP%*15+3
COLOR 14,1 : PRINT USING "###";I%;
IF NAMEUSE$(I%)=1 THEN
COLOR 11,1
PRINT " ";CHR$(16),FUELNAME$(I%),SPACES(10-LEN(FUELNAME$(I%)));
ELSE
COLOR 12,1
PRINT " ";FUELNAME$(I%),SPACES(10-LEN(FUELNAME$(I%)));
END IF
NEXT I%
RETURN

Commands:
COLOR 3,0
LOCATE 25,1 : PRINT SPACES(75);
LOCATE 25,20 : PRINT "Press <O> to quit, <RETURN> to continue";
RETURN
    
```



```

IF TEMPS<>="" THEN FILENAME$(OPTN$(5))=TEMPS
END SELECT
GOTO Startloop3

```

DisplayFile Type:

```

. This is a mini-subroutine to display the file type
IF FILETYPE$(OPTN$(5))=6 THEN COLOR 11,0 ELSE COLOR 12,0
LOCATE (OPTN$(5)-1)*2+8,53
PRINT FILETYPE$(FILETYPE$(OPTN$(5)));TAB(66);
RETURN

```

Code Listing for LCNMR07.INC



This is the subroutine to get the background information.

```

COLOR 10,1
LOCATE 2,14 : PRINT CHR$(216);STRING$(50,106);CHR$(101); ' top line
FOR I%=3 TO 21
LOCATE I%,14 : PRINT CHR$(179);TAB(65);CHR$(179); ' middle
NEXT I%
LOCATE 22,14 : PRINT CHR$(192);STRING$(50,106);CHR$(217); ' bottom line
LOCATE 6,14 : PRINT CHR$(195);STRING$(50,106);CHR$(190); ' middle line
COLOR 10,0
LOCATE 1,12 : PRINT TIMES;
LOCATE 1,58 : PRINT DATES;
COLOR 15,1
LOCATE 4,28 : PRINT "Background information:";
COLOR 14,1
LOCATE 7,34 : PRINT "Source:";
LOCATE 8,30 : PRINT "Blank Name:";
LOCATE 9,28 : PRINT "Smoke Point:";
LOCATE 10,28 : PRINT "Freezing Point:";
LOCATE 11,22 : PRINT "Aromaticity (Vol%):";
LOCATE 12,23 : PRINT "Operator Initials:";
LOCATE 13,25 : PRINT "Instrument Used:";
LOCATE 14,22 : PRINT "<Default = FX-200>:";
LOCATE 16,32 : PRINT "Elemental Analysis:";
LOCATE 17,18 : PRINT "ISC: 1H: 1H (by NMR)";
LOCATE 18,25 : PRINT "Comments (up to 50 characters)";
. Next are commands
COLOR 3,0
LOCATE 24,10
PRINT "Do you wish to use parameters already on file <F>, enter them";
LOCATE 25,10
PRINT "manually <M>, ignore menu <I>, quit <Q>, or continue <RETURN>?";
IF CTRLLOPTN$(3)="Y" THEN GOSUB PrintFileData
. Have got screen, so see which option to use.
Startloop5
AS=INKEY$

```

```

LOCATE 1,58 : PRINT DATES;
COLOR 15,1
LOCATE 4,22 : PRINT "File Name:";
LOCATE 4,55 : PRINT "File Type:";
COLOR 14,1
FOR I%=1 TO 7
COLOR 14,1
LOCATE (I%-1)*2+8,16 : PRINT FILENAME$(I%);
IF FILETYPE$(I%)=8 THEN COLOR 11,1 ELSE COLOR 14,1
LOCATE (I%-1)*2+8,53 : PRINT FILETYPE$(FILETYPE$(I%));
NEXT I%
. Next are commands.
COLOR 3,0
LOCATE 24,11
PRINT "Press <UP,DN> to select, <LEFT,RIGHT> to change file type;";
LOCATE 25,23
PRINT "<Q> to quit, <RETURN> to continue.";
. Have printed screen, so get changes.
COLOR 12,0
LOCATE (OPTN$(5)-1)*2+8,14
PRINT "FILENAME$(OPTN$(5));TAB(63);
GOSUB DisplayFileType
Startloop3:
AS=INKEY$
SELECT CASE AS
CASE "="
COLOR 10,0
LOCATE 1,12 : PRINT TIMES;
CASE "Q", "q", CHR$(27)
GOTO MainMenu
CASE CHR$(13)
RETURN
CASE CHR$(0)+CHR$(72), CHR$(0)+CHR$(80)
COLOR 14,1 : LOCATE (OPTN$(5)-1)*2+8,14
PRINT "FILENAME$(OPTN$(5));TAB(53);
IF FILETYPE$(OPTN$(5))=8 THEN COLOR 11,1 ELSE COLOR 14,1
PRINT FILETYPE$(FILETYPE$(OPTN$(5)));TAB(66);
IF AS=CHR$(0)+CHR$(72) THEN DECR OPTN$(5) ELSE INCR OPTN$(5)
IF OPTN$(5)<1 THEN OPTN$(5)=7
IF OPTN$(5)>7 THEN OPTN$(5)=1
COLOR 12,0 : LOCATE (OPTN$(5)-1)*2+8,14
PRINT "FILENAME$(OPTN$(5));TAB(53);
GOSUB DisplayFileType
CASE CHR$(0)+CHR$(73),CHR$(0)+CHR$(77)
IF AS=CHR$(0)+CHR$(73) THEN
DECR FILETYPE$(OPTN$(5))
ELSE
INCR FILETYPE$(OPTN$(5))
END IF
IF FILETYPE$(OPTN$(5))<1 THEN FILETYPE$(OPTN$(5))=6
IF FILETYPE$(OPTN$(5))>8 THEN FILETYPE$(OPTN$(5))=1
GOSUB DisplayFileType
CASE ELSE
IF ASC(AS)<48 OR ASC(AS)>122 THEN GOTO Startloop3
COLOR 12,0
LOCATE (OPTN$(5)-1)*2+8,14 : PRINT SPACES(33);
LOCATE (OPTN$(5)-1)*2+8,17 : PRINT AS; : LINE INPUT TEMPS
TEMPS=AS+TEMPS

```

```

LOCATE 11,42 : PRINT USING *###.##.###;VAL(D8(137));
LOCATE 12,42 : PRINT D8(141);
LOCATE 13,42 : PRINT D8(142);
LOCATE 18,16 : PRINT USING *###.###.###;VAL(D8(138));
LOCATE 18,33 : PRINT USING *###.###.###;VAL(D8(139));
LOCATE 18,53 : PRINT USING *###.###.###;VAL(D8(140));
LOCATE 20,16 : PRINT LEFT$(D8(144),47);
D8(2)=DATE$
COLOR 15, 0
LOCATE 1,28 : PRINT *
RETURN
    
```

Code Listing for LCNMF08.INC

This is the subroutine to retrieve the blank data.

```

FILENAME$=BLANKDIRS + D8(143) + ".DAT"
GOSUB CheckForFile
OPEN BLANKDIRS + D8(143) + ".DAT" FOR INPUT AS #1
TEMP%=1
WHILE NOT EOF(1) AND TEMP% < 350
  INPUT #1,TEMP$
  IF TEMP% >= 205 AND TEMP% <= 281 THEN BLANK(TEMP%)=VAL(TEMP$)
  INCR TEMP%
WEND
CLOSE 1
RETURN
    
```

Code Listing for LCNMF09.INC

This is the subroutine to read in a NMR file.

```

FILENAME$=FILENAME$(K%)
GOSUB CheckForFile
OPEN FILENAME$(K%) FOR INPUT AS 1
    * Must decide if reading an IBM or JEOL file.
INPUT #1,TEMPS
IF TEMPS$="KEYS" THEN
  WHILE Q$ <> "DATA"
    IF EOF(1) THEN GOTO Problem
    INPUT #1,Q$
    IF Q$="SI L" THEN INPUT #1,SIZE%
    IF Q$="NS L" THEN INPUT #1,NO$C%
  WEND
  INPUT #1,Q$
    * num of pts
    * num of scans
    * IBM file
    
```

```

* no key
* ignore
* quit
* manual
    
```

```

SELECT CASE AS
CASE =
  COLOR 10, 0
  LOCATE 1,12 : PRINT TIMES;
CASE " ",CHR$(13)
  D8(2)=DATE$ : D8(1)=FUELNAME$(L%)
  RETURN
CASE "Q",CHR$(27)
  GOTO MainMenu;
CASE "M","m"
  GOSUB ClearBackgroundData
  COLOR 12, 1
  LOCATE 7,42 : LINE INPUT D8(145)
  LOCATE 9,42 : LINE INPUT D8(143)
  LOCATE 9,42 : LINE INPUT D8(135)
  LOCATE 9,42 : PRINT USING *###.##.###;VAL(D8(135));
  LOCATE 10,42 : LINE INPUT D8(136)
  LOCATE 10,42 : PRINT USING *###.##.###;VAL(D8(136));
  LOCATE 11,42 : LINE INPUT D8(137)
  LOCATE 11,42 : PRINT USING *###.##.###;VAL(D8(137));
  LOCATE 12,42 : LINE INPUT D8(141)
  LOCATE 13,42 : LINE INPUT D8(142)
  IF D8(142)="" THEN D8(142)="FX:200"
  LOCATE 13,42 : PRINT D8(142)
  LOCATE 18,16 : LINE INPUT D8(138)
  LOCATE 18,16 : PRINT USING *###.###.###;VAL(D8(138));
  LOCATE 18,33 : LINE INPUT D8(139)
  LOCATE 18,33 : PRINT USING *###.###.###;VAL(D8(139));
  LOCATE 18,53 : LINE INPUT D8(140)
  LOCATE 18,53 : PRINT USING *###.###.###;VAL(D8(140));
  LOCATE 20,16 : LINE INPUT D8(144)
  D8(2)=DATE$ : D8(1)=FUELNAME$(L%)
CASE "P","p"
  GOSUB PrintFileData
CASE ELSE
  SOUND 1000,3 : SOUND 800,1.5
END SELECT
GOTO Startloops
    
```

```

* file
* oops!
    
```

```

ClearBackgroundData:
    * This is a minisubroutine to clear the background screen.
  COLOR 15,1
  FOR I%=7 TO 13
    LOCATE I%,42 : PRINT SPACES(20);
  NEXT I%
  LOCATE 18,15 : PRINT SPACES(50);
  LOCATE 20,15 : PRINT SPACES(50);
  RETURN
PrintFileData:
  COLOR 15, 4
  LOCATE 1,28 : PRINT * Loading information *;
  GOSUB ClearBackgroundData
  GOSUB GetAvgStrData
  COLOR 12, 1
  LOCATE 7,42 : PRINT D8(145);
  LOCATE 9,42 : PRINT D8(143);
  LOCATE 9,42 : PRINT USING *###.##.###;VAL(D8(135));
  LOCATE 10,42 : PRINT USING *###.##.###;VAL(D8(136));
    
```

Code Listing for LCNMR10.INC

```

MIN&=0 : MAX&=0
FOR I%=1 TO SIZE%2
  IF EOF(I) THEN GOTO Problem
  INPUT #1,D&(I%)
  IF D&(I%)<MIN& THEN MIN&=D&(I%)
  IF D&(I%)>MAX& THEN MAX&=D&(I%)
NEXT I%
RANGE&=MAX&-MIN&
COUNT%=1
CLOSE 1
RETURN
ELSE
  WHILE MID$(TEMP$,6,5) <> "DATA"
  IF EOF(1) THEN GOTO Problem
  INPUT #1,TEMP$
  SELECT CASE TEMP$
    CASE "FILE NAME": INPUT #1,FILENAME$
    CASE "SIZE OF DATA": INPUT #1,SIZE%
    CASE "SPECTRAL WIDTH": INPUT #1,SPECWIDTH%
    CASE "SCANS COMPLETED": INPUT #1,NO$C%
    CASE "FILTER WIDTH": INPUT #1,FILTER%
    CASE "SPECT FREQ": INPUT #1,SPECTFREQ
    CASE "PULSE WIDTH": INPUT #1,PULSEWIDTH
    CASE "SCANS REQUIRED": INPUT #1,SCANSREQ%
    CASE "COMMENT": INPUT #1,COMMENTS$
  END SELECT
  INCR COUNT%
WEND
MAX&=-32768 : MIN&=32768 : COUNT%=1
WHILE TEMP$ <> "TRANSFER SUCCESSFUL"
  IF EOF(1) THEN GOTO Problem
  INPUT #1,TEMP$
  DA(COUNT%)=VAL(TEMP$)
  IF DA(COUNT%)<MIN& THEN MIN&=DA(COUNT%)
  IF DA(COUNT%)>MAX& THEN MAX&=DA(COUNT%)
  INCR COUNT%
WEND
CLOSE 1
RANGE&=MAX&-MIN&
COUNT%=1
RETURN
END IF

```

* min point
* max point

* set counter

* JEOL file

This is the subroutine to draw a NMR file on the screen.

```

SCREEN 12
COLOR DATACOL%,BACKCOL%
WINDOW (1,50):(SIZE%2,500)
YEXPFAC=(500/RANGE&)*GAIN(FILETYPE%(K%))
FOR I%=1 TO SIZE%2
  IF COUNT%=1 THEN D&(I%)=D&(I%)-MIN&
  IF I%>1 THEN
    TEMP1&=DA(I%)*YEXPFAC+YOFFSET%:FILETYPE%(K%)
    TEMP2&=DA(I%+1)*YEXPFAC+YOFFSET%:FILETYPE%(K%)
    LINE (I%,TEMP1&)-(I%+1,TEMP2&),SPECTCL%
  END IF
NEXT I%
INCR COUNT%
RETURN

```

* set colors
* y expansion
* adjust min

Code Listing for LCNMR11.INC

This is the subroutine to draw an axis on a NMR spectrum.

```

SELECT CASE K%
CASE 1,2,3,4,5 : TEMP1%=600 : TEMP2%=SIZE%/2
CASE 6 : TEMP1%=SIZE%/2-1 : TEMP2%=SIZE%/2
CASE 7 : TEMP1%=2465 : TEMP2%=2478
END SELECT
HMDS%=0 : MAX&=0
FOR I%=TEMP1% TO TEMP2%
  IF DA(I%)>MAX& THEN MAX&=DA(I%) : HMDS%=1%
NEXT I%
SELECT CASE K%
CASE 1,2,3,4,5
  TEMP3%=0 : TEMP2%=9
  TEMP3=0.5 : TEMP4=PPMPT2KH
  TEMP5=HMDSHIFT
CASE 6
  TEMP1%=0 : TEMP2%=19
  TEMP3=1.5 : TEMP4=PPMPT8KH
  TEMP5=HMDSHIFT
CASE 7
  TEMP1%=-25 : TEMP2%=250
  TEMP3=-25.0 : TEMP4=PPMPT8KC
  TEMP5=CDCL3SHIFT

```

* find max

* begin, end,
* step, and
* ppm/pt,
* shift ref
* axis scales

```

Problem:
  This is a minisubroutine to print an error message if reading a bad file.
LOCATE 8,5 : PRINT CHR$(201);STRINGS(60,205);CHR$(187);
FOR I%=9 TO 15
  LOCATE I%,5 : PRINT CHR$(186);TAB(75);CHR$(186);
NEXT I%
LOCATE 16,5 : PRINT CHR$(200);STRINGS(60,205);CHR$(186);
TEMP$="Premature EOF while reading file "+FILENAME$
COLOR 31,4 : LOCATE 11,24 : PRINT "" We got a problem here ""
COLOR 14,4 : LOCATE 13,40-5*LEN(TEMP$) : PRINT TEMP$
COLOR 0,3 : LOCATE 24,27 : PRINT " Press any key to continue ";
AS=INPUT$(1)
GOTO MainMenu

```

* set counter

```

CASE 1
LOCATE 1,1 : PRINT CHR$(201),STRINGS$(54,205),CHR$(187);
LOCATE 2,1 : PRINT CHR$(186),STRINGS$(34,32),CHR$(186);
LOCATE 3,1 : PRINT CHR$(186),STRINGS$(54,186),CHR$(182);
LOCATE 4,1 : PRINT CHR$(186),STRINGS$(54,32),CHR$(186);
LOCATE 5,1 : PRINT CHR$(204),STRINGS$(54,205),CHR$(186);
LOCATE 5,9 : PRINT CHR$(208);
LOCATE 5,28 : PRINT CHR$(203);
FOR I%=6 TO 18
LOCATE I%,1 : PRINT CHR$(186),TAB(9),CHR$(179),TAB(26),CHR$(186);
NEXT I%
LOCATE 18,1 : PRINT CHR$(200),STRINGS$(7,205),CHR$(207);
PRINT STRINGS$(18,205),CHR$(186);
LOCATE 7,1 : PRINT CHR$(186),STRINGS$(7,186),CHR$(187);
PRINT STRINGS$(18,186),CHR$(182);
LOCATE 2,5 : PRINT "Xch3"; Xch2 Xch Xcof;
LOCATE 2,15 : PRINT "Xch3"; Xch2 Xch Xcof;
LOCATE 6,12 : PRINT "Shift: Int";
FOR I%=1 TO 8
LOCATE (I%-1)*2+8,3 : PRINT CHR$(I%+64);
LOCATE (I%-1)*2+8,4 : PRINT INTNAMES$(I,I%);
NEXT I%
NEXT I%
* Next is screen for class properties - not currently used.
* LOCATE 5,32 : PRINT CHR$(203);
* LOCATE 5,36 : PRINT CHR$(185);
* FOR I%=6 TO 18
* LOCATE I%,32 : PRINT CHR$(186),TAB(50),CHR$(186);
* NEXT I%
* LOCATE 18,32 : PRINT CHR$(200),STRINGS$(23,205),CHR$(186);
CASE 2,3,4,5
IF FILETYPE$(K%)=2 THEN
TEMP$="Cun Caub Cech3 Cach2Cach *
TEMP$=TEMP$+"Cacq Cabet Cch2>a Cch3>a
ELSE
TEMP$="Cun Caub Cech3 Cbh Cch2>a Cch3>a
TEMP$=TEMP$+"Cacq Cabet Cch2>a Cch3>a
END IF
TEMP%=FILETYPE$(K%)
LOCATE 1,1 : PRINT CHR$(201),STRINGS$(78,205),CHR$(187);
LOCATE 2,1 : PRINT CHR$(186),STRINGS$(78,32),CHR$(186);
LOCATE 3,1 : PRINT CHR$(186),STRINGS$(78,32),CHR$(186);
LOCATE 4,1 : PRINT CHR$(204),STRINGS$(78,205),CHR$(185);
LOCATE 4,24 : PRINT CHR$(208); LOCATE 4,29 : PRINT CHR$(208);
LOCATE 4,52 : PRINT CHR$(208); LOCATE 4,57 : PRINT CHR$(208);
FOR I%=5 TO 13
LOCATE I%,1 : PRINT CHR$(179); LOCATE I%,24 : PRINT CHR$(179);
IF I%<=11 THEN
LOCATE I%,28 : PRINT CHR$(179); LOCATE I%,52 : PRINT CHR$(179);
END IF
LOCATE I%,57 : PRINT CHR$(179); LOCATE I%,80 : PRINT CHR$(179);
NEXT I%
LOCATE 14,1 : PRINT CHR$(182),STRINGS$(22,186),CHR$(217);
LOCATE 12,28 : PRINT CHR$(182),STRINGS$(22,186),CHR$(217);
LOCATE 14,57 : PRINT CHR$(182),STRINGS$(22,186),CHR$(217);
LOCATE 2,5 : PRINT TEMP$
FOR I%=1 TO 5
LOCATE (I%-1)*2+5,3 : PRINT CHR$(I%+64);
IF I%<=4 THEN LOCATE (I%-1)*2+8,4 : PRINT INTNAMES$(TEMP%,I%);
NEXT I%

```

```

CASE ELSE
SCREEN 0 : COLOR 120
LOCATE 12,30 : PRINT "We gotta problem!!";
AS=INPUT$(1)
GOTO MainMenu
END SELECT
ZERO%=HMDS% + INT(TEMP5/TEMP4)
* IF K%=6 OR K%=7 THEN ZERO%=4096
LINE (0,10):(SIZE%2,-10),AXISCOL%
OPEN "CHARACTR.DAT" FOR RANDOM AS #1
DRAW "84"
DRAW "C"+STR$(AXISCOL%)
FOR I=TEMP1% TO TEMP2% STEP TEMP3
IF INT(I/2)=I/2 THEN
TEMP3%=-27
ELSEIF INT(I/1)=I/1 THEN
TEMP3%=-20
ELSE
TEMP3%=-13
END IF
TEMP1=ZERO% - (I/TEMP4)
LINE (TEMP1,-10)-(TEMP1,TEMP3%),AXISCOL%
IF INT(I/2)=I/2 THEN
TEMP4%=PMAP(INT(TEMP1),0,-13)
TEMP1$=STR$(0)
FOR I%=1 TO LEN(TEMP1$)
IF ASC(MID$(TEMP1$,I%,1))>=33 AND ASC(MID$(TEMP1$,I%,1))<=122 THEN
GET #1,ASC(MID$(TEMP1$,I%,1))
DRAW "BM"+STR$(TEMP4%)+",475 TAO "+CHR$(I)
END IF
INCR TEMP4%,10
NEXT I%
END IF
NEXT I
TEMP1$="PPM" : TEMP4%=5
FOR I%=1 TO LEN(TEMP1$)
IF ASC(MID$(TEMP1$,I%,1))>=33 AND ASC(MID$(TEMP1$,I%,1))<=122 THEN
GET #1,ASC(MID$(TEMP1$,I%,1))
DRAW "BM"+STR$(TEMP4%)+",475 TAO "+CHR$(I)
END IF
INCR TEMP4%,12
NEXT I%
CLOSE 1
RETURN

```

Code Listing for LCNMR12.INC

This is the subroutine to draw the average structure screens.

SELECT CASE FILETYPE\$(K%)

```

FOR I%=1 TO LEN(FILETYPE$(FILETYPE$(K%)))
GET #1,ASC(MID$(FILETYPE$(FILETYPE$(K%)),I%,1))
DRAW "BM"+STR$(TEMP%)+";"+TEMP2$+"TAO "+CHARS
INCR TEMP%,12
NEXT I%
CLOSE #1
RETURN

```

```

' get char
' draw type

```

Code Listing for LCNMR13.INC

```

Subroutine to calculate and draw the shift info.

```

```

SELECT CASE FILETYPE$(K%)
CASE 1 : TEMP3%=6 : TEMP1=PPMPT2KH
CASE 2 : TEMP3%=13 : TEMP1=PPMPT2KH
CASE 3 : TEMP3%=13 : TEMP1=PPMPT2KH
CASE 4 : TEMP3%=13 : TEMP1=PPMPT2KH
CASE 5 : TEMP3%=13 : TEMP1=PPMPT2KH
CASE 6 : TEMP3%=4 : TEMP1=PPMPT8KH
CASE 7 : TEMP3%=4 : TEMP1=PPMPT8KG
END SELECT

```

```

' Alkanes
' Monocyclic
' Dicyclic
' Fluorene
' Phenan
' 1H Static
' 13C Static

```

```

' First calc shift divisions in pts and draw shift lines.

```

```

I%=FILETYPE$(K%)
OPEN "CHARACTR DAT" FOR RANDOM AS #1
DRAW "S4 C"+STR$(SHIFTCL%)
FOR I%=1 TO TEMP3%
PT%(I%)=ZERO%INT(PPM(I%)/TEMP1)
PPM(I%)=TEMP1*(ZERO%PT%(I%))
TEMP1%=PT%(I%)
LINE (TEMP1%,-3):(TEMP1%,0)YEXPAC+YOFFSET%(I%)+50,SHIFTCL%
TEMP2%=PMAP(PT%(I%),0)
TEMP1%=PMAP(PT%(I%),0)
GET #1,I%+64
IF TEMP2%<485 AND TEMP2%>1 THEN
DRAW "BM"+STR$(TEMP1%)+";"+STR$(TEMP2%)+TAO "+CHARS" draw char
END IF
NEXT I%
CLOSE #1
RETURN

```

```

' set up for
' labeling
' size - color

```

Code Listing for LCNMR14.INC

```

Subroutine to calculate and draw the baseline info.

```

```

SELECT CASE FILETYPE$(K%)

```

```

FOR I%=5 TO 8
LOCATE (I%-5)*2+5,31 : PRINT CHR$(I%+64);
IF I%<=7 THEN LOCATE (I%-5)*2+6,32 : PRINT INT(TEMP%);
NEXT I%
FOR I%=9 TO 13
LOCATE (I%-9)*2+5,50 : PRINT CHR$(I%+64);
IF I%<=12 THEN LOCATE (I%-9)*2+6,60 : PRINT INT(TEMP%);
NEXT I%
LOCATE 15, 5 : PRINT "Number Of Scans:"

```

```

' Next is screen for class properties - is not currently used.

```

```

LOCATE 13,28 : PRINT CHR$(216);STRINGS(28,100);CHR$(191);
FOR I%=14 TO 17
LOCATE I%,28 : PRINT CHR$(179);TAB(95);CHR$(179);
NEXT I%

```

```

LOCATE 18,28 : PRINT CHR$(192);STRINGS(28,100);CHR$(217);
LOCATE 14,28 : PRINT "Celane"; : LOCATE 14,43 : PRINT "OI";
LOCATE 15,28 : PRINT "Density"; : LOCATE 15,44 : PRINT "Vcl";
LOCATE 16,28 : PRINT "Prop3"; : LOCATE 16,43 : PRINT "Prop6";
LOCATE 17,28 : PRINT "Prop7"; : LOCATE 17,43 : PRINT "Prop8";
CASE 6,7
' Statics
LOCATE 1,10 : PRINT CHR$(201);STRINGS(60,205);CHR$(187);
LOCATE 2,10 : PRINT CHR$(196);STRINGS(60, 32);CHR$(189);
LOCATE 3,10 : PRINT CHR$(188);STRINGS(60, 32);CHR$(188);
LOCATE 4,10 : PRINT CHR$(200);STRINGS(60,205);CHR$(188);
FOR I%=32 TO 55 STEP 23
LOCATE 1,I% : PRINT CHR$(209); : LOCATE 2,I% : PRINT CHR$(179);
LOCATE 3,I% : PRINT CHR$(179); : LOCATE 4,I% : PRINT CHR$(207);
NEXT I%

```

```

LOCATE 5, 1 : PRINT CHR$(219);STRINGS(15, 100);CHR$(191);
FOR I%=6 TO 12
LOCATE I%, 1 : PRINT CHR$(179);STRINGS(15, 32);CHR$(179);
NEXT I%

```

```

LOCATE 13, 1 : PRINT CHR$(192);STRINGS(15, 100);CHR$(217);
LOCATE 2, 2 : PRINT "Scans";
LOCATE 2,13 : PRINT "Aromatic Integral";
LOCATE 2,35 : PRINT "Aliphatic Integral";
LOCATE 2,58 : PRINT "Aromaticity";
FOR I%=1 TO 4
LOCATE (I%-1)*2+6,3 : PRINT CHR$(I%+64);
NEXT I%

```

```

' Will draw file name and integration type on the screen.

```

```

SELECT CASE FILETYPE$(K%)
CASE 1 : TEMP1$="312" : TEMP2$="330"
CASE 2,3,4,5 : TEMP1$="270" : TEMP2$="289"
CASE 6,7 : TEMP1$="220" : TEMP2$="238"
END SELECT

```

```

OPEN "CHARACTR DAT" FOR RANDOM AS #1
DRAW "S4 C"+STR$(LABELCL%)
TEMP%=10
TEMP$=RIGHT$(FILENAME$(K%),LEN(FILENAME$(K%))-LEN(NM$(DIR$)))
FOR I%=1 TO LEN(TEMP$)
GET #1,ASC(MID$(TEMP$,I%,1))
DRAW "BM"+STR$(TEMP%)+";"+TEMP1$+"TAO "+CHARS
INCR TEMP%,12
NEXT I%
TEMP%=10

```

```

' set up for
' labeling
' size - color
' x position

```

```

' get char
' draw filename

```

```

END SELECT

```

```

' Will draw file name and integration type on the screen.

```

```

SELECT CASE FILETYPE$(K%)
CASE 1 : TEMP1$="312" : TEMP2$="330"
CASE 2,3,4,5 : TEMP1$="270" : TEMP2$="289"
CASE 6,7 : TEMP1$="220" : TEMP2$="238"
END SELECT

```

```

OPEN "CHARACTR DAT" FOR RANDOM AS #1
DRAW "S4 C"+STR$(LABELCL%)
TEMP%=10
TEMP$=RIGHT$(FILENAME$(K%),LEN(FILENAME$(K%))-LEN(NM$(DIR$)))
FOR I%=1 TO LEN(TEMP$)
GET #1,ASC(MID$(TEMP$,I%,1))
DRAW "BM"+STR$(TEMP%)+";"+TEMP1$+"TAO "+CHARS
INCR TEMP%,12
NEXT I%
TEMP%=10

```

```

' set up for
' labeling
' size - color
' x position

```

```

' get char
' draw filename

```

```

END SELECT

```

```

CASE 1 : TEMP4% = 4 : TEMP1 = PPMPT2KH
CASE 2 : TEMP4% = 0 : TEMP1 = PPMPT2KH
CASE 3 : TEMP4% = 8 : TEMP1 = PPMPT2KH
CASE 4 : TEMP4% = 6 : TEMP1 = PPMPT2KH
CASE 5 : TEMP4% = 8 : TEMP1 = PPMPT2KH
CASE 6 : TEMP4% = 4 : TEMP1 = PPMPTBKH
CASE 7 : TEMP4% = 4 : TEMP1 = PPMPTBKG
END SELECT

* Next calculate and draw the baselines for integration.
% = FILETYPE%(K%)
FOR % = 1 TO TEMP4% STEP 2
  BEGPT%(K%) = ZERO% * INT(BASEEND(K%, %) / TEMP1)
  BEGAVG%(K%) = ZERO% * INT(BASEEND(K%, %) + 1) / TEMP1
  FOR J% = 15 TO 15
    INCR BEGAVG%(K%, %) , DA / BEGPT%(K%, %) + J%
    INCR ENDAVG%(K%, %) , DA / ENDPT%(K%, %) + J%
  NEXT J%
  BEGAVG%(K%, %) = BEGAVG%(K%, %) / 30
  ENDAVG%(K%, %) = ENDAVG%(K%, %) / 30
  BEGPT%(K%, %) + 1) = BEGPT%(K%, %) : BEGAVG%(K%, %) + 1) = BEGAVG%(K%, %)
  ENDPT%(K%, %) + 1) = ENDPT%(K%, %) : ENDAVG%(K%, %) + 1) = ENDAVG%(K%, %)
  SLOPE = (ENDAVG%(K%, %) - BEGAVG%(K%, %) / (ENDPT%(K%, %) - BEGPT%(K%, %)))
  INTCP = BEGAVG%(K%, %) - (SLOPE * BEGPT%(K%, %))
  FOR J% = BEGPT%(K%, %) TO ENDPT%(K%, %)
    BA(J%) = (SLOPE * J%) + INTCP
    PSET (J%, BA(J%)) * VEYFFAC + YOFFSET%(K%, %) BASECOL%
  NEXT J%
NEXT %
RETURN

* Next are the class physical properties - not currently used.
LOCATE 8.35 PRINT USING "Cetane: %";
LOCATE 8.35 PRINT USING "Density: %";
LOCATE 8.35 PRINT USING "Property 4: %";
LOCATE 10.35 PRINT USING "Property 5: %";
LOCATE 11.35 PRINT USING "Property 6: %";
LOCATE 12.35 PRINT USING "Property 7: %";
LOCATE 13.35 PRINT USING "Property 8: %";
CASE 2
LOCATE 3.4 : PRINT USING "%";
LOCATE 3.11 : PRINT USING "%";
LOCATE 3.18 : PRINT USING "%";
LOCATE 3.25 : PRINT USING "%";
LOCATE 3.32 : PRINT USING "%";
LOCATE 3.38 : PRINT USING "%";
LOCATE 3.47 : PRINT USING "%";
LOCATE 3.55 : PRINT USING "%";
LOCATE 3.63 : PRINT USING "%";
LOCATE 3.70 : PRINT USING "%";
TEMP% = FILETYPE%(K%)
FOR % = 1 TO 5
  LOCATE (%-1)*2+5, 0 : PRINT USING "%";
  IF % <= 4 AND INTNAMES(TEMP%, %) <= " THEN
    LOCATE (%-1)*2+6, 15 : PRINT USING "%";
  END IF
NEXT %
FOR % = 5 TO 8
  LOCATE (%-5)*2+5, 37 : PRINT USING "%";
  IF % <= 7 AND INTNAMES(TEMP%, %) <= " THEN
    LOCATE (%-5)*2+6, 43 : PRINT USING "%";
  END IF
NEXT %
LOCATE 18, 10 : PRINT USING "%";
* Scans

* Next are the class physical properties - not currently used.
LOCATE 14.36 PRINT USING "%";
LOCATE 14.48 PRINT USING "%";
LOCATE 15.37 PRINT USING "%";
LOCATE 15.49 PRINT USING "%";
LOCATE 16.50 PRINT USING "%";
LOCATE 17.38 PRINT USING "%";
LOCATE 17.50 PRINT USING "%";
CASE 3, 4, 5
IF FILETYPE%(K%) = 3 THEN TEMP1% = 0 : TEMP2% = 0 : TEMP3% = 221 : DI
IF FILETYPE%(K%) = 4 THEN TEMP1% = 28 : TEMP2% = 2 : TEMP3% = 233 : FI
IF FILETYPE%(K%) = 5 THEN TEMP1% = 62 : TEMP2% = 4 : TEMP3% = 245 : PHENAN
TEMP% = FILETYPE%(K%)
LOCATE 3.4 : PRINT USING "%";
LOCATE 3.11 : PRINT USING "%";
LOCATE 3.18 : PRINT USING "%";
LOCATE 3.25 : PRINT USING "%";

```

```

* Alkanes
* Monocyclic
* Dicyclic
* Fluorene
* Phenan
* 1H Static
* 13C Static

CASE 1 : TEMP4% = 4 : TEMP1 = PPMPT2KH
CASE 2 : TEMP4% = 0 : TEMP1 = PPMPT2KH
CASE 3 : TEMP4% = 8 : TEMP1 = PPMPT2KH
CASE 4 : TEMP4% = 6 : TEMP1 = PPMPT2KH
CASE 5 : TEMP4% = 8 : TEMP1 = PPMPT2KH
CASE 6 : TEMP4% = 4 : TEMP1 = PPMPTBKH
CASE 7 : TEMP4% = 4 : TEMP1 = PPMPTBKG
END SELECT

* Next calculate and draw the baselines for integration.
% = FILETYPE%(K%)
FOR % = 1 TO TEMP4% STEP 2
  BEGPT%(K%, %) = ZERO% * INT(BASEEND(K%, %) / TEMP1)
  BEGAVG%(K%, %) = ZERO% * INT(BASEEND(K%, %) + 1) / TEMP1
  FOR J% = 15 TO 15
    INCR BEGAVG%(K%, %) , DA / BEGPT%(K%, %) + J%
    INCR ENDAVG%(K%, %) , DA / ENDPT%(K%, %) + J%
  NEXT J%
  BEGAVG%(K%, %) = BEGAVG%(K%, %) / 30
  ENDAVG%(K%, %) = ENDAVG%(K%, %) / 30
  BEGPT%(K%, %) + 1) = BEGPT%(K%, %) : BEGAVG%(K%, %) + 1) = BEGAVG%(K%, %)
  ENDPT%(K%, %) + 1) = ENDPT%(K%, %) : ENDAVG%(K%, %) + 1) = ENDAVG%(K%, %)
  SLOPE = (ENDAVG%(K%, %) - BEGAVG%(K%, %) / (ENDPT%(K%, %) - BEGPT%(K%, %)))
  INTCP = BEGAVG%(K%, %) - (SLOPE * BEGPT%(K%, %))
  FOR J% = BEGPT%(K%, %) TO ENDPT%(K%, %)
    BA(J%) = (SLOPE * J%) + INTCP
    PSET (J%, BA(J%)) * VEYFFAC + YOFFSET%(K%, %) BASECOL%
  NEXT J%
NEXT %
RETURN

This is the subroutine to draw the average structure data.

SELECT CASE FILETYPE%(K%)
CASE 1
  FOR % = 1 TO 6
    LOCATE (%-1)*2+8, 11 : PRINT USING "%";
    IF INTNAMES(TEMP%, %) <= " THEN
      IF % <= 6 THEN
        LOCATE (%-1)*2+9, 17
        PRINT USING "%";
      END IF
    END IF
  NEXT %
LOCATE 4.5 : PRINT USING "%";
LOCATE 4.13 : PRINT USING "%";
LOCATE 4.24 : PRINT USING "%";
LOCATE 4.34 : PRINT USING "%";
LOCATE 4.45 : PRINT USING "%";
* Scans
* Xch3
* Xch2
* Xch
* Xcq

```

Code Listing for LCNMR15.INC

This is the subroutine to draw the average structure data.

Code Listing for LCNMR16.INC

```

LOCATE 3.32 : PRINT USING '#####.VAL(D6( 38+TEMP1%)) : ' Cch2
LOCATE 3.38 : PRINT USING '#####.VAL(D6(151+TEMP2%)) : ' Ccacq
LOCATE 3.47 : PRINT USING '#####.VAL(D6( 32+TEMP1%)) : ' Ccbb
LOCATE 3.55 : PRINT USING '#####.VAL(D6( 40+TEMP1%)) : ' Cch2>a
LOCATE 3.63 : PRINT USING '#####.VAL(D6( 42+TEMP1%)) : ' Cch3>a
LOCATE 3.70 : PRINT USING '#####.VAL(D6(48+TEMP1%)) : ' MW
FOR I%=1 TO 5
  LOCATE (I%-1)*2+5, 0 : PRINT USING '#####.PPM(TEMP%,I%);
  IF I%<=4 AND INTNAME$(TEMP%,I%)<>' THEN
    LOCATE (I%-1)*2+6,15 : PRINT USING '#####.VAL(D6(I%+TEMP3%));
  END IF
NEXT I%
FOR I%=5 TO 8
  LOCATE (I%-5)*2+5,37 : PRINT USING '#####.PPM(TEMP%,I%);
  IF I%<=7 AND INTNAME$(TEMP%,I%)<>' THEN
    LOCATE (I%-5)*2+6,43 : PRINT USING '#####.VAL(D6(I%+TEMP3%));
  END IF
NEXT I%
FOR I%=9 TO 13
  LOCATE (I%-9)*2+5,65 : PRINT USING '#####.PPM(TEMP%,I%);
  IF I%<=12 AND INTNAME$(TEMP%,I%)<>' THEN
    LOCATE (I%-9)*2+6,71 : PRINT USING '#####.VAL(D6(I%+TEMP3%));
  END IF
NEXT I%
LOCATE 10,10 : PRINT USING '#####.NOSC% : ' # Scans

```

```

* Next are the class physical properties - not currently used.
* TEMP%=FILETYPE%(K%)*378
* LOCATE 14,36 : PRINT USING '#####.VAL(D6(173+TEMP%)) : ' Cetane
* LOCATE 14,46 : PRINT USING '#####.VAL(D6(174+TEMP%)) : ' Cl
* LOCATE 15,37 : PRINT USING '#####.VAL(D6(175+TEMP%)) : ' Density
* LOCATE 15,46 : PRINT USING '#####.VAL(D6(176+TEMP%)) : ' Vcal
* LOCATE 16,38 : PRINT USING '#####.VAL(D6(177+TEMP%)) : ' Prop5
* LOCATE 16,50 : PRINT USING '#####.VAL(D6(178+TEMP%)) : ' Prop6
* LOCATE 17,38 : PRINT USING '#####.VAL(D6(179+TEMP%)) : ' Prop7
* LOCATE 17,50 : PRINT USING '#####.VAL(D6(180+TEMP%)) : ' Prop8
CASE 67
TEMP%=FILETYPE%(K%)
IF TEMP%=6 THEN T%=0
IF TEMP%=7 THEN T%=2
LOCATE 3,15 : PRINT USING '#####.VAL(D6(259+T%)) : ' Atom
LOCATE 3,38 : PRINT USING '#####.VAL(D6(258+T%)) : ' Aliph
FOR I%=1 TO 4
  LOCATE (I%-1)*2+6,6
  PRINT USING '#####.PPM(TEMP%,I%);
NEXT I%
LOCATE 3,58
PRINT USING '#####.VAL(D6(133-(TEMP%-6)));
LOCATE 3,2 : PRINT USING '#####.NOSC%
END SELECT
RETURN

```

This is the subroutine to mark the active shift divider.

```

T%=FILETYPE%(K%)
SELECT CASE FILETYPE%(K%)
CASE 1
  LOCATE (ACTIVE%(1,T%)-1)*2+8,5
CASE 2,3,4,5
  IF ACTIVE%(1,T%)>=1 AND ACTIVE%(1,T%)<=4 THEN
    LOCATE (ACTIVE%(1,T%)-1)*2+5, 5
  END IF
IF ACTIVE%(1,T%)>=5 AND ACTIVE%(1,T%)<=8 THEN
  LOCATE (ACTIVE%(1,T%)-5)*2+5,33
END IF
IF ACTIVE%(1,T%)>=9 AND ACTIVE%(1,T%)<=13 THEN
  LOCATE (ACTIVE%(1,T%)-9)*2+5,61
END IF
CASE 67
  LOCATE (ACTIVE%(1,T%)-1)*2+8,5
END SELECT
IF TEMP%='ON' THEN PRINT CHR$(17);CHR$(206);CHR$(16);
IF TEMP%='OFF' THEN PRINT SPACE$(3);
RETURN

```

Code Listing for LCNMR17.INC

This is the subroutine to mark the active baseline endpoints.

```

SELECT CASE FILETYPE%(K%)
CASE 1 : TEMP1%=7 : TEMP1=PPMPT2KH
CASE 2 : TEMP1%=7 : TEMP1=PPMPT2KH
CASE 3 : TEMP1%=7 : TEMP1=PPMPT2KH
CASE 4 : TEMP1%=7 : TEMP1=PPMPT2KH
CASE 5 : TEMP1%=7 : TEMP1=PPMPT2KH
CASE 6 : TEMP1%=22 : TEMP1=PPMPT8KH
CASE 7 : TEMP1%=22 : TEMP1=PPMPT8KH
END SELECT
* First calc shift divisions in pts and draw shift lines.
T%=FILETYPE%(K%)
TEMP%=ZERO*INT(BASEEND(T%,ACTIVE%(2,T%))/TEMP1)
IF TEMP%='ON' THEN TEMP2%=BASECOL%
IF TEMP%='OFF' THEN TEMP2%=BACKCOL%
LINE (TEMP%,11),(TEMP%+TEMP1%-25),TEMP2%

```

* Alkanes
* Monocyclic
* Dicyclic
* Fluorene
* Phenan
* 1H Static
* 13C Static

* calc pt
* set color
* draw mark

```
LINE (TEMP%-11)-(TEMP%+TEMP1%-25),TEMP2%
RETURN
```

Code Listing for LCNMR18.INC

```
Subroutine to draw the summary screen.
```

```
SCREEN 0 : WIDTH 80
COLOR 15, 0 : CLS

* First is heading information.
COLOR 9, 0 : LOCATE 1, 1 : PRINT "Fuel Name";
COLOR 12, 0 : LOCATE 2, 2 : PRINT FUELNAME$(L%);
COLOR 10, 0 : LOCATE 1, 60 : PRINT DATES;
COLOR 10, 0 : LOCATE 2, 70 : PRINT TIMES;

* Next is aromaticity box.
COLOR 0, 4
LOCATE 1, 20 : PRINT CHR$(201);STRINGS(30,205);CHR$(187);
LOCATE 2, 20 : PRINT CHR$(186);STRINGS(30, 32);CHR$(186);
LOCATE 3, 20 : PRINT CHR$(200);STRINGS(30,205);CHR$(188);

* Next is moles and aromaticities box.
COLOR 10, 1
LOCATE 4, 1 : PRINT CHR$(201);STRINGS(70,205);CHR$(187);
FOR I%=5 TO 12
  LOCATE I%, 1 : PRINT CHR$(186);STRINGS(70, 32);CHR$(186);
NEXT I%
LOCATE 13, 1 : PRINT CHR$(200);STRINGS(70,205);CHR$(188);
LOCATE 4, 26 : PRINT CHR$(209) : LOCATE 5, 28 : PRINT CHR$(179);
LOCATE 6, 1 : PRINT CHR$(186);STRINGS(28,186);CHR$(217);
LOCATE 9, 71 : PRINT STRINGS(6,186);
COLOR 11, 1
LOCATE 5, 3 : PRINT "Moles and Aromaticities";

* Next is physical properties box.
COLOR 10, 1
LOCATE 15, 1 : PRINT CHR$(201);STRINGS(70,205);CHR$(187);
FOR I%=16 TO 23
  LOCATE I%, 1 : PRINT CHR$(186);STRINGS(70, 32);CHR$(186);
NEXT I%
LOCATE 24, 1 : PRINT CHR$(200);STRINGS(70,205);CHR$(188);
LOCATE 15, 33 : PRINT CHR$(209) : LOCATE 16, 33 : PRINT CHR$(179);
LOCATE 17, 1 : PRINT CHR$(186);STRINGS(31,186);CHR$(217);
LOCATE 22, 1 : PRINT CHR$(186);STRINGS(78,186);CHR$(182);
FOR I%=13 TO 70 STEP 9
  IF I%>35 THEN TEMP%=16 ELSE TEMP%=18
  FOR J%=TEMP% TO 21
    LOCATE J%, I% : PRINT CHR$(179);
  NEXT J%
NEXT I%
COLOR 11, 1
```

```
LOCATE 16, 3 : PRINT "Physical Properties for Fuel";
* Next are instructions at bottom of screen.
COLOR 3, 0 : LOCATE 25,16
PRINT "Press <O> to quit to Main Menu, <RETURN> to continue";
* Next must draw in the data tables.
COLOR 14, 4
LOCATE 2,23 : PRINT "13C Arom";
LOCATE 2,42 : PRINT "1H Arom";
COLOR 14, 1
LOCATE 8, 4 : PRINT "Alkanes";
LOCATE 9, 4 : PRINT "Monocyclics";
LOCATE 10, 4 : PRINT "Dicyclics";
LOCATE 11, 4 : PRINT "Fluorenes";
LOCATE 12, 4 : PRINT "Phenanthrenes";
LOCATE 7,22 : PRINT "C Aromal": C total:
LOCATE 8,73 : PRINT "fa": fa: F total;
TEMP%=0 : TEMP1%=18 : TEMP2%=41
FOR I%=1 TO 42
  SELECT CASE I%
    CASE 4 : TEMPS="Cetane"
    CASE 5 : TEMPS="50% BP"
    CASE 6 : TEMPS="Pour Pt"
    CASE 8 : TEMPS="Flash Pt"
    CASE 9 : TEMPS="Density"
    CASE 11 : TEMPS="Cloud Pt"
    CASE 12 : TEMPS="Viscosity"
    CASE 13 : TEMPS="Filter"
    CASE 28 : TEMPS="Ht Comb"
    CASE 28 : TEMPS="% Arom"
    CASE 31 : TEMPS="Cat Inhd"
    CASE 32 : TEMPS="Sp Grav"
    CASE 33 : TEMPS="Ht BP"
    CASE 34 : TEMPS="10% BP"
    CASE 35 : TEMPS="80% BP"
    CASE 36 : TEMPS="End BP"
    CASE 37 : TEMPS="Resid C"
    CASE ELSE : TEMPS=""
  END SELECT
  IF TEMP%<=I% THEN
    LOCATE TEMP1%,TEMP2% : PRINT TEMPS;
    INCR TEMP% : INCR TEMP2%
  IF TEMP2%>68 THEN TEMP2%=5 : INCR TEMP1%,2
  END IF
NEXT I%
LOCATE 23, 3 : PRINT "Elemental Analysis";
LOCATE 23,25 : PRINT "C": H: H (NMR)";
* Next must draw in the data.
COLOR 15, 4
LOCATE 2,33 : PRINT USING "#####";VAL(D$(132))
LOCATE 2,51 : PRINT USING "#####";VAL(D$(133))
COLOR 15, 1
TS="#####": AS="#####"
LOCATE 8,36 : PRINT USING TS;VAL(D$(114))
LOCATE 8,59 : PRINT USING AS; VAL(D$(116))
FOR I%=1 TO 4
  SELECT CASE I%
    CASE 1 : I%=0
    " Monocyclics
```


Code Listing for LCNMR19.INC

Subroutine to do the control options from the names menu.

```

CASE 2 : T%=25
CASE 3 : T%=51
CASE 4 : T%=77
END SELECT
LOCATE 1%+8,22 : PRINT USING T6;VAL(D6(24+T%))
LOCATE 1%+8,38 : PRINT USING T8;VAL(D6(25+T%))
LOCATE 1%+8,48 : PRINT USING A5;VAL(D6(26+T%))
LOCATE 1%+8,58 : PRINT USING A6;VAL(D6(27+T%))
NEXT 1%
LOCATE 10,71 : PRINT USING A6;VAL(D6(146))

```

```

TEMP%=0 : TEMP1%=17 : TEMP2%=41
FOR 1%=1 TO 42
IF TEMP%<20 THEN

```

```

SELECT CASE 1%
CASE 4 : TEMPS="*****"
CASE 5 : TEMPS="*****"
CASE 6 : TEMPS="*****"
CASE 8 : TEMPS="*****"
CASE 9 : TEMPS="*****"
CASE 11 : TEMPS="*****"
CASE 12 : TEMPS="*****"
CASE 13 : TEMPS="*****"
CASE 26 : TEMPS="*****"
CASE 28 : TEMPS="*****"
CASE 31 : TEMPS="*****"
CASE 32 : TEMPS="*****"
CASE 33 : TEMPS="*****"
CASE 34 : TEMPS="*****"
CASE 35 : TEMPS="*****"
CASE 36 : TEMPS="*****"
CASE 37 : TEMPS="*****"
CASE ELSE : TEMPS=""

```

```

END SELECT
IF TEMPS<>"" THEN
LOCATE TEMP1%;TEMP2% : PRINT USING TEMP6;VAL(D6(156+1%));
INCR TEMP% : INCR TEMP2%,9
IF TEMP2%>68 THEN TEMP2%=5 : INCR TEMP1%,2
END IF
END IF

```

```

NEXT 1%
LOCATE 23,28 : PRINT USING "*****"; VAL(D6(138));
LOCATE 23,43 : PRINT USING "*****"; VAL(D6(139));
LOCATE 23,63 : PRINT USING "*****"; VAL(D6(140));

```

Have printed everything so see what to do.

```

Startloop8:
A6=INKEY$
SELECT CASE A6
CASE =
COLOR 10,0
LOCATE 2,70 : PRINT TIMES;
CASE "q";CHR$(27)
GOTO MainMenu
CASE CHR$(13)
RETURN
CASE ELSE
SOUND 1000,3 : SOUND 800,1.5
END SELECT
GOTO Startloop8

```

- * Dicyclics
- * Fluorene
- * Phenan
- * C A/Total
- * C total
- * fa
- * Ftotal
- * fa

Code Listing for LCNMR20.INC

This is the subroutine to get the average structure data.

```

IF CTRLLOPTS(1)="Y" THEN
COLOR 31,4
LOCATE 14,1 : PRINT SPACES(80);
LOCATE 14,24 : PRINT *** Filing the Output Data ***;
GOSUB FileAvgStrData
END IF
IF CTRLLOPTS(4)="Y" THEN
COLOR 31,4
LOCATE 14,1 : PRINT SPACES(80);
LOCATE 14,22 : PRINT *** Printing the Integral Data ***;
GOSUB HardCopyIntegrals
END IF
IF CTRLLOPTS(5)="Y" THEN
COLOR 31,4
LOCATE 14,1 : PRINT SPACES(80);
LOCATE 14,22 : PRINT *** Printing the Results Data ***;
GOSUB HardCopyResults
END IF
IF CTRLLOPTS(6)="Y" THEN
COLOR 31,4
LOCATE 14,1 : PRINT SPACES(80);
LOCATE 14,22 : PRINT *** Printing the Property Data ***;
GOSUB HardCopyProps
END IF
RETURN

```

* File Results

* HVC Integral

* HVC Results

* HVC Props

- * Must first check for file to see if present, if it is, then load data from avg str file. If not present, then flash message, and abort the load, but do not generate error message.

```

COLOR 0,0 : LOCATE 1,1
FILENAME$=INPUTDIR$+FUELNAME$(L%)+".DAT"
SHELL "DIR "+FILENAME$+" > "+SCRDIR$+TEMP.ZZZ
OPEN SCRDIR$+TEMP.ZZZ FOR INPUT AS #1
FOR 1%=1 TO 4
LINE INPUT #1,TEMPS

```

- * C %
- * H %
- * H % (NMR)
- * no key
- * quit
- * return
- * oopel

```

LOCATE 2,24 : PRINT * Help Screen for LC-NMR Software *
.
.   Help Menu Options
COLOR 10, 0
LOCATE 4,12 : PRINT *Key:           Function*
COLOR 11, 0
LOCATE 5,13 : PRINT *G* : LOCATE 6,13 : PRINT *P*
LOCATE 7,13 : PRINT *S* : LOCATE 8,13 : PRINT *B*
LOCATE 8,13 : PRINT *M* : LOCATE 10,13 : PRINT *O*
LOCATE 11,10 : PRINT *<Return>*
LOCATE 12,12 : PRINT *<F1>*
LOCATE 14,12 : PRINT *<F2>*
LOCATE 15,11 : PRINT *<+>*
LOCATE 17, 4 : PRINT *<LEFT, RIGHT ARROW>*
LOCATE 16, 8 : PRINT *<CTRL L-R ARROW>*
LOCATE 20, 8 : PRINT *<PgUp, PgDn>*
LOCATE 21, 5 : PRINT *<CTRL PgUp, PgDn>*
LOCATE 23, 8 : PRINT *<UP, DOWN ARROW>*
LOCATE 25, 8 : PRINT *<Insert, Delete>*
COLOR 14, 0
LOCATE 5,22 : PRINT *Change Spectrum Y Gain (vertical expansion)*
LOCATE 6,22 : PRINT *Change Spectrum Y Offset (vertical position)*
LOCATE 7,22 : PRINT *Change Shift Division Step (in spectral points)*
LOCATE 8,22 : PRINT *Change Baseline Endpoint Vertical Step*
LOCATE 9,22 : PRINT *Calls up menu to change currently displayed file*
LOCATE 10,22 : PRINT *Exit Back to the Main Menu*
LOCATE 11,22 : PRINT *Continue on to the Next Spectrum*
LOCATE 12,22 : PRINT *Calls up this help screen*
LOCATE 14,22 : PRINT *Toggles the display of the integral regions*
LOCATE 15,22 : PRINT *Increase/Decrease the integral display gain by 2x*
LOCATE 17,25 : PRINT *Moves the 'active' shift divider to the left/right*
LOCATE 18,25 : PRINT *Moves 'active' shift divider to the 1/4 by 10x*
LOCATE 20,25 : PRINT *Moves baseline endpoint Up-Dn by baseline step*
LOCATE 21,25 : PRINT *Moves baseline endpoint Up-Dn by step times 10*
LOCATE 23,25 : PRINT *Moves the active shift division indicator Up-Dn*
LOCATE 25,25 : PRINT *Moves the active baseline endpoint left-right*
COLOR 14,3
LOCATE 10,78 : PRINT CHR$(216),STRING$(3,196),CHR$(191)
TEMP$="RETURN"
FOR I%=11 TO 18
  LOCATE I%,78
  COLOR 14, 3 : PRINT CHR$(179),*
  COLOR 0, 3 : PRINT MID$(TEMP$,I%-10,1),*
  COLOR 14, 3 : PRINT CHR$(179)
NEXT I%
LOCATE 17,78 : PRINT CHR$(192),STRING$(3,196),CHR$(217)
.
.   Have printed screen, so get return, redraw spectrum, and go back
TS=INKEY$
WHILE TS<>CHR$(13)
  TS=INKEY$
WEND
CLS
GOSUB DisplayNMRFile
GOSUB DisplayAxis
GOSUB DrawAvgScreens
GOSUB CalculateAndDrawShift
GOSUB CalculateAndDrawBase
GOSUB CalculateIntegrals
GOSUB CalculateAverageStructures

```

* File not found

```

NEXT I%
IF EOF(1) THEN
  COLOR 30, 4
  LOCATE 1,28 : PRINT * *** File not found! *** *
  FOR I%=1 TO 2
    SOUND 1000,3 : SOUND 800,1,5 : DELAY 0.4
  NEXT I%
  CLOSE 1 : KILL SCRDIRS+TEMP.ZZZ
  COLOR 15, 0
  LOCATE 1, 1 : PRINT SPACES$(35)
  RETURN
END IF
CLOSE 1 : KILL SCRDIRS+TEMP.ZZZ
OPEN INPUTDIR$+FUELNAME$(L%)+*.DAT FOR INPUT AS #1
I%=1
WHILE NOT EOF(1) AND I%<350
  INPUT #1,D$(I%)
  INCR I%
WEND
DECR I%
CLOSE #1
RETURN

```

Code Listing for LCNMR21.INC

This is the subtm to menu writes the average structure file.

```

FILENAME$=OUTPTDIR$+FUELNAME$(L%)+*.DAT*
OPEN OUTPTDIR$+FUELNAME$(L%)+*.DAT* FOR OUTPUT AS #1
D$(287)="END"
FOR I%=1 TO 287
  PRINT #1,D$(I%)
NEXT I%
CLOSE 1
RETURN

```

Code Listing for LCNMR22.INC

This is the subroutine to draw the help screen.

```

COLOR 15, 0 : SCREEN 0 : CLS
COLOR 15, 4
LOCATE 1, 5 : PRINT CHR$(201),STRING$(88,205),CHR$(187)
LOCATE 2, 5 : PRINT CHR$(188),STRING$(89, 32),CHR$(188)
LOCATE 3, 5 : PRINT CHR$(200),STRING$(89,205),CHR$(188)
.
.   top line
.   ends
.   bottom line

```

Code Listing for LCNMR25.INC

This is the subroutine to get the name of the blank.

```

OPTNS(1)=1) Blank1*
OPTNS(2)=2) Blank2*
OPTNS(3)=3) Blank3*
    * Will draw the screen.
COLOR 15,0 : CLS
COLOR 10,1
LOCATE 5,15 : PRINT CHR$(218),STRING$(49,199),CHR$(191); * top line
FOR I%=6 TO 16
    LOCATE I%,15 : PRINT CHR$(179),TAB(65),CHR$(179); * middle
NEXT I%
LOCATE 17,15 : PRINT CHR$(192),STRING$(49,199),CHR$(217); * bottom line
COLOR 10,1
LOCATE 8,20 : PRINT TIMES;
LOCATE 8,51 : PRINT DATES;
COLOR 15,1
LOCATE 8,28 : PRINT "Blank Name Options Menu.";
COLOR 12,1
LOCATE 10,23 : PRINT "Please select the appropriate name.";
COLOR 14,1
FOR I%=1 TO 3
    LOCATE (I%-1)*2+12,40-(0.5*LEN(OPTNS(I%)))
    COLOR 11,1 : PRINT LEFT$(OPTNS(I%),1);
    COLOR 14,1 : PRINT RIGHT$(OPTNS(I%),LEN(OPTNS(I%))-1);
NEXT I%
    * Next are commands
COLOR 9,0
LOCATE 21,18 : PRINT "Press the highlighted letter or <ENTER> to select.";
LOCATE 22,20 : PRINT "Press the <Q> to return to the Main Menu.";
    * Next see what to do
COLOR 14,0
LOCATE (OPTN%(7)-1)*2+12,38-(0.5*LEN(OPTNS(OPTN%(7))))
PRINT * "OPTNS(OPTN%(7)).";
Startloop8.
AS=INKEY$
SELECT CASE AS
CASE =
    COLOR 10,1
    LOCATE 8,20 : PRINT TIMES;
CASE "Q",q : CHR$(27)
    GOTO MainMenu
CASE CHR$(13)
    RETURN
CASE "*"
    OPTN%(7)=1 : RETURN
CASE "2"
    OPTN%(7)=2 : RETURN
CASE CHR$(0)+CHR$(72), CHR$(0)+CHR$(80)
    * no key
    * Exit
    * return
    * Ed old file
    * Create new
    * up-down
    
```

Code Listing for LCNMR23.INC

Subroutine to wipe out data for an unused recal fraction.

```

SELECT CASE K%
CASE 1 : T1%=106 : T2%=115 : T3%=205 : T4%=209
CASE 2 : T1%= 3 : T2%= 26 : T3%=210 : T4%=221
CASE 3 : T1%= 28 : T2%= 51 : T3%=222 : T4%=233
CASE 4 : T1%= 54 : T2%= 77 : T3%=234 : T4%=245
CASE 5 : T1%= 80 : T2%=103 : T3%=246 : T4%=257
CASE 6 : T1%=133 : T2%=133 : T3%=256 : T4%=256
CASE 7 : T1%=132 : T2%=132 : T3%=260 : T4%=261
END SELECT
FOR I%=T1% TO T2%
    DS(I%)=..
NEXT I%
FOR I%=T3% TO T4%
    DS(I%)=..
NEXT I%
RETURN
    
```

Code Listing for LCNMR24.INC

Subroutine to wipe out the fraction carbon data if necessary.

```

FOR I%=3 TO 27 : DS(I%+T1%)=0 : NEXT I%
FOR I%=0 TO 7 : DS(I%+T2%)=0 : NEXT I%
FOR I%=0 TO 1 : DS(I%+T3%)=0 : NEXT I%
GOTO CalculateTotalCarbon
    
```

```

GOSUB DrawAvgStrData
TEMP$="ON" : GOSUB MarkActiveShift
TEMP$="ON" : GOSUB MarkActiveBase
RETURN
    
```

```

LOCATE (OPTN%(7)-1)*2+12.38-(0.5*LEN(OPTN$(OPTN%(7))))
COLOR 11,1
PRINT * 'LEFTS (OPTN$(OPTN%(7)),1);
COLOR 14,1
PRINT RIGHTS(OPTN$(OPTN%(7)),LEN(OPTN$(OPTN%(7)))-1);
IF AS=CHRS(0)+CHRS(72) THEN DECR OPTN%(7) ELSE INCR OPTN%(7)
IF OPTN%(7)<1 THEN OPTN%(7)=3
IF OPTN%(7)>3 THEN OPTN%(7)=1
COLOR 14,0
LOCATE (OPTN%(7)-1)*2+12.38-(0.5*LEN(OPTN$(OPTN%(7))))
PRINT * 'OPTN$(OPTN%(7))';
CASE CHRS(0)+CHRS(75),CHRS(0)+CHRS(77)
CASE ELSE
SOUND 1000,3 : SOUND 800,1.5
END SELECT
GOTO Startloop8

Code Listing for LCNMR26.INC

Subroutine to change anything on the NMR spectra.

Startloop7:
AS=INKEY$
SELECT CASE AS
CASE =
CASE CHRS(13)
RETURN
CASE 'q','Q',CHRS(27)
GOTO MainMenu
CASE CHRS(0)+CHRS(59)
GOSUB HelpScreen
CASE CHRS(0)+CHRS(80)
IF INTEGRALS='OFF' : TEMPS='OFF' : GOSUB DrawIntegralRegions
ELSE
INTEGRALS='ON' : TEMPS='ON' : GOSUB DrawIntegralRegions
END IF
CASE '+*'
IF INTEXP%(FILETYPE%(K%))<=16382 THEN
IF INTEGRALS='ON' THEN
TEMPS='OFF' : GOSUB DrawIntegralRegions
END IF
INTEXP%(FILETYPE%(K%))=INTEXP%(FILETYPE%(K%))*2
IF INTEGRALS='ON' THEN
TEMPS='ON' : GOSUB DrawIntegralRegions
END IF
END IF
CASE '*.'
IF AS=CHRS(0)+CHRS(72) THEN DECR ACTIVE%(1,T%)
IF AS=CHRS(0)+CHRS(60) THEN INCR ACTIVE%(1,T%)
IF ACTIVE%(1,T%)<1 THEN ACTIVE%(1,T%)=TEMP1%
IF ACTIVE%(1,T%)>TEMP1% THEN ACTIVE%(1,T%)=1
TEMP$='ON' : GOSUB MarkActiveShift
CASE CHRS(0)+CHRS(82),CHRS(0)+CHRS(83)
T%=FILETYPE%(K%)
SELECT CASE FILETYPE%(K%)
CASE 1 : TEMP3%=-4
CASE 2 : TEMP3%=-6
CASE 3,4,5 : TEMP3%=8
CASE 6,7 : TEMP3%=-4
END SELECT
TEMP$='OFF' : GOSUB MarkActiveBase
IF AS=CHRS(0)+CHRS(82) THEN DECR ACTIVE%(2,T%)
IF AS=CHRS(0)+CHRS(83) THEN INCR ACTIVE%(2,T%)
IF ACTIVE%(2,T%)<1 THEN ACTIVE%(2,T%)=TEMP3%
IF ACTIVE%(2,T%)>TEMP3% THEN ACTIVE%(2,T%)=1
TEMP$='ON' : GOSUB MarkActiveBase
CASE '*:':g':y':y'
GainYOffset

INTEXP%(FILETYPE%(K%))=INTEXP%(FILETYPE%(K%))/2
IF INTEGRALS='ON' THEN
TEMP$='ON' : GOSUB DrawIntegralRegions
END IF
CASE 'M','m'
Menu
END IF
SCREEN 0 : WIDTH 80
COLOR 15,0 : CLS : COLOR 10,1
LOCATE 5,20 PRINT CHRS(218),STRINGS(38,188),CHRS(181);
FOR I%=6 TO 18
LOCATE I%,20 : PRINT CHRS(179),STRINGS(38,32),CHRS(178);
NEXT I%
LOCATE 18,20 : PRINT CHRS(182),STRINGS(38,188),CHRS(217);
COLOR 12,1
LOCATE 7,23 PRINT "Please select file no/type to go to"
COLOR 14,1
FOR I%=1 TO 7
LOCATE I%+8,32 : PRINT USING "0%":I% : PRINT FILETYPE$(I%)
NEXT I%
LOCATE 17,38 : PRINT "<Q> Quit";
Startloop20:
AS=INKEY$
SELECT CASE AS
CASE =
CASE 'q','Q',CHRS(27)
GOTO MainMenu
CASE "1:2:3:4:5:6:7"
K%=VAL(AS) : GOTO Startloop19
CASE ELSE
SOUND 1000,3 : SOUND 800,1.5
END SELECT
GOTO Startloop20
CASE CHRS(0)+CHRS(72),CHRS(0)+CHRS(80)
T%=FILETYPE%(K%)
SELECT CASE FILETYPE%(K%)
CASE 1 : TEMP1%=-6
CASE 2,3,4,5 : TEMP1%=-13
CASE 6,7 : TEMP1%=-4
END SELECT
TEMP$='OFF' : GOSUB MarkActiveShift
IF AS=CHRS(0)+CHRS(72) THEN DECR ACTIVE%(1,T%)
IF AS=CHRS(0)+CHRS(80) THEN INCR ACTIVE%(1,T%)
IF ACTIVE%(1,T%)<1 THEN ACTIVE%(1,T%)=TEMP1%
IF ACTIVE%(1,T%)>TEMP1% THEN ACTIVE%(1,T%)=1
TEMP$='ON' : GOSUB MarkActiveShift
CASE CHRS(0)+CHRS(82),CHRS(0)+CHRS(83)
T%=FILETYPE%(K%)
SELECT CASE FILETYPE%(K%)
CASE 1 : TEMP3%=-4
CASE 2 : TEMP3%=-6
CASE 3,4,5 : TEMP3%=8
CASE 6,7 : TEMP3%=-4
END SELECT
TEMP$='OFF' : GOSUB MarkActiveBase
IF AS=CHRS(0)+CHRS(82) THEN DECR ACTIVE%(2,T%)
IF AS=CHRS(0)+CHRS(83) THEN INCR ACTIVE%(2,T%)
IF ACTIVE%(2,T%)<1 THEN ACTIVE%(2,T%)=TEMP3%
IF ACTIVE%(2,T%)>TEMP3% THEN ACTIVE%(2,T%)=1
TEMP$='ON' : GOSUB MarkActiveBase
CASE '*:':g':y':y'
GainYOffset

```

```

T%=FILETYPE%(K%)
SELECT CASE FILETYPE%(K%)
CASE 1 : TEMPI%=22
CASE 2,3,4,5 : TEMPI%=20
CASE 6,7 : TEMPI%=10
END SELECT
IF AS='G' OR AS='g' THEN T8='Gain: ' : T=GAIN(T%)
IF AS='Y' OR AS='y' THEN T8='Y Offset: ' : T=YOFFSET%(T%)
PRINT USING '#####.T';
LOCATE TEMP1%+1,1 : PRINT 'Old ' ;T8;
LOCATE TEMP1%+1,1 : PRINT 'New ' ;T8;
LINE INPUT TEMPS
IF TEMPS<>' ' THEN
IF AS='G' OR AS='g' THEN GAIN(T%)=VAL(TEMPS)
IF AS='Y' OR AS='y' THEN YOFFSET%(T%)=VAL(TEMPS)
CLS
GOSUB DisplayNMPFile
GOSUB DisplayAxis
GOSUB DrawAvgScreens
GOSUB DrawAvgStructs
GOSUB CalculateAndDrawBase
GOSUB CalculateIntegrals
GOSUB CalculateAverageStructures
GOSUB DrawAvgStrData
TEMP8='ON' : GOSUB MarkActiveShift
TEMP8='ON' : GOSUB MarkActiveBase
IF INTEGRALS='ON' THEN
TEMP8='ON' : GOSUB DrawIntegralRegions
END IF
ELSE
LOCATE TEMP1%+0,1 : PRINT SPACES(21);
LOCATE TEMP1%+1,1 : PRINT SPACES(21);
END IF
T%=FILETYPE%(K%)
SELECT CASE FILETYPE%(K%)
CASE 1 : TEMPI%=22
CASE 2,3,4,5 : TEMPI%=20
CASE 6,7 : TEMPI%=10
END SELECT
IF AS='S' OR AS='s' THEN T8='Shift: ' : T=SHIFTSTEP%(T%)
IF AS='B' OR AS='b' THEN T8='Base' : T=BASESTEP%(T%)
LOCATE TEMP1%+0,1 : PRINT 'Old ' ;T8; ' Step: ' ;
PRINT USING '#####.T';
LOCATE TEMP1%+1,1 : PRINT 'New ' ;T8; ' Step: ' ;
LINE INPUT TEMPS
IF TEMPS<>' ' THEN
IF AS='S' OR AS='s' THEN SHIFTSTEP%(T%)=VAL(TEMPS)
IF AS='B' OR AS='b' THEN BASESTEP%(T%)=VAL(TEMPS)
END IF
LOCATE TEMP1%+0,1 : PRINT SPACES(22);
LOCATE TEMP1%+1,1 : PRINT SPACES(22);
CASE CHRS(0)+CHRS(75) ,CHRS(0)+CHRS(77),...
CHRS(0)+CHRS(119),CHRS(0)+CHRS(116)
TEMP%='BACKCOL% : GOSUB MoveActiveShift
IF INTEGRALS='ON' THEN
TEMP8='OFF' : GOSUB DrawIntegralRegions
END IF
T%=FILETYPE%(K%)
IF AS=CHRS(0)+CHRS(75) THEN
TEMP%=BASESTEP%(T%)
ELSEIF AS=CHRS(0)+CHRS(81) THEN
TEMP%=-1*BASESTEP%(T%)
ELSEIF AS=CHRS(0)+CHRS(132) THEN
TEMP%=BASESTEP%(T%)*10
ELSEIF AS=CHRS(0)+CHRS(116) THEN
TEMP%=-10*BASESTEP%(T%)
END IF
IF ACTIVE%(2,T%)/2=INT(ACTIVE%(2,T%)/2) THEN
INCR ENDAVG$(T%,ACTIVE%(2,T%)),TEMP%
ELSE
INCR BEGAVG$(T%,ACTIVE%(2,T%)),TEMP%
TEMP%=BASECOL% : GOSUB MoveActiveBase
GOSUB CalculateIntegrals
GOSUB DrawAvgStrData
IF INTEGRALS='ON' THEN
TEMP8='ON' : GOSUB DrawIntegralRegions
END IF
CASE ELSE
SOUND 1000,3 : SOUND 800,1.5
END SELECT
GOTO Startloop7

```

* Alkanes
* Mono->Phenan
* Statics

* Shift - Base

* Alkanes
* Mono->Phenan
* Statics

* Shift L - R

* Base up - dn

* up

* down

* cdt up

* cdt dn

* even = end pt

* odd = beg pt

* oops!!

Code Listing for LCNMR27.INC

Subroutine to divide blank integrals by the number of scans.

```

FOR I%=1 TO 5
SELECT CASE I%
CASE 1 : TEMP1%=205 : TEMP2%=200
CASE 2,3,4,5
TEMP1%=(I%-2)*12+210 : TEMP2%=(I%-2)*12+221
END SELECT
FOR J%=TEMP1% TO TEMP2%
DS(J%)=STR$( VAL(DS(J%)/SOR(VAL(DS(201+I%)))) )
NEXT J%
RETURN
    
```

* alkane
* mono->phenan

Code Listing for LCNMR28.INC

This is the subroutine to see if need to file the blank data.

```

SCREEN 0 : WIDTH 80
COLOR 15, 0 : CLS
COLOR 14, 4
LOCATE 9,10 : PRINT CHR$(218);STRINGS$(59,198);CHR$(191); ' top line
FOR I%=10 TO 14
LOCATE I%,10 : PRINT CHR$(179);TAB(70);CHR$(179); ' middle
NEXT I%
LOCATE 15,10 : PRINT CHR$(192);STRINGS$(59,198);CHR$(217); ' bottom line
COLOR 31, 4
LOCATE 12,22 : PRINT "OK to file the data for ",FUELNAME$(L%);"? (Y/N)";
Startloop10:
AS=INPUT$(1)
SELECT CASE AS
CASE "N","n","Q","q":CHR$(27)
GOTO MainMenu
CASE "Y","y"
TEMPS=OUTPTDIRS
OUTPTDIRS=BLANKDIRS
GOSUB FileAvgStrData
OUTPTDIRS=TEMPS
RETURN
CASE ELSE
SOUND 1000,3 : SOUND 800,15
END SELECT
GOTO Startloop10
    
```

* exit
* ok to file
* oops!

Code Listing for LCNMR29.INC

This is the subroutine to do the printer menu.

```

OPTN$(1)="IBM ProPrinter"
OPTN$(2)="HP LaserJet Series II"
' Will draw the screen.
COLOR 15, 0 : CLS
COLOR 10,1
LOCATE 5,15 : PRINT CHR$(218);STRINGS$(49,198);CHR$(191); ' top line
FOR I%=9 TO 16
LOCATE I%,15 : PRINT CHR$(179);TAB(65);CHR$(179); ' middle
NEXT I%
LOCATE 17,15 : PRINT CHR$(192);STRINGS$(49,198);CHR$(217); ' bottom line
COLOR 10, 1
LOCATE 9,20 : PRINT TIMES;
LOCATE 9,51 : PRINT DATES;
COLOR 15, 1
LOCATE 8,32 : PRINT "Printer Options*";
COLOR 12, 1
LOCATE 10,21 : PRINT "Please select the appropriate printer.";
COLOR 14,1
FOR I%=1 TO 2
LOCATE (I%-1)*2+12,40-(0.5*LEN(OPTN$(I%)))
COLOR 11,1 : PRINT LEFT$(OPTN$(I%),1);
COLOR 14,1 : PRINT RIGHT$(OPTN$(I%),LEN(OPTN$(I%))-1);
NEXT I%
' Next are commands
COLOR 3,0
LOCATE 21,18 : PRINT "Press the highlighted letter or <ENTER> to select*";
LOCATE 22,20 : PRINT "Press the <Q> to return to the Main Menu*";
' Next see what to do
COLOR 14,0
LOCATE (PRINTER%-1)*2+12,38-(0.5*LEN(OPTN$(PRINTER%)))
PRINT " : OPTN$(PRINTER%)* ";
Startloop16
AS=INKEY$
SELECT CASE AS
CASE " "
COLOR 10,1
LOCATE 6,20 : PRINT TIMES;
CASE "Q","q":CHR$(27)
GOTO MainMenu
CASE CHR$(13)
RETURN
CASE "I","i"
PRINTER%=1 : RETURN
CASE "H","h"
PRINTER%=-2 : RETURN
' no key
' Exit
' return
' IBM Pro
' HP LJII
    
```

```

CASE CHR$(0)+CHR$(72), CHR$(0)+CHR$(80) ' up-down
LOCATE (PRINTER%-1)*2+12,38-(0.5*LEN(OPTNS$(PRINTER%)))
COLOR 11,1
PRINT "LEFTS (OPTNS$(PRINTER%),1);
COLOR 14,1
PRINT RIGHT$(OPTNS$(PRINTER%),LEN(OPTNS$(PRINTER%))-1);
IF AS=CHR$(0)+CHR$(72) THEN DECR PRINTER% ELSE INCR PRINTER%
IF PRINTER%<1 THEN PRINTER%=2
IF PRINTER%>2 THEN PRINTER%=1
COLOR 14,0
LOCATE (PRINTER%-1)*2+12,38-(0.5*LEN(OPTNS$(PRINTER%)))
PRINT "OPTNS$(PRINTER%);
CASE CHR$(0)+CHR$(75),CHR$(0)+CHR$(77) ' left-right
CASE ELSE ' oopel
SOUND 1000,3 : SOUND 800,1.5
END SELECT
GOTO Startloop18
    
```

Code Listing for LCNMR30.INC

This is the subroutine to do the edit integration menu.

```

OPTNS(1)="Edit Data Already on File"
OPTNS(2)="Create a New File for Data"
' Will draw the screen.
COLOR 10,1
LOCATE 5,15 : PRINT CHR$(218),STRING$(49,100),CHR$(191); ' top line
FOR I%=6 TO 16
LOCATE I%,15 : PRINT CHR$(179),TAB(95),CHR$(179); ' middle
NEXT I%
LOCATE 17,15 : PRINT CHR$(192),STRING$(49,100),CHR$(217); ' bottom line
COLOR 10,1
LOCATE 6,20 : PRINT TIMES;
LOCATE 6,51 : PRINT DATES;
COLOR 15,1
LOCATE 6,28 : PRINT "Edit Integration Options";
COLOR 12,1
LOCATE 10,22 : PRINT "Please select the appropriate method";
COLOR 14,1
FOR I%=1 TO 2
LOCATE (I%-1)*2+12,40-(0.5*LEN(OPTNS(I%)))
COLOR 11,1 : PRINT LEFT$(OPTNS(I%),1);
COLOR 14,1 : PRINT RIGHT$(OPTNS(I%),LEN(OPTNS(I%))-1);
NEXT I%
' Next are commands
COLOR 3,0
LOCATE 21,16 : PRINT "Press the highlighted letter or <ENTER> to select";
LOCATE 22,20 : PRINT "Press the <Q> to return to the Main Menu.";
' Next see what to do.
COLOR 14,0
    
```

```

LOCATE (OPTN%(0)-1)*2+12,38-(0.5*LEN(OPTNS$(OPTN%(0))))
PRINT "OPTNS$(OPTN%(0));";
Startloop14.
AS=INKEY$
SELECT CASE AS
CASE "="
COLOR 10,1
LOCATE 6,20 : PRINT TIMES;
CASE "Q",q,CHR$(27)
GOTO MainMenu
CASE CHR$(13)
RETURN
CASE "E",e
' Ed old file
CASE "C",c
' Create new
OPTN%(0)=1 : RETURN
OPTN%(0)=2 : RETURN
CASE CHR$(0)+CHR$(72), CHR$(0)+CHR$(80)
LOCATE (OPTN%(0)-1)*2+12,38-(0.5*LEN(OPTNS$(OPTN%(0))))
COLOR 11,1
PRINT "LEFTS (OPTNS$(OPTN%(0)),1);
COLOR 14,1
PRINT RIGHT$(OPTNS$(OPTN%(0)),LEN(OPTNS$(OPTN%(0))-1);
IF AS=CHR$(0)+CHR$(72) THEN DECR OPTN%(0) ELSE INCR OPTN%(0)
IF OPTN%(0)<1 THEN OPTN%(0)=2
IF OPTN%(0)>2 THEN OPTN%(0)=1
COLOR 14,0
LOCATE (OPTN%(0)-1)*2+12,38-(0.5*LEN(OPTNS$(OPTN%(0))))
PRINT "OPTNS$(OPTN%(0));";
CASE CHR$(0)+CHR$(75),CHR$(0)+CHR$(77) ' left-right
CASE ELSE ' oopel
SOUND 1000,3 : SOUND 800,1.5
END SELECT
GOTO Startloop14
    
```

Code Listing for LCNMR31.INC

This is the subroutine to draw the integration screen.

```

OPTNS(1)="Alkane" OPTNS(2)="Mono" OPTNS(3)="Dicyclic"
OPTNS(4)="Flourene" OPTNS(5)="Phenane" OPTNS(6)="1H Static"
OPTNS(7)="13C Static"
COLOR 15,1 CLS
COLOR 4,3
LOCATE 1,1 : PRINT SPACES(80);
LOCATE 1,31 : PRINT "Fuel Name: "FUELNAME$(L%);
COLOR 1,3
LOCATE 1,3 : PRINT TIMES;
LOCATE 1,69 : PRINT DATES;
COLOR 0,3
LOCATE 25,1 : PRINT SPACES(80);
LOCATE 25,12
PRINT "File <F>, Move <ARROW KEYS>, Quit <Q>, Continue <RETURN>";
    
```

```

COLOR 0,1
FOR I%=2 TO 24
FOR J%=1 TO 8
LOCATE I%,(J%-1)*11+1 : PRINT CHR$(178);
NEXT J%
NEXT I%
FOR I%=1 TO 7
COLOR 12,1
LOCATE 2,(I%-1)*11+3 : PRINT OPT$(I%);
FOR J%=1 TO 11
IF INTRNAMES(I%,J%) < >= THEN
COLOR 11,1
LOCATE (J%-1)*2+3,(I%-1)*11+3
PRINT INTRNAMES(I%,J%);
TEMP1%=J% : TEMP2%=I%
COLOR 15,1
GOSUB HighlightIntegral
END IF
NEXT J%
NEXT I%
RETURN
    
```

Code Listing for LCNMR32.INC

This is the subroutine to edit the displayed integrals.

```

Startloop6:
AS=INKEY$
SELECT CASE AS
CASE "="
COLOR 1, 3
LOCATE 1, 3 : PRINT TIME$;
CASE CHR$(13)
RETURN
CASE "Q";CHR$(27)
GOTO MainMenu
CASE "F";"
COLOR 15, 4
LOCATE 25, 1 : PRINT SPACES(80);
LOCATE 25,24 : PRINT "*** Filing the information ***";
DS(2)=DATE$
GOSUB FileAvgStrData
COLOR 0, 3
LOCATE 25, 1 : PRINT SPACES(80);
LOCATE 25,12
PRINT "File <F>, Move <ARROW KEYS>, Quit <Q>, Continue <RETURN>";
CASE CHR$(0)+CHR$(72), CHR$(0)+CHR$(80)
COLOR 15,1
GOSUB HighlightIntegral
IF AS=CHR$(0)+CHR$(72) THEN DECR TEMP1% ELSE INCR TEMP1%
IF TEMP1% < 1 THEN TEMP1%=11
IF TEMP1% > 11 THEN TEMP1%=1
    
```

```

COLOR 12,0
GOSUB HighlightIntegral
CASE CHR$(0)+CHR$(75),CHR$(0)+CHR$(77)
COLOR 15,1
GOSUB HighlightIntegral
IF AS=CHR$(0)+CHR$(73) THEN DECR TEMP2% ELSE INCR TEMP2%
IF TEMP2% < 1 THEN TEMP2%=7
IF TEMP2% > 7 THEN TEMP2%=1
COLOR 12,0
GOSUB HighlightIntegral
CASE ELSE
IF ASC(AS) < 48 OR ASC(AS) > 57 THEN
SOUND 1000,3 : SOUND 800,1.5
GOTO Startloop6
END IF
COLOR 14,1
LOCATE (TEMP1%-1)*2+4,(TEMP2%-1)*11+2
PRINT SPACES(10)
LOCATE (TEMP1%-1)*2+4,(TEMP2%-1)*11+2
PRINT AS; : LINE INPUT TEMP$
TEMP$=AS+TEMP$
SELECT CASE TEMP2%
CASE 1 : DS(TEMP1%+204)=TEMP$
CASE 2 : DS(TEMP1%+209)=TEMP$
CASE 3 : DS(TEMP1%+221)=TEMP$
CASE 4 : DS(TEMP1%+233)=TEMP$
CASE 5 : DS(TEMP1%+245)=TEMP$
CASE 6 : DS(INT(TEMP1%/3)+258)=TEMP$
CASE 7 : DS(INT(TEMP1%/3)+260)=TEMP$
END SELECT
COLOR 12,0
GOSUB HighlightIntegral
DS(2)=DATE$
END SELECT
GOTO Startloop6
    
```

Code Listing for LCNMR33.INC

This is the subroutine to highlight an integral.

```

LOCATE (TEMP1%-1)*2+4,(TEMP2%-1)*11+2
IF INTRNAMES(TEMP2%,TEMP1%)="" THEN PRINT SPACES(10); : RETURN
SELECT CASE TEMP2%
CASE 1
PRINT USING "#####.###" ;VAL(DS(TEMP1%+204));
CASE 2
PRINT USING "#####.###" ;VAL(DS(TEMP1%+209));
CASE 3
PRINT USING "#####.###" ;VAL(DS(TEMP1%+221));
CASE 4
PRINT USING "#####.###" ;VAL(DS(TEMP1%+233));
CASE 5
PRINT USING "#####.###" ;VAL(DS(TEMP1%+245));
CASE 6
PRINT USING "#####.###" ;VAL(DS(TEMP1%+258));
CASE 7
PRINT USING "#####.###" ;VAL(DS(TEMP1%+260));
    
```

- * no key
- * return
- * quit
- * file data


```

PRINT *
PRINT * 3 2
IF PRINTER% = 1 THEN LPRINT CHR$(27);CHR$(65);CHR$(12);CHR$(27);CHR$(50)
IF PRINTER% = 2 THEN LPRINT CHR$(27);"&18D"
LPRINT *
LPRINT USING "#####.VAL(D5(106)); : LPRINT *
LPRINT USING "#####.VAL(D5(106)); : LPRINT *
LPRINT USING "#####.VAL(D5(110)); : LPRINT *
LPRINT USING "#####.VAL(D5(147)); : LPRINT *
LPRINT : LPRINT

. Monocyclic average structure data
LPRINT TAB(7);"Average Structural Parameters for Monocyclic ";
LPRINT "Aromatic Fraction";
FOR I% = 1 TO 63 : LPRINT TAB(6+I%); : NEXT I% : LPRINT
IF PRINTER% = 1 THEN LPRINT CHR$(27);CHR$(65);CHR$( 6);CHR$(27);CHR$(50)
IF PRINTER% = 2 THEN LPRINT CHR$(27);"&12D"
FOR I% = 1 TO 6 : LPRINT TAB(I%*6-4); : NEXT I%
LPRINT TAB(68); : LPRINT *
FOR I% = 1 TO 8 : LPRINT TAB(I%*6-7); : NEXT I%
LPRINT TAB(69);"MW ADS"
TEMP% = %un sub eCH3 eCH2 eCH BH CH2>a CH3>a
LPRINT TAB(3);TEMP%
IF PRINTER% = 1 THEN LPRINT CHR$(27);CHR$(65);CHR$(12);CHR$(27);CHR$(50)
IF PRINTER% = 2 THEN LPRINT CHR$(27);"&18D"
LPRINT USING "#####.VAL(D5( 54)); : LPRINT *
LPRINT USING "#####.VAL(D5( 66)); : LPRINT *
LPRINT USING "#####.VAL(D5( 80)); : LPRINT *
LPRINT USING "#####.VAL(D5( 82)); : LPRINT *
LPRINT USING "#####.VAL(D5( 94)); : LPRINT *
LPRINT USING "#####.VAL(D5( 98)); : LPRINT *
LPRINT USING "#####.VAL(D5( 66)); : LPRINT *
LPRINT USING "#####.VAL(D5( 80)); : LPRINT *
LPRINT USING "#####.VAL(D5( 82)); : LPRINT *
LPRINT USING "#####.VAL(D5( 94)); : LPRINT *
LPRINT USING "#####.VAL(D5( 98)); : LPRINT *
LPRINT USING "#####.VAL(D5( 72));VAL(D5( 74))
LPRINT : LPRINT

. Phenanthrene Average Structure data
LPRINT TAB(10);"Average Structural Parameters for Phenanthrene ";
LPRINT "Fraction";
FOR I% = 1 TO 63 : LPRINT TAB(6+I%); : NEXT I% : LPRINT : LPRINT
IF PRINTER% = 1 THEN LPRINT CHR$(27);CHR$(65);CHR$( 6);CHR$(27);CHR$(50)
IF PRINTER% = 2 THEN LPRINT CHR$(27);"&12D"
FOR I% = 1 TO 6 : LPRINT TAB(I%*6-4); : NEXT I%
LPRINT TAB(68); : LPRINT *
FOR I% = 1 TO 8 : LPRINT TAB(I%*6-7); : NEXT I%
LPRINT TAB(69);"MW ADS"
TEMP% = %un sub eCH3 eCH2 eCH BH CH2>a CH3>a
LPRINT TAB(3);TEMP%
IF PRINTER% = 1 THEN LPRINT CHR$(27);CHR$(65);CHR$(12);CHR$(27);CHR$(50)
IF PRINTER% = 2 THEN LPRINT CHR$(27);"&18D"
LPRINT USING "#####.VAL(D5( 80)); : LPRINT *
LPRINT USING "#####.VAL(D5( 82)); : LPRINT *
LPRINT USING "#####.VAL(D5( 86)); : LPRINT *
LPRINT USING "#####.VAL(D5( 88)); : LPRINT *
LPRINT USING "#####.VAL(D5( 90)); : LPRINT *
LPRINT USING "#####.VAL(D5( 84)); : LPRINT *
LPRINT USING "#####.VAL(D5( 94)); : LPRINT *
LPRINT USING "#####.VAL(D5( 96)); : LPRINT *
LPRINT : LPRINT
FOR I% = 1 TO 80 : LPRINT * : NEXT I%
LPRINT CHR$(12)

. Have finished 1st so will do second page of printout.

LPRINT Fuel : "DS( 1)
LPRINT Source : "DS(145)
LPRINT : LPRINT
FOR I% = 1 TO 80 : LPRINT * : NEXT I% : LPRINT
IF PRINTER% = 2 THEN LPRINT CHR$(27);"(s3B" ELSE LPRINT
LPRINT TAB(7);"Absolute Number of Moles of Carbon and Fractional "

```

```

PRINT *
IF PRINTER% = 1 THEN LPRINT CHR$(27);CHR$(65);CHR$(12);CHR$(27);CHR$(50)
IF PRINTER% = 2 THEN LPRINT CHR$(27);"&18D"
LPRINT *
LPRINT USING "#####.VAL(D5(106)); : LPRINT *
LPRINT USING "#####.VAL(D5(106)); : LPRINT *
LPRINT USING "#####.VAL(D5(110)); : LPRINT *
LPRINT USING "#####.VAL(D5(147)); : LPRINT *
LPRINT : LPRINT

. Monocyclic average structure data
LPRINT TAB(7);"Average Structural Parameters for Monocyclic ";
LPRINT "Aromatic Fraction";
FOR I% = 1 TO 63 : LPRINT TAB(6+I%); : NEXT I% : LPRINT
IF PRINTER% = 1 THEN LPRINT CHR$(27);CHR$(65);CHR$( 6);CHR$(27);CHR$(50)
IF PRINTER% = 2 THEN LPRINT CHR$(27);"&12D"
FOR I% = 1 TO 6 : LPRINT TAB(I%*6-4); : NEXT I%
LPRINT TAB(68);"MW ADS"
TEMP% = %un sub eCH3 eCH2 eCH BH CH2>a CH3>a
LPRINT TAB(3);TEMP%
IF PRINTER% = 1 THEN LPRINT CHR$(27);CHR$(65);CHR$(12);CHR$(27);CHR$(50)
IF PRINTER% = 2 THEN LPRINT CHR$(27);"&18D"
LPRINT USING "#####.VAL(D5( 3)); : LPRINT *
LPRINT USING "#####.VAL(D5( 9)); : LPRINT *
LPRINT USING "#####.VAL(D5( 9)); : LPRINT *
LPRINT USING "#####.VAL(D5( 11)); : LPRINT *
LPRINT USING "#####.VAL(D5( 13)); : LPRINT *
LPRINT USING "#####.VAL(D5( 19)); : LPRINT *
LPRINT USING "#####.VAL(D5( 15)); : LPRINT *
LPRINT USING "#####.VAL(D5( 17)); : LPRINT *
LPRINT USING "#####.VAL(D5( 21));VAL(D5( 23))
LPRINT : LPRINT

. Dicyclic Average Structure data
LPRINT TAB(8);"Average Structural Parameters for Dicyclic ";
LPRINT "Aromatic Fraction";
FOR I% = 1 TO 63 : LPRINT TAB(6+I%); : NEXT I% : LPRINT : LPRINT
IF PRINTER% = 1 THEN LPRINT CHR$(27);CHR$(65);CHR$( 6);CHR$(27);CHR$(50)
IF PRINTER% = 2 THEN LPRINT CHR$(27);"&12D"
FOR I% = 1 TO 6 : LPRINT TAB(I%*6-4); : NEXT I%
LPRINT TAB(68);"MW ADS"
TEMP% = %un sub eCH3 eCH2 eCH BH CH2>a CH3>a
LPRINT TAB(3);TEMP%
IF PRINTER% = 1 THEN LPRINT CHR$(27);CHR$(65);CHR$(12);CHR$(27);CHR$(50)
IF PRINTER% = 2 THEN LPRINT CHR$(27);"&18D"
LPRINT USING "#####.VAL(D5( 28)); : LPRINT *
LPRINT USING "#####.VAL(D5( 30)); : LPRINT *
LPRINT USING "#####.VAL(D5( 34)); : LPRINT *
LPRINT USING "#####.VAL(D5( 36)); : LPRINT *
LPRINT USING "#####.VAL(D5( 38)); : LPRINT *
LPRINT USING "#####.VAL(D5( 32)); : LPRINT *
LPRINT USING "#####.VAL(D5( 40)); : LPRINT *
LPRINT USING "#####.VAL(D5( 42)); : LPRINT *
LPRINT USING "#####.VAL(D5( 46));VAL(D5( 48))
LPRINT : LPRINT

```

```

LPRINT TAB(4); "Predicted Smoke Point: ";
IF VAL(DS(135)) < > 0 THEN
  IF VAL(DS(135)) < 12 THEN TEMPS = " >> ### << " ELSE TEMPS = " ### "
  LPRINT USING TEMPS; VAL(DS(135)); LPRINT
ELSE
  LPRINT : LPRINT
END IF
LPRINT TAB(4); "Predicted Freezing Point: ";
IF VAL(DS(136)) < > 0 THEN
  LPRINT USING "#####"; VAL(DS(136)); LPRINT
ELSE
  LPRINT : LPRINT
END IF
LPRINT TAB(4); "Aromaticity: ";
IF VAL(DS(137)) < > 0 THEN
  LPRINT USING "#####"; VAL(DS(137))
ELSE
  LPRINT
END IF
LPRINT TAB(6); "< Volume %>"
LPRINT
LPRINT TAB(4); "Elemental Analysis: C H N S Cl Br I F";
LPRINT " H (by NMR)"
IF VAL(DS(138)) < > 0 THEN LPRINT TAB(26); VAL(DS(138));
IF VAL(DS(139)) < > 0 THEN LPRINT TAB(43); VAL(DS(139));
IF VAL(DS(140)) < > 0 THEN LPRINT TAB(65); VAL(DS(140))
LPRINT CHR$(12)
IF PRINTER% = 1 THEN
  LPRINT CHR$(27); CHR$(73); CHR$(0);
END IF
RETURN

" Arom V%
" Smk Pt
" Freez Pt
" if ProPrint
" then select
" font

This is the subroutine to hardcopy the properties.

IF PRINTER% = 1 THEN
  LPRINT CHR$(27); CHR$(73); CHR$(FONT%-1)
END IF
IF PRINTER% = 1 THEN
  LPRINT CHR$(14); TAB(11);
ELSE
  LPRINT CHR$(27); "{s38"; TAB(28);
END IF
LPRINT "Physical Properties"
IF PRINTER% = 2 THEN LPRINT CHR$(27); "{e08";
LPRINT
LPRINT "Fuel: "; DS( 1)
LPRINT "Source: "; DS(145)
LPRINT : LPRINT
FOR I% = 1 TO 65 : LPRINT TAB(6+I%); "; : NEXT I%
LPRINT : LPRINT

" Boldface off

```

Code Listing for LCNMR36.INC

This is the subroutine to hardcopy the properties.

```

LPRINT "Aromaticity Data"
IF PRINTER% = 2 THEN LPRINT CHR$(27); "{e08" ELSE LPRINT
FOR I% = 23 TO 55 : LPRINT TAB(I%); "; : NEXT I% : LPRINT
IF PRINTER% = 1 THEN LPRINT CHR$(27); CHR$(6); CHR$(27); CHR$(50)
IF PRINTER% = 2 THEN LPRINT CHR$(27); "{i120"
LPRINT TAB(21); "C
LPRINT TAB(22); "A: total
LPRINT TAB(23); "Ar: total"
IF PRINTER% = 1 THEN LPRINT CHR$(27); CHR$(69); CHR$(12); CHR$(27); CHR$(50)
IF PRINTER% = 2 THEN LPRINT CHR$(27); "{i60"
FOR I% = 3 TO 73 : LPRINT TAB(I%); "; : NEXT I% : LPRINT
TEMP% = "#####
LPRINT
LPRINT TAB(4); "Alkanes
LPRINT USING TEMPS; VAL(DS(114)); VAL(DS(116))
LPRINT
TEMP% = "#####
FOR I% = 3 TO 73 : LPRINT TAB(I%); "; : NEXT I% : LPRINT
LPRINT
LPRINT TAB(4); "Monocyclic
LPRINT USING TEMPS; VAL(DS(24)); VAL(DS(25)); VAL(DS(26)); VAL(DS(27))
LPRINT TAB(4); "Aromatics
FOR I% = 3 TO 73 : LPRINT TAB(I%); "; : NEXT I% : LPRINT
LPRINT
LPRINT TAB(4); "Cyclic
LPRINT USING TEMPS; VAL(DS(49)); VAL(DS(50)); VAL(DS(51)); VAL(DS(52))
LPRINT TAB(4); "Aromatics
FOR I% = 3 TO 73 : LPRINT TAB(I%); "; : NEXT I% : LPRINT
LPRINT
LPRINT TAB(4); "Fluorenes
LPRINT USING TEMPS; VAL(DS(75)); VAL(DS(76)); VAL(DS(77)); VAL(DS(78))
LPRINT
FOR I% = 3 TO 73 : LPRINT TAB(I%); "; : NEXT I% : LPRINT
LPRINT
LPRINT TAB(4); "Phenanthrenes
LPRINT USING TEMPS; VAL(DS(101)); VAL(DS(102)); VAL(DS(103)); VAL(DS(104))
LPRINT
FOR I% = 3 TO 73 : LPRINT TAB(I%); "; : NEXT I% : LPRINT
LPRINT TAB(63); "r;
IF PRINTER% = 1 THEN
  LPRINT CHR$(27); CHR$(63); CHR$(11); "a; CHR$(27); CHR$(64);
ELSE
  LPRINT "a;
END IF
LPRINT " "
LPRINT USING "#####"; VAL(DS(146))
LPRINT
FOR I% = 23 TO 55 : LPRINT TAB(I%); "; : NEXT I% : LPRINT : LPRINT
LPRINT TAB(4); "Comments: "
LPRINT : LPRINT
LPRINT : LPRINT
FOR I% = 1 TO 80 : LPRINT " "; : NEXT I% : LPRINT
IF PRINTER% = 2 THEN
  LPRINT CHR$(27); "{s38"
ELSE
  LPRINT
END IF
LPRINT TAB(30); "Other Physical Data"
IF PRINTER% = 2 THEN LPRINT CHR$(27); "{e08";
LPRINT
FOR I% = 23 TO 55 : LPRINT TAB(I%); "; : NEXT I% : LPRINT : LPRINT

```

```

LPRINT "Smoke Point:";
IF VAL(D$(135))<>0 THEN
  IF VAL(D$(135))<12 THEN TEMP8=">> Smk Pt
  LPRINT USING TEMP8,VAL(D$(135));
END IF
LPRINT TAB(80);"Freezing Point:";
IF VAL(D$(136))<>0 THEN
  LPRINT USING "#####";VAL(D$(136)); LPRINT: LPRINT
ELSE
  LPRINT: LPRINT: LPRINT
END IF

LPRINT " Property Value Error Units"
LPRINT "-----"
FOR I%=1 TO 42
  SELECT CASE I%
  CASE 4
    TEMP18="Cetane
    TEMP28="± 0.85 Cetane
  CASE 5
    TEMP18="50% Boiling Point
    TEMP28="± 9.91 °C
  CASE 6
    TEMP18="Pour Point
    TEMP28="± 5.18 °C
  CASE 8
    TEMP18="Flash Point
    TEMP28="± 9.47 °C
  CASE 9
    TEMP18="Density
    TEMP28="± 0.005 kg/L
  CASE 11
    TEMP18="Cloud Point
    TEMP28="± 3.77 °C
  CASE 12
    TEMP18="Viscosity
    TEMP28="± 0.27 cSt
  CASE 13
    TEMP18="Filterability
    TEMP28="± 19.1"
  CASE 26
    TEMP18="Heat of Combustion
    TEMP28="± 0.08 MJ/kg
  CASE 28
    TEMP18="Percent Aromatics
    TEMP28="± 1.85 vol %
  CASE 31
    TEMP18="Cetane Index
    TEMP28="± 1.10 Cetane
  CASE 32
    TEMP18="Specific Gravity
    TEMP28="± 0.002 60/60F
  CASE 33
    TEMP18="Initial Boiling Point
    TEMP28="± 5.88 °C
  CASE 34
    TEMP18="10% Boiling Point
    TEMP28="± 6.25 °C
  CASE 35
    TEMP18="90% Boiling Point

```

```

TEMP28="± 18.6 °C
CASE 36
  TEMP18="End Boiling Point
  TEMP28="± 20.6 °C
CASE 37
  TEMP18="Residual Carbon
  TEMP28="± 0.28 vol %
CASE ELSE
  TEMP18="
END SELECT
IF TEMP18<>" THEN
  LPRINT " "
  LPRINT USING TEMP18,VAL(D$(156+I%));
  LPRINT TEMP28
END IF
NEXT I%
LPRINT CHR$(12)
IF PRINTER%=1 THEN
  LPRINT CHR$(27);CHR$(73);CHR$(0);
END IF
RETURN

```

' If ProPrint
' then select
' font

Code Listing for LCNMR37.INC

This is the subroutine to get the printer font.

```

OPTNS(1)="Regular Print
OPTNS(2)="FastFont
OPTNS(3)="Near Letter Quality
COLOR 10,1
FOR I%=11 TO 16
  LOCATE I%,15: PRINT CHR$(179);TAB(85);CHR$(179);
NEXT I%
COLOR 12,1
LOCATE 10,21: PRINT " Please select the appropriate font: ";
COLOR 14,1
FOR I%=1 TO 3
  LOCATE (I%-1)*2+12,40-(0.5*LEN(OPTNS(I%)))
  COLOR 11,1: PRINT LEFT$(OPTNS(I%),1);
  COLOR 14,1: PRINT RIGHT$(OPTNS(I%),LEN(OPTNS(I%))-1);
NEXT I%
' Next see what to do
COLOR 14,0
LOCATE (FONT%-1)*2+12,38-(0.5*LEN(OPTNS(FONT%)))
PRINT " (FONT%);";
Startloop17:
AS=INKEY$
SELECT CASE AS
CASE =
  COLOR 10,1
  LOCATE 6,20: PRINT TIMES;

```

' no key

```

CLOSE 1
' if arc 'undrawing' shift division, will draw spectra and base back
IF TEMP% = BACKCOL% THEN
FOR I% = PT%(I%,ACTIVE%(1,T%))-3 TO PT%(I%,ACTIVE%(1,T%))+3
TEMP1% = DA(I%)*YEXPFC + YOFFSET%(I,T%)
TEMP2% = DA(I%+1)*YEXPFC + YOFFSET%(I,T%)
LINE (I%,TEMP1%),(I%-1,TEMP2%),SPECTCL%
NEXT I%
TEMP1% = PT%(I%,ACTIVE%(1,T%))
PSET (TEMP1%,BA(TEMP1%)*YEXPFC + YOFFSET%(I,T%),BASECOL%)
END IF
RETURN

```

Code Listing for LCNMR39.INC

Subroutine to draw the active baseline.

```

T% = FILETYPE%(K%)
I% = ACTIVE%(2,T%)
IF INT(I%/2) <> I%/2 THEN
BEGAVG%(T%,I%+1) = BEGAVG%(T%,I%)
ENDAVG%(T%,I%+1) = ENDAVG%(T%,I%)
ELSE
BEGAVG%(T%,I%-1) = BEGAVG%(T%,I%)
ENDAVG%(T%,I%-1) = ENDAVG%(T%,I%)
END IF
SLOPE = (ENDAVG%(T%,I%) - BEGAVG%(T%,I%)) / (ENDPT%(T%,I%) - BEGPT%(T%,I%))
INTCP = BEGAVG%(T%,I%) - (SLOPE * BEGPT%(T%,I%))
FOR J% = BEGPT%(T%,I%) TO ENDPT%(T%,I%)
BA(J%) = (SLOPE * J%) + INTCP
PSET (J%,BA(J%)*YEXPFC + YOFFSET%(T%,I%),TEMP%)
IF TEMP% = BACKCOL% THEN
TEMP1% = DA(J%)*YEXPFC + YOFFSET%(T%,I%)
TEMP2% = DA(J%+1)*YEXPFC + YOFFSET%(T%,I%)
LINE (J%,TEMP1%),(J%-1,TEMP2%),SPECTCL%
END IF
NEXT J%
RETURN

```

' clic baseline
' draw base
' if undrawing
' base, must
' redraw spect
' under base

Code Listing for LCNMR40.INC

This is the subroutine to draw the main menu.

OPTNS(1) = 'Change Default Parameters'

```

' Exit
' return
' regular
' fastfont
' NLQ
' up-down
CASE 'Q', 'q', CHRS(27)
GOTO MainMenu
CASE CHRS(13)
RETURN
CASE 'R', 'r'
FONT% = 1 : RETURN
CASE 'F', 'f'
FONT% = 2 : RETURN
CASE 'N', 'n'
FONT% = 2 : RETURN
CASE CHRS(0) + CHRS(72), CHRS(0) + CHRS(80)
LOCATE (FONT% - 1) * 2 + 12, (0.5 * LEN(OPTNS(FONT%)))
COLOR 11, 1
PRINT ' ', LEFT$(OPTNS(FONT%), 1);
COLOR 14, 1
PRINT RIGHT$(OPTNS(FONT%), LEN(OPTNS(FONT%)) - 1); '
IF AS = CHRS(0) + CHRS(72) THEN DECR FONT% ELSE INCR FONT%
IF FONT% < 1 THEN FONT% = 3
IF FONT% > 3 THEN FONT% = 1
COLOR 14, 0
LOCATE (FONT% - 1) * 2 + 12, (0.5 * LEN(OPTNS(FONT%)))
PRINT ' ', OPTNS(FONT%), ' ';
CASE CHRS(0) + CHRS(73), CHRS(0) + CHRS(77)
CASE ELSE
SOUND 1000, 3 : SOUND 800, 15
END SELECT
GOTO Startloop17

```

Code Listing for LCNMR38.INC

Subroutine to draw the active shift divisor.

```

SELECT CASE FILETYPE%(K%)
CASE 1, 2, 3, 4, 5 : TEMP1 = PPMPT2KH
CASE 6 : TEMP1 = PPMPT8KH
CASE 7 : TEMP1 = PPMPT8KC
END SELECT
' First calc shift divisions in ppb and draw shift lines.
T% = FILETYPE%(K%)
OPEN 'CHARACTR.DAT' FOR RANDOM AS #1
FIELD #1, 40 AS CHARS
DRAW 'S4 C' + STR$(TEMP%)
PPM(T%,ACTIVE%(1,T%)) = TEMP1 * (ZERO% - PPT%(T%,ACTIVE%(1,T%)))
TEMP1% = PPT%(T%,ACTIVE%(1,T%))
LINE (TEMP1%, -3) : (TEMP1%, DA(TEMP1%)*YEXPFC + YOFFSET%(T%,I%) + 50), TEMP%
TEMP1% = PMAP(PPT%(T%,ACTIVE%(1,T%)), 0); 3
TEMP2% = PMAP(D$(PPT%(T%,ACTIVE%(1,T%))) * YEXPFC + YOFFSET%(T%,I%) + 55, 1)
GET #1, ACTIVE%(1,T%) + 64
IF TEMP2% < 485 AND TEMP2% > 0 THEN
DRAW 'BM' + STR$(TEMP1%) + ' '; STR$(TEMP2%) + TAO + CHARS : draw char
END IF

```

' Flow Spectra
' 1H Static
' 13C Static

' set up for
' labeling
' size - color

```

OPTN$(1)=2 : GOTO DoOption1
CASE 'R',r
OPTN$(1)=3 : GOTO DoOption1
CASE 'S',s
OPTN$(1)=4 : GOTO DoOption1
CASE 'W',w
OPTN$(1)=5 : GOTO DoOption1
CASE 'P',p
OPTN$(1)=6 : GOTO DoOption1
CASE 'E',e
OPTN$(1)=7 : GOTO DoOption1
CASE 'Q',q
OPTN$(1)=8 : GOTO DoOption1
CASE CHR$(0)+CHR$(72), CHR$(0)+CHR$(80)
LOCATE (OPTN$(1)-1)*2+8,38-(0.5*LEN(OPTN$(OPTN$(1))))
COLOR 1,1
PRINT "LEFTS (OPTN$(OPTN$(1)),1);
PRINT RIGHTS(OPTN$(OPTN$(1)),LEN(OPTN$(OPTN$(1))-1));
IF AS=CHR$(0)+CHR$(72) THEN DECR OPTN$(1) ELSE INCR OPTN$(1)
IF OPTN$(1)<1 THEN OPTN$(1)=8
IF OPTN$(1)>8 THEN OPTN$(1)=1
COLOR 14,0
LOCATE (OPTN$(1)-1)*2+8,38-(0.5*LEN(OPTN$(OPTN$(1))))
PRINT "OPTN$(OPTN$(1));
CASE CHR$(0)+CHR$(73),CHR$(0)+CHR$(77)
CASE ELSE
SOUND 1000,3 : SOUND 800,1.5
END SELECT
GOTO Startloop1
DoOption1
SELECT CASE OPTN$(1)
CASE 1 : GOTO ChangeDefaultParams
CASE 2 : GOTO AnalyzeFuelData
CASE 3 : GOTO Recalculate
CASE 4 : GOTO StackPlot
CASE 5 : GOTO WorkUpBlank
CASE 6 : GOTO PrintReports
CASE 7 : GOTO EditIntegrations
CASE 8
CLOSE : COLOR 12,0 : CLS
GOSUB Logo
LOCATE 1,1 : PRINT "May the Precession be yours..."
END
END SELECT

```

Code Listing for LCNMR41.INC

This is the subroutine which contains the documentation.

Here is a listing of the order in which the calculated

```

OPTN$(2)="Analyze Fuel Data"
OPTN$(3)="Recalculate Fuel Data"
OPTN$(4)="Stack Plot Fuel Data"
OPTN$(5)="Work Up Blank Data"
OPTN$(6)="Print Fuel Reports"
OPTN$(7)="Edit Fuel Integrations"
OPTN$(8)="Quit to DOS"
.
. Will draw the screen.
SCREEN 0 : WIDTH 80
COLOR 15,0 : CLS
COLOR 15,4
LOCATE 1,5 : PRINT CHR$(201),STRING$(99,205);CHR$(187)
LOCATE 2,9 : PRINT CHR$(186),STRING$(99,32);CHR$(186)
LOCATE 3,6 : PRINT CHR$(200),STRING$(99,205);CHR$(186)
LOCATE 1,31 : PRINT CHR$(209);
LOCATE 2,31 : PRINT CHR$(179);
LOCATE 3,31 : PRINT CHR$(207);
LOCATE 2,10 : PRINT "LC-NMR"
LOCATE 2,19 : PRINT VERSNS
LOCATE 2,35 : PRINT "LC-NMR Data Analysis Software ";
.
Main Menu box
COLOR 10,1
LOCATE 5,15 : PRINT CHR$(218),STRING$(49,100);CHR$(191);
FOR I%=6 TO 22
LOCATE I%,15 : PRINT CHR$(179);TAB(95);CHR$(179);
NEXT I%
LOCATE 23,15 : PRINT CHR$(182),STRING$(49,100);CHR$(217);
COLOR 10,1
LOCATE 6,20 : PRINT TIMES;
LOCATE 6,51 : PRINT DATES;
COLOR 15,1
LOCATE 6,35 : PRINT "MAIN MENU:";
COLOR 14,1
FOR I%=1 TO 8
LOCATE (I%-1)*2+8,40-(0.5*LEN(OPTN$(I%)))
COLOR 11,1 : PRINT LEFTS (OPTN$(I%),1);
COLOR 14,1 : PRINT RIGHTS(OPTN$(I%),LEN(OPTN$(I%))-1);
NEXT I%
.
Next are commands.
COLOR 3,0
LOCATE 25,16 : PRINT "Press the highlighted letter or <ENTER> to select.";
.
Next see what to do.
COLOR 14,0
LOCATE (OPTN$(1)-1)*2+8,38-(0.5*LEN(OPTN$(OPTN$(1))))
PRINT "OPTN$(OPTN$(1));";
Startloop1:
AS=INKEY$
SELECT CASE AS
CASE =
COLOR 10,1
LOCATE 6,20 : PRINT TIMES;
CASE CHR$(13)
GOTO DoOption1
CASE 'C',c
OPTN$(1)=1 : GOTO DoOption1
CASE 'A',a

```

parameters are stored in the file. I know that the order is slightly illogical, but I have attempted to make this file compatible with the files from the old LC-NMR program LC-NMR. This file is composed of sequential access records. The first and second strings are the Fuel Name and Data. The strings between 3 and 140 are the calculated results. Then comes a couple of strings to give processing parameters and physical data. The old LC-NMR system stops here with at total of 148 records in the file. As the new system will calculate more than this, the new parameters will come at the end of the file. These parameters include such tidbits as the number of quaternary carbon calculated for each file, both absolute number moles and avg number. It will also include the physical properties for each fraction as well as for the overall fuel mixture. As the length of the file for this pgm will be different from files from the LC-NMR software, files extending past the old limit 148 elements will be terminated with an element which simply says "END". This way, files may be read until either 148 elements have been read, or the END statement is reached. Also, it has become evident that it would be nice to be able to recalculate the data from old integration values. Therefore, the entries from 205 - 256 are the integration values.

Below is a listing of the order of the strings in the file:

```

1: Fuel Name          -- General Data --
2: Data Run          --
3: *Cun              --- Monocyclic Data ---
4: *Cun
5: *Ceub
6: *Ceub
7: *Cbbh
8: *Cbbh
9: *Cach3
10: *Cach3
11: *Cach2
12: *Cach2
13: *Cach
14: *Cach
15: *Cch2>a
16: *Cch2>a
17: *Cch3>a
18: *Cch3>a
19: *Cabst
20: *Cabst
21: Avg Molecular Wt
22: Fraction Bub Sltas
23: ADS
24: Moles Aromatic C
25: Total Moles Carbon
26: Fract Arom
27: Fract Total Carbon

--- Dicyclic Data --- = MONO + 25
The Dicyclic Data is in the same order as the monocyclic data and occupies the numbers 28 - 52 in the files. Number 53 is a spacer between the data sets. (=mono + 25)

--- Fluorene Data --- = MONO + 51
The Fluorene Data is in the same order as the monocyclic data and occupies the numbers 54 - 78 in the files. Number 79 is a spacer between the data sets. (=dl + 26)

--- Phenanthrene Data --- = MONO + 77
The Phenanthrene Data is in the same order as the monocyclic data and occupies the numbers 80 - 104 in the files. Number 105 is a spacer between the data sets. (=fl + 26)

106: *Cch3
107: *Cch3
108: *Cch2
109: *Cch2
110: *Cch
111: *Cch
112: Avg Mol Wt
113: Avg Deg Branching
114: Moles C
115: Moles C (2)
116: Fraction Carbon
117: Fract C: Alkane (2)
118: Fract C: Mono (2)

```

119: Fract C: Naph (2) 120: Fract C: Flou (2)

121: spacer between data sets

... General Data ---

122: Volume Monocyclics

124: Volume Fluorene

126: Volume Alkanes

128: Monocyclic Wt %

130: Fluorene Wt %

132: Carbon Aromaticity

134: Molar Conc HMDS

136: Freezing Point

138: Elemental Analysis Carbon

140: Elemental Analysis H-by NMR

142: Instrument Used

144: Comments

148: Fractional Aromaticity

This is the end of the parameters stored under the old LC-NMR program. From here will be the parameters used by this program. They will be defined and the file extended as needed.

147: *Ccq - Alkane

148: Ccq - Alkane

149: *Ccq - Monocyclic

150: Ccq - Mono

151: *Ccq - Dicyclic

152: Ccq - Dicyclic

153: *Ccq - Fluorene

154: Ccq - Fluorene

155: *Ccq - Phenanthrene

156: Ccq - Phenanth

157: Name

158: Formula

159: Molecular Weight

160: Cetane Number

161: 50% Boiling Point

162: Pour Point

163: Cetane Improvr %

164: Plash Point

165: Density

166: Refractive Index

167: Cloud Point

168: Viscosity

169: Filterability

170: Class (fuel, alk, etc)

171: Average Degree Branching

172: Specific Dispersion

173: Surface Tension

174: Aniline Point

175: Critical Pressure

176: Critical Temperature

177: Critical Volume

178: Heat Capacity

179: Heat of Vaporization

180: Heat of Formation

181: Free Energy of Formation

182: Heat of Combustion

183: Molecular Volume

184: Percent Aromatics

185: Percent Olefins

186: Fuel Type (DF-2, JP 6, etc)

187: Cetane Index

--- Physical Properties ---

--- Uncorrelated Property

--- Uncorrelated Property

--- Uncorrelated Property

cetane

deg C

deg C

deg C

kg/L

--- Uncorrelated Property

deg C

unknown

--- Uncorrelated Property

--- Uncorrelated Property

--- Uncorrelated Property

--- Uncorrelated Property

--- Uncorrelated Property

--- Uncorrelated Property

--- Uncorrelated Property

--- Uncorrelated Property

--- Uncorrelated Property

MJ/kg

--- Uncorrelated Property

volume %

--- Uncorrelated Property

--- Uncorrelated Property

cetane

Code Listing for LCNMR42.INC

This is the subroutine to find the aromaticity.

```

188: Specific Gravity
189: Initial Boiling Point
190: 10% Boiling Point
191: 90% Boiling Point
192: End Boiling Point
193: Residual Carbon
194: Unused Property
196: Unused Property
198: Unused Property
200: Unused Property
202: Unused Property
204: Unused Property
205: Integration Data
207: Alkane HMDS (A-B)
208: Alkane CH2 (C-D)
209: Alkane CH (E-F)
210: Mono HMDS (A-B)
212: Mono >alpha (C-D)
213: Mono <alpha (D-E)
215: Mono <CH2 (E-F)
216: Mono <CH (G-H)
218: Mono AR-1 (I-J)
220: Mono AR-3 (K-L)
222: DI HMDS (A-B)
224: DI >alpha (C-D)
226: DI <alpha (E-F)
228: DI <CH (G-H)
230: DI AR-1 (I-J)
232: DI AR-3 (K-L)
234: FI HMDS (A-B)
236: FI >alpha (C-D)
238: FI <alpha (E-F)
240: FI <CH (G-H)
242: FI AR-1 (I-J)
244: FI AR-3 (K-L)
246: Ph HMDS (A-B)
248: Ph >alpha (C-D)
250: Ph <alpha (E-F)
252: Ph <CH (G-H)
254: Ph AR-1 (I-J)
256: Ph AR-3 (K-L)
258: Static 1H Aliphatic
260: Static 13C Aliphatic
262: Alkane NOSC
264: Dicyclic NOSC
266: Phen NOSC
267: END
RETURN
208: Alkane Unused (B-C)
209: Alkane CH2 (D-E)
211: Mono Unused (B-C)
213: Mono <CH3 (D-E)
215: Mono <TET (F-G)
217: Mono Unused (H-I)
219: Mono AR-2 (J-K)
221: Mono AR-4 (L-M)
223: DI Unused (B-C)
225: DI Unused (D-E)
227: DI <CH2 (F-G)
229: DI Unused (H-I)
231: DI AR-2 (J-K)
233: DI AR-4 (L-M)
235: FI Unused (B-C)
237: FI Unused (D-E)
239: FI <CH2 (F-G)
241: FI Unused (H-I)
243: FI AR-2 (J-K)
245: FI AR-4 (L-M)
247: Ph Unused (B-C)
249: Ph Unused (D-E)
251: Ph <CH2 (F-G)
253: Ph Unused (H-I)
255: Ph AR-2 (J-K)
257: Ph AR-4 (L-M)
259: Static 1H Aromatic
261: Static 13C Aromatic
263: Mono NOSC
265: Fluorene NOSC
267: END
OPTN$(1)="Aromaticity Value"
OPTN$(2)="NMR Integration Areas"
OPTN$(3)="Ignore this section"
OPTN$(4)="Exit this section"
Will draw the screen.
SCREEN 0 : WIDTH 80
COLOR 15, 0 : CLS
GOSUB DrawAromaticityScreen
TEMP3%=TEMP1% : TEMP4%=TEMP2%
TEMP1%=10 : TEMP2%=1
GOSUB DrawFuelName
TEMP1%=TEMP3% : TEMP2%=TEMP4%
Next see what to do.
COLOR 14,0
LOCATE (OPTN$(8)-1)*2+12,38:(0.5*LEN(OPTN$(8)))
PRINT " OPTN$(OPTN$(8)), "
Startup18:
AS=INKEY$
SELECT CASE AS
CASE =
COLOR 10,1
LOCATE 6,20 : PRINT TIMES;
CASE "Q",q,CHRS(27)
GOTO MainMenu
CASE CHRS(13)
GOTO DoOption18
CASE "A",a
OPTN$(8)=1 : GOTO DoOption18
CASE "N",n
OPTN$(8)=2 : GOTO DoOption18
CASE "I",i
OPTN$(8)=3 : GOTO DoOption18
CASE "E",e
OPTN$(8)=4 : GOTO DoOption18
CASE CHRS(0)+CHRS(72), CHRS(0)+CHRS(80)
LOCATE (OPTN$(8)-1)*2+12,38:(0.5*LEN(OPTN$(8)))
COLOR 11,1
PRINT " LEFTS (OPTN$(8)),1);
COLOR 14,1
LOCATE 14,1
PRINT RIGHTS(OPTN$(8)),LEN(OPTN$(8))-1,";
IF AS=CHRS(0)+CHRS(72) THEN DECR OPTN$(8) ELSE INCR OPTN$(8)
IF OPTN$(8)<1 THEN OPTN$(8)=4
IF OPTN$(8)>4 THEN OPTN$(8)=1
COLOR 14,0
LOCATE (OPTN$(8)-1)*2+12,38:(0.5*LEN(OPTN$(8)))
PRINT " OPTN$(OPTN$(8)), "
CASE CHRS(0)+CHRS(75),CHRS(0)+CHRS(77)
CASE ELSE
' no key
' quit
' return
' arom value
' integ value
' ignore
' exit
' up-down
LOCATE (OPTN$(8)-1)*2+12,38:(0.5*LEN(OPTN$(8)))
PRINT " LEFTS (OPTN$(8)),1);
COLOR 14,1
LOCATE 14,1
PRINT RIGHTS(OPTN$(8)),LEN(OPTN$(8))-1,";
IF AS=CHRS(0)+CHRS(72) THEN DECR OPTN$(8) ELSE INCR OPTN$(8)
IF OPTN$(8)<1 THEN OPTN$(8)=4
IF OPTN$(8)>4 THEN OPTN$(8)=1
COLOR 14,0
LOCATE (OPTN$(8)-1)*2+12,38:(0.5*LEN(OPTN$(8)))
PRINT " OPTN$(OPTN$(8)), "
CASE CHRS(0)+CHRS(75),CHRS(0)+CHRS(77)
CASE ELSE
' left-right
' cpsi)

```



```

SOUND 1000,3 : SOUND 800,1,5
END SELECT
GOTO Startloop18
DoOption18:
SELECT CASE OPTN%(8)
CASE 1 : GOSUB GetAromValue : GOTO Startloop18
CASE 2 : GOSUB GetAromIntValue : GOTO Startloop18
CASE 3 : DS(TEMP1%)=0 : DS(TEMP2%)=0 : DS(TEMP2%+1)=0 : RETURN
CASE 4 : RETURN
END SELECT

GetAromValue:
. This is a mini-subroutine to get the aromaticity value.
FOR I%=8 TO 16
LOCATE I%,15 : PRINT CHR$(179);TAB(65);CHR$(179); . middle
NEXT I%
COLOR 3, 0
LOCATE 21,15 : PRINT SPACES(80);
LOCATE 22,15 : PRINT SPACES(80);
COLOR 15, 1
LOCATE 12,23 : LINE INPUT "New Aromaticity Value: ";DS(TEMP1%)
IF VAL(DS(TEMP1%))<>1 THEN
TEMP=VAL(DS(TEMP1%))
AROM=TEMP/(1-TEMP)
END IF
DS(TEMP2%)=STR$(1) : DS(TEMP2%+1)=STR$(AROM)
GOSUB DrawAromaticityScreen
COLOR 14,0
LOCATE (OPTN%(8)-1)*2+12,38,(0.5*LEN(OPTN%(8))))
PRINT " ",OPTN$(OPTN%(8)):" ";
RETURN

GetAromIntValue:
. This is a mini-subroutine to get the aromaticity integrals.
FOR I%=8 TO 16
LOCATE I%,15 : PRINT CHR$(179);TAB(65);CHR$(179); . middle
NEXT I%
COLOR 3, 0
LOCATE 21,15 : PRINT SPACES(80);
LOCATE 22,15 : PRINT SPACES(80);
TEMP1%=Please enter the "+TEMPS+" integrals"
COLOR 14, 1
LOCATE 10,40-0.5*LEN(TEMP1%) : PRINT TEMP1%;
COLOR 15, 1
LOCATE 12,30 : PRINT "Aliphatic: ";
LOCATE 14,30 : PRINT "Aromatic: ";
LOCATE 12,45 : LINE INPUT DS(TEMP2%)
LOCATE 14,45 : LINE INPUT DS(TEMP2%+1)
IF VAL(DS(TEMP2%))+VAL(DS(TEMP2%+1))<>0 THEN
TEMP1=VAL(DS(TEMP2%))
TEMP2=VAL(DS(TEMP2%+1))
DS(TEMP1%)=STR$(TEMP2 / (TEMP1+TEMP2))
END IF
GOSUB DrawAromaticityScreen
COLOR 14,0
LOCATE (OPTN%(8)-1)*2+12,38,(0.5*LEN(OPTN%(8))))
PRINT " ",OPTN$(OPTN%(8)):" ";
RETURN

DrawAromaticityScreen:
. This is a mini-subroutine to draw the screen to get the aromaticity.
COLOR 10, 1
LOCATE 5,15 : PRINT CHR$(218);STRINGS(49,198);CHR$(191); . top line
FOR I%=8 TO 16
LOCATE I%,15 : PRINT CHR$(179);TAB(65);CHR$(179); . middle
NEXT I%
LOCATE 19,15 : PRINT CHR$(192);STRINGS(49,198);CHR$(217); . bottom line
COLOR 10, 1
LOCATE 8,20 : PRINT TIMES;
LOCATE 6,51 : PRINT DATES;
COLOR 12, 1
LOCATE 7,37 : PRINT USING "###.###";VAL(DS(TEMP1%));
IF VAL(DS(TEMP1%))<=0 THEN
COLOR 28, 1
TEMP1%="Current "+TEMPS+" Aromaticity Impossible!"
LOCATE 8,40-0.5*LEN(TEMP1%) : PRINT TEMP1%;
END IF
COLOR 11, 1
TEMP1%="Enter the "+TEMPS+" aromaticity by:"
LOCATE 10,40-0.5*LEN(TEMP1%) : PRINT TEMP1%;
COLOR 14, 1
FOR I%=1 TO 4
LOCATE (I%-1)*2+12,40-(0.5*LEN(OPTN%(I%)))
COLOR 11, 1 : PRINT LEFT$(OPTN$(I%),1);
COLOR 14, 1 : PRINT RIGHT$(OPTN$(I%),LEN(OPTN$(I%))-1);
NEXT I%
. Next are commands
COLOR 3,0
LOCATE 21,16 : PRINT "Press the highlighted letter or <ENTER> to select.";
LOCATE 22,20 : PRINT "Press the <Q> to return to the Main Menu.";
RETURN

```

Code Listing for LCNMR43.INC

This is the subrtn to see if a file is present before opening.

```

SHELL "DIR "+FILENAME$+" > "+SCRDIR$+"TEMP.ZZZ"
OPEN SCRDIR$+"TEMP.ZZZ" FOR INPUT AS #1
FOR I%=1 TO 4
LINE INPUT #1,TEMPS
NEXT I%
IF EOF(1) THEN
CLOSE #1 : KILL SCRDIR$+"TEMP.ZZZ"
SCREEN 0 : COLOR 15, 0 : CLS
COLOR 0, 4
LOCATE 8, 5 : PRINT CHR$(201);STRINGS(69,205);CHR$(187);
FOR I%=8 TO 15
LOCATE I%,5 : PRINT CHR$(186);TAB(75);CHR$(186);

```

```

NEXT I%
LOCATE 16,5 : PRINT CHR$(200),STRING$(60,205);CHR$(188);
COLOR 31,4
LOCATE 11,23 : PRINT "Unable to open the requested file."
COLOR 14,4
TEMP$=">>>"*FILENAMES+" is not in the directory <<<"
LOCATE 13,40-0.5*LEN(TEMP$) : PRINT TEMP$
COLOR 0,3
LOCATE 24,19 : PRINT " Press any key to return to the Main Menu ";
TEMP$=INPUT$(1)
GOTO MainMenu
END IF
CLOSE 1 : KILL SCRDIRS+TEMP.ZZZ
RETURN
    
```

* File found

Code Listing for LCNMR44.INC

This is the subrtn to do the error handling.

```

SCREEN 0 : COLOR 15,0 : CLS
COLOR 0,4
LOCATE 8,5 : PRINT CHR$(201),STRING$(60,205);CHR$(187);
FOR I%=9 TO 15
  LOCATE I%,5 : PRINT CHR$(186);TAB(79);CHR$(186);
NEXT I%
LOCATE 16,5 : PRINT CHR$(200),STRING$(60,205);CHR$(188);
COLOR 31,4
LOCATE 11,28 : PRINT USING ">>> Error ### encountered <<<";ERR#;
COLOR 14,4
TEMP$="See Appendix E, p. 412, in Turbo Basic Manual for full message."
LOCATE 13,9 : PRINT TEMP$;
COLOR 0,3
LOCATE 24,19 : PRINT " Press any key to return to the Main Menu ";
TEMP$=INPUT$(1)
CLOSE
GOTO MainMenu
    
```

Code Listing for LCNMR45.INC

This is the subroutines to display the integral regions.

```

I%=FILETYPE%(K%)
IF TEMP$="ON" THEN TEMP%=INTOOL% ELSE TEMP%=BACKCOL%
SELECT CASE FILETYPE%(K%)
CASE 1 : TEMP1%=5 : TEMP2%=205 : TEMP3%=1
    
```

* Alkanes

```

CASE 2 : TEMP1%=12 : TEMP2%=210 : TEMP3%=1
CASE 3 : TEMP1%=12 : TEMP2%=222 : TEMP3%=1
CASE 4 : TEMP1%=12 : TEMP2%=234 : TEMP3%=1
CASE 5 : TEMP1%=12 : TEMP2%=246 : TEMP3%=1
CASE 6 : TEMP1%=3 : TEMP2%=258 : TEMP3%=2
CASE 7 : TEMP1%=3 : TEMP2%=280 : TEMP3%=2
END SELECT
MAXINT=0
FOR I%=1 TO TEMP1% STEP TEMP3%
  IF I%>=6 THEN TEMP4%=INT(I%/3) ELSE TEMP4%=I%-1
  IF VAL(D$(TEMP2%+TEMP4%))>MAXINT THEN MAXINT=VAL(D$(TEMP2%+TEMP4%))
NEXT I%
FOR I%=1 TO TEMP1% STEP TEMP3%
  IF INTNAMES(I%)(%)<>" THEN
    IF I%>=6 THEN TEMP4%=INT(I%/3) ELSE TEMP4%=I%-1
    TEMP1=0 : TEMP2=0 : TEMP3=100/MAXINT*INTEXP%(I%)
    FOR J%=PT%(I%)(%+1) TO FT%(I%)(%)
      INCR TEMP1,(DA(J%)-BA(J%))/INTNF(I%)
      INCR TEMP2,(DA(J%-1)-BA(J%-1))*INTNF(I%)
    LINE (J%,TEMP1+TEMP3+79)-(J%-1,TEMP2+TEMP3+79),TEMP$
    NEXT J%
  END IF
NEXT I%
RETURN
    
```

- * Monocyclic
- * Dicyclic
- * Fluorene
- * Phenane
- * 1H Static
- * 13C Static

- * loop to find
- * max integral
- * loop to draw
- * if int used

Code Listing for LCNMR46.INC

This is the subrtn to find which files are present on the disk.

```

COLOR 15,4
LOCATE 12,24 : PRINT " Loading Currently Available ";
LOCATE 13,24 : PRINT " files from the disk ";
TEMP$="DIR *NMRDIRS+FUELNAMES(L%)+*.* > *SCRDIRS+TEMP.ZZZ"
SHELL TEMP$
FOR I%=1 TO 7
  TEMP$=FUELNAMES(L%)
  IF I%<6 THEN TEMP$=TEMP$+"S"
  IF I%<6 THEN TEMP$=TEMP$+"F"
  IF I%=7 THEN TEMP$=TEMP$+"C"
  WHILE LEN(TEMP$)<8
    TEMP$=TEMP$+"."
  WEND
  IF I%<6 THEN TEMP$=TEMP$+"T0"+CHR$(48+I%)
  IF I%=6 THEN TEMP$=TEMP$+"T0"
  IF I%=7 THEN TEMP$=TEMP$+"T0"
  OPEN SCRDIRS+TEMP.ZZZ FOR INPUT AS #1
  WHILE NOT EOF(1) AND LEFT$(AS,12)<>TEMP$
    INPUT #1,AS
  WEND
  IF EOF(1) THEN
    FILETYPE%(I%)=8
  ELSE
    
```

* not found

Code Listing for LCNMR48.INC

Subroutine to wipe out data for an fraction <0.25% C

```
FOR I%=T1% TO T2%
  DS(I%)=0
NEXT I%
FOR I%=T3% TO T4%
  DS(I%)=0
NEXT I%
DS(T5%)=0
GOTO CalculateTotalCarbon
```

Code Listing for LCNMR49.INC

This is the subroutine to edit the number of scans.

```
* Will draw the screen.
COLOR 10, 1
LOCATE 6,18 : PRINT CHR$(216),STRINGS(43,106),CHR$(101); * top line
FOR I%=7 TO 18
  LOCATE I%,18 : PRINT CHR$(179),TAB(82),CHR$(179); * middle
NEXT I%
LOCATE 19,18 : PRINT CHR$(192),STRINGS(43,106),CHR$(217); * bottom line
COLOR 10, 1
LOCATE 7,20 : PRINT TIMES;
LOCATE 7,51 : PRINT DATES;
COLOR 15, 1
LOCATE 8,25 : PRINT * Class Number Scans*,
LOCATE 9,25 : PRINT * -----*,
COLOR 14, 1
LOCATE 10,25 : PRINT * Alkane*,
LOCATE 12,25 : PRINT * Monocyclic*,
LOCATE 14,25 : PRINT * Dicyclic*,
LOCATE 16,25 : PRINT * Fluorene*,
LOCATE 18,25 : PRINT *Phenanthrene*,
COLOR 12, 1
FOR I%=1 TO 5
  LOCATE (I%-1)*2+10,45 : PRINT USING "0.000000" ,VAL(DS(261+I%));
NEXT I%
* Next are commands
COLOR 3, 0
```

```
FILETYPE%(I%)=I%
END IF
CLOSE 1
* Note: if doing a recalculate, want to key the file proton files
* off of the number of scans, not the presence of the disk files.
IF OPTN%(1)=3 AND I%<=5 THEN
  IF VAL(DS(261+I%))>0 THEN FILETYPE%(I%)=I% ELSE FILETYPE%(I%)=6
END IF
NEXT I%
KILL SCHDIRS+TEMP.ZZZ
COLOR 15, 0
LOCATE 12,24 : PRINT SPACES(40);
LOCATE 13,24 : PRINT SPACES(40);
RETURN
```

Code Listing for LCNMR47.INC

This is the subroutine to do the fuel property calcs.

```
PROP=MIXCOEFF(1)
INCR PROP,VAL(DS(106))*VAL(DS(116))*MIXCOEFF(2)
INCR PROP,VAL(DS(106))*VAL(DS(116))*MIXCOEFF(3)
INCR PROP,VAL(DS(110))*VAL(DS(116))*MIXCOEFF(4)
INCR PROP,VAL(DS( 3))*VAL(DS( 27))*MIXCOEFF(5)
INCR PROP,VAL(DS( 8))*VAL(DS( 27))*MIXCOEFF(6)
INCR PROP,VAL(DS(11))*VAL(DS( 27))*MIXCOEFF(7)
INCR PROP,VAL(DS(13))*VAL(DS( 27))*MIXCOEFF(8)
INCR PROP,VAL(DS(16))*VAL(DS( 27))*MIXCOEFF(9)
INCR PROP,VAL(DS(15))*VAL(DS( 27))*MIXCOEFF(10)
INCR PROP,VAL(DS( 28))*VAL(DS( 52))*MIXCOEFF(11)
INCR PROP,VAL(DS( 34))*VAL(DS( 52))*MIXCOEFF(12)
INCR PROP,VAL(DS( 36))*VAL(DS( 52))*MIXCOEFF(13)
INCR PROP,VAL(DS( 40))*VAL(DS( 52))*MIXCOEFF(14)
INCR PROP,VAL(DS( 54))*VAL(DS( 78))*MIXCOEFF(15)
INCR PROP,VAL(DS( 60))*VAL(DS( 78))*MIXCOEFF(16)
INCR PROP,VAL(DS( 68))*VAL(DS( 78))*MIXCOEFF(18)
INCR PROP,VAL(DS( 80))*VAL(DS(104))*MIXCOEFF(19)
INCR PROP,VAL(DS( 86))*VAL(DS(104))*MIXCOEFF(20)
INCR PROP,VAL(DS( 88))*VAL(DS(104))*MIXCOEFF(21)
INCR PROP,VAL(DS( 82))*VAL(DS(104))*MIXCOEFF(22)
IF LEFT$(FUNCTIONS,1)='X' THEN PROP=PROP
IF LEFT$(FUNCTIONS,3)='1/X' THEN PROP=1/PROP
PROP=PROP * OFSEFACTOR
PROP=PROP + SLOPEFACTOR
RETURN
```

Listing for Program I.4: LCNMRCFG.BAS

Program Name: LCNMRCFG BAS Ver 1.00 Date Written: 01/04/1988
 Author: Allen Caswell Date Modified: 08/11/1988

The purpose of this program is to service the configuration file for the LC-NMR software. This file contains all of the standard parameters for the LC-NMR program.

First is the section to set up the variables.

COMMON TEMPS

- * First are control parameters for configuration program.
- VERSN\$ = "Ver 1.00"
- OPTNS(1) = "Reset to Default Parameters"
- OPTNS(2) = "Change Selected Parameters"
- OPTNS(3) = "Exit to LC-NMR Program"
- OPTNS(4) = "Quit to DOS"
- OPTNS(1) = 1
- ODRS = "D\LCNMRFPGMS"
- DIM CTRLPTS(8), FILETYPES(7), INTNAMES(7,12), PPM(7,13)
- DIM BASEEND(7,8), FILETYPES(8), SHIFTSTEP(7), GAIN(7)
- DIM YOFFSET(7), BASESTEP(7), INTEXP(7)
- * The constants detailed below are dependent on the exact parameters under which the spectra were taken.
- * For the 2K Proton flow files:
 - SF: 199.5 MHz SW: 2100.0 Hz FW: 1500.0 Hz PW: 4.1 us
- * For the 8K Proton Static Files:
 - SF: 200.13 MHz SW: 4000.0 Hz FW: 5000.0 Hz PW: 1.0 us
- * For the 8K Carbon Static Files:
 - SF: 50.327 MHz SW: 12500.0 Hz FW: 15700.0 Hz PW: 14.0 us
- HMDSHIFT = 0.07
- CDCL3SHIFT = 77.0
- PPMPT2KH = 0.0102796
- PPMPT8KH = 0.0048796
- PPMPT8KC = 0.00606388
- HMDS CONC = 0.000308
- FLOWRATE = 2.94
- SCANTIME = 0.910
- CONVERT = 60000
- * Next are the control parameters for the LC-NMR program.
- Cq = 0.00
- VERS = "Ver 3.30"
- PRINTPR% = 1
- FONT% = 1
- SPECTCL% = 12
- AXISCOL% = 9
- TABLECL% = 13
- * Chemical shift for HMDS
- * chemical shift for CDCL3
- * #PPM/pt for 2K file
- * #PPM/pt for 8K file- 1H
- * #PPM/pt for 8K file- 13C
- * HMDS Concentration
- * Chromato flow rate
- * Time for scan
- * Conversion factor
- * Couant for alkanes
- * Version Number
- * ProPrinter
- * Regular data font
- * Spectrum color
- * Axis color
- * Table color

```

LOCATE 23,16 : PRINT "Press the <ARROW KEYS> to move, <F> to file data,
LOCATE 24,16 : PRINT " <Q> to quit, or <ENTER> to continue. ";
* Have drawn the screen, so highlight data and edit.
COLOR 12,0
LOCATE (OPTN%(9)-1)*2+10,45:PRINT USING "#####"VAL(D$(281)+OPTN%(9));
Startloop2:
AS=INKEY$
SELECT CASE AS
CASE =
    COLOR 10,1 : LOCATE 7,20 : PRINT TIMES;
CASE "Q",7,CHR$(27)
    GOTO MainMenu
CASE CHR$(13)
    RETURN
CASE "F",7
    COLOR 15,4
    LOCATE 21,25 : PRINT " *** Filing the Data *** ";
    GOSUB FileVgStData
    COLOR 15,0
    LOCATE 21,25 : PRINT SPACES(40);
CASE CHR$(9)+CHR$(7,2), CHR$(9)+CHR$(80)
    COLOR 12,1
    LOCATE (OPTN%(9)-1)*2+10,45
    PRINT USING "#####"VAL(D$(281)+OPTN%(9));
    IF AS=CHR$(9)+CHR$(7,2) THEN DEC OPTN%(9) ELSE INC OPTN%(9)
    IF OPTN%(9)<1 THEN OPTN%(9)=5
    IF OPTN%(9)>5 THEN OPTN%(9)=1
    COLOR 12,0
    LOCATE (OPTN%(9)-1)*2+10,45
    PRINT USING "#####"VAL(D$(281)+OPTN%(9));
CASE CHR$(9)+CHR$(7,9),CHR$(9)+CHR$(77)
    COLOR 12,0
    LOCATE (OPTN%(9)-1)*2+10,45
    PRINT USING "#####"VAL(D$(281)+OPTN%(9));
CASE ELSE
    SOUND 1000,3 : SOUND 800,1.5
END SELECT
GOTO Startloop2
    
```

```

SHIFTCL% =14
BASECOL% =15
DATACOL% =11
INTCOL% =10
BACKCOL% =0
INTEGRALS =OFF
NMRDIRS =D:\LCNMR\DATA\ARMY681
INPUTDIRS =D:\LCNMR\DATA\ARMY681
OUTPTDIRS =D:\LCNMR\DATA\ARMY681
BLANKDIRS =D:\LCNMR\DATA\ARMY681
SCORDIRS =F:
PARAMDIRS =D:\LCNMR\PGMS1
CFGDIRS =D:\LCNMR\PGMS1
CTRLLOPTNS(1)=N
CTRLLOPTNS(2)=N
CTRLLOPTNS(3)=N
CTRLLOPTNS(4)=N
CTRLLOPTNS(5)=N
CTRLLOPTNS(6)=N
FILETYPE%(1)=1
FILETYPE%(2)=2
FILETYPE%(3)=3
FILETYPE%(4)=4
FILETYPE%(5)=5
FILETYPE%(6)=6
FILETYPE%(7)=7
INTEXP%(1)=2
INTEXP%(2)=2
INTEXP%(3)=2
INTEXP%(4)=2
INTEXP%(5)=2
INTEXP%(6)=2
INTEXP%(7)=2
FOR %1=1 TO 7
  YOFFSTEP%(%) =0
  SHIFTSTEP%(%)=2
  BASESTEP%(%)=10
NEXT %

```

```

* Shift division color
* Baseline color
* Data foreground color
* Integral display color
* Background color
* Do not display integrals
* NMR spectra directory
* Input data file dir
* Output data file dir
* Blank data directory
* Scratch file directory
* Param dir for prop calcs
* Dir for config file
* Stack Plot command
* Auto File Select command
* Hard Copy Integrals cmd
* Hard Copy Results cmd
* Hard Copy Properties cmd
* File #1 - Alkane
* File #2 - Monocyclic
* File #3 - Dicyclic
* File #4 - Fluorene
* File #5 - Phenanthrene
* File #6 - 1H Static
* File #7 - 13C Static

```

```

* Spectrum vertical offset
* Step for shift movement
* Step for baseline moves
* Alkane -> 13C Static

```

```

* Next are the fraction names.
DATA * Alkane ** Monocyclic ** Dicyclic
DATA * Fluorene ** Phenanthrene ** 1H Static
DATA * 13C Static ** Do Not Use
FOR %1=1 TO 8 : READ FILETYPE%(%) : NEXT %

```

```

* Next are the integration region names for each class
DATA *H1DS,*1,*CH3,*CH2,*CH
DATA *H1DS,*1,*a,*CH3,*CH2,*aTET,*eCH,*AR,*1,*...
DATA *H1DS,*1,*a,*CH3,*CH2,*eCH,*AR,*1,*...
DATA *H1DS,*1,*a,*CH3,*CH2,*eCH,*AR,*1,*...
DATA *H1DS,*1,*a,*CH3,*CH2,*eCH,*AR,*1,*...
DATA *Aliphatic* *Aromatic*
DATA *Aliphatic* *Aromatic*
FOR %1=1 TO 5 : READ INTNAMES(1,%%) : NEXT %
FOR %1=1 TO 12 : READ INTNAMES(2,%%) : NEXT %
FOR %1=1 TO 12 : READ INTNAMES(3,%%) : NEXT %
FOR %1=1 TO 12 : READ INTNAMES(4,%%) : NEXT %
FOR %1=1 TO 12 : READ INTNAMES(5,%%) : NEXT %
FOR %1=1 TO 3 : READ INTNAMES(6,%%) : NEXT %
FOR %1=1 TO 3 : READ INTNAMES(7,%%) : NEXT %

```

```

* Next are the endpoints for the baselines.
DATA 3.0, 0.33, 0.33, -0.5
DATA 8.0, 6.0, 3.5, 0.5,
DATA 9.0, 6.0, 4.0, 2.0,
DATA 9.0, 6.0, 4.0, 2.0,
DATA 16.6, 11.4, 10.8, 4.0
DATA 175.0, 100.0, 68.0, -5.0
FOR %1=1 TO 4 : READ BASEEND(1,%%) : NEXT %
FOR %1=1 TO 6 : READ BASEEND(2,%%) : NEXT %
FOR %1=1 TO 8 : READ BASEEND(3,%%) : NEXT %
FOR %1=1 TO 8 : READ BASEEND(4,%%) : NEXT %
FOR %1=1 TO 8 : READ BASEEND(5,%%) : NEXT %
FOR %1=1 TO 4 : READ BASEEND(6,%%) : NEXT %
FOR %1=1 TO 4 : READ BASEEND(7,%%) : NEXT %

```

```

* Next are the gain settings for displaying the spectra.
DATA 5, 8, 6, 8, 5, 5
FOR %1=1 TO 7 : READ GAIN%(%) : NEXT %

```

```

MainMenu
Next see if restore defaults, or change selected items.

```

```

* Alkane thru 13C Static

```

```

* Alkane
* Monocyclic
* Dicyclic
* Fluorene
* Phenan
* Static 1H
* Static 13C
0.5, -0.5
2.0, 0.6, 0.6, -0.5
2.0, 0.6, 0.6, -0.5
2.0, 0.6, 0.6, -0.5

```

```

* Alkane thru 13C Static

```

```

* Alkane thru 13C Static

```

```

* Alkane thru 13C Static

```

```

* Alkane thru 13C Static

```

```

* Alkane thru 13C Static

```

```
GOTO Startloop1
DoOption1:
SELECT CASE OPTN%(1)
CASE 1
GOTO RestoreDefaults
CASE 2
GOTO EditParameters
CASE 3
CHAIN "LCNMR EXE"
CASE 4
CLOSE
GOSUB Logo
LOCATE 1,1 : PRINT "May your camel never stand upwind..."
AS=INPUT$(1)
END
END SELECT
```

RestoreDefaults:

This is the section to restore the default parameters.

```
GOSUB GetDirectory
COLOR 10,1
LOCATE 7,15 : PRINT CHR$(216);STRING$(49,196);CHR$(191);
FOR I%=6 TO 18
LOCATE I%,15 : PRINT CHR$(179);TAB(95);CHR$(179);
NEXT I%
LOCATE 19,15 : PRINT CHR$(192);STRING$(49,196);CHR$(217);
COLOR 28,1
LOCATE 13,28 : PRINT "**** Writing the file ****";
GOSUB WriteFile
GOTO MainMenu
```

EditParameters:

This is the section to edit selected parameters.

```
GOSUB GetDirectory
COLOR 28,0 : CLS
LOCATE 12,20 : PRINT "**** READING THE CONFIGURATION FILE ****";
GOSUB ReadFile
COLOR 4,0 : CLS
COLOR 4,3
LOCATE 1,20 : PRINT STRING$(40,32);
LOCATE 2,20 : PRINT TAB(24);"Press <RETURN> to accept default";TAB(60);
LOCATE 3,20 : PRINT STRING$(40,32);
*****
COLOR 11,0
```

```
Main Menu box
COLOR 10,1
LOCATE 7,15 : PRINT CHR$(216);STRING$(49,196);CHR$(191);
FOR I%=8 TO 18
LOCATE I%,15 : PRINT CHR$(179);TAB(95);CHR$(179);
NEXT I%
LOCATE 19,15 : PRINT CHR$(192);STRING$(49,196);CHR$(217);
COLOR 10,1
LOCATE 8,20 : PRINT TIMES;
LOCATE 8,51 : PRINT DATES;
COLOR 15,1
LOCATE 9,35 : PRINT "MAIN MENU:";
COLOR 14,1
FOR I%=1 TO 4
LOCATE (I%-1)*2+11,40-(0.5*LEN(OPTN$(I%)))
COLOR 13,1 : PRINT LEFT$(OPTN$(I%),1);
COLOR 14,1 : PRINT RIGHT$(OPTN$(I%),LEN(OPTN$(I%))-1);
NEXT I%
```

* Next are commands.
 COLOR 3,0
 LOCATE 25,18 : PRINT "Press the highlighted letter or <ENTER> to select:";

* Next see what to do.

```
COLOR 14,0
LOCATE (OPTN$(1)-1)*2+11,38-(0.5*LEN(OPTN$(1)))
PRINT " ",OPTN$(OPTN$(1))," ";
```

Startloop1:
 AS=INKEY\$
 SELECT CASE AS

```
CASE =
COLOR 10,1
LOCATE 8,20 : PRINT TIMES;
CASE CHR$(13)
GOTO DoOption1
CASE "R",r
OPTN%(1)=1 : GOTO DoOption1
CASE "C",c
OPTN%(1)=2 : GOTO DoOption1
CASE "E",e
OPTN%(1)=3 : GOTO DoOption1
CASE "Q",q;CHR$(27)
OPTN%(1)=4 : GOTO DoOption1
CASE CHR$(0)+CHR$(72), CHR$(0)+CHR$(80)
LOCATE (OPTN%(1)-1)*2+11,38-(0.5*LEN(OPTN$(1)))
PRINT " ",LEFT$(OPTN$(1),1);
COLOR 14,1
PRINT RIGHT$(OPTN$(1),LEN(OPTN$(1))-1);
IF AS=CHR$(0)+CHR$(72) THEN DECR OPTN%(1) ELSE INCR OPTN%(1)
IF OPTN%(1)<1 THEN OPTN%(1)=4
IF OPTN%(1)>4 THEN OPTN%(1)=1
COLOR 14,0
LOCATE (OPTN%(1)-1)*2+11,38-(0.5*LEN(OPTN$(1)))
PRINT " ",OPTN$(OPTN%(1))," ";
```

* no key
 * return
 * recal
 * change
 * edit: LC-NMR
 * exit: DOS
 * up-down

```
CASE ELSE
SOUND 1000,3 : SOUND 800,1.5
END SELECT
```

* left-right
 * copys!

```

LOCATE 7,20 : PRINT *** NMR and Chromatography Constants ***;
COLOR 10, 0
LOCATE 10,30 : PRINT 'Description of Data.';
LOCATE 14,28 : PRINT 'Old Data.';
LOCATE 16,28 : PRINT 'New Data.';
COLOR 15, 0
LOCATE 11,20 : PRINT 'Chemical Shift of HMDS (in PPM - 1H)';
LOCATE 14,40 : PRINT HMDSHIFT;
LOCATE 16,40 : LINE INPUT TEMP$ : IF TEMP$ <>="" THEN HMDSHIFT=VAL(TEMP$)
GOSUB ClearDat
LOCATE 11,20 : PRINT 'Chemical Shift of C0C3 (in PPM - 13C)';
LOCATE 14,40 : PRINT CDCLSHIF1;
LOCATE 16,40 : LINE INPUT TEMP$ : IF TEMP$ <>="" THEN CDCLSHIF1=VAL(TEMP$)
GOSUB ClearDat
LOCATE 11,20 : PRINT 'PPM per point for 2k Proton Flow File (JEOL)';
LOCATE 14,40 : PRINT PPMPT2KH;
LOCATE 16,40 : LINE INPUT TEMP$ : IF TEMP$ <>="" THEN PPMPT2KH=VAL(TEMP$)
GOSUB ClearDat
LOCATE 11,20 : PRINT 'PPM per point for 8k Proton Static File (BM)';
LOCATE 14,40 : PRINT PPMPT8KH;
LOCATE 16,40 : LINE INPUT TEMP$ : IF TEMP$ <>="" THEN PPMPT8KH=VAL(TEMP$)
GOSUB ClearDat
LOCATE 11,20 : PRINT 'PPM per point for 8k Carbon 13 Static File (BM)';
LOCATE 14,40 : PRINT PPMPT8KC;
LOCATE 16,40 : LINE INPUT TEMP$ : IF TEMP$ <>="" THEN PPMPT8KC=VAL(TEMP$)
GOSUB ClearDat
LOCATE 11,20 : PRINT 'Concentration of HMDS in the solvent.';
LOCATE 14,40 : PRINT HMDSOCONC;
LOCATE 16,40 : LINE INPUT TEMP$ : IF TEMP$ <>="" THEN HMDSOCONC=VAL(TEMP$)
GOSUB ClearDat
LOCATE 11,20 : PRINT 'Liquid Chromatographic Flow Rate (ml/min)';
LOCATE 14,40 : PRINT FLOWRATE;
LOCATE 16,40 : LINE INPUT TEMP$ : IF TEMP$ <>="" THEN FLOWRATE=VAL(TEMP$)
GOSUB ClearDat
LOCATE 11,20 : PRINT 'NMR Scan Repetition Rate (scans/sec)';
LOCATE 14,40 : PRINT SCANTIME;
LOCATE 16,40 : LINE INPUT TEMP$ : IF TEMP$ <>="" THEN SCANTIME=VAL(TEMP$)
GOSUB ClearDat
LOCATE 11,20 : PRINT 'Conversion Factor for Volume Calculation';
LOCATE 14,40 : PRINT CONVERT;
LOCATE 16,40 : LINE INPUT TEMP$ : IF TEMP$ <>="" THEN CONVERT=VAL(TEMP$)
GOSUB ClearDat
*****
COLOR 11, 0
LOCATE 7,10 : PRINT SPACES(65);
LOCATE 7,18 : PRINT *** Control Parameters for LC-NMR Software ***;
COLOR 15, 0
LOCATE 11,20 : PRINT 'Mole Fraction of Quaternary Carbon in Alkanes';
LOCATE 14,40 : PRINT Cq;
LOCATE 16,40 : LINE INPUT TEMP$ : IF TEMP$ <>="" THEN Cq=VAL(TEMP$)
GOSUB ClearDat
LOCATE 11,20 : PRINT 'Version number for LC-NMR software';
LOCATE 14,40 : PRINT VERS;
LOCATE 16,40 : LINE INPUT TEMP$ : IF TEMP$ <>="" THEN VERS=TEMP$
GOSUB ClearDat
LOCATE 11,20 : PRINT 'Default Printer: 1=ProPrinter 2=LaserJet';
LOCATE 14,40 : PRINT PRINTER$;
LOCATE 16,40 : LINE INPUT TEMP$ : IF TEMP$ <>="" THEN PRINTER$=VAL(TEMP$)
GOSUB ClearDat
LOCATE 11,20 : PRINT 'Default Font for ProPrinter: 1=Reg 2=Fast 3=NLO';

```

```

LOCATE 14,40 : PRINT FONT$;
LOCATE 16,40 : LINE INPUT TEMP$ : IF TEMP$ <>="" THEN FONT$=VAL(TEMP$)
GOSUB ClearDat
LOCATE 11,20 : PRINT 'Color for drawing the spectrum (see manual for #)';
LOCATE 14,40 : PRINT SPECTCL%
LOCATE 16,40 : LINE INPUT TEMP$ : IF TEMP$ <>="" THEN SPECTCL%=VAL(TEMP$)
GOSUB ClearDat
LOCATE 11,20 : PRINT 'Color for drawing the axis (see manual for #)';
LOCATE 14,40 : PRINT AXISCOL%
LOCATE 16,40 : LINE INPUT TEMP$ : IF TEMP$ <>="" THEN AXISCOL%=VAL(TEMP$)
GOSUB ClearDat
LOCATE 11,20 : PRINT 'Color for drawing the tables (see manual for #)';
LOCATE 14,40 : PRINT LABELCL%
LOCATE 16,40 : LINE INPUT TEMP$ : IF TEMP$ <>="" THEN LABELCL%=VAL(TEMP$)
GOSUB ClearDat
LOCATE 11,20 : PRINT 'Color for drawing shift dividers (manual for #)';
LOCATE 14,40 : PRINT SHIFTCL%
LOCATE 16,40 : LINE INPUT TEMP$ : IF TEMP$ <>="" THEN SHIFTCL%=VAL(TEMP$)
GOSUB ClearDat
LOCATE 11,20 : PRINT 'Color for drawing the baselines (manual for #)';
LOCATE 14,40 : PRINT BASECOL%
LOCATE 16,40 : LINE INPUT TEMP$ : IF TEMP$ <>="" THEN BASECOL%=VAL(TEMP$)
GOSUB ClearDat
LOCATE 11,20 : PRINT 'The data foreground color (see manual for #)';
LOCATE 14,40 : PRINT DATAOL%
LOCATE 16,40 : LINE INPUT TEMP$ : IF TEMP$ <>="" THEN DATAOL%=VAL(TEMP$)
GOSUB ClearDat
LOCATE 11,20 : PRINT 'The integral display color (see manual for #)';
LOCATE 14,40 : PRINT INTOOL%
LOCATE 16,40 : LINE INPUT TEMP$ : IF TEMP$ <>="" THEN INTOOL%=VAL(TEMP$)
GOSUB ClearDat
LOCATE 11,20 : PRINT 'The screen background color (see manual for #)';
LOCATE 14,40 : PRINT BACKCOL%
LOCATE 16,40 : LINE INPUT TEMP$ : IF TEMP$ <>="" THEN BACKCOL%=VAL(TEMP$)
GOSUB ClearDat
LOCATE 11,20 : PRINT 'Display the integrals graphically <ON, OFF>';
LOCATE 14,40 : PRINT INTEGRALS;
LOCATE 16,40 : LINE INPUT TEMP$ : IF TEMP$ <>="" THEN INTEGRALS=TEMP$
GOSUB ClearDat
LOCATE 11,20 : PRINT 'Default Directory for LC-NMR Spectral Data Files';
LOCATE 14,40 : PRINT NMRDIR$;
LOCATE 16,40 : LINE INPUT TEMP$ : IF TEMP$ <>="" THEN NMRDIR$=TEMP$
GOSUB ClearDat
LOCATE 11,20 : PRINT 'Directory for LC-NMR INPUT (Avg Structure) Files';
LOCATE 14,40 : PRINT INPUTDIR$;
LOCATE 16,40 : LINE INPUT TEMP$ : IF TEMP$ <>="" THEN INPUTDIR$=TEMP$
GOSUB ClearDat
LOCATE 11,20 : PRINT 'Directory for LC-NMR OUTPUT (Avg Structure) Files';
LOCATE 14,40 : PRINT OUTPUTDIR$;
LOCATE 16,40 : LINE INPUT TEMP$ : IF TEMP$ <>="" THEN OUTPUTDIR$=TEMP$
GOSUB ClearDat
LOCATE 11,20 : PRINT 'Directory for LC-NMR BLANK DATA Files';
LOCATE 14,40 : PRINT BLANKDIR$;
LOCATE 16,40 : LINE INPUT TEMP$ : IF TEMP$ <>="" THEN BLANKDIR$=TEMP$
GOSUB ClearDat
LOCATE 11,20 : PRINT 'Dir for SCRATCH WORK (F:=RAMdisk NUL=Current dir)';
LOCATE 14,40 : PRINT SCRDIR$;
LOCATE 16,40 : LINE INPUT TEMP$ : IF TEMP$ <>="" THEN SCRDIR$=TEMP$
GOSUB ClearDat
LOCATE 11,20 : PRINT 'Dir for PROPERTY CALC PARAMETERS (NUL=Current dir)';

```

```

LOCATE 14,40 : PRINT PARAMIDRS;
LOCATE 16,40 : LINE INPUT TEMPS : IF TEMPS<>="" THEN PARAMIDRS=TEMPS
GOSUB ClearDat
FOR I%=1 TO 6
  LOCATE 11,20 : PRINT "Control Option #";I%," Order like control menu.";
  LOCATE 14,40 : PRINT CTRLOPTNS(I%);
  LOCATE 16,40 : LINE INPUT TEMPS : IF TEMPS<>="" THEN CTRLOPTNS(I%)=TEMPS
GOSUB ClearDat
NEXT I%
FOR I%=1 TO 7
  LOCATE 11,20 : PRINT "File Type #";I%,"(1=Alkane, 2=Monocyclic, etc)";
  LOCATE 14,40 : PRINT FILETYPES(I%);
  LOCATE 16,40 : LINE INPUT TEMPS
  IF TEMPS<>="" THEN FILETYPES(I%)=VAL(TEMPS)
GOSUB ClearDat
NEXT I%
FOR I%=1 TO 7
  LOCATE 11,20 : PRINT "y (vertical) offset #";I%,"(in screen pts 1-500)";
  LOCATE 14,40 : PRINT YOFFSETS(I%);
  LOCATE 16,40 : LINE INPUT TEMPS
  IF TEMPS<>="" THEN YOFFSETS(I%)=VAL(TEMPS)
GOSUB ClearDat
NEXT I%
FOR I%=1 TO 7
  LOCATE 11,20 : PRINT "Stop for shift divider #";I%,"(in spectral pts)";
  LOCATE 14,40 : PRINT SHIFTSTEPS(I%);
  LOCATE 16,40 : LINE INPUT TEMPS
  IF TEMPS<>="" THEN SHIFTSTEPS(I%)=VAL(TEMPS)
GOSUB ClearDat
NEXT I%
FOR I%=1 TO 7
  LOCATE 11,20 : PRINT "Step for baseline move #";I%,"(in spectral pts)";
  LOCATE 14,40 : PRINT BASESTEPS(I%);
  LOCATE 16,40 : LINE INPUT TEMPS
  IF TEMPS<>="" THEN BASESTEPS(I%)=VAL(TEMPS)
GOSUB ClearDat
NEXT I%
FOR I%=1 TO 8
  LOCATE 11,20 : PRINT "Name #";I%,"of 8 integration regions in Alkanes";
  LOCATE 14,40 : PRINT INTNAMES(I%);
  LOCATE 16,40 : LINE INPUT TEMPS
  IF TEMPS<>="" THEN INTNAMES(I%)=TEMPS
GOSUB ClearDat
NEXT I%
*****
COLOR 11, 0
LOCATE 7,10 : PRINT SPACES(65);
LOCATE 7,17 : PRINT "Integral Division Shifts for Classes ***";
COLOR 15, 0
FOR I%=1 TO 6
  LOCATE 11,20 : PRINT "Shift #";I%,"of 6 shifts in Alkanes (ppm)";
  LOCATE 14,40 : PRINT PPM(I%);
  LOCATE 16,40 : LINE INPUT TEMPS :IF TEMPS<>="" THEN PPM(I%)=VAL(TEMPS)
GOSUB ClearDat
NEXT I%
FOR I%=1 TO 13
  LOCATE 11,20 : PRINT "Shift #";I%,"of 13 shifts in Monocyclics (ppm)";
  LOCATE 14,40 : PRINT PPM(2,I%);
  LOCATE 16,40 : LINE INPUT TEMPS :IF TEMPS<>="" THEN PPM(2,I%)=VAL(TEMPS)
GOSUB ClearDat
NEXT I%
FOR I%=1 TO 13
  LOCATE 11,20 : PRINT "Shift #";I%,"of 13 shifts in Dicyclics (ppm)";
  LOCATE 14,40 : PRINT PPM(3,I%);
  LOCATE 16,40 : LINE INPUT TEMPS :IF TEMPS<>="" THEN PPM(3,I%)=VAL(TEMPS)
GOSUB ClearDat
NEXT I%
FOR I%=1 TO 13
  LOCATE 11,20 : PRINT "Shift #";I%,"of 13 shifts in Fluorenes (ppm)";
  LOCATE 14,40 : PRINT PPM(4,I%);
  LOCATE 16,40 : LINE INPUT TEMPS :IF TEMPS<>="" THEN PPM(4,I%)=VAL(TEMPS)
GOSUB ClearDat
NEXT I%
FOR I%=1 TO 12
  LOCATE 11,20 : PRINT "Name #";I%,"of 12 int regions in Dicyclics";
  LOCATE 14,40 : PRINT INTNAMES(3,I%);
  LOCATE 16,40 : LINE INPUT TEMPS : IF TEMPS<>="" THEN INTNAMES(3,I%)=TEMPS
GOSUB ClearDat
NEXT I%
FOR I%=1 TO 12
  LOCATE 11,20 : PRINT "Name #";I%,"of 12 int regions in Fluorenes";
  LOCATE 14,40 : PRINT INTNAMES(4,I%);
  LOCATE 16,40 : LINE INPUT TEMPS : IF TEMPS<>="" THEN INTNAMES(4,I%)=TEMPS
GOSUB ClearDat
NEXT I%
FOR I%=1 TO 12
  LOCATE 11,20 : PRINT "Name #";I%,"of 12 int regions in Phenanthrenes";
  LOCATE 14,40 : PRINT INTNAMES(5,I%);
  LOCATE 16,40 : LINE INPUT TEMPS : IF TEMPS<>="" THEN INTNAMES(5,I%)=TEMPS
GOSUB ClearDat
NEXT I%
FOR I%=1 TO 3
  LOCATE 11,20 : PRINT "Name #";I%,"of 3 int regions in Satic Proton";
  LOCATE 14,40 : PRINT INTNAMES(6,I%);
  LOCATE 16,40 : LINE INPUT TEMPS : IF TEMPS<>="" THEN INTNAMES(6,I%)=TEMPS
GOSUB ClearDat
NEXT I%
FOR I%=1 TO 3
  LOCATE 11,20 : PRINT "Name #";I%,"of 3 int regions in Satic Carbon";
  LOCATE 14,40 : PRINT INTNAMES(7,I%);
  LOCATE 16,40 : LINE INPUT TEMPS : IF TEMPS<>="" THEN INTNAMES(7,I%)=TEMPS
GOSUB ClearDat
NEXT I%
*****
COLOR 11, 0
LOCATE 7,10 : PRINT SPACES(65);
LOCATE 7,17 : PRINT "Integral Division Shifts for Classes ***";
COLOR 15, 0
FOR I%=1 TO 6
  LOCATE 11,20 : PRINT "Shift #";I%,"of 6 shifts in Alkanes (ppm)";
  LOCATE 14,40 : PRINT PPM(1,I%);
  LOCATE 16,40 : LINE INPUT TEMPS :IF TEMPS<>="" THEN PPM(1,I%)=VAL(TEMPS)
GOSUB ClearDat
NEXT I%
FOR I%=1 TO 13
  LOCATE 11,20 : PRINT "Shift #";I%,"of 13 shifts in Monocyclics (ppm)";
  LOCATE 14,40 : PRINT PPM(2,I%);
  LOCATE 16,40 : LINE INPUT TEMPS :IF TEMPS<>="" THEN PPM(2,I%)=VAL(TEMPS)
GOSUB ClearDat
NEXT I%
FOR I%=1 TO 13
  LOCATE 11,20 : PRINT "Shift #";I%,"of 13 shifts in Dicyclics (ppm)";
  LOCATE 14,40 : PRINT PPM(3,I%);
  LOCATE 16,40 : LINE INPUT TEMPS :IF TEMPS<>="" THEN PPM(3,I%)=VAL(TEMPS)
GOSUB ClearDat
NEXT I%
FOR I%=1 TO 13
  LOCATE 11,20 : PRINT "Shift #";I%,"of 13 shifts in Fluorenes (ppm)";
  LOCATE 14,40 : PRINT PPM(4,I%);
  LOCATE 16,40 : LINE INPUT TEMPS :IF TEMPS<>="" THEN PPM(4,I%)=VAL(TEMPS)
GOSUB ClearDat
NEXT I%

```



```

FOR I%=1 TO 13
LOCATE 11,20 : PRINT "Shift #",I%,"of 13 shifts in Phenans (ppm)";
LOCATE 14,40 : PRINT PPM(5,I%);
LOCATE 16,40 : LINE INPUT TEMPS :IF TEMPS<>" THEN PPM(5,I%)=VAL(TEMPS)
GOSUB ClearDat
NEXT I%
FOR I%=1 TO 4
LOCATE 11,20 : PRINT "Shift #",I%,"of 4 shifts in Static 1H (ppm)";
LOCATE 14,40 : PRINT PPM(6,I%);
LOCATE 16,40 : LINE INPUT TEMPS :IF TEMPS<>" THEN PPM(6,I%)=VAL(TEMPS)
GOSUB ClearDat
NEXT I%
FOR I%=1 TO 4
LOCATE 11,20 : PRINT "Shift #",I%,"of 4 base shifts in Static 13C (ppm)";
LOCATE 14,40 : PRINT BASEEND(7,I%);
LOCATE 16,40 : LINE INPUT TEMPS :IF TEMPS<>" THEN BASEEND(7,I%)=VAL(TEMPS)
GOSUB ClearDat
NEXT I%
FOR I%=1 TO 7
LOCATE 11,20 : PRINT "Integral display expansion for class #",I%," (units unknown)";
LOCATE 14,40 : PRINT GAIN(I%);
LOCATE 16,40 : LINE INPUT TEMPS :IF TEMPS<>" THEN GAIN(I%)=VAL(TEMPS)
GOSUB ClearDat
NEXT I%
FOR I%=1 TO 7
LOCATE 11,20 : PRINT "Gain setting for class #",I%," (units unknown)";
LOCATE 14,40 : PRINT GAIN(I%);
LOCATE 16,40 : LINE INPUT TEMPS :IF TEMPS<>" THEN GAIN(I%)=VAL(TEMPS)
GOSUB ClearDat
NEXT I%
FOR I%=1 TO 7
LOCATE 11,20 : PRINT "Integral display expansion for class #",I%";
LOCATE 14,40 : PRINT INTEXP(I%);
LOCATE 16,40 : LINE INPUT TEMPS :IF TEMPS<>" THEN INTEXP(I%)=VAL(TEMPS)
GOSUB ClearDat
NEXT I%
FOR I%=1 TO 7
LOCATE 11,20 : PRINT "Have got all data so see if ok to put back into the file";
LOCATE 14,40 : PRINT CHRS(216),STRINGS(60,166),CHRS(161); ' top line
FOR I%=22 TO 24
LOCATE I%, 5 : PRINT CHRS(179);TAB(75);CHRS(179); ' middle
LOCATE 25, 5 : PRINT CHRS(192),STRINGS(60,166),CHRS(217); ' bottom line
LOCATE 28, 1
LOCATE 23,16 : PRINT "Have got all information - OK to file ? (Y/N/C)";
Startloop4
AS=INKEY$
SELECT CASE AS
CASE ""
no key
file it
CASE "Y",Y
GOSUB WriteFile
GOTO MainMenu
CASE "N",n;"C",c;"Q",q;CHRS(27)
' exit
GOTO MainMenu
CASE ELSE
' oops!
SOUND 1000,3 SOUND 800,1,5
END SELECT
GOTO Startloop4
GetTemp
' This is a minisubroutine to get the temp string for editing the file.
LOCATE 16,40 : LINE INPUT TEMPS
RETURN

```

```

Startloop3.
AS=INKEYS
SELECT CASE AS
CASE =
CASE "Q",q,CHRS(27)
GOTO MainMenu
CASE "Y",y
RETURN
CASE "N",n
GOTO GetDirectory
CASE ELSE
SOUND 1000,3 : SOUND 800,1,5
GOTO Startloop3

```

- * no key
- * quit
- * correct
- * Incorrect

WriteFile:

This is the subroutine to write the config file.

```

OPEN ODIRS+"LCNMRCFG.DAT" FOR OUTPUT AS #1
PRINT #1,HMDSHIFT
PRINT #1,CDCL3SHIFT
PRINT #1,PPMPT2KH
PRINT #1,PPMPT8KH
PRINT #1,PPMPT8KC
PRINT #1,HMDSOONC
PRINT #1,FLOWRATE
PRINT #1,SCANTIME
PRINT #1,CONVERT

```

- * chem shift HMDS
- * chem shift CDCL3
- * PPM/pt-2K file
- * PPM/pt-8K 1H
- * PPM/pt-8K 13C
- * HMDS Concentration
- * Chromato flow rate
- * Time for scan
- * Conversion factor

Next are the control parameters for the LC-NMR program.

```

PRINT #1,Cq
PRINT #1,VERS
PRINT #1,PRINTER%
PRINT #1,FONT%
PRINT #1,SPECTCL%
PRINT #1,AXISCOL%
PRINT #1,LABELCL%
PRINT #1,SHIFTCL%
PRINT #1,BASECOL%
PRINT #1,DATACOL%
PRINT #1,INTCOL%
PRINT #1,BACKCOL%
PRINT #1,INTEGRALS
PRINT #1,NMRDIRS
PRINT #1,INPUTDIRS
PRINT #1,OUTPUTDIRS
PRINT #1,BLANKDIRS
PRINT #1,SCORDIRS
PRINT #1,PARAMDIRS
FOR I%=1 TO 6
PRINT #1,CTRLOPTS(I)%
NEXT I%
FOR I%=1 TO 7

```

- * Cquart for alkanes
- * Version Number
- * ProPrinter
- * Regular data font
- * Spectrum color
- * Axis color
- * Label color
- * Shift division color
- * Baseline color
- * Data foreground color
- * Background color
- * Display integrals
- * NMR spectra directory
- * Input data file dir
- * Output data file dir
- * Blank data directory
- * Scratch file directory
- * Params for prop calcs
- * Control Options

ClearDat:

```

* This is a minisubroutine to clear the data between answers.
LOCATE 11,20 : PRINT SPACES(65);
LOCATE 14,40 : PRINT SPACES(35);
LOCATE 16,40 : PRINT SPACES(35);
RETURN

```

GetDirectory:

This is the section to get the config file directory.

```

COLOR 10, 1
LOCATE 7,15 : PRINT CHRS(210);STRINGS(49,190);CHRS(101); * top line
FOR I%=8 TO 16
LOCATE I%,15 : PRINT CHRS(179);TAB(65);CHRS(179); * middle
NEXT I%
LOCATE 19,15 : PRINT CHRS(192);STRINGS(49,190);CHRS(217); * bottom line
COLOR 0, 0
LOCATE 25,15 : PRINT SPACES(63);
COLOR 15, 1
LOCATE 10,26 : PRINT "Configuration File Directory:";
COLOR 14, 1
LOCATE 13,31 : PRINT ODIRS;
COLOR 27, 1
LOCATE 16,28 : PRINT "Is This Correct? (Y/N/Q)";
Startloop2:
AS=INKEYS
SELECT CASE AS
CASE =
CASE "Q",q,CHRS(27)
GOTO MainMenu
CASE "Y",y
GOTO Continue1
CASE "N",n

```

- * no key
- * quit
- * correct
- * Incorrect

```

COLOR 11, 1
LOCATE 16,27 : PRINT "Please enter new directory:";
COLOR 14, 1
LOCATE 13,31 : PRINT SPACES(30);
LOCATE 13,31 : LINE INPUT TEMPS
IF TEMPS<>" " THEN ODIRS=TEMPS
LOCATE 13,31 : PRINT TEMPS
COLOR 27, 1
LOCATE 16,27 : PRINT "Is This Correct? (Y/N/Q) ";
CASE ELSE
SOUND 1000,3 : SOUND 800,1,5
END SELECT
GOTO Startloop2
Continue1:
COLOR 15, 1 : LOCATE 10,26 : PRINT " Configuration File Name: ";
COLOR 14, 1 : LOCATE 13,26 : PRINT ODIRS+"LCNMRCFG.DAT";
COLOR 27, 1 : LOCATE 16,28 : PRINT "Is This Correct? (Y/N/Q)";

```

```

OPEN ODIRS+'LCNMRCFG DAT' FOR INPUT AS #1
INPUT #1,HMDSHIFT
INPUT #1,CDCL3SHIFT
INPUT #1,PPMPT2KH
INPUT #1,PPMPT8KH
INPUT #1,PPMPT8KC
INPUT #1,HMDS CONC
INPUT #1,FLOWRATE
INPUT #1,SCANTIME
INPUT #1,CONVERT

```

. Next are the control parameters for the LC-NMR program.

```

INPUT #1,Cq
INPUT #1,VERS
INPUT #1,PRINTER%
INPUT #1,FONT%
INPUT #1,SPECTCOL%
INPUT #1,AXISCOL%
INPUT #1,LABELCL%
INPUT #1,SHIFTCL%
INPUT #1,BASECOL%
INPUT #1,DATACOL%
INPUT #1,INTCOL%
INPUT #1,BACKCOL%
INPUT #1,INTEGRALS
INPUT #1,NMRDIRS
INPUT #1,INPUTDIRS
INPUT #1,OUTPUTDIRS
INPUT #1,BLANKDIRS
INPUT #1,SCRDIRS
INPUT #1,PARAMDIRS
FOR I%=1 TO 8
  INPUT #1,CTRLOPT$(I%)
NEXT I%
FOR I%=1 TO 7
  INPUT #1,FILETYPE$(I%)
NEXT I%
FOR I%=1 TO 7
  INPUT #1,YOFFSET$(I%)
NEXT I%
FOR I%=1 TO 7
  INPUT #1,SHIFTSTEP$(I%)
NEXT I%
FOR I%=1 TO 7
  INPUT #1,BASESTEP$(I%)
NEXT I%

```

. Next are the fraction names.

```

FOR I%=1 TO 8 : PRINT #1, FILETYPE$(I%) : NEXT I%

```

. Next are the integration region names for each class.

```

FOR I%=1 TO 5 : PRINT #1,INTNAMES(1,I%) : NEXT I%
FOR I%=1 TO 12 : PRINT #1,INTNAMES(2,I%) : NEXT I%
FOR I%=1 TO 12 : PRINT #1,INTNAMES(3,I%) : NEXT I%
FOR I%=1 TO 12 : PRINT #1,INTNAMES(4,I%) : NEXT I%
FOR I%=1 TO 12 : PRINT #1,INTNAMES(5,I%) : NEXT I%
FOR I%=1 TO 3 : PRINT #1,INTNAMES(6,I%) : NEXT I%
FOR I%=1 TO 3 : PRINT #1,INTNAMES(7,I%) : NEXT I%

```

. Next are the integral divisions in PPM for each class.

```

FOR I%=1 TO 6 : PRINT #1,PPM(1,I%) : NEXT I%
FOR I%=1 TO 13 : PRINT #1,PPM(2,I%) : NEXT I%
FOR I%=1 TO 13 : PRINT #1,PPM(3,I%) : NEXT I%
FOR I%=1 TO 13 : PRINT #1,PPM(4,I%) : NEXT I%
FOR I%=1 TO 13 : PRINT #1,PPM(5,I%) : NEXT I%
FOR I%=1 TO 4 : PRINT #1,PPM(6,I%) : NEXT I%
FOR I%=1 TO 4 : PRINT #1,PPM(7,I%) : NEXT I%

```

. Next are the endpoints for the baselines.

```

FOR I%=1 TO 4 : PRINT #1,BASEEND(1,I%) : NEXT I%
FOR I%=1 TO 6 : PRINT #1,BASEEND(2,I%) : NEXT I%
FOR I%=1 TO 8 : PRINT #1,BASEEND(3,I%) : NEXT I%
FOR I%=1 TO 8 : PRINT #1,BASEEND(4,I%) : NEXT I%
FOR I%=1 TO 8 : PRINT #1,BASEEND(5,I%) : NEXT I%
FOR I%=1 TO 4 : PRINT #1,BASEEND(6,I%) : NEXT I%
FOR I%=1 TO 4 : PRINT #1,BASEEND(7,I%) : NEXT I%

```

. Next are the gain settings for displaying the spectra.

```

FOR I%=1 TO 7 : PRINT #1,GAIN(I%) : NEXT I%

```

. Next are the gain settings for displaying the integrals.

```

FOR I%=1 TO 7 : PRINT #1,INTEXP$(I%) : NEXT I%
CLOSE #1
RETURN

```

ReadFile:

```


```

```


```

```


```

```


```

```


```

```


```

```


```

```


```

```


```

```


```

```


```

```


```

```


```

```


```

* File Types

* Spectrum vertical offset

* Step for shift movement

* Step for baseline moves

* Alkane -> 13C

* Alkane

* Monocyclic

* Dicyclic

* Fluorene

* Phenanthrene

* 1H Static

* 13C Static

* Alkane

* Monocyclic

* Dicyclic

* Fluorene

* Phenan

* Static 1H

* Static 13C

* Alkane - 13C Static

* Alkane - 13C Static

. Next are the fraction names.

```

FOR I%=1 TO 8 : INPUT #1, FILETYPE$(I%) : NEXT I%

```

. Next are the integration region names for each class.

```

FOR I%=1 TO 5 : INPUT #1,INTNAMES(1,I%) : NEXT I%
FOR I%=1 TO 12 : INPUT #1,INTNAMES(2,I%) : NEXT I%
FOR I%=1 TO 12 : INPUT #1,INTNAMES(3,I%) : NEXT I%
FOR I%=1 TO 12 : INPUT #1,INTNAMES(4,I%) : NEXT I%
FOR I%=1 TO 12 : INPUT #1,INTNAMES(5,I%) : NEXT I%
FOR I%=1 TO 3 : INPUT #1,INTNAMES(6,I%) : NEXT I%
FOR I%=1 TO 3 : INPUT #1,INTNAMES(7,I%) : NEXT I%

```

. Next are the integral divisions in PPM for each class

```


```

```


```

chemical shift for HMDS

chemical shift for CDCl3

ppm/pt for 2K file

ppm/pt for 8K file

ppm/pt for 8K file

HMDS Concentration

Chromato flow rate

Time for scan

Conversion factor

* Quant for alkanes

* Version Number

* Prof/Printer

* Regular data font

* Spectrum color

* Axis color

* Label color

* Shift division color

* Baseline color

* Data foreground color

* Integral display color

* Background color

* Display Integrals

* NMR spectra directory

* Input data file dir

* Blank data directory

* Scratch file directory

* Params for prop calcs

* Control Options

* File Types

* Spectrum vertical offset

* Step for shift movement

* Step for baseline moves

* Alkane -> 13C

* Alkane

* Monocyclic

* Dicyclic

* Fluorene

* Phenanthrene

* 1H Static

* 13C Static

This is the subroutine to read the configuration file.

```

LINE (%:30)-(27,TEMP),C2
DECR TEMP,(60/54)*8
NEXT %
.
. Next is AC in center.
PI#=#4*ATN(1)
CIRCLE (13,0),15,C3,,,1,25
PAINT ( 0,0),CHRS(&HFF)
LINE (-3,5,-22)-(1,22),C3,B
LINE (-3,25,-21)-(0,75,21),C4,BF
CIRCLE (17,0),15,C3,PI#/#4,7*PI#/#4,1,25
CIRCLE (17,0),22,C3,PI#/#4,7*PI#/#4,1,25
LINE ( 28,7, 15,9)-(23,5, 10,2)
LINE ( 28,7,-15,9)-(23,5,-10,2)
PAINT (5,0),CHRS(&HFF)
.
. Next is software table.
LOCATE 10,31 : PRINT "Software - Software";
LOCATE 21,31 : PRINT "Software - Software";
TEMP#="Software"
FOR %#=1 TO LEN(TEMP#)
LOCATE 11+%:27 : PRINT MID$(TEMP#,%,1);
LOCATE 11+%:54 : PRINT MID$(TEMP#,%,1);
NEXT %
RETURN

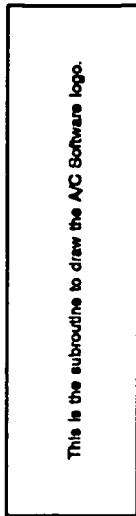
```

```

. Alkane
. Monocyclic
. Dicyclic
. Fluorene
. Phenane
. Static 1H
. Static 13C
.
. Alkane
. Monocyclic
. Dicyclic
. Fluorene
. Phenane
. Static 1H
. Static 13C
.
. Alkane - 13C Static
.
. Alkane - 13C Static
.
FOR %#=1 TO 8 : INPUT #1,PPM(1,%): NEXT %
FOR %#=1 TO 13 : INPUT #1,PPM(2,%): NEXT %
FOR %#=1 TO 13 : INPUT #1,PPM(3,%): NEXT %
FOR %#=1 TO 13 : INPUT #1,PPM(4,%): NEXT %
FOR %#=1 TO 13 : INPUT #1,PPM(5,%): NEXT %
FOR %#=1 TO 4 : INPUT #1,PPM(6,%): NEXT %
FOR %#=1 TO 4 : INPUT #1,PPM(7,%): NEXT %
.
. Next are the endpoints for the baselines.
FOR %#=1 TO 4 : INPUT #1,BASEND(1,%): NEXT %
FOR %#=1 TO 6 : INPUT #1,BASEND(2,%): NEXT %
FOR %#=1 TO 6 : INPUT #1,BASEND(3,%): NEXT %
FOR %#=1 TO 6 : INPUT #1,BASEND(4,%): NEXT %
FOR %#=1 TO 6 : INPUT #1,BASEND(5,%): NEXT %
FOR %#=1 TO 4 : INPUT #1,BASEND(6,%): NEXT %
FOR %#=1 TO 4 : INPUT #1,BASEND(7,%): NEXT %
.
. Next are the gain settings for displaying the spectra.
FOR %#=1 TO 7 : INPUT #1,GAIN(%): NEXT %
.
. Next are the gain settings for displaying the integrals.
FOR %#=1 TO 7 : INPUT #1,INTEXP%(%): NEXT %
CLOSE #1
RETURN
Logo:
$INCLUDE "LOGO.BAS"

```

Listing for Code LOGO.BAS



```

SCREEN 12
COLOR 11,0
WINDOW (-100,-100)-(100,100)
C1=15 : C2=12 : C3=15 : C4=1 : C5=1 : C6=190
. First are boxes.
LINE (-41,-43)-( 41, 43),C1,B
LINE (-41,-31)-( 41,-31),C1
LINE (-41, 31)-( 41, 31),C1
LINE (-28,-43)-(28, 43),C1
LINE ( 28,-43)-(28, 43),C1
PAINT (-39,-40),CHRS(C8)
PAINT ( 39, 40),CHRS(C6)
PAINT (-39,-40),CHRS(C6)
. Next are web lines
TEMP=30
FOR %#=-27 TO 27 STEP 6
LINE (%:27,TEMP)-(%:-30),C2

```

. outer box
. inner lines
. corner boxes

Listing for Program I.5: NMR

```

10 CLS
15 DIM D(35)
20 OUT 195,129
30 DATA 1,2,3,4,5,6,7,9,16,17,19,20,21,22,23,24,25
40 DATA 32,33,34,35,36,37,39,40,41,49
50 FOR I=1 TO 30 : READ D(I) : NEXT I
55 PRINT : PRINT : PRINT : PRINT : PRINT
60 INPUT * PLEASE ENTER THE BEGINNING AND ENDING GAINS *;B,E
70 INPUT * PLEASE ENTER THE NUMBER FOR THE GAIN CHANGE *;N
75 CLS : OUT 192,D(B)
78 PRINT @ 366,SYSTEM WILL START WHEN BUSY LIGHT COMES ON*
79 A=INP(194) : PRINT @ 733,A
75 IF A=1 THEN 74
80 CLS
82 PRINT : PRINT : PRINT
83 PRINT * BEGINNING RECEIVER GAIN: *;B;
84 PRINT * ENDING RECEIVER GAIN: *;E
90 PRINT @ 400,NUMBER OF BLINKS: *;C
100 PRINT @ 828,NUMBER TO CHANGE ON: *;N
105 PRINT @ 846,CURRENT RECEIVER GAIN: *;B
130 A=INP(194) : PRINT @ 733,A
132 PRINT @ R+64,*; : PRINT @ R,CHR$(123) : R=R+64
133 IF R<64 THEN R=665
140 IF A=0 THEN 130
160 C=C+1 : PRINT @ 421,C
170 IF C=N THEN OUT 192,D(E) : PRINT @ 668,E
175 GOSUB 190
180 GOTO 130
180 REM
180 REM THIS IS THE SUBROUTINE TO ADVANCE THE FRACTION
200 REM
210 REM
220 FOR I=1 TO 2000 : NEXT I
230 OUT 193,1 : FOR I=1 TO 500 : NEXT I : OUT 193,0
240 RETURN

```

Appendix II

Introduction

This appendix contains the program listings for the correlations software package. This software package consists of seven individual files and three data files. All of these programs are chained together into one complete package, making the individual programs invisible to the user. In doing so, the data files mentioned above are used to store the parameters which are passed from program to program, eliminating the need to reenter the individual parameters for each program. The individual program names and a brief description of each program is as follows: (Please note that the 5 appended to the program names indicates that they are Version 5.xx of that program. Versions predating 5.xx were developed on the IBM CS9000 and have been replaced by the software presented herein.)

Program II.1: PROP5.BAS This program is a data base manager which maintains the files which contain the physical property information for each compound or fuel.

Program II.2: REG5.BAS This piece of software reads the physical property and average structure files for each compound or fuel, then performs a multiple regression analysis to calculate the mixing coefficients.

Program II.3: CORR5.BAS Along with REG5.BAS, this program forms the core of the correlations software. The CORR5 program reads the physical property and average structure files, utilizing the mixing coefficients which are calculated in the REG5 program to calculate the predicted physical property of each compound or fuel. This program also does a statistical analysis to determine the distribution of errors, the distribution of products (fuels only), and contains an abbreviated version of the GRAPH.BAS program which calculates the correlation plots, the correlation coefficients, standard deviation of residuals, etc.

Program II.4: GRAPH.BAS This program is designed to graphically present the information generated by the other correlations software. It also allows the operator to use a pointer to select a specific point. Once the point is selected, the data is then searched and the nearest data point to the arrow is determined and displayed in a window. The displayed information includes the observed and calculated data values as well as the compound or fuel name and file name.

Program II.5: GRAF_ED.BAS This piece of software works in conjunction with GRAPH.BAS, editing the graphing file, giving the ability to "throw out" data points.

Program II.6: ERROR.BAS This program reads the correlations graphing files and calculates the absolute error, percent error, and relative precision of each data point along with the minimum, maximum, and average percent error and relative precision for the entire file.

Program II.7: EZ_PLOT.BAS This program generates correlation files by reading the average structure and physical property files for each compound or fuel and plotting a specific physical property against a specific average structural parameter.

Additionally, there are three data files which must be either in the default directory or in the path for this software to operate properly. These files are CORRCFG.DAT which contains the configuration data for the REG5.BAS and CORR5.BAS programs, FUELPARM.DAT which contains the constants for the fuel correlation equations, and CHARACTER.DAT which contains a character set for displaying alphanumeric data on graphics screens.

Listing for Program II.1: PROPS.BAS

Program Name: PROPERTY.BAS Ver 5.10 Date Written: 0/02/1987
 Author: Allen Caswell Date Modified: 04/07/1988

This is version 3.00 of the property program. This program will service the property files for the correlations basis set. Ver 3.0 means that this program works with the sequential access files. There is a file named PNUM.DAT which contains the number of compounds for which there is property data. The data itself is stored in sequential access files under its number. This replaces the old system of keeping the data in a random access file. This system is much more efficient.

The order of the data in the files is as follows:

- 1: Name
- 2: Formula
- 3: Mol Wt
- 4: Cetane #
- 5: Boil Pt - 50%
- 6: Pour Pt
- 7: Improv %
- 8: Flash Pt
- 9: Density
- 10: Ref Indx
- 11: Cloud Pt
- 12: Viscos
- 13: Filter
- 14: Class
- 15: ADB
- 16: Sp. Disp
- 17: Surf Ten
- 18: Aniline
- 19: Crit P
- 20: Crit T
- 21: Crit V
- 22: Heat Cap
- 23: Ht Vapor
- 24: Ht. Form
- 25: Free E F
- 26: Ht. Comb
- 27: Mol Vol
- 28: Aromatic
- 29: Olefins
- 30: Fuel Type
- 31: Cetane Ind
- 32: Sp. Grav
- 33: BP - IBP
- 34: BP - 10%
- 35: BP - 90%
- 36: BP - EP
- 37: C Residue
- 38: empty
- 39: empty
- 40: empty
- 41: empty
- 42: empty

First is the section to set up the variables.

```
COMMON ODIRE,OFILS
DIM F$(50),D$(50)
VERSION$ = "Ver 5.10"
HOOPLY$ = ""
SEARCH = 1
DISP = 1
BEGSRCH = 1
SRCHCLASS$ = "ALKANE"
PDRIVES = "D"
RMSDK$ = ""
CLASS$ = 1
OPTINI% = 2
OPTI2% = 1
TEMP$ = "Main Menu"
ROW1% = 1
COL1% = 1
```

Next are names for fields in file.
 DATA "Name", "Formula", "Mol Wt", "Cetane #", "BP - 50%", "Pour Pt",
 DATA "Improv%",
 DATA "Flash Pt", "Density", "Ref Indx", "Cloud Pt", "Viscosit", "Filter"
 DATA "Class"
 DATA "Ag Dq Br", "Sp. Disp", "Surf Ten", "Aniline", "Cr Press", "Cr Temp"
 DATA "Crit Vol"
 DATA "Heat Cap", "Ht Vapor", "Ht. Form", "Free E F", "Ht. Comb", "Mol Vol"

```
DATA "% Arom"  

DATA "% Olefin", "FuelType", "Cet Indx", "Sp. Grav", "BP - IBP", "BP - 10%",  

DATA "BP - 90%",  

DATA "BP - End", "C Resid",  

DATA  

FOR I%=1 TO 42 : READ F$(I%) : NEXT I%  

Next are names for main menu options.  

DATA "Exit to DOS", "Edit a File", "Directory"  

DATA "Run REGS", "Run CORRS", "Run ERROR"  

DATA "Run GRAPH", "Run GRAF ED", "Run EZ_PLOT"  

FOR I%=1 TO 9 : READ OPTN$(I%) : NEXT I%  

Next are names for edit menu options.  

DATA "Edit by Number", "Edit by Name"  

DATA "Add a File", "EXIT"  

FOR I%=1 TO 4 : READ OPTN$(2,I%) : NEXT I%  

Next are names for classes on main menu.  

DATA "ALKANE", "ALKENE", "MODELIM", "CYCLOHEX", "DECALIN"  

DATA "MONO", "DICYCLIC", "TETRALIN", "FUEL"  

FOR I%=1 TO 9 : READ CLASS$(I%) : NEXT I%
```

This is the MAIN MENU.

```
MAINMENU:  

COLOR 15,0 : CLS  

First will draw the screen - first is the title box.  

COLOR 15,4  

LOCATE 1, 5 : PRINT CHR$(201);STRINGS$(99,209);CHR$(167) 'top line  

LOCATE 2, 5 : PRINT CHR$(166);STRINGS$(99,32);CHR$(166) 'ends  

LOCATE 3, 5 : PRINT CHR$(200);STRINGS$(99,209);CHR$(166) 'bottom line  

LOCATE 1, 31 : PRINT CHR$(209); 'top junct  

LOCATE 2, 31 : PRINT CHR$(179); 'middle line  

LOCATE 3, 31 : PRINT CHR$(207); 'bottom junct  

LOCATE 2, 10 : PRINT "Property";  

LOCATE 2, 18 : PRINT VERSION$;  

LOCATE 2, 38 : PRINT "Data Base Management Software";
```

Next are RAM, Compounds boxes.
 COLOR 0,7
 TEMP%=8
 FOR I%=1 TO 2
 LOCATE TEMP%+0.60 : PRINT CHR\$(216);STRINGS\$(12,196);CHR\$(191); 'top
 LOCATE TEMP%+2.60 : PRINT CHR\$(166);STRINGS\$(12,205);CHR\$(181); 'middle
 LOCATE TEMP%+4.60 : PRINT CHR\$(182);STRINGS\$(12,196);CHR\$(217); 'bottom
 LOCATE TEMP%+1.60 : PRINT CHR\$(179);TAB(73);CHR\$(179); 'side
 LOCATE TEMP%+3.60 : PRINT CHR\$(179);TAB(73);CHR\$(179); 'side
 TEMP%=TEMP%+8
 NEXT I%
 LOCATE 9.63 : PRINT "Compounds";


```

LOCATE 11,66 : PRINT USING "###" NumOfCompounds;
LOCATE 17,63 : PRINT "RAM Disk";
LOCATE 19,67 : PRINT RMDSK$;

' Next is compounds box.
COLOR 15,1
LOCATE 6,33 : PRINT CHR$(218);STRINGS(14,196);CHR$(191); ' top
LOCATE 8,33 : PRINT CHR$(196);STRINGS(14,205);CHR$(191); ' middle
LOCATE 22,33 : PRINT CHR$(192);STRINGS(14,196);CHR$(217); ' bottom
LOCATE 7,33 : PRINT CHR$(179);TAB(46);CHR$(179); ' side
FOR I%=9 TO 21
  LOCATE I%,33 : PRINT CHR$(179);TAB(46);CHR$(179);
NEXT I%
LOCATE 7, 38 : PRINT "Close";
FOR I%=1 TO 9
  LOCATE I% +10,37 : PRINT CLASS$(I%);
NEXT I%

' Next is options box
COLOR 0,15
LOCATE 10,7 : PRINT CHR$(218);STRINGS(15,196);CHR$(191); ' top
LOCATE 11,7 : PRINT CHR$(179);SPACES(15) ;CHR$(179); ' side
LOCATE 12,7 : PRINT CHR$(196);STRINGS(15,205);CHR$(191); ' middle
LOCATE 22,7 : PRINT CHR$(192);STRINGS(15,196);CHR$(217); ' bottom
FOR I%=13 TO 21
  LOCATE I%,7 : PRINT CHR$(179);SPACES(15);CHR$(179); ' side
  LOCATE I%,8 : PRINT OPTN$(I%,12);
NEXT I%
LOCATE 11,11 : PRINT "Main Menu";
COLOR 3, 0
LOCATE 25,21 : PRINT "Press <R> to toggle use of the RAM disk.";

' Have printed screen, so determine which key has been pressed.
IF RMDSK$="" THEN
  DIR$=PDIVES+"CORRY"+CLASS$(CLASS%)+";"
ELSE
  DIR$="F:"
END IF
FILES=PDIVES+"CORRY"+CLASS$(CLASS%)+";PNUM.DAT"
OPEN FILES FOR INPUT AS #1
  INPUT #1,NumOfCompounds
CLOSE #1
COLOR 14,0 : LOCATE CLASS%+10,35 : PRINT " ",CLASS$(CLASS%); " ";
COLOR 14,0 : LOCATE OPTN1%+12,8 : PRINT OPTN$(I,OPTN1%);
IF TEMP$="" THEN
  COLOR 15,12 : LOCATE 7,36 : PRINT TEMP$;
END IF
IF TEMP$="" THEN
  COLOR 15,12 : LOCATE 11,66 : PRINT USING "##" NumOfCompounds;
GOTO Startloop1
END IF
IF TEMP$="" THEN
  COLOR 0,15 : LOCATE 11,9 : PRINT TEMP$;
END IF

' RAM disk
CASE CHR$(0)+CHR$(72);CHR$(0)+CHR$(80) ' up-down
  IF TEMP$="" THEN
    COLOR 15,1 : LOCATE 7,38 : PRINT TEMP$;
  END IF
  TEMP$=""
  GOTO Startloop1
END IF
CASE CHR$(0)+CHR$(72);CHR$(0)+CHR$(80) ' up-down
  IF TEMP$="" THEN
    COLOR 0,15 : LOCATE OPTN1%+12,8 : PRINT OPTN$(I,OPTN1%);
    IF AS=CHR$(0)+CHR$(72) THEN DECR OPTN1% ELSE INCR OPTN1%
  ELSE
    IF OPTN1% < 1 THEN OPTN1%=9
    IF OPTN1% > 9 THEN OPTN1%=1
  END IF
  COLOR 14,0 : LOCATE OPTN1%+12,8 : PRINT OPTN$(I,OPTN1%);
  GOTO Startloop1
END IF
IF TEMP$="" THEN
  COLOR 15,1 : LOCATE CLASS%+10,35
  PRINT " ",CLASS$(CLASS%); " ";
  IF AS=CHR$(0)+CHR$(72) THEN DECR CLASS% ELSE INCR CLASS%
  IF CLASS% < 1 THEN CLASS%=9
  IF CLASS% > 9 THEN CLASS%=1
  COLOR 14,0 : LOCATE CLASS%+10,35
  PRINT " ",CLASS$(CLASS%); " ";
  FILES=PDIVES+"CORRY"+CLASS$(CLASS%)+";PNUM.DAT"
  DIR$=PDIVES+"CORRY"+CLASS$(CLASS%)+";"
  OPEN FILES FOR INPUT AS #1
    INPUT #1,NumOfCompounds
  CLOSE #1
  COLOR 0,15 : LOCATE 11,66 : PRINT USING "##" NumOfCompounds;
  GOTO Startloop1
END IF
IF TEMP$="" THEN
  SOUND 1000,3 : SOUND 800,1.5
  GOTO Startloop1
END SELECT

```

```

DoOption1:
SELECT CASE OPTN$(I,OPTN1%)
CASE " " : Exit to DOS
CLOSE
GOSUB Logo
LOCATE 1,1 : PRINT "It's your Kim Lucky day..."
AS=INPUT$(1)
END
CASE " " : Edit a File
GOTO EditFile

Startloop1:
AS=INKEY$
SELECT CASE AS
CASE =
  GOTO Startloop1
CASE CHR$(13)
  GOTO DoOption1
CASE "X","Y","O","I",CHR$(27)
  ' exit to DOS

```

```

DoOption1:
SELECT CASE OPTN$(I,OPTN1%)
CASE " " : Exit to DOS
CLOSE
GOSUB Logo
LOCATE 1,1 : PRINT "It's your Kim Lucky day..."
AS=INPUT$(1)
END
CASE " " : Edit a File
GOTO EditFile

```

```

FOR I%=0 TO 6
FOR J%=0 TO 5
IF I%<>0 OR J%<>0 THEN
COLOR 10,1 : LOCATE I%*3+4,J%*13+4 : PRINT FS(I%+(J%*7)+1);
END IF
NEXT J%
NEXT I%
COLOR 13,1
LOCATE 25,20 : PRINT DIRS;
LOCATE 25,69 : PRINT USING "###" NumOfCompounds;

EditMenu:
COLOR 12,1
LOCATE 25, 6 : PRINT "Directory: ";
LOCATE 25,47 : PRINT "Number of Compounds: ";
FOR I%=1 TO 4
LOCATE 1,(I%-1)*19+3 : PRINT OPTN$(2,I%);
NEXT I%
OPEN DIRS+"PNUM.DAT" FOR INPUT AS #1
INPUT #1,NumOfFiles
CLOSE #1
COLOR 13,1
LOCATE 25,20 : PRINT DIRS;
LOCATE 25,69 : PRINT USING "###" NumOfCompounds;

```

```

* Have got screen, so see what to do.
COLOR 14,0
LOCATE 1,(OPTN2%-1)*19+3 : PRINT OPTN$(2,OPTN2%);
Startloop2:
AS=INKEY$
SELECT CASE AS
CASE =
GOTO Startloop2
CASE CHR$(13)
GOTO DoOption2
CASE " ", "U", "V"
OPTN2%=1 : GOTO DoOption2
CASE "N", "n"
OPTN2%=2 : GOTO DoOption2
CASE "A", "a"
OPTN2%=3 : GOTO DoOption2
CASE "X", "x", "O", "o", CHR$(27)
OPTN2%=4 : GOTO DoOption2
CASE CHR$(0)+CHR$(75),CHR$(0)+CHR$(77)
COLOR 12,1
LOCATE 1,(OPTN2%-1)*19+3 : PRINT OPTN$(2,OPTN2%);
IF AS=CHR$(0)+CHR$(75) THEN DECR OPTN2% ELSE INCR OPTN2%
IF OPTN2%<1 THEN OPTN2%=4
IF OPTN2%>4 THEN OPTN2%=1
COLOR 14,0
LOCATE 1,(OPTN2%-1)*19+3 : PRINT OPTN$(2,OPTN2%);
GOTO Startloop2
CASE ELSE
SOUND 1000,3 : SOUND 800,1,5
GOTO Startloop2
coops!
END SELECT
DoOption2:

```

```

CASE * Directory *
GOTO Directory
CASE * Run REGS *
CHAIN "REGS.EXE"
CASE * Run CORR5 *
CHAIN "CORRS.EXE"
CASE * Run ERROR *
CHAIN "ERROR.EXE"
CASE * Run GRAPH *
CHAIN "GRAPH.EXE"
CASE * Run GRAF ED *
CHAIN "GRAF_ED.EXE"
CASE * Run EZ_PLOT *
CHAIN "EZ_PLOT.EXE"
END SELECT

EditFile:

```



```

* Will first have to draw the screen.
COLOR 15,1 : CLS : COLOR 0,1
FOR I%=1 TO 25
LOCATE I%, 2 : PRINT CHR$(179);
LOCATE I%,78 : PRINT CHR$(179);
IF I%>=4 AND I%<=23 THEN
FOR J%=0 TO 5
LOCATE I%, 2+J%*13 : PRINT CHR$(179);
LOCATE I%,13+J%*13 : PRINT CHR$(179);
NEXT J%
END IF
NEXT I%
LOCATE 3, 2+J%*13 : PRINT CHR$(209);
LOCATE 24,2 : PRINT CHR$(189);STRINGS$(75,209);CHR$(181);
LOCATE 24,2 : PRINT CHR$(189);STRINGS$(75,209);CHR$(181);
LOCATE 24,40 : PRINT CHR$(209); : LOCATE 25,40 : PRINT CHR$(179);
LOCATE 2,60 : PRINT CHR$(179); : LOCATE 3,60 : PRINT CHR$(207);
FOR J%=1 TO 5
LOCATE 3, 2+J%*13 : PRINT CHR$(209);
LOCATE 24, 2+J%*13 : PRINT CHR$(207);
NEXT J%
FOR J%=0 TO 4
LOCATE 3,13+J%*13 : PRINT CHR$(209);
LOCATE 24,13+J%*13 : PRINT CHR$(207);
NEXT J%
FOR I%=6 TO 21 STEP 3
LOCATE I%,J%*13+2
PRINT CHR$(185);STRINGS$(10,186);CHR$(180);
NEXT J%
NEXT I%
COLOR 10,1
LOCATE 2, 6 : PRINT "Name: ";
LOCATE 2,63 : PRINT "Number: ";

```

```

SELECT CASE OPTN$(2,OPTN2%)
CASE * Edit by Number *
  GOTO EditByNumber
CASE * Edit by Name *
  GOTO EditByName
CASE * Add a File *
  GOTO AddFile
CASE * EXIT *
  GOTO MainMenu
CASE ELSE
  SOUND 1000,3 : SOUND 800,1.5
  GOTO Startloop2
END SELECT
  
```

EditByNumber:

This is the section to EDIT BY NUMBER.

```

GOSUB ClearData
COLOR 15,1 : LOCATE 1, 2 : PRINT SPACES(77);
COLOR 14,0 : LOCATE 1,13
PRINT * Please enter the number of compound you wish to edit *;
COLOR 28,1 : LOCATE 2,63 : PRINT "Number: ";
GetNum:
  COLOR 15,1 : LOCATE 2,73 : LINE INPUT SNUM$
  IF SNUM$="" THEN SNUM$="0"
  TEM$=LEFT$(SNUM$,1)
  IF ASC(TEM$)<48 OR ASC(TEM$)>57 OR VAL(SNUM$)>NumOfCompounds THEN
    LOCATE 2,73 : PRINT SPACES(4);
    SOUND 1000,3 : SOUND 800,1.5
    GOTO GetNum
  END IF
  SNUM=VAL(SNUM$)
  IF SNUM<=0 THEN GOTO EditMenu
  FILE$=DIR$+"P"+SNUM$+".DAT"
  OPEN FILE$ FOR INPUT AS #1 : INPUT #1,D$(1)
  LOCATE 2,73 : PRINT SPACES(4);
  LOCATE 2,73 : PRINT USING "@##";SNUM;
  GOTO DisplayAndEdit
  
```

EditByName:

This is the section to EDIT BY NAME.

```

GOSUB ClearData
COLOR 15,1 : LOCATE 1, 2 : PRINT SPACES(77);
COLOR 14,0 : LOCATE 1,14
PRINT * Please enter the name of compound you wish to edit *;
  
```

```

COLOR 28,1 : LOCATE 2, 6 : PRINT "Name: ";
COLOR 15,1 : LOCATE 2,13 : LINE INPUT SNAME$
FOR I%=1 TO NumOfCompounds
  AS=INKEY$
  IF AS=CHRS(27) THEN GOTO DidNotFind
  FILE$=DIR$+"P"+RIGHT$(STR$(I%),LEN(STR$(I%))-1)+".DAT"
  OPEN FILE$ FOR INPUT AS #1
  INPUT #1,D$(1)
  LOCATE 2,73 : PRINT USING "@##";I%;
  SNUM=I%
  IF LEFT$(D$(1),LEN(SNAME$))=SNAME$ THEN GOTO DisplayAndEdit
  CLOSE #1
NEXT I%

DidNotFind:
  Did not find name in file.
  CLOSE #1
COLOR 15,1 : LOCATE 1, 2 : PRINT SPACES(77);
COLOR 15,4 : LOCATE 1,19
PRINT * *** That name is not in the file *** *;
COLOR 10,1 : LOCATE 2, 6 : PRINT "Name: ";
AS=INKEY$
WHILE AS=""
  AS=INKEY$
WEND
COLOR 15,1 : LOCATE 1, 2 : PRINT SPACES(77);
LOCATE 2,13 : PRINT SPACES(45);
LOCATE 2,73 : PRINT SPACES(4);
GOTO EditMenu

DisplayAndEdit:
  * Have found compound so get data and continue.
  COLOR 12,1 : LOCATE 1,10
  PRINT "Press <ARROW KEYS>, <PgUp><PgDn>, <F1> to file, <ESC> to exit";
  COLOR 10,1
  LOCATE 2, 6 : PRINT "Name: ";
  LOCATE 2,63 : PRINT "Number: ";
  COLOR 15,1
  LOCATE 2,12 : PRINT SPACES(47);
  LOCATE 2,73 : PRINT USING "@##";SNUM;
  LOCATE 2,13 : PRINT D$(1)
  FOR I%=2 TO 42
    INPUT #1,D$(I%)
    IF LEN(D$(I%))>8 THEN D$(I%)=LEFT$(D$(I%),8)
    WHILE LEN(D$(I%))<8
      D$(I%)=D$(I%)+*
    WEND
  NEXT I%
  CLOSE #1
  FOR I%=0 TO 8
    FOR J%=0 TO 5
      IF I%<>0 OR J%<>0 THEN
        TEM%=I% + (J%*7)+1
        LOCATE I%-3+5,J%*13+4 : PRINT D$(TEM%);
      END IF
    NEXT J%
  NEXT I%
  * Have printed data, so edit.
  
```

```

TEMP$="OFF"
GOSUB HighlightData
Startloop3:
AS=INKEY$
SELECT CASE AS
CASE "=" : CHR$(13)
CASE CHR$(27)
COLOR 12,1 : LOCATE 1,10 : PRINT SPACES(65);
GOTO EditMenu
CASE CHR$(0)+CHR$(73):CHR$(0)+CHR$(81)
IF AS=CHR$(0)+CHR$(73) THEN DECR SNUM
IF AS=CHR$(0)+CHR$(81) THEN INCR SNUM
IF SNUM=NumOfCompounds THEN INCR SNUM=1
IF SNUM<1 THEN SNUM=NumOfCompounds
SNUM$=MID$(STR$(SNUM),2,3)
FILES=DIR$+"P"+SNUM$+".DAT"
OPEN FILES FOR INPUT AS #1
INPUT #1,D$(1)
COLOR 15, 1
LOCATE 2,72 : PRINT USING "###" SNUM;
GOTO DisplayAndEdit
CASE CHR$(0)+CHR$(99)
COLOR 13,4 : LOCATE 1,10
PRINT "Press <ARROW KEYS>, <PgUp><PgDn>,";
PRINT "Press <F1> to file, <ESC> to exit,";
COLOR 15,1
OPEN FILES FOR OUTPUT AS #1
FOR I%=1 TO 42
PRINT #1,D$(I%)
NEXT I%
CLOSE #1
COLOR 12,1 : LOCATE 1,10
PRINT "Press <ARROW KEYS>, <PgUp><PgDn>,";
PRINT "Press <F1> to file, <ESC> to exit,";
COLOR 15,1
CASE CHR$(0)+CHR$(75):CHR$(0)+CHR$(77)
GOSUB HighlightData
IF AS=CHR$(0)+CHR$(75) THEN DECR COL1% ELSE INCR COL1%
IF COL1%<1 THEN COL1%=8
IF COL1%>8 THEN COL1%=1
GOSUB HighlightData
CASE CHR$(0)+CHR$(72):CHR$(0)+CHR$(80)
GOSUB HighlightData
IF AS=CHR$(0)+CHR$(72) THEN DECR ROW1% ELSE INCR ROW1%
IF ROW1%<1 THEN ROW1%=7
IF ROW1%>7 THEN ROW1%=1
GOSUB HighlightData
CASE CHR$(8)
IF ROW1%=1 AND COL1%=1 THEN
D$(1)=SPACES(45)
COLOR 15,0 : LOCATE 2,12 : PRINT "D$(1)";
ELSE
TEMP%=(ROW1%-1) + ((COL1%-1)*7)+1
D$(TEMP%)=SPACES(6)
COLOR 14,0 : LOCATE (ROW1%-1)*3+5,(COL1%-1)*13+3
PRINT "D$(TEMP%)";
END IF
CASE ELSE
IF ROW1%=1 AND COL1%=1 THEN
COLOR 14,0 : LOCATE 1,13
PRINT "Please enter the data for the compound, null to exit."
OPEN DIR$+"PNUM.DAT" FOR INPUT AS #1
INPUT #1,NumOfCompounds
CLOSE #1
SNUM=NumOfCompounds + 1

```

```

PRINT SPACES(47);
LOCATE 2,13 : PRINT AS;
LOCATE 2,14 : LINE INPUT TEMP1$
D$(1)=AS+TEMP1$
IF LEN(D$(1))>45 THEN D$(1)=LEFT$(D$(1),45)
WHILE LEN(D$(1))<45
D$(1)=D$(1)+" "
WEND
LOCATE 2,12 : PRINT "D$(1)";
ELSE
TEMP%=(ROW1%-1) + ((COL1%-1)*7)+1
LOCATE (ROW1%-1)*3+5,(COL1%-1)*13+3
COLOR 14,0 : PRINT SPACES(10);
LOCATE (ROW1%-1)*3+5,(COL1%-1)*13+4
PRINT AS; : LINE INPUT TEMP1$
D$(TEMP%)=AS+TEMP1$
IF LEN(D$(TEMP%))>8 THEN D$(TEMP%)=LEFT$(D$(TEMP%),8)
WHILE LEN(D$(TEMP%))<8
D$(TEMP%)=D$(TEMP%)+""
WEND
LOCATE (ROW1%-1)*3+5,(COL1%-1)*13+3
PRINT "D$(TEMP%)";
END IF
END SELECT
GOTO Startloop3

```

```

HighlightData

```

```

' This is a minisubroutine to inverse video the data.
IF TEMP$="OFF" THEN
COLOR 14,0 : TEMP$="ON"
ELSE
COLOR 15,1 : TEMP$="OFF"
END IF
IF ROW1%=1 AND COL1%=1 THEN
LOCATE 2,12 : PRINT "D$(1)"; : RETURN
ELSE
TEMP%=(ROW1%-1) + ((COL1%-1)*7)+1
LOCATE (ROW1%-1)*3+5,(COL1%-1)*13+3 : PRINT "D$(TEMP%)";
RETURN
END IF

```

```

AddFile:

```

```

' Clear data
GOSUB ClearData
COLOR 15,1 : LOCATE 1,2 : PRINT SPACES(77);
COLOR 14,0 : LOCATE 1,13
PRINT "Please enter the data for the compound, null to exit."
OPEN DIR$+"PNUM.DAT" FOR INPUT AS #1
INPUT #1,NumOfCompounds
CLOSE #1
SNUM=NumOfCompounds + 1

```

```

' Highlight

```

```

' no key
' exit

```

```

' PgUp;PgDn

```

```

' File name

```

```

' file data

```

```

' left-right

```

```

' up-down

```

```

' backspace

```

```

' edit data

```

```

' Clear data

```

```

' Please enter the data for the compound, null to exit.

```

```

' NumOfCompounds

```

```

' NumOfCompounds + 1

```

```

' This section to add a file to the files.

```

```

' Clear data

```

```

' Please enter the data for the compound, null to exit.

```

```

' NumOfCompounds

```

```

' NumOfCompounds + 1

```

```

COLOR 15,1 : LOCATE 2,73 : PRINT USING "###SNUM;
FLES=DIR$+P$+RIGHT$(STR$(SNUM),LEN$(STR$(SNUM))-1)+"DAT
.
.
. Have got preliminaries so get data.
LOCATE 2,13 : LINE INPUT D$(1)
IF D$(1)="" THEN
GOTO EditMenu
END IF
FOR I%=0 TO 6
FOR J%=0 TO 6
IF I%<>0 OR J%<>0 THEN
TEMP%=J% + (I%*7)+1
COLOR 15,1 : LOCATE J%*3+5,I%*13+4
LINE INPUT D$(TEMP%)
END IF
NEXT J%
NEXT I%
.
. Have got data so see if put into file.
COLOR 15,1 : LOCATE 1,2 : PRINT SPACES(77);
COLOR 15,4 : LOCATE 1,2
PRINT "OK to file this info? Yes No "FLES";
TEMP28=" No "; COLOR 30,0 : LOCATE 1,36 : PRINT TEMP28;
FOR I%=1 TO 60 : AS=INKEY$: NEXT I%
Startloop4:
AS=INKEY$
SELECT CASE AS
CASE =
GOTO Startloop4
CASE CHR$(13)
GOTO DoOption4
CASE "y,Y"
TEMP28=" Yes "
GOTO DoOption4
CASE "n,N"
TEMP28=" No "
GOTO DoOption4
CASE CHR$(0)+CHR$(75),CHR$(0)+CHR$(77)
IF TEMP28=" No " THEN
COLOR 15,4 : LOCATE 1,36 : PRINT TEMP28;
TEMP28=" Yes "
COLOR 30,0 : LOCATE 1,28 : PRINT TEMP28;
GOTO Startloop4
END IF
IF TEMP28=" Yes " THEN
COLOR 15,4 : LOCATE 1,28 : PRINT TEMP28;
TEMP28=" No "
COLOR 30,0 : LOCATE 1,36 : PRINT TEMP28;
GOTO Startloop4
END IF
CASE ELSE
SOUND 1000,3 : SOUND 800,1.5
GOTO Startloop4
END SELECT
DoOption4:
SELECT CASE TEMP28
CASE " Yes "
. Have got data so put in file

```

```

COLOR 15,1 : LOCATE 1,1 : PRINT SPACES(79);
COLOR 15,4 : LOCATE 1,13
PRINT " Please enter the data for the compound, null to exit."
OPEN FLES FOR OUTPUT AS #1
PRINT #1,D$(I%)
NEXT I%
CLOSE #1
.
. Must reset the number of compounds in file.
OPEN DIR$+"PNUM.DAT" FOR OUTPUT AS #1
PRINT #1,SNUM
CLOSE #1
COLOR 13,1
LOCATE 25,69 : PRINT USING "###SNUM;
COLOR 14,0 : LOCATE 1,13
PRINT " Please enter the data for the compound, null to exit."
GOTO AddFile
CASE " No "
GOTO AddFile
END SELECT

```

Directory:

This is the section to give a directory.

```

COLOR 15,0 : CLS
OPEN DIR$+"PNUM.DAT" FOR INPUT AS #1
INPUT #1,NumOfFiles
CLOSE #1
BEGSRCH%=1 : ENDSRCH%=NumOfFiles : SRCHCLASS%=CLASS$(CLASS%)
.
. First is num of compounds box
COLOR 0,15
LOCATE 2,18 : PRINT CHR$(201),STRING$(43,205),CHR$(187) 'top line
LOCATE 3,18 : PRINT CHR$(186),STRING$(43,32),CHR$(186) 'ends
LOCATE 4,18 : PRINT CHR$(186),STRING$(43,32),CHR$(186) 'ends
LOCATE 5,18 : PRINT CHR$(200),STRING$(43,205),CHR$(186) 'bottom line
LOCATE 3,24 : PRINT "Number of compounds in file: ";
LOCATE 4,27 : PRINT "Directory: ";
LOCATE 3,53 : PRINT USING "###S",NumOfCompounds;
LOCATE 4,39 : PRINT DIR$
.
. Next is Search By Box - Print Box
COLOR 15,1
LOCATE 7,10 : PRINT CHR$(218),STRING$(28,186),CHR$(191) 'top
LOCATE 7,49 : PRINT CHR$(218),STRING$(19,186),CHR$(191)
FOR I%=8 TO 15
LOCATE I%,10 : PRINT CHR$(179),STRING$(28,32),CHR$(179);
LOCATE I%,49 : PRINT CHR$(179),STRING$(19,32),CHR$(179);
NEXT I%
LOCATE 9,10 : PRINT CHR$(185),STRING$(28,186),CHR$(180); 'cross
LOCATE 9,49 : PRINT CHR$(185),STRING$(19,186),CHR$(180);
LOCATE 14,10 : PRINT CHR$(195),STRING$(28,186),CHR$(180); 'cross

```

```

LOCATE 14,49 : PRINT CHR$(195);STRINGS(19,196);CHR$(160);
LOCATE 16,10 : PRINT CHR$(192);STRINGS(26,196);CHR$(217);
LOCATE 16,49 : PRINT CHR$(192);STRINGS(18,196);CHR$(217);
LOCATE 6,19 : PRINT "Print";
LOCATE 6,56 : PRINT "Search By";
LOCATE 11,14 : PRINT "Number" From:;
LOCATE 15,15 : PRINT "Class";
LOCATE 11,53 : PRINT "Name, Number";
LOCATE 12,53 : PRINT " Class";
LOCATE 15,55 : PRINT "All Data";
LOCATE 11,30 : PRINT USING "#####";BEGSRCH%;
LOCATE 12,30 : PRINT USING "#####";ENDSRCH%;
LOCATE 15,27 : PRINT SRCHCLASS$;
.
. Next is hardcopy box.
COLOR 15,1
LOCATE 19,31 : PRINT CHR$(216);STRINGS(16,196);CHR$(101) ' top
FOR I%=20 TO 22
LOCATE I%,31 : PRINT CHR$(179);STRINGS(16, 32);CHR$(179);
NEXT I%
LOCATE 23,31 : PRINT CHR$(192);STRINGS(16,196);CHR$(217); ' bottom
LOCATE 21,37 : PRINT "Hardcopy";
.
. Next are instructions.
COLOR 3,0 : LOCATE 25,19
PRINT "Press <H> to toggle Hardcopy, <ESC> to EXIT;";
.
. Have got screen, see what to do.
SEARCH=1 : DISP=1 : TEMP3$="" Search By:
COLOR 15,4
FOR I%=10 TO 13
LOCATE I%,11 : PRINT STRINGS(26,32);
LOCATE I%,50 : PRINT STRINGS(19,32);
NEXT I%
LOCATE 11,14 : PRINT "Number" From:; : PRINT USING "#####";BEGSRCH%;
LOCATE 12,14 : PRINT " To: "; : PRINT USING "#####";ENDSRCH%;
LOCATE 11,53 : PRINT "Name, Number";
LOCATE 12,53 : PRINT " Class";
COLOR 15, 5 : LOCATE 6,17 : PRINT TEMP3$;
Startloops;
AS=INKEY$
SELECT CASE AS
CASE "="
GOTO Startloops
CASE CHR$(27)
GOTO MainMenu
CASE CHR$(13)
GOTO DoOptions
CASE "H", "h"
GOSUB ChangeHcopy
IF HCOOPY$="Y" THEN HCOOPY$="N" ELSE HCOOPY$="Y"
GOSUB ChangeHcopy
GOTO Startloops
CASE CHR$(0)+CHR$(75);CHR$(0)+CHR$(77)
IF TEMP3$="" Search By: THEN
COLOR 15,1 : LOCATE 6,17 : PRINT TEMP3$
TEMP3$="" Print:
COLOR 15,5 : LOCATE 6,54 : PRINT TEMP3$
GOTO Startloops

```

```

ELSE
COLOR 15,1 : LOCATE 6,54 : PRINT TEMP3$
TEMP3$="" Search By:
COLOR 15,5 : LOCATE 6,17 : PRINT TEMP3$
GOTO Startloops
END IF
CASE CHR$(0)+CHR$(72);CHR$(0)+CHR$(60)
IF TEMP3$="" Print: THEN
IF DISP=1 THEN
COLOR 15,1
FOR I%=10 TO 13
LOCATE I%,50 : PRINT STRINGS(19,32);
NEXT I%
LOCATE 11,53 : PRINT "Name, Number";
LOCATE 12,53 : PRINT " Class";
COLOR 15,4
LOCATE 15,50 : PRINT STRINGS(19,32);
LOCATE 15,55 : PRINT "All Data";
DISP=2
GOTO Startloops
ELSE
COLOR 15,1
LOCATE 15,50 : PRINT STRINGS(19,32);
LOCATE 15,55 : PRINT "All Data";
COLOR 15,4
FOR I%=10 TO 13
LOCATE I%,50 : PRINT STRINGS(19,32);
NEXT I%
LOCATE 11,53 : PRINT "Name, Number";
LOCATE 12,53 : PRINT " Class";
DISP=1
GOTO Startloops
END IF
ELSE
IF SEARCH=1 THEN
. Clear old screen.
COLOR 15,1
FOR I%=10 TO 13
LOCATE I%,11 : PRINT STRINGS(26,32);
NEXT I%
LOCATE 11,14 : PRINT "Number" From:;
PRINT USING "#####";BEGSRCH%;
LOCATE 12,14 : PRINT " To: ";
PRINT USING "#####";ENDSRCH%;
. Draw new screen.
T6=SRCHCLASS$
COLOR 15,4 : LOCATE 15,11 : PRINT STRINGS(26,32);
COLOR 31,4 : LOCATE 15,15 : PRINT "Class";
COLOR 15,4 : LOCATE 15,27 : LINE INPUT SRCHCLASS$
IF SRCHCLASS$="" THEN SRCHCLASS$="1$
IF LEN(SRCHCLASS$)>8 THEN SRCHCLASS$=LEFT$(SRCHCLASS$,8)
WHILE LEN(SRCHCLASS$)<8
SRCHCLASS$=SRCHCLASS$+""
WEND
COLOR 15,4 : LOCATE 15,15 : PRINT "Class";
COLOR 15,4 : LOCATE 15,27 : PRINT SRCHCLASS$
SEARCH=2
GOTO Startloops

```

```

. bottom
. exit
. return
. hardcopy
. left-right

```

```

ELSE
  * Clear old screen.
  COLOR 15,1 : LOCATE 15,11 : PRINT STRINGS$(20,32)
  LOCATE 15,15 : PRINT "Class";
  LOCATE 15,27 : PRINT SRCHCLASS$;
  * Get new screen.
  COLOR 15, 4
  FOR I%=10 TO 13
    LOCATE I%,11 : PRINT STRINGS$(20,32);
  NEXT I%
  LOCATE 11,14 : PRINT "Number From: ";
  LOCATE 12,14 : PRINT " To: ";
  COLOR 31, 4 : LOCATE 11,24 : PRINT "From: ";
  LINE INPUT T$
  IF T$<>="" THEN BEGRCH%=VAL(T$)
  COLOR 15, 4 : LOCATE 11,24
  PRINT USING "From: ###" BEGRCH%;
  COLOR 31, 4 : LOCATE 12,24 : PRINT " To: ";
  LINE INPUT T$
  IF T$<>="" THEN ENDRCH%=VAL(T$)
  COLOR 15, 4 : LOCATE 12,24
  PRINT USING " To: ###" ENDRCH%;
  BEGRCH=1
  GOTO Startloop$
END IF
END IF
CASE ELSE
  SOUND 1000,3 : SOUND 800,1.5
  GOTO Startloop$
END SELECT
ChangeHcopy:
  * This is a miniaubroutine to do the hardcopy coloring.
  FOR I%=20 TO 22
    LOCATE I%,32 : PRINT STRINGS$(16,32);
  NEXT I%
  LOCATE 21,37 : PRINT "Hardcopy".
  RETURN
DoOptions:
  COLOR 31,4 : LOCATE 16,14
  PRINT * Begin the directory - <RET> = Yes <ESC> = No *;
  Startloop$:
  AS=INKEY$
  SELECT CASE AS
    CASE =
      GOTO Startloop$
    CASE CHR$(27)
      COLOR 15,0 : LOCATE 16,10 : PRINT SPACES$(65);
      GOTO Startloop$
    CASE CHR$(13)
      GOTO DoDirectory
    CASE ELSE
      SOUND 1000,3 : SOUND 800,1.5
      GOTO Startloop$
  END SELECT
DoDirectory:
  * This is the section to do the directory
  COLOR 15, 0 : CLS
  COLOR 0,15 : LOCATE 1,7
  PRINT * Press <ESC> to EXIT Pass: ### of: ### *;
  FOR I%=1 TO 42
    D$(I%)=""
  NEXT I%
  IF HCOPI%="" THEN
    LPRINT "Contents of Compound Property File *.DATES* *TIMES
    LPRINT
    FOR I%=1 TO 79 : LPRINT "=: NEXT I% : LPRINT
    END IF
  IF DISP=1 THEN
    COLOR 14,0
    LOCATE 2, 6 : PRINT "Number:";
    LOCATE 2,24 : PRINT "Name:";
    LOCATE 2,69 : PRINT "Class:";
    LOCATE 3, 1 : PRINT STRINGS$(80,209);
    IF HCOPI%="" THEN
      LPRINT TAB(6);"Number";TAB(24);"Name";TAB(69);"Class"
      FOR I%=1 TO 79 : LPRINT "=: NEXT I% : LPRINT : LPRINT
      END IF
    END IF
    * Start loop to get data.
    IF SEARCH=2 THEN ENDRCH%=NumOfCompounds : BEGRCH%=1
    NUMFOUND%=0 : LINE%=4
    COLOR 0,15 : LOCATE 1,67 : PRINT USING "###" NUMFOUND%;
    COLOR 0,15 : LOCATE 1,48 : PRINT USING "###" ENDRCH%;
  FOR I%=BEGSRCH% TO ENDRCH%
    AS=INKEY$
    IF AS=CHR$(27) THEN GOTO EndDirectory
    COLOR 0,15 : LOCATE 1,37 : PRINT USING "###" I%;
    PINM$="P" + RIGHT$(STR$(I%),LEN(STR$(I%))-1)
    FILE$=DIR$ + P$ + RIGHT$(STR$(I%),LEN(STR$(I%))-1) + ".DAT"
    OPEN FILE$ FOR INPUT AS #1
    J%=1
    WHILE NOT EOF(1) AND J%<=42
      INPUT #1, D$(J%)
      IF J%>1 THEN
        WHILE LEN(D$(J%))<8
          D$(J%)=D$(J%) + " "
        WEND
        IF LEN(D$(J%))>8 THEN D$(J%)=LEFT$(D$(J%),8)
      END IF
      INCR J%
    WEND
    CLOSE #1
    IF SEARCH=2 AND SRCHCLASS<>D$(14) THEN GOTO NextCompound
    NUMFOUND%=NUMFOUND%+1
    COLOR 0,15 : LOCATE 1,67 : PRINT USING "###" NUMFOUND%;
  * Section to print name, number, class.
  IF DISP=1 THEN
    COLOR 15,0

```

```

LOCATE LINE%, 7 : PRINT PNUM$;
LOCATE LINE%,16 : PRINT D6(1);
LOCATE LINE%,66 : PRINT D6(14);
IF HCOOPY$="Y" THEN
  LPRINT TAB(7);PNUM$;TAB(16);D6(1);TAB(66);D6(14)
END IF
INCR LINE%
IF LINE%>25 THEN
  LOCATE J%,1 : PRINT SPACES(60);
  NEXT J%
  LINE%=4
END IF
GOTO NextCompound
END IF

```

• Section to print all data.
COLOR 15, 0 : LOCATE 4,1
COLOR 11, 0 : PRINT "Name: "; COLOR 15,0 : PRINT D6(1);TAB(65);
COLOR 11, 0 : PRINT "Number: "; COLOR 15,0 : PRINT PNUM\$
FOR J%=2 TO 42
 IF F\$(J%)<>" " THEN
 COLOR 10,0 : PRINT F\$(J%); ;
 COLOR 15,0 : PRINT D6(J%), ;
 END IF
 NEXT J%
IF HCOOPY\$="Y" THEN
 LPRINT "Name: ";D6(1);TAB(65);"Num: ";PNUM\$
 FOR J%=2 TO 42
 IF F\$(J%)<>" " THEN LPRINT F\$(J%); ;D6(J%),
 NEXT J%
 LPRINT : LPRINT
 END IF
NextCompound:
NEXT %
EndDirectory:
• Have done everything so return.
IF HCOOPY\$="Y" THEN LPRINT CHR\$(12)
COLOR 15,4
FOR I%=14 TO 16
 LOCATE I%,16 : PRINT SPACES(40);
NEXT I%
LOCATE 15,16 : PRINT " *** Press any key to exit this section. *** ";
AS=INKEY\$
WHILE AS=""
 AS=INKEY\$
WEND
GOTO Directory
ClearData:

LOCATE 15, 1
LOCATE 2,12 : PRINT SPACES(47);
LOCATE 2,73 : PRINT SPACES(4);
FOR I%=0 TO 6
 FOR J%=0 TO 5
 IF I%>0 OR J%<0 THEN
 COLOR 15,1 : LOCATE I%*3+5,J%*13+3 : PRINT SPACES(10);
 END IF
 NEXT J%
 NEXT I%
 FOR I%=1 TO 42 : D6(I%)="" : NEXT I%
 RETURN
 • clear array

Logo:
\$INCLUDE "LOGO.BAS"
• T.T.T.'That's all Folks!!!!
• Code listing for LOGO.BAS
•
• • This is the subroutine to draw the AC software logo at x,y
•
SCREEN 12
COLOR 11,0
WINDOW (-100,-100):(100,100)
C1=15 : C2=12 : C3=15 : C4=1 : C5=1 : C6=106
• First are boxes
LINE (-41,-43)-(-41, 43),C1;B
LINE (-41,-31)-(-41,-31),C1
LINE (-41, 31)-(-41, 31),C1
LINE (-28,-43)-(-28, 43),C1
LINE (-28,-43)-(-28, 43),C1
PAINT (-39,-40),CHR\$(C6)
PAINT (-39, 40),CHR\$(C6)
PAINT (-39, 40),CHR\$(C6)
• Next are web lines
TEMP=30
FOR I%=27 TO 27 STEP 6
 LINE (27,TEMP)-(-%,30),C2
 LINE I%,30)-(27,TEMP),C2
 DEGR TEMP,(60/54)*6
NEXT I%
• Next is AC in center.
PI#="4*ATN(1)
CIRCLE (-13,0),15,C3,,,1.25
CIRCLE (-13,0),22,C3,,,1.25
PAINT (-13,0),CHR\$(6)HEX
LINE (-3,5,22)-(-1,22),C3;B
LINE (-3,25,-21)-(-7,25),C4;B
CIRCLE (-17,0),15,C3,PI#/4,7*PI#/4,1.25
CIRCLE (-17,0),22,C3,PI#/4,7*PI#/4,1.25
• outer box
• inner lines
• corner boxes
• calc PI
• draws A
• draws C

This is the section to clear the data on the screen.

Listing for Program II.2: REG5.BAS

```

LINE (20.7,15.5):(23.5,10.2)
LINE (20.7,15.5):(23.5,10.2)
PRINT (5.0),CHR$(8)HF)
.
. Next is software table.
LOCATE 10,31 : PRINT "Software - Software";
LOCATE 21,31 : PRINT "Software - Software";
TEMP$="Software"
FOR I%=1 TO LEN(TEMP$)
  LOCATE 11+I%,27 : PRINT MID$(TEMP$,I%,1);
  LOCATE 11+I%,54 : PRINT MID$(TEMP$,I%,1);
NEXT I%
RETURN
.
. This is a pgm to do a multiple regression analysis on the fuel
. and compound properties which are stored in the files. This
. pgm takes the NMR properties of each fuel or compound to give a
. physical property of the fuel or compound. A Multiple Regression
. Analysis on this gives the coefficients for a linear combination
. of the NMR properties to be used for predictions. Unlike Ver 1.0,
. this version uses the calculated average structure properties to
. arrive at the regression analysis. Before, the integration values
. were used. Ver 2.00 also gets all the information it needs out of
. the expanded LC-NMR files.
. Version 3.00 uses the expanded basis set files. Instead of 9
. properties in the basis set, there are now 42 possible properties.
. These files are sequential access rather than random access and
. are accessed in the same way as the LC-NMR files. The number of
. compounds in the files is stored in a file called PNUM.DAT.
.
. This is version 5.0 - is was written for the PS/2 Model 80. There
. are no major changes from ver 3.10, except for the machine on which
. it runs.
.
. Program Name: REGRESS BAS Ver 5.00 Date Written: 08/23/1988
. Author: Allen Caswell Date Modified: 08/13/1988
.
.
. First is the section to set up the variables.
.
.
COMMON ODIRS, OFILES
ON KEY(1) GOSUB WriteConfigFile
KEY(1) ON
ON KEY(2) GOSUB WriteFuelParams
KEY(2) ON
PROPR$="D" : LCDRV$="D" : HCOOPY$="N" : RMDSK$="N"
OPTN1%=1 : OPTN2%=1 : OPTN3%=1
OPTN4%=1 : OPTN5%=1 : OPTN6%=1
CLASS%=1 : PROP%=4
ACT$ ="* Class * : VERSN$="Ver 5.00" : CFGDIR$="D:\CORRPGMS"
.
. Next dimension the variables
DIM PROP$(50), NME$(15), CLASS$(10), D$(42), OD$(350), INPU(400,22)
DIM PROPERTY(400), A(22,22), G(22,22), B(22,22), INVA(22,22), T(22)
DIM CLUSE%(8,201), CPAGE%(8), OPTN3%(8), FRACTION$(5)
DIM MIXCOEFF$(22), T$(22)
.
. Next are names for classes of compounds.
DATA "ALKANE", "ALKENE", "MODELIN", "CYCLOHEX", "DECALIN",
DATA "MONO", "DICYCLIC", "TETRALIN", "FUEL",
FOR I%=1 TO 8 : READ CLASS$(I%) : NEXT I%
.
. Next are names of properties to match.
DATA "Name", "Formula", "Mol Wt", "Cetane #", "BP - 50%", "Pour Pt",
DATA "Improv%",
DATA "Flash Pt", "Density", "Ref Indx", "Cloud Pt", "Viscosit", "Filter",

```

```

DATA * Class *
DATA 'Ag Dq Br', 'Sp. Disp', 'Suff Tent', 'Aniline', 'Cr Press', 'Cr Temp'
DATA 'Crtt Vol'
DATA 'Heat Cap', 'Ht Vapor', 'Ht Form', 'Free E F', 'Ht Comb', 'Mol Vol'
DATA * % Atom *
DATA * % Olefin * : fuelType, 'Cat Inct', 'Sp. Grav', 'BP - IBP', 'BP - 10%'
DATA 'BP - End', 'C. Resid', * * * * *
DATA *
FOR I%=1 TO 42 : READ PROPS(I%) : NEXT I%
* Next are names for options on menu.
DATA * Exit To DOS * : Run GRAF ED * : Run CORR5 * : Run PROPS *
DATA * Run GRAPH * : Run ERROR * : Run EZ_PLOT * : Restart *
FOR I%=1 TO 8 : READ OPTNS(I%) : NEXT I%
* Next are names of fractions for fuels.
DATA 'Alkane *', 'Monocyclic *', 'Dicyclic *', 'Flourane *'
DATA 'Phenanthrene'
FOR I%=1 TO 5 : READ FRACTIONS(I%) : NEXT I%
* Next are names for fuel classes.
DATA 'All *', 'JP-5 *', 'JP-8 *', 'DF-2 *'
FOR I%=1 TO 5 : READ FUELCLASSES(I%) : NEXT I%
* Next are defaults.
FOR I%=1 TO 9
CPAGE%(I%)=1 : OPTN3%(I%)=1
FOR J%=1 TO 200
CUSE%(I%,J%)=1
NEXT J%
NEXT I%
GOSUB ReadConfigFile
StartOfProgram:
*
*
* The next order of business is get class and property to sort by.
*
* First are Compound, Hardcopy, and Time Boxes.
COLOR 15,0 : CLS
COLOR 0,7
TEMP%=5
FOR I%=1 TO 4
LOCATE TEMP%+0,1 : PRINT CHR$(219);STRINGS(11,198);CHR$(191); 'top
LOCATE TEMP%+2,1 : PRINT CHR$(198);STRINGS(11,205);CHR$(191); 'middle
LOCATE TEMP%+4,1 : PRINT CHR$(182);STRINGS(11,188);CHR$(217); 'bottom
LOCATE TEMP%+1,1 : PRINT CHR$(179);TAB(13);CHR$(179); 'side
LOCATE TEMP%+3,1 : PRINT CHR$(179);TAB(13);CHR$(179); 'side
TEMP%=TEMP%+5
NEXT I%
LOCATE 6,3 : PRINT 'Hardcopy:'
LOCATE 6,7 : PRINT 'HCOOPY';
LOCATE 11,3 : PRINT 'Compounds';
LOCATE 13,6 : PRINT USING '###',NUMCOMPOUNDS;

```

```

LOCATE 16,3 : PRINT 'RAM Disk';
LOCATE 16,7 : PRINT RMDSKS;
LOCATE 21,5 : PRINT 'Time';
* Next is top box - for the title.
COLOR 15,4
LOCATE 1,5 : PRINT CHR$(201);STRINGS(99,206);CHR$(187) 'top line
LOCATE 2,5 : PRINT CHR$(186);STRINGS(99,32);CHR$(186) 'ends
LOCATE 3,5 : PRINT CHR$(200);STRINGS(99,205);CHR$(186) 'bottom line
LOCATE 1,31 : PRINT CHR$(209); 'top junct
LOCATE 2,31 : PRINT CHR$(179); 'middle line
LOCATE 3,31 : PRINT CHR$(207); 'bottom junct
LOCATE 2,10 : PRINT 'REGRESS'
LOCATE 2,18 : PRINT 'VERSNS'
LOCATE 2,35 : PRINT 'Multiple Regression Analysis Software';
* Next are Class and Property Boxes
COLOR 15,1
FOR I%=5 TO 21
LOCATE I%,18 : PRINT SPACES(13);
LOCATE I%,37 : PRINT SPACES(30);
LOCATE I%,18 : PRINT CHR$(179);
LOCATE I%,31 : PRINT CHR$(179);
FOR J%=0 TO 3
LOCATE I%,J%*13+37 : PRINT CHR$(179);
NEXT J%
NEXT I%
LOCATE 4,18 : PRINT STRINGS(13,199); 'top lines
LOCATE 4,37 : PRINT STRINGS(36,199); 'double lines
LOCATE 6,18 : PRINT STRINGS(13,205); 'bottom lines
LOCATE 6,37 : PRINT STRINGS(36,205);
LOCATE 21,18 : PRINT STRINGS(13,199);
LOCATE 21,37 : PRINT STRINGS(36,199);
FOR I%=0 TO 1
LOCATE 4,I%*19+18 : PRINT CHR$(218); 'ul corner
LOCATE 4,I%*45+31 : PRINT CHR$(191); 'ur corner
LOCATE 21,I%*19+18 : PRINT CHR$(192); 'll corner
LOCATE 21,I%*45+31 : PRINT CHR$(217); 'lr corner
LOCATE 6,I%*19+18 : PRINT CHR$(186); 'joints
LOCATE 6,I%*45+31 : PRINT CHR$(181);
LOCATE 8,I%*13+50 : PRINT CHR$(206);
LOCATE 21,I%*13+50 : PRINT CHR$(193);
NEXT I%
LOCATE 5,50 : PRINT **
LOCATE 5,63 : PRINT **
LOCATE 5,22 : PRINT 'Class',
LOCATE 5,53 : PRINT 'Property';
FOR I%=1 TO 9
LOCATE I%+8,21
PRINT CLASS$(I%);
NEXT I%
FOR I%=1 TO 14
LOCATE I%*1+8,40 : PRINT PROPS(I%);
LOCATE I%*1+6,53 : PRINT PROPS(I%+14);
LOCATE I%*1+6,66 : PRINT PROPS(I%+28);
NEXT I%
* Next are the command statements.
COLOR 3,0
LOCATE 23,25 : PRINT * Press <RET> to begin execution.
LOCATE 24,25 : PRINT *Press <H> to toggle hardcopy, <R> for RAM disk *;

```

```

LOCATE 25,25 : PRINT *      Press <O> for Options, <Q> to quit * ;
* Have got screen, so get the information from the keyboard.
FILES=PROPRV$+ICORR1+CLASS$(CLASS%) + \PNUM.DAT
OPEN FILES FOR INPUT AS #1
INPUT #1,NumOfCompounds
CLOSE #1
COLOR 0,7 : LOCATE 13, 6 : PRINT USING "##";NumOfCompounds;
IF ACT$=" Class * THEN
  COLOR 15, 1 : LOCATE CLASS%+6,19
  PRINT * "CLASS$(CLASS%)" ;
  IF AS=CHRS(0)+CHRS(72) THEN DECR CLASS% ELSE INCR CLASS%
  IF CLASS%<1 THEN CLASS%=0
  IF CLASS%>8 THEN CLASS%=1
  COLOR 14, 0 : LOCATE CLASS%+6,19
  PRINT * "CLASS$(CLASS%)" ;
  FILES=PROPRV$+ICORR1+CLASS$(CLASS%) + \PNUM.DAT
  OPEN FILES FOR INPUT AS #1
  INPUT #1,NumOfCompounds
  CLOSE #1
  COLOR 0,7 : LOCATE 13, 6 : PRINT USING "##";NumOfCompounds;
  GOTO Startloop
END IF
IF ACT$=" Property * THEN
  COL%=INT((PROP%-1)/14) : ROW%=PROP% - (COL%*14)
  COLOR 15, 1 : LOCATE ROW%+6,COL%*13 + 38
  PRINT * "PROPS$(PROP%)" ;
  IF AS=CHRS(0)+CHRS(72) THEN DECR PROP% ELSE INCR PROP%
  IF PROP%<1 THEN PROP%=1
  IF PROP%>42 THEN PROP%=42
  COL%=INT((PROP%-1)/14) : ROW%=PROP% - (COL%*14)
  COLOR 14, 0 : LOCATE ROW%+6,COL%*13 + 38
  PRINT * "PROPS$(PROP%)" ;
  GOTO Startloop
END IF
CASE ELSE
  SOUND 1000,3 : SOUND 800,1,5
  GOTO STARTLOOP
END SELECT

```

GetData:

Will now start the loop to get the data from the desired files.

```

* Will first get some background info.
GOSUB GetCompoundUse
IF CLASS%=9 THEN
  GOSUB ReadFuelParams
  GOSUB GetFractionsToUse
  GOSUB GetFuelType
  GOSUB GetFuelParams
  IF PROP%=4 THEN GOSUB GetCellLevel
* Must find the first fraction turned on.
FUSE%=0
WHILE FRACTION%(FUSE%)<>1 AND FUSE%<=8 : INCR FUSE% : WEND
IF FUSE%>5 THEN
  SOUND 1000,3 : SOUND 800,1,5
  COLOR 12, 0 : CLS
  LOCATE 11,31 : PRINT *** YOU IDIOT ***,
  LOCATE 12,22 : PRINT "You did not select any fuel classes!!";

```

```

LOCATE 25,25 : PRINT *      Press <O> for Options, <Q> to quit * ;
* Have got screen, so get the information from the keyboard.
FILES=PROPRV$+ICORR1+CLASS$(CLASS%) + \PNUM.DAT
OPEN FILES FOR INPUT AS #1
INPUT #1,NumOfCompounds
CLOSE #1
COLOR 0,7 : LOCATE 13, 6 : PRINT USING "##";NumOfCompounds;
IF ACT$=" Class * THEN
  COLOR 15, 5 : LOCATE 5, 21 : PRINT ACT$;
ELSE
  COLOR 15, 5 : LOCATE 5, 52 : PRINT ACT$;
END IF
COLOR 14, 0 : LOCATE CLASS%+6,19
PRINT * "CLASS$(CLASS%)" ;
COL%=INT((PROP%-1)/14) : ROW%=PROP% - (COL%*14)
COLOR 14, 0 : LOCATE ROW%+6,COL%*13 + 38
PRINT * "PROPS$(PROP%)" ;
FILES=PROPRV$+ICORR1+CLASS$(CLASS%) + \PNUM.DAT
OPEN FILES FOR INPUT AS #1
INPUT #1,NumOfCompounds
CLOSE #1

```

```

Startloop:
AS=INKEY$
SELECT CASE AS
CASE =
  COLOR 0,7
  LOCATE 23,4 : PRINT TIMES;
  GOTO Startloop
CASE CHRS(13)
  GOTO GetData
CASE "0","0","0","0",CHRS(27)
  GOTO Options
CASE "r","r"
  LPRINT CHRS(12)
  GOTO Startloop
CASE "h","h"
  IF HCOOPY$="Y" THEN HCOOPY$="N" ELSE HCOOPY$="Y"
  COLOR 0,7 : LOCATE 8,7 : PRINT HCOOPY$;
  GOTO Startloop
CASE "r","r"
  IF RMDSK$="Y" THEN RMDSK$="N" ELSE RMDSK$="Y"
  COLOR 0,7 : LOCATE 18,7 : PRINT RMDSK$;
  GOTO Startloop
CASE CHRS(0)+CHRS(75)+CHRS(0)+CHRS(77)
  IF ACT$=" Class * THEN
    COLOR 15, 1 : LOCATE 5, 21 : PRINT ACT$;
    ACT$=" Property *
    COLOR 15, 5 : LOCATE 5, 52 : PRINT ACT$;
  GOTO Startloop
END IF
IF ACT$=" Property * THEN
  COLOR 15, 1 : LOCATE 5, 52 : PRINT ACT$;
  ACT$=" Class *
  COLOR 15, 5 : LOCATE 5, 21 : PRINT ACT$;
  GOTO Startloop
END IF
CASE CHRS(0)+CHRS(72), CHRS(0)+CHRS(60)
  * no key
  * return
  * options
  * form feed
  * hardcopy
  * RAM disk
  * left-right
  * up-down

```

```

AS=INPUT$(1)
GOTO StartOffProgram
END IF
.
.
. Will first set up the screen.
SELECT CASE CLASS$
CASE 1 : TEMPs=" Xch3 Xch2 Xch "
CASE 2 : TEMPs=" Xch3 Xch2 Xch "
CASE 3 : TEMPs=" Xch3 Xch2 Xch "
CASE 4 : TEMPs=" Ceub sCH2 sCH "
CASE 5 : TEMPs=" Ceub sCH3 sCH2 sCH "
CASE 6 : TEMPs=" Cun Ach3 Ach2 Ach Cat CH2>A"
CASE 7 : TEMPs=" Cun Ach3 Ach2 CH2>A"
CASE 8 : TEMPs=" Ach3 Ach2 CH2>A"
CASE 9 : TEMPs=" "
END SELECT
IF RMDSK$="" THEN
TEMP16="F:"
ELSE
TEMP16="PRDRV$+\"CORRY"+CLASS$(CLASS$)+\"
END IF
COLOR 15, 0 : CLS
COLOR 11, 0
LOCATE 1, 1 : PRINT LEFT$(TEMP16;27);
LOCATE 2, 1 : PRINT "Class: "CLASS$(CLASS$);
LOCATE 3, 1 : PRINT "Property: "PROPs$(PROp$);
LOCATE 1,60 : PRINT TIMES;
LOCATE 1,70 : PRINT DATES;
LOCATE 3,60 : PRINT "Run Time: sec";
IF CLASS%=9 THEN
LOCATE 2,22 : PRINT "Fuel Classes: ";
FOR I%=1 TO 5
IF FRACTION$(I%)=1 THEN PRINT LEFT$(FRACTIONS$(I%),6);
NEXT I%
END IF
COLOR 12, 7
LOCATE 1,31
PRINT USING " Pass ### of ### ";I%,NumOfCompounds;
COLOR 14, 0
LOCATE 4, 1
PRINT TAB(2);"Name":TAB(10);TEMPs;TAB(67);PROPs$(PROp$)
PRINT STRING$(60,205)
COLOR 15, 0 : LINECNT%=0
.
. Will set up the printer if doing a hardcopy.
IF HCOOPY$="" THEN
LPRINT "Multiple Regression Analysis "DATES; "TIMES
LPRINT : LPRINT "
LPRINT "Class used: "CLASS$(CLASS$);
LPRINT "Property used: "PROPs$(PROp$)
IF CLASS%=9 THEN
LPRINT "Fuel Classes: ";
FOR I%=1 TO 5
IF FRACTION$(I%)=1 THEN LPRINT LEFT$(FRACTIONS$(I%),10);
NEXT I%
END IF
LPRINT : LPRINT STRING$(79,205)
LPRINT TAB(2);"Name":TAB(10);TEMPs;TAB(67);PROPs$(PROp$)
LPRINT STRING$(79,205)
END IF
END IF
. Have got screen, so get the data.
TOTALObs%=0 : COUNTER%=1
RunTime=TIMER
FOR I%=1 TO NumOfCompounds
AS=INKEY$
IF AS=CHR$(27) THEN GOTO EndOfLoop
IF AS="C" OR AS="V" THEN GOTO StartOfProgram
COLOR 0, 7 : LOCATE 1,31
PRINT USING " Pass ### of ### ";I%,NumOfCompounds;
COLOR 12, 0 : LOCATE 3,71
PRINT USING "### #";TIMER-RunTime;
.
. Will see if use this compound and if so, continue.
IF CUSE$(CLASS%,I%)=1 THEN
.
. Will get property data and see if continue.
SELECT CASE RMDSK$
CASE "F"
PNUMs=PRDRV$+\"CORRY"+CLASS$(CLASS$)+\"
PNUMs=PNUMs+\"P"+RIGHT$(STR$(I%),LEN(STR$(I%))-1)+\"DAT\"
CASE "V"
PNUMs="F:"+"P"+RIGHT$(STR$(I%),LEN(STR$(I%))-1)+\"DAT\"
END SELECT
OPEN PNUMs FOR INPUT AS #1
D$(1)=" : INPUT #1,D$(1)
J%=2
WHILE NOT EOF(1) AND J%<=42
D$(J%)=" : INPUT #1,D$(J%)
IF LEN(D$(J%))>6 THEN D$(J%)=LEFT$(D$(J%),6)
WHILE LEN(D$(J%))<6
D$(J%)=D$(J%)+\"
WEND
INCR J%
WEND
CLOSE #1
.
. Have got prop data so see if classes match and data not empty.
Proceeds="NO"
IF D$(14)=CLASS$(CLASS%) AND D$(PROp%)<>
. THEN Proceeds="YES"
.
. If doing fuels, must match class type and cetane improver.
IF CLASS%=9 AND Proceeds="YES" THEN
Proceeds="NO"
IF FUELCLASS$(1)=1 THEN
Proceeds="YES"
ELSE
FOR K%=2 TO 5
IF FUELCLASS$(K%)=1 AND FUELCLASS$(K%)=D$(30) THEN
Proceeds="YES"
END IF
NEXT K%
END IF
IF PROp%=4 AND Proceeds="YES" THEN
Proceeds="NO"
SELECT CASE CETLEVEL$
CASE " : Proceeds="YES"
CASE D$(7) : Proceeds="YES"
END SELECT
. match cetane
. all cetanes
. matches

```

```

END IF
END IF
IF Proceed$='YES' THEN
    ' Will get integration data.
    CNAME$='C'+RIGHT$(STR$(%LEN(STR$(%))-1)
    SELECT CASE RMDISK$
    CASE 'H'
        CNUM$=LCORR$+'CORR'+CLASS$(CLASS$)+'*'
        CNUM$=CNUM$+CNAME$+'*DAT*'
    CASE 'R'
        CNUM$='F'+CNAME$+'*DAT*'
    END SELECT
    OPEN CNUM$ FOR INPUT AS #1
    J%=1
    WHILE NOT EOF(1) AND OD$(J%) <> 'END' AND J% < 350
        INPUT #1,OD$(J%)
        IF OD$(J%)='7.7777' THEN OD$(J%)='0'
        IF OD$(J%)='*'.+*+*+*+* THEN OD$(J%)='0'
        INCR J%
    WEND
    CLOSE #1
    ' Will set in the observed property.
    PROPERTY(COUNTER%)=VAL(OD$(PROP%))
    IF CLASS$='9' THEN
        TEMP=VAL(OD$(PROP%)) + OFFSETFACTR
        IF LEFT$(FUNCTION$,1)='X' THEN PROPERTY(COUNTER%)=TEMP
        IF LEFT$(FUNCTION$,3)='1/X' THEN PROPERTY(COUNTER%)=1/TEMP
        IF LEFT$(FUNCTION$,3)='LOG' THEN PROPERTY(COUNTER%)=LOG(TEMP)
    END IF
    ' Have got data so will put in matrix.
    SELECT CASE CLASS$
    CASE 1
        VAR%=3
        INPUT(COUNTER%,1)=VAL(OD$(106))
        INPUT(COUNTER%,2)=VAL(OD$(108))
        INPUT(COUNTER%,3)=VAL(OD$(110))
        INPUT(COUNTER%,4)=VAL(OD$(147))
    CASE 3
        VAR%=2
        INPUT(COUNTER%,1)=VAL(OD$(106))
        INPUT(COUNTER%,2)=VAL(OD$(113))
    CASE 4
        VAR%=3
        INPUT(COUNTER%,1)=VAL(OD$(106))
        INPUT(COUNTER%,2)=VAL(OD$(113))
        INPUT(COUNTER%,3)=VAL(OD$(206))
    CASE 5
        VAR%=2
        INPUT(COUNTER%,1)=VAL(OD$(106))
        INPUT(COUNTER%,2)=VAL(OD$(113))
    CASE 8
        VAR%=5
        INPUT(COUNTER%,1)=VAL(OD$( 3))
        INPUT(COUNTER%,1)=VAL(OD$( 9))
        INPUT(COUNTER%,2)=VAL(OD$( 11))
        INPUT(COUNTER%,3)=VAL(OD$( 13))
        INPUT(COUNTER%,4)=VAL(OD$(149))
    ' hard disk
    ' RAM disk
    ' Mono
    ' Cch3
    ' Cch2
    ' Cch
    ' Ccq
    ' INPUT(COUNTER%,5)=VAL(OD$( 19))
    ' INPUT(COUNTER%,5)=VAL(OD$( 15))
    ' Cct
    ' Cch2>
CASE 7
    VAR%=4
    INPUT(COUNTER%,1)=VAL(OD$( 26))
    INPUT(COUNTER%,2)=VAL(OD$( 34))
    INPUT(COUNTER%,3)=VAL(OD$( 36))
    INPUT(COUNTER%,4)=VAL(OD$( 40))
    CASE 8
        VAR%=3
        INPUT(COUNTER%,1)=VAL(OD$( 15))
        INPUT(COUNTER%,2)=VAL(OD$(211))
        INPUT(COUNTER%,3)=VAL(OD$( 23))
    CASE 9
        INPUT(COUNTER%,1)=VAL(OD$(106))"VAL(OD$(116))
        INPUT(COUNTER%,2)=VAL(OD$(106))"VAL(OD$(116))
        INPUT(COUNTER%,3)=VAL(OD$(110))"VAL(OD$(116))
        INPUT(COUNTER%,4)=VAL(OD$( 3))"VAL(OD$( 27))
        INPUT(COUNTER%,5)=VAL(OD$( 9))"VAL(OD$( 27))
        INPUT(COUNTER%,6)=VAL(OD$( 11))"VAL(OD$( 27))
        INPUT(COUNTER%,7)=VAL(OD$( 13))"VAL(OD$( 27))
        INPUT(COUNTER%,8)=VAL(OD$( 16))"VAL(OD$( 27))
        INPUT(COUNTER%,9)=VAL(OD$( 15))"VAL(OD$( 27))
        INPUT(COUNTER%,10)=VAL(OD$( 26))"VAL(OD$( 52))
        INPUT(COUNTER%,11)=VAL(OD$( 34))"VAL(OD$( 52))
        INPUT(COUNTER%,12)=VAL(OD$( 36))"VAL(OD$( 52))
        INPUT(COUNTER%,13)=VAL(OD$( 46))"VAL(OD$( 52))
        INPUT(COUNTER%,14)=VAL(OD$( 54))"VAL(OD$( 78))
        INPUT(COUNTER%,15)=VAL(OD$( 60))"VAL(OD$( 78))
        INPUT(COUNTER%,16)=VAL(OD$( 62))"VAL(OD$( 78))
        INPUT(COUNTER%,17)=VAL(OD$( 66))"VAL(OD$( 78))
        INPUT(COUNTER%,18)=VAL(OD$( 60))"VAL(OD$(104))
        INPUT(COUNTER%,19)=VAL(OD$( 68))"VAL(OD$(104))
        INPUT(COUNTER%,20)=VAL(OD$( 68))"VAL(OD$(104))
        INPUT(COUNTER%,21)=VAL(OD$( 62))"VAL(OD$(104))
        IF FRACTION%(1)=1 THEN VARR%= 3
        IF FRACTION%(2)=1 THEN VARR%= 9
        IF FRACTION%(3)=1 THEN VARR%=13
        IF FRACTION%(4)=1 THEN VARR%=17
        IF FRACTION%(9)=1 THEN VARR%=21
    END SELECT
    ' Have got everything so will print to screen.
    ' First set up print fields.
    FOR J%=1 TO VAR% : T(J%)=INPUT(COUNTER%,J%) : NEXT J%
    T(9)=PROPERTY(COUNTER%)
    TEMPS=-
    FOR J%=1 TO VAR%
        TEMPS=TEMPS+'*'+*****
    NEXT J%
    IF LEN(TEMPS)>53 THEN TEMPS=LEFT$(TEMPS,53)
    WHILE LEN(TEMPS)<53 : TEMPS=TEMPS+'*' : WEND
    TEMPS=TEMPS+'*'+*****
    ' Will do the printing
    LOCATE LINECNT%,1 : COLOR 15,0
    PRINT CNAME$TAB(6);
    IF VAL(OD$( 78))>0.00001 THEN COLOR 10.0 : PRINT 'F'; : COLOR 15.0
    IF VAL(OD$(104))>0.00001 THEN COLOR 12.0 : PRINT 'P'; : COLOR 15.0

```

```

LOCATE 13, 10 : PRINT CHR$(200),STRING$(59,205);CHR$(188) 'bottom line
LOCATE 12, 21 : PRINT """" CALCULATING REGRESSION ANALYSIS """"
.
. Will find all zero column and warn user.
GOSUB CheckForError
.
N%=COUNTER%-1
FOR ROW%=1 TO VAR%+1
  FOR COL%=1 TO VAR%+1
    SUM=0
    FOR I%=1 TO N%
      SUM=SUM+INPU(I%,ROW%-1)*INPU(I%,COL%-1)
      IF ROW%=1 THEN SUM=SUM+INPU(I%,COL%-1)
      IF COL%=1 THEN SUM=SUM+INPU(I%,ROW%-1)
    NEXT I%
    A(ROW%,COL%)=SUM
  NEXT COL%
  AT(1,1)=N%
  FOR ROW%=1 TO VAR%+1
    SUM=0
    FOR I%=1 TO N%
      IF ROW%<>1 THEN SUM=SUM+INPU(I%,ROW%-1)*PROPERTY(I%)
      IF ROW%=1 THEN SUM=SUM+PROPERTY(I%)
    NEXT I%
    G(ROW%,1)=SUM
  NEXT ROW%
.
. Will find the inverse of the matrix a (order=var%+1) MAT INVA=INV(A)
ORDER%=VAR%+1
FOR I%=1 TO ORDER%
  FOR J%=1 TO ORDER%
    B(I%,J%)=0
    NEXT J%
    B(I%,I%)=1
  NEXT I%
. Elimination Routine
FOR I%=1 TO ORDER%
  . Find largest coefficient on or below main diagonal.
  MX=-1
  FOR K%=I% TO ORDER%
    IF ABS(A(K%,I%))>MX THEN
      MX=ABS(A(K%,I%))
      R%=K%
    END IF
  NEXT K%
  . Swap equation at row R% with that at Ith row
  FOR K%=1 TO ORDER%
    T=A(I%,K%) : TB=B(I%,K%)
    A(I%,K%)=A(R%,K%) : B(I%,K%)=B(R%,K%)
    A(R%,K%)=T : B(R%,K%)=TB
  NEXT K%
. Perform elimination
FOR J%=1 TO ORDER%
  IF J%<>I% THEN
    M=A(J%,I%)/A(I%,I%)
    FOR K%=1 TO ORDER%
      A(J%,K%)=A(J%,K%)-M*A(I%,K%)
      B(J%,K%)=B(J%,K%)-M*B(I%,K%)
    NEXT K%
. PROP match
. CAUSE match
. crmpd loop
. Form feed
. Start timer
RunTime=TIME
. Will print a message to user
COLOR 15,4
LOCATE 11, 10 : PRINT CHR$(201),STRING$(59,205);CHR$(187) 'top line
LOCATE 12, 10 : PRINT CHR$(166),STRING$(59, 32);CHR$(188) 'ends
.
. Have got data so must do multiple regression.
.
. Have got data so get next compound.
INCR COUNTRY%
END IF
END IF
NEXT I%
EndOfLoop:
.
.
.
.

```

```

COLOR 14,4
PRINT USING "b(##) = ;%1;
COLOR 15,4
PRINT USING "#####.#####.###(%1);
NEXT %
* Next is hardcopy instruction.
COLOR 3, 0
LOCATE 24,25 : PRINT "Press <H> to hardcopy the results";
LOCATE 25, 2 : PRINT "Press <O> to exit w/o storing params.";
IF HOOPY$="Y" THEN GOSUB Hardcopy
Startloop4
AS=INKEY$
SELECT CASE AS
CASE "="
COLOR 0,4 : LOCATE 5,6 : PRINT TIME$; : GOTO Startloop4
CASE "H"
GOSUB Hardcopy
CASE "O" : GOTO Options
CASE ELSE
IF CLASS%=9 THEN
COLOR 0, 3
LOCATE 10,20 : PRINT CHR$(201);STRING$(99,205);CHR$(167);
FOR %1=11 TO 13
LOCATE %1,20 : PRINT CHR$(166);TAB(90);CHR$(166);
NEXT %1
LOCATE 14,20 : PRINT CHR$(200);STRING$(99,205);CHR$(166);
COLOR 4, 3
LOCATE 12,29 : PRINT "Writing file";
COLOR 14, 3 : PRINT "Params File";
FOR %1=1 TO 22
MIXCOEFF(%)=B(%1)
NEXT %1
GOSUB WriteFuelParams
END IF
GOTO Options
END SELECT
GOTO Startloop4

```

Printout:

Have now gotten coefficients so will print out.

```

* First is results box.
COLOR 15, 0 : CLS
COLOR 0, 4
LOCATE 2,10 : PRINT CHR$(201);STRING$(99,205);CHR$(167) ' top line
FOR %1=3 TO 21
LOCATE %1,10 : PRINT CHR$(166);TAB(70);CHR$(166); ' slides
NEXT %1
LOCATE 22,10 : PRINT CHR$(200);STRING$(99,205);CHR$(168) ' bottom line
LOCATE 4,10 : PRINT CHR$(204);STRING$(99,205);CHR$(165) ' middle line
LOCATE 10,10 : PRINT CHR$(166);STRING$(99,166);CHR$(162) ' middle line
COLOR 27, 4
LOCATE 3,22 : PRINT " *** RESULTS *** "
COLOR 0, 4
LOCATE 5,15 : PRINT DATES;
LOCATE 5,58 : PRINT TIME$;
COLOR 11, 4
LOCATE 6,25 : PRINT "Class Searched: ;CLASS$(CLASS%);
LOCATE 7,25 : PRINT "Property Searched: ;PROP$(PROP%);
LOCATE 8,25 : PRINT "Number of Variables: ;VAR%";
LOCATE 9,25 : PRINT "Number of Observations: ";N%
COLOR 11, 0
LOCATE 1,19 : PRINT "Time for Regression Calculation: ;sec";
COLOR 12, 0
LOCATE 1,52 : PRINT USING "###.###";TIMER-RunTime;
COLOR 15, 4
FOR %1=1 TO ORDER%
SELECT CASE %1
CASE 1, 2, 3, 4, 5, 6, 7, 8, 9,10,11 : LOCATE 10+%1,%15
CASE 12,13,14,15,16,17,18,19,20,21,22 : LOCATE -1+%1,%42
END SELECT

```

This is the section to print the options menu.

```

COLOR 0,15
LOCATE 14,1 : PRINT CHR$(216);STRING$(15,166);CHR$(191); ' top
LOCATE 15,1 : PRINT CHR$(179);SPACES$(15) ;CHR$(179); ' side
LOCATE 16,1 : PRINT CHR$(166);STRING$(15,205);CHR$(181); ' middle
LOCATE 25,1 : PRINT CHR$(182);STRING$(15,166);CHR$(217); ' bottom
FOR %1=17 TO 24
LOCATE %1,1 : PRINT CHR$(179);SPACES$(19);CHR$(179); ' side
LOCATE %1,3 : PRINT OPTN$(%1-16);
NEXT %1
LOCATE 15,6 : PRINT "Options";

```

```

CHAIN "GRAPH EXE"
CASE 6
CHAIN "ERROR EXE"
CASE 7
CHAIN "EZ_PLOT EXE"
CASE 8
GOTO StartOfProgram
END SELECT

```

```

* ERROR
* EZ_PLOT
* restart

```

Hardcopy:

This is the subroutine to hardcopy the results of the search.

```

LPRINT "Results of Multiple Regression Analysis " ,DATES," ,TIMES
LPRINT : LPRINT
LPRINT "Class searched: " ,CLASS$(CLASS%)
LPRINT "Property searched: " ,PROP$(PROP%)
LPRINT "Number of variables: " ,VAR%
LPRINT "Number of observations: " ,N%
IF CLASS%=9 THEN
LPRINT " Fuel Classes Searched:"
FOR I%=1 TO 5
IF FRACTION$(I%)=1 THEN LPRINT TAB(10),FRACTIONS(I%)
NEXT I%
END IF
LPRINT : LPRINT
LPRINT "The Linear Coefficients are"
FOR I%=1 TO ORDER%
LPRINT TAB(10) : LPRINT USING "b(##) = %f%-1;
LPRINT USING "#####.#####.###(I%);
NEXT I%
LPRINT CHR$(12)
RETURN

```

DrawCmpdScreen:

This is the subroutine to draw the compound use screen.

```

* First is box for compounds.
COLOR 2,1
LOCATE 5,4 : PRINT CHR$(201);STRING$(71,205);CHR$(187);
FOR J%=8 TO 17
LOCATE J%,4 : PRINT CHR$(186);STRING$(71,32);CHR$(186);
NEXT J%
LOCATE 18,4 : PRINT CHR$(200);STRING$(71,205);CHR$(188);
LOCATE 7,4 : PRINT CHR$(189);STRING$(71,186);CHR$(182);
COLOR 14,1

```

```

COLOR 14,0 : LOCATE OPTN%+18,3 : PRINT OPTN$(OPTN%);
* Have got menu, so see which selection.
Startloop3:
BS=INKEY$
SELECT CASE BS
CASE "="
GOTO Startloop3
CASE CHR$(13)
GOTO DoOption3
CASE CHR$(0)+CHR$(72);CHR$(0)+CHR$(80)
COLOR 0,15 : LOCATE OPTN%+18,3
PRINT OPTN$(OPTN%);
IF BS=CHR$(0)+CHR$(72) THEN DECR OPTN% ELSE INCR OPTN%
IF OPTN%<1 THEN OPTN%=8
IF OPTN%>8 THEN OPTN%=1
COLOR 14,0 : LOCATE OPTN%+18,3
PRINT OPTN$(OPTN%);
GOTO Startloop3
CASE CHR$(0)+CHR$(75);CHR$(0)+CHR$(77)
GOTO Startloop3
CASE ELSE
SOUND 1000,3 : SOUND 800,1,5
GOTO Startloop3
END SELECT
DoOption3:
* Will automatically write the config file.
IF OPTN%<=8 THEN
COLOR 0,3
LOCATE 10,20 : PRINT CHR$(201);STRING$(39,205);CHR$(187);
FOR I%=11 TO 13
LOCATE I%,20 : PRINT CHR$(186);TAB(60);CHR$(186);
NEXT I%
LOCATE 14,20 : PRINT CHR$(200);STRING$(39,205);CHR$(188);
COLOR 4,3
LOCATE 12,28 : PRINT "Writing the " : COLOR 14,3 : PRINT "Config File";
GOSUB WriteConfigFile
END IF
* Have selected option, so must do it.
SELECT CASE OPTN%
CASE 1
CLOSE
GOSUB Logo
LOCATE 1,1
PRINT "May the Force be with you..."
AS=INKEY$
WHILE AS=""
AS=INKEY$
WEND
END
CASE 2
CHAIN "GRAF_ED EXE"
CASE 3
CHAIN "CORR5 EXE"
CASE 4
CHAIN "PROPS EXE"
CASE 5

```

* exit

* GRAF_ED
* CORR5
* PROPS
* GRAPH


```

CNAMES="C"+RIGHT$(STR$(OPTN3%(I%)),LEN(STR$(OPTN3%(I%)))-1)
TEMP%=INT((OPTN3%(I%)-(CPAGE%(I%)-1)*100-1)/10)
LOCATE (OPTN3%(I%)-(CPAGE%(I%)-1)*100-TEMP%*7+5
IF OPTN3%(I%)<=NumOfCompounds THEN
  IF CUSE%(I%,OPTN3%(I%))=1 THEN
    IF BKGND%=0 THEN TEMP%=12 ELSE TEMP%=10
    COLOR TEMP%,BKGND%
    PRINT " ",CHR$(16),CNAMES$,SPACES$(3-LEN(CNAMES));
  ELSE
    IF BKGND%=0 THEN TEMP%=14 ELSE TEMP%=15
    COLOR TEMP%,BKGND%
    PRINT " ",CNAMES$,SPACES$(3-LEN(CNAMES));
  END IF
ELSE
  COLOR 15, BKGND% : PRINT SPACES(7);
END IF
END IF
RETURN

```

GetCompoundUse:

This is the section to see which compounds to use.

```

COLOR 15,0 : CLS
FOR I%=1 TO 9
  IF I%=<CLASS% THEN
    FILES=PROVS+"CORRY"+CLASS$(I%)*"PNUM.DAT
    OPEN FILES FOR INPUT AS #1
    INPUT #1,NumOfCompounds
    CLOSE #1
    . Next will draw screen for each class.
    GOSUB DrawCmpdScreen
    GOSUB PageOfNames
    BKGND%=0 : GOSUB MarkCompoundName
    Startloop%
    AS=INKEY$
    SELECT CASE AS
      CASE " "
        GOTO StartOfProgram
      CASE CHR$(13)
        GOTO Continue%
      CASE "O"
        GOTO Options
      CASE ""
        FOR J%=1 TO NumOfCompounds
          CUSE%(I%,J%)=1
        NEXT J%
        GOSUB PageOfNames
        BKGND%=0 : GOSUB MarkCompoundName
      CASE "*"
        FOR J%=1 TO NumOfCompounds
          CUSE%(I%,J%)=0
        NEXT J%
    . no key
    . quit
    . return
    . options
    . mark all
    . unmark all

```

```

LOCATE 6,9 : PRINT "Class: ";
LOCATE 6,32 : PRINT "Number of Compounds: ";
LOCATE 6,66 : PRINT "Page: ";
COLOR 11,1 : LOCATE 6,16 : PRINT CLASS$(I%);
COLOR 11,1 : LOCATE 6,53 : PRINT USING "###"NumOfCompounds;
COLOR 12,1 : LOCATE 6,71 : PRINT USING "###"CPAGE%(I%);
. Next is header/footer information.
COLOR 10,0
LOCATE 3,16 : PRINT "Please indicate the compounds to use in this run.";
COLOR 3,0
LOCATE 20,6 : PRINT "Press <*> to mark all, <-> to unmark all, ";
PRINT "<SPACE> to toggle mark.";
LOCATE 21,10 : PRINT "<ARROW KEYS> to move cursor, <PG UP><PG DN> ";
PRINT "to change pages.";
LOCATE 22,6 : PRINT "<H> to hardcopy, <P> to form feed, ";
PRINT "<RETURN> to continue, <Q> to quit.";
RETURN

```

PageOfNames:

This is the subroutine to draw a page of compound names.

```

FOR J%=CPAGE%(I%)-1*100+1 TO CPAGE%(I%)*100
  IF J%<=NumOfCompounds THEN
    TEMP%=INT((J%-(CPAGE%(I%)-1)*100-1)/10)
    LOCATE (J%-(CPAGE%(I%)-1)*100-TEMP%*7+5
    CNAMES="C"+RIGHT$(STR$(J%),LEN(STR$(J%))-1)
    IF CUSE%(I%,J%)=1 THEN
      COLOR 10,1
      PRINT " ",CHR$(19),CNAMES$,SPACES$(3-LEN(CNAMES));
    ELSE
      COLOR 15,1
      PRINT " ",CNAMES$,SPACES$(3-LEN(CNAMES));
    END IF
  ELSE
    COLOR 15,1
    TEMP%=INT((J%-(CPAGE%(I%)-1)*100-1)/10)
    LOCATE (J%-(CPAGE%(I%)-1)*100-TEMP%*7+5
    PRINT SPACES(7);
  END IF
NEXT J%
RETURN

```

MarkCompoundName:

This is the subroutine to mark a compound name.

```

IF CPAGE%(I%)=INT((OPTN3%(I%)-1)/100)+1 THEN

```

```

NEXT J%
GOSUB PageOfNames
BKGNDF%=0 : GOSUB MarkCompoundName
CASE *
  BKGNDF%=1 : GOSUB MarkCompoundName
  TEMP%=CUSE%(I%OPTN3%(I%))
  IF TEMP%=1 THEN TEMP%=0 ELSE TEMP%=1
  CUSE%(I%OPTN3%(I%))=TEMP%
  BKGNDF%=0 : GOSUB MarkCompoundName
  CASE CHR$(0)+CHR$(72), CHR$(0)+CHR$(80)
  BKGNDF%=1 : GOSUB MarkCompoundName
  IF AS=CHR$(0)+CHR$(72) THEN DECR OPTN3%(I%) ELSE INCR OPTN3%(I%)
  TEMP1%=(CPAGE%(I%)-1)*100 + 1
  TEMP2%=(CPAGE%(I%)) *100
  IF OPTN3%(I%)<TEMP1% THEN OPTN3%(I%)=TEMP2%
  IF OPTN3%(I%)>TEMP2% THEN OPTN3%(I%)=TEMP1%
  BKGNDF%=0 : GOSUB MarkCompoundName
  CASE CHR$(0)+CHR$(73), CHR$(0)+CHR$(81)
  IF CPAGE%(I%)=1 THEN
    CPAGE%(I%)=2 : INCR OPTN3%(I%),100
  ELSE
    CPAGE%(I%)=1 : DECR OPTN3%(I%),100
  END IF
  COLOR 12,1 : LOCATE 6,71 : PRINT USING "#.#;CPAGE%(I%);
GOSUB PageOfNames
BKGNDF%=0 : GOSUB MarkCompoundName
CASE "t", "h"
  LPRINT "Summary of compounds not used: ",DATE$
  LPRINT "      Class being searched: ",CLASS$(CLASS%)
  LPRINT "      Property being searched: ",PROP$(PROP%)
  LPRINT "      Number of Compounds: ",NumOfCompounds
  FOR I%=1 TO NumOfCompounds
    IF CUSE%(CLASS%(I%))=0 THEN
      CHAMES="C"+RIGHT$(STR$(I%),LEN(STR$(I%))-1)
      LPRINT CHAMES,
    END IF
  NEXT I%
  LPRINT : LPRINT
CASE "1","2","3"
  COLOR 31,4
  LOCATE 23,25 : PRINT " Press <*> ON, or <-> for OFF ";
  TEMPS=INPUT$(1)
  SELECT CASE TEMPS
  CASE CHR$(27),"Q","q"
    COLOR 15,0
    LOCATE 23,25 : PRINT SPACES(30);
    GOTO StartOfProgram
  CASE *
    CASE ELSE
      SOUND 1000,3 : SOUND 800,1.5
      GOTO Startloop8
  END SELECT
  SELECT CASE AS
  CASE "1" : TEMP1%=1 : TEMP2%=20
  CASE "2" : TEMP1%=21 : TEMP2%=40
  CASE "3" : TEMP1%=41 : TEMP2%=100
  END SELECT
  FOR J%=TEMP1% TO TEMP2%
  IF J%<=NumOfCompounds THEN
    IF TEMPS="" THEN CUSE%(I%,J%)=1 ELSE CUSE%(I%,J%)=0

```

```

END IF
NEXT J%
GOSUB PageOfNames
COLOR 15,0
LOCATE 23,25 : PRINT SPACES(30);
BKGNDF%=0 : GOSUB MarkCompoundName
CASE "1","p"
  LPRINT CHR$(12)
  CASE ELSE
    SOUND 1000,3 : SOUND 800,1.5
  END SELECT
  GOTO Startloop8
Continue:
END IF
NEXT I%
RETURN

```

GetFractionsToUse:

This is the subroutine to get the fractions to use for fuels.

```

Options box
SCREEN 0 : WIDTH 80
COLOR 15,0 : CLS
COLOR 10,1
LOCATE 7,15 : PRINT CHR$(210),STRINGS(40,100),CHR$(191); ' top line
FOR I%=8 TO 18
  LOCATE I%,15 : PRINT CHR$(179),TAB(65),CHR$(179); ' middle
NEXT I%
LOCATE 17,15 : PRINT CHR$(192),STRINGS(40,100),CHR$(217); ' bottom line
COLOR 10,0
LOCATE 6,15 : PRINT TIMES;
LOCATE 6,56 : PRINT DATES;
COLOR 12,1
LOCATE 9,20 : PRINT "Please mark the fractions of fuels to use";
GOSUB PrintFractions
Next are commands
COLOR 3,0
LOCATE 21,17 : PRINT " Press <SPACE> to toggle the mark ";
LOCATE 22,17 : PRINT "Press <RET> to continue, <O> for options menu.";
Next see what to do.
BKGNDF%=0 : GOSUB MarkFraction
Startloop8
AS=INKEY$
SELECT CASE AS
CASE *
  COLOR 10,0 : LOCATE 6,15 : PRINT TIMES;
  GOTO Startloop8
CASE CHR$(13)
  RETURN
CASE "Q","q",CHR$(27)
  exit

```

```

GOTO StartOfProgram
CASE 'O', 'o'
  GOTO Options
CASE '*'
  FOR I%=1 TO 5
    FRACTION%(I%)=1
  NEXT I%
  GOSUB PrintFractions
  BKGND%=0 : GOSUB MarkFraction
CASE '.'
  FOR I%=1 TO 5
    FRACTION%(I%)=0
  NEXT I%
  GOSUB PrintFractions
  BKGND%=0 : GOSUB MarkFraction
CASE '!'
  BKGND%=1 : GOSUB MarkFraction
  TEMP%=FRACTION%(OPTN5%)
  IF TEMP%=1 THEN TEMP%=0 ELSE TEMP%=1
  FRACTION%(OPTN5%)=TEMP%
  BKGND%=0 : GOSUB MarkFraction
CASE 'R'+'(0)+'CHR$(72), CHR$(60)+'CHR$(60)
  BKGND%=1 : GOSUB MarkFraction
  IF AS=CHR$(0)+'CHR$(72) THEN DECOR OPTN5% ELSE INCR OPTN5%
  IF OPTN5%<1 THEN OPTN5%=5
  IF OPTN5%>5 THEN OPTN5%=1
  BKGND%=0 : GOSUB MarkFraction
CASE ELSE
  SOUND 1000,3 : SOUND 800,1.5
END SELECT
GOTO Startboop9
PrintFractions:
  * This is a mini-subroutine to draw a page of fuel class names.
  FOR I%=1 TO 5
    LOCATE 10+I%,34
    COLOR 14,1 : PRINT USING '#)' I%;
    IF FRACTION%(I%)=0 THEN
      COLOR 15,1 : PRINT '* ',FRACTIONS(I%);
    ELSE
      COLOR 10,1 : PRINT CHR$(16);FRACTIONS(I%);
    END IF
  NEXT I%
  RETURN
MarkFraction:
  * This is a mini-subroutine to mark a fuel class for use.
  LOCATE 10+OPTN5%,37
  IF FRACTION%(OPTN5%)=0 THEN
    COLOR 15,BKGND% : PRINT '* ',FRACTIONS(OPTN5%);
  ELSE
    COLOR 10,BKGND% : PRINT '* ',CHR$(16);FRACTIONS(OPTN5%);
  END IF
  RETURN
ReadConfigFile:
  * Will write message to the user.
  COLOR 0,3
  LOCATE 10,20 : PRINT CHR$(201);STRINGS$(30,205);CHR$(187);
  FOR I%=11 TO 13
    LOCATE I%,20 : PRINT CHR$(186);TAB(60);CHR$(186);
  NEXT I%
  LOCATE 14,20 : PRINT CHR$(200);STRINGS$(30,205);CHR$(189);
  COLOR 4,3
  LOCATE 12,28 : PRINT "Reading the "; COLOR 14,3 : PRINT "Config File";
  * Must next read the file.
  OPEN CFGDIR$+"CORRCFG.DAT" FOR INPUT AS #4
  INPUT #4, ODIR$
  INPUT #4, OFILES$
  INPUT #4, HOOPY$
  INPUT #4, RMDISK$
  INPUT #4, CLASS$
  INPUT #4, PROP%
  INPUT #4, OPTN%
  INPUT #4, OPTN2%
  INPUT #4, OPTN4%
  INPUT #4, OPTN5%
  INPUT #4, OPTN6%
  INPUT #4, OPTN7%
  INPUT #4, OPTN8%
  INPUT #4, OPTN9%
  FOR KKK%=1 TO 9 : INPUT #4, OPTN3%(KKK%) : NEXT KKK%
  FOR KKK%=1 TO 9 : INPUT #4, CPAGE$(KKK%) : NEXT KKK%
  FOR KKK%=1 TO 10 : INPUT #4, CUSE$(KKK%) : NEXT KKK%
  FOR KKK%=1 TO 5 : INPUT #4, FUELCLASS$(KKK%) : NEXT KKK%
  FOR KKK%=1 TO 5 : INPUT #4, FRACTION%(KKK%) : NEXT KKK%
  WHILE NOT EOF(4)
    INPUT #4,TEMP1%
    INPUT #4,TEMP2%
    CUSE%(TEMP1%,TEMP2%)=0
  WEND
  CLOSE #4
  RETURN
WriteConfigFile:
  * This is the subroutine to write the config file.

```

This is the subroutine to read the config file.

This is the subroutine to write the config file.

OPEN CFGDIR\$+"CORRCFG.DAT" FOR OUTPUT AS #4

```

OPEN CFGDIRS+'FUELPARM.DAT' FOR RANDOM AS #5 LEN=728
FIELD #5, 25 AS SS, 25 AS IS, 25 AS OS, 25 AS FS, 25 AS TS(1),
25 AS TS(2), 25 AS TS(3), 25 AS TS(4), 25 AS TS(5), 25 AS TS(6),
25 AS TS(7), 25 AS TS(8), 25 AS TS(9), 25 AS TS(10), 25 AS TS(11),
25 AS TS(12), 25 AS TS(13), 25 AS TS(14), 25 AS TS(15), 25 AS TS(16),
25 AS TS(17), 25 AS TS(18), 25 AS TS(19), 25 AS TS(20), 25 AS TS(21),
25 AS TS(22)
LSET SS=STR$(SLOPEFACTOR)
LSET IS=STR$(INTCPFACTOR)
LSET OS=STR$(OFFSETPACTR)
LSET FS=FUNCTIONS
FOR J% = 1 TO 22
    LSET TS(J%) = STR$(MIXCOEFF(J%))
NEXT J%
PUT 5, PROP%
CLOSE #5
RETURN

```

CheckForError:



```

IF COUNTER%-1=0 THEN GOTO GoAntError
FOR I%=1 TO VAR%
    SUM=0
    FOR J%=1 TO COUNTER%-1
        INCR SUM, INPU(J%, I%)
    NEXT J%
    IF SUM<0.00001 THEN TEMP%=I% : GOTO GoAntError
NEXT I%
RETURN
GoAntError:
COLOR 15,0 : CLS
COLOR 10,1
LOCATE 9,10 : PRINT CHR$(218);STRINGS$(59,108);CHR$(191); ' top line
FOR I%=10 TO 14
    LOCATE I%,10 : PRINT CHR$(179);TAB(70);CHR$(179); ' middle
NEXT I%
LOCATE 15,10 : PRINT CHR$(192);STRINGS$(59,108);CHR$(217); ' bottom line
COLOR 26,1
LOCATE 11,31 : PRINT *** WARNING ***;
COLOR 14,1
LOCATE 13,18 : PRINT 'Column is empty! Regression will crash!';
COLOR 15,1 : LOCATE 13,25 : PRINT USING '@#';TEMP%;

```

```

' Next ate commands
COLOR 3,0
LOCATE 22,17 : PRINT 'Press <RET> to continue, <O> for options menu';
AS=INPUT$(1)
IF AS='O' OR AS='o' THEN GOTO Options
GOTO StartOfProgram

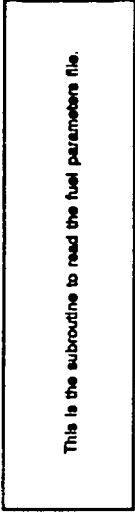
```

```

PRINT #4, ODIRS
PRINT #4, OFILES
PRINT #4, HOOPYE
PRINT #4, RMDISIG
PRINT #4, CLASS%
PRINT #4, PROP%
PRINT #4, OPTN%
PRINT #4, OPTN2%
PRINT #4, OPTN4%
PRINT #4, OPTN5%
PRINT #4, OPTN6%
PRINT #4, OPTN7%
PRINT #4, OPTN8%
PRINT #4, OPTN9%
FOR KKK%=1 TO 9 : PRINT #4, ORPT3%(KKK%) : NEXT KKK%
FOR KKK%=1 TO 9 : PRINT #4, CPAGE%(KKK%) : NEXT KKK%
FOR KKK%=1 TO 10 : PRINT #4, CUSER%(KKK%) : NEXT KKK%
FOR KKK%=1 TO 5 : PRINT #4, FUELCASS%(KKK%) : NEXT KKK%
FOR KKK%=1 TO 5 : PRINT #4, FRACTION%(KKK%) : NEXT KKK%
FOR KKK%=1 TO 9
    FOR JJ%=1 TO 200
        IF CUSER%(KKK%, JJ%)=0 THEN PRINT #4, KKK%, ' ; JJ%;
    NEXT JJ%
NEXT KKK%
CLOSE #4
RETURN

```

ReadFuelParams:

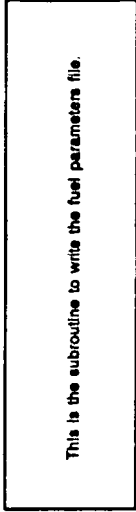


```

OPEN CFGDIRS+'FUELPARM.DAT' FOR RANDOM AS #5 LEN=728
FIELD #5, 25 AS SS, 25 AS IS, 25 AS OS, 25 AS FS, 25 AS TS(1),
25 AS TS(2), 25 AS TS(3), 25 AS TS(4), 25 AS TS(5), 25 AS TS(6),
25 AS TS(7), 25 AS TS(8), 25 AS TS(9), 25 AS TS(10), 25 AS TS(11),
25 AS TS(12), 25 AS TS(13), 25 AS TS(14), 25 AS TS(15), 25 AS TS(16),
25 AS TS(17), 25 AS TS(18), 25 AS TS(19), 25 AS TS(20), 25 AS TS(21),
25 AS TS(22)
GET 5, PROP%
SLOPEFACTOR=VAL$(S) : INTCPFACTOR=VAL$(I)
OFFSETPACTR=VAL$(O) : FUNCTIONS=FS
FOR J%=1 TO 22
    MIXCOEFF(J%)=VAL$(TS(J%))
NEXT J%
CLOSE #5
RETURN

```

WriteFuelParams:



```

This is the subroutine to write the fuel parameters file.

```

GetFuelParams:

This is the subroutine to get mixing coeff parameters.

```

* Options box
COLOR 15,0 : CLS
COLOR 10,1
LOCATE 7,15 : PRINT CHR$(219);STRING$(49,196);CHR$(191); ' top line
FOR I%=8 TO 16
    LOCATE I%,15 : PRINT CHR$(179);TAB(65);CHR$(179); ' middle
NEXT I%
LOCATE 17,15 : PRINT CHR$(182);STRING$(49,196);CHR$(217); ' bottom line
COLOR 10,0
LOCATE 6,15 : PRINT TIMES;
LOCATE 6,56 : PRINT DATES;
COLOR 12,1
LOCATE 9,19 : PRINT "Please make any changes that are necessary";
COLOR 14,1
LOCATE 11,27 : PRINT "Slope";
LOCATE 12,27 : PRINT "Intcp";
LOCATE 13,27 : PRINT "Offset";
LOCATE 14,27 : PRINT "f(q)";
COLOR 15,1
LOCATE 11,37 : PRINT SLOPEFACTOR;
LOCATE 12,37 : PRINT INTCPFACTOR;
LOCATE 13,37 : PRINT OFFSETFACTR;
LOCATE 14,37 : PRINT FUNCTIONS;

```

```

* Next are commands.
COLOR 3,0
LOCATE 22,17 : PRINT "Press <RET> to continue, <O> for options menu";
* Next see what to do.
BKGND%=0 : GOSUB MainFuelParam
Startloop12:
AS=INKEY$
SELECT CASE AS
CASE "=" ' no key
    COLOR 10,0 : LOCATE 6,15 : PRINT TIMES;
    GOTO Startloop12
CASE CHR$(13) ' return
    RETURN
CASE "O", "o" CHR$(27) ' exit
    GOTO StartOfProgram
CASE "O", "o" ' options
    GOTO Options
CASE CHR$(0)+CHR$(72), CHR$(0)+CHR$(80) ' up-down
    BKGND%=1 : GOSUB MainFuelParam
    IF AS=CHR$(0)+CHR$(72) THEN DECR OPTN% ELSE INCR OPTN%
    IF OPTN%<1 THEN OPTN%=4
    IF OPTN%>4 THEN OPTN%=1
    BKGND%=0 : GOSUB MainFuelParam
CASE ELSE
    ' edit

```

```

COLOR 15,1
LOCATE 10+OPTN%,35 : PRINT SPACES(26);
LOCATE 10+OPTN%,37 : PRINT AS; : LINE INPUT TEMPS
SELECT CASE OPTN%
CASE 1 : SLOPEFACTOR=VAL(AS+TEMPS)
CASE 2 : INTCPFACTOR=VAL(AS+TEMPS)
CASE 3 : OFFSETFACTR=VAL(AS+TEMPS)
CASE 4 : FUNCTIONS=AS+TEMPS
END SELECT
BKGND%=0 : GOSUB MainFuelParam
END SELECT
GOTO Startloop12
MainFuelParam:
* This is a mini-subroutine to mark a fuel class for use.
LOCATE 10+OPTN%,35
COLOR 15,BKGND%
SELECT CASE OPTN%
CASE 1 : PRINT " : SLOPEFACTOR";
CASE 2 : PRINT " : INTCPFACTOR";
CASE 3 : PRINT " : OFFSETFACTR";
CASE 4 : PRINT " : FUNCTIONS";
END SELECT
RETURN

```

GetCetLevel:

This is the subroutine to get the cetane improver level.

```

* Options box
SCREEN 0 : WIDTH 80
COLOR 15,0 : CLS
COLOR 10,1
LOCATE 7,15 : PRINT CHR$(219);STRING$(49,196);CHR$(191); ' top line
FOR I%=8 TO 16
    LOCATE I%,15 : PRINT CHR$(179);TAB(65);CHR$(179); ' middle
NEXT I%
LOCATE 17,15 : PRINT CHR$(182);STRING$(49,196);CHR$(217); ' bottom line
COLOR 10,0
LOCATE 6,15 : PRINT TIMES;
LOCATE 6,56 : PRINT DATES;
COLOR 14,1
LOCATE 9,23 : PRINT "Please Enter the Improver level for";
LOCATE 10,29 : PRINT "the Cetane Calculations";
COLOR 12,1
LOCATE 15,27 : PRINT "<NUL> = all improver levels";
* Next will get level
COLOR 15,1
LOCATE 13,38 : LINE INPUT CETLEVEL$
IF CETLEVEL$<>="" THEN
    WHILE LEN(CETLEVEL$)<8

```


RETURN

Log: \$INCLUDE "LOGO.BAS"

T-T-T:Thats all folks!!!

Listing for Program II.3: CORR5.BAS

This is the correlation program. It will open the data files from the LC-NMR pgm, getting both the integration data and the average structure data which are contained in the files under the compound or fuel name. It will also access the physical property files. Once the information has been read, it then calculates the physical property (ie, cetane #) for the desired compounds or fuels and places the data into the output file as well giving hardcopy when desired. The pgm then jumps to a shortened version of the graphing program to display the results graphically. The order of data in the graph file is as follows:

- line name - title 1 - title 2 - x label - y label
- 1) observed property 2) calculated property
- 3) use toggle function 4) compound number
- 5) compound name 6) point number

Program Name: CORR5.BAS Ver 5.10 Date Written: 06/03/1988
 Author: Allen Caswell Date Modified: 07/10/1988

First is the section to set up the variables.

```

* First are default parameters for program.
COMMON ODIR$,OFILES
ON KEY(1) GOSUB WriteConfigFile
KEY(1) ON
KEY(2) GOSUB WriteFuelParams
KEY(2) ON
PRDRV$="D": LCDRV$="D": HCOPT$="N": RMDOS$="N"
SCALE$="Y": FITCONS="Y": STAT$="Y": SIND$="N"
CLASS%=1: PROP%=4: GOPTN%=1: PAGE%=1
OPTN2%=1: X%=350: Y%=240: OPTN4%=1
OPTN5%=1: OPTN6%=1: OPTN7%=1
VERNS$="Ver 5.00": CFGDIR$="D:\CORR5\PGMSY"
IF ODIR$="" THEN ODIR$="D:\CORR5\RESULT"
IF OFILES="" THEN OFILES="TEST.DAT"
ACTIVES="Class"
PP$="#####"

* Next will dimension the necessary matrices
DIM FRACTIONS(5), MINCOEFF(21), PROP$(42), OD(350), DS(42)
DIM FUELCLASS$(5), FRACTION$(5), CUSE$(10), ODS(350), R(500)
DIM FUELCLASS$(5), VARNAME$(21), CPAGE%(10), OBS(500), TS(22)
DIM MIXCOEFF(22), MAXCOEFF(21), OPTN3%(10), PROF(21), ZS(10)
DIM POINTE%(100), PIX%(2820), CALC(600)
DIM AVGCoeff(21), CLASS$(10), DIFF(500)
DIM CUSE%(10,200), USE%(500)

* Next are names for classes of compounds.
DATA "ALKANE", "ALKENE", "MODELIX", "CYCLOHEX", "DECALIN"
DATA "MONO", "DICYCLIC", "TETRALIN", "FUEL"
FOR I%=1 TO 6: READ CLASS$(I%): NEXT I%

```

```

Startloop.
AS=INKEY$
SELECT CASE AS
CASE =
    COLOR 0,7
    LOCATE 23,4 : PRINT TIME$;
    GOTO Startloop
CASE CHRS(13)
    GOTO GetData
CASE "0","0","0","0","0","0","0","0","0","0"
    GOTO Options
CASE "P","P"
    LPRINT CHRS(12)
    GOTO Startloop
CASE "G","G"
    COLOR 15,0 : CLS
    GOTO Graph
CASE "B","B"
    GOTO BarGraphAndPieChart
CASE "E","E"
    GOTO Statistics
CASE "H","H"
    IF HCOOPY$="Y" THEN HCOOPY$="N" ELSE HCOOPY$="Y"
    IF RMDSK$="Y" THEN RMDSK$="N" ELSE RMDSK$="Y"
    COLOR 0,7 : LOCATE 18,7 : PRINT HCOOPY$;
    GOTO Startloop
CASE "R","R"
    IF RMDSK$="Y" THEN RMDSK$="N" ELSE RMDSK$="Y"
    COLOR 10,0 : LOCATE 25,3
    PRINT "Sound = "SND$;
    IF SND$="Y" THEN SOUND 800,2 ELSE SOUND 300,4
    DELAY 0.5
    COLOR 15,0 : LOCATE 25,3
    PRINT SPACES(15);
    GOTO Startloop
CASE "D","D"
    COLOR 31,8
    LOCATE 23,20 : PRINT "Directory?";
    COLOR 14,6
    LOCATE 23,32 : PRINT SPACES(21);
    LOCATE 23,32 : LINE INPUT TEMPS
    IF TEMPS<>" " THEN ODIRS=UCASE$(TEMPS)+1
    LOCATE 23,32 : PRINT SPACES(21);
    LOCATE 23,32 : PRINT ODIRS
    LOCATE 23,20 : COLOR 12,6 : PRINT "D";
    COLOR 15,6 : PRINT "Directory?";
    GOTO Startloop
CASE "F","F"
    COLOR 31,8
    LOCATE 23,56 : PRINT "File?";
    COLOR 14,6
    LOCATE 23,62 : PRINT SPACES(13);
    LOCATE 23,62 : LINE INPUT TEMPS
    IF TEMPS<>" " THEN OFILES=TEMPS
    LOCATE 23,62 : PRINT SPACES(13);
    LOCATE 23,62 : PRINT OFILES;
    LOCATE 23,56 : COLOR 12,6 : PRINT "F";

```

```

* Next are names of properties to match.
DATA "Name","Formula","Mol Wt","Cetane #","BP - 50%","Pour Pt."
DATA "Improv'n"
DATA "Flash Pt." : Density,"Ref Indx","Cloud Pt","Viscoat","Filler"
DATA "Class"
DATA "Ag Dg Br","Sp. Disp","Surf Tnt","Aniline","Cr Press","Cr Temp"
DATA "Crt Vol"
DATA "Heat Cap","Ht Vapor","Ht. Form","Free E F","Ht. Comb","Mol Vol"
DATA "% Atom"
DATA "% Olefin","FuelType","Cat Indr","Sp. Grav","BP - IBP","BP - 10%"
DATA "BP - End","C Reakt"
DATA
FOR I%=1 TO 42 : READ PROP$(I%) : NEXT I%

* Next are options for end of program.
DATA "Edit to DOS","Run GRAF-ED"
DATA "Run ERROR","Run GRAPH","Run EZ_PLOT","Restart"
FOR I%=1 TO 8 : READ OPTN$(I%) : NEXT I%

* Next are names for fuel classes.
DATA "Al","JP-5","JP-8","DF-2"
FOR I%=1 TO 5 : READ FUELCLASS$(I%) : NEXT I%

* Next are names of fuel fractions.
DATA "Alkane","Monocyclic","Dicyclic","Flourene"
DATA "Phenanthrene"
FOR I%=1 TO 5 : READ FRACTION$(I%) : NEXT I%

* Next are names for mixing coeff variables.
DATA "b(0)"
DATA "Xch3","Xch2","Xch"
DATA "Cun","Cch3","Cch2","Cch","Ccat","Cch2>"
DATA "Cun","Cch3","Cch2","Cch2>"
DATA "Cun","Cch3","Cch2","Cch2>"
DATA "Cun","Cch3","Cch2","Cch2>"
FOR I%=0 TO 21 : READ VARNAME$(I%) : NEXT I%

* Must set up the class use options.
FOR I%=1 TO 10 : CUSE$(I%)="Y" : NEXT I%
FOR I%=1 TO 10
    CPAGE$(I%)=1 : OPTN3$(I%)=1
    FOR J%=1 TO 200 : CUSE$(I%,J%)=1 : NEXT J%
NEXT I%
FOR I%=1 TO 5 : FUELCLASS$(I%)=0 : NEXT I%
GOSUB ReadConfigFile

StartOfProgram:

```

The next order of business is get class and property to sort by.

First are Compound, Hardcopy, and Time Boxes.
GOSUB DrawMainMenuScreen


```

COLOR 14, 0 : LOCATE ROW%+6,COL%*13 + 38
PRINT " :PROPS(PROP%);" ;
GOTO Startloop
END IF
CASE ELSE
SOUND 1000,3 : SOUND 800,1,5
GOTO Startloop
END SELECT

```

GetData:

Next will get the information out of the files.

```

* First see if did not select any classes.
I%=1
DO UNTIL CUSE$(I%)="Y" OR I%=10
  INCR I%
LOOP
IF I%>=10 THEN GOTO Youdidit

* Will next get the various operating parameters.
GOSUB GetCompoundUse
IF CUSE$(0)="Y" THEN
  GOSUB GetFuelType
  GOSUB GetReactionsToUse
  GOSUB ReadFuelParams
  GOSUB GetFuelParams
  IF PROP%=4 THEN GOSUB GetCetLevel
  GOSUB DisplayMixCoef
END IF
GOSUB SetUpScreenAndPrinter
COUNT%=1
FOR I%=0 TO 21
  AVGCoeff(I%)=0 : MINCOEFF(I%)=0 : MAXCOEFF(I%)=0
  AS=INKEY$
NEXT I%
RunTime=TIMER

* Will start loop to get all data.
FOR I%=1 TO 10
  AS=INKEY$
  IF AS=CHR$(27) OR AS="Q" OR AS="q" THEN GOTO ExitLoop
  IF CUSE$(I%)="Y" THEN
    GOSUB GetNumberOfCompounds

* Next is loop for compounds in class.
FOR J%=1 TO NumOfCompounds
  COLOR 0,15
  LOCATE 1,43 : PRINT USING "###,J%";
  COLOR 12, 0
  LOCATE 3,71 : PRINT USING "###.###";TIMER-RunTime;
  AS=INKEY$
  IF AS=CHR$(27) OR AS="Q" OR AS="q" THEN GOTO ExitLoop
  * print timer
  * early exit
  * class loop
  * Init counter
  * Init ranges
  * flush buffer
  * Init timer
  * get compounds
  * fuel class
  * fuel fractn
  * fuel params
  * read params
  * fuel mix coef
  * Cetane Impv
  * Initialize
  * Init counter
  * Init ranges
  * flush buffer
  * Init timer
  * class loop
  * early exit
  * print pass #
  * cmpd loop
  * print timer
  * early exit
  IF AS=CHR$(27) OR AS="Q" OR AS="q" THEN GOTO ExitLoop

```

```

COLOR 15, 0 : PRINT "le";
GOTO Startloop
CASE **
  * mark-unmark
  IF CUSE$(CLASS%)="N" THEN
    COLOR 12,0 : LOCATE CLASS%+8,19
    PRINT " :CHR$(16),CLASS$(CLASS%);" ;
  ELSE
    COLOR 14,0 : LOCATE CLASS%+8,19
    PRINT " :CLASS$(CLASS%);" ;
  END IF
GOTO Startloop
CASE CHR$(0)+CHR$(72),CHR$(0)+CHR$(77)
  IF ACTIVE="Class" THEN
    COLOR 15, 1 : LOCATE 5, 21 : PRINT ACTIVE;
    ACTIVE="Property"
  COLOR 15, 5 : LOCATE 5, 52 : PRINT ACTIVE;
  GOTO Startloop
END IF
IF ACTIVE="Property" THEN
  COLOR 15, 1 : LOCATE 5, 52 : PRINT ACTIVE;
  ACTIVE="Class"
  COLOR 15, 5 : LOCATE 5, 21 : PRINT ACTIVE;
  GOTO Startloop
END IF
CASE CHR$(0)+CHR$(72), CHR$(0)+CHR$(80)
  IF ACTIVE="Class" THEN
    IF CUSE$(CLASS%)="N" THEN
      COLOR 15, 1 : LOCATE CLASS%+8,19
      PRINT " :CLASS$(CLASS%);" ;
    ELSE
      COLOR 10,1 : LOCATE CLASS%+8,19
      PRINT " :CHR$(16),CLASS$(CLASS%);" ;
    END IF
  IF AS=CHR$(0)+CHR$(72) THEN DECR CLASS% ELSE INCR CLASS%
  IF CLASS%<1 THEN CLASS%=0
  IF CLASS%>9 THEN CLASS%=1
  IF CUSE$(CLASS%)="N" THEN
    COLOR 14, 0 : LOCATE CLASS%+8,19
    PRINT " :CLASS$(CLASS%);" ;
  ELSE
    COLOR 12,0 : LOCATE CLASS%+8,19
    PRINT " :CHR$(16),CLASS$(CLASS%);" ;
  END IF
  FILES=PROPV%+100RRY+CLASS$(CLASS%)+1PNUM.DAT
  OPEN FILES FOR INPUT AS #1
  INPUT #1,NumOfCompounds
  CLOSE #1
  COLOR 0,7 : LOCATE 13, 0 : PRINT USING "###";NumOfCompounds;
  GOTO Startloop
END IF
IF ACTIVE="Property" THEN
  COLOR %=INT((PROP%-1)/14) : ROW%=PROP% - (COL%*14)
  COLOR 15, 1 : LOCATE ROW%+6,COL%*13 + 38
  PRINT " :PROPS(PROP%);" ;
  IF AS=CHR$(0)+CHR$(72) THEN DECR PROP% ELSE INCR PROP%
  IF PROP%<1 THEN PROP%=42
  IF PROP%>42 THEN PROP%=1
  COLOR %=INT((PROP%-1)/14) : ROW%=PROP% - (COL%*14)

```

```

* Will first see if compound use is on or not
FOR K%=1 TO 42 : D6(K%)=" : NEXT K%
IF GUSE%(K,J%)=1 THEN
  GOSUB GetPropData
  Proceeds="NO"
* Have got prop data so see if classes match and data not empty.
IF D6(14)=CLASS$(K%) AND D6(PROP%)<>" * THEN Proceeds="YES"
* If doing fuels, must match class type and cetane improver.
IF I%=9 AND Proceeds="YES" THEN
  Proceeds="NO"
  * doing fuels
IF FUELCLASS%(I)=1 THEN
  Proceeds="YES"
  * match class
ELSE
  Proceeds="YES"
  * all classes
FOR K%=2 TO 5
  IF FUELCLASS%(K%)=1 AND FUELCLASS$(K%)=D6(30) THEN
    Proceeds="YES"
  END IF
NEXT K%
END IF
IF PROP%=4 AND Proceeds="YES" THEN
  Proceeds="NO"
SELECT CASE CETLEVELS
CASE " : Proceeds="YES"
CASE D6(7) : Proceeds="YES"
END SELECT
END IF
IF Proceeds="YES" THEN
* Found a match, so get integration data and do corr.
* Will first get integration data.
CNAME$="C"+RIGHT$(STR$(J%),LEN$(STR$(J%))-1)
SELECT CASE RMDIS$(
CASE "N"
  CNUM$=LCORV$+ACORR'+CLASSES%(K%)+I"
  CNUM$=CNUM$+CNAME$+"DAT"
CASE "P"
  CNUM$="F"+CNAME$+"DAT"
END SELECT
OPEN CNAME$ FOR INPUT AS #1
K%=1
WHILE NOT EOF(1) AND OD6(K%)<>"END" AND K%<350
  INPUT #1,OD6(K%)
  IF OD6(K%)="?????" THEN OD6(K%)="0"
  IF OD6(K%)="+.+++++" THEN OD6(K%)="0"
  INCR K%
WEND
CLOSE #1
Num=K%-1
FOR K%=3 TO 140 : OD(K%)=VAL(OD6(K%)) : NEXT K%
FOR K%=148 TO Num : OD(K%)=VAL(OD6(K%)) : NEXT K%
* Have got data, so put into variables and do corr.
OBS(COUNT%)=VAL(D$(PROP%))
SMPLNUM$=D$(I)
SMPLNUM$=CNAME$

```

* Have got data so will do calc - in subroutines

```

SELECT CASE PROP%
CASE 4 : GOSUB Cetane
CASE 5 : GOSUB BoilingPoint
CASE 6 : GOSUB PourPoint
CASE 8 : GOSUB FlashPoint
CASE 9 : GOSUB Density
CASE 10 : GOSUB RefractiveIndex
CASE 11 : GOSUB CloudPoint
CASE 12 : GOSUB Viscosity
CASE 13 : GOSUB Filterability
CASE 18 : GOSUB SpecificDispersion
CASE 17 : GOSUB SurfaceTension
CASE 18 : GOSUB AnilinePoint
CASE 19 : GOSUB CriticalPressure
CASE 20 : GOSUB CriticalTemperature
CASE 21 : GOSUB CriticalVolume
CASE 22 : GOSUB HeatCapacity
CASE 23 : GOSUB HeatOfVaporization
CASE 24 : GOSUB HeatOfFormation
CASE 25 : GOSUB FreeEnergyOfFormation
CASE 28 : GOSUB HeatOfCombustion
CASE 27 : GOSUB MolecularVolume
CASE 28 : GOSUB Aromatics
CASE 29 : GOSUB Olefins
CASE 31 : GOSUB CetaneIndex
CASE 32 : GOSUB SpecificGravity
CASE 33 : GOSUB InitialBoilPoint
CASE 34 : GOSUB BoilingPointTenPercent
CASE 35 : GOSUB BoilingPointLineyPercent
CASE 36 : GOSUB BoilingPointEndPoint
CASE 37 : GOSUB ResidualCarbon
CASE ELSE
  COLOR 15,4 : CLS
  LOCATE 12,28 : PRINT "*** UNCORRELATABLE PROPERTY ***";
  AS=INPUT$(1)
  CLOSE
  GOTO StartOfProgram
END SELECT
* Will calculated difference between calc and observed
DIFF(COUNT%)=CALC(COUNT%)-OBS(COUNT%)
* Have got data so print, etc.
COLOR 15,0 : LOCATE LINECNT%,1
PRINT USING "##.#":COUNT%;
PRINT TAB(5);SMPLNUM$;TAB(10);
IF VAL(OD$(78))>0.00001 THEN COLOR 10,0 : PRINT "F"; COLOR 15,0
IF VAL(OD$(104))>0.00001 THEN COLOR 12,0 : PRINT "P"; COLOR 15,0
PRINT TAB(13);LEFT$(SMPLNUM$,25);TAB(40);
PRINT USING PP%;OBS(COUNT%);CALC(COUNT%);DIFF(COUNT%);
INCR LINECNT%
IF LINECNT%>25 THEN
  COLOR 15,0
  FOR K%=6 TO 25 : LOCATE K%,1 : PRINT SPACES(80); : NEXT K%
  LINECNT%*=8
END IF
IF HCOPIYS="Y" THEN
  LPRINT USING "###":COUNT%;

```

```

WINDOW (0,0)-(640,480)
C1%=12
C2%=14
C3%=10
C4%=11
C5%=15
LINE (15,222)-(455,222),C1%
LINE (15,84)-(455,381),C1%,B
TEMP%="Distribution of Products"
DRAW "C"+STR$(C2%)+TAO"
GOSUB DrawString
TEMP%="AI Mono Di Fi Ph"
DRAW "C"+STR$(C2%)+TAO"
TEMP%="60 : TEMPY%=478 : TEMP1$="X"
GOSUB DrawString
TEMP%="Product"
DRAW "C"+STR$(C2%)+TAO"
TEMP%="0 : TEMPY%=230 : TEMP1$="Y"
GOSUB DrawString
TEMP1%=C3%
FOR J%=0 TO 21
TEMP%="VARNAMES(J%)"
DRAW "C"+STR$(TEMP1%)+TAO"
TEMP%="(J%+1)*20 : TEMPY%=420 : TEMP1$="Y"
GOSUB DrawString
INCR TEMP1% : IF TEMP1%>15 THEN TEMP1%=10
NEXT J%
FOR K%=1 TO 2
IF K%=1 THEN TEMP%="LEFT$(STR$(1*MAX),5) : TEMPY%=85
IF K%=2 THEN TEMP%="LEFT$(STR$(1*MAX),5) : TEMPY%=400
TEMP%="0 : TEMP1$="Y"
DRAW "C"+STR$(C4%)+TAO"
GOSUB DrawString
NEXT K%
FOR K%=1 TO 4
IF K%=1 THEN TEMP%="Fn : +FUNCTION$ : TEMPY%=420
IF K%=2 THEN TEMP%="Oa : +STR$(OFFSETFAC) : TEMPY%=438
IF K%=3 THEN TEMP%="m : +STR$(SLOPEFACTOR) : TEMPY%=458
IF K%=4 THEN TEMP%="b : +STR$(INTGPFAC) : TEMPY%=474
DRAW "C"+STR$(C4%)+TAO"
TEMP%="484 : TEMP1$="X"
GOSUB DrawString
NEXT K%
FOR K%=1 TO 2
IF K%=1 THEN TEMP%="Property : +PROP$(PROP%) : TEMPY%=35
IF K%=2 THEN TEMP%="Classes : +SCLASS$ : TEMPY%=55
DRAW "C"+STR$(C4%)+TAO"
TEMP%="320 6*LEN(TEMP%) : TEMP1$="X"
GOSUB DrawString
NEXT K%
LINE (35,63)-(35,0),15 : LINE (85,63)-(85,0),15
LINE (215,63)-(215,0),15 : LINE (285,63)-(285,0),15

```

- axis color
- title color
- data color
- scale color
- min and max
- X-axis
- Y-axis
- title

- X-label
- Y-label
- X-scale

- Y-scale

- Labels

- Titles
- dividing
- lines

```

LPRINT TAB(5);SMPLNUM$;TAB(10);
IF VAL(ODS(76))>0.00001 THEN LPRINT "F";
IF VAL(ODS(104))>0.00001 THEN LPRINT "P";
LPRINT TAB(119);LEFT$(SMPLNUM$;25);TAB(40);
LPRINT USING PP%;OBS(COUNT%);CALC(COUNT%);DIFF(COUNT%);
END IF
• Will put results on file for graphics program - or LOTUS.
USE$(COUNT%)=1
TEMP%="STR$(OBS(COUNT%))+STR$(CALC(COUNT%))+";
TEMP%="TEMP%+STR$(OBS(COUNT%))+";
TEMP%="TEMP%+STR$(USE$(COUNT%))+";
TEMP%="TEMP%+CHR$(34)+SMPLNUM$+CHR$(34)+";
TEMP%="TEMP%+CHR$(34)+SMPLNUM$+CHR$(34)+";
TEMP%="TEMP%+STR$(COUNT%)
PRINT #3,TEMP%
• Must increment the counter for number found.
INCR COUNT%
END IF
NEXT J%
NEXT K%
NEXT L%
NEXT M%
NEXT N%
NEXT O%
NEXT P%
NEXT Q%
NEXT R%
NEXT S%
NEXT T%
NEXT U%
NEXT V%
NEXT W%
NEXT X%
NEXT Y%
NEXT Z%
NEXT AA%
NEXT AB%
NEXT AC%
NEXT AD%
NEXT AE%
NEXT AF%
NEXT AG%
NEXT AH%
NEXT AI%
NEXT AJ%
NEXT AK%
NEXT AL%
NEXT AM%
NEXT AN%
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NEXT ZP%
NEXT ZQ%
NEXT ZR%
NEXT ZS%
NEXT ZT%
NEXT ZY%
NEXT ZZ%

```

- proceed=Y/N
- case%=1/0
- next compd
- case\$= Y/N
- next class
- early exit
- close all
- correct crt

- Will calc and display min, max, and average errors.
- IF CLASS%<>0 THEN
- FOR I%=1 TO 21 : AVGCoeff(I%)=1 : NEXT I%
- END IF
- FOR I%=0 TO 21 : AVGCoeff(I%)=AVGCoeff(I%)/COUNT% : NEXT I%
- GOSUB MinAndMax

This is the section to draw in the bar graph.

```

• Must find MIN and MAX coefficients
AVGCoeff(0)=MIXCOEFF(1)
MAXCOEFF(0)=MIXCOEFF(1)
MINCOEFF(0)=MIXCOEFF(1)
MAX=ABS(MAXCOEFF(0))
FOR I%=1 TO 21
IF ABS(MAXCOEFF(I%))>MAX THEN MAX=ABS(MAXCOEFF(I%))
IF ABS(MINCOEFF(I%))>MAX THEN MAX=ABS(MINCOEFF(I%))
IF ABS(AVGCoeff(I%))>MAX THEN MAX=ABS(AVGCoeff(I%))
NEXT I%
IF MIN>0 THEN MIN=0
YEXPAC=315/(2*MAX)
• Must set up the screen.
CLS : SCREEN 12 : COLOR 11,0

```

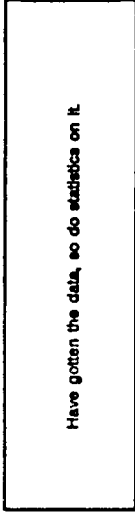
```

LINE (375, 63)-(375, 0),15 : LINE (455, 63)-(455, 0),15
* Next must draw in the data.
FOR I%=0 TO 21
TEMP1=AVGCOEFF(I%)*YEXPAC+Z22
TEMP2=MINCOEFF(I%)*YEXPAC+Z22
TEMP3=MAXCOEFF(I%)*YEXPAC+Z22
LINE ((I%+1)*20+3,TEMP1)-((I%+1)*20+7,Z22),C3%,BF
LINE ((I%+1)*20,TEMP2)-((I%+1)*20+10,TEMP2),C3%
LINE ((I%+1)*20,TEMP3)-((I%+1)*20+10,TEMP3),C5%
NEXT I%
* Have drawn in the bar graph, so draw the pie chart.
TEMP8 = Fraction of
TEMPX%=480 : TEMPY%=150 : TEMP18=X
DRAW 'C'+STR$(C2%)+'.TAD'
GOSUB DrawString
TEMP9 = 'Total'
TEMPX%=530 : TEMPY%=375 : TEMP18=X
DRAW 'C'+STR$(C2%)+'.TAD'
GOSUB DrawString
SUM1=0
FOR I%=0 TO 21
INCR SUM1,ABS(AVGCOEFF(I%))
NEXT I%
PI=4*ATN(1)
TEMP1=0.00001 : SUM2=0 : TEMPX%=C3%
FOR I%=0 TO 21
INCR SUM2,ABS(AVGCOEFF(I%))
TEMP2=SUM2/SUM1*PI*2
CIRCLE (535,Z22), 65,TEMPX%,-TEMP1,-TEMP2
TEMP1=TEMP2 : INCR TEMPX%
IF TEMPX%>15 THEN TEMPX%=10
NEXT I%
* Have done everything so see what to do next.
Startloop14:
AS=INKEY$
SELECT CASE AS
CASE = : GOTO Startloop14
CASE 'p','y' : LPRINT CHR$(12)
CASE 'H','Y' : GOSUB HardCopy/BarGraph
CASE 'E','y' : GOTO Statistics
CASE 'G','y' : GOTO Graph
CASE 'B','y' : GOTO BarGraphAndPieChart
CASE 'F','y' : GOSUB FileBarChartData
CASE 'O','y' : SCREEN 0 : GOTO Options
CASE 'Q','y',CHR$(27) : GOTO StartOfProgram
CASE ELSE : GOTO Statistics
END SELECT
GOTO Startloop14

```

- * no key
- * form feed
- * hardcopy
- * edit
- * graph
- * bar chart
- * write file
- * options
- * QUIT

Statistics:



```

* Will do bubble sort to get Error Distribution.
SCREEN 0 : WIDTH 80 : COLOR 4,2
LOCATE 15,15 : PRINT CHR$(216);STRINGS$(49,196);CHR$(191); 'top
LOCATE 16,15 : PRINT CHR$(179);TAB(65) ;CHR$(179); 'side
LOCATE 17,15 : PRINT CHR$(182);STRINGS$(49,196);CHR$(217); 'bottom
COLOR 31,2
LOCATE 16,28 : PRINT *** SORTING THE DATA ***;
FOR I%=1 TO COUNT%
P%=0
FOR K%=1 TO COUNT%-1
IF OBS(K%)>OBS(K%+1) THEN
SWAP OBS(K%), OBS(K%+1)
SWAP CALC(K%), CALC(K%+1)
SWAP DIFF(K%), DIFF(K%+1)
P%=1
END IF
NEXT K%
IF P%=0 THEN GOTO ErrorDistribution
NEXT I%
ErrorDistribution:
* Have sorted so will print error distribution.
* Will catch errors - no points loaded.
IF COUNT%<=1 THEN
SOUND 1000,3 : SOUND 800,1.5
SCREEN 0 : WIDTH 80 : COLOR 15,0 : CLS
COLOR 11,4
LOCATE 10,15 : PRINT CHR$(216);STRINGS$(49,196);CHR$(191); 'top
FOR I%=11 TO 14
LOCATE I%,15 : PRINT CHR$(179);TAB(65) ;CHR$(179); 'side
NEXT I%
LOCATE 15,15 : PRINT CHR$(182);STRINGS$(49,196);CHR$(217); 'bottom
COLOR 31,4 : LOCATE 12,34 : PRINT *** ERROR ***;
COLOR 14,4 : LOCATE 13,33 : PRINT 'Data Not Loaded';
COLOR 3,0
LOCATE 22,22 : PRINT 'Press any key to return to main menu';
AS=INPUT$(1)
GOTO StartOfProgram
END IF
CLS : SCREEN 12
COLOR 11,0
WINDOW (1,-1*ABSMAX) : (COUNT%,ABSMAX)
TEMP=1
FOR I=1 TO COUNT% STEP (COUNT%-1)/10
LINE (I,-1*ABSMAX)-(I,ABSMAX),12
NEXT I
FOR I=0 TO ABSMAX STEP (2*ABSMAX)/10
LINE (I,-(COUNT%/I),12

```

- * set window
- * draw grid
- * draw grid

```

LINE (1,0)-(COUNT%,0),12
NEXT 1
LOCATE 1,32 : PRINT "X Scale: 1 -> 1" : PRINT USING "###",COUNT%
LOCATE 2,21
PRINT USING "Y Scale: ##### to #####" : PRINT USING "###",ABSMAX,ABSMAX
LOCATE 3,25 : PRINT USING "Standard Deviation: #####SD" :
LOCATE 25,26 : PRINT "Low to High Observed" : PRINT USING "###",SD
LINE (1,0)-(COUNT%,0),14
LINE (1,1*SD)-(COUNT%,1*SD),11
LINE (1,-1*SD)-(COUNT%,-1*SD),11
FOR I%=1 TO COUNT%
LINE (I%,0)-(I%,DIFF(I%+1)),10
NEXT I%
.
. Have printed, so see if continue.
Startloop15:
AS=INKEY%
SELECT CASE AS
CASE = : GOTO Startloop15
CASE "P": LPRINT CHR$(12)
CASE "E": GOTO Statistics
CASE "G": GOTO Graph
CASE "B": GOTO BarGraphAndPieChart
CASE "O": SCREEN 0 : GOTO Options
CASE "V": GOSUB FileErrorData
CASE "Q": CHR$(27) : GOTO StartOfProgram
CASE ELSE : GOTO Graph
END SELECT
GOTO Startloop15

Graph:
SCREEN 0 : WIDTH 80
GOSUB GetFile
$INCLUDE 'CORRS12 INC'

Options:
$INCLUDE 'CORRS04 INC'

DrawMainMenuScreen:
$INCLUDE 'CORRS13 INC'

RegressionAnalysis:
$INCLUDE 'CORRS01 INC'

HardCopyStats:
$INCLUDE 'CORRS02 INC'

GetFile:
$INCLUDE 'CORRS03 INC'

FindPrint:
$INCLUDE 'CORRS05 INC'

SetUpScreenAndPrinter:
$INCLUDE 'CORRS06 INC'

GetCompoundUse:
$INCLUDE 'CORRS07 INC'

GetFuelType
$INCLUDE 'CORRS08 INC'

GetFuelParams:
$INCLUDE 'CORRS15 INC'

GetCetLevel:
$INCLUDE 'CORRS08 INC'

GetFractionsToUse
$INCLUDE 'CORRS10 INC'

MinAndMax:
$INCLUDE 'CORRS14 INC'

DisplayMixCoeff:
$INCLUDE 'CORRS16 INC'

$INCLUDE 'CORRS11 INC' . Youdlist, GetNumberOfCompounds, GetPropData
. ReadConfigFile, WriteConfigFile
. ReadFuelParams, WriteFuelParams
. HardCopyBarGraph, DrawString
. FileBarChartData, FileErrorData

Logo:
$INCLUDE 'LOGO.BAS'

Cetane:
. This is the subrn to do the CETANE calcs Prop: 4
SELECT CASE CLASS$(I%)
CASE 'ALKANE' .
CALC(COUNT%)=34.20285034
INCR CALC(COUNT%),52.41819873*OD(106)
INCR CALC(COUNT%),51.98441147*OD(108)
INCR CALC(COUNT%),-1.47859760*OD(110)
CALC(COUNT%)=CALC(COUNT%)*1.888413477 - 30.437546
CASE 'ALKENE' .
CALC(COUNT%)=73.903886 + 1.1741538*OD(106) - 38.146161*OD(113)
CASE 'DIENE' .
CALC(COUNT%)=23.50 + 0.25*OD(108)
CASE 'CYCLOHEX'
CALC(COUNT%)=-0.3679898 + 2.0359103*OD(106) + 13.86508*OD(113)
CALC(COUNT%)=CALC(COUNT%) - 2.8867358*OD(206)
CASE 'DECALIN'
CALC(COUNT%)=55.10918 - 1.2055341*OD(108) - 7.5804484*OD(113)
CASE 'MONO' .
CALC(COUNT%)=1118.91408250
INCR CALC(COUNT%),VAL(OD6( 3))*.1424742784 . Mono Cui
INCR CALC(COUNT%),VAL(OD6( 6))*.218630242 . Cch3
INCR CALC(COUNT%),VAL(OD6(11))*.24.68393788 . Cch2
INCR CALC(COUNT%),VAL(OD6(13))*.1.18313050 . Cch
INCR CALC(COUNT%),VAL(OD6(19))*.0 . Clet
INCR CALC(COUNT%),VAL(OD6(15))*.3.41954255 . Cch2>
CALC(COUNT%)=CALC(COUNT%)*1.233727349 - 1479.178077
CASE 'DICYCLIC'
CALC(COUNT%)=7263.43852344
INCR CALC(COUNT%),VAL(OD6(28))*.2.73911858 . DI Cui
INCR CALC(COUNT%),VAL(OD6(34))*.12.41802518 . Cch3
INCR CALC(COUNT%),VAL(OD6(36))*.7.01429224 . Cch2
INCR CALC(COUNT%),VAL(OD6(40))*.1.88352842 . Cch2>
CALC(COUNT%)=CALC(COUNT%)*0.880451753 - 7094.843750

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```

CASE 'TETRALIN'
CALC(COUNT%)=0.2273608 + 1.6332365*OD( 15) + 3.463368*OD(211)
CASE 'FUEL'
CALC(COUNT%)=OD(157)*OD(116) + OD(165)*OD( 27)
CALC(COUNT%)=CALC(COUNT%) + OD(173)*OD( 52) + OD(161)*OD( 76)
CALC(COUNT%)=CALC(COUNT%) + OD(189)*OD(104)
SELECT CASE D6(7)
CASE '<0.030' : CALC(COUNT%)=1.012131407*CALC(COUNT%) + 12.753746
CASE '0.030' : CALC(COUNT%)=0.874242865*CALC(COUNT%) + 13.487256
CASE ' ' : CALC(COUNT%)=0.689674282*CALC(COUNT%) + 10.645872
END.SELECT
GOSUB DefFuelCalc
END SELECT
RETURN
    
```

```

BoilingPoint:
. This is the subrn to do the BOILING PT calca Prop: 5
SELECT CASE CLASS$(%)
CASE 'ALKANE'
CALC(COUNT%)= 18.8686 - 18.8622*OD(106) - 18.8677*OD(108)
CALC(COUNT%)=CALC(COUNT%) - 18.8728*OD(110) - 18.8778*OD(147)
CALC(COUNT%)=1.1661188*(1/CALC(COUNT%) - 250) - 24.0481
CASE 'MONO'
CALC(COUNT%)=68.32607687
INCR CALC(COUNT%), 28.94813728*OD( 9)
INCR CALC(COUNT%), 43.90350342*OD( 11)
INCR CALC(COUNT%), 59.59009657*OD( 13)
INCR CALC(COUNT%), 80.11620168*OD(146)
INCR CALC(COUNT%), 20.86387489*OD( 15)
CALC(COUNT%)=1.030359544*CALC(COUNT%) - 6.814421
CASE 'DICYCLIC'
REM Average Structures Method
CALC(COUNT%)=157.827 + 42.4365*OD( 34) + 95.0166*OD( 36)
CALC(COUNT%)=CALC(COUNT%) + 110.169*OD( 38)
CALC(COUNT%)=CALC(COUNT%) + 14.1824*OD( 40)
CALC(COUNT%)=1*CALC(COUNT%) + 0
CASE 'FUEL'
GOSUB DefFuelCalc
END SELECT
RETURN
    
```

```

PourPoint:
. This is the subrn to do the FOUR PT calca Prop: 6
SELECT CASE CLASS$(%)
CASE 'ALKANE'
REM Alkane Calculation
CALC(COUNT%)=43.6760 + 43.68046*OD(106) + 43.6777*OD(108)
CALC(COUNT%)=CALC(COUNT%) + 43.6763*OD(110) + 43.6728*OD(147)
CALC(COUNT%)=1.2764687*1/CALC(COUNT%) - 608.363
CASE 'MONO'
REM Mono Calculation
CALC(COUNT%)=68.6831 + 16.088*OD( 9) - 6.76148*OD( 11)
CALC(COUNT%)=CALC(COUNT%) - 4.87162*OD( 13)
CALC(COUNT%)=CALC(COUNT%) - 12.82*OD(148)
CALC(COUNT%)=CALC(COUNT%) + 3.28633*OD( 15)
CASE 'DICYCLIC'
REM Dicyclic Calculation
CALC(COUNT%)= 25.7878 + 7.23272*OD( 34) - 30.9269*OD( 36)
CALC(COUNT%)=CALC(COUNT%) - 61.3087*OD(151)
    
```

```

CALC(COUNT%)=CALC(COUNT%) + 2.02359*OD( 40)
CALC(COUNT%)=1*CALC(COUNT%) + 0
CASE 'FUEL'
GOSUB DefFuelCalc
END SELECT
RETURN
FlashPoint:
. This is the subrn to do the FLASH PT calca Prop: 6
SELECT CASE CLASS$(%)
CASE 'ALKANE'
CALC(COUNT%)=210 - 744*OD(106) - 8*OD(108)
CALC(COUNT%)=CALC(COUNT%) + 1448*OD(110) + 0*OD(147)
CASE 'MONO'
TEMP=6 + OD(8) + OD(11) + OD(13) + OD(146) + OD(15) + OD(17)
CALC(COUNT%)=134.81 + 19.9731*TEMP + 1.49348*OD(9)
CALC(COUNT%)=1.0137885*CALC(COUNT%) - 1.07834
CASE 'FUEL'
GOSUB DefFuelCalc
END SELECT
RETURN
    
```

```

$SEGMENT
Density:
. This is the subrn to do the DENSITY calca Prop: 9
SELECT CASE CLASS$(%)
CASE 'ALKANE'
CALC(COUNT%)=1688.5001 + 1686.7285*OD(106) + 1687.3565*OD(108)
CALC(COUNT%)=CALC(COUNT%) + 1688.0271*OD(110) + 1688.7404*OD(147)
CALC(COUNT%)=1.0378129*CALC(COUNT%) - 2.64012E-02
CASE 'DIENE'
CALC(COUNT%)=0.7899 + 0.0026*OD(106)
CASE 'CYCLOHEX'
CALC(COUNT%)=0.7513501 + 4.1668464E-03*OD(106) + 1.9600687E-02*OD(113)
CALC(COUNT%)=CALC(COUNT%) - 1.7211739E-02*OD(206)
CASE 'DECALIN'
CALC(COUNT%)=0.630487 + 4.2884609E-03*OD(106) + 1.4154704E-02*OD(113)
CASE 'MONO'
CALC(COUNT%)=0.856488 + 8.73778E-03*OD( 9) + 4.48975E-03*OD( 11)
CALC(COUNT%)=CALC(COUNT%) + 3.49110E-03*OD( 13)
CALC(COUNT%)=CALC(COUNT%) + 1.82681E-02*OD(148)
CALC(COUNT%)=CALC(COUNT%) - 4.18890E-04*OD( 15)
CASE 'DICYCLIC'
CALC(COUNT%)=0.887182 + 3.8733E-03*OD( 34) - 9.63778E-03*OD( 36)
CALC(COUNT%)=CALC(COUNT%) - 1.48817E-02*OD( 38)
CALC(COUNT%)=CALC(COUNT%) - 1.18222E-02*OD(151)
CALC(COUNT%)=CALC(COUNT%) - 7.84452E-03*OD( 40)
CASE 'TETRALIN'
CALC(COUNT%)=0.9594468 - 5.2357546E-03*OD( 15) - 4.5328914E-03*OD(211)
CASE 'FUEL'
MODEL MIX
GOSUB DefFuelCalc
END SELECT
RETURN
    
```

```

RefractiveIndex:
. This is the subrn to do the REF INDEX calca Prop: 10
SELECT CASE CLASS$(%)
    
```

```

CASE 'ALKANE' *
CALC(COUNT%) = -1277.53 + 1278.99*OD(106) + 1279.00*OD(108)
CALC(COUNT%) = CALC(COUNT%) + 1279.33*OD(110) + 1279.68*OD(147)
CALC(COUNT%) = 1.9684942*CALC(COUNT%) - 0.1214265
CASE 'MONO' *
CALC(COUNT%) = 1.46634 + 0.80762E-03*OD( 9) + 4.43701E-03*OD( 11)
CALC(COUNT%) = CALC(COUNT%) + 2.18346E-03*OD( 13)
CALC(COUNT%) = CALC(COUNT%) + 7.82145E-03*OD(149)
CALC(COUNT%) = CALC(COUNT%) - 7.35969E-04*OD( 15)
CALC(COUNT%) = 1.203549*CALC(COUNT%) - 0.304689
CASE 'DICYCLIC'
REM 'Dicyclic Calculation
CALC(COUNT%) = 1.60684 - 1.76428E-04*OD( 34) - 1.35068E-02*OD( 36)
CALC(COUNT%) = CALC(COUNT%) - 0.018491*OD( 38)
CALC(COUNT%) = CALC(COUNT%) - 0.020157*OD(151)
CALC(COUNT%) = CALC(COUNT%) - 6.76552E-03*OD( 40)
CALC(COUNT%) = 1.0536997*CALC(COUNT%) - 8.45376E-02
END SELECT
RETURN

CloudPoint:
. This is the subrn to do the CLOUD PT calcs Prop: 11
SELECT CASE CLASS$(%)
CASE 'ALKANE' *
CALC(COUNT%) = 0 + 0*OD(106) + 0*OD(108)
CALC(COUNT%) = CALC(COUNT%) + 0*OD(110) + 0*OD(147)
CASE 'FUEL' *
GOSUB DoFuelCalc
END SELECT
RETURN

Viscosity:
. This is the subrn to do the VISCOSITY calcs Prop: 12
SELECT CASE CLASS$(%)
CASE 'ALKANE' *
CALC(COUNT%) = 0 + 0*OD(106) + 0*OD(108)
CALC(COUNT%) = CALC(COUNT%) + 0*OD(110) + 0*OD(147)
CASE 'MONO' *
TEMP = 6 + OD(9) + OD(11) + OD(13) + OD(149) + OD(15) + OD(17)
CALC(COUNT%) = -0.219648 + 0.120416*TEMP - 7.64261E-02*OD(9)
CALC(COUNT%) = 1.0601879*CALC(COUNT%) - 4.16122E-02
CASE 'FUEL' *
GOSUB DoFuelCalc
END SELECT
RETURN

Filterability:
. This is the subrn to do the FILTERABILITY calcs Prop: 13
SELECT CASE CLASS$(%)
CASE 'FUEL' *
GOSUB DoFuelCalc
END SELECT
RETURN

SpecificDispersion:
. This is the subrn to do the SP. DISP. calcs Prop: 16
SELECT CASE CLASS$(%)
CASE 'ALKANE' *
CALC(COUNT%) = -220627 + 221029*OD(106) + 221023*OD(108)
CALC(COUNT%) = CALC(COUNT%) + 221018*OD(110) + 221013*OD(147)

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CALC(COUNT%) = -19.157639*CALC(COUNT%) - 1765.8608
CASE 'MONO' *
CALC(COUNT%) = 187.679 - 3.29317*OD(9) - 10.6503*OD(11)
CALC(COUNT%) = CALC(COUNT%) - 19.4555*OD(13)
CALC(COUNT%) = CALC(COUNT%) - 28.3787*OD(149)
CALC(COUNT%) = CALC(COUNT%) - 8.53621*OD(15)
CALC(COUNT%) = 1.022244*CALC(COUNT%) - 3.80623
END SELECT
RETURN

SurfaceTension:
. This is the subrn to do the SURFACE TENSION calcs Prop: 17
SELECT CASE CLASS$(%)
CASE 'ALKANE' *
CALC(COUNT%) = 19582.3 - 18603.1*OD(106) - 16560.6*OD(108)
CALC(COUNT%) = CALC(COUNT%) - 19320.2*OD(110) - 19480.1*OD(147)
CALC(COUNT%) = 1.2331308*CALC(COUNT%) - 4.68244
CASE 'MONO' *
CALC(COUNT%) = 27.742 + 0.484*OD( 9) + 0.63*OD( 11)
CALC(COUNT%) = CALC(COUNT%) - 0.062*OD( 13)
CALC(COUNT%) = CALC(COUNT%) + 0.078*OD( 15)
CALC(COUNT%) = 3.1153327*CALC(COUNT%) - 60.5514
END SELECT
RETURN

AnilinePoint:
. This is the subrn to do the ANILINE calcs Prop: 18
SELECT CASE CLASS$(%)
CASE 'ALKANE' *
CALC(COUNT%) = -762137 + 762227*OD(106) + 762207*OD(108)
CALC(COUNT%) = CALC(COUNT%) + 762189*OD(110) + 762151*OD(147)
END SELECT
RETURN

CriticalPressure:
. This is the subrn to do the CRITICAL PRESS calcs Prop: 19
SELECT CASE CLASS$(%)
CASE 'ALKANE' *
CALC(COUNT%) = -4.77345E6 + 4.77601E08*OD(106) + 4.77344E08*OD(108)
CALC(COUNT%) = CALC(COUNT%) + 4.7711E08*OD(110) + 4.76854E08*OD(147)
TEMP = 0.227*OD(106) + 0.227*OD(108) + 0.210*OD(110) + 0.210*OD(147)
CALC(COUNT%) = VAL(D$(3))/(0.34 + TEMP)^2
CASE 'MONO' *
TEMP = 6 + OD(9) + OD(11) + OD(13) + OD(149) + OD(15) + OD(17)
CALC(COUNT%) = 68.4255 - 3.85583*TEMP - 0.806247*OD(9)
CALC(COUNT%) = 1.0978126*CALC(COUNT%) - 2.84441
CALC(COUNT%) = 45.8035 - 4.68159*OD(9) - 9.79832*OD(11)
CALC(COUNT%) = CALC(COUNT%) - 12.6361*OD(13)
CALC(COUNT%) = CALC(COUNT%) - 16.3439*OD(149)
CALC(COUNT%) = CALC(COUNT%) - 3.07235*OD(15)
CALC(COUNT%) = 1.0725809*CALC(COUNT%) - 2.34544
TEMP = 0.34 + 0.164*OD(11)+OD(15)) + 0.162*OD(13) + 0.154*OD(149)
CALC(COUNT%) = VAL(D$(3))/TEMP^2
END SELECT
RETURN

CriticalTemperature:
. This is the subrn to do the CRITICAL TEMP calcs Prop: 20
SELECT CASE CLASS$(%)

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CASE 'ALKANE'
  Average Structure Method
  CALC(COUNT%) = -1.34084E08 + 1.34034E08*OD(108) + 1.34114E08*OD(108)
  CALC(COUNT%) = CALC(COUNT%) + 1.34191E08*OD(110)
  CALC(COUNT%) = CALC(COUNT%) + 1.34289E08*OD(147)
  CALC(COUNT%) = 1.0360809*CALC(COUNT%) - 10.5801
  Boiling Point Method
  TEMP = 0.020*OD(108) + 0.020*OD(108) + 0.012*OD(110) + 0.00*OD(147)
  CALC(COUNT%) = VAL(06(5))/(0.578 + TEMP * TEMP ^ 2)
  CALC(COUNT%) = 0.7385033*CALC(COUNT%) + 145.886
CASE 'MONO'
  Carbon Number - ADS Method
  TEMP = 6 + OD(9) + OD(11) + OD(13) + OD(149) + OD(15) + OD(17)
  CALC(COUNT%) = 152.062 + 23.5092*TEMP + 4.60963*OD(5)
  CALC(COUNT%) = 1.0991419*CALC(COUNT%) - 38.7584
  Average Structure Method
  CALC(COUNT%) = 283.831 + 27.8109*OD(9) + 50.8221*OD(11)
  CALC(COUNT%) = CALC(COUNT%) + 77.4144*OD(13)
  CALC(COUNT%) = CALC(COUNT%) + 83.3687*OD(149)
  CALC(COUNT%) = CALC(COUNT%) + 22.6388*OD(15)
  CALC(COUNT%) = 1.0848573*CALC(COUNT%) - 33.1863
  Boiling Point Method
  TEMP = 0.013*OD(11) + OD(15) + 0.012*OD(13) - 0.007*OD(149)
  CALC(COUNT%) = VAL(06(5))/(0.578 + TEMP * TEMP ^ 2)
  CALC(COUNT%) = 0.6730634*CALC(COUNT%) + 186.868
END SELECT
RETURN

CriticalVolume:
  This is the subrn to do the CRITICAL VOLUME calcs Prop 21
SELECT CASE CLASS$(%)
CASE 'ALKANE'
  CALC(COUNT%) = -14359.3 + 14366.4*OD(108) + 14359.6*OD(108)
  CALC(COUNT%) = CALC(COUNT%) + 14353.2*OD(110) + 14348.7*OD(147)
  CALC(COUNT%) = 1.0845822*1/CALC(COUNT%) - 4.46028E-02
  CALC(COUNT%) = 40 + 55*OD(108) + 51*OD(110) + 41*OD(147)
CASE 'MONO'
  TEMP = 6 + OD(9) + OD(11) + OD(13) + OD(149) + OD(15) + OD(17)
  CALC(COUNT%) = -4.79784E-02 + 5.18911E-02*TEMP + 6.33648E-03*OD(5)
  CALC(COUNT%) = 1.0219639*CALC(COUNT%) - 9.03398E-03
  CALC(COUNT%) = 0.282001 + 5.83743E-02*OD(9) + 0.115389*OD(11)
  CALC(COUNT%) = CALC(COUNT%) + 0.182851*OD(13)
  CALC(COUNT%) = CALC(COUNT%) + 0.198999*OD(149)
  CALC(COUNT%) = CALC(COUNT%) + 5.28144E-02*OD(15)
  CALC(COUNT%) = 1.0157028*CALC(COUNT%) - 6.6716E-03
  CALC(COUNT%) = 40 + 44.5*OD(11) + OD(15) + 49*OD(13) + 31*OD(149)
END SELECT
RETURN

HeatCapacity:
  This is the subrn to do the HEAT CAPACITY calcs Prop 22
SELECT CASE CLASS$(%)
CASE 'ALKANE'
  CALC(COUNT%) = 151.38 - 151.322*OD(108) - 151.377*OD(108)
  CALC(COUNT%) = CALC(COUNT%) - 151.431*OD(110) - 151.484*OD(147)
  CALC(COUNT%) = 1.1133138*1/CALC(COUNT%) - 5.58737
CASE 'MONO'
  TEMP = 6 + OD(9) + OD(11) + OD(13) + OD(149) + OD(15) + OD(17)
  CALC(COUNT%) = 3.58220 + 5.97422*TEMP + 0.278831*OD(5)
  CALC(COUNT%) = 1.0100408*CALC(COUNT%) - 0.506899

HeatOfEvaporization:
  This is the subrn to do the HEAT OF VAPOR calcs Prop 23
SELECT CASE CLASS$(%)
CASE 'ALKANE'
  CALC(COUNT%) = 309.488 - 309.099*OD(108) - 309.491*OD(108)
  CALC(COUNT%) = CALC(COUNT%) - 309.882*OD(110) - 310.252*OD(147)
  CALC(COUNT%) = 0.9831473*1/CALC(COUNT%) + 6.77238E-03
CASE 'MONO'
  TEMP = 6 + OD(9) + OD(11) + OD(13) + OD(149) + OD(15) + OD(17)
  CALC(COUNT%) = 1.8208 + 0.894279*TEMP + 0.428863*OD(5)
  CALC(COUNT%) = 1.0360811*CALC(COUNT%) - 0.424342
CASE ELSE
  END SELECT
RETURN

HeatOfFormation:
  This is the subrn to do HEAT OF FORMATION calcs Prop 24
SELECT CASE CLASS$(%)
CASE 'ALKANE'
  CALC(COUNT%) = -89.3276 + 89.4799*OD(108) + 89.5217*OD(108)
  CALC(COUNT%) = CALC(COUNT%) + 89.5848*OD(110) + 89.6077*OD(147)
  CALC(COUNT%) = 1.1042493*1/CALC(COUNT%) + 6.77805
CASE 'MONO'
  TEMP = 6 + OD(9) + OD(11) + OD(13) + OD(149) + OD(15) + OD(17)
  CALC(COUNT%) = 48.0728 - 6.07028*TEMP - 2.86568*OD(5)
  CALC(COUNT%) = 1.002847*CALC(COUNT%) + 1.89813E-02
CASE ELSE
  END SELECT
RETURN

FreeEnergyOfFormation:
  This is the subrn to do the FREE E. OF FORM calcs Prop 25
SELECT CASE CLASS$(%)
CASE 'ALKANE'
  CALC(COUNT%) = -5671.32 + 5671.71*OD(108) + 5671.31*OD(108)
  CALC(COUNT%) = CALC(COUNT%) + 5670.91*OD(110) + 5670.5*OD(147)
  CALC(COUNT%) = 1.3381489*1/CALC(COUNT%) - 10 + 0.188807
CASE 'MONO'
  TEMP = 6 + OD(9) + OD(11) + OD(13) + OD(149) + OD(15) + OD(17)
  CALC(COUNT%) = 23.4941 + 0.853167*TEMP - 2.41353*OD(5)
  CALC(COUNT%) = 1.0816181*CALC(COUNT%) - 1.87917
RETURN
CASE ELSE
  END SELECT
RETURN

HeatOfCombustion:
  This is the subrn to do the HEAT OF COMBUST calcs Prop 28
SELECT CASE CLASS$(%)
CASE 'ALKANE'
  CALC(COUNT%) = 1.07228 - 1.08808*OD(108) - 1.07225*OD(108)
  CALC(COUNT%) = CALC(COUNT%) - 1.07541*OD(110) - 1.07857*OD(147)
  CALC(COUNT%) = 1.0203915*1/CALC(COUNT%) - 15.487781
CASE 'MONO'
  TEMP = 6 + OD(9) + OD(11) + OD(13) + OD(149) + OD(15) + OD(17)
  CALC(COUNT%) = -127.579 + 148.085*TEMP - 2.75543*OD(5)
  CALC(COUNT%) = 1.000015*CALC(COUNT%) - 3.7306777E-02

```



```

CASE FUEL
  GOSUB DoFuelCalc
END SELECT
RETURN

MolecularVolume:
  This is the subrn to do the MOLECULAR VOLUME calcs Prop 27
SELECT CASE CLASS$(%)
CASE 'ALKANE'
CALC(COUNT%)= 29.5995 - 29.5493*OD(106) - 29.5982*OD(108)
CALC(COUNT%)=CALC(COUNT%) - 29.5668*OD(110)
CALC(COUNT%)=CALC(COUNT%) - 29.6049*OD(147)
CALC(COUNT%)=1.1081339*1/CALC(COUNT%) - 18.809
CASE 'MONO'
CALC(COUNT%)= 82.3559 + 14.7988*OD(9) + 31.2141*OD(11)
CALC(COUNT%)=CALC(COUNT%) + 47.8291*OD(13)
CALC(COUNT%)=CALC(COUNT%) + 63.0310*OD(149)
CALC(COUNT%)=CALC(COUNT%) + 18.7311*OD(15)
CALC(COUNT%)=1.0075088*CALC(COUNT%) - 1.22483
CASE 'DICYCLIC'
CALC(COUNT%)=128.785 + 13.4959*OD(34) + 28.2471*OD(36)
CALC(COUNT%)=CALC(COUNT%) + 44.5998*OD(38)
CALC(COUNT%)=CALC(COUNT%) + 18.8543*OD(40)
CALC(COUNT%)=1.0003922*CALC(COUNT%) - 8.26236E-02
RETURN
CASE ELSE
END SELECT
RETURN

Aromatics:
  This is the subrn to do the PERCENT AROMATICS calcs Prop 28
SELECT CASE CLASS$(%)
CASE 'FUEL'
  GOSUB DoFuelCalc
  CALC(COUNT%)=(OD(27) + OD(52) + OD(78) + OD(104)) * 100
  CALC(COUNT%)=OD(132)*100
CASE ELSE
END SELECT
RETURN

Olefins:
  This is the subrn to do the PERCENT OLEFINS calcs Prop 29
SELECT CASE CLASS$(%)
CASE 'FUEL'
  GOSUB DoFuelCalc
  CALC(COUNT%)=(OD(27) + OD(52) + OD(78) + OD(104)) * 100
  CALC(COUNT%)=OD(132)*100
CASE ELSE
END SELECT
RETURN

CetaneIndex:
  This is the subrn to do the CETANE INDEX calcs Prop 31
SELECT CASE CLASS$(%)
CASE 'ALKANE'
CALC(COUNT%)=2.58598E07 - 2.58598E07*OD(106) - 2.58598E07*OD(108)
CALC(COUNT%)=CALC(COUNT%) - 2.58598E07*OD(110)
CALC(COUNT%)=CALC(COUNT%) - 2.58598E07*OD(147)
CALC(COUNT%)=1.4078022*CALC(COUNT%) - 32.7867
CASE 'ALKENE'
CALC(COUNT%)=73.803698 + 1.1741538*OD(106) - 38.146181*OD(113)
CASE 'DIENE'
CALC(COUNT%)=23.50 + 0.25*OD(108)
CASE 'CYCLOHEX'
CALC(COUNT%)=-0.3978699 + 2.0359103*OD(108) + 13.86508*OD(113)
CALC(COUNT%)=CALC(COUNT%) - 2.8887356*OD(206)
CASE 'DECALIN'
CALC(COUNT%)=53.10918 - 1.2055341*OD(108) - 7.5904484*OD(113)
CASE 'MONO'
CALC(COUNT%)=5.71407 - 10.6485*OD(9) - 8.13829E-02*OD(11)
CALC(COUNT%)=CALC(COUNT%) - 6.75867*OD(13)
CALC(COUNT%)=CALC(COUNT%) - 36.3951*OD(149)
CALC(COUNT%)=CALC(COUNT%) + 5.32162*OD(15)
CALC(COUNT%)=1.1225058*CALC(COUNT%) - 3.87011
CASE 'DICYCLIC'
CALC(COUNT%)=82.4839 - 82.4839*OD(34) - 79.8955*OD(36)
CALC(COUNT%)=CALC(COUNT%) - 24.7108*OD(151)
CALC(COUNT%)=CALC(COUNT%) + 1.88253*OD(40)
CALC(COUNT%)=1*CALC(COUNT%) - 0
CASE 'TETRALIN'
CALC(COUNT%)=-0.2273609 + 1.8332365*OD(15) + 3.483368*OD(211)
CASE 'FUEL'
  GOSUB DoFuelCalc
CASE ELSE
END SELECT
RETURN

SpecificGravity:
  This is the subrn to do the SPECIFIC GRAVITY calcs Prop 32
SELECT CASE CLASS$(%)
CASE 'ALKANE'
CALC(COUNT%)=-1888.5001 + 1888.7285*OD(106) + 1887.3565*OD(108)
CALC(COUNT%)=CALC(COUNT%) + 1998.0271*OD(110) + 1888.7404*OD(147)
CALC(COUNT%)=1.0379129*CALC(COUNT%) - 2.84012E-02
CASE 'ALKENE'
CALC(COUNT%)=-0.7155571 + 5.1788149E-03*OD(106) + 1.236882E-02*OD(113)
CASE 'DIENE'
CALC(COUNT%)=0.7898 + 0.0028*OD(108)
CASE 'CYCLOHEX'
CALC(COUNT%)=0.7513501 + 4.1888484E-03*OD(108) + 1.8800687E-02*OD(113)
CALC(COUNT%)=CALC(COUNT%) - 1.7211739E-02*OD(206)
CASE 'DECALIN'
CALC(COUNT%)=0.830487 + 4.2994609E-03*OD(108) + 1.4154704E-02*OD(113)
CASE 'MONO'
CALC(COUNT%)=0.898488 + 8.73778E-03*OD(9) + 4.49879E-03*OD(11)
CALC(COUNT%)=CALC(COUNT%) + 3.49110E-03*OD(13)
CALC(COUNT%)=CALC(COUNT%) + 1.82951E-02*OD(149)
CALC(COUNT%)=CALC(COUNT%) - 4.18880E-04*OD(15)
CALC(COUNT%)=1.8508524*CALC(COUNT%) - 0.740225
CASE 'DICYCLIC'
CALC(COUNT%)=0.987182 + 3.8733E-03*OD(34) - 9.83778E-03*OD(36)
CALC(COUNT%)=CALC(COUNT%) - 1.48817E-02*OD(38)
CALC(COUNT%)=CALC(COUNT%) - 1.18222E-02*OD(151)
CALC(COUNT%)=CALC(COUNT%) - 7.84452E-03*OD(40)
CALC(COUNT%)=1.071507*CALC(COUNT%) - 6.80288E-02
CASE 'TETRALIN'
CALC(COUNT%)=0.9594488 - 5.2357546E-03*OD(15) - 4.5328914E-03*OD(211)
CASE 'FUEL'
  GOSUB DoFuelCalc
CASE ELSE

```

```

PROP(16) = VAL(ODS( 62)) * VAL(ODS( 78)) * MIXCOEFF(17)
PROP(17) = VAL(ODS( 66)) * VAL(ODS( 76)) * MIXCOEFF(18)
PROP(18) = VAL(ODS( 80)) * VAL(ODS(104)) * MIXCOEFF(19)
PROP(19) = VAL(ODS( 86)) * VAL(ODS(104)) * MIXCOEFF(20)
PROP(20) = VAL(ODS( 88)) * VAL(ODS(104)) * MIXCOEFF(21)
PROP(21) = VAL(ODS( 82)) * VAL(ODS(104)) * MIXCOEFF(22)
CALC(COUNT%) = 0
IF COUNT% = 1 THEN
  FOR K% = 1 TO 21
    MAXCOEFF(K%) = PROP(K%) : MINCOEFF(K%) = PROP(K%)
  NEXT K%
END IF
FOR K% = 0 TO 21
  INCR CALC(COUNT%), PROP(K%)
  INCR AVGCOEFF(K%), PROP(K%)
  IF PROP(K%) > MAXCOEFF(K%) THEN MAXCOEFF(K%) = PROP(K%)
  IF PROP(K%) < MINCOEFF(K%) THEN MINCOEFF(K%) = PROP(K%)
NEXT K%
IF LEFT$(FUNCTIONS,1) = "X" THEN CALC(COUNT%) = CALC(COUNT%)
IF LEFT$(FUNCTIONS,3) = "1/" THEN CALC(COUNT%) = 1 / CALC(COUNT%)
IF LEFT$(FUNCTIONS,3) = "LOG" THEN CALC(COUNT%) = LOG(CALC(COUNT%))
CALC(COUNT%) = CALC(COUNT%) - OFFSETFACTOR
CALC(COUNT%) = CALC(COUNT%) * SLOPEFACTOR
CALC(COUNT%) = CALC(COUNT%) + INTGPFACOR
RETURN

```

```

MAXCOEFF(K%) = PROP(K%) : MINCOEFF(K%) = PROP(K%)
NEXT K%
END IF
FOR K% = 0 TO 21
  INCR CALC(COUNT%), PROP(K%)
  INCR AVGCOEFF(K%), PROP(K%)
  IF PROP(K%) > MAXCOEFF(K%) THEN MAXCOEFF(K%) = PROP(K%)
  IF PROP(K%) < MINCOEFF(K%) THEN MINCOEFF(K%) = PROP(K%)
NEXT K%

```

```

IF LEFT$(FUNCTIONS,1) = "X" THEN CALC(COUNT%) = CALC(COUNT%)
IF LEFT$(FUNCTIONS,3) = "1/" THEN CALC(COUNT%) = 1 / CALC(COUNT%)
IF LEFT$(FUNCTIONS,3) = "LOG" THEN CALC(COUNT%) = LOG(CALC(COUNT%))
CALC(COUNT%) = CALC(COUNT%) - OFFSETFACTOR
CALC(COUNT%) = CALC(COUNT%) * SLOPEFACTOR
CALC(COUNT%) = CALC(COUNT%) + INTGPFACOR
RETURN

```

```

T-T-T-That's all folks ! ! ! !

```

Code Listing for CORR501.INC

This is a subroutine do the regression analysis for corr coef.

```

S1=0 : S2=0 : S3=0 : S4=0 : S5=0 : S6=0 : S7=0 : S8=0 : S9=0 : C%=0
FOR J%=1 TO COUNT%
  IF USE%(J%) = 1 THEN
    S1 = S1 + OBS(J%)
    S2 = S2 + CALC(J%)
    S3 = S3 + OBS(J%) * CALC(J%)
    S4 = S4 + OBS(J%) ^ 2
    S5 = S5 + CALC(J%) ^ 2
    INCR C%
  END IF
NEXT J%
D = C% * S4 * S1 ^ 2
AA1 = (C% * S3 * S1 * S2) / D
AA2 = (S4 * S2 * S1 * S3) / D
FOR J% = 1 TO C%
  R(J%) = CALC(J%) * AA1 * OBS(J%) * AA2
  IF R(J%) < 1E-10 AND R(J%) > -1E-10 THEN R(J%) = 0
  SS = SS + R(J%) ^ 2
NEXT J%

```

```

END SELECT
RETURN

```

```

InitialBoilPoint:
. This is the subrn to do the INITIAL BP calcs
SELECT CASE CLASS$(I%)
CASE "FUEL"
  GOSUB DoFuelCalc
END SELECT
RETURN

```

```

BoilingPointTenPercnt:
. This is the subrn to do the 10% BOIL POINT calcs
SELECT CASE CLASS$(I%)
CASE "FUEL"
  GOSUB DoFuelCalc
END SELECT
RETURN

```

```

BoilingPointInetyPercnt:
. This is the subrn to do the 90% BOIL POINT calcs
SELECT CASE CLASS$(I%)
CASE "FUEL"
  GOSUB DoFuelCalc
END SELECT
RETURN

```

```

BoilingPointEndPoint:
. This is the subrn to do the END BOIL POINT calcs
SELECT CASE CLASS$(I%)
CASE "FUEL"
  GOSUB DoFuelCalc
END SELECT
RETURN

```

```

ResidualCarbon:
. This is the subrn to do the RESIDUAL CARBON calcs
SELECT CASE CLASS$(I%)
CASE "FUEL"
  GOSUB DoFuelCalc
END SELECT
RETURN

```

```

DoFuelCalc:
PROP( 0) = MIXCOEFF(1)
PROP( 1) = VAL(ODS(106)) * VAL(ODS(116)) * MIXCOEFF( 2)
PROP( 2) = VAL(ODS(108)) * VAL(ODS(116)) * MIXCOEFF( 3)
PROP( 3) = VAL(ODS(110)) * VAL(ODS(116)) * MIXCOEFF( 4)
PROP( 4) = VAL(ODS( 3)) * VAL(ODS( 27)) * MIXCOEFF( 5)
PROP( 5) = VAL(ODS( 6)) * VAL(ODS( 27)) * MIXCOEFF( 6)
PROP( 6) = VAL(ODS(11)) * VAL(ODS( 27)) * MIXCOEFF( 7)
PROP( 7) = VAL(ODS(13)) * VAL(ODS( 27)) * MIXCOEFF( 8)
PROP( 8) = VAL(ODS(18)) * VAL(ODS( 27)) * MIXCOEFF( 9)
PROP( 9) = VAL(ODS(15)) * VAL(ODS( 27)) * MIXCOEFF(10)
PROP(10) = VAL(ODS(28)) * VAL(ODS(52)) * MIXCOEFF(11)
PROP(11) = VAL(ODS(34)) * VAL(ODS(52)) * MIXCOEFF(12)
PROP(12) = VAL(ODS(38)) * VAL(ODS(52)) * MIXCOEFF(13)
PROP(13) = VAL(ODS(40)) * VAL(ODS(52)) * MIXCOEFF(14)
PROP(14) = VAL(ODS(54)) * VAL(ODS(78)) * MIXCOEFF(15)
PROP(15) = VAL(ODS( 60)) * VAL(ODS( 78)) * MIXCOEFF(16)

```

Prop: 33

Prop: 34

Prop: 35

Prop: 36

Prop: 37

Xch3
Cch2
Xch
Cun
Cch3
Cch2
Cch
Cch2
Cch2
Cun
Cch3
Cch2
Cch2
Cun
Cch3

```

LPRINT "Time: ",TIMES," Date:",DATES
LPRINT "Statistics for file: ",ODIRS+OFILES$
LPRINT "Line name ",LINENAMES$
LPRINT "Property: ",PROPS(PROF%)
LPRINT "Class: ",SCLASS$
LPRINT USING "Number of Points: ###.C%";C%
LPRINT USING "Slope: #####.#####";AA1
LPRINT USING "Intercept: #####.#####";AA2
LPRINT
LPRINT "Standard Deviation of Residuals: ";
LPRINT USING "#####.#####";S
LPRINT "Expected error in slope (95% confidence): ";
LPRINT USING "#####.#####";E1
LPRINT "Expected error in intercept (95% confidence): ";
LPRINT USING "#####.#####";E2
LPRINT USING "Correlation Coefficient: #####.###";R2
RETURN

```

Code Listing for CORR503.INC

This is a subroutine to read the data from a graphing file.

```

COUNT%=1
OPEN ODIRS+OFILES FOR INPUT AS #1
IF NOT EOF(1) THEN INPUT #1,LINENAMES
IF NOT EOF(1) THEN INPUT #1,TITLE1$
IF NOT EOF(1) THEN INPUT #1,TITLE2$
IF NOT EOF(1) THEN INPUT #1,XLABELS
IF NOT EOF(1) THEN INPUT #1,YLABELS
WHILE NOT EOF(1)
INPUT #1,OBS(COUNT%)
INPUT #1,CALC(COUNT%)
INPUT #1,USE%(COUNT%)
INPUT #1,TEMPS
INPUT #1,TEMPS
INCR COUNT%
WEND
CLOSE #1
DECR COUNT%
RETURN

```

Code Listing for CORR504.INC

This is the section to do the options.

```

S=SQR(S3/(C%-2))
E1=SQR(C%/D1)*1.96*S
E2=SQR(S4/D1)*1.96*S
R2=(C%-S3-S1^2-S2^2)/(C%*94-S1^2+C%*98-S2^2)
IF E1<1E-10 AND E1>1E-10 THEN E1=0
IF E2<1E-10 AND E1>1E-10 THEN E2=0
IF R2<1E-10 AND R2>1E-10 THEN R2=0
R2=SQR(R2)
* Have done calcs, so print to the screen, printer.
COLOR 2, 1
LOCATE 1, 8 : PRINT CHR$(201);STRINGS(63,206);CHR$(197)
FOR I%=2 TO 12
LOCATE I%,8;PRINT CHR$(198);STRINGS(63, 32);CHR$(196)
NEXT I%
LOCATE 13, 8 : PRINT CHR$(200);STRINGS(63,206);CHR$(196)
COLOR 15, 1
LOCATE 2,11 : PRINT TIMES;
LOCATE 2,60 : PRINT DATES;
LOCATE 3,16 : PRINT "Statistics for file:";
LOCATE 4,16 : PRINT "Line Name:";
LOCATE 5,16 : PRINT "Property:";
LOCATE 6,16 : PRINT "Class:";
LOCATE 7,30 : PRINT "Number of Points:";
LOCATE 8,11 : PRINT "Slope:";
LOCATE 8,46 : PRINT "Intercept:";
LOCATE 9,11 : PRINT "Standard Deviation of Residuals:";
LOCATE 10,11 : PRINT "Expected Error in Slope (95% confidence)";
LOCATE 11,11 : PRINT "Expected Error in Intercept (95% confidence)";
LOCATE 12,23 : PRINT "Correlation Coefficient:";
COLOR 14, 1
LOCATE 3,38 : PRINT ODIRS+OFILES;
LOCATE 4,30 : PRINT LINENAMES;
LOCATE 5,26 : PRINT PROF$(PROF%);
LOCATE 6,25 : PRINT SCLASS$;
LOCATE 7,48 : PRINT USING "###.C%";C%;
LOCATE 8,16 : PRINT USING "#####.#####";AA1;
LOCATE 8,57 : PRINT USING "#####.#####";AA2;
LOCATE 9,57 : PRINT USING "#####.#####";S;
LOCATE 10,57 : PRINT USING "#####.#####";E1;
LOCATE 11,57 : PRINT USING "#####.#####";E2;
LOCATE 12,49 : PRINT USING "#####.#####";R2;
* Will play tape if sound is on and corr coeff < 0.5
IF SND%=0 AND R2<0.5 THEN
PLAY "T120MBOZL4CCL2ELBCLBEL4GL9LCL8EL4GL4GL2BL4GL2CL4CCL2E"
END IF
RETURN

```

Code Listing for CORR502.INC

Subroutine to hardcopy the stats on the printer.

LPRINT

```

. Options section.
.
COLOR 0,15
LOCATE 14,1 : PRINT CHR$(216),STRING$(15,196),CHR$(101);
LOCATE 15,1 : PRINT CHR$(179),SPACES(15) ,CHR$(179);
LOCATE 16,1 : PRINT CHR$(198),STRING$(15,205),CHR$(181);
LOCATE 25,1 : PRINT CHR$(192),STRING$(15,196),CHR$(217);
FOR I%=17 TO 24
LOCATE I%,1 : PRINT CHR$(179),SPACES(15),CHR$(179);
NEXT I%
LOCATE 15,6 : PRINT 'Options';
.
. Have got screen so see what to do.
COLOR 14,0 : LOCATE 16+OPTN2%,3 : PRINT OPTN$(OPTN2%);
Startloop:
AS=INKEY$
SELECT CASE AS
CASE =
GOTO Startloop6
CASE CHR$(0)+CHR$(72),CHR$(0)+CHR$(80)
COLOR 0,15 : LOCATE 16+OPTN2%,3
PRINT OPTN$(OPTN2%);
IF AS=CHR$(0)+CHR$(72) THEN DECOR OPTN2% ELSE INCR OPTN2%
IF OPTN2%<1 THEN OPTN2%=8
IF OPTN2%>8 THEN OPTN2%=1
COLOR 14,0 : LOCATE 16+OPTN2%,3
PRINT OPTN$(OPTN2%);
GOTO Startloop6
CASE CHR$(13)
GOTO DoOption
CASE CHR$(0)+CHR$(75),CHR$(0)+CHR$(77)
GOTO Startloop6
CASE ELSE
SOUND 1000,3 : SOUND 800,1,5
GOTO Startloop6
END SELECT
DoOption:
IF OPTN2%<>8 THEN
COLOR 0,3
LOCATE 10,20 : PRINT CHR$(201),STRING$(36,205),CHR$(167);
FOR I%=11 TO 13
LOCATE I%,20 : PRINT CHR$(166),TAB(60),CHR$(166);
NEXT I%
LOCATE 14,20 : PRINT CHR$(200),STRING$(36,205),CHR$(168);
COLOR 4,3
LOCATE 12,29 : PRINT 'Writing the * : COLOR 14,3 : PRINT 'Config File';
GOSUB WriteConfigFile
END IF
SELECT CASE OPTN2%
CASE 1
CLOSE
GOSUB Logo
LOCATE 1,1
PRINT 'And it don't rain in Indianapolis in the summertime...'
AS=INKEY$
WHILE AS=-
AS=INKEY$
WEND
END
.
. Must find matching point.
TEMP%=1
OPEN ODIFS+OFIL$ FOR INPUT AS #1
IF NOT EOF(1) THEN INPUT #1,LINENAMES
IF NOT EOF(1) THEN INPUT #1,TITLE$
IF NOT EOF(1) THEN INPUT #1,XLABEL$
IF NOT EOF(1) THEN INPUT #1,YLABEL$
WHILE NOT EOF(1)
INPUT #1,OBS(TEMP%)
INPUT #1,CALC(TEMP%)
INPUT #1,USE%(TEMP%)
INPUT #1,SMPLNUM$
INPUT #1,POINTNO$
IF OBS(TEMP%)=TEMP1 AND CALC(TEMP%)=TEMP2 THEN GOTO Found
INCR TEMP%
WEND
Found
CLOSE #1
.
. This is a subroutine to find the closest match to the point.
WINDOW (0,460)-(640,0)
GET (0,417)-(175,480),PIX%
TEMP3=(I%-XOFFSET)/XOFFAC : TEMP4=(J%-YOFFSET)/YOFFAC
DIFF=ABS(TEMP3-OBS(1)) + ABS(TEMP4-CALC(1))
TEMP1=OBS(1) : TEMP2=CALC(1)
FOR I%=1 TO COUNT%
TEMP=ABS(TEMP3-OBS(I%)) + ABS(TEMP4-CALC(I%))
IF TEMP<DIFF THEN
DIFF=TEMP : TEMP1=OBS(I%) : TEMP2=CALC(I%)
END IF
NEXT I%
.
.

```

Code Listing for CORR505.INC

This is a subroutine to find the closest match to the point.

```

WINDOW (0,460)-(640,0)
GET (0,417)-(175,480),PIX%
TEMP3=(I%-XOFFSET)/XOFFAC : TEMP4=(J%-YOFFSET)/YOFFAC
DIFF=ABS(TEMP3-OBS(1)) + ABS(TEMP4-CALC(1))
TEMP1=OBS(1) : TEMP2=CALC(1)
FOR I%=1 TO COUNT%
TEMP=ABS(TEMP3-OBS(I%)) + ABS(TEMP4-CALC(I%))
IF TEMP<DIFF THEN
DIFF=TEMP : TEMP1=OBS(I%) : TEMP2=CALC(I%)
END IF
NEXT I%
.
. Must find matching point.
TEMP%=1
OPEN ODIFS+OFIL$ FOR INPUT AS #1
IF NOT EOF(1) THEN INPUT #1,LINENAMES
IF NOT EOF(1) THEN INPUT #1,TITLE$
IF NOT EOF(1) THEN INPUT #1,XLABEL$
IF NOT EOF(1) THEN INPUT #1,YLABEL$
WHILE NOT EOF(1)
INPUT #1,OBS(TEMP%)
INPUT #1,CALC(TEMP%)
INPUT #1,USE%(TEMP%)
INPUT #1,SMPLNUM$
INPUT #1,POINTNO$
IF OBS(TEMP%)=TEMP1 AND CALC(TEMP%)=TEMP2 THEN GOTO Found
INCR TEMP%
WEND
Found
CLOSE #1

```

```

LPRINT STRINGS(79,81)
LPRINT "No. CNo: Name: ";
LPRINT "Observed: Calculated: Difference: ";
LPRINT STRINGS(79,81)
END IF
.
.
.
. Must set up the screen.
COLOR 15,0 : CLS : COLOR 11,0
LOCATE 1,1 : PRINT LEFT$(ODIR$+OFILES,25);
LOCATE 1,60 : PRINT TIMES; "DATES: ";
LOCATE 2,1 : PRINT "Classes: "SCLASS$
LOCATE 3,1 : PRINT "Property: "PROPS$(PROP%);
LOCATE 3,60 : PRINT "Run Time: sec";
COLOR 14,0
LOCATE 4,1 : PRINT "No. CNo: Name: ";
PRINT "Observed: Calculated: Difference."
LOCATE 5,1 : PRINT STRINGS(80,166);
LINECNT%=6
.
.
.
. Have set up, so open output file and go to it!
OPEN ODIR$+OFILES FOR OUTPUT AS #3
PRINT #3,LINENAMES
PRINT #3,TITLE1$
PRINT #3,TITLE2$
PRINT #3,XLABEL$
PRINT #3,YLABEL$
RETURN

```

' init line ct

Code Listing for CORR507.INC

This is the section to see which compounds to use.

```

COLOR 15,0 : CLS
FOR I%=1 TO 9
IF CUSE$(I%)="Y" THEN
FILES=PRDIR$+"\CORR"+CLASS$(I%)+APNUM.DAT
OPEN FILES FOR INPUT AS #1
INPUT #1,NumOfCompounds
CLOSE #1
.
. Next will draw screen for each class.
GOSUB DrawCmpdScreen
GOSUB PageOfNames
BKGDND%=0 : GOSUB MarkCompoundName
Startloop8
AS=INKEY$
SELECT CASE AS
CASE =
CASE "O" OR CHR$(27)
GOTO StartOfProgram
CASE CHR$(13)
GOTO Continue8
.
. class loop
.
. get number
. compounds for
. this class
.
. no key
. quit
. return

```

```

. Will put a box around the point, display results.
WINDOW (-50,-50)-(530,525)
TEMP3=TEMP1*YEXPFA + XOFFSET : TEMP4=TEMP2*YEXPFA + YOFFSET
LINE (TEMP3-6,TEMP4-5)-(TEMP3+5,TEMP4+6),13,B
FOR I%=1 TO 4
LOCATE I%,1 : PRINT SPACES(22);
NEXT I%
LOCATE 1,1 : PRINT "O: "TEMP1;
LOCATE 2,1 : PRINT "C: "TEMP2;
LOCATE 3,1 : PRINT "P: "SMPLNUM$;
LOCATE 4,1 : PRINT "N: "LEFT$(SMPLNUM$,16);
WINDOW (0,480)-(640,0)
LINE (0,417)-(175,480),10,B
WINDOW (-50,-50)-(530,525)
AS=INKEY$
WHILE AS=" "
AS=INKEY$
WEND
LINE (TEMP3-6,TEMP4-5)-(TEMP3+5,TEMP4+6),0,B
FOR I%=1 TO 4
LOCATE I%,1 : PRINT SPACES(22);
NEXT I%
WINDOW (0,480)-(640,0)
PUT (0,480),PIX%
WINDOW (-50,-50)-(530,525)
RETURN

```

Code Listing for CORR506.INC

This is the subroutine to initialize the screen and the printer.

```

. Next will get search property.
IF SND$="Y" THEN PLAY "MB T200 L6 C3 DEFG P6 D L2 G"
SCLASS$=""
FOR I%=1 TO 10
IF CUSE$(I%)="Y" THEN SCLASS$=SCLASS$+CLASS$(I%)+". "
NEXT I%
LINENAMES=CHR$(34) + "Group Property " + PROPS$(PROP%) + CHR$(34)
XLABEL$ =CHR$(34) + "Observed " + PROPS$(PROP%) + CHR$(34)
YLABEL$ =CHR$(34) + "Calculated " + PROPS$(PROP%) + CHR$(34)
TITLE1$ =CHR$(34) + "Predicted vs Observed " + PROPS$(PROP%) + CHR$(34)
TITLE2$ =CHR$(34) + " " + CHR$(34)
.
. Will setup the screen and printer.
.
. Must print headings if hardcopy is on.
IF HCOPI$="Y" THEN
LPRINT PROPS$(PROP%); "predictions: "TIMES; "DATES"
LPRINT " "
LPRINT SCLASS$

```

```

CASE 'O','o'
GOTO Options
CASE 'P','p'
LPRINT CHR$(12)
CASE 'G','g'
GOTO Graph
CASE 'B','b'
GOTO BarGraphAndPieChart
CASE 'E','e'
GOTO Statistics
CASE '-'
FOR J%=1 TO NumOfCompounds
  CUSE$(J%,J%)=1
NEXT J%
GOSUB PageOfNames
BKGNDF%=0 : GOSUB MarkCompoundName
CASE '.'
FOR J%=1 TO NumOfCompounds
  CUSE$(J%,J%)=0
NEXT J%
GOSUB PageOfNames
BKGNDF%=0 : GOSUB MarkCompoundName
CASE '*'
BKGNDF%=1 : GOSUB MarkCompoundName
TEMP%=CUSE$(J%,OPTN3$(J%))
IF TEMP%=1 THEN TEMP%=0 ELSE TEMP%=1
CUSE$(J%,OPTN3$(J%))=TEMP%
BKGNDF%=0 : GOSUB MarkCompoundName
CASE 'C','c'
BKGNDF%=1 : GOSUB MarkCompoundName
IF A$=CHR$(0)+CHR$(72) THEN DECR OPTN3$(J%) ELSE INCR OPTN3$(J%)
TEMP1%=(CPAGE$(J%)-1)*100 + 1
TEMP2%=(CPAGE$(J%)-1)*100
IF OPTN3$(J%)<TEMP1% THEN OPTN3$(J%)=TEMP2%
IF OPTN3$(J%)>TEMP2% THEN OPTN3$(J%)=TEMP1%
BKGNDF%=0 : GOSUB MarkCompoundName
CASE CHR$(0)+CHR$(73), CHR$(0)+CHR$(81)
IF CPAGE$(J%)=1 THEN
  CPAGE$(J%)=2 : INCR OPTN3$(J%),100
ELSE
  CPAGE$(J%)=1 : DECR OPTN3$(J%),100
END IF
COLOR 12,1 : LOCATE 6,71 : PRINT USING "#.#":CPAGE$(J%),
GOSUB PageOfNames
BKGNDF%=0 : GOSUB MarkCompoundName
CASE 'H','h'
LPRINT "Summary of compounds not used: ",DATE$
LPRINT " Class being searched: ",CLASS$(J%)
LPRINT " Property being searched: ",PROP$(PROP%)
LPRINT " Number of Compounds: ",NumOfCompounds
LPRINT " Output file: ",ODIR$,OFILES$
FOR J%=1 TO NumOfCompounds
  IF CUSE$(J%,J%)=0 THEN
    CNAME$="C"+RIGHT$(STR$(J%),LEN(STR$(J%))-1)
    LPRINT CNAME$,
  END IF
NEXT J%
LPRINT : LPRINT
CASE '1','2','3'
COLOR 31,4

```

```

LOCATE 23,25 : PRINT " Press <*> ON, or <-> for OFF ";
TEMP%=INPUT$(1)
SELECT CASE TEMP%
CASE CHR$(27),"*",'^'
  ' Exit
COLOR 15,0
LOCATE 23,25 : PRINT SPACES$(30);
GOTO StartOfProgram
CASE '...',.'
  ' ok
CASE ELSE
  SOUND 1000,3 : SOUND 800,1,5
  GOTO Startloop6
END SELECT
SELECT CASE A$
CASE '1' : TEMP1%=1 : TEMP2%=20
CASE '2' : TEMP1%=21 : TEMP2%=40
CASE '3' : TEMP1%=41 : TEMP2%=100
END SELECT
FOR J%=TEMP1% TO TEMP2%
  IF J%<=NumOfCompounds THEN
    IF TEMP%="" THEN CUSE$(J%,J%)=1 ELSE CUSE$(J%,J%)=0
  END IF
NEXT J%
GOSUB PageOfNames
COLOR 15,0
LOCATE 23,25 : PRINT SPACES$(30);
BKGNDF%=0 : GOSUB MarkCompoundName
CASE ELSE
  SOUND 1000,3 : SOUND 800,1,5
END SELECT
GOTO Startloop6
Continued:
NEXT 1%
RETURN
DrawCmpdScreen:
This is the subroutine to draw the compound use screen.

```

```

' First is box for compounds
COLOR 2,1
LOCATE 5,4 : PRINT CHR$(201);STRINGS$(71,205);CHR$(187);
FOR J%=6 TO 17
  LOCATE J%,4 : PRINT CHR$(186);STRINGS$(71,32);CHR$(186);
NEXT J%
LOCATE 18,4 : PRINT CHR$(200);STRINGS$(71,205);CHR$(188);
LOCATE 7,4 : PRINT CHR$(189);STRINGS$(71,166);CHR$(182);
COLOR 14,1
LOCATE 6,9 : PRINT "Class: ";
LOCATE 6,32 : PRINT "Number of Compounds: ";
LOCATE 6,68 : PRINT "Page: ";
COLOR 11,1 : LOCATE 6,16 : PRINT CLASS$(J%);
COLOR 11,1 : LOCATE 6,53 : PRINT USING "#.#":NumOfCompounds;

```

```

LOCATE (OPTN3%(I%)-(CPAGE%(I%)-1)*100)-TEMP%*10+7,TEMP%*7+5
IF OPTN3%(I%) <= NumOfCompounds THEN
  IF CUSE%(I%,OPTN3%(I%))=1 THEN
    IF BKGND%=0 THEN TEMP%=12 ELSE TEMP%=10
    COLOR TEMP%,BKGND%
    PRINT *,CHR$(19),CNAME$(I-LEN(CNAMES));
  ELSE
    IF BKGND%=0 THEN TEMP%=14 ELSE TEMP%=15
    COLOR TEMP%,BKGND%
    PRINT *,CNAME$(I-LEN(CNAMES));
  END IF
ELSE
  COLOR 15, BKGND% : PRINT SPACES(7);
END IF
END IF
RETURN

```

Code Listing for CORR508.INC

This is the subroutine to get the class of fuels to use.

```

* Options box
SCREEN 0 : WIDTH 80
COLOR 15,0 : CLS
COLOR 10,1
LOCATE 7,15 : PRINT CHR$(216),STRINGS$(49,199),CHR$(191); ' top line
FOR I%=6 TO 16
  LOCATE I%,15 : PRINT CHR$(179),TAB(65),CHR$(179); ' middle
NEXT I%
LOCATE 17,15 : PRINT CHR$(192),STRINGS$(49,199),CHR$(217); ' bottom line
COLOR 10,0
LOCATE 8,15 : PRINT TIMES;
LOCATE 8,58 : PRINT DATES;
COLOR 12,1
LOCATE 8,20 : PRINT 'Please mark the classes of fuels to use.';
GOSUB PrintFuelClasses
* Next are commands
COLOR 3,0
LOCATE 21,17 : PRINT ' Press <SPACE> to toggle the mark. ' ;
LOCATE 22,17 : PRINT 'Press <RET> to continue, <O> for options menu.';
COLOR 12,0
TEMP%=Output File '+ODIR$+OFIL$
LOCATE 25,40-0 5*LEN(TEMP%) : PRINT TEMP%;
* Next see what to do.
BKGND%=0 : GOSUB MarkFuelClass
Startloop10.
AS=INKEY$
SELECT CASE AS
CASE =

```

```

COLOR 12,1 : LOCATE 8,71 : PRINT USING '#':CPAGE%(I%);
* Next is header/footer information.
COLOR 10,0
LOCATE 3,18 : PRINT 'Please indicate the compounds to use in this run.';
COLOR 3,0
LOCATE 20,8 : PRINT 'Press <+> to mark all, <-> to unmark all.';
PRINT '<SPACE>' to toggle mark.';
PRINT '<ARROW KEYS>' to move cursor, <PG UP><PG DN>' ;
LOCATE 21,10 : PRINT 'to change pages.';
LOCATE 22,8 : PRINT '<H>' to hardcopy, <P> to form feed.';
PRINT '<RETURN>' to continue, <Q> to quit.';
COLOR 12,0
TEMP%=Output File '+ODIR$+OFIL$
LOCATE 25,40-0 5*LEN(TEMP%) : PRINT TEMP%;
RETURN

```

PageCNAMES:

This is the subroutine to draw a page of compound names.

```

FOR J%=(CPAGE%(I%)-1)*100+1 TO CPAGE%(I%)*100
IF J%<=NumOfCompounds THEN
  TEMP%=INT(J%/(CPAGE%(I%)-1)*100-1)/10
  LOCATE (J%-(CPAGE%(I%)-1)*100)-TEMP%*10+7,TEMP%*7+5
  CNAME$='C'+RIGHT$(STR$(J%),LEN(STR$(J%))-1)
  IF CUSE%(I%,J%)=1 THEN
    COLOR 10,1
    PRINT *,CHR$(19),CNAME$(I-LEN(CNAMES));
  ELSE
    COLOR 15,1
    PRINT *,CNAME$(I-LEN(CNAMES));
  END IF
ELSE
  COLOR 15,1
  TEMP%=INT(J%/(CPAGE%(I%)-1)*100-1)/10
  LOCATE (J%-(CPAGE%(I%)-1)*100)-TEMP%*10+7,TEMP%*7+5
  PRINT SPACES(7);
END IF
NEXT J%
RETURN

```

MarkCompoundName:

This is the subroutine to mark a compound name.

```

IF CPAGE%(I%)=INT((OPTN3%(I%)-1)/100)+1 THEN
  CNAME$='C'+RIGHT$(STR$(OPTN3%(I%)),LEN(STR$(OPTN3%(I%)))-1)
  TEMP%=INT((OPTN3%(I%)-(CPAGE%(I%)-1)*100-1)/10)

```

```

COLOR 10,0 : LOCATE 8,15 : PRINT TIMES;
GOTO Startloop10
CASE CHR$(13)
RETURN
CASE "Q", "q", CHR$(27)
GOTO StartOfProgram
CASE "O", "o"
GOTO Options
CASE "G", "g"
GOTO Graph
CASE "B", "b"
GOTO BarGraphAndPieChart
CASE "E", "e"
GOTO Statistics
CASE ""
FOR I%=1 TO 5
FUELCLASS%(I%)=1
NEXT I%
GOSUB PrintFuelClasses
BKGN%D%=0 : GOSUB MarkFuelClass
CASE ""
FOR I%=1 TO 5
FUELCLASS%(I%)=0
NEXT I%
GOSUB PrintFuelClasses
BKGN%D%=0 : GOSUB MarkFuelClass
CASE ""
BKGN%D%=1 : GOSUB MarkFuelClass
TEMP%:=FUELCLASS%(OPTN4%)
IF TEMP%=1 THEN TEMP%=0 ELSE TEMP%=1
FUELCLASS%(OPTN4%)=TEMP%
BKGN%D%=0 : GOSUB MarkFuelClass
BKGN%D%=1 : GOSUB MarkFuelClass
IF AS=CHR$(0)+CHR$(72), CHR$(0)+CHR$(80)
IF OPTN4%<1 THEN OPTN4%=5
IF OPTN4%>5 THEN OPTN4%=1
BKGN%D%=0 : GOSUB MarkFuelClass
CASE ELSE
SOUND 1000,3 : SOUND 800,1,5
END SELECT
GOTO Startloop10

PrintFuelClasses:
. This is a mini-subroutine to draw a page of fuel class names.
FOR I%=1 TO 5
LOCATE 10+I%,34
COLOR 14,1 : PRINT USING "#) ",I%;
IF FUELCLASS%(I%)=0 THEN
COLOR 15,1 : PRINT " ",FUELCLASS%(I%);
ELSE
COLOR 10,1 : PRINT CHR$(16);FUELCLASS%(I%);
END IF
NEXT I%
RETURN
MarkFuelClass:
. This is a mini-subroutine to mark a fuel class for use
LOCATE 10+OPTN4%,37
IF FUELCLASS%(OPTN4%)=0 THEN
COLOR 15,BKGN%D% : PRINT " ",FUELCLASS$(OPTN4%); " ";
ELSE
COLOR 10,BKGN%D% : PRINT " ",CHR$(16);FUELCLASS$(OPTN4%); " ";
END IF
RETURN

```

Code Listing for CORR509.INC

This is the subroutine to get the cetane improver level.

```

. Options box
SCREEN 0 : WIDTH 80
COLOR 15,0 : CLS
COLOR 10,1
LOCATE 7,15 : PRINT CHR$(216);STRINGS$(49,190);CHR$(191); ' top line
FOR I%=8 TO 16
LOCATE I%,15 : PRINT CHR$(179);TAB(85);CHR$(179); ' middle
NEXT I%
LOCATE 17,15 : PRINT CHR$(192);STRINGS$(49,190);CHR$(217); ' bottom line
COLOR 10,0
LOCATE 6,15 : PRINT TIMES;
LOCATE 8,96 : PRINT DATES;
COLOR 14,1
LOCATE 9,23 : PRINT "Please Enter the Improver level for";
LOCATE 10,28 : PRINT "the Cetane Calculations";
COLOR 12,1
LOCATE 15,27 : PRINT "<NUL> = all Improver levels";
COLOR 12,0
TEMP%="Output File "+ODIR$+OFIL$
LOCATE 25,40-0.5*LEN(TEMP%) : PRINT TEMP%;
. Next will get level
COLOR 15,1
LOCATE 13,38 : LINE INPUT CETLEVELS
IF CETLEVELS<>" " THEN
WHILE LEN(CETLEVELS)<8
CETLEVELS=CETLEVELS+" "
WEND
END IF
LOCATE 19,0
LOCATE 22,15 : PRINT "Is this correct? <RET>=Yes, <N>=No, <Q>=quit, <O>=phone";
Startloop11:
AS=INKEY$
SELECT CASE AS
CASE ""
CASE "Y", "y", CHR$(13)
RETURN
CASE "N", "n"
GOTO GetCellLevel
. no key
. correct
. incorrect

```



```

COLOR 15,BKGNDR% : PRINT * "FRACTIONS(OPTN5%)" * ;
ELSE
COLOR 10,BKGNDR% : PRINT * "CHRS(10);FRACTIONS(OPTN5%)" * ;
END IF
RETURN
    
```

Code Listing for CORR511.INC

You did not:

This is the subrtn to for those who forgot to select any classes.

```

COLOR 15,4 : CLS
LOCATE 11,31 : PRINT *** YOU IDIOT ***
LOCATE 12,24 : PRINT "you forgot to select any classes!";
SOUND 1000,3 : SOUND 800,1.5
AS=INKEYS
WHILE AS=""
AS=INKEYS
WEND
GOTO StartOfProgram
    
```

GetNumberOfCompounds:

This is the subrtn to read num of compounds in the directory.

```

FILES=PRDRVS+"CORR"+CLASS$(I%)+^PNUM.DAT
OPEN FILES FOR INPUT AS #1
INPUT #1,NumOfCompounds
CLOSE #1
COLOR 0,15 : LOCATE 1,20
PRINT USING " Class: # Pass ### of ### " ;I%,J%,NumOfCompounds,
RETURN
    
```

GetPropData:

This is the subroutine to read a property file.

```

SELECT CASE RMDSKS
CASE "H"
PNUMS=PRDRVS+"CORR"+CLASS$(I%)+^*
PNUMS=PNUMS+^P+^RIGHT$(STR$(J%),LEN(STR$(J%))-1)+^DAT
    
```

```

CASE "V"
PNUMS=F+^P+^RIGHT$(STR$(J%),LEN(STR$(J%))-1)+^DAT
END SELECT
OPEN PNUMS FOR INPUT AS #1
DS(1)=" : INPUT #1,DS(1)
K%=2
WHILE NOT EOF(1) AND K%<=42
DS(K%)=" : INPUT #1,DS(K%)
IF LEN(DS(K%))>8 THEN DS(K%)=LEFT$(DS(K%),8)
WHILE LEN(DS(K%))<8
DS(K%)=DS(K%)+*
WEND
INCR K%
WEND
CLOSE #1
RETURN
    
```

ReadConfigFile:

This is the subroutine to read the config file.

```

* Will write message to the user.
COLOR 0,3
LOCATE 10,20 : PRINT CHR$(201);STRING$(30,205);CHR$(167);
FOR I%=11 TO 13
LOCATE I%,20 : PRINT CHR$(168);TAB(60);CHR$(169);
NEXT I%
LOCATE 14,20 : PRINT CHR$(200);STRING$(30,205);CHR$(169);
COLOR 4,3
LOCATE 12,29 : PRINT "Reading the "; COLOR 14,3 : PRINT "Config File";
    
```

```

* Must next read the file
OPEN CFGDIRS+"CORRCFG.DAT" FOR INPUT AS #4
INPUT #4,ODIRS
INPUT #4,OFILES
INPUT #4,HCOOPY$
INPUT #4,RMDSKS
INPUT #4,CLASS$
INPUT #4,PROP%
INPUT #4,OPTN%
INPUT #4,OPTN2%
INPUT #4,OPTN4%
INPUT #4,OPTN5%
INPUT #4,OPTN6%
INPUT #4,OPTN7%
INPUT #4,OPTN8%
INPUT #4,OPTN9%
FOR KKK%=1 TO 9 : INPUT #4,OPNT3%(KKK%) : NEXT KKK%
FOR KKK%=1 TO 8 : INPUT #4,CPAGE$(KKK%) : NEXT KKK%
FOR KKK%=1 TO 10 : INPUT #4,CUSE$(KKK%) : NEXT KKK%
FOR KKK%=1 TO 5 : INPUT #4,FUELCLASS$(KKK%) : NEXT KKK%
FOR KKK%=1 TO 5 : INPUT #4,FRACTION$(KKK%) : NEXT KKK%
WHILE NOT EOF(4)
    
```

* RAM disk
* open file
* read name
* read data
* make all
* fields =
* len of 8

* get number
* compounds for
* this class

* hard disk

```

25 AS T$(22)
GET 5 PROP%
SLOPEFACTOR=VAL(S$) : INTCPFACTOR=VAL(I$)
OFFSETFACR=VAL(O$) : FUNCTION$=F$
FOR J%=1 TO 22
    MIXCOEFF(J%)=VAL(T$(J%))
NEXT J%
CLOSE #5
RETURN
    
```

WriteFuelParams:

This is the subroutine to write the fuel parameters file.

```

OPEN CFGDIR$+FUELPARM.DAT FOR RANDOM AS #5 LEN=729
FIELD #5, 25 AS S$, 25 AS I$, 25 AS O$, 25 AS F$, 25 AS T$( 1),_
25 AS T$( 2), 25 AS T$( 3), 25 AS T$( 4), 25 AS T$( 5), 25 AS T$( 6),_
25 AS T$( 7), 25 AS T$( 8), 25 AS T$( 9), 25 AS T$(10), 25 AS T$(11),_
25 AS T$(12), 25 AS T$(13), 25 AS T$(14), 25 AS T$(15), 25 AS T$(16),_
25 AS T$(17), 25 AS T$(18), 25 AS T$(19), 25 AS T$(20), 25 AS T$(21),_
25 AS T$(22)
LSET S$=STR$(SLOPEFACTOR)
LSET I$=STR$(INTCPFACTOR)
LSET O$=STR$(OFFSETFACR)
LSET F$=FUNCTION$
FOR J%=1 TO 22
    LSET T$(J%)=STR$(MIXCOEFF(J%))
NEXT J%
PUT #5, PROP%
CLOSE #5
RETURN
    
```

DrawString:

This is a subroutine to draw a string on the graphics screen.

```

OPEN CHARACTER.DAT FOR RANDOM AS #1
FIELD #1, 40 AS CHARS
TEMP% = LEN(TEMP$)
FOR I%=1 TO TEMP%
    IF ASC(MID$(TEMP$,I%,1)) >= 33 AND ASC(MID$(TEMP$,I%,1)) <= 122 THEN
        GET #1,ASC(MID$(TEMP$,I%,1))
        DRAW "BM"+STR$(TEMP%)+","+STR$(TEMP%)+CHARS
        draw char
    END IF
    IF TEMP1$="X" THEN INCR TEMP%:12 ELSE INCR TEMP%:12
NEXT I%
CLOSE #1
RETURN
    
```

```

INPUT #4,TEMP1%
INPUT #4,TEMP2%
CUSE$(TEMP1%,TEMP2%)=0
WEND
CLOSE #4
RETURN
    
```

WriteConfigFile:

This is the subroutine to write the config file.

```

OPEN CFGDIR$+CORROFG.DAT FOR OUTPUT AS #4
PRINT #4, ODIR$
PRINT #4, OFILES$
PRINT #4, HCOPI$
PRINT #4, RMDSK$
PRINT #4, CLASS$
PRINT #4, PROP%
PRINT #4, OPTN%
PRINT #4, OPTN2%
PRINT #4, OPTN4%
PRINT #4, OPTN5%
PRINT #4, OPTN6%
PRINT #4, OPTN7%
PRINT #4, OPTN8%
PRINT #4, OPTN9%
FOR KKK%=1 TO 9 : PRINT #4, OPTN3%(KKK%) : NEXT KKK%
FOR KKK%=1 TO 9 : PRINT #4, CPAGES%(KKK%) : NEXT KKK%
FOR KKK%=1 TO 10 : PRINT #4, CUSE$(KKK%) : NEXT KKK%
FOR KKK%=1 TO 5 : PRINT #4, FUELCCLASS%(KKK%) : NEXT KKK%
FOR KKK%=1 TO 5 : PRINT #4, FRACTION%(KKK%) : NEXT KKK%
FOR JJJ%=1 TO 200
    IF CUSE$(KKK%,JJJ%)=0 THEN PRINT #4,KKK%+","+JJJ%
NEXT JJJ%
NEXT KKK%
CLOSE #4
RETURN
    
```

ReadFuelParams:

This is the subroutine to read the fuel parameters file.

```

OPEN CFGDIR$+FUELPARM.DAT FOR RANDOM AS #5 LEN=729
FIELD #5, 25 AS S$, 25 AS I$, 25 AS O$, 25 AS F$, 25 AS T$( 1),_
25 AS T$( 2), 25 AS T$( 3), 25 AS T$( 4), 25 AS T$( 5), 25 AS T$( 6),_
25 AS T$( 7), 25 AS T$( 8), 25 AS T$( 9), 25 AS T$(10), 25 AS T$(11),_
25 AS T$(12), 25 AS T$(13), 25 AS T$(14), 25 AS T$(15), 25 AS T$(16),_
25 AS T$(17), 25 AS T$(18), 25 AS T$(19), 25 AS T$(20), 25 AS T$(21),_
25 AS T$(22)
    
```


Code Listing for CORR512.INC

Section to draw the graph of the data.

```

* Have got stats, so draw graph of data.
IF PTCOIN$="Y" AND COUNT%>0 THEN GOSUB RegressionAnalysis ' calc stats
* First is menu of graph choices.
COLOR 2, 4
LOCATE 15, 5 : PRINT CHR$(201);STRING$(90,205);CHR$(187); ' top line
FOR I%=19 TO 21
LOCATE I%,5;PRINT CHR$(188);STRING$(90, 32);CHR$(186); ' ends
NEXT I%
LOCATE 22, 6 : PRINT CHR$(200);STRING$(90,205);CHR$(186); ' bottom line
LOCATE 15,45 : PRINT CHR$(209); ' top junct
LOCATE 22,45 : PRINT CHR$(207); ' bottom junct
FOR I%=19 TO 21 : LOCATE I%,45 : PRINT CHR$(179); : NEXT I% 'center line
COLOR 15, 4
LOCATE 16,10 : COLOR 11,4 : PRINT "F"; COLOR 15, 4 : PRINT "f";
LOCATE 17,10 : COLOR 11,4 : PRINT "D"; COLOR 15, 4 : PRINT "d";
LOCATE 18,10 : COLOR 11,4 : PRINT "T"; COLOR 15, 4 : PRINT "t";
LOCATE 19,10 : COLOR 11,4 : PRINT "X"; COLOR 15, 4 : PRINT "x";
LOCATE 20,10 : COLOR 11,4 : PRINT "Y"; COLOR 15, 4 : PRINT "y";
LOCATE 21,10 : COLOR 11,4 : PRINT "L"; COLOR 15, 4 : PRINT "l";
LOCATE 16,49 : PRINT "Auto Scale";
LOCATE 17,49 : PRINT "Point Connect";
LOCATE 18,49 : PRINT "Display Stat";
COLOR 14, 4
LOCATE 16,21 : PRINT LEFT$(OFIL$
LOCATE 17,21 : PRINT LEFT$(ODIR$
LOCATE 18,21 : PRINT LEFT$(TITLE$
LOCATE 19,21 : PRINT LEFT$(XLAB$
LOCATE 20,21 : PRINT LEFT$(YLAB$
LOCATE 21,21 : PRINT LEFT$(LINENAMES;22);
LOCATE 16,70 : PRINT SCALES;
LOCATE 17,70 : PRINT PTCOIN$;
LOCATE 18,70 : PRINT STAT$;
COLOR 3, 0
LOCATE 24, 7 : PRINT "Press <LETTER> to change the field,";
LOCATE 25,10 : PRINT "<ARROW KEYS> to change option,";
PRINT "<P> to Form Feed, <Q> to quit,";
* Have got the screen drawn, so see what to do.
IF GOPTN%=1 THEN TEMP%=SCALES
IF GOPTN%=2 THEN TEMP%=PTCOIN$
IF GOPTN%=3 THEN TEMP%=STAT$
COLOR 14, 0 : LOCATE GOPTN%+15,99
PRINT " ",TEMP%;";
Startloop2:
AS=INKEY$
SELECT CASE AS

```

```

CASE " " : LOCATE 2,11 : PRINT TIMES : GOTO Startloop2
CASE "Q",q' : quit
CLOSE : GOTO StartOfProgram
CASE "O",o' : options
CASE CHR$(13) : enter
CASE "H",h' : hcopy stats
GOSUB HardCopyStats
GOTO Startloop2
CASE "P",p' : form feed
LPRINT CHR$(12)
GOTO Startloop2
CASE "E",e' : error dist
CASE "B",b' : bar chart
GOTO BarGraphAndPieChart
CASE "S",s' : sound
IF SND$="Y" THEN SND$="N" ELSE SND$="Y"
COLOR 10,0 : LOCATE 23,3
PRINT "Sound = " ;SND$;
IF SND$="Y" THEN SOUND 800,2 ELSE SOUND 300,4
DELAY 0.5
COLOR 15,0 : LOCATE 23,3
PRINT SPACES$(15);
GOTO Startloop2
CASE "D",d' : directory
COLOR 31, 4
LOCATE 17,10 : PRINT "Directory";
COLOR 14, 4
LOCATE 17,21 : PRINT SPACES$(21);
LOCATE 17,21 : LINE INPUT ODIR$
ODIR$=UCASE$(ODIR$)+";"
LOCATE 17,21 : PRINT ODIR$;
LOCATE 17,10 : COLOR 11,4 : PRINT "D";
COLOR 15, 4 : PRINT "Directory";
GOTO Startloop2
CASE "T",t' : title
COLOR 31, 4
LOCATE 16,10 : PRINT "Title";
COLOR 14, 4
LOCATE 16,21 : PRINT SPACES$(21);
LOCATE 16,21 : LINE INPUT TITLE$
LOCATE 16,10 : COLOR 11,4 : PRINT "T";
COLOR 15, 4 : PRINT "Title";
GOTO Startloop2
CASE "X",x' : X label
COLOR 31, 4
LOCATE 16,10 : PRINT "X Label";
COLOR 14, 4
LOCATE 16,21 : PRINT SPACES$(21);
LOCATE 16,21 : LINE INPUT XLABEL$
LOCATE 16,10 : COLOR 11,4 : PRINT "X";
COLOR 15, 4 : PRINT "Label";
GOTO Startloop2
CASE "Y",y' : Y label
COLOR 31, 4
LOCATE 20,10 : PRINT "Y Label";
COLOR 14, 4

```

```

LOCATE 20,21 : PRINT SPACES(21);
LOCATE 20,21 : LINE INPUT YLABLES
LOCATE 20,10 : COLOR 11,4 : PRINT "Y";
COLOR 15, 4 : PRINT " Lable";
GOTO Startloop2
CASE "L",*
COLOR 31, 4
LOCATE 21,10 : PRINT "Line Name";
COLOR 14, 4
LOCATE 21,21 : PRINT SPACES(21);
LOCATE 21,21 : LINE INPUT LINENAMES$
LOCATE 21,10 : COLOR 11,4 : PRINT "L";
COLOR 15, 4 : PRINT "Line Name";
GOTO Startloop2
CASE "F",*
TEMP$=OFILF$
COLOR 31,4
LOCATE 16,10 : PRINT "File";
COLOR 14,4
LOCATE 16,21 : PRINT SPACES(22);
LOCATE 16,21 : LINE INPUT OFILF$
IF OFILF$="" THEN
OFILF$=TEMP$
LOCATE 16,21 : PRINT OFILF$
END IF
GOSUB GetFile
GOTO Graph
CASE CHR$(0)+CHR$(75),CHR$(0)+CHR$(77)
SELECT CASE GOPTN%
CASE 1
IF SCALES="" THEN SCALES="N" ELSE SCALES="Y"
TEMP$=SCALES
CASE 2
SELECT CASE PTOONS$
CASE "Y"
PTOONS$="N" : TEMPS$=PTOONS$
CASE "N"
PTOONS$="Y" : TEMPS$=PTOONS$
CASE "*"
PTOONS$="Y" : TEMPS$=PTOONS$
END SELECT
CASE 3
IF STAT$="" THEN STAT$="N" ELSE STAT$="Y"
TEMP$=STAT$
END SELECT
COLOR 14, 0 : LOCATE GOPTN%+15,66
PRINT " ",TEMP$," ";
GOTO Startloop2
CASE CHR$(0)+CHR$(72), CHR$(0)+CHR$(60)
IF GOPTN%=1 THEN TEMPS$=SCALES$
IF GOPTN%=2 THEN TEMPS$=PTOONS$
IF GOPTN%=3 THEN TEMPS$=STAT$
COLOR 14, 4 : LOCATE GOPTN%+15,66
PRINT " ",TEMP$," ";
IF AS=CHR$(0)+CHR$(72) THEN DECR GOPTN%
IF AS=CHR$(0)+CHR$(60) THEN INCR GOPTN%
IF GOPTN%<1 THEN GOPTN%=3
IF GOPTN%>3 THEN GOPTN%=1
IF GOPTN%=1 THEN TEMPS$=SCALES$
IF GOPTN%=2 THEN TEMPS$=PTOONS$

```

```

IF GOPTN%=3 THEN TEMPS$=STAT$
COLOR 14, 0 : LOCATE GOPTN%+15,66
PRINT " ",TEMP$," ";
GOTO Startloop2
CASE ELSE
SOUND 1000,3 : SOUND 800,1.5
GOTO Startloop2
END SELECT
DrawGraph;
* Will catch stupid mistakes. (no data file loaded into memory)
IF COUNT%=<1 THEN
COLOR 15,0 : CLS
LOCATE 11,21 : PRINT "*** OK, Stupid - Load a data file! ***";
SOUND 1000,3 : SOUND 800,1.5
AS=INKEY$
WHILE AS=""
AS=INKEY$
WEND
COLOR 15,0 : CLS
GOTO Graph
END IF
* First must find the max and min values in file.
IF SCALES="" THEN
MAXY=OBS(1) : MINX=OBS(1)
MAXY=CALC(1) : MINY=CALC(1)
FOR I%=1 TO COUNT%
IF OBS(I%) < MINX THEN MINX=OBS(I%)
IF OBS(I%) > MAXY THEN MAXY=OBS(I%)
IF CALC(I%) < MINY THEN MINY=CALC(I%)
IF CALC(I%) > MAXY THEN MAXY=CALC(I%)
NEXT I%
IF MAXY>0 THEN MAXY=MAXY+.05*MAXX ELSE MAXY=MAXY-.05*MAXX
IF MINX<0 THEN MINX=MINX-.05*MINX ELSE MINX=MINX+.05*MINX
IF MAXY>0 THEN MAXY=MAXY+.05*MAXY ELSE MAXY=MAXY-.05*MAXY
IF MINY<0 THEN MINY=MINY-.05*MINY ELSE MINY=MINY+.05*MINY
ELSE
* Must draw screen for min and max data.
COLOR 15, 0 : CLS : COLOR 2,4
LOCATE 7,15 : PRINT CHR$(201),STRINGS$(48,205),CHR$(187); 'top line
FOR I%=6 TO 16
LOCATE I%,15 : PRINT CHR$(186),STRINGS$(48, 32),CHR$(186); 'ends
NEXT I%
LOCATE 17,15 : PRINT CHR$(200),STRINGS$(48,205),CHR$(188); 'bottom line
COLOR 15, 4
LOCATE 9,27 : PRINT "Minimum X Value";
LOCATE 10,27 : PRINT "Maximum X Value";
LOCATE 11,27 : PRINT "Minimum Y Value";
LOCATE 12,27 : PRINT "Maximum Y Value";
LOCATE 14,24 : PRINT "Position Cursor to change a value ";
COLOR 14, 4
LOCATE 9,44 : PRINT MINX;
LOCATE 10,44 : PRINT MAXX;
LOCATE 11,44 : PRINT MINY;
LOCATE 12,44 : PRINT MAXY;
* Must see what to do
TEMP%=1 : LOCATE 8+TEMP%,44 : COLOR 14,0 : PRINT MINX;

```

```

Startloop3:
AS=INKEY$
SELECT CASE AS
CASE =
GOTO Startloop3
CASE '0', '1'
COLOR 15,0 : CLS
GOTO Graph
CASE '0', '1'
GOTO Options
CASE CHR$(13)
GOTO Continue3
CASE ' ','1','2','3','4','5','6','7','8','9'
COLOR 14,4
LOCATE 8+TEMP%,44 : PRINT SPACES(20);
COLOR 14,0 : LOCATE 8+TEMP%,44 : PRINT AS;
SELECT CASE TEMP%
CASE 1
LINE INPUT TEMP%
MINX=VAL(AS+TEMP%)
GOTO Startloop3
CASE 2
LINE INPUT TEMP%
MAXX=VAL(AS+TEMP%)
GOTO Startloop3
CASE 3
LINE INPUT TEMP%
MINY=VAL(AS+TEMP%)
GOTO Startloop3
CASE 4
LINE INPUT TEMP%
MAXY=VAL(AS+TEMP%)
GOTO Startloop3
CASE ELSE
SOUND 1000,3 : SOUND 800,1.5
GOTO Startloop3
END SELECT
CASE CHR$(0)+CHR$(72), CHR$(0)+CHR$(80)
COLOR 14,4
LOCATE 8+TEMP%,44
IF TEMP%=1 THEN PRINT MINX;
IF TEMP%=2 THEN PRINT MAXX;
IF TEMP%=3 THEN PRINT MINY;
IF TEMP%=4 THEN PRINT MAXY;
IF AS=CHR$(0)+CHR$(72) THEN DECOR TEMP% ELSE INCR TEMP%
IF TEMP%<1 THEN TEMP%=4
IF TEMP%>4 THEN TEMP%=1
COLOR 14,0
LOCATE 8+TEMP%,44
IF TEMP%=1 THEN PRINT MINX;
IF TEMP%=2 THEN PRINT MAXX;
IF TEMP%=3 THEN PRINT MINY;
IF TEMP%=4 THEN PRINT MAXY;
GOTO Startloop3
CASE ELSE
SOUND 1000,3 : SOUND 800,1.5
GOTO Startloop3
END SELECT
END IF
Continue3:
Startloop3:
XORANGE =MAXX-MINX
YORANGE =MAXY-MINY
XEXPFACTOR=500/XORANGE
YEXPFACTOR=500/YORANGE
XOFFSET=(0-MINX)*XEXPFACTOR
YOFFSET=(0-MINY)*YEXPFACTOR
.
. Will set up the screen.
OPEN "CHARACTR.DAT" FOR RANDOM AS #1
FIELD #1, 40 AS CHARS
SCREEN 12
COLOR 11,0
C1%=12
C2%=14
C3%=10
C4%=11
C5%=15
DRAW 'BM 350,240 C12'
DRAW 'S8 D8 E2 F3 E2 H3 E2 L6'
DRAW 'B2 P4,12'
GET (350,232)-(381,240),POINTER%
DRAW 'S4'
CLS
WINDOW (-50,-50)-(630,620)
DRAW 'C'+STRS(C2%)
TEMP%=350-(8*LEN(TITLE18))
FOR I%=1 TO LEN(TITLE18)
IF ASC(MID$(TITLE18,I%,1))>=33 AND ASC(MID$(TITLE18,I%,1))<=122 THEN
GET #1,ASC(MID$(TITLE18,I%,1))
DRAW 'BM'+STRS(TEMP%)+', 11 TAB '+CHR$(I%)
END IF
INCR TEMP%,12
NEXT I%
TEMP%=350-(8*LEN(TITLE28))
FOR I%=1 TO LEN(TITLE28)
IF ASC(MID$(TITLE28,I%,1))>=33 AND ASC(MID$(TITLE28,I%,1))<=122 THEN
GET #1,ASC(MID$(TITLE28,I%,1))
DRAW 'BM'+STRS(TEMP%)+', 28 TAB '+CHR$(I%)
END IF
INCR TEMP%,12
NEXT I%
TEMP%=350-(8*LEN(XLABEL$))
FOR I%=1 TO LEN(XLABEL$)
IF ASC(MID$(XLABEL$,I%,1))>=33 AND ASC(MID$(XLABEL$,I%,1))<=122 THEN
GET #1,ASC(MID$(XLABEL$,I%,1))
DRAW 'BM'+STRS(TEMP%)+', 475 TAB '+CHR$(I%)
END IF
INCR TEMP%,12
NEXT I%
TEMP%=240-(8*LEN(YLABEL$))
FOR I%=1 TO LEN(YLABEL$)
IF ASC(MID$(YLABEL$,I%,1))>=33 AND ASC(MID$(YLABEL$,I%,1))<=122 THEN
GET #1,ASC(MID$(YLABEL$,I%,1))
DRAW 'BM 10'+STRS(TEMP%)+TA270 '+CHR$(I%)
END IF
INCR TEMP%,12
NEXT I%
LINE ( 0, 0)-(500, 0),C1%
LINE ( 0, 0)-( 0,500),C1%
DRAW 'C'+STRS(C4%)
. set scale cfr
. X axis
. Y axis
. set scale cfr
. data ranges
. exp factors
. offsets

```



```

END SELECT
'bottom lines
LOCATE 21,18 : PRINT STRING$(13,196);
LOCATE 21,37 : PRINT STRING$(39,196);
FOR J%=0 TO 1
  LOCATE 4,1%*19+18 : PRINT CHR$(218);
  LOCATE 4,1%*45+31 : PRINT CHR$(191);
  LOCATE 21,1%*19+18 : PRINT CHR$(182);
  LOCATE 21,1%*45+31 : PRINT CHR$(217);
  LOCATE 6,1%*19+18 : PRINT CHR$(196);
  LOCATE 6,1%*45+31 : PRINT CHR$(181);
  LOCATE 6,1%*13+50 : PRINT CHR$(209);
  LOCATE 21,1%*13+50 : PRINT CHR$(183);
NEXT J%
LOCATE 5,50 : PRINT " ";
LOCATE 5,63 : PRINT " ";
LOCATE 5,22 : PRINT "Class";
LOCATE 5,53 : PRINT "Property";
FOR I%=1 TO 9
  LOCATE I%,8,21
  PRINT CLASS$(I%);
NEXT I%
FOR I%=1 TO 14
  LOCATE I%*1+8,40 : PRINT PROP$(I%);
  LOCATE I%*1+8,53 : PRINT PROP$(I%+14);
  LOCATE I%*1+8,66 : PRINT PROP$(I%+28);
NEXT I%
' Next is output file box.
COLOR 15,6
LOCATE 22,18 : PRINT CHR$(218),STRING$(37,196),CHR$(181);
LOCATE 23,18 : PRINT CHR$(179),TAB(7) ,CHR$(179);
LOCATE 24,18 : PRINT CHR$(182),STRING$(37,196),CHR$(217);
LOCATE 22,34 : PRINT CHR$(184);
LOCATE 23,54 : PRINT CHR$(179);
LOCATE 24,54 : PRINT CHR$(183);
LOCATE 23,20 : COLOR 12,6 : PRINT "D";
LOCATE 23,56 : COLOR 12,6 : PRINT "F";
LOCATE 15,6 : PRINT "rectory";
COLOR 14,8
LOCATE 23,32 : PRINT OFILES;
LOCATE 23,62 : PRINT OFILES;
' Next are the command statements.
COLOR 3,0
LOCATE 7,78 : PRINT "OPT";
LOCATE 8,78 : PRINT STRING$(3,196);
LOCATE 9,78 : PRINT "<H>";
LOCATE 10,78 : PRINT "<R>";
LOCATE 11,78 : PRINT "<S>";
LOCATE 12,78 : PRINT "<D>";
LOCATE 13,78 : PRINT "<F>";
LOCATE 14,78 : PRINT "<S>";
LOCATE 15,78 : PRINT "<G>";
LOCATE 16,78 : PRINT "<O>";
LOCATE 17,78 : PRINT "<P>";
LOCATE 18,78 : PRINT "<J>";
' Have got screen, so get the information from the keyboard.
FILES=PRDRV$+"CORR"+CLASS$(CLASS%)+".PNUM.DAT"
OPEN FILES FOR INPUT AS #1
INPUT #1,NumOfCompounds
CLOSE #1
COLOR 0,7 : LOCATE 13,6 : PRINT USING "###",NumOfCompounds;
IF CLUES$(CLASS%)="Y" THEN
  COLOR 12,0 : LOCATE CLASS%+8,19
  PRINT " ,CHR$(16),CLASS$(CLASS%)" ;
ELSE

```

Code Listing for CORR513.INC

```

This is the subroutine to draw the main menu on the screen.

```

```

SCREEN 0 : WIDTH 80
COLOR 15,0 : CLS
COLOR 0,7
TEMP%=5
FOR I%=1 TO 4
  LOCATE TEMP%+0,1 : PRINT CHR$(218),STRING$(11,196),CHR$(181);
  LOCATE TEMP%+2,1 : PRINT CHR$(186),STRING$(11,205),CHR$(181);
  LOCATE TEMP%+4,1 : PRINT CHR$(182),STRING$(11,196),CHR$(217);
  LOCATE TEMP%+1,1 : PRINT CHR$(179),TAB(13),CHR$(179);
  LOCATE TEMP%+3,1 : PRINT CHR$(179),TAB(13),CHR$(179);
  TEMP%=TEMP%+6
NEXT I%
LOCATE 6,3 : PRINT "Hardcopy";
LOCATE 6,7 : PRINT "COPY";
LOCATE 11,3 : PRINT "Compounds";
LOCATE 13,6 : PRINT USING "###",NUMCOMPOUNDS;
LOCATE 16,3 : PRINT "RAM Disk";
LOCATE 16,7 : PRINT "RAMDISK";
LOCATE 21,5 : PRINT "Time";
' Next is top box - for the title.
COLOR 15,4
LOCATE 1,6 : PRINT CHR$(201),STRING$(69,205),CHR$(187)
LOCATE 2,6 : PRINT CHR$(186),STRING$(69,32),CHR$(186)
LOCATE 3,6 : PRINT CHR$(200),STRING$(69,205),CHR$(188)
LOCATE 1,31 : PRINT CHR$(209);
LOCATE 2,31 : PRINT CHR$(179);
LOCATE 3,31 : PRINT CHR$(207);
LOCATE 2,10 : PRINT " CORR ";
LOCATE 2,19 : PRINT "VERNS"
LOCATE 2,35 : PRINT "Physical Property Correlation Software";
' Next are Class and Property Boxes
COLOR 15,1
FOR I%=5 TO 21
  LOCATE I%,18 : PRINT SPACES(13);
  LOCATE I%,37 : PRINT SPACES(38);
  LOCATE I%,18 : PRINT CHR$(179);
  LOCATE I%,31 : PRINT CHR$(179);
  FOR J%=0 TO 3
    LOCATE I%,J%*13+37 : PRINT CHR$(179);
  NEXT J%
NEXT I%
LOCATE 4,18 : PRINT STRING$(13,196);
LOCATE 4,37 : PRINT STRING$(39,196);
LOCATE 6,18 : PRINT STRING$(13,205);
LOCATE 6,37 : PRINT STRING$(39,205);

```

```

IF HCOPI%="Y" THEN
LPRINT TAB(11);
LPRINT USING "Maximum Error: #####.#####";MAX;
LPRINT TAB(41);
LPRINT USING "Maximum Abs Error: #####.#####";ABSMAX;
LPRINT TAB(11);
LPRINT USING "Minimum Error: #####.#####";MIN;
LPRINT TAB(41);
LPRINT USING "Minimum Abs Error: #####.#####";ABSMIN;
LPRINT TAB(19);
LPRINT USING "No Points: ###";COUNT%;
LPRINT TAB(38);
LPRINT USING "Avg Error: #####.#####";AVG;
LPRINT TAB(24);
LPRINT USING "Standard Deviation: #####.#####";SD;
END IF
COLOR 31,4
LOCATE 13,19 : PRINT " Press <F> to form feed, any key to continue. ";
AS=INPUT$(1)
IF AS="F" OR AS="Y" THEN LPRINT CHR$(12) ' form feed
IF AS="O" OR AS="V" OR AS=CHR$(27) THEN GOTO StartOfProgram ' bug out
IF AS="O" OR AS="V" THEN GOTO Options
COLOR 15,4
LOCATE 13,19 : PRINT " Press <F> to form feed, any key to continue. ";
RETURN

```

Code Listing for CORR515.INC

This is the subroutine to get mixing coeff parameters.

```

Options box
COLOR 10,1
LOCATE 7,15 : PRINT CHR$(218);STRING$(49,199);CHR$(191); ' top line
FOR I%=8 TO 16
LOCATE I%,15 : PRINT CHR$(179);TAB(85);CHR$(179); ' middle
NEXT I%
LOCATE 17,15 : PRINT CHR$(192);STRING$(49,199);CHR$(217); ' bottom line
COLOR 10,0
LOCATE 6,15 : PRINT TIMES;
LOCATE 6,58 : PRINT DATES;
COLOR 12, 1
LOCATE 9,19 : PRINT "Please make any changes that are necessary.";
COLOR 14, 1
LOCATE 11,27 : PRINT " Slope.";
LOCATE 12,27 : PRINT " Intcp.";
LOCATE 13,27 : PRINT "Offset.";
LOCATE 14,27 : PRINT " f(x)";
COLOR 15, 1
LOCATE 11,37 : PRINT SLOPEFACTOR;
LOCATE 12,37 : PRINT INTCFACTOR;
LOCATE 13,37 : PRINT OFFSEIFACTR;

```

```

COLOR 14,0 : LOCATE CLASS%+8,10 : PRINT " ,CLASS$(CLASS%);" ;
END IF
IF ACTVES="Class" THEN
COLOR 15, 5 : LOCATE 5,21 : PRINT ACTVES;
ELSE
COLOR 15, 5 : LOCATE 5,52 : PRINT ACTVES;
END IF
COLOR 14,0
COL%=INT((PROP%-1)/14) : ROW%=PROP% - (COL%*14)
LOCATE ROW%+8,COL%*13 + 38 : PRINT " ,PROPS(PROP%);" ;
FILES=PRDRV%+"CORR"+CLASS$(CLASS%)+".PNUM.DAT"
FOR I%=1 TO 10
IF CUSES(I%)="Y" AND I%<>CLASS% THEN
COLOR 10,1 : LOCATE I%,8,10
PRINT " :CHR$(16);CLASS$(I%);" ;
END IF
NEXT I%
OPEN FILES FOR INPUT AS #1
INPUT #1,NumOfCompounds
CLOSE #1
RETURN

```

Code Listing for CORR514.INC

This is the subroutine to find the minimum and maximum.

```

MIN=10000 : MAX=-10000 : ABSMIN=10000 : ABSMAX=-10000 : TOT=0 : TOT2=0
IF COUNT%<>0 THEN
FOR I%=1 TO COUNT%
IF DIFF(I%)<MIN THEN MIN=DIFF(I%)
IF DIFF(I%)>MAX THEN MAX=DIFF(I%)
IF ABS(DIFF(I%))<ABSMIN THEN ABSMIN=ABS(DIFF(I%))
IF ABS(DIFF(I%))>ABSMAX THEN ABSMAX=ABS(DIFF(I%))
TOT =TOT +DIFF(I%)
TOT2=TOT2+DIFF(I%)^2
NEXT I%
AVG=TOT/COUNT%
SD =SQRT(TOT2/COUNT%-AVG^2)
END IF
COLOR 15,4
LOCATE 7,7 : PRINT CHR$(201);STRING$(87,203);CHR$(187) ' top line
FOR I%=8 TO 12
LOCATE I%,7;PRINT CHR$(186);STRING$(87, 32);CHR$(186) ' ends
NEXT I%
LOCATE 13,7 : PRINT CHR$(200);STRING$(87,205);CHR$(188) ' bottom line
LOCATE 9,11 : PRINT USING "Maximum Error: #####.#####";MAX;
LOCATE 10,11 : PRINT USING "Minimum Error: #####.#####";MIN;
LOCATE 9,41 : PRINT USING "Maximum Abs Error: #####.#####";ABSMAX;
LOCATE 10,41 : PRINT USING "Minimum Abs Error: #####.#####";ABSMIN;
LOCATE 11,19 : PRINT USING "No. Points: ###";COUNT%;
LOCATE 11,38 : PRINT USING "Avg Error: #####.#####";AVG;
LOCATE 12,28 : PRINT USING "Standard Deviation: #####.#####";SD;

```

Code Listing for CORR516.INC

```

LOCATE 14,37 : PRINT FUNCTIONS;
.
. Next are commands.
COLOR 3,0
LOCATE 22,17 : PRINT *Press <RET> to continue, <O> for options menu.;
COLOR 12, 0
TEMP$="Output File: "+ODIR$+OFIL$
LOCATE 25,40-0.5*LEN(TEMP$) : PRINT TEMP$;
.
. Next see what to do.
BKGNDF%=0 : GOSUB MarkFuelParam
Startloop12:
AS=INKEY$
SELECT CASE AS
CASE ""
COLOR 10,0 : LOCATE 6,15 : PRINT TIMES;
GOTO Startloop12
CASE CHR$(13)
RETURN
CASE "O";"t";CHR$(27)
GOTO StartOfProgram
CASE "O";"v"
GOTO Options
CASE "O";"g"
GOTO Graph
CASE "B";"b"
GOTO BarGraphAndPieChart
CASE "E";"e"
GOTO Statistics
CASE CHR$(0)+CHR$(72), CHR$(0)+CHR$(80)
BKGNDF%=1 : GOSUB MarkFuelParam
IF AS=CHR$(0)+CHR$(72) THEN DECR OPTN6% ELSE INCR OPTN6%
IF OPTN6%<1 THEN OPTN6%=1
IF OPTN6%>4 THEN OPTN6%=4
BKGNDF%=0 : GOSUB MarkFuelParam
CASE ELSE
COLOR 15, 1
LOCATE 10+OPTN6%.35 : PRINT SPACE$(20);
LOCATE 10+OPTN6%.37 : PRINT AS; : LINE INPUT TEMP$
SELECT CASE OPTN6%
CASE 1 : SLOPEFACTOR=VAL(AS+TEMP$)
CASE 2 : INTCPFACTOR=VAL(AS+TEMP$)
CASE 3 : OFFSETFACTOR=VAL(AS+TEMP$)
CASE 4 : FUNCTIONS=AS+TEMP$
END SELECT
BKGNDF%=0 : GOSUB MarkFuelParam
END SELECT
GOTO Startloop12
MarkFuelParam:
. This is a mini-subroutine to mark a fuel class for use.
LOCATE 10+OPTN6%.35
COLOR 15,BKGNDF%
SELECT CASE OPTN6%
CASE 1 : PRINT * "SLOPEFACTOR";
CASE 2 : PRINT * "INTCPFACTOR";
CASE 3 : PRINT * "OFFSETFACTOR";
CASE 4 : PRINT * "FUNCTIONS";
END SELECT
RETURN
. Options box.
COLOR 15,0 : CLS
COLOR 10,1
LOCATE 2, 5 : PRINT CHR$(219),STRING$(99,199),CHR$(191); ' top line
FOR I%=3 TO 21
LOCATE I%, 5 : PRINT CHR$(179);TAB(75);CHR$(179); ' middle
NEXT I%
LOCATE 22, 5 : PRINT CHR$(192),STRING$(99,199),CHR$(217); ' bottom line
LOCATE 9, 5 : PRINT CHR$(192),STRING$(99,199),CHR$(190); ' middle line
COLOR 10, 1
LOCATE 3,15 : PRINT TIMES;
LOCATE 3,56 : PRINT DATES;
COLOR 12, 1
LOCATE 3,35 : PRINT *Parameters*;
LOCATE 10,30 : PRINT *Mixing Coefficients*.;
COLOR 14, 1
LOCATE 4,27 : PRINT *Property*.;
LOCATE 5,27 : PRINT * Slope*.;
LOCATE 6,27 : PRINT * Intcp*.;
LOCATE 7,27 : PRINT * Offset*.;
LOCATE 8,27 : PRINT * f(x)*.;
FOR I%=1 TO 22
IF I%<=11 THEN LOCATE I%+10,10 ELSE LOCATE I%-1,45
PRINT USING "b,(.##)=-,|%-1,
NEXT I%
COLOR 15, 1
LOCATE 4,37 : PRINT PROP$(PROP%);
LOCATE 5,37 : PRINT SLOPEFACTOR;
LOCATE 6,37 : PRINT INTCPFACTOR;
LOCATE 7,37 : PRINT OFFSETFACTR;
LOCATE 8,37 : PRINT FUNCTIONS;
FOR I%=1 TO 22
IF I%<=11 THEN LOCATE I%+10,18 ELSE LOCATE I%-1,53
PRINT USING "#####.#####"; MIXCOEFF(I%);
NEXT I%
. Next are commands
COLOR 3, 0
LOCATE 23,30 : PRINT *Press <H> to hardcopy*.;
LOCATE 24,17 : PRINT *Press <RET> to continue, <O> for options menu*.;
COLOR 12, 0
TEMP$="Output File: "+ODIR$+OFIL$
LOCATE 25,40-0.5*LEN(TEMP$) : PRINT TEMP$;
.
. Next see what to do
BKGNDF%=0 : GOSUB MarkActiveParam
Startloop13

```

This is the subroutine to show the mixing coeff parameters

Listing for Program II.4: GRAPH.BAS

```

AS=INKEY$
SELECT CASE AS
CASE =
  COLOR 10,1 : LOCATE 3,15 : PRINT TIMES;
  GOTO Startloop13
CASE CHR$(13)
  RETURN
CASE "Q", "q", CHR$(27)
  GOTO StartOPProgram
CASE "O", "o"
  GOTO Options
CASE "P", "p"
  LPRINT CHR$(12)
CASE "G", "g"
  GOTO Graph
CASE "E", "e"
  GOTO Statistics
CASE "B", "b"
  GOTO BarGraphAndPieChart
CASE CHR$(0)+CHR$(72), CHR$(0)+CHR$(80)
  BKGND%=1 : GOSUB MarkActiveParam
  IF AS=CHR$(0)+CHR$(72) THEN DECR OPTN7% ELSE INCR OPTN7%
  IF OPTN7%< 1 THEN OPTN7%=22
  IF OPTN7%>22 THEN OPTN7%=1
  BKGND%=0 : GOSUB MarkActiveParam
CASE "H", "h"
  LPRINT "Summary of Mixing Coefficient Parameters "; TIMES; " : DATES
  LPRINT " Property: PROP% (PROP%)
  LPRINT " Slope: SLOPEFACTOR
  LPRINT " Intcp: INTCPFACTOR
  LPRINT " Offset: OFFSETFACTR
  LPRINT " f(x): FUNCTIONS
  TEMPS = " & *****.*****
  FOR I%=1 TO 22
    LPRINT USING TEMPS; I%-1, MIXCOEFF(I%)
  NEXT I%
CASE ELSE
  COLOR 15, 1
  IF OPTN7%<=11 THEN LOCATE OPTN7%+10,16 ELSE LOCATE OPTN7%-1,51
  PRINT SPACES(20);
  IF OPTN7%<=11 THEN LOCATE OPTN7%+10,18 ELSE LOCATE OPTN7%-1,53
  PRINT AS; : LINE INPUT TEMPS
  MIXCOEFF(OPTN7%)=VAL(AS+TEMPS)
  BKGND%=0 : GOSUB MarkActiveParam
END SELECT
GOTO Startloop13
MarkActiveParam:
  . This is a mini-subroutine to mark a fuel class for use
  IF OPTN7%<=11 THEN LOCATE OPTN7%+10,16 ELSE LOCATE OPTN7%-1,51
  COLOR 15,BKGND%
  PRINT USING " *****.***** "; MIXCOEFF(OPTN7%);
  RETURN

```

```

' no lury

```

```

' return

```

```

' exit

```

```

' options

```

```

' form feed

```

```

' graph

```

```

' error dist

```

```

' bar chart

```

```

' up-down

```

```

' hardcopy

```

```

' DATES

```

```

. This is a program designed to graph the files written by the correlations
. software. It is essentially the same as the graphing program which is
. part of the correlations program CORR5.

```

```

. Program Name: GRAPH.BAS Ver 6.10      Date Written: 12/20/1987
. Author: Allen Caswell                Date Modified: 05/18/1988

```

```

First is the section to set up the variables.

```

```

. First are default parameters for program.

```

```

COMMON ODIRS, OFILES

```

```

. Next will dimension the necessary matrices.

```

```

DIM RPTS$(10), SDRS$(10), COUNT$(10), CALC(10,500), OBS(10,500)
DIM ERRSL(10), ERRIN(10), TITLE1$(10), USE$(10,500), POINTER$(100)
DIM SLOPE(10), NME$(10), TITLE2$(10), PIX$(2820), LINENAMES(10)
DIM INTCP(10), CORR(10), XLABLE$(10), YLABLE$(10), PTCOONS(10)
DIM R(500)

```

```

. Next are options for end of program.

```

```

DATA * Exit to DOS **: Run GRAF_ED **: Run PROPS **: Run REGS *
DATA * Run ERROR **: Run CORR5 **: Run EZ_PLOT **: Restart *
FOR I%=1 TO 8 READ OPTN$(I%) : NEXT I%

```

```

. Next are defaults for parameters.

```

```

RestoreDefaults
SCALES=Y% : PTCOONS=Y% : STATIS=Y%
FULLCS=Y% : HCSTIS=N% : HCPTIS=N%
GOPTN%=1 : OPTN2%=1 : OPTN3%=1
X%=350 : Y%=240 : NumFiles%=1
SND$ =N% : SCRDIR$=F% : VERSNS=V%R 6.10
FOR I%=1 TO 10
  RPTS$(I%)=0 : SLOPE(I%)=0 : INTCP(I%)=0 : SDRS(I%)=0
  ERRSL(I%)=0 : ERRIN(I%)=0 : CORR(I%)=0 : COUNT$(I%)=0
  NME$(I%)="" : TITLE1$(I%)="" : TITLE2$(I%)="" : LINENAMES(I%)=""
  XLABLE$(I%)="" : YLABLE$(I%)="" : PTCOONS(I%)=""
NEXT I%
IF ODIRS="" THEN ODIRS="D:\CORR\RESULT"
IF OFILES="" THEN OFILES="TEST.DAT"

```

```

Next is the opening screen.

```

```

SCREEN 0 : WIDTH 80 : COLOR 15, 0 : CLS
COLOR 6, 7
LOCATE 1,38 : PRINT CHR$(201),STRINGS$(41,205),CHR$(187);
FOR %1=2 TO 12
    LOCATE %1,38 : PRINT CHR$(186),TAB(80),CHR$(186);
NEXT %1
LOCATE 13,38 : PRINT CHR$(200),STRINGS$(41,205),CHR$(188);
LOCATE 6,38 : PRINT CHR$(186),STRINGS$(41,186),CHR$(182);
COLOR 11,7
LOCATE 3,57 : PRINT "GRAPHY";
LOCATE 4,53 : PRINT VERSNS;
COLOR 14,7
LOCATE 8,57 : PRINT "THE ";
COLOR 15,7
LOCATE 10,48 : PRINT "Scientific Graphing Software";
COLOR 0,7
LOCATE 12,54 : PRINT "A/C Software";
    
```

```

SCREEN 0 : WIDTH 80 : COLOR 15, 0 : CLS
COLOR 6, 7
LOCATE 1,38 : PRINT CHR$(201),STRINGS$(41,205),CHR$(187);
FOR %1=2 TO 12
    LOCATE %1,38 : PRINT CHR$(186),TAB(80),CHR$(186);
NEXT %1
LOCATE 13,38 : PRINT CHR$(200),STRINGS$(41,205),CHR$(188);
LOCATE 6,38 : PRINT CHR$(186),STRINGS$(41,186),CHR$(182);
COLOR 11,7
LOCATE 3,57 : PRINT "GRAPHY";
LOCATE 4,53 : PRINT VERSNS;
COLOR 14,7
LOCATE 8,57 : PRINT "THE ";
COLOR 15,7
LOCATE 10,48 : PRINT "Scientific Graphing Software";
COLOR 0,7
LOCATE 12,54 : PRINT "A/C Software";
    
```

DrawGraph.

Section to draw the graph of the data.

StartOfProgram:

Section to the Main Menu.

```

CASE CHR$(0)+CHR$(73),CHR$(0)+CHR$(81)
    GOSUB PageUpPageDown
CASE CHR$(0)+CHR$(75),CHR$(0)+CHR$(77)
    GOSUB LeftRight
CASE CHR$(0)+CHR$(72), CHR$(0)+CHR$(80)
    GOSUB UpDown
CASE ELSE
    SOUND 1000,3 : SOUND 800,1,5
END SELECT
GOTO Startloop2
    
```

```

GOSUB DrawMainMenu
    
```

```

* Will get the actual number of files need in.
IF NumFiles<9 THEN File%=NumFiles%-1 ELSE File%=NumFiles%
* Will catch stupid mistakes. (no data file loaded into memory)
TEMP%=0
FOR %1=1 TO File%
    INCR TEMP%,COUNT%(%1)
NEXT %1
IF TEMP%<=1 THEN
    COLOR 15,0 : CLS : COLOR 12,0
    LOCATE 11,21 : PRINT "*** OK, Stupid - Load a data file ***";
    SOUND 1000,3 : SOUND 800,1,5
    AS=INKEYS
    WHILE AS=""
        AS=INKEY$
    WEND
    COLOR 15,0 : CLS
    GOTO StartofProgram
END IF
    
```

```

* Have got the screen drawn, so see what to do.
Startloop2:
AS=INKEY$
SELECT CASE AS
CASE " "
    COLOR 10,1 : LOCATE 2,22 : PRINT TIMES;
CASE "O", "o", "Q", "q", CHR$(27)
    GOTO Options
CASE CHR$(13)
    GOTO DrawGraph
CASE "H", "h"
    GOSUB HeroCopyStats
CASE "P", "p"
    LPRINT CHR$(12)
CASE "S", "s"
    GOSUB ToggleSound
CASE "D", "d"
    GOSUB ChangeDirectory
CASE "T", "t"
    GOSUB ChangeTitle
CASE "X", "x"
    GOSUB ChangeXLabel
CASE "Y", "y"
    GOSUB ChangeYLabel
CASE "L", "l"
    GOSUB ChangeLineNumber
CASE "F", "f"
    GOSUB GetAnotherFile
CASE " "
    GOSUB DoDirectory
    
```

```

* First must find the max and min values in file.
GOSUB FindMinMax
X RANGE =MAXX-MINX
Y RANGE =MAXY-MINY
XEXPFACTOR=500/XRANGE
YEXPFACTOR=(0-MINY)*XEXPFACTOR
YOFFSET=(0-MINY)*YEXPFACTOR
    
```

```

* Will set up the screen.
OPEN "CHARACTER.DAT" FOR RANDOM AS #1
FIELD #1, 40 AS CHARS
SCREEN 12
IF FULLCS="" THEN COLOR 11,0 ELSE COLOR 15,0
C1%=12
C2%=14
C3%=10
C4%=11
    
```

```

* pgup - pgdn
* left right
* up-down
* data ranges
* exp factors
* offsets
* axis color
* title color
* data color
* scale color
    
```

```

* no key
* options
* enter
* hcopy stats
* form feed
* sound
* directory
* title
* X label
* Y label
* Line name
* file
* list files
    
```

```

C5% = 15
DRAW 'BM 350,240 C12'
DRAW 'S8 D8 E2 F3 E2 H3 E2 L8'
DRAW 'B2 P4,12'
GET (350,242)-(381,240),POINTER%
DRAW '84'
CLS
WINDOW (-50,-105)-(530,525)
IF FULLCS='Y' THEN TEMP% = C2% ELSE TEMP% = 15
DRAW 'C'+STR$(TEMP%)
TEMP% = 350 - (6*LEN(TITLE$(OPTN3%)))
FOR I% = 1 TO LEN(TITLE$(OPTN3%))
    TEMP% = MIDS(TITLE$(OPTN3%),I%,1)
    IF ASC(TEMP%) >= 33 AND ASC(TEMP%) <= 122 THEN
        GET #1,ASC(TEMP%)
        DRAW 'BM'+STR$(TEMP%)+', 11 TAO '+CHAR%
    END IF
    INCR TEMP%,12
NEXT I%
TEMP% = 350 - (6*LEN(TITLE$(OPTN3%)))
FOR I% = 1 TO LEN(TITLE$(OPTN3%))
    TEMP% = MIDS(TITLE$(OPTN3%),I%,1)
    IF ASC(TEMP%) >= 33 AND ASC(TEMP%) <= 122 THEN
        GET #1,ASC(TEMP%)
        DRAW 'BM'+STR$(TEMP%)+', 26 TAO '+CHAR%
    END IF
    INCR TEMP%,12
NEXT I%
TEMP% = 350 - (6*LEN(LABEL$(OPTN3%)))
FOR I% = 1 TO LEN(LABEL$(OPTN3%))
    TEMP% = MIDS(LABEL$(OPTN3%),I%,1)
    IF ASC(TEMP%) >= 33 AND ASC(TEMP%) <= 122 THEN
        GET #1,ASC(TEMP%)
        DRAW 'BM'+STR$(TEMP%)+', 434 TAO '+CHAR%
    END IF
    INCR TEMP%,12
NEXT I%
TEMP% = 240 - (6*LEN(YLABEL$(OPTN3%)))
FOR I% = 1 TO LEN(YLABEL$(OPTN3%))
    TEMP% = MIDS(YLABEL$(OPTN3%),I%,1)
    IF ASC(TEMP%) >= 33 AND ASC(TEMP%) <= 122 THEN
        GET #1,ASC(TEMP%)
        DRAW 'BM 10,'+STR$(TEMP%)+',TA270 '+CHAR%
    END IF
    INCR TEMP%,12
NEXT I%
IF FULLCS='Y' THEN TEMP5% = C1% ELSE TEMP5% = 15
LINE ( 0, 0)-(500, 0),TEMP5%
LINE ( 0, 0)-( 0,500),TEMP5%
IF FULLCS='Y' THEN TEMP% = C4% ELSE TEMP% = 15
DRAW 'C'+STR$(TEMP%)
TEMP% = (I%-1)*125
LINE (TEMP%,0)-(TEMP%,5),TEMP5%
LINE (0,TEMP%)-(-5,TEMP%),TEMP5%
TEMP = MINX + (I%-1)*(RANGE/4)
FOR J% = 1 TO 5
    IF J% <= LEN(STR$(TEMP)) THEN
        TEMP2% = ASC(MIDS(STR$(TEMP),J%,1))
        IF TEMP2% >= 33 AND TEMP2% <= 122 THEN
            ' pt connect
            ' read pointer
            ' arrow into
            ' array
            ' POINTER%
            ' set window
            ' set title c
            ' draw title1
            ' get char
            ' draw char
            ' draw title2
            ' get char
            ' draw char
            ' draw ylable
            ' get char
            ' draw char
            ' draw ylable
            ' get char
            ' draw char
            ' X axis
            ' Y axis
            ' set scale cir
            ' X tic marks
            ' Y tic marks
            ' X scale
            ' Will draw graph
            ' FOR J% = 1 TO File%
            ' TEMP1 = XEYFAC*OBS(J%,I%) + XOFFSET
            ' TEMP2 = YEXFAC*CALC(J%,I%) + YOFFSET
            ' IF TEMP1 >= 25 AND TEMP1 <= 525 THEN
            ' IF TEMP2 >= 25 AND TEMP2 <= 525 THEN
            ' Will x out the bad points.
            ' IF PTCOBS(J%) < > ' THEN GOSUB DrawPoint
            ' IF USE%(J%,I%) = 0 THEN
            ' IF FULLCS='Y' THEN TEMP% = C1% ELSE TEMP% = 1
            ' LINE (TEMP1-4,TEMP2-4)-(TEMP1+4,TEMP2+4),TEMP%
            ' LINE (TEMP1+4,TEMP2-4)-(TEMP1-4,TEMP2+4),TEMP%
            ' END IF
            ' END IF
            ' END IF
            ' Have drawn the graph so must draw the line names.
            GOSUB LabelLines
            NEXT J%
            ' Will connect points
            ' FOR J% = 1 TO File%
            ' IF FULLCS='Y' THEN
            ' SELECT CASE J%
            ' CASE 1,2,3,4,5,6 : TEMP% = C3% + (J%-1)
            ' CASE 7,8,9 : TEMP% = C3% + (J%-7)
            ' 1st select
            ' full color
        
```

```

CASE CHR$(27),CHR$(13),CHR$(10)
SCREEN 0 : WIDTH 60
COLOR 15,0 : CLS
IF FITCONS="Y" THEN GOSUB PrintRegressionResults
GOTO StartProgram
CASE CHR$(0)+CHR$(72),CHR$(0)+CHR$(60)
PUT (X%,Y%),POINTERS% : up-down
IF AS=CHR$(0)+CHR$(72) THEN INCR Y%,4 ELSE DECR Y%,4
IF Y%<=35 THEN Y%=525
IF Y%>525 THEN Y%=-35
PUT (X%,Y%),POINTERS%
GOTO Startloop5
CASE CHR$(0)+CHR$(75),CHR$(0)+CHR$(77)
PUT (X%,Y%),POINTERS% : left-right
IF AS=CHR$(0)+CHR$(75) THEN DECR X%,4 ELSE INCR X%,4
IF X%<=50 THEN X%=315
IF X%>515 THEN X%=-50
PUT (X%,Y%),POINTERS%
GOTO Startloop5
CASE "*"
GOSUB FindPoint
GOTO Startloop5
CASE ELSE
SOUND 1000,3 : SOUND 600,1.5
GOTO Startloop5
END SELECT

Options
This is the section to do the options.

COLOR 0,15
LOCATE 14,1 : PRINT CHR$(216),STRING$(15,166),CHR$(161), : top
LOCATE 15,1 : PRINT CHR$(179),SPACE$(15),CHR$(179); : side
LOCATE 16,1 : PRINT CHR$(180),STRING$(15,200),CHR$(181); : middle
LOCATE 25,1 : PRINT CHR$(162),STRING$(15,166),CHR$(217); : bottom
FOR I%=17 TO 24
LOCATE I%,1 : PRINT CHR$(179),SPACE$(15),CHR$(179); : side
LOCATE I%,3 : PRINT OPTN$(I%-16);
NEXT I%
LOCATE 15,6 : PRINT "Options";

Have got screen so see what to do.
COLOR 14,0 : LOCATE 16+OPTN2%,3 : PRINT OPTN$(OPTN2%);
Startloop8
AS=INKEY$
SELECT CASE AS
CASE =
GOTO Startloop8
CASE CHR$(0)+CHR$(72),CHR$(0)+CHR$(60)
COLOR 0,15 : LOCATE 16+OPTN2%,3
PRINT OPTN$(OPTN2%);
IF AS=CHR$(0)+CHR$(72) THEN DECR OPTN2% ELSE INCR OPTN2%
GOTO Startloop5
CASE =
: no key
CASE CHR$(0)+CHR$(75),CHR$(0)+CHR$(60)
: up-down
PRINT OPTN$(OPTN2%);
END SELECT

END SELECT
ELSE
TEMP%=15
END IF
SELECT CASE FITCONS(J%)
CASE "Y",L
TEMP1=MIN(XEYFAC)+XOFFSET
TEMP2=YEYFAC*(MIN(SLOPE(J%)+INTCP(J%)))+YOFFSET
TEMP3=MAX(XEYFAC)+XOFFSET
TEMP4=XEYFAC*(MAX(SLOPE(J%)+INTCP(J%)))+YOFFSET
LINE (TEMP1,TEMP2)-(TEMP3,TEMP4),TEMP%
CASE "P"
FOR I%=2 TO COUNT(J%)
TEMP1=XEYFAC*OBS(J%,I%) +XOFFSET
TEMP2=XEYFAC*CALC(J%,I%) +YOFFSET
TEMP3=XEYFAC*OBS(J%,I%-1) +XOFFSET
TEMP4=XEYFAC*CALC(J%,I%-1)+YOFFSET
LINE (TEMP1,TEMP2)-(TEMP3,TEMP4),TEMP%
NEXT I%
END SELECT
NEXT J%

Will put in stats.
IF STATSS="Y" THEN
DRAW "C"+STR$(TEMP%)
FOR KKK%=1 TO 3
SELECT CASE KKK%
CASE 1
TEMP%="Points" : TEMP1=RPT$(OPTN3%)
TEMPX%=445 : TEMPY%=356
CASE 2
TEMP%="Corr" : TEMP1=CORR(OPTN3%)
TEMPX%=400 : TEMPY%=373
CASE 3
TEMP%="Std(0)" : TEMP1=SDRES(OPTN3%)
TEMPX%=365 : TEMPY%=360
END SELECT
GOSUB FindExponent
TEMP%="TEMP%+LEFT$(STR$(TEMP),6)
IF TEMP%>=2 THEN TEMP%=1
IF KKK%>1 THEN TEMP%="TEMP%+x10 "+STR$(TEMP%)
IF LEN(TEMP%)<10 THEN TEMP2%="LEN(TEMP%)" ELSE TEMP2%="19" : string length
FOR I%=1 TO TEMP2%
IF ASC(MID$(TEMP%,I,1))>=33 AND ASC(MID$(TEMP%,I,1))<=122 THEN
GET #1,ASC(MID$(TEMP%,I,1))
DRAW "BM"+STR$(TEMPX%)+","++STR$(TEMPY%)
DRAW "TAO "+CHAR$
END IF
INCR TEMPX%,12
NEXT I%
NEXT KKK%
END IF
CLOSE #1
PUT (X%,Y%),POINTERS%
Startloop5
AS=INKEY$
SELECT CASE AS
CASE =
GOTO Startloop5

```

```

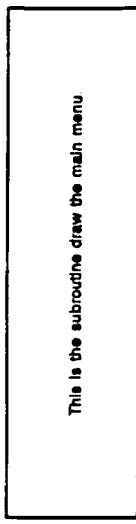
LOCATE 3, 1 : PRINT CHR$(186);STRING$(14,186);CHR$(182) ' middle line
COLOR 1, 3
LOCATE 2, 8 : PRINT "Files";
COLOR 4, 3
FOR I%=1 TO NumFiles%
    LOCATE I%+3,3 : PRINT NME$(I%);
NEXT I%
COLOR 12, 0
LOCATE OPTN3%+3,2 : PRINT " : NME$(OPTN3%);TAB(16);
' Next is menu of graph choices.
COLOR 2, 4
LOCATE 15, 5 : PRINT CHR$(201);STRING$(90,200);CHR$(187); ' top line
FOR I%=18 TO 21
    LOCATE I%,5 PRINT CHR$(186);STRING$(90, 32);CHR$(186); ' ends
NEXT I%
LOCATE 22, 5 : PRINT CHR$(200);STRING$(90,200);CHR$(188); ' bottom line
LOCATE 15,45 : PRINT CHR$(209); ' top junct
LOCATE 22,45 : PRINT CHR$(207); ' bottom junct
FOR I%=18 TO 21 : LOCATE I%,45 : PRINT CHR$(179); : NEXT I% 'center line
COLOR 15, 4
LOCATE 18,10 : COLOR 11,4 : PRINT "F"; : COLOR 15, 4 : PRINT "file.";
LOCATE 17,10 : COLOR 11,4 : PRINT "D"; : COLOR 15, 4 : PRINT "directory.";
LOCATE 18,10 : COLOR 11,4 : PRINT "T"; : COLOR 15, 4 : PRINT "file.";
LOCATE 19,10 : COLOR 11,4 : PRINT "X"; : COLOR 15, 4 : PRINT "Label.";
LOCATE 20,10 : COLOR 11,4 : PRINT "Y"; : COLOR 15, 4 : PRINT "Label.";
LOCATE 21,10 : COLOR 11,4 : PRINT "L"; : COLOR 15, 4 : PRINT "line Name.";
LOCATE 16,49 : PRINT "Auto Scale.....";
LOCATE 17,49 : PRINT "Point Connect.....";
LOCATE 18,49 : PRINT "Display Stats.....";
LOCATE 19,49 : PRINT "Hard Copy Stats.....";
LOCATE 20,49 : PRINT "Hard Copy Points.....";
LOCATE 21,49 : PRINT "Full Color.....";
COLOR 14, 4
LOCATE 16,21 : PRINT LEFT$(OFILES
LOCATE 17,21 : PRINT LEFT$(ODIRS
LOCATE 18,21 : PRINT LEFT$(DTITLE$(OPTN3%)
LOCATE 19,21 : PRINT LEFT$(DLABLE$(OPTN3%)
LOCATE 20,21 : PRINT LEFT$(VLABLE$(OPTN3%)
LOCATE 21,21 : PRINT LEFT$(UNENAMES$(OPTN3%);22);TAB(44);
LOCATE 16,70 : PRINT SCALES;
LOCATE 17,70 : PRINT PTCOIN$(OPTN3%);
LOCATE 18,70 : PRINT STATIS;
LOCATE 19,70 : PRINT HCSITIS;
LOCATE 20,70 : PRINT HCSPTIS;
LOCATE 21,70 : PRINT FULLCS;
IF GOPTN%=1 THEN TEMPS=SCALES
IF GOPTN%=2 THEN TEMPS=PTCOIN$(OPTN3%)
IF GOPTN%=3 THEN TEMPS=STATIS
IF GOPTN%=4 THEN TEMPS=HCSITIS
IF GOPTN%=5 THEN TEMPS=HCSPTIS
IF GOPTN%=6 THEN TEMPS=FULLCS
COLOR 14, 0
LOCATE GOPTN%+15,68 : PRINT " : TEMPS";
COLOR 3, 0
LOCATE 24, 7 : PRINT "Press <LETTER> to change the field, ;
PRINT "←-ARROW KEYS> to change option";
LOCATE 25, 1 : PRINT "Press <H> to Hard Copy stats, <P> to Form Feed, ;
PRINT "←\> for Directory, <Q> to quit.";
RETURN

```

```

IF OPTN2%<1 THEN OPTN2%=8
IF OPTN2%>8 THEN OPTN2%=1
COLOR 14,0 : LOCATE 16+OPTN2%,3
PRINT OPTN$(OPTN2%);
GOTO Startloop8
CASE CHR$(13)
GOTO DoOption
CASE CHR$(9)+CHR$(75);CHR$(9)+CHR$(77)
GOTO Startloop8
CASE ELSE
SOUND 1000,3 : SOUND 800,1.5
GOTO Startloop8
END SELECT
DoOption:
SELECT CASE OPTN2%
CASE 1
CLOSE
GOSUB Logo
LOCATE 1,1
PRINT "Here's something happening here,"
PRINT "And what it ain't exactly clear...";
AS=INPUT$(1)
END
CASE 2
CHAIN "GRAF_ED.EXE"
CASE 3
CHAIN "PROPS.EXE"
CASE 4
CHAIN "REGS.EXE"
CASE 5
CHAIN "ERROR.EXE"
CASE 6
CHAIN "CORPS.EXE"
CASE 7
CHAIN "EZ_PLOT.EXE"
CASE 8
GOTO RestoreDefaults
END SELECT
DrawMainMenu:
' First is menu of file names
COLOR 0, 3
LOCATE 1, 1 : PRINT CHR$(201);STRING$(14,205);CHR$(187) ' top line
FOR I%=2 TO 12
    LOCATE I%, 1 : PRINT CHR$(186);TAB(16);CHR$(186) ' ends
NEXT I%
LOCATE 13, 1 : PRINT CHR$(200);STRING$(14,205);CHR$(188) ' bottom line

```



These are the subroutines from main menu to do all options.

```

ToggleSound:
IF SND$="Y" THEN SND$="N" ELSE SND$="Y"
COLOR 10,0 : LOCATE 23,3
PRINT "Sound = "SND$;
IF SND$="Y" THEN SOUND 600,2 ELSE SOUND 300,4
DELAY 0.9
COLOR 15,0 : LOCATE 23,3
PRINT SPACES(15);
RETURN

ChangeDirectory:
COLOR 31, 4
LOCATE 17,10 : PRINT "Directory:";
COLOR 14, 4
LOCATE 17,21 : PRINT SPACES(24);
LOCATE 17,21 : LINE INPUT ODIF$;
ODIF$=UCASE$(ODIF$)*"Y"
LOCATE 17,10 : COLOR 11,4 : PRINT "D";
COLOR 14, 4
LOCATE 17,21 : PRINT LEFT$(ODIF$,22);TAB(44);
RETURN

ChangeTitle:
COLOR 31, 4
LOCATE 16,10 : PRINT "Title:";
COLOR 14, 4
LOCATE 16,21 : PRINT SPACES(24);
LOCATE 16,21 : LINE INPUT TITLE$(OPTN3%)
LOCATE 16,10 : COLOR 11,4 : PRINT "T";
COLOR 15, 4 : PRINT "Title:";
RETURN

ChangeYLabel:
COLOR 31, 4
LOCATE 19,10 : PRINT "Y Label:";
COLOR 14, 4
LOCATE 19,21 : PRINT SPACES(24);
LOCATE 19,21 : LINE INPUT YLABEL$(OPTN3%)
LOCATE 19,10 : COLOR 11,4 : PRINT "Y";
COLOR 15, 4 : PRINT "Y Label:";
RETURN

ChangeYLabel:
COLOR 31, 4
LOCATE 20,10 : PRINT "Y Label:";
COLOR 14, 4
LOCATE 20,21 : PRINT SPACES(24);
LOCATE 20,21 : LINE INPUT YLABEL$(OPTN3%)
LOCATE 20,10 : COLOR 11,4 : PRINT "Y";
COLOR 15, 4 : PRINT "Y Label:";
RETURN

ChangeLineName:
COLOR 31, 4
LOCATE 21,10 : PRINT "Line Name:";
COLOR 14, 4
LOCATE 21,21 : PRINT SPACES(24);
LOCATE 21,21 : LINE INPUT LINENAME$(OPTN3%)
LOCATE 21,10 : COLOR 11,4 : PRINT "L";
COLOR 15, 4 : PRINT "Line Name:";
RETURN

GetAnotherFile:
COLOR 31,4
LOCATE 16,10 : PRINT "File:";
COLOR 14,4
LOCATE 16,21 : PRINT SPACES(24);
LOCATE 16,21 : LINE INPUT TEMPS
IF TEMPS<>" " THEN
  OFILES=UCASE$(TEMPS)
ELSE
  IF NIMES(OPTN3%)<>" " THEN OFILES=NIMES(OPTN3%)
END IF
LOCATE 16,21 : PRINT OFILES
GOSUB GetFile
IF PTCOON$="Y" AND COUNT$(OPTN3%)>0 THEN GOSUB RegressionAnalysis
IF HCSITTS="Y" THEN GOSUB HardCopyStats
IF HCPTSS$="Y" THEN GOSUB HardCopyPoints
COLOR 11,4
LOCATE 16,10 : PRINT "F"; : COLOR 15, 4 : PRINT "File:";
COLOR 14, 4
LOCATE 16,21 : PRINT LEFT$(OFILES, 22);TAB(44);
LOCATE 17,21 : PRINT LEFT$(ODIF$, 22);TAB(44);
LOCATE 18,21 : PRINT LEFT$(TITLE$,22);TAB(44);
LOCATE 19,21 : PRINT LEFT$(YLABEL$(OPTN3%), 22);TAB(44);
LOCATE 20,21 : PRINT LEFT$(YLABEL$(OPTN3%), 22);TAB(44);
LOCATE 21,21 : PRINT LEFT$(LINENAME$(OPTN3%),22);TAB(44);
IF GOFTN%=2 THEN COLOR 14,0 ELSE COLOR 14,4
LOCATE 17,69 : PRINT ":",PTCOON$(OPTN3%);" ";
NIMES(OPTN3%)=OFILES
INCR OPTN3%
IF OPTN3%>9 THEN OPTN3%=0
IF OPTN3%>=NumFiles% THEN NumFiles%=OPTN3%
COLOR 4, 3
FOR I%=1 TO NumFiles%
  LOCATE I%+3,2 : PRINT ":",NIMES(I%);TAB(16);
NEXT I%
COLOR 12, 0
LOCATE OPTN3%+3,2 : PRINT ":",NIMES(OPTN3%);TAB(16);
RETURN

DoDirectory:
COLOR 16, 3
LOCATE 23, 1 : PRINT SPACES(80);
LOCATE 23,10 : PRINT "Please enter mask for Directory: ";
COLOR 1, 3 : LINE INPUT TEMPS
IF TEMPS="" THEN TEMPS=ODIF$
COLOR 10, 0 : CLS
FILES TEMPS
COLOR 12, 0
PRINT TAB(20)," *** Press any key to Continue *** ";
AS=INPUT$(1)
COLOR 15, 0 : CLS
GOTO StartOfProgram
PageUpPageDown:
COLOR 4, 3

```

```

LOCATE OPTN3%+3.2 : PRINT "NAMES(OPTN3%),TAB(19);
IF AS=CHRS(0)+CHRS(73) THEN DECR OPTN3% ELSE INCR OPTN3%
IF OPTN3%<1 THEN OPTN3%=NumFiles%
IF OPTN3%>NumFiles% THEN OPTN3%=1
COLOR 12,0
LOCATE OPTN3%+3.2 : PRINT "NAMES(OPTN3%),TAB(19);
OFILES=NAMES(OPTN3%)
COLOR 14,4
LOCATE 16,21 : PRINT LEFT$(OFILES ,22);TAB(44);
LOCATE 17,21 : PRINT LEFT$(ODIRS ,22);TAB(44);
LOCATE 18,21 : PRINT LEFT$(TITLE$(OPTN3%) ,22);TAB(44);
LOCATE 19,21 : PRINT LEFT$(LABEL$(OPTN3%) ,22);TAB(44);
LOCATE 20,21 : PRINT LEFT$(VARIABLE$(OPTN3%) ,22);TAB(44);
LOCATE 21,21 : PRINT LEFT$(LINENAME$(OPTN3%) ,22);TAB(44);
IF GOPTN%=2 THEN COLOR 14,0 ELSE COLOR 14,4
LOCATE 17,69 : PRINT "PTCONS(OPTN3%) " ;
IF PTCONS="" THEN GOSUB PrintRegressionResults
RETURN
LeRight:
SELECT CASE GOPTN%
CASE 1
IF SCALES="" THEN SCALES="" ELSE SCALES=""
TEMP%=SCALES
CASE 2
SELECT CASE PTCONS(OPTN3%)
CASE ""
PTCONS(OPTN3%)="" : TEMP%=PTCONS(OPTN3%)
CASE "P"
PTCONS(OPTN3%)="P" : TEMP%=PTCONS(OPTN3%)
CASE "L"
PTCONS(OPTN3%)="L" : TEMP%=PTCONS(OPTN3%)
CASE "I"
PTCONS(OPTN3%)="I" : TEMP%=PTCONS(OPTN3%)
END SELECT
CASE 3
IF STATSS="" THEN STATSS="" ELSE STATSS=""
TEMP%=STATSS
CASE 4
IF HCSITTS="" THEN HCSITTS="" ELSE HCSITTS=""
TEMP%=HCSITTS
CASE 5
IF HCPTSS="" THEN HCPTSS="" ELSE HCPTSS=""
TEMP%=HCPTSS
CASE 6
IF FULLCS="" THEN FULLCS="" ELSE FULLCS=""
TEMP%=FULLCS
END SELECT
COLOR 14,0 : LOCATE GOPTN%+15,69
PRINT " ",TEMP%," ";
RETURN
UpDown:
IF GOPTN%=1 THEN TEMP%=SCALES
IF GOPTN%=2 THEN TEMP%=PTCONS(OPTN3%)
IF GOPTN%=3 THEN TEMP%=STATSS
IF GOPTN%=4 THEN TEMP%=HCSITTS
IF GOPTN%=5 THEN TEMP%=HCPTSS
IF GOPTN%=6 THEN TEMP%=FULLCS
COLOR 14,4 : LOCATE GOPTN%+15,69
PRINT " ",TEMP%," ";
IF AS=CHRS(0)+CHRS(72) THEN DECR GOPTN%

```

```

IF AS=CHRS(0)+CHRS(80) THEN INCR GOPTN%
IF GOPTN%<1 THEN GOPTN%=6
IF GOPTN%>8 THEN GOPTN%=1
IF GOPTN%=1 THEN TEMP%=SCALES
IF GOPTN%=2 THEN TEMP%=PTCONS(OPTN3%)
IF GOPTN%=3 THEN TEMP%=STATSS
IF GOPTN%=4 THEN TEMP%=HCSITTS
IF GOPTN%=5 THEN TEMP%=HCPTSS
IF GOPTN%=6 THEN TEMP%=FULLCS
COLOR 14,0 : LOCATE GOPTN%+15,69
PRINT " ",TEMP%," ";
RETURN

```

FindMinMax.

This is the subroutine to find the min and max data points.

```

IF SCALES="" THEN
MAXX=OBS(1,1) : MINX=OBS(1,1)
MAXY=CALC(1,1) : MINY=CALC(1,1)
FOR J%=1 TO File%
IF OBS(J%,1%)<MINX THEN MINX=OBS(J%,1%)
IF OBS(J%,1%)>MAXX THEN MAXX=OBS(J%,1%)
IF CALC(J%,1%)<MINY THEN MINY=CALC(J%,1%)
IF CALC(J%,1%)>MAXY THEN MAXY=CALC(J%,1%)
NEXT J%
IF MAXX>0 THEN MAXX=MAXX+.05*MAXX ELSE MAXX=MAXX-.05*MAXX
IF MINX>0 THEN MINX=MINX-.05*MINX ELSE MINX=MINX+.05*MINX
IF MAXY>0 THEN MAXY=MAXY+.05*MAXY ELSE MAXY=MAXY-.05*MAXY
IF MINY>0 THEN MINY=MINY-.05*MINY ELSE MINY=MINY+.05*MINY
RETURN
ELSE
. Must draw screen for min and max data.
COLOR 15,0 : CLS : COLOR 2,4
LOCATE 7,10 : PRINT CHRS(201);STRING$(56,209);CHRS(167); 'top line
FOR I%=6 TO 16
LOCATE I%,10 PRINT CHRS(186);STRING$(56,32);CHRS(186); 'ends
NEXT I%
LOCATE 17,10 : PRINT CHRS(200);STRING$(56,209);CHRS(186); 'bottom line
COLOR 15,4
LOCATE 9,27 : PRINT "Minimum X Value";
LOCATE 10,27 : PRINT "Maximum X Value";
LOCATE 11,27 : PRINT "Minimum Y Value";
LOCATE 12,27 : PRINT "Maximum Y Value";
LOCATE 14,24 : PRINT "Position Cursor to change a value ";
COLOR 14,4
LOCATE 9,44 : PRINT MINX;
LOCATE 10,44 : PRINT MAXX;
LOCATE 11,44 : PRINT MINY;
LOCATE 12,44 : PRINT MAXY;

```

```

* Must see what to do.
TEMP%=1 : LOCATE 8+TEMP%,44 : COLOR 14,0 : PRINT MINX;
Startloop3:
AS=INKEY%
SELECT CASE AS
CASE =
GOTO Startloop3
CASE 'Q','q',CHR$(27)
COLOR 15,0 : CLS
GOTO StartProgram
CASE 'O','o'
GOTO Options
CASE CHR$(13)
RETURN
CASE ' ','0','1','2','3','4','5','6','7','8','9'
COLOR 14,4
LOCATE 8+TEMP%,44 : PRINT SPACES(24);
COLOR 14,0 : LOCATE 8+TEMP%,44 : PRINT AS;
SELECT CASE TEMP%
CASE 1
LINE INPUT TEMP%
MINX=VAL(AS+TEMP%)
GOTO Startloop3
CASE 2
LINE INPUT TEMP%
MAXX=VAL(AS+TEMP%)
GOTO Startloop3
CASE 3
LINE INPUT TEMP%
MINY=VAL(AS+TEMP%)
GOTO Startloop3
CASE 4
LINE INPUT TEMP%
MAXY=VAL(AS+TEMP%)
GOTO Startloop3
CASE ELSE
SOUND 1000,3 : SOUND 800,1.5
GOTO Startloop3
END SELECT
CASE CHR$(0)+CHR$(72), CHR$(0)+CHR$(80)
COLOR 14,4
LOCATE 8+TEMP%,44
IF TEMP%=1 THEN PRINT MINX;
IF TEMP%=2 THEN PRINT MAXX;
IF TEMP%=3 THEN PRINT MINY;
IF TEMP%=4 THEN PRINT MAXY;
IF AS=CHR$(0)+CHR$(72) THEN DECR TEMP% ELSE INCR TEMP%
IF TEMP%<1 THEN TEMP%=4
IF TEMP%>4 THEN TEMP%=1
COLOR 14,0
LOCATE 8+TEMP%,44
IF TEMP%=1 THEN PRINT MINX;
IF TEMP%=2 THEN PRINT MAXX;
IF TEMP%=3 THEN PRINT MINY;
IF TEMP%=4 THEN PRINT MAXY;
GOTO Startloop3
CASE ELSE
SOUND 1000,3 : SOUND 800,1.5
GOTO Startloop3
END SELECT

```

```

* no key
* quit
* options
* enter
* edit
* up-down
* copall

```

```

RegressionAnalysis:
* This is a subroutine do the regression analysis for corr coeff.
S1=0 : S2=0 : S3=0 : S4=0 : S5=0 : S6=0 : S7=0 : S8=0 : S9=0 : C%=0
FOR J%=1 TO COUNT%(OPTN3%)
IF USE%(OPTN3%,J%)=1 THEN
S1=S1+OBS(OPTN3%,J%)
S2=S2+CALC(OPTN3%,J%)
S3=S3+OBS(OPTN3%,J%)*CALC(OPTN3%,J%)
S4=S4+OBS(OPTN3%,J%)^2
S5=S5+CALC(OPTN3%,J%)^2
INCR C%
END IF
NEXT J%
D=C%*S4-S1^2
AA1=(C%*S3-S1*S2)/D
AA2=(S4*S2-S1*S3)/D
IF AA2<1E-10 AND AA2>-1E-10 THEN AA2=0
FOR J%=1 TO C%
R(J%)=CALC(OPTN3%,J%)-AA1*OBS(OPTN3%,J%)-AA2
IF R(J%)<1E-10 AND R(J%)>1E-10 THEN R(J%)=0
S5=S5+R(J%)^2
NEXT J%
S=SQR(S5/(C%-2))
E1=SQR(C%/D)*1.96*S
E2=SQR(S4/D)*1.96*S
R2=(C%*S3-S1*S2)^2/((C%*S4-S1^2)*(C%*S6-S2^2))
IF E1<1E-10 AND E1>1E-10 THEN E1=0
IF E2<1E-10 AND E2>1E-10 THEN E2=0
IF R2<1E-10 AND R2>1E-10 THEN R2=0
RPTS%(OPTN3%)=C%
SLOPE(OPTN3%)=AA1
INTCP(OPTN3%)=AA2
SDRES(OPTN3%)=S
ERRSL(OPTN3%)=E1
ERRIN(OPTN3%)=E2
CORR(OPTN3%)=R2
GOSUB PrintRegressionResults
RETURN
PrintRegressionResults
* This is a subroutine do the print the regression results.

```

```

LPRINT USING " Slope: #####.#####;AA1
LPRINT USING " Intercept: #####.#####;AA2
LPRINT "Standard Deviation of Residuals:
LPRINT USING "#####;B
LPRINT "Expected error in slope (95% confidence):
LPRINT USING "#####;E1
LPRINT "Expected error in intercept (95% confidence):
LPRINT USING "#####;E2
LPRINT USING "Correlation Coefficient: #####;R2
LPRINT
RETURN
    
```

HardCopyPoints:

Subroutine to hardcopy the points on the printer.

```

LPRINT "Time: ",TIME$, " Date: ",DATE$
LPRINT " File Name: ",ODIR$+OFILES
LPRINT " Line Name: ",LINENAME$(OPTN3%)
LPRINT " Title Line #1: ",TITLE1$(OPTN3%)
LPRINT " Title Line #2: ",TITLE2$(OPTN3%)
LPRINT " X Axis Label: ",XLABEL$(OPTN3%)
LPRINT " Y Axis Label: ",YLABEL$(OPTN3%)
LPRINT " Number of Pts: ",COUNT$(OPTN3%)
FOR %I=1 TO COUNT$(OPTN3%)
    LPRINT OBS(OPTN3%,%I),"",CALC(OPTN3%,%I),"",USE$(OPTN3%,%I)
NEXT %I
LPRINT
RETURN
    
```

DrawPoint:

This is the subroutine to draw in the data point.

```

IF FULLCS="Y" THEN
SELECT CASE %J%
CASE 1,2,3,4,5,6 : TEMP%=C3%+(%J%-1)
CASE 7,8,9       : TEMP%=C3%+(%J%-7)
END SELECT
ELSE
TEMP%=15
END IF
SELECT CASE %J%
CASE 1           : CIRCLE (TEMP1-1,TEMP2-1),2,TEMP%
CASE 2           : BOX (TEMP1-3,TEMP2-3),(TEMP1+3,TEMP2+3),TEMP%,B
CASE 3           : CROSS
    
```

```

* Have done calcs, so print to the screen, printer.
COLOR 2,1
LOCATE 1,20 : PRINT CHR$(201);STRINGS(59,205);CHR$(187) 'top line
FOR %I=2 TO 12
    LOCATE %I,20:PRINT CHR$(186);STRINGS(59, 32);CHR$(186) 'ends
NEXT %I
LOCATE 13,20 : PRINT CHR$(200);STRINGS(59,205);CHR$(186) 'bottom line
COLOR 10,1
LOCATE 2,22 : PRINT TIMES;
LOCATE 2,66 : PRINT DATES;
COLOR 15,1
LOCATE 3,25 : PRINT "Statistics for file:";
LOCATE 4,25 : PRINT "Line Name:";
LOCATE 5,25 : PRINT "Property:";
LOCATE 6,25 : PRINT "Class:";
LOCATE 7,35 : PRINT "Number of Points:";
LOCATE 8,22 : PRINT "Slope:";
LOCATE 9,22 : PRINT "Intercept:";
LOCATE 10,22 : PRINT "Standard Deviation of Residuals:";
LOCATE 11,22 : PRINT "Expected Error in Slope (95% confidence):";
LOCATE 11,22 : PRINT "Expected Error in Intercept (95% confid)";
LOCATE 12,30 : PRINT "Correlation Coefficient:";
COLOR 14,1
LOCATE 3,46 : PRINT LEFT$(ODIR$+OFILES,31);TAB(76);
LOCATE 4,37 : PRINT LEFT$(LINENAME$(OPTN3%),40);TAB(76);
LOCATE 6,31 : PRINT PROP$(PROP%);TAB(76);
LOCATE 7,55 : PRINT USING "#####;RPTS$(OPTN3%);
LOCATE 8,30 : PRINT USING "#####;SLOPE(OPTN3%);
LOCATE 9,65 : PRINT USING "#####;INTCP(OPTN3%);
LOCATE 9,65 : PRINT USING "#####;SDRES(OPTN3%);
LOCATE 10,65 : PRINT USING "#####;ERRSL(OPTN3%);
LOCATE 11,65 : PRINT USING "#####;ERRRN(OPTN3%);
LOCATE 12,65 : PRINT USING "#####;CORR(OPTN3%);
    
```

```

* Will play tape if sound is on and corr coeff < 0.5
IF SND6="Y" AND R2<0.5 THEN
PLAY "T120MBO2L4OCL2EL6CL6EL4G16CL6EL4G14G12BL4GEL2CL4OCL2E"
END IF
RETURN
    
```

HardCopyStats:

Subroutine to hardcopy the stats on the printer.

```

LPRINT "Time: ",TIME$, " Date: ",DATE$
LPRINT "Statistics for file: ",ODIR$+OFILES
LPRINT " Line Name: ",LINENAME$(OPTN3%)
LPRINT " Title Line #1: ",TITLE1$(OPTN3%)
LPRINT " Title Line #2: ",TITLE2$(OPTN3%)
LPRINT " X Axis Label: ",XLABEL$(OPTN3%)
LPRINT " Y Axis Label: ",YLABEL$(OPTN3%)
LPRINT USING " Number of Points: ###;C%
    
```

```

LINE (TEMP1,TEMP2-3):(TEMP1,TEMP2+3),TEMP%,TEMP%
LINE (TEMP1-3,TEMP2):(TEMP1+3,TEMP2),TEMP%
CASE 4
LINE (TEMP1-3,TEMP2-3):(TEMP1+3,TEMP2+3),TEMP%,BF
CASE 5
LINE (TEMP1-3,TEMP2-3):(TEMP1,TEMP2+3),TEMP%
LINE (TEMP1,TEMP2+3):(TEMP1+3,TEMP2-3),TEMP%
LINE (TEMP1+3,TEMP2-3):(TEMP1-3,TEMP2-3),TEMP%
CASE 6
CIRCLE (TEMP1-1,TEMP2-1),3,TEMP%
PAINT (TEMP1,TEMP2),TEMP%
CASE 7
LINE (TEMP1-3,TEMP2-3):(TEMP1,TEMP2+3),TEMP%
LINE (TEMP1,TEMP2+3):(TEMP1+3,TEMP2-3),TEMP%
LINE (TEMP1+3,TEMP2-3):(TEMP1-3,TEMP2-3),TEMP%
PAINT (TEMP1,TEMP2),TEMP%
CASE 8
LINE (TEMP1,TEMP2-3):(TEMP1,TEMP2+3),TEMP%
LINE (TEMP1-3,TEMP2):(TEMP1+3,TEMP2),TEMP%
LINE (TEMP1+3,TEMP2-3):(TEMP1+3,TEMP2-3),TEMP%
CASE 9
CIRCLE (TEMP1,TEMP2),4,TEMP%
LINE (TEMP1,TEMP2-3):(TEMP1,TEMP2+3),TEMP%
LINE (TEMP1-3,TEMP2):(TEMP1+3,TEMP2),TEMP%
END SELECT
RETURN

```

Labelines:
 * filled box
 * triangle
 * filled circle
 * filled tri
 * asterisk
 * cross&circle

This is the subroutine to draw in the line names.

```

IF FULLCS="Y" THEN
SELECT CASE J%
CASE 1,2,3,4,5,6 : TEMP%=C3%+(J%-1)
CASE 7,8,9 : TEMP%=C3%+(J%-7)
END SELECT
ELSE
TEMP%=15
END IF
SELECT CASE File%
CASE 1,2,3
SELECT CASE J%
CASE 1 : TEMP23="449"
CASE 2 : TEMP23="484"
CASE 3 : TEMP23="479"
END SELECT
TEMP33=LEFT$(LINENAMES(J%),50)
TEMP18=STR$(350-9*LEN(TEMP33))
TEMP1 =PMAP(VAL(TEMP18)-9,2)
TEMP2 =PMAP(VAL(TEMP23)-3,3)
CASE 4,5,6
SELECT CASE J%
CASE 1 : TEMP18="350" : TEMP23="449"
CASE 2 : TEMP18="32" : TEMP23="449"
CASE 3 : TEMP18="350" : TEMP23="484"
CASE 4 : TEMP18="32" : TEMP23="484"
CASE 5 : TEMP18="32" : TEMP23="479"
CASE 6 : TEMP18="350" : TEMP23="479"
END SELECT
TEMP33=LEFT$(LINENAMES(J%),25)
TEMP1 =PMAP(VAL(TEMP18)-9,2)
TEMP2 =PMAP(VAL(TEMP23)-3,3)
CASE 7,8,9
SELECT CASE J%
CASE 1 : TEMP1=-30 : TEMP2=-60 : TEMP18="32" : TEMP23="449"
CASE 2 : TEMP1=165 : TEMP2=-60 : TEMP18="248" : TEMP23="449"
CASE 3 : TEMP1=-355 : TEMP2=-60 : TEMP18="457" : TEMP23="449"
CASE 4 : TEMP1=-30 : TEMP2=-60 : TEMP18="32" : TEMP23="484"
CASE 5 : TEMP1=165 : TEMP2=-60 : TEMP18="248" : TEMP23="484"
CASE 6 : TEMP1=-355 : TEMP2=-60 : TEMP18="457" : TEMP23="484"
CASE 7 : TEMP1=-30 : TEMP2=-100 : TEMP18="32" : TEMP23="479"
CASE 8 : TEMP1=165 : TEMP2=-100 : TEMP18="248" : TEMP23="479"
CASE 9 : TEMP1=-355 : TEMP2=-100 : TEMP18="457" : TEMP23="479"
END SELECT
TEMP33=LEFT$(LINENAMES(J%),19)
END SELECT
IF TEMP33<>" THEN
GOSUB DrawFont
* Must draw in the line name.
DRAW "C"+STR$(TEMP%)
TEMP%=VAL(TEMP18)
FOR I%=1 TO LEN(TEMP33)
TEMP%=MID$(TEMP33,I%,1)
IF ASC(TEMP%)>=33 AND ASC(TEMP%)<=122 THEN
GET #1,ASC(TEMP%)
DRAW "BM"+STR$(TEMP%)+";"+TEMP23+"TAO "+CHARS
* get char
* draw char
END IF
INCR TEMP%,12
NEXT I%
END IF
RETURN
GetFile:
This is a subroutine to read the data from a graphing file.
GOSUB CheckForFile
COUNT%(OPTN3%)=1
OPEN ODIFS+OFIL$ FOR INPUT AS #1
IF NOT EOF(1) THEN INPUT #1,LINENAMES(OPTN3%)
IF NOT EOF(1) THEN INPUT #1,TITLE1$(OPTN3%)
IF NOT EOF(1) THEN INPUT #1,TITLE2$(OPTN3%)
IF NOT EOF(1) THEN INPUT #1,XLABEL$(OPTN3%)
IF NOT EOF(1) THEN INPUT #1,YLABEL$(OPTN3%)
WHILE NOT EOF(1)
INPUT #1,OBIS(OPTN3%),COUNT%(OPTN3%)

```

* 1st select
 * full color
 * black&white

```

FOR I%=1 TO 4
  LOCATE I%,1 : PRINT SPACES(22);
NEXT I%
LOCATE 1,1 : PRINT "O.":TEMP1;
LOCATE 2,1 : PRINT "C.":TEMP2;
LOCATE 3,1 : PRINT "P.":SMPLNUMS;
LOCATE 4,1 : PRINT "N.":LEFT$(SMPLNUMS,10);
WINDOW (0,480)-(640,0)
LINE (0,417)-(175,480),10,B
WINDOW (-50,-105)-(530,525)
AS=INKEY$
WHILE AS$=""
  AS=INKEY$
WEND
LINE (TEMP3*6,TEMP4*5)-(TEMP3*6,TEMP4*6),0,B
FOR I%=1 TO 4
  LOCATE I%,1 : PRINT SPACES(22);
NEXT I%
WINDOW (0,480)-(640,0)
PUT (0,480),PIX%
WINDOW (-50,-105)-(530,525)
RETURN

```

This is the subrtn to do the error handling.

ErrorMessage:

```

SCREEN 0 : COLOR 15, 0 : CLS
COLOR 0, 4
LOCATE 8, 5 : PRINT CHR$(201);STRINGS(99,205);CHR$(187);
FOR I%=9 TO 15
  LOCATE I%,5 : PRINT CHR$(186);TAB(79);CHR$(186);
NEXT I%
LOCATE 16,5 : PRINT CHR$(200);STRINGS(99,205);CHR$(188);
COLOR 31, 4
LOCATE 11,28 : PRINT USING " >>> Error ### encountered <<<";ERR;
TEMP$="See Appendix E, p. 412, in Turbo Basic Manual for full message"
LOCATE 13, 9 : PRINT TEMP$;
COLOR 0, 3
LOCATE 24,19 : PRINT " Press any key to return to the Main Menu ";
TEMP$=INPUT$(1)
CLOSE
COLOR 15, 0 : CLS
GOTO StartOfProgram
CheckForFile:

```

This is the subrtn to see if a file is present before opening.

```

INPUT #1,CALC(OPTN3%,COUNT$(OPTN3%))
INPUT #1,USE$(OPTN3%,COUNT$(OPTN3%))
INPUT #1,TEMP$
INPUT #1,TEMP$
INCR COUNT$(OPTN3%)
WEND
CLOSE #1
DECR COUNT$(OPTN3%)
RETURN

```

This is a subroutine to find the closest match to the point.

```

WINDOW (0,480)-(640,0)
GET (0,417)-(175,480),PIX%
TEMP3=0%-XOFFSET)/YEXPAC : TEMP4=(Y%-YOFFSET)/YEXPAC
DIFF=ABS(TEMP3-OBS(1,1)) + ABS(TEMP4-CALC(1,1))
TEMP1=OBS(1,1) : TEMP2=CALC(1,2) : FLE%=1
FOR J%=1 TO FILE%
  TEMP=ABS(TEMP3-OBS(J%,1%)) + ABS(TEMP4-CALC(J%,1%))
  IF TEMP < DIFF THEN
    DIFF=TEMP : TEMP1=OBS(J%,1%) : TEMP2=CALC(J%,1%) : FLE%=J%
  END IF
NEXT J%
NEXT PIX%

```

```

* Must find matching point.
TEMP%=1
OPEN ODR$+NM$(FLE%) FOR INPUT AS #1
IF NOT EOF(1) THEN INPUT #1,LINENAMES$(FLE%)
IF NOT EOF(1) THEN INPUT #1,TITLE$(FLE%)
IF NOT EOF(1) THEN INPUT #1,TITLE2$(FLE%)
IF NOT EOF(1) THEN INPUT #1,XLABEL$(FLE%)
IF NOT EOF(1) THEN INPUT #1,YLABEL$(FLE%)
WHILE NOT EOF(1)
  INPUT #1,OBS(FLE%,TEMP%)
  INPUT #1,CALC(FLE%,TEMP%)
  INPUT #1,USE$(FLE%,TEMP%)
  INPUT #1,SMPLNUMS
  INPUT #1,SMPLNMES
  INPUT #1,POINTNO%
  IF OBS(FLE%,TEMP%)=TEMP1 AND CALC(FLE%,TEMP%)=TEMP2 THEN GOTO Found
  INCR TEMP%
WEND
Found:
CLOSE #1

```

```

* Will put a box around the point, display results.
WINDOW (-50,-105)-(530,525)
TEMP3=TEMP1*XEXPAC + XOFFSET : TEMP4=TEMP2*YEXPAC + YOFFSET
LINE (TEMP3*6,(TEMP4*5)-(TEMP3*5,TEMP4*6),13,B

```

Listing for Program II.5: GRAF_ED.BAS

This program is designed to edit the graphing files. That is, it pulls the file from the disk, displays it, allows it to be edited, and returns the file to the disk. With this program, you can delete points from the graph, etc.

Program Name: GRAF ED Ver 5.00 Date Written: 12/14/1987
 Author: Allen Caswell Date Modified: 12/20/1987

First is the section to set up the variables.

```
COMMON ODIRS, OFILES
VERFNS="5 00"
OPTN1%=1
OPTN2%=1
PAGE%=1
IF ODIRS="" THEN ODIRS = "D:\CORR\RESULT"
IF OFILES="" THEN OFILES = "TEST.DAT"
DIM OBS(500), CALC(500), USE%(500), SMP(LNME$(500)
DIM SMP(LNME$(500), POINTNO%(500)
. Next are options for end of program.
DATA * Exit to DOS ** Run CORR ** Run PROPS ** Run REGS *
DATA * Run ERROR ** Run GRAPH ** Run EZ_PLOT ** Restart *
FOR I%=1 TO 8 : READ OPTN$(I%) : NEXT I%
```

StartOfProgram

This is the section for the opening screen, dir and file data.

```
. Top box - for the title
COLOR 15,0 : CLS
COLOR 15,4
LOCATE 1, 5 : PRINT CHR$(201);STRING$(89,205);CHR$(167)
LOCATE 2, 5 : PRINT CHR$(186);STRING$(89, 32);CHR$(186)
LOCATE 3, 5 : PRINT CHR$(200);STRING$(89,205);CHR$(188)
LOCATE 1,31 : PRINT CHR$(208);
LOCATE 2,31 : PRINT CHR$(178);
LOCATE 3,31 : PRINT CHR$(207);
LOCATE 2,10 : PRINT "GRAF ED"
LOCATE 2,20 : PRINT VERFNS
LOCATE 2,40 : PRINT "Graph File Editing Software";
. Directory and File box
COLOR 10,1
```

```
SHELL "DIR "+ODIRS+OFILES+" > "+SCRDIRS+TEMP.ZZZ
OPEN SCRDIRS+TEMP.ZZZ FOR INPUT AS #1
FOR I%=1 TO 4
LINE INPUT #1,TEMP$
NEXT I%
IF EOF(1) THEN
CLOSE 1 : KILL SCRDIRS+TEMP.ZZZ
SCREEN 0 : COLOR 15, 0 : CLS
COLOR 0, 4
LOCATE 8, 5 : PRINT CHR$(201);STRING$(89,205);CHR$(167);
FOR I%=9 TO 15
LOCATE I%,5 : PRINT CHR$(186);TAB(79);CHR$(186);
NEXT I%
LOCATE 16,5 : PRINT CHR$(200);STRING$(89,205);CHR$(188);
COLOR 31, 4
LOCATE 11,23 : PRINT "Unable to open the requested file."
COLOR 14, 4
TEMP$=">>>"+ODIRS+OFILES+" is not in the directory <<<"
LOCATE 13,40-5*LEN(TEMP$) : PRINT TEMP$
COLOR 0, 3
LOCATE 24,19 : PRINT * Press any key to return to the Main Menu *;
TEMP$=INPUT$(1)
GOTO StartOfProgram
END IF
CLOSE 1 : KILL SCRDIRS+TEMP.ZZZ
RETURN
```

FindExponent:

```
. This is a miniaubroutine to find the exponent of a number.
TEMP=0.0000000000000001 : TEMP%=-18
WHILE TEMP<TEMP1 AND TEMP%<38
TEMP=TEMP*10 : INCR TEMP%
WEND
RETURN
```

Logo:

```
$INCLUDE "LOGO.BAS"
```

T-T-T-That's all folks ! ! ! !

```

LOCATE 7,15 : PRINT CHR$(218);STRING$(49,199);CHR$(191); ' top line
FOR I%=8 TO 16
  LOCATE I%,15 : PRINT CHR$(179);TAB(69);CHR$(179); ' middle
NEXT I%
LOCATE 17,15 : PRINT CHR$(192);STRING$(49,199);CHR$(217); ' bottom line
COLOR 15,1
LOCATE 10,24 : PRINT TIMES;
LOCATE 10,47 : PRINT DATES;
LOCATE 12,24 : PRINT "Directory:";
LOCATE 14,24 : PRINT "File:";
COLOR 14,1
LOCATE 12,36 : PRINT ODIRS;
LOCATE 14,36 : PRINT OFILES;
.
.
.
. Next are commands.
COLOR 3,0
LOCATE 22,17 : PRINT * Press <SPACE> to edit highlighted data. *;
LOCATE 23,17 : PRINT *Press <RET> to continue, <O> for options menu.*;
.
. Next see what to do.
COLOR 14,0
LOCATE 12+(OPTN1%-1)*2,36 : PRINT *;TEMP%; *;
LOCATE 12+(OPTN1%-1)*2,36 : PRINT *;TEMP%; *;
Startloop1:
AS=INKEY$
SELECT CASE AS
CASE =
  COLOR 15,1
  LOCATE 10,24 : PRINT TIMES;
  GOTO Startloop1
CASE CHR$(13)
  GOTO EditData
CASE "O";"O";"Q";"q";CHR$(27)
  GOTO Options
CASE CHR$(0)+CHR$(72), CHR$(0)+CHR$(60)
  IF OPTN1%=1 THEN TEMPS=ODIRS ELSE TEMPS=OFILES
  LOCATE 12+(OPTN1%-1)*2,36 : PRINT *;TEMP%; *;
  IF OPTN1%=1 THEN OPTN1%=2 ELSE OPTN1%=1
  COLOR 14,0
  IF OPTN1%=1 THEN TEMPS=ODIRS ELSE TEMPS=OFILES
  LOCATE 12+(OPTN1%-1)*2,36 : PRINT *;TEMP%; *;
  GOTO Startloop1
CASE CHR$(0)+CHR$(75),CHR$(0)+CHR$(77)
  GOTO Startloop1
CASE ELSE
  IF ASC(AS) >= 65 AND ASC(AS) <= 122 THEN
    COLOR 3,1,1
    SELECT CASE OPTN1%
      CASE 1 : TEMPS="Directory:"
      CASE 2 : TEMPS="File:"
    END SELECT
    LOCATE 12+(OPTN1%-1)*2,24 : PRINT TEMPS;
    COLOR 12,1
    LOCATE 12+(OPTN1%-1)*2,36 : PRINT SPACES(25);
    LOCATE 12+(OPTN1%-1)*2,38 : PRINT AS;
    LOCATE 12+(OPTN1%-1)*2,38 : LINE INPUT TEMPS
    SELECT CASE OPTN1%
      CASE 1 : ODIRS =UCASES(AS)+UCASE$(TEMP$)+";" : TEMPS=ODIRS
      CASE 2 : OFILES=UCASES(AS)+UCASE$(TEMP$) : TEMPS=OFILES
    END SELECT
  ELSE
    COLOR 15,0 : CLS
    COLOR 0,1
    LOCATE 1,1 : PRINT CHR$(201);STRING$(78,209);CHR$(187); ' top
    FOR I%=2 TO 24
      LOCATE I%,1 : PRINT CHR$(186);TAB(80);CHR$(186); ' slides
    NEXT I%
    LOCATE 25,1 : PRINT CHR$(200);STRING$(78,209);CHR$(186); ' bottom
    LOCATE 3,1 : PRINT CHR$(199);STRING$(78,199);CHR$(182); ' cross bar
    LOCATE 5,1 : PRINT CHR$(199);STRING$(78,199);CHR$(182); ' cross bar
    LOCATE 23,1 : PRINT CHR$(199);STRING$(78,199);CHR$(182); ' cross bar
    COLOR 10,1
    LOCATE 2,5 : PRINT "File:";
    LOCATE 2,67 : PRINT "Page:";
    LOCATE 4,9 : PRINT "Observed";
    LOCATE 4,28 : PRINT "Calculated";
    LOCATE 4,42 : PRINT "Use";
    LOCATE 4,46 : PRINT "Number";
    LOCATE 4,60 : PRINT "Name";
    LOCATE 4,74 : PRINT "Point";
    LOCATE 24,15 : PRINT "Press <SPACE> to edit, <F1> to File, <ESC> to Quit";
    COLOR 12,1
    LOCATE 2,12 : PRINT ODIRS,OFILES;
    LOCATE 2,73 : PRINT USING "###";PAGE%;
  .
  . Have got page, so get data, so edit it!
  GOSUB GetFile
  GOSUB PrintPage
  TEMP1%=1 : TEMP2%=1
  COLOR 11,0 : GOSUB MarkData
  Startloop4:
  AS=INKEY$
  SELECT CASE AS
  CASE =
    GOTO Startloop4
  .
  . get data
  . print data
  . mark data
  . no key

```

This is the section to edit the data.


```

CASE CHR$(27) + CHR$(7)
COLOR 31,4
LOCATE 24, 2 : PRINT SPACES(20);
PRINT 'Are you sure? (Y/N)';
PRINT SPACES(30);
Startloop5:
ABS=INKEY$
SELECT CASE ABS
CASE =
GOTO Startloop5
CASE "Y", "y", "O", "o", "Y", "y", "O", "o" : CHR$(27)
GOTO StartOfProgram
CASE "N", "n"
COLOR 10,1
LOCATE 24, 2 : PRINT SPACES(19);
PRINT 'Press <SPACE> to edit, <F> to File, <ESC> to Quit';
PRINT SPACES(13);
GOTO Startloop4
CASE ELSE
SOUND 1000,3 : SOUND 800,1.5
GOTO Startloop5
END SELECT
CASE CHR$(0) + CHR$(56)
COLOR 31,4
LOCATE 24, 2 : PRINT SPACES(19);
PRINT '***** Filling the Data *****';
PRINT SPACES(13);
GOSUB FillData
COLOR 10,1
LOCATE 24, 2 : PRINT SPACES(19);
PRINT 'Press <SPACE> to edit, <F1> to File, <ESC> to Quit';
PRINT SPACES(13);
GOTO Startloop4
CASE CHR$(0) + CHR$(75), CHR$(0) + CHR$(77)
COLOR 15,1
GOSUB MarkData
IF AS=CHR$(0) + CHR$(75) THEN DECR TEMP2% ELSE INCR TEMP2%
IF TEMP2% < 1 THEN TEMP2%=0
IF TEMP2% > 6 THEN TEMP2%=1
COLOR 11,0
GOSUB MarkData
GOTO Startloop4
CASE CHR$(0) + CHR$(72), CHR$(0) + CHR$(60)
COLOR 15,1
GOSUB MarkData
IF AS=CHR$(0) + CHR$(72) THEN DECR TEMP1% ELSE INCR TEMP1%
IF TEMP1% < 1 THEN TEMP1%=17
IF TEMP1% > 17 THEN TEMP1%=1
COLOR 11,0
GOSUB MarkData
GOTO Startloop4
CASE CHR$(0) + CHR$(73), CHR$(0) + CHR$(61)
GOSUB ClearPage
IF AS=CHR$(0) + CHR$(73) THEN DECR PAGE% ELSE INCR PAGE%
IF PAGE% < 1 THEN PAGE%=29
IF PAGE% > 29 THEN PAGE%=1
COLOR 12, 1
LOCATE 2,73 : PRINT USING "###", PAGE%;
GOSUB PrintPage
COLOR 11,0 : GOSUB MarkData
quit
**
GOTO Startloop4
CASE **
COLOR 12,1
SELECT CASE TEMP2%
CASE 1
LOCATE TEMP1%+5,2
PRINT SPACES(LEN(SITRS)+OBS)(TEMP1%+(PAGE%-1)*17))+3);
LOCATE TEMP1%+5,3 : LINE INPUT TEMP$
OBS=(TEMP1%+(PAGE%-1)*17)=VAL(TEMP$)
CASE 2
LOCATE TEMP1%+5,22
PRINT SPACES(LEN(SITRS)+CALC)(TEMP1%+(PAGE%-1)*17))+3);
LOCATE TEMP1%+5,23 : LINE INPUT TEMP$
CALC=(TEMP1%+(PAGE%-1)*17)=VAL(TEMP$)
CASE 3
LOCATE TEMP1%+5,41
PRINT SPACES(6);
IF USE%(TEMP1%+(PAGE%-1)*17)=1 THEN
USE%(TEMP1%+(PAGE%-1)*17)=0
ELSE
USE%(TEMP1%+(PAGE%-1)*17)=1
END IF
CASE 4
LOCATE TEMP1%+5,45
PRINT SPACES(LEN(SMPLNUM$)(TEMP1%+(PAGE%-1)*17))+4);
LOCATE TEMP1%+5,47
LINE INPUT SMPLNUM$(TEMP1%+(PAGE%-1)*17)
CASE 5
LOCATE TEMP1%+5,51
PRINT SPACES(24);
LOCATE TEMP1%+5,53
LINE INPUT SIMPLNUM$(TEMP1%+(PAGE%-1)*17)
CASE 6
LOCATE TEMP1%+5,73
PRINT SPACES(7);
LOCATE TEMP1%+5,75 : LINE INPUT TEMP$
POINTNO%(TEMP1%+(PAGE%-1)*17)=VAL(TEMP$)
CASE ELSE
SOUND 1000,3 : SOUND 800,1.5
RETURN
END SELECT
COLOR 11,0 : GOSUB MarkData
GOTO Startloop4
CASE ELSE
SOUND 1000,3 : SOUND 800,1.5
GOTO Startloop4
END SELECT
Options:

```

This is the section to do the options.

COLOR 0,15
LOCATE 14,1 : PRINT CHR\$(219),STRINGS\$(15,196),CHR\$(191); ' top


```

COUNT%=1
OPEN OOIRS+OFILES$ FOR INPUT AS #1
IF NOT EOF(1) THEN INPUT #1,LINENAMES
IF NOT EOF(1) THEN INPUT #1,TITLE1$
IF NOT EOF(1) THEN INPUT #1,TITLE2$
IF NOT EOF(1) THEN INPUT #1,XLABELS
IF NOT EOF(1) THEN INPUT #1,YLABELS
WHILE NOT EOF(1)
  INPUT #1,OBS(COUNT%)
  INPUT #1,CALC(COUNT%)
  INPUT #1,USE%(COUNT%)
  INPUT #1,SMPLNUM$(COUNT%)
  INPUT #1,SMPLNMS(COUNT%)
  INPUT #1,POINTNO%(COUNT%)
  INCR COUNT%
WEND
CLOSE #1
DECR COUNT%
RETURN

```

Logo: \$INCLUDE *LOGO.BAS*

T-T-T:That's all folks!!!

```

RETURN
CASE 3
LOCATE TEMP1%+5,41
IF USE%(TEMP1%+(PAGE%-1)*17)=1 THEN TEMP%="Y" ELSE TEMP%="N"
PRINT " :TEMP%," ;
RETURN
CASE 4
LOCATE TEMP1%+5,45
PRINT " *SMPLNUM$(TEMP1%+(PAGE%-1)*17),"; ;
RETURN
CASE 5
LOCATE TEMP1%+5,51
PRINT " *LEFT$(SMPLNMS(TEMP1%+(PAGE%-1)*17),20),"; ;
RETURN
CASE 6
LOCATE TEMP1%+5,573
PRINT USING " ### "POINTNO%(TEMP1%+(PAGE%-1)*17);
RETURN
CASE ELSE
SOUND 1000,3 : SOUND 800,1.5
RETURN
END SELECT
RETURN

```

FileData:

This is a subroutine to put the data back into the file.

```

OPEN OOIRS+OFILES$ FOR OUTPUT AS #1
PRINT #1,LINENAMES
PRINT #1,TITLE1$
PRINT #1,TITLE2$
PRINT #1,XLABELS
PRINT #1,YLABELS
FOR I%=1 TO COUNT%
  TEMP%=STR$(OBS(I%))+STR$(CALC(I%))+";"
  TEMP%+TEMP$+STR$(USE%(I%))+";"
  TEMP%+TEMP$+CHR$(34)+SMPLNUM$(I%)+CHR$(34)+";"
  TEMP%+TEMP$+CHR$(34)+SMPLNMS(I%)+CHR$(34)+";"
  TEMP%+TEMP$+STR$(POINTNO%(I%))
  PRINT #1,TEMP%
NEXT I%
CLOSE #1
RETURN

```

GetFile:

This is a subroutine to read the data from a graphing file

Listing for Program II.6: ERROR.BAS

Program Name: ERROR.BAS Ver 1.00 Date Written: 06/10/1987
 Author: Allen Caswell Date Modified: 12/20/1987

The purpose of this program is to calculate the percentage errors in the correlations files generated by the Correlations programs. It reads the graphic files, then calculates the percentage error on each compound and then gives the overall average error.

First is the section to set up the variables.

```
COMMON ODIR$, OFILES$
DEFDBL A-Z
DIM XDAT(500), YDAT(500), USE%(500), CNUM$(500)
DIM ER(500), DI(500), RP(500)
VERSIN$="5 00"
OPTN% = 1
OPTN1% = 1
PAUSE = 0
HOOPY$ = ""
IF OFILES$="" THEN OFILES$="TEST.DAT"
IF ODIR$="" THEN ODIR$="D:\CORR\RESULT"

' Next are names for options on menu.
DATA " Exit To DOS **: Run GRAF ED **: Run CORR **: Run REGS *"
DATA " Run PROP'S **: Run GRAFH **: Run EZ-PILOT **: Restart *"
FOR I%=1 TO 8 : READ OPTN$(I%) : NEXT I%

' Next is editing for print using statement.
ABS=ABS+"##### 000,000,000000 ##### 000,000,000000"
BeginPgm:
```

Next will get the operational parameters.

```
' Will draw the screen.
COLOR 15,0 : CLS
COLOR 15,4
LOCATE 1,5 : PRINT CHR$(201);STRINGS$(66,205);CHR$(187)
LOCATE 2,5 : PRINT CHR$(186);STRINGS$(66,32);CHR$(186)
LOCATE 3,5 : PRINT CHR$(200);STRINGS$(66,205);CHR$(186)
LOCATE 1,31 : PRINT CHR$(209);
LOCATE 2,31 : PRINT CHR$(179);

' top line
' ends
' bottom line
' top junct
' middle line
```

```
LOCATE 3,31 : PRINT CHR$(207);
LOCATE 2,10 : PRINT "ERROR"
LOCATE 2,18 : PRINT VERSIN$
LOCATE 2,35 : PRINT "Statistical Error Analysis Software";

' Directory and File box.
COLOR 10,1
LOCATE 7,15 : PRINT CHR$(218);STRINGS$(49,199);CHR$(191);
FOR I%=8 TO 18
  LOCATE I%,15 : PRINT CHR$(179);TAB(65);CHR$(179);
NEXT I%
LOCATE 19,15 : PRINT CHR$(182);STRINGS$(49,199);CHR$(217);
COLOR 15,1
LOCATE 10,24 : PRINT TIMES;
LOCATE 10,47 : PRINT DATES;
LOCATE 12,24 : PRINT "Directory:";
LOCATE 14,24 : PRINT "File:";
LOCATE 16,24 : PRINT "Hard Copy:";
COLOR 14,1
LOCATE 12,36 : PRINT ODIRS;
LOCATE 14,38 : PRINT OFILES;
LOCATE 16,38 : PRINT HOOPY$;

' Next are commands
COLOR 3,0
LOCATE 22,17 : PRINT " Press <LETTER> to edit highlighted data. ";
LOCATE 23,6 : PRINT "Press <RET> to continue, <\> for directory, ";
LOCATE 24,6 : PRINT "<O> for options menu.";

' Next see what to do.
COLOR 14,0
IF OPTN1%=1 THEN TEMPS=ODIRS
IF OPTN1%=2 THEN TEMPS=OFILES
IF OPTN1%=3 THEN TEMPS=HOOPY$
LOCATE 12+(OPTN1%-1)*2,36 : PRINT " ;TEMPS:";
Startloop1:
AS=INKEY$
SELECT CASE AS
CASE =
  COLOR 15,1
  LOCATE 10,24 : PRINT TIMES;
  GOTO Startloop1
CASE CHR$(13)
  GOTO GetData
CASE "O", "o", "O", "o", "q", CHR$(27)
  GOTO Options
CASE CHR$(0)+CHR$(75),CHR$(0)+CHR$(77)
  GOTO Startloop1
CASE CHR$(0)+CHR$(72), CHR$(0)+CHR$(80)
  COLOR 14,1
  SELECT CASE OPTN1%
  CASE 1 : TEMPS=ODIRS
  CASE 2 : TEMPS=OFILES
  CASE 3 : TEMPS=HOOPY$
  END SELECT
  LOCATE 12+(OPTN1%-1)*2,36 : PRINT " ;TEMPS:";
  IF AS=CHR$(0)+CHR$(72) THEN DECR OPTN1% ELSE INCR OPTN1%
  IF OPTN1%<1 THEN OPTN1%=3
  IF OPTN1%>3 THEN OPTN1%=1
  COLOR 14,0
' no key
' return
' exit
' left-right
' up-down
```

GetData: Have gotten instructions so will get data and calculate.

```

SELECT CASE OPTN1%
CASE 1 : TEMPS=ODIRS
CASE 2 : TEMPS=OFILES
CASE 3 : TEMPS=HCOOPY%
END SELECT
LOCATE 12+(OPTN1%-1)*2,36 : PRINT " ",TEMPS," ";
GOTO Startloop1
CASE " "
COLOR 16, 4
LOCATE 24, 1 : PRINT SPACES(80);
LOCATE 24,10 : PRINT "Please enter mask for Directory: ";
COLOR 15, 4 : LINE INPUT TEMPS
IF TEMPS="" THEN TEMPS=ODIRS
COLOR 10, 0 : CLS
FILES TEMPS
COLOR 12, 0
PRINT TAB(20); " *** Press any key to Continue *** ";
AS=INPUT$(1)
COLOR 15,0 : CLS
GOTO BeginPgm
CASE ELSE
IF ASC(AS)>=65 AND ASC(AS)<=122 THEN
COLOR 31,1
SELECT CASE OPTN1%
CASE 1 : TEMPS="Directory;"
CASE 2 : TEMPS="File;"
CASE 3 : TEMPS="Hard Copy;"
END SELECT
LOCATE 12+(OPTN1%-1)*2,24 : PRINT TEMPS;
IF OPTN1%=3 THEN
SELECT CASE HCOOPY%
CASE "Y" : HCOOPY%="Y" : TEMPS=HCOOPY%
CASE "F" : HCOOPY%="F" : TEMPS=HCOOPY%
CASE "H" : HCOOPY%="H" : TEMPS=HCOOPY%
END SELECT
ELSE
COLOR 12,1
LOCATE 12+(OPTN1%-1)*2,36 : PRINT SPACES(25);
LOCATE 12+(OPTN1%-1)*2,36 : PRINT AS;
LOCATE 12+(OPTN1%-1)*2,39 : LINE INPUT TEMPS
SELECT CASE OPTN1%
CASE 1 : ODIRS=UCASE$(AS)+UCASE$(TEMPS)+" " : TEMPS=ODIRS
CASE 2 : OFILES=UCASE$(AS)+UCASE$(TEMPS) : TEMPS=OFILES
END SELECT
END IF
COLOR 14,0
LOCATE 12+(OPTN1%-1)*2,36 : PRINT " ",TEMPS," ";
COLOR 15,1
SELECT CASE OPTN1%
CASE 1 : TEMPS="Directory;"
CASE 2 : TEMPS="File;"
CASE 3 : TEMPS="Hard Copy;"
END SELECT
LOCATE 12+(OPTN1%-1)*2,24 : PRINT TEMPS;
ELSE
SOUND 1000,3 : SOUND 800,1,5
END IF
GOTO Startloop1
END SELECT

```

```

* Print message to user.
COLOR 4,2
LOCATE 22,15 : PRINT CHR$(218);STRINGS(40,106);CHR$(191); 'top
LOCATE 23,15 : PRINT CHR$(179);TAB(85) ;CHR$(179); 'side
LOCATE 24,15 : PRINT CHR$(182);STRINGS(40,106);CHR$(217); 'bottom
COLOR 31,2
LOCATE 23,28 : PRINT " *** READING THE DATA *** ";
* Will first get the data from the file.
TOTPE=0 : TOTRP=0
BIGPE=-999999 : LITPE=999999
BIGRP=-999999 : LITRP=999999
MAXPRNG=-999999 : MINPRNG=999999
C%=1
OPEN ODIRS+OFILES FOR INPUT AS #1
IF NOT EOF(1) THEN INPUT #1,LINENAMES
IF NOT EOF(1) THEN INPUT #1,TITLE1$
IF NOT EOF(1) THEN INPUT #1,TITLE2$
IF NOT EOF(1) THEN INPUT #1,XLABELS
IF NOT EOF(1) THEN INPUT #1,YLABELS
WHILE NOT EOF(1)
INPUT #1,XDAT(C%)
INPUT #1,YDAT(C%)
INPUT #1,USE$(C%)
INPUT #1,CNUM$(C%)
INPUT #1,TEMPS
INPUT #1,TEMP%
IF USE$(C%)=1 THEN
IF XDAT(C%)>MAXPRNG THEN MAXPRNG=XDAT(C%)
IF XDAT(C%)<MINPRNG THEN MINPRNG=XDAT(C%)
INCR C%
END IF
WEND
CLOSE #1
PTS%=C%-1
* Will now draw the screen.
COLOR 15, 0 : CLS
COLOR 0, 7 : LOCATE 1,31
PRINT USING " Pass ### of ### " ;PTS%;
COLOR 11, 0
LOCATE 1, 1 : PRINT ODIRS+OFILES;
LOCATE 1,90 : PRINT TIMES," ,DATES;
COLOR 14, 0
LOCATE 2, 3 : PRINT "Number Observed Calculated
PRINT "Difference % Error % R.P."
LOCATE 3, 1 : PRINT STRINGS(90,196);
LINECNT%=4
* Must see if hardcopy, if so, then print headings

```

```

LPRINT "Percent Error:"
LPRINT USING TEMPS\LITPE,BIGPE,AVGPE
LPRINT "Relative Precision:"
LPRINT USING TEMPS\LITRP,BIGRP,AVGRP
LPRINT : LPRINT CHR$(12)
END IF

* Will pause before continuing.
AS=INPUT$(1)

Options.
This is the section to print the options menu

COLOR 0,15
LOCATE 14,1 : PRINT CHR$(216),STRING$(15,196),CHR$(191);
LOCATE 15,1 : PRINT CHR$(179),SPACES(19) ,CHR$(179);
LOCATE 16,1 : PRINT CHR$(196),STRING$(15,206),CHR$(191);
LOCATE 25,1 : PRINT CHR$(192),STRING$(15,199),CHR$(217);
FOR I%=17 TO 24
LOCATE I%,1 : PRINT CHR$(179),SPACES(15),CHR$(179);
LOCATE I%,3 : PRINT OPTN$(I%-16);
NEXT I%
LOCATE 15,6 : PRINT "Options";
LOCATE 14,0 : LOCATE OPTN%+16,3 : PRINT OPTN$(OPTN%);

* Have got menu, so see which selection.
Startloop3
BS=INKEY$
SELECT CASE BS
CASE =
GOTO Startloop3
CASE CHR$(13)
GOTO DoOption3
CASE CHR$(0)+CHR$(72),CHR$(0)+CHR$(80)
COLOR 0,15 : LOCATE OPTN%+16,3
PRINT OPTN$(OPTN%);
IF BS=CHR$(0)+CHR$(72) THEN DECR OPTN% ELSE INCR OPTN%
IF OPTN%<1 THEN OPTN%=6
IF OPTN%>6 THEN OPTN%=1
COLOR 14,0 : LOCATE OPTN%+16,3
PRINT OPTN$(OPTN%);
GOTO Startloop3
CASE CHR$(0)+CHR$(75),CHR$(0)+CHR$(77)
GOTO Startloop3
CASE ELSE
SOUND 1000,3 : SOUND 800,15
GOTO Startloop3
END SELECT

DoOption3
* Have selected option, so must do it
SELECT CASE OPTN%

```

```

IF HCOOPY$="Y" OR HCOOPY$="R" THEN
LPRINT "Results of Percent Error Analysis " "DATES:" "TIMES
LPRINT "Filename:" "ODRS+OFILES;" "Linename:" "LINENAMES
IF HCOOPY$<"R" THEN
FOR I%=1 TO 79 : LPRINT "I:"; NEXT I% : LPRINT
LPRINT TAB(3);
LPRINT "Number Observed Calculated ";
LPRINT "Difference % Error % R.P."
FOR I%=1 TO 79 : LPRINT "I:"; NEXT I% : LPRINT
END IF
END IF

* Have got data so do calc and print
RANGE=ABS(MAXRNG-MINRNG)
FOR I%=1 TO PTS%
COLOR 0,7 : LOCATE 1,38
PRINT USING "###.###";
BS=INKEY$
IF BS=CHR$(27) THEN GOTO CalcAvg
IF BS="S" OR BS="Y" THEN INCR PAUSE, 0.1
IF BS="P" OR BS="F" THEN DECR PAUSE, 0.1
IF PAUSE<0 THEN PAUSE=0
DELAY PAUSE
DI(I%)=XDAT(I%) - YDAT(I%)
IF XDAT(I%)<>0 THEN ER(I%)=ABS(DI(I%) / XDAT(I%)) * 100
RP(I%)=ABS(DI(I%) / RANGE ) * 100
TOTPE=TOTPE + ER(I%) : TOTRP=TOTRP + RP(I%)
IF ER(I%)>BIGPE THEN BIGPE=ER(I%)
IF RP(I%)>BIGRP THEN BIGRP=RP(I%)
IF RP(I%)<LITRP THEN LITRP=RP(I%)
COLOR 15,0 : LOCATE LINECNT%,1
PRINT USING ABS;XDAT(I%),YDAT(I%),DI(I%),ER(I%),RP(I%)
INCR LINECNT%
IF LINECNT%>25 THEN GOSUB ClearData
IF HCOOPY$="Y" THEN
LPRINT CNUM$(I%);TAB(10);
LPRINT USING ABS;XDAT(I%),YDAT(I%),DI(I%),ER(I%),RP(I%)
END IF
NEXT I%

CalcAvg:
* Have finished getting data, calc average and end.
AVGPE=TOTPE/PTS% : AVGRP=TOTRP/PTS%
IF LINECNT%>19 THEN GOSUB ClearData
LOCATE LINECNT%,1 : COLOR 11,0
PRINT
PRINT "Number of points:";PTS%
PRINT "Range of Observed Data:";MINRNG,"->"MAXRNG,"="RANGE
TEMP$="Min:##### Max:##### Average:#####"
PRINT "Percent Error:"
PRINT USING TEMPS\LITPE,BIGPE,AVGPE
PRINT "Relative Precision:"
LPRINT "Number of points:";PTS%
LPRINT "Range of Observed Data:";MINRNG,"->"MAXRNG,"="RANGE

```

This is the section to print the options menu

Listing for Program II.7: EZ_PLOT.BAS

```

CASE 1
CLOSE
GOSUB Logo
LOCATE 1,1
PRINT "So whadda you expect ... a meda?!!!"
AS=INKEY%
WHILE AS=
AS=INKEY%
WEND
END
CASE 2
CHAIN "GRAF_ED EXE"
CASE 3
CHAIN "CORRS EXE"
CASE 4
CHAIN "REGS EXE"
CASE 5
CHAIN "PROPS EXE"
CASE 6
CHAIN "GRAPH EXE"
CASE 7
CHAIN "EZ_PLOT EXE"
CASE 8
GOTO BeginPgm
END SELECT

```

ClearData:

This is a subroutine to clear the screen of data.

```

COLOR 15,0
FOR J%=4 TO 25
LOCATE J%,1 : PRINT SPACES(70);
NEXT J%
LINECTN%=4
RETURN
Logo:
$INCLUDE "LOGO.BAS"
T-T-T-That's all folks !!!

```

This program is designed to allow for the plotting of one property against another. That is, the LC-NMR property of a fuel may be plotted on the x-axis against the physical property on the y-axis. An example would be the ch2>a for monocyclics vs density, etc.

Program Name: EZ_PLOT.BAS Ver 6.00 Date Written: 12/20/1987
 Author: Allen Caswell Date Modified: 05/12/1988

First is the section to set up the variables.

```

* First are default parameters for program.
COMMON ODIRS, OFILES
PRDRVS="D"; LCDRV$="D"; HCOOPY$="N"; RMDSK$="N"
SND$="N"; CLASS%=1; PROP%=4; GOPTN%=1
PAGE%=1; OPTN2%=1; LCNMR%=3; ACTVES="Class"
VERNS$="Ver 5.00"
IF ODIRS="" THEN ODIRS="D:\CORR\RESULTV"
IF OFILES="" THEN OFILES="TEST.DAT"

* Next will dimension the necessary matrices.
DIM PROPS(42), CLASS$(10), DS(42), OD$(350), OD(C350), CUSE$(10)

* Next are names for classes of compounds
DATA "ALKANE", "ALKENE", "MODELIM", "CYCLOHEX", "DECALIN"
DATA "MONO", "DICYCLOC", "TETRALIN", "FUEL"
FOR I%=1 TO 9 : READ CLASS$(I%) : NEXT I%

* Next are names of properties to match.
DATA "Name", "Formula", "Mol Wt", "Catane #", "BP - 50%", "Pour Pt"
DATA "Improv%", "Density", "Ref Indx", "Cloud Pt", "Viscoat", "Filter"
DATA "Class"
DATA "Ag Dg Br", "Sp Disp", "Surf Ten", "Aniline", "Cr Press", "Cr Temp"
DATA "Cirt Vol"
DATA "Heat Cap", "Ht Vapor", "Ht Form", "Free E F", "Ht Comb", "Mol Vol"
DATA "% Atom"
DATA "% Olerin", "FuelType", "Cet Indx", "Sp. Grav", "BP - IBP", "BP - 10%"
DATA "BP - End", "C Resist"
DATA *
FOR I%=1 TO 42 : READ PROPS(I%) : NEXT I%

* Next are options for end of program.
DATA "Exit to DOS", "Run GRAF_ED", "Run PROPS", "Run REGS"
DATA "Run ERROR", "Run GRAPH", "Run CORRS", "Restart"
FOR I%=1 TO 8 : READ OPTNS(I%) : NEXT I%

* Must set up the class use options
FOR I%=1 TO 10 : CUSE$(I%)="N" : NEXT I%

```

StartOfProgram:

The next order of business is get class and property to sort by.

```

SCREEN 0 : WIDTH 80
COLOR 15,0 : CLS
COLOR 0,7
TEMP%=5
FOR I%=1 TO 4
LOCATE TEMP%+0,1 : PRINT CHR$(218);STRINGS(11,199);CHR$(191); 'top
LOCATE TEMP%+2,1 : PRINT CHR$(198);STRINGS(11,205);CHR$(181); 'middle
LOCATE TEMP%+4,1 : PRINT CHR$(192);STRINGS(11,199);CHR$(217); 'bottom
LOCATE TEMP%+1,1 : PRINT CHR$(179);TAB(13);CHR$(179); 'side
LOCATE TEMP%+3,1 : PRINT CHR$(179);TAB(13);CHR$(179); 'side
TEMP%=TEMP%+5
NEXT I%
LOCATE 6,3 : PRINT "Hardcopy";
LOCATE 6,7 : PRINT "Hcopy";
LOCATE 11,3 : PRINT "Compounds";
LOCATE 13,6 : PRINT USING "@##";NUMCOMPOUNDS;
LOCATE 16,3 : PRINT "RAM Disk";
LOCATE 16,7 : PRINT "RAMDISK";
LOCATE 21,3 : PRINT "LC-NMR";
LOCATE 23,6 : PRINT USING "@##";LCNMR%;
    ' Next is top box - for the title.
COLOR 15,4
LOCATE 1,5 : PRINT CHR$(201);STRINGS(98,205);CHR$(167) 'top line
LOCATE 2,5 : PRINT CHR$(168);STRINGS(98,32);CHR$(166) 'ends
LOCATE 3,5 : PRINT CHR$(168);STRINGS(98,205);CHR$(166) 'bottom line
LOCATE 1,31 : PRINT CHR$(206); 'top junct
LOCATE 2,31 : PRINT CHR$(179); 'middle line
LOCATE 3,31 : PRINT CHR$(207); 'bottom junct
LOCATE 2,10 : PRINT "EZ_PLOT";
LOCATE 2,19 : PRINT "VERSIONS"
LOCATE 2,35 : PRINT "LC-NMR - Physical Property Software";
    ' Next are Class and Property Boxes
COLOR 15,1
FOR I%=5 TO 21
LOCATE I%,18 : PRINT SPACES(13);
LOCATE I%,37 : PRINT SPACES(39);
LOCATE I%,18 : PRINT CHR$(179);
LOCATE I%,31 : PRINT CHR$(179);
FOR J%=0 TO 3
LOCATE I%,J%*13+37 : PRINT CHR$(179);
NEXT J%
NEXT I%
LOCATE 4,18 : PRINT STRINGS(13,198);
LOCATE 4,37 : PRINT STRINGS(39,198);
LOCATE 6,18 : PRINT STRINGS(13,205);
LOCATE 6,37 : PRINT STRINGS(39,205);
LOCATE 21,18 : PRINT STRINGS(13,198);
LOCATE 21,37 : PRINT STRINGS(39,198);
    
```

```

FOR I%=0 TO 1
LOCATE 4,I%*19+18 : PRINT CHR$(218); 'ul corner
LOCATE 4,I%*45+31 : PRINT CHR$(191); 'ur corner
LOCATE 21,I%*19+18 : PRINT CHR$(192); 'll corner
LOCATE 21,I%*45+31 : PRINT CHR$(217); 'lr corner
LOCATE 6,I%*19+18 : PRINT CHR$(198); 'joints
LOCATE 6,I%*45+31 : PRINT CHR$(181);
LOCATE 6,I%*13+50 : PRINT CHR$(206);
LOCATE 21,I%*13+50 : PRINT CHR$(193);
NEXT I%
LOCATE 5,50 : PRINT " ";
LOCATE 5,63 : PRINT " ";
LOCATE 5,22 : PRINT "Clear";
LOCATE 5,53 : PRINT "Property";
FOR I%=1 TO 9
LOCATE I%,8,21
PRINT CLASS$(I%);
NEXT I%
FOR I%=1 TO 14
LOCATE I%*1+6,40 : PRINT PROP$(I%);
LOCATE I%*1+6,53 : PRINT PROP$(I%+14);
LOCATE I%*1+6,66 : PRINT PROP$(I%+28);
NEXT I%
    ' Next is output file box.
COLOR 15,6
LOCATE 22,18 : PRINT CHR$(218);STRINGS(57,199);CHR$(191); 'top
LOCATE 23,18 : PRINT CHR$(179);TAB(7) 'side
LOCATE 24,18 : PRINT CHR$(192);STRINGS(57,199);CHR$(217); 'bottom
LOCATE 22,54 : PRINT CHR$(194); 'top junct
LOCATE 23,54 : PRINT CHR$(179); 'middle
LOCATE 24,54 : PRINT CHR$(193); 'bottom junct
LOCATE 23,20 : COLOR 12,6 : PRINT "D"; COLOR 15,6 : PRINT "factory.";
LOCATE 23,56 : COLOR 12,6 : PRINT "F"; COLOR 15,6 : PRINT "le.";
COLOR 14,6
LOCATE 23,32 : PRINT "ODRS";
LOCATE 23,62 : PRINT "FILES";
    ' Next are the command statements.
COLOR 3,0
LOCATE 7,78 : PRINT "OPT"; LOCATE 9,78 : PRINT STRINGS(9,198);
LOCATE 9,78 : PRINT "<H>"; LOCATE 10,78 : PRINT "<R>";
LOCATE 11,78 : PRINT "< >"; LOCATE 12,78 : PRINT "<D>";
LOCATE 13,78 : PRINT "<F>"; LOCATE 14,78 : PRINT "<S>";
LOCATE 15,78 : PRINT "<N>"; LOCATE 16,78 : PRINT "<O>";
LOCATE 17,78 : PRINT "<->";
    ' Have got screen, so get the information from the keyboard.
FILES=PRDRV$+"CORP"+CLASS$(CLASS%)+"PRNUM.DAT
OPEN FILES FOR INPUT AS #1
INPUT #1,NumOfCompounds
CLOSE #1
COLOR 0,7 : LOCATE 13,6 : PRINT USING "@##";NumOfCompounds;
IF CUSE$(CLASS%)="Y" THEN
COLOR 12,0 : LOCATE CLASS%+8,19
PRINT " ";CHR$(16);CLASS$(CLASS%); " ";
ELSE
COLOR 14,0 : LOCATE CLASS%+8,19 : PRINT " ";CLASS$(CLASS%); " ";
END IF
    
```



```

IF ACTIVES="Class" THEN
  COLOR 15, 5 : LOCATE 5,21 : PRINT ACTIVES;
ELSE
  COLOR 15, 5 : LOCATE 5,52 : PRINT ACTIVES;
END IF
COLOR 14,0
COL,%=INT((PROP%-1)/14) : ROW%=-PROP% - (COL%*14)
LOCATE ROW%+6,COL%*13 + 38 : PRINT "PROP$(PROP%)" ;
FILES=PRDRVS+"CORR"+CLASS$(CLASS%)+".PNUM.DAT
FOR I%=1 TO 10
  IF CUSE$(I%)="Y" AND I%<>CLASS% THEN
    COLOR 10,1 : LOCATE I%+8,19
    PRINT "CHR$(16),CLASS$(I%)" ;
  END IF
NEXT I%
OPEN FILES FOR INPUT AS #1
INPUT #1,NumOfCompounds
CLOSE #1
Startloop:
AS=INKEY$
SELECT CASE AS
CASE "="
  GOTO Startloop
CASE CHR$(13)
  GOTO GetData
CASE "O","o"
  GOTO Options
CASE "H","h"
  IF HCOPI%="Y" THEN HCOPI%="N" ELSE HCOPI%="Y"
  COLOR 0,7 : LOCATE 0,7 : PRINT HCOPI% ;
  GOTO Startloop
CASE "R","r"
  IF RMDSK%="Y" THEN RMDSK%="N" ELSE RMDSK%="Y"
  COLOR 0,7 : LOCATE 18,7 : PRINT RMDSK% ;
  GOTO Startloop
CASE "N","n","L","l"
  COLOR 18,7
  LOCATE 21, 3 : PRINT "LC-NMR #";
  COLOR 0,7
  LOCATE 23, 6 : PRINT " ";
  IF TEMP%<>">" THEN LCNMR%=VAL(TEMP%)
  LOCATE 23, 6 : PRINT USING "@##",LCNMR%
  COLOR 0,7
  LOCATE 21,3 : PRINT "LC-NMR #";
  GOTO Startloop
CASE "S","s"
  IF SNDS%="Y" THEN SNDS%="N" ELSE SNDS%="Y"
  COLOR 10,0 : LOCATE 25,3
  PRINT "Sound =" ;SNDS;
  IF SNDS%="Y" THEN SOUND 800,2 ELSE SOUND 300,4
  DELAY 0,5
  COLOR 15,0 : LOCATE 25,3
  PRINT SPACES(15);
  GOTO Startloop
CASE "D","d"
  COLOR 31,8
  LOCATE 23,20 : PRINT "Directory";
  COLOR 14,6
  LOCATE 23,32 : PRINT SPACES(21);
  ' no key
  ' return
  ' options
  ' hardcopy
  ' RAM disk
  ' LC-NMR #
  ' sound
  ' output dir
  ' output file
  ' mark-unmark
  ' left-right
  ' up-down
  LOCATE 23,32 : LINE INPUT TEMPS
  IF TEMP%<>">" THEN ODIRS%=TEMPS
  LOCATE 23,32 : PRINT SPACES(21);
  LOCATE 23,32 : PRINT ODIRS
  LOCATE 23,20 : COLOR 12,6 : PRINT "D";
  COLOR 15,8 : PRINT "Directory";
  GOTO Startloop
CASE "F","f"
  COLOR 31,8
  LOCATE 23,56 : PRINT "File";
  COLOR 14,6
  LOCATE 23,62 : PRINT SPACES(13);
  LOCATE 23,62 : LINE INPUT TEMPS
  IF TEMP%<>">" THEN OFILES%=TEMPS
  LOCATE 23,62 : PRINT SPACES(13);
  LOCATE 23,62 : PRINT OFILES;
  LOCATE 23,56 : COLOR 12,6 : PRINT "F";
  COLOR 15, 6 : PRINT "file";
  GOTO Startloop
CASE "*"
  GOTO Startloop
CASE "."
  IF CUSE$(CLASS%)="Y" THEN
    COLOR 12,0 : LOCATE CLASS%+8,19
    PRINT "CHR$(16),CLASS$(CLASS%)" ;
  ELSE
    CUSE$(CLASS%)="Y"
  END IF
  COLOR 14,0 : LOCATE CLASS%+8,19
  PRINT "CHR$(16),CLASS$(CLASS%)" ;
  CUSE$(CLASS%)="Y"
END IF
GOTO Startloop
CASE CHR$(0)+CHR$(75),CHR$(0)+CHR$(77)
  IF ACTIVES="Class" THEN
    COLOR 15, 1 : LOCATE 5, 21 : PRINT ACTIVES;
  ACTIVES="Property"
  COLOR 15, 5 : LOCATE 5, 52 : PRINT ACTIVES;
  GOTO Startloop
END IF
IF ACTIVES="Property" THEN
  COLOR 15, 1 : LOCATE 5, 52 : PRINT ACTIVES;
  ACTIVES="Class"
  GOTO Startloop
END IF
CASE CHR$(0)+CHR$(72), CHR$(0)+CHR$(80)
  IF ACTIVES="Class" THEN
    COLOR 10,1 : LOCATE CLASS%+8,19
    PRINT "CHR$(16),CLASS$(CLASS%)" ;
  ELSE
    COLOR 10,1 : LOCATE CLASS%+8,19
    PRINT "CHR$(16),CLASS$(CLASS%)" ;
  END IF
  IF AS=CHR$(0)+CHR$(72) THEN DECR CLASS% ELSE INCR CLASS%
  IF CLASS%<1 THEN CLASS%=0
  IF CLASS%>9 THEN CLASS%=1
  IF CUSE$(CLASS%)="Y" THEN
    COLOR 14, 0 : LOCATE CLASS%+8,19
    PRINT "CHR$(16),CLASS$(CLASS%)" ;
  ELSE
    COLOR 12,0 : LOCATE CLASS%+8,19

```

```

PRINT *,CHR$(16);CLASS$(CLASS%);* ;
END IF
FILES=PROPRM+*CORR+CLASS$(CLASS%)+*PNUM.DAT
OPEN FILES FOR INPUT AS #1
INPUT #1,NumOfCompounds
CLOSE #1
GOTO Startloop
COLOR 0,7 : LOCATE 13, 8 : PRINT USING "###",NumOfCompounds;
END IF
IF ACTIVES= Property * THEN
COL%=INT((PROPR%-1)/14) : ROW%=PROPR% - (COL%*14)
COLOR 15, 1 : LOCATE ROW%+8,COL%*13 + 36
PRINT *,PROPR$(PROPR%);* ;
IF AS=CHR$(9)+CHR$(72) THEN DECR PROPR% ELSE INCR PROPR%
IF PROPR%<1 THEN PROPR%=42
IF PROPR%>42 THEN PROPR%=1
COL%=INT((PROPR%-1)/14) : ROW%=PROPR% - (COL%*14)
COLOR 14, 0 : LOCATE ROW%+8,COL%*13 + 36
PRINT *,PROPR$(PROPR%);* ;
GOTO Startloop
END IF
CASE ELSE
SOUND 1000,3 : SOUND 600,1,5
GOTO Startloop
END SELECT
END SELECT
GetData:
Next will get the information out of the files.
* First see if did not select any classes.
I%=1
DO UNTIL CUSE$(I%)="Y" OR I%=10
INCR I%
LOOP
IF I%>=10 THEN
COLOR 15,4 : CLS
LOCATE 11,31 : PRINT "" YOU IDIOT ""
LOCATE 12,24 : PRINT "You forgot to select any classes!";
AS=INKEY$
WHILE AS=" "
AS=INKEY$
WEND
GOTO StartOfProgram
END IF
* Next will get search property.
IF SNDS="Y" THEN PLAY "MB T200 LB O3 DEFG P8 D L2 G"
SCLASS$=""
FOR I%=1 TO 10
IF CUSE$(I%)="Y" THEN SCLASS$=SCLASS$+CLASS$(I%)+*
NEXT I%
LINENAMES="LC-NMR Prop #"+STR$(LCNMR%)+* vs * + PROPR$(PROPR%)
XLABLE$="LC-NMR Number"+STR$(LCNMR%)
YLABLE$=PROPR$(PROPR%)
TITLE1$="LC-NMR #"+STR$(LCNMR%)+* vs *+PROPR$(PROPR%)
TITLE2$=""
* Will setup the screen and printer.
* Must print headings if hardcopy is on.
IF HCOPI%="Y" THEN
LPRINT "LC-NMR #":LCNMR%;*vs *PROPR$(PROPR%);* :TIMES;* :DATES
LPRINT * The following classes were searched: * ;
LPRINT SCLASS$
LPRINT STRING$(79,61)
LPRINT "No. C-Number: Name";
LPRINT TAB(58),"LC-NMR":TAB(60);PROPR$(PROPR%)
LPRINT STRING$(79,61)
END IF
* Must set up the screen.
COLOR 15, 0 : CLS : COLOR 11,0
LOCATE 1,1 : PRINT LEFT$(ODIR$+OFIL$,25);
LOCATE 1,60 : PRINT TIMES$; * :DATES;
LOCATE 2,1 : PRINT "Classes: "SCLASS$
LOCATE 3,1 : PRINT "Property: "PROPR$(PROPR%);
LOCATE 3,60 : PRINT "Run Time: sec";
COLOR 14,0
LOCATE 4,1 : PRINT "No. C-Number: Name";
LOCATE 4,58 : PRINT "LC-NMR":TAB(60);PROPR$(PROPR%);
LOCATE 5,1 : PRINT STRING$(60,100);
LINECNT%=6
* Have set up, so open output file and go to it!
LINENAMES="Aromaticity Check"
TITLE1$="Aromaticity Check"
TITLE2$=""
XLABLE$="Calculated 13C Aromaticity"
YLABLE$="Measured 13C Aromaticity"
OPEN ODIR$+OFIL$ FOR OUTPUT AS #3
PRINT #3,LINENAMES
PRINT #3,TITLE1$
PRINT #3,TITLE2$
PRINT #3,XLABLE$
PRINT #3,YLABLE$
COUNT%=1
FOR I%=1 TO 20 : AS=INKEY$ : NEXT I%
RunTime=TIMER
* Will start loop to get all data.
FOR I%=1 TO 10
AS=INKEY$ : IF AS=CHR$(27) THEN GOTO ExitLoop
IF CUSE$(I%)="Y" THEN
FILES=PROPRM+*CORR+CLASS$(I%)+*PNUM.DAT
OPEN FILES FOR INPUT AS #1
INPUT #1,NumOfCompounds
CLOSE #1
COLOR 0,15 : LOCATE 1,26
PRINT USING " Class: # Pass ### of ### ",I%,J%,NumOfCompounds,

```


Appendix III

Introduction

This appendix contains the program listings for the physical property calculation software. This package consists of three separate programs. These programs utilize the equations developed in the correlations software package to calculate the physical properties of hydrocarbons, fuels, and fuel mixtures. The programs included in this package are as follows:

Program III.1: PHYSPROP.BAS This software calculates the physical properties of alkane, monocyclic, and dicyclic aromatic hydrocarbons. The carbon structural information for a compound is entered and the physical properties are calculated.

Program III.2: FUELCALC.BAS This software calculates the physical properties of a fuel mixture. The average structural information for the fuel are entered and the physical properties are calculated after each structure is entered.

Program III.3: FUELMIX.BAS This software calculates the physical properties of a mixture of two fuels. The average structural information for each fuel is loaded from disk files and the fuels are mixed on a volume percent basis. The operator may edit any of the average structural information as well as the percent composition of the mix. The operator also has the option of filing either of the mixture components or the mixture results. This allows later recall allows for the generation of tertiary mixtures.

Additionally, the programs FUELCALC.BAS and FUELMIX.BAS require that the data file FUELPARAM.DAT be either in the current directory or in the path for proper execution. This data file contains the constants for the equations utilized to calculate the physical properties of the fuels.

Listing for Program III.1: PHYSPROP.BAS

Program Name: PHYSPROP Ver 1.10 Date Written: 07/13/1988
 Author: Allen Caswell Date Modified: 07/25/1988

This program is designed to calculate the physical properties of alkane, monocyclic, and bicyclic aromatic compounds from the chemical structures of the compounds. To do the calculations, the operator enters the number of each structure present in the fuel, and the properties are updated after each structure is entered

First will set up the variables.

```
ON ERROR GOTO ErrorMessage
DIM OPTN$(4), ALKANE$(4), MOLEFRACTION(4), MONO%(7), DICYCLIC%(5)
* Next are the options of the menus.
FOR I%=1 TO 4
  OPTN$(I%)=1
NEXT I%
* Next are the constants
VERSNS="Ver 1.10"
```

This is the section to do the MAIN MENU.

```
MainMenu:
OPTN$(1)="Alkane Property Calculation"
OPTN$(2)="Monocyclic Property Calculation"
OPTN$(3)="Bicyclic Property Calculation"
OPTN$(4)="Quit to DOS"
GOSUB DrawMainMenu
* Next see what to do.
COLOR 14,0
LOCATE (OPTN$(1)-1)*2+12,38:(0.5*LEN(OPTN$(1)))
PRINT " ",OPTN$(OPTN$(1)):" ";
Startloop1:
AS=INKEY$
SELECT CASE AS
CASE =
  COLOR 10,1 : LOCATE 9,20 : PRINT TIMES;
CASE CHR$(13)
  GOTO DoOption1
CASE "A";"a"
  * no key
  * return
  * alkane
```

```
OPTN$(1)=1 : GOTO DoOption1
CASE "M";"m"
  OPTN$(1)=2 : GOTO DoOption1
CASE "D";"d"
  OPTN$(1)=3 : GOTO DoOption1
CASE "C";"c",CHR$(27)
  OPTN$(1)=4 : GOTO DoOption1
CASE CHR$(0)+CHR$(7), CHR$(9)+CHR$(8)
  LOCATE (OPTN$(1)-1)*2+12,38:(0.5*LEN(OPTN$(1)))
  COLOR 11,1
  PRINT " ",LEFT$(OPTN$(1)),1);
  COLOR 14,1
  PRINT RIGHT$(OPTN$(1)),LEN(OPTN$(1))-1);" ";
  IF AS=CHR$(0)+CHR$(7) THEN DECR OPTN$(1) ELSE INCR OPTN$(1)
  IF OPTN$(1)<1 THEN OPTN$(1)=4
  IF OPTN$(1)>4 THEN OPTN$(1)=1
  COLOR 14,0
  LOCATE (OPTN$(1)-1)*2+12,38:(0.5*LEN(OPTN$(1)))
  PRINT " ",OPTN$(OPTN$(1)):" ";
CASE CHR$(0)+CHR$(7),CHR$(9)+CHR$(7)
CASE ELSE
  SOUND 1000,3 : SOUND 800,1.5
END SELECT
GOTO Startloop1
DoOption1:
SELECT CASE OPTN$(1)
CASE 1 : GOTO AlkaneCalculation
CASE 2 : GOTO MonocyclicCalculation
CASE 3 : GOTO BicyclicCalculation
CASE 4
  COLOR 12,0 : CLS
  LOCATE 1,1
  PRINT "PHYSPROP ",VERSNS;" Terminated.....Press any key to continue"
  AS=INPUT$(1)
END
END SELECT
```

This is the section to do the Alkane Physical Property Calcs.

```
AlkaneCalculation:
GOSUB DrawAlkaneScreen
* Will draw in the alkane group information.
FOR I%=1 TO 4
  COLOR 15,1
  LOCATE 4,(I%-1)*15+18 : PRINT USING "###" *ALKANEX(I%);
NEXT I%
CLASS$="ALKANE"
GOSUB CalculateMoleFractions
GOSUB CalculateProperties
* Must get group information and do calculations.
COLOR 10,0
```

```

LOCATE 4,(OPTN%(2)-1)*15+16 : PRINT USING "###" *ALKANE%(OPTN%(2));
Startloop2:
AS=INKEY$
SELECT CASE AS
CASE " "
' no key
' quit
CASE "q",Q,CHR$(27)
' hardcopy
GOTO MainMenu
CASE CHR$(0)+CHR$(56)
' reset
CASE "r",R
' reset
COLOR 15, 1
FOR I%=1 TO 4
MONO%(I%)=0
LOCATE 4,(I%-1)*15+16 : PRINT USING "###" *ALKANE%(I%);
NEXT I%
GOSUB CalculateMoleFractions
GOSUB CalculateProperties
COLOR 10, 0
LOCATE 4,(OPTN%(2)-1)*15+16 : PRINT USING "###" *ALKANE%(OPTN%(2));
CASE CHR$(0)+CHR$(75),CHR$(0)+CHR$(77)
' left-right
COLOR 15, 1
LOCATE 4,(OPTN%(2)-1)*15+16 : PRINT USING "###" *ALKANE%(OPTN%(2));
IF AS=CHR$(0)+CHR$(75) THEN DECR OPTN%(2) ELSE INCR OPTN%(2)
IF OPTN%(2) > 4 THEN OPTN%(2)=1
IF OPTN%(2) < 1 THEN OPTN%(2)=4
COLOR 10, 0
LOCATE 4,(OPTN%(2)-1)*15+16 : PRINT USING "###" *ALKANE%(OPTN%(2));
CASE "1",1,"2",2,"3",3,"4",4,"5",5,"6",6,"7",7,"8",8
' number
COLOR 10, 0
LOCATE 4,(OPTN%(2)-1)*15+16 : PRINT " " ;
LOCATE 4,(OPTN%(2)-1)*15+16 : PRINT AS;
LINE INPUT TEMP$
ALKANE%(OPTN%(2))=VAL(AS+TEMP$)
COLOR 10, 0
LOCATE 4,(OPTN%(2)-1)*15+16 : PRINT USING "###" *ALKANE%(OPTN%(2));
GOSUB CalculateMoleFractions
GOSUB CalculateProperties
CASE ELSE
' copoll
SOUND 1000,3 : SOUND 800,1,5
END SELECT
GOTO Startloop2

```

DicyclicCalculation

This is the section to do the Dicyclic Phys Property Calca.

```

GOSUB DrawDicyclicScreen
' Will draw in the monocyclic group information.
FOR I%=1 TO 5

```

```

LOCATE 4,(OPTN%(2)-1)*15+16 : PRINT USING "###" *ALKANE%(OPTN%(2));
Startloop2:
AS=INKEY$
SELECT CASE AS
CASE " "
' no key
' quit
CASE "q",Q,CHR$(27)
' hardcopy
GOTO MainMenu
CASE CHR$(0)+CHR$(56)
' reset
CASE "r",R
' reset
COLOR 15, 1
FOR I%=1 TO 4
ALKANE%(I%)=0
LOCATE 4,(I%-1)*15+16 : PRINT USING "###" *ALKANE%(I%);
NEXT I%
GOSUB CalculateMoleFractions
GOSUB CalculateProperties
COLOR 10, 0
LOCATE 4,(OPTN%(2)-1)*15+16 : PRINT USING "###" *ALKANE%(OPTN%(2));
CASE CHR$(0)+CHR$(75),CHR$(0)+CHR$(77)
' left-right
COLOR 15, 1
LOCATE 4,(OPTN%(2)-1)*15+16 : PRINT USING "###" *ALKANE%(OPTN%(2));
IF AS=CHR$(0)+CHR$(75) THEN DECR OPTN%(2) ELSE INCR OPTN%(2)
IF OPTN%(2) > 4 THEN OPTN%(2)=1
IF OPTN%(2) < 1 THEN OPTN%(2)=4
COLOR 10, 0
LOCATE 4,(OPTN%(2)-1)*15+16 : PRINT USING "###" *ALKANE%(OPTN%(2));
CASE "1",1,"2",2,"3",3,"4",4,"5",5,"6",6,"7",7,"8",8
' number
COLOR 10, 0
LOCATE 4,(OPTN%(2)-1)*15+16 : PRINT " " ;
LOCATE 4,(OPTN%(2)-1)*15+16 : PRINT AS;
LINE INPUT TEMP$
ALKANE%(OPTN%(2))=VAL(AS+TEMP$)
COLOR 10, 0
LOCATE 4,(OPTN%(2)-1)*15+16 : PRINT USING "###" *ALKANE%(OPTN%(2));
GOSUB CalculateMoleFractions
GOSUB CalculateProperties
CASE ELSE
' copoll
SOUND 1000,3 : SOUND 800,1,5
END SELECT
GOTO Startloop2

```

MonocyclicCalculation:

This is the section to do the Monocyclic Phys Property Calca.

GOSUB DrawMonocyclicScreen

```

' Will draw in the monocyclic group information.
FOR I%=1 TO 7
COLOR 15, 1
LOCATE 5,(I%-1)*9+11 : PRINT USING "###" *MONO%(I%);
NEXT I%
CLASS$="MONOC"
GOSUB CalculateADS

```

DrawMainMenu:

This is the subroutine to draw the Main Menu.

```

COLOR 15,1
LOCATE 5,(%-1)*11+15 : PRINT USING *###* ,DICYCLUC%(I%);
NEXT I%
CLASS$="DICYCLUC"
GOSUB CalculateTotalDicyclic
GOSUB CalculateProperties
.
. Must get group information and do calculations.
COLOR 10,0
LOCATE 5,(OPTN%(4)-1)*11+15 : PRINT USING *###* ,DICYCLUC%(OPTN%(4));
Startloop4:
AS=INKEY$
SELECT CASE AS
CASE " "
CASE "Q","q",CHR$(27)
GOTO MainMenu
CASE CHR$(0)+CHR$(59)
GOSUB HardCopy
CASE "R","r"
COLOR 15,1
FOR I%=1 TO 5
DICYCLUC%(I%)=0
LOCATE 5,(%-1)*11+15 : PRINT USING *###* ,DICYCLUC%(I%);
NEXT I%
COLOR 10,0
LOCATE 5,(OPTN%(4)-1)*11+15 : PRINT USING *###* ,DICYCLUC%(OPTN%(4));
GOSUB CalculateTotalDicyclic
GOSUB CalculateProperties
CASE CHR$(0)+CHR$(75),CHR$(0)+CHR$(77)
COLOR 15,1
LOCATE 5,(OPTN%(4)-1)*11+15 : PRINT USING *###* ,DICYCLUC%(OPTN%(4));
IF AS=CHR$(0)+CHR$(75) THEN DECR OPTN%(4) ELSE INCR OPTN%(4)
IF OPTN%(4)>5 THEN OPTN%(4)=1
IF OPTN%(4)<1 THEN OPTN%(4)=5
COLOR 10,0
LOCATE 5,(OPTN%(4)-1)*11+15 : PRINT USING *###* ,DICYCLUC%(OPTN%(4));
CASE "0","1","2","3","4","5","6","7","8","9"
COLOR 10,0
LOCATE 5,(OPTN%(4)-1)*11+15 : PRINT * ";
LOCATE 5,(OPTN%(4)-1)*11+16 : PRINT AS;
LINE INPUT TEMPS
DICYCLUC%(OPTN%(4))=VAL(AS+TEMPS)
COLOR 10,0
LOCATE 5,(OPTN%(4)-1)*11+15 : PRINT USING *###* ,DICYCLUC%(OPTN%(4));
GOSUB CalculateTotalDicyclic
GOSUB CalculateProperties
CASE ELSE
SOUND 1000,3 : SOUND 800,15
END SELECT
GOTO Startloop4:
.
.
.
.
. Will draw the screen.
SCREEN 0 : WIDTH 80
COLOR 15,0 : CLS
COLOR 0,4
LOCATE 1,5 : PRINT CHR$(201),STRINGS$(60,205),CHR$(187)
LOCATE 2,5 : PRINT CHR$(186),STRINGS$(60,32),CHR$(186)
LOCATE 3,5 : PRINT CHR$(186),STRINGS$(60,32),CHR$(186)
LOCATE 4,5 : PRINT CHR$(200),STRINGS$(60,205),CHR$(186)
LOCATE 1,31 : PRINT CHR$(209);
LOCATE 2,31 : PRINT CHR$(179);
LOCATE 3,31 : PRINT CHR$(179);
LOCATE 4,31 : PRINT CHR$(207);
COLOR 15,4
LOCATE 2,10 : PRINT "PHYSPROP";
LOCATE 2,19 : PRINT VERSNS;
LOCATE 3,14 : PRINT "July 1988";
LOCATE 2,35 : PRINT "Physical Property Calculation Software";
LOCATE 3,35 : PRINT * " Alien Carwell, Virginia Tech * ";
.
. Main Menu box.
COLOR 10,1
LOCATE 8,15 : PRINT CHR$(218),STRINGS$(49,186),CHR$(191);
FOR I%=9 TO 18
LOCATE I%,15 : PRINT CHR$(179),TAB$(65),CHR$(179);
NEXT I%
LOCATE 19,15 : PRINT CHR$(192),STRINGS$(49,186),CHR$(217);
COLOR 10,1
LOCATE 9,20 : PRINT TIMES;
LOCATE 9,51 : PRINT DATES;
COLOR 15,1
LOCATE 10,35 : PRINT "MAIN MENU";
COLOR 14,1
FOR I%=1 TO 4
LOCATE (I%-1)*2+12,40,5*,LEN(OPTNS(I%))
COLOR 11,1 : PRINT LEFT$(OPTNS(I%),1);
COLOR 14,1 : PRINT RIGHT$(OPTNS(I%),LEN(OPTNS(I%))-1);
NEXT I%
.
. Next eye commands.
COLOR 3,0
LOCATE 23,20 : PRINT * " Press the highlighted letter, or ";
LOCATE 24,20 : PRINT * "use the arrow keys and <ENTER> to select.";
RETURN
    
```

* top line
* ends
* bottom line
* top junct
* middle line
* middle line
* bottom junct


```

DrawAlkaneScreen:
LOCATE 2,10 : PRINT CHR$(201);STRINGS$(56,205);CHR$(187); ' top line
FOR %i=3 TO 5
  LOCATE %i,10 : PRINT CHR$(186);TAB(70);CHR$(188); ' middle
NEXT %i
LOCATE 6,10 : PRINT CHR$(200);STRINGS$(56,205);CHR$(188); ' bottom line
COLOR 11,1
LOCATE 3,28 : PRINT "Dicyclic Structural Data.";
COLOR 14,1
LOCATE 4,15 : PRINT "Cch3 Cch2 Cch Cchq Cch2>C"
COLOR 31,4
LOCATE 7,5 : PRINT SPACES(70);
LOCATE 7,8 : PRINT "WARNING - Dicyclic calculations are based on a ";
GOSUB DrawPropertyBox
RETURN
DrawPropertyBox:

```

This is the subroutine to do draw the Physical Property Box.

```

COLOR 10,1
LOCATE 8,1 : PRINT CHR$(216);STRINGS$(78,198);CHR$(191); ' top line
FOR %i=9 TO 21
  LOCATE %i,1 : PRINT CHR$(179);TAB(80);CHR$(179); ' middle
NEXT %i
LOCATE 22,1 : PRINT CHR$(182);STRINGS$(78,198);CHR$(217); ' bottom line
COLOR 11,1
LOCATE 9,25 : PRINT "Calculated Physical Properties.";
LOCATE 21,32 : PRINT "(Note: m = mole)";
COLOR 14,1
LOCATE 10,3 : PRINT " Cetane Number      Boiling Point ";
LOCATE 10,42 : PRINT " Freezing Point      Flash Point ";
LOCATE 13,3 : PRINT " Density          Refractive Index ";
LOCATE 13,42 : PRINT " Surface Tension  Critical Pressure ";
LOCATE 16,3 : PRINT " Critical Temp     Critical Volume ";
LOCATE 16,42 : PRINT " Heat Capacity     Ht. Vaporization ";
LOCATE 18,3 : PRINT " Free Energy Form  Heat Combustion ";
LOCATE 18,42 : PRINT " Molecular Volume  Heat of Formation ";
Next are comments
COLOR 3,0
LOCATE 24,15 : PRINT "Press <ARROW KEYS> to change highlighted variable.";
LOCATE 25,15 : PRINT " <R> to reset, <F1> to print properties, <Q> quit.";
RETURN
DrawPhysicalProperties

```

This is the subroutine to draw the physical properties.

```

DrawAlkaneScreen:
LOCATE 15,0 : CLS
COLOR 10,1
LOCATE 2,7 : PRINT CHR$(201);STRINGS$(65,205);CHR$(187); ' top line
FOR %i=3 TO 5
  LOCATE %i,7 : PRINT CHR$(186);TAB(73);CHR$(188); ' middle
NEXT %i
LOCATE 6,7 : PRINT CHR$(200);STRINGS$(65,205);CHR$(188); ' bottom line
COLOR 11,1
LOCATE 3,29 : PRINT "Alkane Structural Data.";
COLOR 14,1
LOCATE 4,12 : PRINT "Cch3: Cch2: Cch: Ccq:"
LOCATE 5,12 : PRINT "Xch3: Xch2: Xch: Xcq:"
GOSUB DrawPropertyBox
RETURN
DrawMonocyclicScreen:

```

This is the subroutine to draw in the monocyclic screen.

```

COLOR 15,0 : CLS
COLOR 10,1
LOCATE 2,7 : PRINT CHR$(201);STRINGS$(65,205);CHR$(187); ' top line
FOR %i=3 TO 5
  LOCATE %i,7 : PRINT CHR$(186);TAB(73);CHR$(188); ' middle
NEXT %i
LOCATE 6,7 : PRINT CHR$(200);STRINGS$(65,205);CHR$(188); ' bottom line
COLOR 11,1
LOCATE 3,27 : PRINT "Monocyclic Structural Data.";
COLOR 14,1
LOCATE 4,11 : PRINT "Cch3 Cch2 Cch Cchq "
PRINT "Cch2>C Cch3>C ADS";
GOSUB DrawPropertyBox
RETURN
DrawDicyclicScreen:

```

This is the subroutine to draw in the dicyclic screen.

```

COLOR 15,0 : CLS
COLOR 10,1

```

COLOR 28, 0
 LOCATE 23,29 : PRINT "Printing Property Data";
 LPRINT "Results of Physical Property Calculations: ",TIMES; ",DATES"
 LPRINT

. Must select class and print
 SELECT CASE CLASS\$
 CASE 'ALKANE'
 LPRINT * Compound Class: Alkane
 LPRINT USING * Total Number C: ##,###;TOTALALKANE%
 LPRINT USING * Cch3: ## ;*ALKANE%(1);
 LPRINT USING * Xch3: ##,### ;*MOLEFRACTION(1)
 LPRINT USING * Cch2: ## ;*ALKANE%(2);
 LPRINT USING * Xch2: ##,### ;*MOLEFRACTION(2)
 LPRINT USING * Cch: ## ;*ALKANE%(3);
 LPRINT USING * Xch: ##,### ;*MOLEFRACTION(3)
 LPRINT USING * Ccq: ## ;*ALKANE%(4);
 LPRINT USING * Xcq: ##,### ;*MOLEFRACTION(4)
 LPRINT
 LPRINT * Calculated Physical Properties:
 TEMP016\$= * Cetane: ##,###,### ;
 TEMP025\$= * Boiling Point: ##,###,### ;
 TEMP035\$= * Freezing Point: ##,###,### ;
 TEMP045\$= * Flash Point: ##,###,### ;
 TEMP055\$= * Density: ##,###,### ;
 TEMP065\$= * Refractive Index: ##,###,### ;
 TEMP075\$= * Surface Tension: ##,###,### ;
 TEMP085\$= * Critical Pressure: ##,###,### ;
 TEMP088\$= * Critical Temperature: ##,###,### ;
 TEMP105\$= * Critical Volume: ##,###,### ;
 TEMP115\$= * Heat Capacity: ##,###,### ;
 TEMP125\$= * Heat of Vaporization: ##,###,### ;
 TEMP135\$= * Free Energy Formation: ##,###,### ;
 TEMP145\$= * Heat of Combustion: ##,###,### ;
 TEMP155\$= * Heat of Formation: ##,###,### ;
 TEMP165\$= * Molecular Volume: ##,###,### ;
 LPRINT USING TEMP016\$ CETANE; : LPRINT *± 10.3 cetane*
 LPRINT USING TEMP025\$ BOILPT; : LPRINT *± 12.0 °C*
 LPRINT USING TEMP035\$ FREEZPT; : LPRINT *± 25.7 °C*
 LPRINT USING TEMP045\$ FLASHPT; : LPRINT *± 0.25 °C*
 LPRINT USING TEMP055\$ DENSITY; : LPRINT *± 0.011 g/m³*
 LPRINT USING TEMP065\$ REFINDX; : LPRINT *± 0.005 nD20*
 LPRINT USING TEMP075\$ SURFTEN; : LPRINT *± 0.94 dyne/cm (25°C)*
 LPRINT USING TEMP085\$ CRITP; : LPRINT *± 1.47 atm*
 LPRINT USING TEMP088\$ CRITT; : LPRINT *± 8.14 °C*
 LPRINT USING TEMP105\$ CRITV; : LPRINT *± 0.015 l/mole*
 LPRINT USING TEMP115\$ HEATCAP; : LPRINT *± 1.38 cal/mole (25°C)*
 LPRINT USING TEMP125\$ HTVAPOR; : LPRINT *± 0.168 kcal/mole (25°C)*
 LPRINT USING TEMP135\$ FREEEF; : LPRINT *± 0.848 kcal/mole (25°C)*
 LPRINT USING TEMP145\$ HTCOMB; : LPRINT *± 1.80 kcal/mole (25°C)*
 LPRINT USING TEMP155\$ HTFORM; : LPRINT *± 0.848 kcal/mole (25°C)*
 LPRINT USING TEMP165\$ MOLVOL; : LPRINT *± 4.01 ml/mole*
 LPRINT CHR\$(12)
 CASE 'MONO'
 LPRINT * Compound Class: Monocyclic Aromatic*
 LPRINT USING * Total Number C: ##,###;TOTALMONO%
 LPRINT USING * Cch3: ##;MONO%(1)
 LPRINT USING * Cch2: ##;MONO%(2)
 LPRINT USING * Cch: ##;MONO%(3)
 LPRINT USING * Ccq: ##;MONO%(4)

COLOR 15, 1
 LOCATE 11, 2 : PRINT SPACES(76);
 LOCATE 14, 2 : PRINT SPACES(76);
 LOCATE 17, 2 : PRINT SPACES(76);
 LOCATE 20, 2 : PRINT SPACES(76);
 SELECT CASE CLASS\$
 CASE 'ALKANE','MONO'
 LOCATE 11, 3 : PRINT USING "##### cat" CETANE;
 LOCATE 11,23 : PRINT USING "##### °C" BOILPT;
 LOCATE 11,43 : PRINT USING "##### °C" FREEZPT;
 LOCATE 11,62 : PRINT USING "##### °C" FLASHPT;
 LOCATE 14, 4 : PRINT USING "##### g/m³" DENSITY;
 LOCATE 14,26 : PRINT USING "##### " REFINDX;
 LOCATE 14,41 : PRINT USING "##### dyne/cm" SURFTEN;
 LOCATE 14,63 : PRINT USING "##### atm" CRITP;
 LOCATE 17, 3 : PRINT USING "##### °C" CRITT;
 LOCATE 17,23 : PRINT USING "##### l/m³" CRITV;
 LOCATE 17,42 : PRINT USING "##### cal/m³" HEATCAP;
 LOCATE 17,62 : PRINT USING "##### kcal/m³" HTVAPOR;
 LOCATE 20, 3 : PRINT USING "##### kcal/m³" FREEEF;
 LOCATE 20,23 : PRINT USING "##### kcal/m³" HTCOMB;
 LOCATE 20,43 : PRINT USING "##### ml/m³" MOLVOL;
 LOCATE 20,62 : PRINT USING "##### kcal/m³" HTFORM;
 CASE 'CYCLIC'
 LOCATE 11,23 : PRINT USING "##### °C" BOILPT;
 LOCATE 11,43 : PRINT USING "##### °C" FREEZPT;
 LOCATE 14, 4 : PRINT USING "##### g/m³" DENSITY;
 LOCATE 14,26 : PRINT USING "##### " REFINDX;
 LOCATE 20,43 : PRINT USING "##### ml/m³" MOLVOL;

END SELECT
 RETURN
 WipeOut:
 This is the subroutine to erase the physical properties data.

CETANE=0 : BOILPT=0 : FREEZPT=0 : FLASHPT=0 : DENSITY=0
 REFINDX=0 : SURFTEN=0 : CRITP=0 : CRITT=0 : CRITV=0
 HEATCAP=0 : HTVAPOR=0 : FREEEF=0 : HTCOMB=0 : MOLVOL=0
 HTFORM=0
 COLOR 15, 1
 LOCATE 11, 2 : PRINT SPACES(76);
 LOCATE 14, 2 : PRINT SPACES(76);
 LOCATE 17, 2 : PRINT SPACES(76);
 LOCATE 20, 2 : PRINT SPACES(76);
 RETURN
 HardCopy:

This is the subroutine to hard copy data.


```
LOCATE 5,(%*1)*15+18 : PRINT USING "###.###",MOLEFRACTION(1%);
NEXT 1%
RETURN
```

CalculateADS:

```
This is the subroutine to calculate the monocyclic ADS.
```

```
MONO%(7)=0 : TOTALMONO%=0
FOR 1%=1 TO 6
IF 1%<=4 THEN INCR MONO%(7),MONO%(1%)
INCR TOTALMONO%,MONO%(1%)
NEXT 1%
* Will also calculate the Cch3>=4
MONO%(6)=MONO%(2) + 2*MONO%(3) + 3*MONO%(4)
COLOR 15,1
LOCATE 5,56 : PRINT USING "###.###",MONO%(6);
* Will draw in the ADS information.
COLOR 15,1
LOCATE 5,65 : PRINT USING "###.###",MONO%(7);
RETURN
```

CalculateTotalDicyclic:

```
This is the subroutine to calculate the dicyclic carbon.
```

```
TOTALDICYCLIC%=10
FOR 1%=1 TO 5
INCR TOTALDICYCLIC%,DICYCLIC(1%)
NEXT 1%
RETURN
```

CalculateProperties:

```
This is the subroutine to calculate the physical properties
```

```
* First is section to do the alkane physical property calculations
IF CLASS$="ALKANE" AND TOTALALKANE%<=0 THEN GOSUB WipeOut : RETURN
IF CLASS$="MONO" AND TOTALMONO%<=5 THEN GOSUB WipeOut : RETURN
IF CLASS$="DICYCLIC" AND TOTALDICYCLIC%<=0 THEN GOSUB WipeOut : RETURN
SELECT CASE CLASS$
```

CASE "ALKANE"

```
CETANE = 2.59566E07
INCR CETANE, -2.59566E07*MOLEFRACTION(1)
INCR CETANE, -2.58565E07*MOLEFRACTION(2)
INCR CETANE, -2.58565E07*MOLEFRACTION(3)
INCR CETANE, -2.58565E07*MOLEFRACTION(4)
CETANE = 1.4078022*CETANE - 32.7867
BOLPT = 18.8689
INCR BOLPT, -18.8622*MOLEFRACTION(1)
INCR BOLPT, -18.8677*MOLEFRACTION(2)
INCR BOLPT, -18.8728*MOLEFRACTION(3)
INCR BOLPT, -18.8778*MOLEFRACTION(4)
BOLPT = 1.1661168*(1/BOLPT) - 250 - 24.9491
FREEZEPT = -43.8780
INCR FREEZEPT, 43.69048*MOLEFRACTION(1)
INCR FREEZEPT, 43.67770*MOLEFRACTION(2)
INCR FREEZEPT, 43.67630*MOLEFRACTION(3)
INCR FREEZEPT, 43.67280*MOLEFRACTION(4)
FREEZEPT = 1.2784687*(1/FREEZEPT) - 608.383
FLASHPT = 210
INCR FLASHPT, -7.44*MOLEFRACTION(1)
INCR FLASHPT, -8*MOLEFRACTION(2)
INCR FLASHPT, 14.48*MOLEFRACTION(3)
INCR FLASHPT, 0*MOLEFRACTION(4)
FLASHPT = 1.07*FLASHPT - 1.84
DENSITY = -1688.5001
INCR DENSITY, 1688.7285*MOLEFRACTION(1)
INCR DENSITY, 1687.3565*MOLEFRACTION(2)
INCR DENSITY, 1688.0271*MOLEFRACTION(3)
INCR DENSITY, 1688.7404*MOLEFRACTION(4)
DENSITY = 1.0379129*DENSITY - 2.84012E-02
REFINDX = -1.277.53
INCR REFINDX, 1278.98*MOLEFRACTION(1)
INCR REFINDX, 1279.00*MOLEFRACTION(2)
INCR REFINDX, 1279.33*MOLEFRACTION(3)
INCR REFINDX, 1279.68*MOLEFRACTION(4)
REFINDX = 1.0884342*REFINDX - 0.1214285
SURFTEN = 19592.3
INCR SURFTEN, -19603.1*MOLEFRACTION(1)
INCR SURFTEN, -19560.8*MOLEFRACTION(2)
INCR SURFTEN, -19520.2*MOLEFRACTION(3)
INCR SURFTEN, -19480.1*MOLEFRACTION(4)
SURFTEN = 1.2331308*SURFTEN - 4.86244
CRITP = 28.48660660
INCR CRITP, 28.03883852*MOLEFRACTION(1)
INCR CRITP, -8.57350254*MOLEFRACTION(2)
INCR CRITP, -42.72133255*MOLEFRACTION(3)
INCR CRITP, -88.38150024*MOLEFRACTION(4)
CRITP = 1.25038293*CRITP - 11.833322
CRITV = -1.34084E08
INCR CRITV, +1.34034E08*MOLEFRACTION(1)
INCR CRITV, +1.34114E08*MOLEFRACTION(2)
INCR CRITV, +1.34191E08*MOLEFRACTION(3)
INCR CRITV, +1.34266E08*MOLEFRACTION(4)
CRITV = 1.0340809*CRITV - 10.5801
CRITV = -14359.3
INCR CRITV, 14388.4*MOLEFRACTION(1)
INCR CRITV, 14359.8*MOLEFRACTION(2)
INCR CRITV, 14353.2*MOLEFRACTION(3)
INCR CRITV, 14346.7*MOLEFRACTION(4)
```

```

CRITY=1.0645622*ICRITY - 4.40026E-02
HEATCAP=151.36
INCR HEATCAP, -151.322*MOLEFRACTION(1)
INCR HEATCAP, -151.377*MOLEFRACTION(2)
INCR HEATCAP, -151.431*MOLEFRACTION(3)
INCR HEATCAP, -151.484*MOLEFRACTION(4)
HEATCAP=1.1135138*HEATCAP - 5.58737
HTVAPOR= 309.486
INCR HTVAPOR, -309.088*MOLEFRACTION(1)
INCR HTVAPOR, -309.491*MOLEFRACTION(2)
INCR HTVAPOR, -309.882*MOLEFRACTION(3)
INCR HTVAPOR, -310.252*MOLEFRACTION(4)
HTVAPOR=0.9831473*HTVAPOR + 6.77238E-03
HTFORM=-66.8276
INCR HTFORM, 66.4799*MOLEFRACTION(1)
INCR HTFORM, 66.5217*MOLEFRACTION(2)
INCR HTFORM, 66.5649*MOLEFRACTION(3)
INCR HTFORM, 66.6077*MOLEFRACTION(4)
HTFORM=1.1042493*HTFORM + 6.77806
FREEEF=-5671.32
INCR FREEEF, 5671.71*MOLEFRACTION(1)
INCR FREEEF, 5671.31*MOLEFRACTION(2)
INCR FREEEF, 5670.91*MOLEFRACTION(3)
INCR FREEEF, 5670.50*MOLEFRACTION(4)
FREEEF=1.3381489*(FREEEF - 10) + 0.168607
HTCOMB=1.07229
INCR HTCOMB, -1.06809*MOLEFRACTION(1)
INCR HTCOMB, -1.07225*MOLEFRACTION(2)
INCR HTCOMB, -1.07541*MOLEFRACTION(3)
INCR HTCOMB, -1.07857*MOLEFRACTION(4)
HTCOMB=1.0203918*HTCOMB - 15.467761
MOLVOL= 26.5695
INCR MOLVOL, -26.5493*MOLEFRACTION(1)
INCR MOLVOL, -26.5692*MOLEFRACTION(2)
INCR MOLVOL, -26.5886*MOLEFRACTION(3)
INCR MOLVOL, -26.6049*MOLEFRACTION(4)
MOLVOL=1.1061336*1/MOLVOL - 16.606
;
; Next is section to do phys prop calcs for monocyclics.
;
CASE 'MONO'
CETANE=5.71407
INCR CETANE, -10.8465 *MONO%(1)
INCR CETANE, -8.13929E-02*MONO%(2)
INCR CETANE, -8.75987 *MONO%(3)
INCR CETANE, -36.39510 *MONO%(4)
INCR CETANE, 5.32182 *MONO%(5)
CETANE=1.1225058*CETANE - 3.87011
BOILPT=88.32607867
INCR BOILPT, 26.94813728*MONO%(1)
INCR BOILPT, 45.90350342*MONO%(2)
INCR BOILPT, 58.58008957*MONO%(3)
INCR BOILPT, 60.11920166*MONO%(4)
INCR BOILPT, 20.89387468*MONO%(5)
BOILPT=1.03035954*BOILPT - 5.814421
FREEZEPT= 69.6631
INCR FREEZEPT, 16.08600*MONO%(1)
INCR FREEZEPT, -6.78148*MONO%(2)
INCR FREEZEPT, -4.87162*MONO%(3)
INCR FREEZEPT, -12.82000*MONO%(4)

```

```

INCR FREEZEPT, 3.28933*MONO%(5)
FREEZEPT=2.4233007*FREEZEPT + 67.62355
FLASHPT=-134.61
INCR FLASHPT, 19.87310*TOTALMONO%
INCR FLASHPT, 1.46346*MONO%(7)
FLASHPT=1.0137885*FLASHPT - 1.07834
DENSITY=0.856468
INCR DENSITY, 6.73776E-03*MONO%(1)
INCR DENSITY, 4.46875E-03*MONO%(2)
INCR DENSITY, 3.49110E-03*MONO%(3)
INCR DENSITY, 1.62951E-02*MONO%(4)
INCR DENSITY, -4.16860E-04*MONO%(5)
DENSITY=1.8506524*DENSITY - 0.740225
REFINDEX=1.46634
INCR REFINDEX, 6.80782E-03*MONO%(1)
INCR REFINDEX, 4.43701E-03*MONO%(2)
INCR REFINDEX, 2.16348E-03*MONO%(3)
INCR REFINDEX, 7.52143E-03*MONO%(4)
INCR REFINDEX, -7.35685E-04*MONO%(5)
REFINDEX=1.203349*REFINDEX - 0.304689
SURETEN=21.742
INCR SURFTEEN, 0.484*MONO%(1)
INCR SURFTEEN, 0.630*MONO%(2)
INCR SURFTEEN, 0.082*MONO%(3)
INCR SURFTEEN, 0.000*MONO%(4)
INCR SURFTEEN, 0.078*MONO%(5)
SURETEN=3.1153327*SURFTEEN - 90.5514
CRITP=45.6035
INCR CRITP, -4.66159*MONO%(1)
INCR CRITP, -9.78632*MONO%(2)
INCR CRITP, -12.6381*MONO%(3)
INCR CRITP, -16.3435*MONO%(4)
INCR CRITP, -3.07235*MONO%(5)
CRITP=1.0725608*CRITP - 2.34544
CRITV=293.631
INCR CRITV, 27.8109*MONO%(1)
INCR CRITV, 50.8221*MONO%(2)
INCR CRITV, 77.4144*MONO%(3)
INCR CRITV, 63.3687*MONO%(4)
INCR CRITV, 22.9388*MONO%(5)
CRITV=0.262001
INCR CRITV, 5.83743E-02*MONO%(1)
INCR CRITV, 0.115398 *MONO%(2)
INCR CRITV, 0.162851 *MONO%(3)
INCR CRITV, 0.188989 *MONO%(4)
INCR CRITV, 5.26144E-02*MONO%(5)
CRITV=1.0157028*CRITV - 6.8716E-03
HEATCAP=-3.58220
INCR HEATCAP, 5.974220*TOTALMONO%
INCR HEATCAP, 0.278931*MONO%(7)
HEATCAP=1.0100408*HEATCAP - 0.50899
HTVAPOR=1.8208
INCR HTVAPOR, 0.984278*TOTALMONO%
INCR HTVAPOR, 0.426593*MONO%(7)
HTVAPOR=1.0366011*HTVAPOR - 0.424342
HTFORM=48.0728
INCR HTFORM, -8.07026*TOTALMONO%
INCR HTFORM, -2.66568*MONO%(7)
HTFORM=1.002647*HTFORM + 1.95813E-02

```

```

; m-b
; Xch3
; Xch2
; Xch
; Xcq
; m-b
; Xch3
; Xch2
; Xch
; Xcq
; m-b
; Xch3
; Xch2
; Xch
; Xcq
; m-b
; Xch3
; Xch2
; Xch
; Xcq
; m-b
; Xch3
; Xch2
; Xch
; Xcq
; m-b
; Cch3
; Cch2
; Cch
; Ccq
; Cch2>
; m-b
; Cch3
; Cch2
; Cch
; Ccq
; Cch2>
; m-b
; Cch3
; Cch2
; Cch
; Ccq

```

```

; Cch2>
; m-b
; C total
; ADS
; m-b
; Cch3
; Cch2
; Ccq
; Cch2>
; m-b
; Cch3
; Cch2
; Ccq
; Cch2>
; m-b
; Cch3
; Cch2
; Ccq
; Cch2>
; m-b
; C total
; ADS
; m-b
; C total
; ADS
; m-b
; C total
; ADS
; m-b

```

Listing for Program III.2: FUELCAL.C.BAS

Program Name: FUELCALC Ver 1.00 Date Written: 07/19/1988
 Author: Allen Caswell Date Modified: 07/19/1988

This program is designed to calculate the physical properties of middle distillate fuels. The mixing coefficients for the calculation are read in from the file written by the correlation program. This file must be in the default directory in order for the program to run. To operate the program, the operator enters the average structures for the fuel into the leftmost box, and the physical properties are automatically updated in the rightmost box. The file which contains the mixing coefficients is named FUELPARAM.DAT and MUST be in the default directory.

First will set up the variables.

```
ON ERROR GOTO ErrorMessage
DIM SLOPEFACTOR(42), INTCPPFACTOR(42), OFFSETFACTOR(42), FUNCTION$(42)
DIM MIXCOEFF(42,22), PROPS(42), TS(22), PROF(42), AVGSTRI(16)
```

```
Next are the constants
VERNS$ =Ver 100
OPTN%(1)=1
CFGDIR$ ="
```

```
Must read in the parameters.
GOSUB ReadFuelParams
```

MainMenu

This is the section to do the main menu.

GOSUB DrawMainMenu

```
Next see what to do
COLOR 10,0
LOCATE OPTN%(1)+7,19 : PRINT USING "###.###" *AVGSTRI(OPTN%(1));
Startloop:
AS=INKEY$
SELECT CASE AS
CASE =
    COLOR 10,0 : LOCATE 5,20 : PRINT TIMES;
CASE "Q",q : CHFS(27)
    GOTO EndProgram
CASE CHFS(0) + CHFS(69)
    no key
    quit
    hardcopy
```

```
FREEEF=23.4941
INCR FREEEF, 0.955167*TOTALMONO%
INCR FREEEF, -2.41353*MONO%(7)
FREEEF=1.0316191*FREEEF - 1.87917
HTCOMB=-127.879
INCR HTCOMB,146.063*TOTALMONO%
INCR HTCOMB, -2.75543*MONO%(7)
HTCOMB=1.000015*HTCOMB - 3.730677E-02
MOLVOL=92.3659
INCR MOLVOL, 14.7668*MONO%(1)
INCR MOLVOL, 31.2141*MONO%(2)
INCR MOLVOL, 47.6201*MONO%(3)
INCR MOLVOL, 63.0310*MONO%(4)
INCR MOLVOL, 16.7311*MONO%(5)
MOLVOL=1.0075069*MOLVOL - 1.22463
```

Next is section to do phys prop calca for dicyclics.

```
CASE "DICYCLIC"
BOILPT=229.24151611
INCR BOILPT, 18.30818668*DICYCLIC%(1)
INCR BOILPT, 28.21828215*DICYCLIC%(2)
INCR BOILPT, 41.73328580*DICYCLIC%(3)
INCR BOILPT,-149.27979690*DICYCLIC%(4)
INCR BOILPT, 16.32395254*DICYCLIC%(5)
BOILPT=1.00755972*BOILPT - 2.165405
FREEZEPT=-30.94892159
INCR FREEZEPT, 4.85980164*DICYCLIC%(1)
INCR FREEZEPT, -36.21059273*DICYCLIC%(2)
INCR FREEZEPT, -30.78991518*DICYCLIC%(3)
INCR FREEZEPT, -65.75940704*DICYCLIC%(4)
INCR FREEZEPT, 1.95241804*DICYCLIC%(5)
FREEZEPT=2.504740221*FREEZEPT - 22.199685
DENSITY=0.997182
INCR DENSITY, 3.87330E-03*DICYCLIC%(1)
INCR DENSITY, -9.63778E-03*DICYCLIC%(2)
INCR DENSITY, -1.48817E-02*DICYCLIC%(3)
INCR DENSITY, -1.19222E-02*DICYCLIC%(4)
INCR DENSITY, -7.84452E-03*DICYCLIC%(5)
DENSITY=1.071507*DENSITY - 8.90286E-02
REFINDX=1.60694
INCR REFINDX, -1.76428E-04*DICYCLIC%(1)
INCR REFINDX, -1.35098E-02*DICYCLIC%(2)
INCR REFINDX, -0.018481 *DICYCLIC%(3)
INCR REFINDX, -0.020157 *DICYCLIC%(4)
INCR REFINDX, -6.76552E-03*DICYCLIC%(5)
REFINDX=1.0536997*REFINDX - 8.43578E-02
MOLVOL=128.755
INCR MOLVOL, 13.4659*DICYCLIC%(1)
INCR MOLVOL, 28.2471*DICYCLIC%(2)
INCR MOLVOL, 44.5689*DICYCLIC%(3)
INCR MOLVOL, 16.6543*DICYCLIC%(5)
MOLVOL=1.0003922*MOLVOL - 8.26236E-02
END SELECT
```

```
Have calculated properties, so display them.
GOSUB DrawPhysicalProperties
RETURN
```

T.T.T-That's all folks!!!!!!!

```

INCR PROP(1%)*AVGSTR(7)*AVGSTR(5)*MIXCOEFF(1%,6)
INCR PROP(1%)*AVGSTR(6)*AVGSTR(5)*MIXCOEFF(1%,7)
INCR PROP(1%)*AVGSTR(9)*AVGSTR(5)*MIXCOEFF(1%,8)
INCR PROP(1%)*AVGSTR(10)*AVGSTR(5)*MIXCOEFF(1%,9)
INCR PROP(1%)*AVGSTR(11)*AVGSTR(5)*MIXCOEFF(1%,10)
INCR PROP(1%)*AVGSTR(13)*AVGSTR(12)*MIXCOEFF(1%,11)
INCR PROP(1%)*AVGSTR(14)*AVGSTR(12)*MIXCOEFF(1%,12)
INCR PROP(1%)*AVGSTR(15)*AVGSTR(12)*MIXCOEFF(1%,13)
INCR PROP(1%)*AVGSTR(16)*AVGSTR(12)*MIXCOEFF(1%,14)
IF LEFT$(FUNCTION$(1%),1)='X' THEN PROP(1%)=PROP(1%)
IF LEFT$(FUNCTION$(1%),3)='1/A' THEN PROP(1%)=1/PROP(1%)
IF LEFT$(FUNCTION$(1%),3)='LOG' THEN PROP(1%)=LOG(PROP(1%))
PROP(1%)=PROP(1%)-OFFSETFACTR(1%)
PROP(1%)=PROP(1%)*SLOPEFACTOR(1%)
PROP(1%)=PROP(1%)+INTCFACR(1%)
NEXT 1%
GOSUB DrawResults
RETURN
    
```

DrawMainMenu:

This is the subroutine to draw the Main Menu.

```

* Will draw the screen.
SCREEN 0: WIDTH 80
COLOR 15,0:CLS
COLOR 0,4
LOCATE 1,5:PRINT CHR$(201);STRING$(99,205);CHR$(187)
LOCATE 2,5:PRINT CHR$(186);STRING$(99,32);CHR$(186)
LOCATE 3,5:PRINT CHR$(186);STRING$(99,32);CHR$(186)
LOCATE 4,5:PRINT CHR$(200);STRING$(99,205);CHR$(188)
LOCATE 1,31:PRINT CHR$(209);
LOCATE 2,31:PRINT CHR$(179);
LOCATE 3,31:PRINT CHR$(179);
LOCATE 4,31:PRINT CHR$(207);
COLOR 15,4
LOCATE 2,10:PRINT "FUELCALC";
LOCATE 2,19:PRINT "VERNS";
LOCATE 3,14:PRINT "July 1988";
LOCATE 2,35:PRINT "Physical Property Calculation Software";
LOCATE 3,35:PRINT "Allen Caswell, Virginia Tech";
    
```

```

* Average Structure Box
COLOR 10,1
LOCATE 6,1:PRINT CHR$(201);STRING$(28,205);CHR$(187);
FOR I%=7 TO 23
LOCATE I%,1:PRINT CHR$(186);TAB(28);CHR$(186);
NEXT I%
LOCATE 24,1:PRINT CHR$(200);STRING$(28,205);CHR$(188);
COLOR 11,1
LOCATE 7,6:PRINT "Average Structures";
COLOR 14,1
LOCATE 9,4:PRINT "Alkane";
    
```

```

* reset
GOSUB Hardcopy
CASE "R"
COLOR 15,1
FOR I%=1 TO 16
AVGSTR(I%)=0
LOCATE I%+7,19:PRINT USING "#####"AVGSTR(I%);
NEXT I%
GOSUB PerformCalc
COLOR 10,0
LOCATE OPTN%(1)+7,19:PRINT USING "#####"AVGSTR(OPTN%(1));
CASE CHR$(0)+CHR$(72),CHR$(0)+CHR$(80)
COLOR 15,1
LOCATE OPTN%(1)+7,19:PRINT USING "#####"AVGSTR(OPTN%(1));
IF AS=CHR$(0)+CHR$(72) THEN DECR OPTN%(1) ELSE INCR OPTN%(1)
IF OPTN%(1)<1 THEN OPTN%(1)=16
IF OPTN%(1)>16 THEN OPTN%(1)=1
COLOR 10,0
LOCATE OPTN%(1)+7,19:PRINT USING "#####"AVGSTR(OPTN%(1));
CASE CHR$(0)+CHR$(75),CHR$(0)+CHR$(77)
CASE "L","2","3","4","5","6","7","8","9","*","."
COLOR 15,1
LOCATE OPTN%(1)+7,19:PRINT SPACES(9);
LOCATE OPTN%(1)+7,20:PRINT AS;
LINE INPUT TEMP$
AVGSTR(OPTN%(1))=VAL(AS+TEMP$)
COLOR 10,0
LOCATE OPTN%(1)+7,19:PRINT USING "#####"AVGSTR(OPTN%(1));
GOSUB PerformCalc
CASE ELSE
SOUND 1000,3: SOUND 800,1.5
END SELECT
GOTO Startloop
    
```

PerformCalc:

This is the section to do the Physical Property Calc.

```

* Must first check if array empty, if so clear results and return.
TOTAL=0
FOR I%=1 TO 16
INCR TOTAL AVGSTR(I%)
NEXT I%
IF TOTAL<=0 THEN
GOSUB ClearResults
RETURN
END IF
FOR I%=4 TO 42
PHOP(I%)=MIXCOEFF(I%,1)
INCR PROP(1%)*AVGSTR(2)*AVGSTR(1)*MIXCOEFF(1%,2)
INCR PROP(1%)*AVGSTR(3)*AVGSTR(1)*MIXCOEFF(1%,3)
INCR PROP(1%)*AVGSTR(4)*AVGSTR(1)*MIXCOEFF(1%,4)
INCR PROP(1%)*AVGSTR(6)*AVGSTR(5)*MIXCOEFF(1%,5)
    
```

* top line
* ends
* bottom line
* top junct
* middle line
* bottom junct

* ocpal

* Xch3
* Xch2
* Xch
* Cun

DrawResults:

This is the subroutine to draw the physical property results.

```

LOCATE 8,11 : PRINT " fc:" ; LOCATE 9,11 : PRINT " Xch3:" ;
LOCATE 10,11 : PRINT " Xch2:" ; LOCATE 11,11 : PRINT " Xch:" ;
COLOR 15, 1
LOCATE 15, 5 : PRINT "Mono" ; LOCATE 16, 4 : PRINT "Cyclic";
LOCATE 12,11 : PRINT " fc:" ; LOCATE 13,11 : PRINT " Cunt";
LOCATE 14,11 : PRINT " Cch3:" ; LOCATE 15,11 : PRINT " Cch2:" ;
LOCATE 16,11 : PRINT " Cch:" ; LOCATE 17,11 : PRINT " Cch2>at";
LOCATE 18,11 : PRINT "Cch2>at";
COLOR 14, 1
LOCATE 21, 5 : PRINT "Df" ; LOCATE 22, 3 : PRINT "Cyclic";
LOCATE 19,11 : PRINT " fc:" ; LOCATE 20,11 : PRINT " Cunt";
LOCATE 21,11 : PRINT " Cch3:" ; LOCATE 22,11 : PRINT " Cch2:" ;
LOCATE 23,11 : PRINT "Cch2>at";
COLOR 15, 1
FOR I%=1 TO 16
    LOCATE I%+7,20 : PRINT USING "#####"AVGSTR(I%);
NEXT I%
    . Physical Property Box
COLOR 10,1
LOCATE 6,32 : PRINT CHR$(218);STRING$(47,196);CHR$(191); ' top line
FOR I%=7 TO 16
    LOCATE I%,32 : PRINT CHR$(179);TAB(60);CHR$(179); ' middle
NEXT I%
LOCATE 19,32 : PRINT CHR$(182);STRING$(47,196);CHR$(217); ' bottom line
COLOR 11, 1
LOCATE 7,46 : PRINT "Physical Properties"
COLOR 14, 1
    . First Row
LOCATE 8,36 : PRINT "Cetane" ; LOCATE 8,46 : PRINT "Cet Index";
LOCATE 8,56 : PRINT "Density" ; LOCATE 8,66 : PRINT "Sp Grav";
    . Second Row
LOCATE 11,36 : PRINT "Pour Pt" ; LOCATE 11,47 : PRINT "Flash Pt";
LOCATE 11,56 : PRINT "Cloud Pt" ; LOCATE 11,70 : PRINT "Viscos";
    . Third Row
LOCATE 14,36 : PRINT "H Comb" ; LOCATE 14,46 : PRINT "Filter";
LOCATE 14,60 : PRINT "% Arom" ; LOCATE 14,70 : PRINT "C resid";
    . Fourth Row
LOCATE 17,37 : PRINT "IBP" ; LOCATE 17,44 : PRINT "10% BP";
LOCATE 17,53 : PRINT "50% BP" ; LOCATE 17,62 : PRINT "90% BP";
LOCATE 17,71 : PRINT "END BP";
COLOR 10,0
LOCATE 5,20 : PRINT TIMES;
LOCATE 5,51 : PRINT DATES;
    . Next are commands.
COLOR 3,0
LOCATE 21,39 : PRINT " Press <O> to quit, <F1> to hardcopy";
LOCATE 22,39 : PRINT "<R> to reset, < ; CHR$(24);"; CHR$(25);
    PRINT "> to move the cursor";
LOCATE 23,39 : PRINT " or <O-B> to enter a numeric value";
RETURN
    
```

```

    . clear screen
GOSUB ClearResults
COLOR 15, 1
LOCATE 9,34 : PRINT USING "#####"PROP(4);
LOCATE 9,45 : PRINT USING "#####"PROP(31);
LOCATE 9,56 : PRINT USING "#####"PROP(9);
LOCATE 9,68 : PRINT USING "#####"PROP(32);
LOCATE 12,35 : PRINT USING "#####"PROP(6);
LOCATE 12,47 : PRINT USING "#####"PROP(8);
LOCATE 12,59 : PRINT USING "#####"PROP(11);
LOCATE 12,69 : PRINT USING "#####"PROP(12);
LOCATE 15,34 : PRINT USING "#####"PROP(26);
LOCATE 15,47 : PRINT USING "#####"PROP(13);
LOCATE 15,56 : PRINT USING "#####"PROP(28);
LOCATE 15,69 : PRINT USING "#####"PROP(37);
LOCATE 18,34 : PRINT USING "#####"PROP(33);
LOCATE 18,43 : PRINT USING "#####"PROP(34);
LOCATE 18,52 : PRINT USING "#####"PROP(3);
LOCATE 18,61 : PRINT USING "#####"PROP(35);
LOCATE 18,70 : PRINT USING "#####"PROP(36);
RETURN
    
```

ClearResults:

This is the subroutine to clear the physical property results.

```

COLOR 15, 1
FOR I%=9 TO 16 STEP 3
    LOCATE I%,34 : PRINT SPACES(44);
NEXT I%
RETURN
    
```

EndProgram:

This is the section to end the program.

```

COLOR 12, 0 : CLS
LOCATE 1, 1
PRINT "FUELCALC ",VER$; "Terminated...Press any key to continue"
AS=INPUT$(1)
END
    
```



```

LPRINT USING TEM03$:PROP(12); : LPRINT *± 0.27 cS*
LPRINT USING TEM03$:PROP(26); : LPRINT *± 0.06 MJ/kg*
LPRINT USING TEM11$:PROP(13); : LPRINT *± 19.1*
LPRINT USING TEM11$:PROP(28); : LPRINT *± 1.85 volume %*
LPRINT USING TEM12$:PROP(37); : LPRINT *± 5.88 °C*
LPRINT USING TEM13$:PROP(33); : LPRINT *± 5.88 °C*
LPRINT USING TEM14$:PROP(34); : LPRINT *± 0.25 °C*
LPRINT USING TEM15$:PROP(5); : LPRINT *± 9.91 °C*
LPRINT USING TEM16$:PROP(35); : LPRINT *± 18.6 °C*
LPRINT USING TEM17$:PROP(36); : LPRINT *± 20.6 °C*
LPRINT CHR$(12)
COLOR 15, 0
LOCATE 24,50 : PRINT SPACES(25);
RETURN

```

ReadFuelParams:

This is the subroutine to read the fuel parameters file.

```

Will write message to the user.
COLOR 0, 3
LOCATE 10,20 : PRINT CHR$(201);STRINGS(30,205);CHR$(167);
FOR I%=11 TO 13
LOCATE I%,20 : PRINT CHR$(166);TAB(60);CHR$(166);
NEXT I%
LOCATE 14,20 : PRINT CHR$(200);STRINGS(30,205);CHR$(168);
COLOR 4, 3
LOCATE 12,26 : PRINT "Reading the ", : COLOR 14,3 : PRINT "Params File";
OPEN CGDIR$+"FUEL\PARAM.DAT" FOR RANDOM AS #5 LEN=729
FIELD #5, 25 AS S$, 25 AS I$, 25 AS O$, 25 AS F$, 25 AS T$(1),
25 AS T$(2), 25 AS T$(3), 25 AS T$(4), 25 AS T$(5), 25 AS T$(6),
25 AS T$(7), 25 AS T$(8), 25 AS T$(9), 25 AS T$(10), 25 AS T$(11),
25 AS T$(12), 25 AS T$(13), 25 AS T$(14), 25 AS T$(15), 25 AS T$(16),
25 AS T$(17), 25 AS T$(18), 25 AS T$(19), 25 AS T$(20), 25 AS T$(21),
25 AS T$(22)
FOR I%=1 TO 42
GET 5 I%
SLOPEFACTOR(I%)=VAL(S$) : INTOPFACTOR(I%)=VAL(I$)
OFFSETFACR(I%)=VAL(O$) : FUNCTION$(I%)=F$
FOR J%=1 TO 22
MIXCOEFF(I%,J%)=VAL(T$(J%))
NEXT J%
NEXT I%
CLOSE #5
RETURN

```

```

* Viscos
* Ht Comb
* Filter
* % Atom
* C resid
* IBP
* 10% BP
* 50% BP
* 90% BP
* END BP

```

Hardcopy:

This is the subroutine to hardcopy the Physical Properties.

```

COLOR 28, 0
LOCATE 24,50 : PRINT "Printing Fuel Data";
LPRINT "Results of Fuel Property Calculation: " ;DATES; *TIMES
LPRINT
LPRINT * Average Structural Information:
LPRINT USING * Alkane fc: ##### *AVGSTR( 1)
LPRINT USING * Xch3: ##### *AVGSTR( 2)
LPRINT USING * Xch2: ##### *AVGSTR( 3)
LPRINT USING * Xch: ##### *AVGSTR( 4)
LPRINT
LPRINT USING * Monocyclic fc: ##### *AVGSTR( 5)
LPRINT USING * Cun: ##### *AVGSTR( 6)
LPRINT USING * Cch3: ##### *AVGSTR( 7)
LPRINT USING * Cch2: ##### *AVGSTR( 8)
LPRINT USING * Cch: ##### *AVGSTR( 9)
LPRINT USING * Ccat: ##### *AVGSTR(10)
LPRINT USING * Cch2>a: ##### *AVGSTR(11)
LPRINT
LPRINT USING * Dicyclic fc: ##### *AVGSTR(12)
LPRINT USING * Cun: ##### *AVGSTR(13)
LPRINT USING * Cch3: ##### *AVGSTR(14)
LPRINT USING * Cch2: ##### *AVGSTR(15)
LPRINT USING * Cch2>a: ##### *AVGSTR(16)
LPRINT
LPRINT * Calculated Physical Properties:
TEM016$="#####*
TEM025$="#####*
TEM035$="#####*
TEM045$="#####*
TEM055$="#####*
TEM065$="#####*
TEM075$="#####*
TEM085$="#####*
TEM095$="#####*
TEM105$="#####*
TEM115$="#####*
TEM125$="#####*
TEM135$="#####*
TEM145$="#####*
TEM155$="#####*
TEM165$="#####*
TEM175$="#####*
LPRINT USING TEM01$:PROP(4); : LPRINT *± 0.85 Cetane*
LPRINT USING TEM02$:PROP(31); : LPRINT *± 1.10 Cetane*
LPRINT USING TEM03$:PROP(9); : LPRINT *± 0.005 kg/L*
LPRINT USING TEM04$:PROP(32); : LPRINT *± 0.002 60/60°F*
LPRINT USING TEM05$:PROP(6); : LPRINT *± 5.18 °C*
LPRINT USING TEM06$:PROP(8); : LPRINT *± 9.47 °C*
LPRINT USING TEM07$:PROP(11); : LPRINT *± 3.77 °C*

```

* Cetane
* Cell Index
* Density
* Sp Gravity
* Pour Pt
* Flash Pt
* Cloud Pt

Listing for Program III.3: FUELMIX.BAS

Program Name: FUELMIX Ver 1.00 Date Written: 07/24/1988
 Author: Allen Caswell Date Modified: 07/29/1989

This program is designed to calculate the physical properties of mixtures of middle distillate fuels. The mixing coefficients for the calculation are read in from the file written by the correlation program. This file must be in the default directory in order for the program to run. To operate the program, the operator enters the names for the fuels from menus and then enters the relative amount of each fuel to be added together in a mixture. Once these are entered, then average structures for the fuels are shown in the outermost boxes and the physical properties are calculated. It is then possible to edit the average structures of each fuel and the physical properties are automatically updated. The file which contains the mixing coefficients is named FUELPARM.DAT and MUST be in the default directory.

First will set up the variables.

```

ON ERROR GOTO ErrorMessage
DIM INTOFFACTOR(42), FUELNAME$(2,250), NAMEUSE%(2), DE(3,350)
DIM SLOPEFACTOR(42), FUNCTION$(42), OPTN$(4), PAGE%(2)
DIM OFFSEFFACTR(42), MIXCOEFF(42,22), OPTN%(6), T$(22)

' Next are the constants
VERSN$ = "Ver 1.00"
CFGDIR$ = ""
MIX% = 1
PAGE%(1) = 1
PAGE%(2) = 1
SCDRIVES$ = "F:\\"
DIRECTORY$(1) = "D:\LCNMRDATA\ARMY68\*"
DIRECTORY$(2) = "D:\LCNMRDATA\ARMY66\*"
FOR I%=1 TO 8
  OPTN%(I%) = 1
NEXT I%

' Must read in the parameters.
GOSUB ReadFuelParams
MainMenu.
  
```

This is the section to do the main menu.

ErrorMessage:

This is the subrn to do the error handling.

```

SCREEN 0 : COLOR 15, 0 : CLS
COLOR 0, 4
LOCATE 6, 5 : PRINT CHR$(201); STRING$(69, 206); CHR$(187);
FOR I%=9 TO 15
  LOCATE I%, 5 : PRINT CHR$(196); TAB(75); CHR$(186);
NEXT I%
LOCATE 16, 5 : PRINT CHR$(200); STRING$(69, 206); CHR$(186);
COLOR 31, 4
LOCATE 11, 26 : PRINT USING ">>> Error ### encountered <<<"; ERR;
COLOR 14, 4
TEMP$ = "See Appendix E, p. 412, in Turbo Basic Manual for full message."
LOCATE 13, 9 : PRINT TEMP$;
COLOR 0, 3
LOCATE 24, 19 : PRINT " Press any key to return to the Main Menu ";
TEMP$ = INPUT$(1)
CLOSE
GOTO MainMenu
  
```

```
OPTNS(1)="Select fuel files"
OPTNS(2)="Mix selected fuels"
OPTNS(3)="Quit to DOS"
GOSUB DrawMainMenu
```

SelectFuelFiles:

This is the subroutine to get the fuel names and parameters.

```
StartOfSelectFuelFiles:
  First is section to get the directories.
  GOSUB GetDirectoriesMenu
  Next is section to get the fuel files.
  GOSUB GetFuelFilesMenu
```

PerformMixing:

This is the section to do the mixing.

```
First must draw the screen.
IF AMTMIX(1)+AMTMIX(2)<>100 THEN AMTMIX(1)=100-AMTMIX(2)
GOSUB DrawMixMenu
GOSUB PerformCalcs
GOTO MainMenu
```

FileResults:

This is the section to file the mixing results.

```
First must see which data to file
OPTNS(1)="A - Mixture Component A"
OPTNS(2)="B - Mixture Component B"
OPTNS(3)="R - Mixing Results"
OPTNS(4)="Quit to Mixing Menu"
GOSUB DrawFileWhichDataMenu
GOTO FileDataMenu
GOTO MainMenu
```

PerformCalcs:

This is the section to do the Physical Property Calcs.

```
Must first check if array empty, if so clear results and return.
TOTAL=0
FOR I%=1 TO 2
  INCR TOTAL,VAL(DS(I,116))
  INCR TOTAL,VAL(DS(I,27))
  INCR TOTAL,VAL(DS(I,52))
NEXT I%
IF TOTAL<=0 THEN
  FOR I%=1 TO 350 : DS(I,1%)="": NEXT I%
  GOSUB ClearResults
  RETURN
END IF
```

Next must perform the mixing of the two arrays.

```
COLOR 28,0
LOCATE 24,47 : PRINT "Calculating Mixture Properties"
DS(3,116)=STRS(VAL(DS(1,116))*AMTMIX(1)/100 + VAL(DS(2,116))*AMTMIX(2)/100)
DS(3,106)=STRS(VAL(DS(1,106))*AMTMIX(1)/100 + VAL(DS(2,106))*AMTMIX(2)/100)
DS(3,108)=STRS(VAL(DS(1,108))*AMTMIX(1)/100 + VAL(DS(2,108))*AMTMIX(2)/100)
DS(3,110)=STRS(VAL(DS(1,110))*AMTMIX(1)/100 + VAL(DS(2,110))*AMTMIX(2)/100)
DS(3,27)=STRS(VAL(DS(1,27))*AMTMIX(1)/100 + VAL(DS(2,27))*AMTMIX(2)/100)
DS(3,31)=STRS(VAL(DS(1,31))*AMTMIX(1)/100 + VAL(DS(2,31))*AMTMIX(2)/100)
DS(3,9)=STRS(VAL(DS(1,9))*AMTMIX(1)/100 + VAL(DS(2,9))*AMTMIX(2)/100)
DS(3,11)=STRS(VAL(DS(1,11))*AMTMIX(1)/100 + VAL(DS(2,11))*AMTMIX(2)/100)
DS(3,13)=STRS(VAL(DS(1,13))*AMTMIX(1)/100 + VAL(DS(2,13))*AMTMIX(2)/100)
DS(3,18)=STRS(VAL(DS(1,18))*AMTMIX(1)/100 + VAL(DS(2,18))*AMTMIX(2)/100)
DS(3,15)=STRS(VAL(DS(1,15))*AMTMIX(1)/100 + VAL(DS(2,15))*AMTMIX(2)/100)
DS(3,52)=STRS(VAL(DS(1,52))*AMTMIX(1)/100 + VAL(DS(2,52))*AMTMIX(2)/100)
DS(3,28)=STRS(VAL(DS(1,28))*AMTMIX(1)/100 + VAL(DS(2,28))*AMTMIX(2)/100)
DS(3,34)=STRS(VAL(DS(1,34))*AMTMIX(1)/100 + VAL(DS(2,34))*AMTMIX(2)/100)
DS(3,36)=STRS(VAL(DS(1,36))*AMTMIX(1)/100 + VAL(DS(2,36))*AMTMIX(2)/100)
DS(3,40)=STRS(VAL(DS(1,40))*AMTMIX(1)/100 + VAL(DS(2,40))*AMTMIX(2)/100)
```

Next must calculate the physical properties.

```
FOR I%=4 TO 42
  PROP=MIXCOEFF(I%,1)
  INCR PROP,VAL(DS(3,106))*VAL(DS(3,116))*MIXCOEFF(I%,2) * Xch3
  INCR PROP,VAL(DS(3,108))*VAL(DS(3,116))*MIXCOEFF(I%,3) * Xch2
  INCR PROP,VAL(DS(3,110))*VAL(DS(3,116))*MIXCOEFF(I%,4) * Xch
  INCR PROP,VAL(DS(3,31))*VAL(DS(3,27))*MIXCOEFF(I%,5) * Cch
  INCR PROP,VAL(DS(3,6))*VAL(DS(3,27))*MIXCOEFF(I%,6) * Cch3
  INCR PROP,VAL(DS(3,11))*VAL(DS(3,27))*MIXCOEFF(I%,7) * Cch2
  INCR PROP,VAL(DS(3,13))*VAL(DS(3,27))*MIXCOEFF(I%,8) * Cch
  INCR PROP,VAL(DS(3,18))*VAL(DS(3,27))*MIXCOEFF(I%,9) * Cch1
  INCR PROP,VAL(DS(3,15))*VAL(DS(3,27))*MIXCOEFF(I%,10) * Cch2>
  INCR PROP,VAL(DS(3,28))*VAL(DS(3,52))*MIXCOEFF(I%,11) * Cch
  INCR PROP,VAL(DS(3,34))*VAL(DS(3,52))*MIXCOEFF(I%,12) * Cch3
  INCR PROP,VAL(DS(3,36))*VAL(DS(3,52))*MIXCOEFF(I%,13) * Cch2
  INCR PROP,VAL(DS(3,40))*VAL(DS(3,52))*MIXCOEFF(I%,14) * Cch2>
```

```

IF LEFT$(FUNCTION$(%),1)="" THEN PROP=PROP
IF LEFT$(FUNCTION$(%),3)="1/" THEN PROP=1/PROP
IF LEFT$(FUNCTION$(%),3)="LOG" THEN PROP=LOG(PROP)
PROP=PROP * OFFSETFACTR(%)
PROP=PROP * SLOPEFACTOR(%)
PROP=PROP + INTCPFACTOR(%)
.
.   Have calculated property, so place in output array.
Ds(3,150+%)=STR$(PROP)
NEXT %
GOSUB DrawResults
COLOR 15,0
LOCATE 24,47 : PRINT *
RETURN

DrawMainMenu:
.
.   This is the subroutine to draw the Main Menu.
.
.
.
.   Will draw the screen.
SCREEN 0 : WIDTH 80
COLOR 15,0 : CLS
LOCATE 0,4
LOCATE 1,5 : PRINT CHR$(201),STRING$(90,200),CHR$(167)
LOCATE 2,5 : PRINT CHR$(166),STRING$(90,32),CHR$(166)
LOCATE 3,5 : PRINT CHR$(166),STRING$(90,32),CHR$(166)
LOCATE 4,5 : PRINT CHR$(200),STRING$(90,200),CHR$(166)
LOCATE 1,31 : PRINT CHR$(209);
LOCATE 2,31 : PRINT CHR$(179);
LOCATE 3,31 : PRINT CHR$(179);
LOCATE 4,31 : PRINT CHR$(207);
COLOR 15,4
LOCATE 2,10 : PRINT "FUELMIX";
LOCATE 2,19 : PRINT VERSNS;
LOCATE 3,14 : PRINT "July 1988";
LOCATE 2,35 : PRINT "Physical Property Calculation Software";
LOCATE 3,35 : PRINT *   Allen Caswell, Virginia Tech *;
.
.   Main Menu box.
COLOR 10,1
LOCATE 9,15 : PRINT CHR$(218),STRING$(49,190),CHR$(191);
FOR %=-9 TO 18
LOCATE %,15 : PRINT CHR$(179);TAB(65),CHR$(179);
NEXT %
LOCATE 19,15 : PRINT CHR$(182),STRING$(49,190),CHR$(217);
COLOR 10,1
LOCATE 9,20 : PRINT TIMES;
LOCATE 9,51 : PRINT DATES;
COLOR 15,1
LOCATE 11,35 : PRINT "MAIN MENU";
COLOR 14,1
LOCATE (%-1)*2+13,40-(0.5*LEN(OPTN$(%)))

COLOR 11,1 : PRINT LEFT$(OPTN$(%),1);
COLOR 14,1 : PRINT RIGHT$(OPTN$(%),LEN(OPTN$(%))-1);
NEXT %
.
.   Next are commands.
COLOR 3,0
LOCATE 23,20 : PRINT *   Press the highlighted letter, or
LOCATE 24,20 : PRINT *   use the arrow keys and <ENTER> to select*;
.
.   Next see what to do
COLOR 14,0
LOCATE (OPTN$(1)-1)*2+13,38-(0.5*LEN(OPTN$(OPTN$(1))))
PRINT * ,OPTN$(OPTN$(1));* *;
Startloop1:
AS=INKEY$
SELECT CASE AS
CASE ""
COLOR 10,1 : LOCATE 9,20 : PRINT TIMES;
CASE CHR$(13)
GOTO DoOption1
CASE "S",",",*
OPTN$(1)=1 : GOTO DoOption1
CASE "M",",",*
OPTN$(1)=2 : GOTO DoOption1
CASE "O",",",*
OPTN$(1)=3 : GOTO DoOption1
CASE CHR$(0)+CHR$(72), CHR$(0)+CHR$(80)
LOCATE (OPTN$(1)-1)*2+13,38-(0.5*LEN(OPTN$(OPTN$(1))))
COLOR 11,1
PRINT * ,LEFT$(OPTN$(OPTN$(1)),1);
COLOR 14,1
PRINT RIGHT$(OPTN$(OPTN$(1)),LEN(OPTN$(OPTN$(1))-1)*);
IF AS=CHR$(0)+CHR$(72), THEN DECR OPTN$(1) ELSE INCR OPTN$(1)
IF OPTN$(1)<1 THEN OPTN$(1)=3
IF OPTN$(1)>3 THEN OPTN$(1)=1
COLOR 14,0
LOCATE (OPTN$(1)-1)*2+13,38-(0.5*LEN(OPTN$(OPTN$(1))))
PRINT * ,OPTN$(OPTN$(1));* *;
CASE CHR$(0)+CHR$(79),CHR$(0)+CHR$(77)
.   left:right
.   oopal
CASE ELSE
SOUND 1000,3 : SOUND 800,15
END SELECT
GOTO Startloop1
DoOption1:
SELECT CASE OPTN$(1)
CASE 1 : GOTO SelectFuelFiles
CASE 2 : GOTO PerformMixing
CASE 3
COLOR 12,0 : CLS
LOCATE 1,1
PRINT "FUELMIX ",VERSNS;* Terminated....Press any key to continue*
AS=INPUT$(1)
END
END SELECT

```

GetDirectoriesMenu:

This is the subroutine to get the fuel directories.

```

SCREEN 0 : WIDTH 80
COLOR 15, 0 : CLS
COLOR 10, 1
LOCATE 6,15 : PRINT CHR$(216);STRING$(49,196);CHR$(191); ' top line
FOR %I=9 TO 10
    LOCATE %I,15 : PRINT CHR$(179);TAB(65);CHR$(179); ' middle
NEXT %I
LOCATE 17,15 : PRINT CHR$(192);STRING$(49,196);CHR$(217); ' bottom line
COLOR 10, 1
LOCATE 9,20 : PRINT TIMES;
LOCATE 9,51 : PRINT DATES;
COLOR 11, 1
LOCATE 10,27 : PRINT "Directories for Fuel Files.";
COLOR 14, 1
LOCATE 12,23 : PRINT "Directory for Mixture Component A";
LOCATE 15,23 : PRINT "Directory for Mixture Component A";
COLOR 12, 1
LOCATE 13,30 : PRINT "DIRECTORIES(1)";
LOCATE 16,30 : PRINT "DIRECTORIES(2)";
' Next are commands.
COLOR 3,0
LOCATE 23,22 : PRINT " Press <:CHR$(24);:CHR$(25);
PRINT "> to move the cursor";
LOCATE 24,22 : PRINT "<Q> to quit, or <ENTER> to continue";
' Next must see what to do.
COLOR 12, 0
LOCATE (OPTN%(2)-1)*3+13,30 : PRINT "DIRECTORIES(OPTN%(2))";
Startloop2:
AS=INKEY$
SELECT CASE AS
CASE =
    COLOR 10, 1
    LOCATE 9,20 : PRINT TIMES;
CASE 'Q','q',CHR$(27)
    GOTO MainMenu
CASE CHR$(13)
    RETURN
CASE CHR$(0)+CHR$(72), CHR$(0)+CHR$(80)
    COLOR 12, 1
    LOCATE (OPTN%(2)-1)*3+13,30 : PRINT "DIRECTORIES(OPTN%(2))";
    IF AS=CHR$(0)+CHR$(72) THEN INCR OPTN%(2) ELSE DECR OPTN%(2)
    IF OPTN%(2)>2 THEN OPTN%(2)=1
    IF OPTN%(2)<1 THEN OPTN%(2)=2
    COLOR 12, 0
    LOCATE (OPTN%(2)-1)*3+13,30 : PRINT "DIRECTORIES(OPTN%(2))";
CASE ELSE
    COLOR 12, 1
    LOCATE (OPTN%(2)-1)*3+13,30 : PRINT SPACES(60);
    
```

```

LOCATE (OPTN%(2)-1)*3+13,31 : PRINT AS;
LINE INPUT TEMPS
DIRECTORIES(OPTN%(2))=LUCASE$(AS+TEMPS+"")
NAMEUSE%(OPTN%(2))=0
COLOR 12, 0
LOCATE (OPTN%(2)-1)*3+13,30 : PRINT "DIRECTORIES(OPTN%(2))";
END SELECT
GOTO Startloop2
    
```

GetFuelFilesMenu:

This is the subroutine to get the fuel files for mixing.

```

' First is top names box.
COLOR 15,0 : CLS
COLOR 10,1
LOCATE 1,1 : PRINT CHR$(216);STRING$(78,196);CHR$(191);
FOR %I=2 TO 8
    LOCATE %I,1 : PRINT CHR$(179);TAB(80);CHR$(179);
NEXT %I
LOCATE 9, 1 : PRINT CHR$(192);STRING$(78,196);CHR$(217);
COLOR 11, 1
LOCATE 2,24 : PRINT "Fuel File for Mixture Component A";
LOCATE 2,65 : PRINT "Page";
LOCATE 3,20 : PRINT "File Directory: ";DIRECTORIES(1);
COLOR 10, 1
LOCATE 2,71 : PRINT USING "#";PAGE%(1);
TEMPMIX%=MIX% : MIX%=1 : GOSUB LoadNames : MIX%=TEMPMIX%
TEMPMIX%=MIX% : MIX%=1 : GOSUB PageOfNames : MIX%=TEMPMIX%
' Next is bottom names box.
COLOR 10,1
LOCATE 16,1 : PRINT CHR$(216);STRING$(78,196);CHR$(191);
FOR %I=17 TO 23
    LOCATE %I,1 : PRINT CHR$(179);TAB(80);CHR$(179);
NEXT %I
LOCATE 24, 1 : PRINT CHR$(192);STRING$(78,196);CHR$(217);
COLOR 11, 1
LOCATE 17,24 : PRINT "Fuel File for Mixture Component B";
LOCATE 17,65 : PRINT "Page";
LOCATE 18,20 : PRINT "File Directory: ";DIRECTORIES(2);
COLOR 10, 1
LOCATE 17,71 : PRINT USING "#";PAGE%(2);
TEMPMIX%=MIX% : MIX%=2 : GOSUB LoadNames : MIX%=TEMPMIX%
TEMPMIX%=MIX% : MIX%=2 : GOSUB PageOfNames : MIX%=TEMPMIX%
' Next are commands
COLOR 3,0
LOCATE 11,18 : PRINT "Press <F1> to toggle between Mix A and Mix B";
LOCATE 12, 8 : PRINT "Press <:CHR$(24);:CHR$(25);" > to move cursor, ";
PRINT "<PGUP,PGDN> to page names, <O> to quit";
LOCATE 13,23 : PRINT "Press <RETURN> to load a fuel file";
LOCATE 14,17 : PRINT "Note: Files already loaded are marked with ";
    
```



```

GOSUB DrawMixDataScreen
    . Physical Property Box
    COLOR 10, 1
    LOCATE 3,44 : PRINT CHR$(219);STRING$(35,198);CHR$(191); ' top line
    FOR I%=4 TO 16
        LOCATE I%,44 : PRINT CHR$(179);TAB(80);CHR$(179); ' middle
    NEXT I%
    LOCATE 17,44 : PRINT CHR$(162);STRING$(35,198);CHR$(217); ' bottom line
    COLOR 11, 1
    LOCATE 4,53 : PRINT "Physical Properties";
    COLOR 14, 1
    . First Row
    LOCATE 5,47 : PRINT "Octane"; : LOCATE 6,56 : PRINT "Octane Index";
    LOCATE 6,71 : PRINT "Density";
    . Second Row
    LOCATE 7,46 : PRINT "Sp Grav"; : LOCATE 7,56 : PRINT "Pour Pt";
    LOCATE 7,71 : PRINT "Flash Pt";
    . Third Row
    LOCATE 9,46 : PRINT "Cloud Pt"; : LOCATE 9,59 : PRINT "Viscos";
    LOCATE 9,71 : PRINT "Ht Comb";
    . Fourth Row
    LOCATE 11,47 : PRINT "Filter"; : LOCATE 11,59 : PRINT "% Arom";
    LOCATE 11,71 : PRINT "C resid";
    . Fifth Row
    LOCATE 13,46 : PRINT "IBP"; : LOCATE 13,56 : PRINT "10% BP";
    LOCATE 13,72 : PRINT "50% BP";
    . Sixth Row
    LOCATE 15,47 : PRINT "90% BP"; : LOCATE 15,56 : PRINT "END BP";
    . Next are commands.
    COLOR 3,0
    LOCATE 20,44 : PRINT "Press <Q> to quit, <F1> to hardcopy,";
    LOCATE 21,44 : PRINT " <F2> to file data, <R> to reset,";
    LOCATE 22,44 : PRINT "<;CHR$(27);";CHR$(24);";CHR$(25);";CHR$(26);
    PRINT "> to move the highlight bar,";
    LOCATE 23,45 : PRINT "or <0-9> to enter a numeric value,";
    RETURN
PerformMixMenu:
    . Next see what to do.
    TEMP1%=0 : GOSUB HighlightMix
    Startloop4:
    AS=INKEY$
    SELECT CASE AS
    CASE " "
        . no key
    CASE "Q" : LOCATE 2,44 : PRINT TIMES;
    CASE "q" : CHR$(27)
    RETURN
    CASE CHR$(0)+CHR$(58)
        GOSUB Hardcopy
    CASE CHR$(0)+CHR$(80)
        GOTO FileResults
    CASE "R" : "r"
        . reset
        FUELNAMES(MIX%,NAMEUSE%(MIX%))=
        FOR I%=1 TO 350 : D$(MIX%,I%)= : NEXT I%
        NAMEUSE%(MIX%)=0
        SELECT CASE MIX%
        CASE 1 : AMTMIX(1)=0 : AMTMIX(2)=100
        CASE 2 : AMTMIX(1)=100 : AMTMIX(2)=0
        END SELECT
        GOSUB DrawMixDataScreen
        GOSUB PerformCalcs
        TEMP1%=0 : GOSUB HighlightMix
        CASE CHR$(0)+CHR$(72), CHR$(0)+CHR$(80)
            TEMP1%=1 : GOSUB HighlightMix
        CASE CHR$(0)+CHR$(72) THEN DECR OPTN%(MIX%+4) ELSE INCR OPTN%(MIX%+4)
        IF AS=CHR$(0)+CHR$(72) THEN DECR OPTN%(MIX%+4)=19
        IF OPTN%(MIX%+4)<1 THEN OPTN%(MIX%+4)=1
        IF OPTN%(MIX%+4)>19 THEN OPTN%(MIX%+4)=1
        TEMP1%=0 : GOSUB HighlightMix
        CASE CHR$(0)+CHR$(75);CHR$(0)+CHR$(77)
            TEMP1%=1 : GOSUB HighlightMix
        IF MIX%=1 THEN MIX%=2 ELSE MIX%=1
        TEMP1%=0 : GOSUB HighlightMix
        CASE ELSE
            TEMP1%=1 : GOSUB EraseMixData
        IF OPTN%(MIX%+4)>2 THEN PRINT BRACES(6); ELSE PRINT SPACES(26);
        PRINT " ";AS;
        LINE INPUT TEMPS
        SELECT CASE OPTN%(MIX%+4)
        CASE 1 : FUELNAMES(MIX%,NAMEUSE%(MIX%))=AS+TEMPS
        CASE 2 : D$(MIX%,144)=AS+TEMPS
        CASE 3
            AMTMIX(MIX%)=VAL(AS+TEMPS)
        IF AMTMIX(1)+AMTMIX(2)>100 THEN
            IF MIX%=1 THEN AMTMIX(2)=100-AMTMIX(1)
            IF MIX%=2 THEN AMTMIX(1)=100-AMTMIX(2)
            GOSUB DrawMixDataScreen
        END IF
        CASE ELSE : GOSUB EraseMixData : D$(MIX%,TEMP%)=AS+TEMPS
        END SELECT
        IF MIX%=2 AND OPTN%(MIX%+4)=2 THEN GOSUB DrawMixMenu
        TEMP1%=0 : GOSUB HighlightMix
        GOSUB PerformCalcs
        GOTO Startloop4
    END SELECT

```

This is the subroutine to do the Mixing Menu.

Next see what to do.
 TEMP1%=0 : GOSUB HighlightMix
 Startloop4:
 AS=INKEY\$

DrawFileWhichDataMenu:

This is the subroutine to figure out which data to file.

```

SCREEN 0 : WIDTH 80
COLOR 15, 0 : CLS
COLOR 10,1
LOCATE 6,15 : PRINT CHR$(218);STRING$(49,196);CHR$(191); ' top line
FOR %A=0 TO 18
    LOCATE %A,15 : PRINT CHR$(179);TAB(65);CHR$(179); ' middle
NEXT %A
LOCATE 19,15 : PRINT CHR$(192);STRING$(49,196);CHR$(217); ' bottom line
COLOR 10,1
LOCATE 9,20 : PRINT TIMES;
LOCATE 9,51 : PRINT DATES;
COLOR 15,1
LOCATE 11,35 : PRINT "FILE MENU:";
COLOR 14,1
FOR %A=1 TO 4
    LOCATE (%A-1)*2+12,40-(0.5*LEN(OPTN$(%A)))
    COLOR 11,1 : PRINT LEFT$(OPTN$(%A),1);
    COLOR 14,1 : PRINT RIGHT$(OPTN$(%A),LEN(OPTN$(%A))-1);
NEXT %A
    
```

```

' Next are commands.
COLOR 3,0
LOCATE 5,17 : PRINT "Please select the Data which you wish to file:";
LOCATE 23,20 : PRINT " Press the highlighted letter, or ";
LOCATE 24,20 : PRINT " use the arrow keys and <ENTER> to select;"
    
```

```

' Next see what to do.
COLOR 14,0
LOCATE (OPTN$(7)-1)*2+12,38-(0.5*LEN(OPTN$(OPTN$(7))))
PRINT " *OPTN$(OPTN$(7))." ;
Startloop$:
AS=INKEY$
SELECT CASE AS
CASE =
    ' no key
    ' return
    ' component A
    ' component B
    ' mix result
    ' quit
    ' up-down
CASE OPTN$(7)-1 : LOCATE 9,20 : PRINT TIMES;
    RETURN
CASE "A",a
    OPTN$(7)=1 : RETURN
CASE "B",b
    OPTN$(7)=2 : RETURN
CASE "R",r
    OPTN$(7)=3 : RETURN
CASE "Q",q,CHR$(27)
    GOTO PerformMixing
CASE CHR$(0)+CHR$(72), CHR$(0)+CHR$(80)
    LOCATE (OPTN$(7)-1)*2+12,38-(0.5*LEN(OPTN$(OPTN$(7))))
    COLOR 11,1
    PRINT " *LEFT$(OPTN$(OPTN$(7)),1);
    COLOR 14,1
    
```

```

PRINT RIGHT$(OPTN$(OPTN$(7)),LEN(OPTN$(OPTN$(7)))-1); '
IF AS=CHR$(0)+CHR$(72) THEN DECR OPTN$(7) ELSE INCR OPTN$(7)
IF OPTN$(7)<1 THEN OPTN$(7)=4
IF OPTN$(7)>4 THEN OPTN$(7)=1
COLOR 14,0
LOCATE (OPTN$(7)-1)*2+12,38-(0.5*LEN(OPTN$(OPTN$(7))))
PRINT " *OPTN$(OPTN$(7))." ;
CASE CHR$(0)+CHR$(75);CHR$(0)+CHR$(77)
CASE ELSE
    SOUND 1000,3 : SOUND 800,1.5
END SELECT
GOTO Startloops
    
```

' left-right
' coopal

FileDataMenu:

This is the subroutine to file the selected mixing data.

```

SELECT CASE OPTN$(7)
CASE 1
    OD$(1)=DIRECTORY$(1) : OFILES=FUELNAME$(1,NAMEUSE$(1))+".DAT"
    COMMS=DS(1,144)
CASE 2
    OD$(2)=DIRECTORY$(2) : OFILES=FUELNAME$(2,NAMEUSE$(2))+".DAT"
    COMMS=DS(2,144)
CASE 3
    OD$(3)=DIRECTORY$(1) : OFILES=FUELNAME$(1,NAMEUSE$(1))+".DAT"
    COMMS=STR$(AMTMIX(1))+">% of "+FUELNAME$(1,NAMEUSE$(1))+".F"
    COMMS=COMMS+STR$(AMTMIX(2))+">% of "+FUELNAME$(2,NAMEUSE$(2))
END SELECT
' Must draw the menu
SCREEN 0 : WIDTH 80
COLOR 15, 0 : CLS
COLOR 10, 1
LOCATE 8, 5 : PRINT CHR$(218);STRING$(99,196);CHR$(191); ' top line
FOR %A=0 TO 17
    LOCATE %A, 5 : PRINT CHR$(179);TAB(75);CHR$(179); ' middle
NEXT %A
LOCATE 18, 5 : PRINT CHR$(192);STRING$(99,196);CHR$(217); ' bottom line
COLOR 10,1
LOCATE 9,20 : PRINT TIMES;
LOCATE 9,51 : PRINT DATES;
COLOR 14,1
LOCATE 11,10 : PRINT "Directory:";
LOCATE 13,10 : PRINT "File Name:";
LOCATE 15,10 : PRINT " Comment:";
COLOR 12, 1
LOCATE 11,22 : PRINT LEFT$(OD$(50);
LOCATE 13,22 : PRINT LEFT$(OFILES$50);
LOCATE 15,22 : PRINT LEFT$(COMMS$50);
' Next are commands
COLOR 3,0
LOCATE 6,22 : PRINT " Output File Information: ";
    
```



```
LOCATE 14.45 : PRINT USING "#####" ;VAL(D5(3,189));      * IBP
LOCATE 14.55 : PRINT USING "#####" ;VAL(D5(3,190));      * 10% BP
LOCATE 14.67 : PRINT USING "#####" ;VAL(D5(3,161));      * 50% BP
LOCATE 16.45 : PRINT USING "#####" ;VAL(D5(3,191));      * 90% BP
LOCATE 16.55 : PRINT USING "#####" ;VAL(D5(3,192));      * END BP
RETURN
```

ClearResults:

This is the subroutine to clear the physical property results.

```
COLOR 15, 1
FOR I%=9 TO 16 STEP 2
LOCATE I%,45 : PRINT SPACES(34);
NEXT I%
RETURN
EndProgram;
```

This is the section to end the program.

```
COLOR 12, 0 : CLS
LOCATE 1, 1
PRINT "FUELPROP :VERSNS:" Terminated....Press any key to continue"
AS=INPUT$(1)
END
```

HardCopy:

This is the subroutine to hardcopy the Physical Properties

```
COLOR 28, 0
LOCATE 24,54 : PRINT "Printing Fuel Data";
LPRINT
LPRINT "Results of Fuel Property Calculation:  *DATES*  *TIMES$
LPRINT *
LPRINT * Component A Fuel Name:  *FUELNAME$(1,NAMEUSE$(1))
LPRINT * Component A Comment: *LEFT$(D5(1,144), 50)
LPRINT * Component B Fuel Name:  *FUELNAME$(2,NAMEUSE$(2))
LPRINT * Component B Comment:  *LEFT$(D5(2,144), 50)
LPRINT *
LPRINT * Average Structural Information.*
LPRINT *
```

```
LOCATE 23.22 : PRINT * Press the <ENTER> to file data. *;
LOCATE 24.22 : PRINT * <Q> to quit, or <F>CHRS(24) *;
PRINT CHRS(23);CHRS(28);> to select;
* Next see what to do.
TEMP%=0 : GOSUB HighlightFileInfo
Startloop$:
AS=INKEY$
SELECT CASE AS
CASE =
* no key
CASE CHR$(13)
* return
GOSUB FileMIData
CASE "q", "Q", CHRS(27)
* quit
GOTO FileResults
CASE CHR$(0) + CHR$(72), CHR$(0) + CHR$(60)
* up-down
TEMP%=1 : GOSUB HighlightFileInfo
IF AS=CHR$(0) + CHR$(72) THEN DECR OPTN%(8) ELSE INCR OPTN%(8)
IF OPTN%(8) < 1 THEN OPTN%(8) = 3
IF OPTN%(8) > 3 THEN OPTN%(8) = 1
TEMP%=0 : GOSUB HighlightFileInfo
CASE CHR$(0) + CHR$(75), CHR$(0) + CHR$(77)
* left right
CASE ELSE
* edit
COLOR 15, 1
LOCATE (OPTN%(8)-1)*2+11, 21 : PRINT SPACES(32);
LOCATE (OPTN%(8)-1)*2+11, 21 : PRINT * *AS;
LINE INPUT TEMP$
SELECT CASE OPTN%(8)
CASE 1 : ODIRS = UCASE$(AS + TEMP$ + 1)
CASE 2 : OFILES = UCASE$(AS + TEMP$)
CASE 3 : COMMS = UCASE$(AS + TEMP$)
END SELECT
TEMP%=0 : GOSUB HighlightFileInfo
END SELECT
GOTO Startloop$
```

This is the subroutine to draw the physical property results

```
GOSUB ClearResults
COLOR 15, 1
LOCATE 6.45 : PRINT USING "#####" ;VAL(D5(3,180));      * Cetane
LOCATE 6.55 : PRINT USING "#####" ;VAL(D5(3,187));      * Cet Index
LOCATE 6.70 : PRINT USING "#####" ;VAL(D5(3,165));      * Density
LOCATE 6.49 : PRINT USING "#####" ;VAL(D5(3,186));      * Sp Gravity
LOCATE 6.53 : PRINT USING "#####" ;VAL(D5(3,182));      * Pour Pt
LOCATE 6.67 : PRINT USING "#####" ;VAL(D5(3,164));      * Flash Pt
LOCATE 10.45 : PRINT USING "#####" ;VAL(D5(3,167));      * Cloud Pt
LOCATE 10.55 : PRINT USING "#####" ;VAL(D5(3,168));      * Viscos
LOCATE 10.87 : PRINT USING "#####" ;VAL(D5(3,192));      * HT Comb
LOCATE 12.45 : PRINT USING "#####" ;VAL(D5(3,169));      * Filter
LOCATE 12.55 : PRINT USING "#####" ;VAL(D5(3,184));      * % Arom
LOCATE 12.68 : PRINT USING "#####" ;VAL(D5(3,193));      * C resid
```

DrawResults:

This is the subroutine to draw the physical property results

```
GOSUB ClearResults
COLOR 15, 1
LOCATE 6.45 : PRINT USING "#####" ;VAL(D5(3,180));      * Cetane
LOCATE 6.55 : PRINT USING "#####" ;VAL(D5(3,187));      * Cet Index
LOCATE 6.70 : PRINT USING "#####" ;VAL(D5(3,165));      * Density
LOCATE 6.49 : PRINT USING "#####" ;VAL(D5(3,186));      * Sp Gravity
LOCATE 6.53 : PRINT USING "#####" ;VAL(D5(3,182));      * Pour Pt
LOCATE 6.67 : PRINT USING "#####" ;VAL(D5(3,164));      * Flash Pt
LOCATE 10.45 : PRINT USING "#####" ;VAL(D5(3,167));      * Cloud Pt
LOCATE 10.55 : PRINT USING "#####" ;VAL(D5(3,168));      * Viscos
LOCATE 10.87 : PRINT USING "#####" ;VAL(D5(3,192));      * HT Comb
LOCATE 12.45 : PRINT USING "#####" ;VAL(D5(3,169));      * Filter
LOCATE 12.55 : PRINT USING "#####" ;VAL(D5(3,184));      * % Arom
LOCATE 12.68 : PRINT USING "#####" ;VAL(D5(3,193));      * C resid
```

```

LPRINT USING TEM015,VAL(D5(3,160)):: LPRINT "± 0.85 Cetane" * Cetane *
LPRINT USING TEM023,VAL(D5(3,187)):: LPRINT "± 1.10 Cetane" * Cet Ind
LPRINT USING TEM035,VAL(D5(3,185)):: LPRINT "± 0.005 kg/L" * Density
LPRINT USING TEM045,VAL(D5(3,166)):: LPRINT "± 0.002 60/60F" * Sp Grav
LPRINT USING TEM055,VAL(D5(3,162)):: LPRINT "± 5.18 °C" * Pour Pt
LPRINT USING TEM065,VAL(D5(3,164)):: LPRINT "± 9.47 °C" * Flash Pt
LPRINT USING TEM075,VAL(D5(3,167)):: LPRINT "± 3.77 °C" * Cloud Pt
LPRINT USING TEM085,VAL(D5(3,166)):: LPRINT "± 0.27 cSt" * Viscos
LPRINT USING TEM095,VAL(D5(3,166)):: LPRINT "± 0.08 MJ/kg" * Ht Comb
LPRINT USING TEM105,VAL(D5(3,166)):: LPRINT "± 19.1" * Filter
LPRINT USING TEM115,VAL(D5(3,164)):: LPRINT "± 1.65 volume %" * Atom
LPRINT USING TEM125,VAL(D5(3,163)):: LPRINT "± 0.29 volume %" * C resid
LPRINT USING TEM135,VAL(D5(3,166)):: LPRINT "± 5.68 °C" * IBP
LPRINT USING TEM145,VAL(D5(3,160)):: LPRINT "± 8.25 °C" * 10% BP
LPRINT USING TEM155,VAL(D5(3,161)):: LPRINT "± 9.91 °C" * 50% BP
LPRINT USING TEM165,VAL(D5(3,161)):: LPRINT "± 18.6 °C" * 80% BP
LPRINT USING TEM175,VAL(D5(3,162)):: LPRINT "± 20.6 °C" * END BP
COLOR 15, 0
LOCATE 24,54 : PRINT SPACES(25);
RETURN

```

ReadFuelParams:

This is the subroutine to read the fuel parameters file.

```

* Will write message to the user.
COLOR 0, 3
LOCATE 10,20 : PRINT CHR$(201),STRINGS(39,205),CHR$(167);
FOR I%=11 TO 13
  LOCATE I%,20 : PRINT CHR$(166),TAB(60),CHR$(166);
NEXT I%
LOCATE 14,20 : PRINT CHR$(200),STRINGS(39,205),CHR$(168);
COLOR 4, 3
LOCATE 12,29 : PRINT "Reading the * : COLOR 14,3 : PRINT "Params File";
OPEN CF$DIRS+"FUELPARM.DAT" FOR RANDOM AS #5 LEN=729
FIELD #5, 25 AS SS, 25 AS I$, 25 AS O$, 25 AS F$, 25 AS T$(1),
25 AS T$(2), 25 AS T$(3), 25 AS T$(4), 25 AS T$(5), 25 AS T$(6),
25 AS T$(7), 25 AS T$(8), 25 AS T$(9), 25 AS T$(10), 25 AS T$(11),
25 AS T$(12), 25 AS T$(13), 25 AS T$(14), 25 AS T$(15), 25 AS T$(16),
25 AS T$(17), 25 AS T$(18), 25 AS T$(19), 25 AS T$(20), 25 AS T$(21),
25 AS T$(22)
FOR I%=1 TO 42
  GET 5,I%
  SLOPEFACTOR(I%)=VAL(SS) : INTOFFFACTOR(I%)=VAL(O$)
  OFFSEIFACTOR(I%)=VAL(O$) : FUNCTION$(I%)=F$
  FOR J%=1 TO 22
    MIXCOEFF(I%,J%)=VAL(T$(J%))
  NEXT J%
NEXT I%
CLOSE #5
RETURN

```

LPRINT *	Mix Component A	Mix Component B	Result
LPRINT *	% Mix Component:
TEM015="	Alkane I%:
TEM023="	Xch3:
TEM035="	Xch2:
TEM045="	Xch:
TEM055="	Monocyclic I%:
TEM065="	Cun:
TEM075="	Cch3:
TEM085="	Cch2:
TEM105="	Cch:
TEM115="	Catz:
TEM125="	Cch2>a:
TEM135="	Dicyclic I%:
TEM145="	Cun:
TEM155="	Cch3:
TEM165="	Cch2:
TEM175="	Cch2>a:
LPRINT USING TEM015,AMTMIX(1);	AMTMIX(2)		
LPRINT USING TEM025,VAL(D5(1,116));	VAL(D5(2,116));	VAL(D5(3,116))	
LPRINT USING TEM035,VAL(D5(1,106));	VAL(D5(2,106));	VAL(D5(3,106))	
LPRINT USING TEM045,VAL(D5(1,108));	VAL(D5(2,108));	VAL(D5(3,108))	
LPRINT USING TEM055,VAL(D5(1,110));	VAL(D5(2,110));	VAL(D5(3,110))	
LPRINT USING TEM065,VAL(D5(1,27));	VAL(D5(2,27));	VAL(D5(3,27))	
LPRINT USING TEM075,VAL(D5(1,3));	VAL(D5(2,3));	VAL(D5(3,3))	
LPRINT USING TEM085,VAL(D5(1,9));	VAL(D5(2,9));	VAL(D5(3,9))	
LPRINT USING TEM095,VAL(D5(1,11));	VAL(D5(2,11));	VAL(D5(3,11))	
LPRINT USING TEM105,VAL(D5(1,13));	VAL(D5(2,13));	VAL(D5(3,13))	
LPRINT USING TEM115,VAL(D5(1,19));	VAL(D5(2,19));	VAL(D5(3,19))	
LPRINT USING TEM125,VAL(D5(1,15));	VAL(D5(2,15));	VAL(D5(3,15))	
LPRINT USING TEM135,VAL(D5(1,52));	VAL(D5(2,52));	VAL(D5(3,52))	
LPRINT USING TEM145,VAL(D5(1,28));	VAL(D5(2,28));	VAL(D5(3,28))	
LPRINT USING TEM155,VAL(D5(1,34));	VAL(D5(2,34));	VAL(D5(3,34))	
LPRINT USING TEM165,VAL(D5(1,36));	VAL(D5(2,36));	VAL(D5(3,36))	
LPRINT USING TEM175,VAL(D5(1,40));	VAL(D5(2,40));	VAL(D5(3,40))	
LPRINT			
LPRINT *	Calculated Physical Properties*		
LPRINT			
TEM015="	Cetane Number
TEM025="	Cetane Index
TEM035="	Density
TEM045="	Specific Gravity
TEM055="	Pour Point
TEM065="	Flash Point
TEM075="	Cloud Point
TEM085="	Viscosity
TEM095="	Heat of Combustion
TEM105="	Filtrability
TEM115="	Percent Aromatics
TEM125="	Residual Carbon
TEM135="	Initial Boiling Point
TEM145="	10% Boiling Point
TEM155="	50% Boiling Point
TEM165="	80% Boiling Point
TEM175="	End Boiling Point

ReadAvgStuFile:

This is the subroutine to get the average structure data.

```

COLOR 31,4
LOCATE 15,24 : PRINT * *** Loading Fuel File *** ;
OPEN DIRECTORY$(MIX%)+FUELNAME$(MIX%,OPTN%(MIX%+2))+".DAT" FOR INPUT AS #1
COUNT%=1
WHILE NOT EOF(1) AND COUNT%<350
  INPUT #1,DS(MIX%,COUNT%)
  INCR COUNT%
WEND
DECR COUNT%
CLOSE #1
COLOR 15,0
LOCATE 15,24 : PRINT SPACES(40);
RETURN

```

FileMixData:

This is the subroutine to file the mixture data.

```

* First print a message to the user.
COLOR 28,0
LOCATE 21,31 : PRINT "Filing Output Data";

* Next set the variables in the output array.
DS(OPTN%(7),144)=COMM$
DS(3,1)=LEFT$(OFILES,8)
DS(3,2)=DATE$
END IF
DS(OPTN%(7),287)="END"

* Next file the data.
OPEN CONIR$+OFILES FOR OUTPUT AS #1
TEMP%=1
WHILE DS(OPTN%(7),TEMP%)<>"END"
  PRINT #1,DS(OPTN%(7),TEMP%)
  INCR TEMP%
WEND
PRINT #1,"END"
CLOSE
COLOR 15,0
LOCATE 21,31 : PRINT SPACES(50);
RETURN

```

LoadNames:

This is a subroutine to load a directory of fuel names.

```

COLOR 31,4
LOCATE 15,24 : PRINT * *** Loading File Names *** ;
FOR I%=1 TO 100
  FUELNAME$(MIX%,I%)=""
NEXT I%
SHELL "DIR "+DIRECTORY$(MIX%)+".DAT" >"+SCRDRIVES+TEMP.ZZZ"
OPEN SCRDRIVES+TEMP.ZZZ FOR INPUT AS #1
TEMP%=1
WHILE NOT EOF(1) AND TEMP%<251
  INPUT #1,TEMP%
  IF MIDS(TEMP%,10,3)=".DAT" THEN
    FUELNAME$(MIX%,TEMP%)=LEFT$(TEMP%,8)
    INCR TEMP%
  END IF
WEND
CLOSE 1
KILL SCRDRIVES+TEMP.ZZZ
COLOR 15,0
LOCATE 15,24 : PRINT SPACES(40);
RETURN

```

DrawMixDataScreen:

This is a subroutine to draw the mixture data.

```

COLOR 15,1
LOCATE 2,13 : PRINT FUELNAME$(1,NAMEUSE%(1));TAB(40);
LOCATE 3,13 : PRINT LEFT$(DS(1,144),20);TAB(40);
LOCATE 23,13 : PRINT FUELNAME$(2,NAMEUSE%(2));TAB(40);
LOCATE 24,13 : PRINT LEFT$(DS(2,144),25);TAB(40);
FOR J%=1 TO 2
  LOCATE 5,(J%-1)*14+16 : PRINT USING "#####"AMTMIX(J%);
  LOCATE 6,(J%-1)*14+16 : PRINT USING "#####"VAL(DS(J%,118));
  LOCATE 7,(J%-1)*14+16 : PRINT USING "#####"VAL(DS(J%,108));
  LOCATE 8,(J%-1)*14+16 : PRINT USING "#####"VAL(DS(J%,108));
  LOCATE 8,(J%-1)*14+16 : PRINT USING "#####"VAL(DS(J%,108));
  LOCATE 8,(J%-1)*14+16 : PRINT USING "#####"VAL(DS(J%,110));
  LOCATE 10,(J%-1)*14+16 : PRINT USING "#####"VAL(DS(J%,27));
  LOCATE 11,(J%-1)*14+16 : PRINT USING "#####"VAL(DS(J%,3));
  LOCATE 12,(J%-1)*14+16 : PRINT USING "#####"VAL(DS(J%,9));
  LOCATE 13,(J%-1)*14+16 : PRINT USING "#####"VAL(DS(J%,11));
  LOCATE 14,(J%-1)*14+16 : PRINT USING "#####"VAL(DS(J%,13));
  LOCATE 15,(J%-1)*14+16 : PRINT USING "#####"VAL(DS(J%,15));
  LOCATE 16,(J%-1)*14+16 : PRINT USING "#####"VAL(DS(J%,15));
  LOCATE 17,(J%-1)*14+16 : PRINT USING "#####"VAL(DS(J%,52));
  LOCATE 18,(J%-1)*14+16 : PRINT USING "#####"VAL(DS(J%,28));

```

```

LOCATE 10,(J%-1)*14+16 : PRINT USING '#####',VAL(D5(J%, 34));
LOCATE 20,(J%-1)*14+16 : PRINT USING '#####',VAL(D5(J%, 36));
LOCATE 21,(J%-1)*14+16 : PRINT USING '#####',VAL(D5(J%, 40));
NEXT J%
RETURN
Highlight:

```

This is a subroutine to highlight the selection.

```

TEMP%=INT(OPTN%(MIX%+2):(PAGE%(MIX%-1)*25)-(1)/3)
LOCATE (OPTN%(MIX%+2):(PAGE%(MIX%-1)*25)-TEMP%*3+(MIX%-1)*15+3,TEMP%*15+3
COLOR 14,1 : PRINT USING '###:OPTN%(MIX%+2);
TEMP% = @-LEN(FUELNAME$(MIX%,OPTN%(MIX%+2))
IF OPTN%(MIX%+2)=NAMEUSE%(MIX%) THEN
COLOR 11,TEMP1%
PRINT ' ',CHR$(16),FUELNAME$(MIX%,OPTN%(MIX%+2)),SPACES(TEMP%);
ELSE
COLOR 12,TEMP1%
PRINT ' ',FUELNAME$(MIX%,OPTN%(MIX%+2)),SPACES(TEMP%);
END IF
RETURN
HighlightMix:

```

This is a subroutine to highlight the selection.

```

COLOR 15,TEMP1%
J%=MIX%
SELECT CASE OPTN%(MIX%+4)
CASE 1
IF MIX%=1 THEN
LOCATE 2,12 : PRINT ' ',FUELNAME$(1,NAMEUSE%(1)),TAB(40);
ELSE
LOCATE 23,12 : PRINT ' ',FUELNAME$(2,NAMEUSE%(2)),TAB(40);
END IF
CASE 2
IF MIX%=1 THEN
LOCATE 3,12 : PRINT ' ',LEFT$(D$(1,144),25),TAB(40);
ELSE
LOCATE 24,12 : PRINT ' ',LEFT$(D$(2,144),25),TAB(40);
END IF
CASE 3 : LOCATE 5,(J%-1)*14+15 :PRINT USING '#####',AMTMIX(J%);
CASE 4 : LOCATE 6,(J%-1)*14+15 :PRINT USING '#####',VAL(D5(J%,116));
CASE 5 : LOCATE 7,(J%-1)*14+15 :PRINT USING '#####',VAL(D5(J%,108));
CASE 6 : LOCATE 8,(J%-1)*14+15 :PRINT USING '#####',VAL(D5(J%,108));
CASE 7 : LOCATE 9,(J%-1)*14+15 :PRINT USING '#####',VAL(D5(J%,110));
CASE 8 : LOCATE 10,(J%-1)*14+15 :PRINT USING '#####',VAL(D5(J%,27));
CASE 9 : LOCATE 11,(J%-1)*14+15 :PRINT USING '#####',VAL(D5(J%, 3));

```

```

CASE 10 :LOCATE 12,(J%-1)*14+15 :PRINT USING '#####',VAL(D5(J%, 8));
CASE 11 :LOCATE 13,(J%-1)*14+15 :PRINT USING '#####',VAL(D5(J%, 11));
CASE 12 :LOCATE 14,(J%-1)*14+15 :PRINT USING '#####',VAL(D5(J%, 13));
CASE 13 :LOCATE 15,(J%-1)*14+15 :PRINT USING '#####',VAL(D5(J%, 18));
CASE 14 :LOCATE 16,(J%-1)*14+15 :PRINT USING '#####',VAL(D5(J%, 19));
CASE 15 :LOCATE 17,(J%-1)*14+15 :PRINT USING '#####',VAL(D5(J%, 52));
CASE 16 :LOCATE 18,(J%-1)*14+15 :PRINT USING '#####',VAL(D5(J%, 26));
CASE 17 :LOCATE 19,(J%-1)*14+15 :PRINT USING '#####',VAL(D5(J%, 34));
CASE 18 :LOCATE 20,(J%-1)*14+15 :PRINT USING '#####',VAL(D5(J%, 36));
CASE 19 :LOCATE 21,(J%-1)*14+15 :PRINT USING '#####',VAL(D5(J%, 40));
END SELECT
RETURN
HighlightFileInfo:

```

This is the subroutine to highlight the file information.

```

COLOR 12,TEMP1%
LOCATE (OPTN%(8)-1)*2+11, 21
SELECT CASE OPTN%(8)
CASE 1 : PRINT ' ',LEFT$(OOIRS,50),TAB(73);
CASE 2 : PRINT ' ',LEFT$(OFILES,50),TAB(73);
CASE 3 : PRINT ' ',LEFT$(COMMS,50),TAB(73);
END SELECT
RETURN
EraseMixData:

```

This is a subroutine to locate a mix data file for editing.

```

COLOR 15,TEMP1%
SELECT CASE OPTN%(MIX%+4)
CASE 1 : IF MIX%=1 THEN LOCATE 2,12 ELSE LOCATE 23,12
CASE 2 : IF MIX%=1 THEN LOCATE 3,12 ELSE LOCATE 24,12
CASE 3 : LOCATE 5,(MIX%-1)*14+15
CASE 4 : LOCATE 6,(MIX%-1)*14+15 : TEMP%=110
CASE 5 : LOCATE 7,(MIX%-1)*14+15 : TEMP%=108
CASE 6 : LOCATE 8,(MIX%-1)*14+15 : TEMP%=108
CASE 7 : LOCATE 9,(MIX%-1)*14+15 : TEMP%=110
CASE 8 : LOCATE 10,(MIX%-1)*14+15 : TEMP%=27
CASE 9 : LOCATE 11,(MIX%-1)*14+15 : TEMP%= 3
CASE 10 : LOCATE 12,(MIX%-1)*14+15 : TEMP%= 9
CASE 11 : LOCATE 13,(MIX%-1)*14+15 : TEMP%= 11
CASE 12 : LOCATE 14,(MIX%-1)*14+15 : TEMP%= 13
CASE 13 : LOCATE 15,(MIX%-1)*14+15 : TEMP%= 18
CASE 14 : LOCATE 16,(MIX%-1)*14+15 : TEMP%= 15
CASE 15 : LOCATE 17,(MIX%-1)*14+15 : TEMP%= 52
CASE 16 : LOCATE 18,(MIX%-1)*14+15 : TEMP%= 28
CASE 17 : LOCATE 19,(MIX%-1)*14+15 : TEMP%= 34

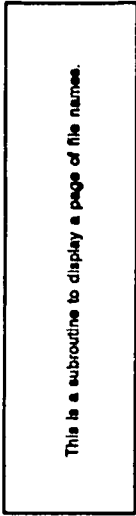
```

```

CASE 18 : LOCATE 20,(MIX%-1)*14+15 : TEMP%= 36
CASE 19 : LOCATE 21,(MIX%-1)*14+15 : TEMP%= 40
END SELECT
RETURN

```

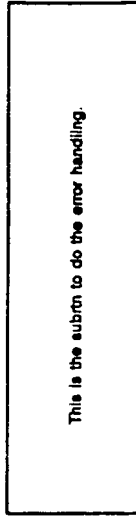
PageOfNames:



```

FOR I%= (PAGE%(MIX%-1)*25+1 TO PAGE%(MIX%)*25
TEMP%=INT((I%-(PAGE%(MIX%-1)*25)-1)/5)
LOCATE I%-(PAGE%(MIX%-1)*25)-TEMP%*5+(MIX%-1)*15+3,TEMP%*15+3
COLOR 14,1 : PRINT USING "###.###":I%
TEMP%=10-LEN(FUELNAMES(MIX%,I%))
IF I%=NAMEUSE%(MIX%,I%) THEN
COLOR 11,1
PRINT "":CHR$(16);FUELNAMES(MIX%,I%);SPACES(TEMP%);
ELSE
COLOR 12,1
PRINT "":FUELNAMES(MIX%,I%);SPACES(TEMP%);
END IF
NEXT I%
RETURN

```



ErrorMessage:

```

SCREEN 0 : COLOR 15,0 : CLS
COLOR 0,4
LOCATE 8,5 : PRINT CHR$(201);STRINGS(66,205);CHR$(167);
FOR I%=9 TO 15
LOCATE I%,5 : PRINT CHR$(166);TAB(75);CHR$(166);
NEXT I%
LOCATE 16,5 : PRINT CHR$(200);STRINGS(66,205);CHR$(168);
COLOR 31,4
LOCATE 11,28 : PRINT USING ">>> Error ### encountered <<<";ERR;
COLOR 14,4
TEMP%="See Appendix E, p. 412, in Turbo Basic Manual for full message."
LOCATE 13,9 : PRINT TEMP%;
COLOR 0,3
LOCATE 24,19 : PRINT " Press any key to return to the Main Menu ";
TEMP%="INPUT$(1)";
CLOSE
GOTO MainMenu

```

T-T-T:That's all folks!!!!

**The vita has been removed from
the scanned document**