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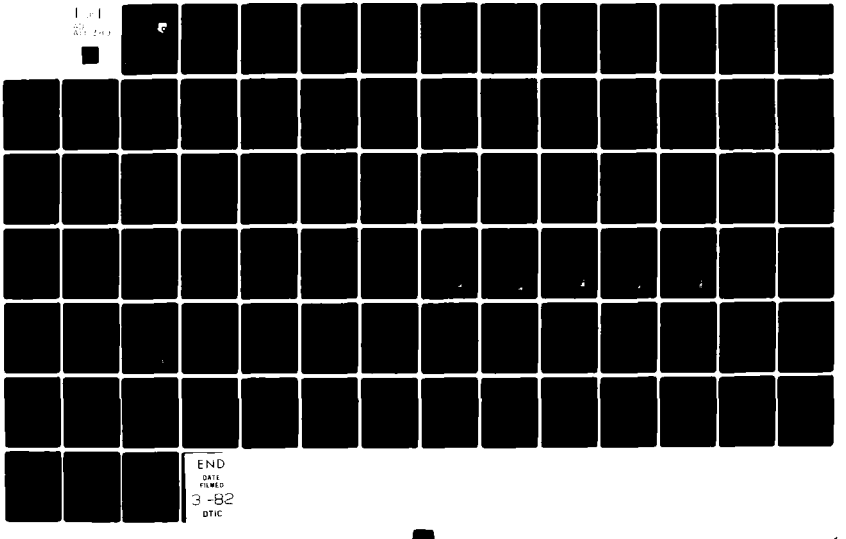

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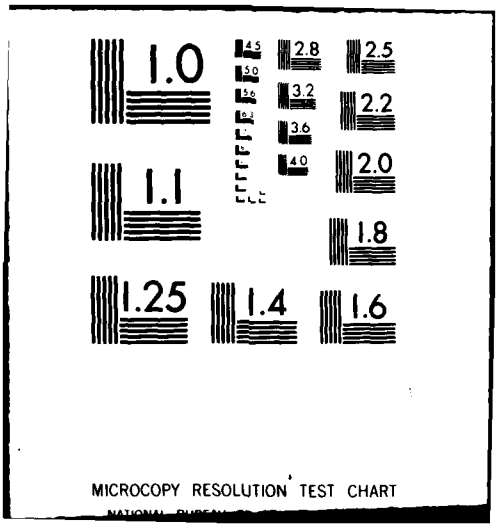
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KOVATS INDICES AS A TOOL IN CHARACTERIZING HYDROCARBON FUELS IN TEMPERATURE PROGRAMMED GLASS CAPILLARY GAS CHROMATOGRAPHY

PART 1. QUALITATIVE IDENTIFICATION

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Edward W. Pitzer

Fuels and Lubrication Division
Fuels Branch

November 1981

Final Report for Period December 1979 - September 1980

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This technical report has been reviewed and is approved for publication.

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) Kovats Indices are used as a tool to identify the major components of several aircraft jet fuels of the JP-4 type. Glass capillary gas chromatography in the temperature programmed mode was the technique of choice. The first phase of the effort involved optimization of the capillary system for the maximum resolution between a selected pair of normal hydrocarbons in an acceptable analysis time. Peak resolution was investigated as a function of carrier capillary pressure, temperature programming rate, and initial column temperature. Eleven qualitatively known and quantitatively accurate calibration solutions were	

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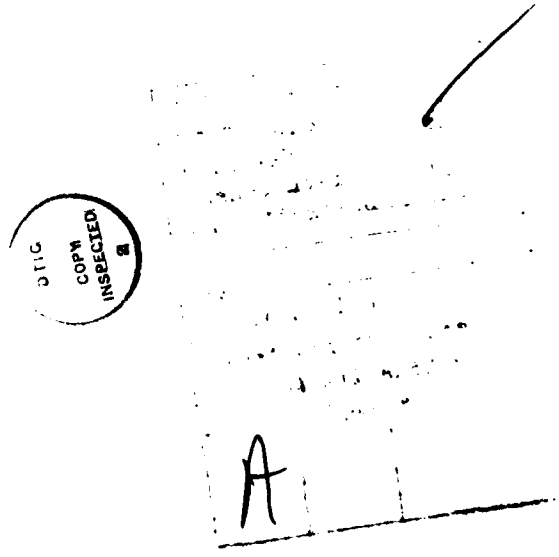
prepared to include over 200 different hydrocarbons. Kovats Indices were generated for these solutions in a statistically reliable fashion on two capillary columns of different polarities. Thus, each hydrocarbon standard had its own unique set of two Kovats Indices. Several petroleum, as well as shale derived, JP-4 samples were subsequently chromatographed on the same two capillary columns. Peaks were given tentative identification by matching of Kovats Indices.

B

FOREWORD

This technical report describes work performed under the In-House Work Unit 30480591 administered by the Fuels Branch (POSF), Fuels and Lubrication Division (POS), Air Force Wright Aeronautical Laboratories, Aero Propulsion Laboratory (AFWAL/PO). Project scientists and co-authors of this investigation were Mr. Paul C. Hayes, Jr. (AFWAL/POSF) and Mr. Edward W. Pitzer (AFWAL/POFF). A substantial contribution was provided by Stephan M. Wolanczyk a student aid, who prepared all the mini-blends, calibration standards, and fuel samples as well as calculated Kovats Indices. Valuable assistance was also given by Ms Elizabeth Tate and Dwayne Burns, also student aids, in calculating indices for the unknown fuel samples. Ms Lynne Schoen also made a substantial contribution in reducing and tabulating data for the final results of this report. Mr. Curtis R. Reeves (AFWAL/POSF), with the help of Ms Tate and Mr. Burns, developed a computer program that greatly facilitated data reduction. Particular gratitude is extended to Mr. Wayne R. Ruby, a chromatographer with the University of Dayton Research Institute, Dayton, Ohio. His stimulating lectures and guidance in avoiding experimental pitfalls were greatly appreciated.



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LIST OF ABBREVIATIONS

ABBREVIATION/SYMBOL	DEFINITION
$(GC)^2$	Glass Capillary Gas Chromatography
t_R	Component's absolute retention time
$t_R{}^1$	Component's corrected retention time (absolute t_R minus t_R of methane)
w_h	Peak width at half height
R	Resolution between two peaks
n^1	Capillary Column's number of effective theoretical plates
I_{PT}^{OV-101}	Retention Index on OV-101 Capillary Column under Conditions of linear temperature programming
I_{PT}^{OV-17}	Retention Index on OV-17 Capillary Column under Conditions of linear temperature programming
m	meters
mm	millimeters
ml	milliliters
µl	microliters
JP-4	Jet propulsion fuel, wide-distillate cut, conforming to MIL-T-5624L

SECTION I

INTRODUCTION

1. THE NEED FOR FUELS CHARACTERIZATIONS

Commercial hydrocarbon products such as gasoline, kerosene, and jet fuels are deceptively simple in appearance but are actually a blend of literally thousands of individual hydrocarbons. Though produced in incomprehensible millions of gallons per year, the total chemical analysis of these familiar products, i.e., the complete qualitative identification and quantitative determination of their constituents, is still elusive to the analytical chemist. Knowledge of the chemistry of these products, however, can yield an immense wealth of practical information. Bulk properties and characteristics such as a combustion behavior, storage stability, ignitability, toxicological effects, as well as physical and generalized chemical properties can all be predicted from a thorough chemical breakdown of a fuel's hydrocarbon composition.

Unfortunately, this Herculean task of detailing the myriad of hydrocarbon components in these products is unassailable by any single, though sophisticated, state-of-the-art analytical technique. What is required is a judicious meshing of highly advanced chromatographic and spectroscopic techniques applied in a sequential mode of attack. This approach is not an original idea. Dr Ronald D. Butler (AFWAL/POSF) has outlined "a unified system for the detailed analysis of aircraft fuels, both conventional and experimental, without regard to their type or complexity" in a research prospectus of February 1980 (Reference 1). His analytical scheme consists of five distinct steps that include a fuel fractionation procedure followed by high resolution glass capillary gas chromatographic analysis and proton and carbon-13 Fourier Transform NMR of the individual fractions.

Petroleum and shale-derived jet fuels are too complex to be unraveled in a single pass by even the most efficient gas chromatographic technique. However, multi-dimensional gas chromatography which heart-cuts desired

segments of the total hydrocarbon profile and diverts this fraction automatically from one capillary column to another having greater selectivity appears very promising. Unfortunately, few preparative scale work-ups from multi-dimensional cuts for subsequent analyses by NMR, IR, etc. have been published.

The purpose of the experimental study described in this report was to establish an optimization procedure and generate statistically reliable and chromatographically sound libraries of qualitative information on a large variety of pure reference hydrocarbons. Libraries containing what are known as Kovats Indices can be used to assign, with high probability, tentative identifications of the major components in JP-4 aircraft fuel. Furthermore, the indices can provide an authoritative judgement as to the integrity of separated fractions from any proposed preparative method of fractionating hydrocarbon fuels.

2. GLASS CAPILLARY GAS CHROMATOGRAPHY AS A SEPARATION TOOL

Glass capillary gas chromatography $(GC)^2$ represents a new era in chromatographic separation techniques. $(GC)^2$ is expected to become the most commonly used method of doing gas chromatography in the near future. The technique is only now becoming reliable, reproducible, accurate, and amenable to routine use in analytical laboratories. Special techniques, injectors, detectors, accessories and instrumentation are now commercially available. Furthermore, the literature abounds with papers demonstrating the proven capabilities of the technique, particularly in the petrochemical field. In chromatography, the resolving power of the glass capillary column set it as a cornerstone for the ultimate prediction of the physical and chemical properties of hydrocarbon fuels from a detailed analysis of their individual components and the application of the appropriate physical chemical equations. The first phase of this effort was the set-up and optimization of the $(GC)^2$ system. Optimization would be realized with the maximum resolution between a selected pair of normal hydrocarbons in an acceptably short analysis time. Such optimization would ensure good

resolution of other hydrocarbons throughout the fuel's $(GC)^2$ profile and provide well-defined and repeatable Kovats Indices.

As stated above, the analytical method of choice was high resolution capillary gas chromatography. A short digression into the meaning and emergence of this technique to the forefront of analytical chemistry is warranted.

Even before Tswett discovered and developed chromatography in 1903, techniques had already been utilized to analyze crude petroleum samples. Shortly before the turn of the century, David Talbot Day, Chief of the Division of Mineral Resources of the American Geological Survey, applied the process of filtration to separate Pennsylvania petroleum. His experiments demonstrated that crude oil forced upward through a column of powdered limestone was changed in color and composition (Reference 2). Spanning the 75 years since these humble beginnings, chromatography has established itself as a valuable tool: in routine analyses to control refining operations, in research separation, and in analytical research.

A particular mode of chromatography, i.e., glass capillary gas chromatography has distinct advantages as applied to the petrochemical industry. These advantages are speed of analysis, resolution of complex samples into individual components, sensitivity for trace analysis on very small sample volumes, and versatility to glean both qualitative and quantitative information from a wide variety of mixtures. In general, gas chromatography is the physical means of separating a sample into its individual components via distribution of the sample between two phases; a stationary phase (i.e., column's liquid coating) and a mobile phase (i.e., carrier gas). The process requires that the sample be sufficiently volatile to be carried through the column (Reference 3). Due to the wide boiling character of conventional hydrocarbon fuels and fuel blends, temperature programming of the column is necessary, i.e., the linear increase of column temperature with time. Using the proper programming

rate, components that elute or emerge early from the column can be well resolved and later emerging peaks made to be sharp and uniformly distributed throughout the chromatogram. When the stationary phase is nonpolar, sample components are separated according to their relative volatility, akin to, but not strictly following, their atmospheric boiling point order. Wall coated open tubular columns, i.e., glass capillary columns, have a thin film of liquid phase deposited on the inner surface of the glass. The film thickness usually varies from 0.2 micron to 0.7 micron depending on the column type. The technique of producing a high efficiency column involves a number of carefully controlled processes including treatment of the glass and the liquid phase. For most phases, the inner wall of the glass capillary is roughened to provide good mechanical stability for the liquid phase allowing use of the column up to high temperatures and giving it a long and useful lifetime. This chemical roughening enables films up to 0.4 micron to be formed in small bore columns and films up to 0.7 micron in wide bore capillary columns.

Glass capillary columns represent a new technology and expanded capabilities for gas chromatographic separations. The efficiency of an exceptionally well-packed conventional 1/8" stainless steel column may be the same as for a well-coated glass capillary column used in this study in terms of the number of effective theoretical plates per meter. However, because the pressure drop across the capillary column is so low, a much longer capillary column can be utilized. Consequently, the total number of theoretical plates in the capillary column may be a factor of 10 to even 100 greater than in conventional 1/8" packed columns (Reference 4). Resolving power is proportional to the total number of column plates. This project takes advantage of the vastly increased number of plates available in glass capillary gas chromatography. Recent advances in capillary column preparation have enabled the transfer of $(GC)^2$ from research to routine analysis, particularly in the petrochemical field. Such complex mixtures as gasoline, naphtha, reformate, and similar products require a high resolution column to separate, tentatively

identify, and quantitate individual components via retention data. Essentially what has made $(GC)^2$ a practical technique are (Reference 5):

a. commerical availability of both polar and nonpolar capillary columns with guaranteed efficiencies;

b. chemically inert and thermally stable capillary columns and stationary phases;

c. low dead volume detectors, accessories, and instrumentation that preserves the resolution and efficiency of these columns:

d. more and more capillary chromatography applications appearing in the literature.

With the significant improved resolution available with glass capillary columns, retention time data can be of greater qualitative value with increased reliability. However, a distinction should be made as to the nature of that retention data. The absolute retention time of a particular component or peak is the time from the point of injection to the peak maximum as displayed on the recorder or logged by an integrator. The same peak on the same column under the same conditions will always have the same retention time. However, slight deviations of any of the operating conditions, or for that matter, the quality or state of the column, can change this absolute retention time. Retention times relative to closely eluting reference hydrocarbons, i.e., Kovats Indices, are far more reliable and repeatable from day to day. Whatever alters the retention time of the reference components will also affect the nearby components in a similar manner.

3. THE KOVATS RETENTION INDEX AS AN IDENTIFICATION TOOL

As early as 1952, James and Martin disclosed in their historic and fundamental paper on gas chromatography that both the retention volume and the retention time of a compound are characteristic values for its identification (Reference 6). Since the main purpose of any

chromatographic system is to resolve mixtures of compounds into less complex mixtures or ultimately into pure compounds, it follows that a properly optimized and controlled system can provide retention data which can serve as complementary information for the positive identification of resolved components. It is generally accepted practice that excellent retention data correlation between an unknown and a selected reference compound on two columns of different polarity is sufficient for positive identification of the unknown, although additional spectometric evidence lends weight to the argument (Reference 7). For practical application, only systems based on "relative retention" data are useful. To obtain relative retention data, the retention behavior of a component is compared with that of one or more standard compounds. The retention parameters of both standards and the unknown are measured under identical conditions. Ideally, the reference standards are actually contained in the sample of interest.

The Retention Index system introduced by Kovats is one of the most widely accepted methods of reporting data (Reference 8). Retention is determined relative to a series of homologous n-hydrocarbons. The Kovats system has proven so useful that the Discussion Group of the Institute of Petroleum has recommended its use in the standardization of retention data (Reference 9).

In Kovats' System, under conditions of linear temperature programming, an approximately linear relationship exists between n-alkane carbon number and retention of an unknown compound of interest (Reference 7):

$$I_{PT}^{OV\text{-}101} = 100 \left[\frac{t_{R(unknown)} - t_{R(C_z)}}{t_{R(C_z+1)} - t_{R(C_z)}} \right] + 100\,z$$

where: a) $I_{PT}^{OV\text{-}101}$ is the retention index of the unknown compound as determined on OV-101 stationary phase under conditions of linear

temperature programming, b) ^{t}R(unknown) is the absolute retention time of the unknown compound, c) $^{t}R(C_z)$ is the absolute retention time for the normal alkane that elutes prior to the unknown, d) $^{t}R(C_z+1)$ is the absolute retention time for the normal alkane that elutes just after the unknown, and e) z is the number of carbon atoms in the n-alkane standard that elutes just prior to the substance of interest. This Kovats' Index unit is characteristically determined by the type of stationary phase liquid and the molecular structure of the component of interest. However, several homologous series of organic compounds can be used as standards, even though originally n-paraffins were used exclusively. Alternate homologous series of standards enables the use of detectors which are not sensitive to hydrocarbons, e.g., n-alkyltrichloroacetates with an electron capture detector or n-alkylbenzenes for an ultraviolet detector (Reference 10).

Unfortunately, the real accuracy or reliability of published Kovats' Data is sometimes quite poor. Several sources of significant error are responsible for this. It was considered crucial to determine how each of these errors could influence the measured data. The principal sources of error in retention index measurement (on capillary columns) include the influence of unstable carrier gas flow and temperature control, inaccurate measurements of retention, too large a sample size, incomplete peak separation, and impure stationary phase. As will be detailed in Section II, Part 1, "System Description," the microprocessor controlled instrument that produced the data for this report demonstrated excellent retention time repeatability, thus eliminating concern for possible drifts in carrier gas flow and temperature programming rate. The computing integrator that controlled the $(GC)^2$ system also could measure the retention times of peaks as sharp as one second peak width, i.e., capillary column peaks, with excellent repeatability. Overloading of columns, expecially in the case of capillary columns with their low capacity, had to be avoided. Overloading causes typical "leading" peak shapes, and the measurement of retention times via peak maxima can lead to incorrect index

values. Symmetrical peaks can be obtained by lowering the sample load. Schomburg defined the "linear dynamic range of precise index determination" as the range limited by the smallest sample the detector can see (usually taken as twice the noise level) and the maximum sample load which does not give asymmetric peaks (Reference 11). To this end, solutions of standards and solutions of fuels were diluted nearly 100:1 in a relatively noninterfering solvent (CS_2) to limit the amount of the most predominant hydrocarbon species to less than 10 nanograms each. It has been pointed out that for identification using Kovats Indices at high precision, open tubular columns of high resolution with effective theoretical plates of at least 50,000 should be used (Reference 12). For this experimental study, the columns exhibited nearly five times this number of plates. At optimum resolution, good capillary columns will completely separate two substances with an index unit difference of about one unit.

On capillary columns the largest errors in retention index reproducibility are due to impure stationary phase. In the calculation of retention indices it is assumed that the retention times of semi-polar substances are related only to the retaining of the sample molecules in a particular kind of stationary phase. This is true if that stationary phase is pure. However, if the phase is contaminated with even a trace amount of a polar species, the retention times of not only the n-paraffins but the semi-polar compounds of interest will also change, and the retention indices determined will be altered. Since this laboratory does not at present fabricate and coat its own capillary columns, a commercial manufacturer of glass capillary columns with a demonstrated record of producing high quality, i.e., high efficiency, inert columns of a purified stationary phase, was used as a source. Test chromatograms showed very little tailing for such compounds as pentanone, octanol, and 2,6-dimethyl-aniline. This substantiated the success of their glass surface deactivation procedure. In these ways, the experimental study documented herein attempted to avoid the common pitfalls that plague those attempting the generation of reliable retention index libraries.

The method of applying the Kovats Indices used in this report is to identify substances by matching their indices as determined on two capillary columns of different polarity against two corresponding libraries of over 200 standard hydrocarbons each. An identification window was established for each standard hydrocarbon on each polarity column and applied to suspect peaks in unknown fuel samples. Of course, all such qualitative judgements on compound identity were tentative and will later be checked by gas chromatography-mass spectrometry. It was also feasible to predict the identity of major hydrocarbon fuel components that had not been included in the standards. The plots of retention indices versus carbon numbers of different homologous groups in Section IV, Part 2, e.g., 2-methyl alkanes, n-alkyl benzene, 1-olefins, etc. display a high degree of correlation. These assignments can be considered entirely reasonable, but acquisition of the pure standard is always the final confirming route.

The next section outlines the experimental system, the quality of the columns, and the operating conditions used in this study.

SECTION II

EXPERIMENTAL APPROACH

1. SYSTEM DESCRIPTION

The basic analytical instrumentation utilized in this study was the Varian Model 3700 Capillary Gas Chromatograph equipped with dual flame ionization detectors. The chromatograph was factory-modified to accept glass capillary columns, and also fitted with a Varian Model 8000 Automatic Liquid Sampler. A Varian Model CDS-111 Computer Integrator controlled the automatic liquid sampler, the temperature programming, and the data collection and continuously monitored the system parameters.

The Varian chromatograph was equipped with a Varian 1070 all glass injection and detection system with dead volumes eliminated or reduced to a practical minimum by design and/or carrier purging. The system provided a choice of sampling-injection modes of which the normal split mode was used in this project. The capillary pneumatics was a pressure regulated system, with all the active components thermostatted to better than +/-1°C for maximum retention time repeatability and detector baseline stability. The injector-splitter featured a true positive septum purge which effectively eliminated septum bleed (Reference 13). Other undesirable organic impurities can originate from the gas supply or from back-diffused sample. Delayed release of these impurities can disrupt the output baseline and introduce ghost peaks, particularly in temperature programmed analyses. Air, as well as moisture in the carrier gas, can appreciably decrease column lifetime. Capillary columns are far more sensitive than conventional packed columns to a given oxygen content of the carrier since they contain far less stationary phase and since a slight alteration of phase chemistry can produce observable changes in column characteristics at a much earlier stage of column demise.

To avoid potential contamination problems, ultra-high purity helium (99.999) was used as the carrier gas. The helium was passed through a Hydrox Purifier, Model 8301, Matheson Gas Products, to remove residual oxygen and/or water vapor present to less than 0.1 parts per million each. The pressure regulator is an essential part of every gas chromatograph equipped with capillary columns since the entire flow system is pressure controlled. All regulators contain an elastic diaphragm which separates the controlled gas from the ambient air. The permeation of air and moisture and organic contamination, i.e., back-diffusion, through an elastic membrane such as rubber, was eliminated by the use of metallic diaphragms. Such diffusion-free regulators can permit a drastic increase in lifetime and upper temperature limit with many capillary stationary phases (Reference 14).

2. FINALIZED OPERATING CONDITIONS

The glass capillary columns used in this work were manufactured by Quadrex, Incorporated. Two columns of different polarity were used; their specifications are included in Table 1.

TABLE 1

$(GC)^2$ COLUMN SPECIFICATIONS

Column Characteristic	Non-Polar	Polar
Stationary Phase	OV-101	OV-17
Column Length	108 m	117 m
Internal Diameter	0.25 mm	0.25 mm
Effective Theoretical Plates	226,000	226,000
Film Thickness	0.2 micron	0.2 micron

The column efficiency was measured on each column prior to use. A 0.1% solution of tridecane in carbon disulfide was used to make the measurement. The solution was run under the same conditions used by the manufacturer to specify the column's efficiencies.

A typical calculation of efficiency on the 108m OV-101 column, operated isothermally at 120°C and an inlet pressure of 45 psig, yielded 225,000 effective theoretical plates. The manufacturer's specification for that column was 226,000 effective theoretical plates. The equation used for calculating the column's effective theoretical plates (n') was:

$$n' = 5.545 \left[\frac{(t_r')}{w_h}\right]^2$$

where: a) t_r' = the adjusted retention time of n-C_{13}, i.e., its absolute retention time minus the column dead volume time (for unretained normal methane);

b) w_h = peak width at half height

The linear gas velocity (cm/sec) is the time taken for an unretained component to move through the column at the initial temperature of the run. Methane is usually selected as the least retained compound. Optimum flow rates can be set for a column by measuring the linear velocity or the actual column outlet flow rate as determined with a bubble meter. For the kinds of columns employed in this study, typical rates should fall within values listed in Table 2.

TABLE 2

THEORETICAL OPTIMUM FLOW RATES FOR $(GC)^2$ COLUMNS USED IN THIS STUDY

Optimum Flow Rates	Wall Coated Open Tubular Column (0.25 mm I.D.)
ml/min (H_2 or He)	0.6 - 1.0
cm/sec	25 - 35

The final, optimized $(GC)^2$ operating parameters for injection, detection, carrier flow, etc., for this study are as listed in Table 3.

TABLE 3

OPTIMIZED $(GC)^2$ RUN PARAMETERS

$(GC)^2$ PARAMETERS	OV-101	OV-17
Initial Temp. (^oC)	35	35
Program Rate (^oC/min)	1	1
Final Temp. (^oC)	200	200
Injector Temp. (^oC)	300	300
Detector Temp. (^oC)	300	300
Capillary Press. (psig)	48	54
CH_4 Ret. Time (min)	6.225	7.690
Linear Velocity (cm/sec)	29.18	25.38
Split Ratio	50:1	50:1
Septum Purge Flow (ml/min)	25	25
Make-Up Flow (ml/min)	30	30
Hydrogen Flow (ml/min)	30	30
Air Flow (ml/min)	300	300
Electrometer Range (amps/millivolt)	10^{-12}	10^{-12}

SECTION III

GENERAL METHODOLOGY FOR KOVATS LIBRARY GENERATION

1. $(GC)^2$ OPTIMIZATION CRITERION

In the qualitative analysis of a complex mixture of individual components, the positive identification of the peaks emerging from a column is very difficult. There are two primary obstacles to identification: 1) the peaks represent only nano- or pico-grams of material, and 2) chromatographic retention times, be they absolute or relative, are not unique. It is possible for two compounds to have identical, if not very close, retention times; hence the need for the maximum resolution possible from a chromatographic system. To reiterate, retention time is not sufficient to positively identify particular peaks, since the data is characteristic, but not definitive.

The use of high resolution glass capillary columns for the most probable assignment of hydrocarbons in a complex mixture, requires the components of a gas chromatographic system, i.e., the oven, inlet, detector, pneumatics, and integrator to be stable and re-setable. Given the unprecedented resolving power of capillary columns and the state-of-the-art microprocessor controlled $(GC)^2$ systems, retention time reliability can be excellent and subsequent peak assignments given a high probability of accuracy.

Resolution was the fundamental yardstick used in this report to evaluate system optimization for the eventual separation of as many fuel hydrocarbon components as possible. Simply, resolution is the quantitative measure of the separation between two peaks. The term resolution shall be here defined as the difference in the absolute retention times of any two peaks divided by the average of their peak widths, i.e.,

$$R = \frac{2\,(t_{r1} - t_{r2})}{1.7\,(w_{h1} + w_{h2})}$$

where:

a) R = resolution between peak #1 and peak #2

b) t_{r1} = absolute retention time of peak #1

t_{r2} = absolute retention time of peak #2

c) w_{h1} = peak width at half height for peak #1

w_{h2} = peak width at half height for peak #2

d) all measurements in the same unit, i.e. time or millimeters.

For reference, an "R" value of 1.5 or greater means baseline separation between two peaks.

The optimum carrier gas pressure, temperature programming rate, and initial column temperature should give the best compromise of high resolution between two hydrocarbon components and an acceptably short analysis time. The central portion of the distillation range of a typical JP-8 fuel, i.e., middle of its $(GC)^2$ profile, has historically displayed the poorest baseline resolution. A pair of normal hydrocarbons was selected whose retention times fell in the middle of the raised section of that JP-8 profile. It was theorized that the maximum resolution between the hydrocarbons could ensure the best resolution of interlying peaks in the profile. The hydrocarbon pair chosen was normal C-11 and normal C-12 with literature boiling points (atmospheric) of 195.890°C and 216.278°C, respectively.

2. OPTIMIZATION EXPERIMENTS

Optimum resolution conditions were determined on a 108 m OV-101 column by observing the change in calculated resolution under varying conditions of initial temperature, program rate, and capillary pressure.

The resolution runs were made under the following constant conditions:

Injector Temp. = 280°C	Make-Up Flow = 30 ml/min
Detector Temp. = 300°C	Split Ratio = 1:200
Air Flow = 300 ml/min	Attenuation = 16 X 10^{-12}
H_2 Flow = 30 ml/min	Chart Speed = 10 cm/min

A solution of .1% by volume undecane and dodecane in high purity hexanes was used to make the resolution determinations. The resulting calculations in Table 4 indicate that for a constant initial temperature and program rate, resolution increased as capillary pressure increased to an upper limit. That limit was noted on the increase in pressure from 48 psig to 60 psig possibly due to exceeding the optimum flow characteristics of helium on this column at 60 psig. Therefore, 48 psig was chosen as the optimum pressure for maximum efficiency in separating the hydrocarbon pair. Table 4 also indicates that for a constant initial temperature and capillary pressure, resolution increased as program rate decreased. Although a higher resolution was obtained at 0.2°C/min, in order to prevent excessively long sample times, 0.5°C/min was chosen as the optimum program rate.

Additional resolution was gained by lowering the initial temperature from 75°C to 50°C. It was concluded that the optimum resolution conditions for the 108 m OV-101 column were an initial temperature of 50°C, a program rate of 0.5°C/min and a capillary pressure of 48 psig.

Next, numerous samples of JP-4, JP-4 in CS_2 (10% by volume), n-alkanes in CS_2 (1% by volume), and n-alkanes in CS_2 (0.1% by volume) were run under the previously determined optimum resolution conditions. It was noted at this time that the diluted JP-4 and the 0.1% n-alkane samples yielded the most Gaussian peak shapes. The initial temperature was lowered from 50°C to 35°C to facilitate better separation of the early eluting peaks

TABLE 4

RESOLUTION AS A FUNCTION OF INITIAL $(GC)^2$ COLUMN TEMPERATURE, PROGRAMMING RATE, AND CAPILLARY INLET PRESSURE

Run #	Date	Init. Col. Temp. (Deg.-C)	Program Rate (Deg.-C/min)	Column Inlet Press. (psig)	Distance Between Peak Apexes (cm)	W_{h1} (cm)	W_{h2} (cm)	Resolution "R"
1	2/29	75	2.0	60	63.1	0.55	0.60	64.55
2	2/29	75	2.0	60	63.0	0.55	0.60	64.55
3	2/29	75	2.0	60	63.1	0.55	0.60	64.55
4	2/29	75	2.0	48	65.5	0.50	0.55	73.39
5	2/29	75	2.0	48	65.5	0.50	0.55	73.39
6	2/29	75	2.0	48	65.5	0.50	0.55	73.39
7	3/3	75	2.0	36	68.5	0.65	0.68	60.59
8	3/3	75	2.0	36	68.5	0.65	0.68	60.59
9	3/3	75	2.0	36	68.5	0.65	0.68	60.59
10	3/3	75	2.0	24	72.8	1.00	1.00	42.82
11	3/3	75	2.0	24	72.9	1.00	1.00	42.88
12	3/3	75	2.0	24	73.0	1.00	1.00	42.94
13	3/4	75	2.0	12	82.0	3.10	3.15	15.44
14	3/4	75	2.0	12	82.8	3.10	3.20	15.46
15	3/4	75	2.0	12	82.7	3.20	3.40	14.74
16	3/4	75	1.0	48	112.7	0.80	0.95	75.76
17	3/4	75	1.0	48	112.6	0.80	0.90	77.92
18	3/4	75	1.0	48	112.5	0.80	0.90	77.85
19	3/4	75	0.5	48	180.0	1.10	1.45	83.04
20	3/5	75	0.5	48	180.8	1.10	1.50	81.81
21	3/5	75	0.5	48	179.6	1.10	1.35	86.24
22	3/5	75	0.2	48	287.9	1.55	2.40	85.75
23	3/5	75	0.2	48	288.0	1.60	2.30	86.88
24	3/5	75	0.2	48	288.1	1.60	2.40	84.78
25	3/5	50	0.5	48	258.2	1.50	1.80	92.05
26	3/5	50	0.5	48	258.4	1.60	1.70	92.12
27	3/6	50	0.5	48	258.9	1.65	1.65	92.30

in JP-4. The program rate was raised from 0.5°C/min to 1.0°C/min to shorten the overall sample time though still providing sharp, nontailing peaks in the boiling range of n-octadecane.

Resolution was calculated under these new conditions. The resulting "R" value of 76.25 was remarkably close to the resolutions calculated using a 1°C/min program rate and 48 psig capillary pressure during the resolution study. The finalized results are listed in Section II.

3. STANDARD HYDROCARBON SOLUTIONS

The first step in preparing the master stock solutions containing the 200+ standard hydrocarbons was to assemble hydrocarbons likely to appear in a typical JP-4 jet propulsion fuel. These hydrocarbons were then grouped into their respective classes (i.e., alkyl benzenes, saturated cyclics, etc.) by boiling point. Those compounds whose boiling points could not be found were later assigned an approximate boiling point interpolated from their retention time on a plot of retention times versus boiling point for the normal alkanes run under the specific conditions previously determined for this investigation (see Figure 1).

Each class of compounds was then divided into smaller groups of five to ten compounds each of widely different boiling points. These groups of compounds were then prepared in solutions at approximately 0.1% by volume and chromatographed under the previously determined specific conditions. These runs indicated both the purity of the compounds and the retention times of the compounds under the specific conditions. Once all the retention time data was gathered the compound classes were then ordered by retention times. These classes were divided into two or three smaller groups when necessary to prevent overlapping of elution times. Each compound in a group of compounds was then weighed into solution along with an aliquot of a solution of normal alkanes from pentane through octadecane, including an internal standard for

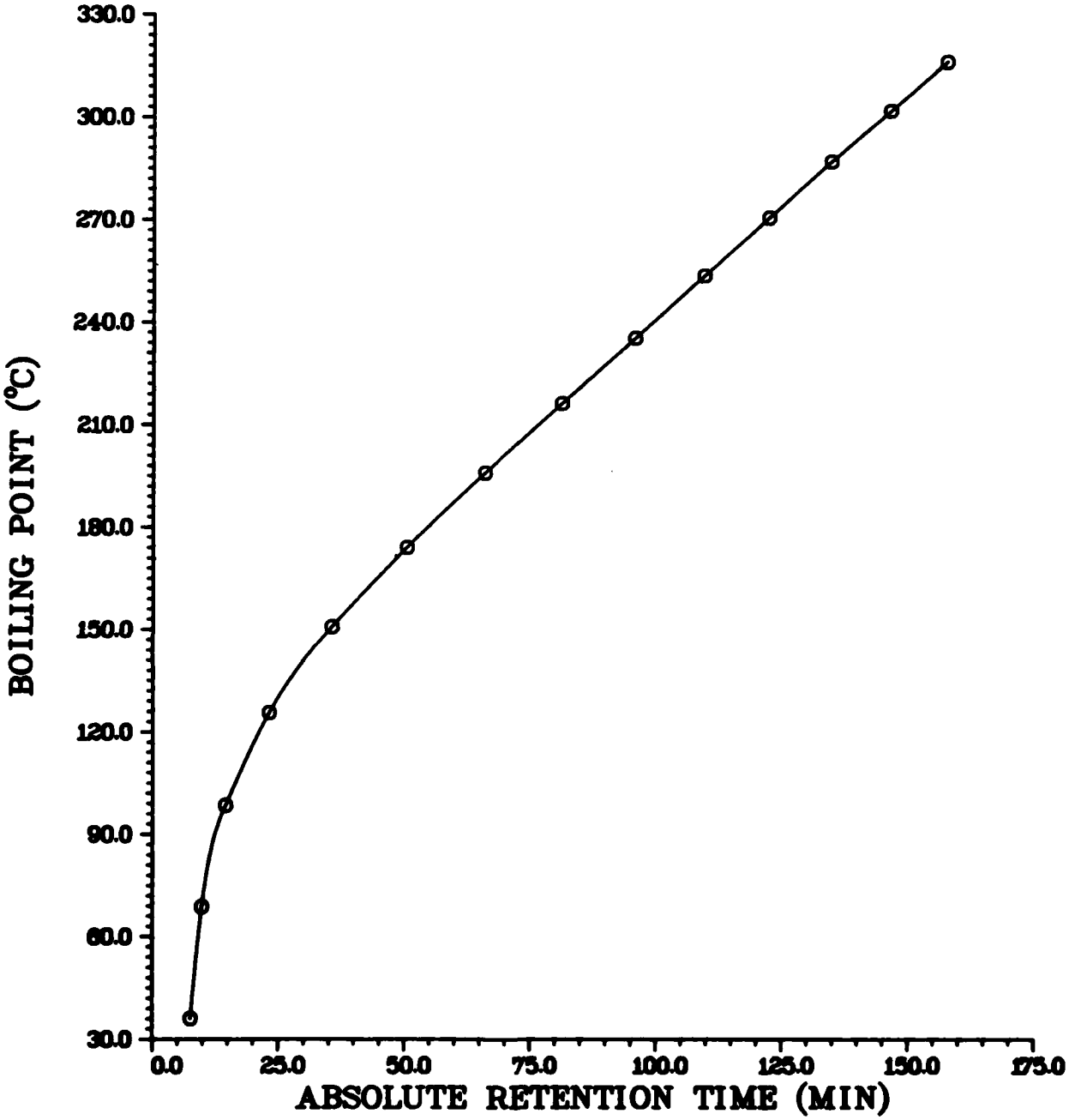

Figure 1. Absolute Retention Time vs. Boiling Point for N-Alkanes C_5 to C_{18}.

subsequent relative response factor determination. The amount of each compound to add to the solutions was determined by its relative amount in a typical JP-4 as determined by previous gas chromatograph and mass spectral analyses.

4. LIBRARIES OF KOVATS RETENTION INDICES

The libraries of Kovats retention indices for both the OV-101 and the OV-17 columns are listed in Table 5. The compounds are listed numerically by their OV-101 Kovats Indices. "K.I.-101" and "K.I.-17" indicate the mean value of the Kovats Indices from five $(GC)^2$ runs. These numbers are accompanied by their standard deviations and 95% confidence levels for five determinations.

A Kovats Index could not be computed for all compounds on both columns, due to peak coelution with other standard compounds, normal alkanes, or the solvent.

The overall precision for these computations is indicated by the mean values of the 95% confidence levels, i.e., $\pm$0.06 for the OV-101 column and $\pm$0.09 for the OV-17 column. It should be noted that the 95% confidence levels of the low boiling compounds are much larger than those of the other compounds. This is a direct result of the shorter retention times of the low boiling compounds, where a slight difference in retention times for repeat runs has a larger effect on the standard deviations than the same difference has for higher boiling components with much longer retention times.

TABLE 5

KOVATS INDICES GENERATED ON TWO QUADREX CAPILLARY COLUMNS:
COLUMN #510B, 108M OV-101; COLUMN #1029A, 117M OV-17

HYDROCARBON NAME	K.I.-101	σ	95% C.L.	K.I.-17	σ	95% C.L.
2-Methylbutane	464.94	0.35	0.43	462.44	0.49	0.60
2,2-Dimethylbutane				512.96	0.19	0.24
Cyclopentane	557.40	0.12	0.15	559.80	0.55	0.68
2,3-Dimethylbutane	557.92	0.25	0.31	532.93	0.33	0.41
2-Methylpentane	561.64	0.11	0.14	534.27	0.22	0.28
3-Methylpentane	578.11	0.22	0.27	549.70	0.48	0.60
1-Hexene	585.17	0.23	0.29			
2,2-Dimethylpentane	617.92	0.06	0.08	559.72	0.41	0.51
Methylcyclopentane	620.07	0.04	0.05	623.49	0.28	0.35
2,4-Dimethylpentane	622.82	0.02	0.03			
2,2,3-Trimethylbutane	627.82	0.07	0.09	606.81	0.43	0.53
Benzene	642.11	0.06	0.08	739.24	0.09	0.11
3,3-Dimethylpentane	646.27	0.06	0.08	628.32	0.23	0.29
Cyclohexane	650.27	0.10	0.12	687.73	0.20	0.25
2-Methylhexane	659.24	0.06	0.07	638.62	0.16	0.20
2,3-Dimethylpentane	661.36	0.04	0.05	649.08	0.39	0.48
Cyclohexene	667.29	0.10	0.12	722.96	0.08	0.10
3-Methylhexane	669.11	0.07	0.08	655.49	0.15	0.18
3-Ethylpentane	681.54	0.08	0.10	678.53	0.46	0.57
1-Heptene	684.69	0.15	0.18	705.53	0.15	0.18
2,2,4-Trimethylpentane	685.74	0.01	0.02	663.92	0.39	0.48
1-cis-2-Dimethylcyclopentane	714.85	0.03	0.05	737.03	0.08	0.10
Methylcyclohexane	715.63	0.05	0.06	739.15	0.10	0.13
2,2-Dimethylhexane	717.70	0.03	0.03	710.36	0.09	0.11
Ethylcyclopentane	725.43	0.05	0.06	749.43	0.10	0.12
2,5-Dimethylhexane	726.53	0.05	0.06	717.57	0.15	0.18
2,4-Dimethylhexane	728.30	0.04	0.04	720.98	0.08	0.11
3,3-Dimethylhexane	734.72	0.05	0.06	731.49	0.14	0.18
2,3,4-Trimethylpentane	743.05	0.06	0.08	743.58	0.10	0.12
2,3,3-Trimethylpentane	747.10	0.03	0.04	751.82	0.05	0.06
Methylbenzene	747.63	0.03	0.04	845.42	0.04	0.05
2,3-Dimethylhexane	754.03	0.05	0.06	751.82	0.13	0.17
3-Ethyl-2-Methylpentane	755.34	0.06	0.08	755.33	0.07	0.09
1-Methylcyclohexene	757.60	0.06	0.08	812.30	0.04	0.05
2-Methylheptane	760.60	0.07	0.09	753.77	0.05	0.06
4-Methylheptane	762.04	0.04	0.05	757.35	0.10	0.13
3-Ethyl-3-Methylpentane	763.72	0.04	0.05	769.33	0.07	0.08
3,4-Dimethylhexane	763.74	0.07	0.08	765.11	0.03	0.04
2,2,4,4-Tetramethylpentane	765.88	0.07	0.08	759.30	0.17	0.21
3-Methylheptane	768.75	0.06	0.08	765.12	0.12	0.15
3-Ethylhexane	769.84	0.07	0.08	768.08	0.07	0.09
cis-1,3-Dimethylcyclohexane	769.96	0.05	0.06	794.50	0.12	0.14
trans-1,4-Dimethylcyclohexane	772.00	0.04	0.05	795.36	0.07	0.09
1,1-Dimethylcyclohexane	778.06	0.06	0.08	806.05	0.01	0.01
cis-1,4-Dimethylcyclohexane				822.91	0.06	0.08
2,2,5-Trimethylhexane	781.15	0.04	0.05	763.42	0.07	0.09
1-Octene	785.76	0.02	0.03	805.81	0.05	0.06
2,2,4-Trimethylhexane	788.87	0.04	0.05	777.93	0.08	0.09
trans-1,2-Dimethylcyclohexane	791.91	0.05	0.07	815.18	0.03	0.03

NOTE: 95% CONFIDENCE LIMIT FOR 5 DETERMINATIONS = $\frac{(\sigma)(2.776)}{(2.236)}$

TABLE 5 (Continued)

KOVATS INDICES GENERATED ON TWO QUADREX CAPILLARY COLUMNS:
COLUMN #510B, 108M OV-101; COLUMN #1029A, 117M OV-17

HYDROCARBON NAME	K.I.-101	σ	95% C.L.	K.I.-17	σ	95% C.L.
trans-1,3-Dimethylcyclohexane				823.87	0.07	0.09
n-Propylcyclopentane				848.84	0.05	0.06
Ethylcyclohexane				854.06	0.06	0.07
2,2-Dimethylheptane	817.31	0.05	0.06	808.09	0.08	0.10
cis-1,2-Dimethylcyclohexane	820.39	0.04	0.05	851.27	0.04	0.05
2,2,3-Trimethylhexane	820.61	0.04	0.05	817.84	0.10	0.13
2,4-Dimethylheptane	821.03	0.06	0.07	812.35	0.08	0.10
4,4-Dimethylheptane	822.58	0.02	0.03	817.64	0.02	0.02
cis,cis,cis-1,3,5-Trimethylcyclohexane	825.38	0.04	0.05	838.47	0.04	0.05
2,6-Dimethylheptane	827.06	0.03	0.04	816.99	0.06	0.07
1,1,3-Trimethylcyclohexane	830.35	0.05	0.06	846.55	0.08	0.11
1,1,4-Trimethylcyclohexane	832.51	0.04	0.05	846.25	0.05	0.06
2,4-Dimethyl 3-Ethylpentane	833.05	0.03	0.04	833.39	0.07	0.09
2,5-Dimethylheptane	833.18	0.04	0.05	825.03	0.02	0.03
2,3,3-Trimethylhexane	833.66	0.05	0.06	834.40	0.08	0.11
3,3-Dimethylheptane	834.68	0.03	0.04	830.23	0.08	0.10
Ethylbenzene	843.07	0.04	0.05	944.10	0.04	0.05
cis,trans,trans-1,2,4-Trimethylcyclohexane	844.82	0.03	0.04	861.39	0.08	0.09
cis,cis,trans-1,3,5-Trimethylcyclohexane	848.69	0.03	0.04	868.09	0.06	0.07
m-Xylene	851.82	0.02	0.03	950.03	0.06	0.08
p-Xylene	852.80	0.04	0.05	948.44	0.02	0.03
2,3-Dimethylheptane	853.26	0.06	0.07	849.82	0.06	0.07
4-Ethylheptane	858.32	0.06	0.07	853.31	0.08	0.10
4-Methyloctane	861.46	0.07	0.08	856.49	0.05	0.06
2-Methyloctane	862.66	0.06	0.07	856.17	0.06	0.07
cis,trans,cis-1,2,3-Trimethylcyclohexane	867.35	0.04	0.04	892.49	0.08	0.10
3-Ethylheptane	867.96	0.05	0.06	865.54	0.06	0.07
cis,trans,cis-1,2,4-Trimethylcyclohexane	869.09	0.03	0.03	894.23	0.07	0.09
3-Methyloctane	869.43	0.06	0.08	865.52	0.04	0.05
2,4,6-Trimethylheptane	874.13	0.03	0.03	856.84	0.06	0.07
o-Xylene	874.53	0.03	0.03	981.56	0.04	0.05
cis-1-Ethyl-3-Methylcyclohexane	881.29	0.04	0.05	906.01	0.01	0.01
1-Nonene	887.15	0.04	0.05	906.46	0.00	0.00
trans-1-Ethyl-2-Methylcyclohexane	901.06	0.04	0.05	927.63	0.05	0.07
1-Ethyl-1-Methylcyclohexane	903.14	0.05	0.06	933.95	0.04	0.05
cis-1-Ethyl-4-Methylcyclohexane	903.98	0.03	0.04	930.25	0.04	0.05
Cumene	908.92	0.04	0.05	1006.06	0.06	0.08
Isopropylcyclohexane	912.85	0.04	0.04	943.24	0.06	0.08
2,2-Dimethyloctane	917.78	0.03	0.04	908.18	0.08	0.10
4,4-Dimethyloctane	919.84	0.03	0.03	914.32	0.04	0.05
cis-1-Ethyl-2-Methylcyclohexane	920.98	0.04	0.05	954.58	0.04	0.05
n-Propylcyclohexane	923.29	0.01	0.01	950.92	0.06	0.08
(+)-γ-Pinene	926.55	0.04	0.05	964.40	0.02	0.03

NOTE: 95% CONFIDENCE LIMIT FOR 5 DETERMINATIONS = $\frac{(\sigma)(2.776)}{(2.236)}$

TABLE 5 (Continued)

KOVATS INDICES GENERATED ON TWO QUADREX CAPILLARY COLUMNS:
COLUMN #510B, 108M OV-101; COLUMN #1029A, 117M OV-17

HYDROCARBON NAME	K.I.-101	σ	95% C.L.	K.I.-17	σ	95% C.L.
2,7-Dimethyloctane	929.14	0.03	0.04	919.33	0.02	0.03
2,6-Dimethyloctane	933.62	0.04	0.05	925.44	0.04	0.05
3,3-Dimethyloctane	934.14	0.03	0.04	928.72	0.07	0.08
n-Propylbenzene	937.01	0.04	0.05	1035.65	0.05	0.06
3,4-Diethylhexane	937.44	0.05	0.06	936.07	0.03	0.04
3-Ethyl-3-Methylheptane	940.32	0.04	0.05	946.53	0.04	0.05
1-Ethyl-3-Methylbenzene	944.83	0.02	0.02	1046.12	0.03	0.03
4-Propylheptane	944.91	0.05	0.06	937.76	0.06	0.07
3-Ethyl-2-Methylheptane	946.34	0.04	0.05			
1,3,5-Trimethylbenzene	952.83	0.02	0.02	1051.36	0.04	0.05
2,3-Dimethyloctane	953.33	0.02	0.03	949.98	0.06	0.07
4-Methylnonane	954.97	0.05	0.06	950.20	0.06	0.07
5-Methylnonane	959.55	0.05	0.06	954.84	0.03	0.04
4-Ethyloctane	961.30	0.03	0.04	956.33	0.05	0.06
1-Ethyl-2-Methylbenzene	961.45	0.03	0.04	1070.46	0.05	0.07
2-Methylnonane	963.97	0.05	0.06	957.96	0.04	0.05
(-)-B-Pinene	965.11	0.03	0.04	1025.80	0.01	0.01
3-Ethyloctane	966.99	0.01	0.01	964.56	0.06	0.07
trans-1-Methyl-4-Isopropylcyclohexane	969.71	0.03	0.04	992.19	0.08	0.10
3-Methylnonane	970.32	0.04	0.06	966.96	0.04	0.05
3,3,4,4-Tetramethylhexane	970.78	0.02	0.03	993.77	0.03	0.04
tert-Butylbenzene	975.93	0.02	0.03	1073.60	0.02	0.03
1,2,4-Trimethylbenzene	976.91	0.03	0.03	1080.84	0.02	0.02
cis-1-Methyl-4-Isopropylcyclohexane	983.78	0.03	0.03	1012.55	0.07	0.07
1-Decene	987.87	0.02	0.03	1006.67	0.03	0.04
Isobutylbenzene	992.48	0.03	0.04	1082.90	0.03	0.04
3-Ethylnonane	992.53	0.00	0.00	1064.57	0.03	0.04
sec-Butylbenzene	995.09	0.03	0.04	1090.33	0.07	0.09
1,2,3-Trimethylbenzene	1003.68	0.03	0.04	1120.33	0.05	0.06
1-Methyl-3-Isopropylbenzene	1006.59	0.03	0.04	1103.84	0.03	0.04
p-Cymene	1009.38	0.03	0.04	1104.61	0.05	0.07
Indan	1013.44	0.03	0.03	1147.39	0.02	0.02
D-Limonene	1018.23	0.01	0.01	1083.41	0.05	0.07
n-Butylcyclohexane	1025.65	0.04	0.05	1054.03	0.01	0.01
1,3-Diethylbenzene	1032.94	0.03	0.04			
1-Methyl-3-Propylbenzene	1035.51	0.04	0.05	1134.57	0.03	0.04
1,4-Diethylbenzene	1038.88	0.02	0.02	1142.00	0.03	0.03
1-Methyl-4-Propylbenzene	1039.05	0.03	0.04			
n-Butylbenzene	1039.90	0.02	0.03	1139.89	0.04	0.05
1,3-Dimethyl-5-Ethylbenzene	1042.81	0.04	0.05	1144.78	0.05	0.06
trans-Decalin	1042.88	0.02	0.02	1102.06	0.03	0.04
neopentylbenzene	1048.25	0.03	0.03	1135.95	0.03	0.03
1-Methyl-2-Propylbenzene	1049.75	0.04	0.05	1154.98	0.06	0.07
1,4-Dimethyl-2-Ethylbenzene	1060.58	0.01	0.02	1166.50	0.04	0.04
4-Methyldecane	1061.06	0.01	0.02	1056.61	0.00	0.00
1,3-Dimethyl-4-Ethylbenzene	1062.14	0.02	0.02	1168.99	0.03	0.04
2-Methyldecane	1064.77	0.01	0.002	1059.14	0.06	0.07
2,2,4,6,6-Pentamethylheptane	1066.61	0.04	0.05	971.86	0.06	0.07
1,2-Dimethyl-4-Ethylbenzene	1068.04	0.02	0.03	1176.59	0.03	0.03

NOTE: 95% CONFIDENCE LIMIT FOR 5 DETERMINATIONS = $\frac{(\sigma)(2.776)}{(2.236)}$

TABLE 5 (Continued)

KOVATS INDICES GENERATED ON TWO QUADREX CAPILLARY COLUMNS:
COLUMN #510B, 108M OV-101; COLUMN #1029A, 117M OV-17

HYDROCARBON NAME	K.I.-101	σ	95% C.L.	K.I.-17	σ	95% C.L.
1,2-Dimethylpropylbenzene	1068.81	0.03	0.04	1161.92	0.02	0.03
1-Ethylpropylbenzene	1071.03	0.02	0.02			
1-tert-Butyl-3-Methylbenzene	1071.55	0.02	0.03	1167.39	0.01	0.02
1,3-Dimethyl-2-Ethylbenzene	1073.15	0.04	0.04	1187.93	0.03	0.04
tert-Pentylbenzene	1076.00	0.02	0.03	1176.49	0.03	0.04
p-tert-Butyltoluene	1076.12	0.05	0.06	1170.49	0.01	0.02
cis-Decalin	1084.51	0.05	0.06	1158.23	0.04	0.05
1-Methylbutylbenzene	1086.41	0.04	0.05	1182.26	0.02	0.03
1,2,4,5-Tetramethylbenzene				1208.65	0.04	0.05
1,2-Dimethyl-3-Ethylbenzene	1086.88	0.03	0.04	1206.44	0.03	0.04
1-Undecene	1088.37	0.04	0.05	1106.70	0.03	0.04
1-Ethyl-3-Isopropylbenzene	1088.54	0.03	0.04	1186.05	0.03	0.04
2-Methylbutylbenzene	1101.75	0.06	0.07	1197.03	0.00	0.00
1,2,3,5-Tetramethylbenzene	1102.85	0.04	0.04	1216.82	0.02	0.03
3-Methylbutylbenzene	1106.52	0.06	0.07	1201.01	0.03	0.04
1-tert-Butyl-2-Methylbenzene	1114.57	0.07	0.08	1228.54	0.03	0.04
2,6-Dimethyldecane	1119.35	0.04	0.06	1109.50	0.03	0.04
1,2,3,4-Tetramethylbenzene	1132.90	0.02	0.02	1257.40	0.04	0.05
Tetralin	1136.43	0.02	0.02	1288.39	0.05	0.06
1,3-Diisopropylbenzene	1138.86	0.06	0.07	1231.47	0.02	0.02
n-Pentylbenzene	1141.13	0.03	0.04	1242.74	0.02	0.03
Naphthalene	1156.25	0.06	0.07	1344.95	0.05	0.06
1,4-Diisopropylbenzene	1157.71	0.01	0.02	1257.77	0.05	0.06
1-tert-Butyl-3,5-Dimethylbenzene	1163.06	0.03	0.04	1258.21	0.02	0.02
2-Methylundecane	1164.88	0.05	0.06	1159.30	0.05	0.06
1-tert-Butyl-4-Ethylbenzene	1165.62	0.02	0.03	1266.63	0.04	0.05
1-Dodecene	1188.62	0.03	0.04	1206.80	0.04	0.05
2-Methylpentylbenzene	1190.88	0.03	0.04	1285.14	0.03	0.04
1,3,5-Triethylbenzene	1206.13	0.04	0.05	1312.11	0.04	0.05
2,6-Dimethylundecane	1215.87	0.07	0.09	1205.25	0.05	0.07
1,2,4-Triethylbenzene	1223.09	0.04	0.05	1334.53	0.04	0.05
n-Hexylbenzene	1243.89	0.04	0.05	1345.67	0.04	0.04
Pentamethylbenzene	1261.35	0.05	0.06	1392.52	0.00	0.01
2-Methylnaphthalene	1267.22	0.08	0.09	1458.02	0.03	0.03
1,1-Diethylpropylbenzene	1274.63	0.05	0.07	1382.32	0.07	0.08
1-Methylnaphthalene	1281.76	0.13	0.16	1484.30	0.01	0.01
1-Tridecene	1288.83	0.03	0.03	1306.95	0.05	0.07
Phenylcyclohexane	1296.28	0.05	0.06	1442.07	0.03	0.04
1-tert-Butyl-3,4,5-Trimethylbenzene	1306.82	0.06	0.07	1421.50	0.04	0.05
n-Heptylbenzene	1347.56	0.02	0.03	1450.47	0.04	0.05
Biphenyl	1349.53	0.09	0.11	1563.26	0.02	0.02
2-Ethylnaphthalene	1366.22	0.09	0.11	1559.59	0.02	0.02
1-Ethylnaphthalene	1367.46	0.05	0.06	1572.55	0.03	0.04
2,6-Dimethylnaphthalene	1377.27	0.03	0.03	1570.18	0.03	0.04

NOTE: 95% CONFIDENCE LIMIT FOR 5 DETERMINATIONS = $\frac{(\sigma)(2.776)}{(2.236)}$

TABLE 5 (Concluded)

KOVATS INDICES GENERATED ON TWO QUADREX CAPILLARY COLUMNS:
COLUMN #510B, 108M OV-101; COLUMN #1029A, 117M OV-17

HYDROCARBON NAME	K.I.-101	σ	95% C.L.	K.I.-17	σ	95% C.L.
1-Tetradecene	1389.14	0.07	0.08	1407.42	0.04	0.04
1,3-Dimethylnaphthalene	1391.04	0.07	0.09	1594.52	0.07	0.08
1,4-Dimethylnaphthalene	1408.81	0.10	0.12	1621.95	0.03	0.04
2,3-Dimethylnaphthalene	1410.50	0.06	0.08	1616.16	0.06	0.08
Hexamethylbenzene	1430.72	0.04	0.05	1583.98	0.04	0.05
n-Octylbenzene	1451.16	0.02	0.02	1555.23	0.04	0.05
n-Nonylbenzene	1555.41	0.06	0.08	1660.62	0.04	0.05
n-Decylbenzene	1659.28	0.05	0.06	1765.55	0.08	0.10
Hexaethylbenzene	1682.39	0.06	0.08			

NOTE: 95% CONFIDENCE LIMIT FOR 5 DETERMINATIONS = $\frac{(\sigma)(2.776)}{(2.236)}$

SECTION IV

FUELS CHARACTERIZATION

1. LIBRARY MATCHING

Samples of both petroleum derived and shale derived jet propulsion fuels were prepared in solution with carbon disulfide at a dilution ratio of 100:1. These samples were then analyzed three times each on both the OV-101 and the OV-17 columns under the same conditions used for the standard solutions to generate the Kovats Libraries.

The Kovats Index for each peak of the fuel samples was then calculated and statistically analyzed at the 95% confidence level for three determinations.

Prior to actually matching the Kovats Index of an unknown compound in a fuel sample to the Kovats Index of a known compound in a sample of standard solution it became necessary to decide with what assurance the two indices matched. During the preparation of the standard solutions it was noticed that the $(GC)^2$ system, under the conditions of this experiment, could not resolve two compounds, placed in the same solution, whose Kovats Index differed by less than one units Therefore an assurance limit of ± 0.5 Kovats Indices unit was used for matching indices.

"After all peak assignments were completed, a precision survey was performed on fuel 15B (table 9): The resulting deviations of assignments of ±0.127 for the OV-101 and ±0.180 for the the OV-17 indicate that the assignments were well within the ±0.5 assurance limit.

The following tables list the five jet propulsion fuels selected for analysis in this report. The peaks identified in each fuel are listed numerically by their OV-101 library indices. "K.I. - samp." represents the mean Kovats Index for the three runs of a sample on the particular column and is accompanied by the standard deviation and 95% confidence level for three determinations. "K.I.-101" and "K.I.-17" represent library Kovats Index values for the known reference standards. "A%" indicates the area percent of an identified peak from the first run of the fuel sample.

TABLE 6

PETROLEUM DERIVED JP-4 FUEL TB-792009

	OV-101					OV-17				
HYDROCARBON NAME	K.I.-101	K.I. SAMP.	σ	95% C.L.	A%	K.I.-17	K.I. SAMP.	σ	95% C.L.	A%
2-Methylbutane	464.94	465.10	0.68	1.69	0.98	462.44	461.97	0.46	1.14	0.98
2-Methylpentane	561.64	562.08	0.10	0.26	2.41	534.27	534.06	0.20	0.49	2.79
3-Methylpentane	578.11	578.24	0.22	0.54	2.01	549.70	549.92	0.29	0.72	1.87
Methylcyclopentane	620.07	620.06	0.13	0.32	0.84	623.49	623.62	0.00	0.00	0.83
2,2,3-Trimethylbutane	627.82	627.74	0.00	0.00	0.07	606.81	607.04	0.00	0.00	0.12
Benzene	642.11	641.83	0.00	0.00	0.48	739.24	739.10	0.16	0.41	(739.15)*
Cyclohexane	650.27	650.11	0.00	0.00	0.98	687.73	687.44	0.00	0.00	0.96
2-Methylhexane	659.24	659.06	0.00	0.00	5.14	638.62	638.86	0.58	1.44	5.01
2,3-Dimethylpentane	661.36	661.30	0.00	0.00	1.88	649.08	649.58	0.29	0.72	1.78
3-Methylhexane	669.11	669.13	0.00	0.00	6.63	655.49	655.78	0.00	0.00	6.67
3-Ethylpentane	681.54	681.36	0.13	0.32	0.93	678.53	678.39	0.00	0.00	0.78
2,2,4-Trimethylpentane	685.74	685.53	0.13	0.32	0.11	663.92	663.65	0.29	0.72	0.11
Methylcyclohexane	715.63	715.56	0.05	0.14	1.00	739.15*	739.10	0.16	0.41	1.44
2,2-Dimethylhexane	717.70	717.57	0.05	0.13	0.47	710.36	710.26	0.19	0.48	0.40
Ethylcyclopentane	725.43	725.35	0.05	0.11	0.15	749.43	749.12	0.09	0.22	0.31
2,5-Dimethylhexane	726.53	726.44	0.05	0.11	0.68	717.57	717.53	0.08	0.21	0.90
2,4-Dimethylhexane	728.30	728.17	0.09	0.22	1.16	720.98	720.98	0.09	0.23	1.10
3,3-Dimethylhexane	734.72	734.54	0.04	0.10	0.36	731.49	731.36	0.17	0.43	0.36
2,3,4-Trimethylpentane	743.05	742.89	0.04	0.09	0.17	743.58	743.43	0.04	0.11	0.12
Methylbenzene	747.63	747.48	0.04	0.09	1.57	845.42	845.41	0.09	0.23	1.49
2,3-Dimethylhexane	754.03	753.89	0.04	0.09	0.84	751.82	751.76	0.15	0.37	0.76
2-Methylheptane	760.60	760.42	0.04	0.09	2.83	753.77	753.75	0.18	0.45	2.90
4-Methylheptane	762.04	762.03	0.05	0.11	1.35	757.35	757.39	0.14	0.36	1.37
3-Methylheptane	768.75	768.56	0.04	0.09	3.31	765.12	765.12	0.14	0.34	3.59
3-Ethylhexane	769.84*	769.77	0.04	0.09	1.01	768.08	767.94	0.13	0.33	0.90
cis-1,3-Dimethylcyclohexane	769.96	769.77	0.04	0.09	(769.84)*	794.50	794.55	0.18	0.44	0.40
1,1-Dimethylcyclohexane	778.06	778.07	0.05	0.12	0.05	806.05	806.47	0.06	0.14	0.15
trans-1,2-Dimethylcyclohexane	791.91	791.98	0.06	0.15	0.16	815.18	815.11	0.01	0.02	0.13
2,2-Dimethylheptane	817.31	817.19	0.04	0.09	0.10	808.09	807.93	0.06	0.14	0.18
2,4-Dimethylheptane	821.03	820.88	0.03	0.08	0.24	812.35	812.25	0.01	0.02	0.24
2,6-Dimethylheptane	827.06	827.01	0.06	0.15	0.21	816.99	816.92	0.05	0.14	0.13
2,5-Dimethylheptane	833.18	833.09	0.05	0.14	0.44	825.03	824.98	0.10	0.26	0.41
3,3-Dimethylheptane	834.68	834.35	0.03	0.07	0.15	830.23	830.12	0.02	0.04	0.08
Ethylbenzene	843.07	842.99	0.02	0.06	0.60	944.10	944.04	0.04	0.11	0.51
cis,trans,trans-1,2,4-Trimethylcyclohexane	844.82	844.85	0.02	0.06	0.09	861.39	861.27	0.04	0.09	0.08
m-Xylene	851.82	851.75	0.02	0.06	1.25	950.03	950.04	0.04	0.09	1.52
p-Xylene	852.80*	852.79	0.04	0.10	0.75	948.44	948.54	0.04	0.10	0.46
2,3-Dimethylheptane	853.26	852.79	0.04	0.10	(852.80)*	849.82	849.76	0.03	0.07	0.31
4-Methyloctane	861.46	861.41	0.03	0.08	0.49	856.49	856.26	0.03	0.08	1.09
3-Methyloctane	869.43	869.38	0.03	0.06	0.66	865.52	865.42	0.08	0.20	0.78
o-Xylene	874.53	874.44	0.05	0.13	0.87	981.56	981.73	0.02	0.06	0.76
cis-1-Ethyl-3-Methylcyclohexane	881.29	881.34	0.05	0.12	0.11	906.01	906.00	0.01	0.02	0.15
Cumene	908.92	908.83	0.00	0.01	0.23	1006.06	1006.19	0.04	0.09	0.26
2,6-Dimethyloctane	933.62	933.61	0.01	0.03	0.21	925.44	925.44	0.06	0.15	0.18
3,4-Diethylhexane	937.44	937.02	0.02	0.06	0.29	936.07	936.24	0.05	0.12	0.14
1,3,5-Trimethylbenzene	952.83	952.76	0.02	0.05	0.50	1051.36	1051.54	0.04	0.09	0.43
4-Ethyloctane	961.30	961.39	0.02	0.04	(961.45)*	956.33	956.34	0.03	0.08	0.15
1-Ethyl-2-Methylbenzene	961.45*	961.39	0.02	0.04	0.57	1070.46	1070.63	0.04	0.09	0.41
2-Methylnonane	963.97	963.97	0.03	0.09	0.21	957.96	958.06	0.03	0.08	0.18
3-Methylnonane	970.32	970.38	0.05	0.12	0.18	966.96	967.06	0.03	0.07	0.18
1,2,4-Trimethylbenzene	976.91	976.86	0.01	0.02	1.62	1080.84	1081.02	0.08	0.19	1.55
Isobutylbenzene	992.48*	992.49	0.04	0.10	0.05	1082.90	1083.25	0.04	0.09	0.08
3-Ethylnonane	992.53	992.49	0.04	0.10	(992.48)*	1064.57	1064.75	0.04	0.09	0.07
1,2,3-Trimethylbenzene	1003.68	1003.65	0.00	0.01	0.48	1120.33	1120.56	0.00	0.00	0.14
1-Methyl-3-Isopropylbenzene	1006.59	1006.61	0.03	0.08	0.14	1103.84	1104.03	0.04	0.09	0.12
Indan	1013.44	1013.39	0.02	0.06	0.08	1147.39	1147.75	0.04	0.09	0.07
n-Butylcyclohexane	1025.65	1025.71	0.02	0.05	0.08	1054.03	1054.12	0.08	0.19	0.08
1-Methyl-3-Propylbenzene	1035.51	1035.57	0.02	0.06	0.47	1134.57	1134.80	0.04	0.09	0.05
1,4-Diethylbenzene	1038.88	1039.11	0.01	0.04	0.33	1142.00	1142.30	0.04	0.09	0.14
n-Butylbenzene	1039.90	1039.96	0.01	0.03	0.11	1139.89	1140.16	0.07	0.19	0.21
1-Methyl-2-Propylbenzene	1049.75	1049.78	0.04	0.09	0.25	1154.98	1155.12	0.07	0.19	0.15
4-Methyldecane	1061.06*	1060.60	0.03	0.07	0.47	1056.61	1056.72	0.08	0.19	0.18
1,4-Dimethyl-2-Ethylbenzene	1060.58	1060.60	0.03	0.07	(1061.06)*	1166.50	1166.69	0.04	0.09	0.41
1,3-Dimethyl-4-Ethylbenzene	1062.14	1062.15	0.04	0.10	0.29	1168.99	1169.12	0.07	0.19	0.30
2-Methyldecane	1064.77	1064.84	0.02	0.06	0.26	1059.14	1059.20	0.04	0.09	0.22
1,2-Dimethyl-4-Ethylbenzene	1068.04	1068.12	0.02	0.06	0.46	1176.59	1176.73	0.00	0.00	0.44
1,2-Dimethyl-3-Ethylbenzene	1086.88	1086.72	0.02	0.06	0.16	1206.44	1206.60	0.04	0.11	0.17
1-Ethyl-3-Isopropylbenzene	1088.54	1088.70	0.03	0.06	0.13	1187.05	1187.22	0.07	0.19	0.06
1,2,3,5-Tetramethylbenzene	1102.85	1102.78	0.07	0.19	0.34	1216.82	1217.00	0.06	0.16	0.44

NOTE: 95% Confidence Limit for 3 Determinations = $\frac{(\sigma)(4.303)}{(1.732)}$

TABLE 6 (Concluded)

HYDROCARBON NAME	K.I.-101	K.I. SAMP.	σ	95% C.L.	A%	K.I.-17	K.I. SAMP.	σ	95% C.L.	A%
2,6-Dimethyldecane	1119.35	1119.29	0.02	0.06	0.13	1109.50	1109.61	0.07	0.19	0.18
Tetralin	1136.43	1136.65	0.07	0.17	0.21	1288.39	1288.54	0.11	0.26	0.18
n-Pentylbenzene	1141.13	1141.25	0.06	0.15	0.05	1242.74	1242.57	0.33	0.83	0.08
Naphthalene	1156.25	1156.71	0.07	0.16	0.30	1344.95	1345.32	0.04	0.09	(1345.67)*
1,4-Diisopropylbenzene	1157.71	1157.98	0.04	0.10	0.10	1256.77	1257.66	0.04	0.11	0.32
2-Methylundecane	1164.88	1164.95	0.03	0.07	0.32	1159.30	1159.51	0.07	0.19	0.08
1,2,4-Triethylbenzene	1223.09	1223.42	0.05	0.11	0.13	1334.53	1334.77	0.08	0.20	0.06
n-Hexylbenzene	1243.89	1243.81	0.03	0.09	0.09	1345.67*	1345.32	0.04	0.09	0.19
2-Methylnaphthalene	1267.22	1267.29	0.07	0.18	0.23	1458.02	1458.01	0.02	0.04	0.18
1-Methylnaphthalene	1281.76	1281.81	0.03	0.08	0.26	1484.30	1484.28	0.04	0.09	0.07
Butane					0.32					0.31
Pentane					0.82					0.86
Hexane					3.72					3.88
Heptane					7.26					7.17
Octane					3.04					3.34
Nonane					1.17					1.13
Decane					1.03					0.91
Undecane					1.92					2.20
Dodecane					2.42					2.36
Tridecane					2.17					1.98
Tetradecane					1.47					1.30
Pentadecane					0.63					0.57
Hexadecane					0.17					0.17
Heptadecane					0.05					0.05
TOTAL					79.45					79.30

TABLE 7

PETROLEUM DERIVED JP-4 FUEL 1B-49B-792009

	OV-101					OV-17				
HYDROCARBON NAME	K.I.-101	K.I. SAMP.	σ	95% C.L.	A%	K.I.-17	K.I. SAMP.	σ	95% C.L.	A%
2-Methylbutane	464.94	465.11	0.41	1.01	1.02	462.44	462.05	0.30	0.74	1.01
3-Methylpentane	578.11	578.18	0.25	0.62	1.27	549.70	549.57	0.15	0.37	1.32
Benzene	642.11	641.92	0.18	0.44	0.38	739.24	739.11	0.00	0.00	(739.15)*
Cyclohexane	650.27	650.19	0.17	0.42	1.20	687.73	687.82	0.00	0.00	1.22
2-Methylhexane	659.24	659.12	0.17	0.42	2.38	638.62	639.09	0.00	0.00	2.42
3-Methylhexane	669.11	669.10	0.15	0.37	3.19	655.49	656.01	0.29	0.73	3.33
2,2,4-Trimethylpentane	685.74	685.63	0.13	0.32	0.06	663.92	664.13	0.29	0.73	0.06
Methylcyclohexane	715.63	715.66	0.04	0.09	2.73	739.15*	739.11	0.00	0.00	3.58
2,2-Dimethylhexane	717.70	718.15	0.08	0.20	0.47	710.36	710.24	0.10	0.26	0.21
Ethylcyclopentane	725.43	725.46	0.03	0.09	0.37	749.43	749.11	0.00	0.00	1.21
2,5-Dimethylhexane	726.53	726.43	0.03	0.09	0.34	717.57	717.56	0.21	0.51	0.46
2,4-Dimethylhexane	728.30	728.23	0.04	0.09	0.57	720.98	720.95	0.10	0.26	0.57
3,3-Dimethylhexane	734.72	734.62	0.04	0.10	0.16	731.49	731.43	0.00	0.00	0.20
2,3,4-Trimethylpentane	743.05	742.97	0.07	0.18	0.08	743.58	743.39	0.00	0.00	0.05
2,3,3-Trimethylpentane	747.10	747.51	0.06	0.16	(747.63)*	751.82	751.67	0.10	0.26	(751.82)*
Methylbenzene	747.63*	747.51	0.06	0.16	1.14	845.42	845.65	0.05	0.14	0.89
2,3-Dimethylhexane	754.03	753.98	0.01	0.02	0.59	751.82*	751.67	0.10	0.26	0.44
2-Methylheptane	760.60	760.44	0.05	0.12	2.11	753.77	753.75	0.18	0.44	2.35
4-Methylheptane	762.04	762.01	0.08	0.19	0.80	757.35	757.38	0.10	0.26	0.88
3,4-Dimethylhexane	763.74	763.49	0.03	0.08	0.26	765.11	765.00	0.00	0.00	(765.12)*
3-Methylheptane	768.75	768.63	0.04	0.09	1.80	765.12*	765.00	0.00	0.00	2.18
3-Ethylhexane	769.84	770.00	0.05	0.12	(769.96)*	768.08	767.86	0.00	0.00	0.53
cis-1,3-Dimethylcyclohexane	769.96*	770.00	0.05	0.12	1.57	794.50	794.70	0.21	0.51	1.35
2,2-Dimethylheptane	817.31	817.18	0.02	0.05	0.08	808.09	808.07	0.11	0.27	0.14
cis-1,2-Dimethylcyclohexane	820.39	820.81	0.02	0.06	(821.03)*	851.27	851.22	0.06	0.15	0.15
2,4-Dimethylheptane	821.03*	820.81	0.02	0.06	0.41	812.35	812.30	0.05	0.13	0.37
cis,cis,cis-1,3,5-Trimethylcyclohexane	825.38	825.20	0.03	0.08	1.12	838.47	838.34	0.05	0.11	0.07
2,6-Dimethylheptane	827.06	827.00	0.03	0.08	0.52	816.99	816.90	0.02	0.05	0.61
1,1,3-Trimethylcyclohexane	830.35	830.30	0.02	0.04	0.82	846.55	846.41	0.06	0.16	1.35
2,5-Dimethylheptane	833.18	833.05	0.04	0.10	0.46	825.03	824.87	0.05	0.13	0.35
3,3-Dimethylheptane	834.68	834.28	0.04	0.11	0.10	830.23	830.02	0.05	0.13	0.16
Ethylbenzene	843.07	843.03	0.05	0.13	0.84	944.10	944.03	0.06	0.15	0.51
cis,trans,trans-1,2,4-Trimethylcyclohexane	844.82	844.81	0.04	0.09	0.40	861.39	861.25	0.05	0.11	0.42
m-Xylene	851.82	851.68	0.04	0.11	1.03	950.03*	950.06	0.06	0.14	1.18
p-Xylene	852.80	852.93	0.02	0.03	(853.26)*	948.44	948.60	0.04	0.09	0.42
2,3-Dimethylheptane	853.26*	852.93	0.02	0.03	0.84	849.82	849.71	0.06	0.15	0.53
4-Methyloctane	861.46	861.39	0.04	0.09	0.55	856.49	856.06	0.07	0.17	(856.17)*
2-Methyloctane	862.50	862.66	0.06	0.07	0.67	856.17*	856.06	0.07	0.17	1.42
cis,trans, cis-1,2,3-Trimethylcyclohexane	867.35*	867.58	0.02	0.04	0.35	892.49	892.44	0.06	0.14	0.22
3-Ethylheptane	867.96	867.58	0.02	0.04	(867.35)*	865.54*	865.27	0.07	0.17	1.23
cis,trans,cis-1,2,4-Trimethylcyclohexane	869.09	869.29	0.02	0.04	(869.43)*	894.23	893.99	0.11	0.28	0.11
3-Methyloctane	869.43*	869.29	0.02	0.04	0.95	865.52	865.27	0.07	0.17	(865.54)*
o-Xylene	874.53	874.34	0.03	0.08	0.77	981.56	981.76	0.05	0.11	0.78
1-Nonene	887.15	886.61	0.04	0.09	0.06	906.46	905.94	0.04	0.10	0.76
trans-1-Ethyl-2-Methylcyclohexane	901.06	901.05	0.08	0.20	0.43	927.63	927.47	0.02	0.05	0.37
1-Ethyl-1-Methylcyclohexane	903.14	903.08	0.00	0.01	0.06	933.95	933.76	0.07	0.16	0.32
cis-1-Ehtyl-4-Methylcyclohexane	903.98	903.92	0.04	0.11	0.05	930.25	930.09	0.03	0.07	0.06
Cumene	908.92	908.72	0.05	0.12	0.18	1006.06	1006.20	0.03	0.08	0.28
Isopropylcyclohexane	912.85	912.73	0.04	0.11	0.19	943.24	943.09	0.04	0.11	0.18
2,2-Dimethyloctane	917.78	918.09	0.04	0.10	0.19	908.18	908.05	0.04	0.10	0.12
n-Propylcyclohexane	923.29	923.21	0.06	0.16	0.61	950.92	950.82	0.02	0.05	1.43
2,7-Dimethyloctane	929.14	929.50	0.07	0.17	0.25	919.33	919.22	0.03	0.08	0.09
2,6-Dimethyloctane	933.62	933.53	0.03	0.07	0.72	925.44	925.31	0.07	0.18	0.63
n-Propylbenzene	937.01	936.88	0.08	0.19	0.24	1035.65	1035.95	0.01	0.03	0.18
3-Ethyl-3-Methylheptane	940.32	940.23	0.05	0.13	0.89	946.53	946.72	0.04	0.10	0.21
1-Ethyl-3-Methylbenzene	944.83*	944.74	0.03	0.08	0.66	1046.12	1046.14	0.04	0.10	1.12
4-Propylheptane	944.91	944.74	0.03	0.08	(944.83)*	937.76	937.61	0.06	0.16	0.13
1,3,5-Trimethylbenzene	952.83	952.69	0.07	0.18	0.75	1051.36	1051.63	0.00	0.00	0.13
4-Methylnonane	954.97	954.85	0.04	0.09	0.15	950.20	950.06	0.06	0.14	(950.03)*
5-Methylnonane	959.55	959.41	0.03	0.07	0.21	954.84	954.59	0.06	0.14	0.32
4-Ethyloctane	961.30*	961.25	0.03	0.07	0.76	956.33	956.15	0.04	0.11	0.53
1-Ethyl-2-Methylbenzene	961.45	961.25	0.03	0.07	(961.30)*	1070.46	1070.78	0.02	0.06	0.33
2-Methylnonane	963.97	963.87	0.04	0.11	0.62	957.96	957.86	0.02	0.06	0.56
3-Ethyloctane	966.99	966.72	0.03	0.09	0.21	964.56	964.38	0.03	0.07	0.28
trans-1-Methyl-4-Isopropylcyclohexane	969.71	970.23	0.05	0.11	(970.32)*	992.19	992.25	0.04	0.11	0.19
3-Methylnonane	970.32*	970.23	0.05	0.11	0.54	966.96	966.84	0.05	0.12	0.53

NOTE: 95% Confidence Limit for 3 Determinations = $\frac{(\sigma)\ (4.303)}{(1.732)}$

TABLE 7 (Concluded)

HYDROCARBON NAME	K.I.-101	K.I. SAMP.	σ	95% C.L.	A%	K.I.-17	K.I. SAMP.	σ	95% CL	A%
1,2,4-Trimethylbenzene	976.91	976.72	0.06	0.14	1.24	1080.84	1081.18	0.02	0.06	1.18
3-Ethylnonane	992.53	992.37	0.04	0.10	0.06	1064.57	1064.64	0.01	0.03	0.14
sec-Butylbenzene	995.09	994.85	0.04	0.11	0.24	1090.33	1090.64	0.01	0.02	0.09
1,2,3-Trimethylbenzene	1003.68	1003.50	0.04	0.10	0.50	1120.33	1120.73	0.01	0.02	0.61
p-Cymene	1009.38	1009.33	0.07	0.16	0.09	1104.61	1104.21	0.00	0.00	0.27
n-Butylcyclohexane	1025.65	1025.62	0.03	0.07	0.25	1054.03	1054.08	0.00	0.01	0.29
1-Methyl-3-Propylbenzene	1035.51	1035.47	0.02	0.06	0.33	1134.57	1134.98	0.01	0.03	0.26
1,4-Diethylbenzene	1038.88	1039.13	0.02	0.06	0.42	1142.00	1142.50	0.02	0.04	0.11
1,3-Dimethyl-5-Ethylbenzene	1042.81	1042.84	0.02	0.05	(1042.88)*	1144.78	1145.15	0.02	0.04	0.05
trans-Decalin	1042.88*	1042.84	0.02	0.05	0.45	1102.06	1102.22	0.08	0.19	0.33
Neopentylbenzene	1048.25	1048.13	0.05	0.12	0.05	1135.95	1136.49	0.03	0.08	0.11
1-Methyl-2-Propylbenzene	1049.75	1049.70	0.05	0.12	0.24	1154.98	1155.39	0.02	0.05	0.21
1,4-Dimethyl-2-Ethylbenzene	1060.58*	1060.79	0.01	0.04	0.43	1166.50	1166.92	0.03	0.06	0.15
4-Methyldecane	1061.06	1060.79	0.01	0.04	(1060.58)*	1156.61	1156.29	0.02	0.05	0.14
1,3-Dimethyl-4-Ethylbenzene	1062.14	1062.09	0.01	0.04	0.18	1168.99	1169.40	0.03	0.08	0.19
1,2-Dimethyl-4-Ethylbenzene	1068.04	1068.05	0.07	0.17	0.35	1176.59	1176.96	0.03	0.07	0.20
cis-Decalin	1084.51	1084.54	0.01	0.01	0.09	1158.23	1158.30	0.02	0.05	0.09
1,2-Dimethyl-3-Ethylbenzene	1086.88	1086.69	0.01	0.01	0.26	1206.44	1206.25	0.02	0.05	0.12
2,6-Dimethyldecane	1119.35	1119.34	0.02	0.04	0.11	1109.50	1109.59	0.00	0.01	0.11
1,2,3,4-Tetramethylbenzene	1132.90	1132.81	0.04	0.10	0.18	1257.40	1257.21	0.20	0.50	0.09
1,4-Diisopropylbenzene	1157.71	1158.05	0.01	0.02	0.08	1257.77	1258.16	0.18	0.45	0.05
2-Methylundecane	1164.88	1164.91	0.00	0.00	0.28	1159.30	1159.53	0.02	0.06	0.23
Butane					0.27					0.26
Pentane					1.28					1.26
Hexane					2.73					2.88
Heptane					4.62					4.72
Octane					4.05					3.53
Nonane					3.21					3.40
Decane					2.64					3.07
Undecane					2.09					1.88
Dodecane					1.04					1.06
Tridecane					0.73					0.81
[illegible]					0.50					0.46
[illegible]					0.20					0.25
[illegible]					0.07					0.06
					70.82					71.69

TABLE 8

PETROLEUM DERIVED JP-4 FUEL 1B-62B-792009

	OV-101					OV-17				
HYDROCARBON NAME	K.I.-101	K.I. SAMP.	σ	95% C.L.	A%	K.I.-17	K.I. SAMP.	σ	95% C.L.	A%
2-Methylbutane	464.94	464.98	0.24	0.59	0.93	462.44	462.15	0.77	1.92	0.91
2-Methylpentane	561.64	561.86	0.04	0.10	1.07	534.27	534.34	0.17	0.43	1.21
3-Methylpentane	578.11	577.88	0.18	0.46	0.82	549.70	550.17	0.15	0.36	0.56
Benzene	642.11	641.98	0.08	0.21	0.29	739.24	739.09	0.06	0.15	(739.15)*
2-Methylhexane	659.24	659.22	0.07	0.18	0.85	638.62	639.17	0.31	0.77	0.86
Methylcyclohexane	715.63	715.65	0.01	0.03	3.30	739.15*	739.09	0.06	0.15	4.15
Ethylcyclopentane	725.43	725.49	0.10	0.25	0.55	749.43	748.98	0.13	0.14	1.83
2,5-Dimethylhexane	726.53	726.46	0.04	0.10	0.13	717.57	717.55	0.02	0.04	0.14
2,4-Dimethylhexane	728.30	728.24	0.04	0.10	0.22	720.98	720.89	0.16	0.39	0.22
3,3-Dimethylhexane	734.72	734.69	0.02	0.05	0.04	731.49	731.36	0.07	0.17	0.05
2,3,3-Trimethylpentane	747.10	747.52	0.05	0.13	0.80	751.82	751.73	0.05	0.12	0.23
2,3-Dimethylhexane	754.03	754.09	0.03	0.08	0.37	751.82	751.73	0.05	0.12	0.23
2-Methylheptane	760.60	760.47	0.03	0.07	1.71	753.77	753.66	0.05	0.12	0.52
4-Methylheptane	762.04	761.96	0.05	0.12	0.48	757.35	757.23	0.13	0.32	1.22
3,4-Dimethylhexane	763.74	763.61	0.02	0.05	0.17	765.11	764.95	0.12	0.31	(765.12)*
3-Methylheptane	768.75	768.58	0.03	0.07	0.95	765.12*	764.95	0.12	0.31	0.23
3-Ethylhexane	769.84*	770.03	0.03	0.08	1.82	768.08	767.82	0.09	0.22	1.66
cis-1,3-Dimethylcyclohexane	769.96	770.03	0.03	0.08	(769.84)*	794.50	794.50	0.10	0.25	1.13
1,1-Dimethylcyclohexane	778.06	778.14	0.06	0.14	0.18	806.05	806.52	0.00	0.00	0.32
cis-1,2-Dimethylcyclohexane	820.39	820.56	0.06	0.15	(821.03)*	851.27	851.07	0.00	0.00	2.24
2,4-Dimethylheptane	821.03*	820.56	0.06	0.15	0.47	812.35	812.23	0.00	0.00	0.86
cis,cis,cis,-1,3,5-Trimethylcyclohexane	825.38	825.16	0.03	0.08	1.64	838.47	838.23	0.10	0.25	2.37
2,6-Dimethylheptane	827.06	826.91	0.02	0.06	0.72	816.99	816.82	0.00	0.00	0.29
1,1,3-Trimethylcyclohexane	830.35	830.28	0.03	0.07	1.31	846.55*	846.38	0.10	0.25	0.43
1,1,4-Trimethylcyclohexane	832.51*	832.96	0.04	0.10	0.43	846.25	846.38	0.10	0.25	(846.55)*
2,5-Dimethylheptane	833.18	832.96	0.04	0.10	(832.51)*	825.03	824.87	0.00	0.00	0.20
3,3-Dimethylheptane	834.68	835.15	0.01	0.03	0.19	830.23	829.87	0.00	0.00	0.08
Ethylbenzene	843.07	843.03	0.01	0.03	1.07	944.10	943.77	0.04	0.09	0.43
cis,trans,trans-1,2,4-Trimethylcyclohexane	844.82	844.76	0.01	0.04	0.58	861.39	861.16	0.00	0.00	1.2
m-Xylene	851.82	851.57	0.09	0.22	0.77	950.03	949.90	0.02	0.05	(950.20)*
p-Xylene	852.80	852.94	0.02	0.05	0.88	948.44	948.40	0.02	0.06	0.31
4-Ethylheptane	858.32	858.69	0.01	0.03	0.15	853.31	853.82	0.00	0.00	1.37
4-Methyloctane	861.46	861.29	0.04	0.10	0.60	856.49	856.07	0.10	0.25	0.56
2-Methyloctane	862.66	862.41	0.04	0.10	0.71	856.17	856.07	0.10	0.25	0.56
cis,trans,cis-1,2,3-Trimethylcyclohexane	867.35	867.40	0.02	0.04	0.51	892.49	892.18	0.06	0.15	0.63
3-Methyloctane	869.43	869.20	0.02	0.05	1.13	865.52	865.24	0.00	0.00	0.36
cis-1-Ethyl-3-Methylcyclohexane	881.29	881.17	0.06	0.15	0.75	906.01	905.82	0.08	0.21	0.45
trans-1-Ethyl-2-Methylcyclohexane	901.06	901.03	0.07	0.17	0.65	927.63	927.30	0.01	0.03	0.51
1-Ethyl-1-Methylcyclohexane	903.14	903.02	0.07	0.18	0.07	933.95	933.65	0.07	0.18	0.08
cis-1-Ethyl-4-Methylcyclohexane	903.98	903.91	0.00	0.01	0.07	930.25	929.97	0.04	0.10	0.08
Cumene	908.92	908.69	0.04	0.11	0.20	1006.06	1005.94	0.04	0.09	0.25
Isopropylcyclohexane	912.85	912.67	0.05	0.13	0.27	943.24	943.07	0.08	0.20	0.24
2,2-Dimethyloctane	917.98	918.02	0.05	0.12	0.24	908.18	908.03	0.00	0.91	0.14
cis-1-Ethyl-2-Methylcyclohexane	920.98	920.83	0.05	0.12	0.11	954.58	954.53	0.02	0.06	(954.84)*
n-Propylcyclohexane	923.29	923.23	0.05	0.13	0.90	950.92	950.80	0.02	0.05	2.06
2-7-Dimethyloctane	929.14	929.43	0.03	0.08	0.34	919.32	919.17	0.04	0.10	0.13
2,6-Dimethyloctane	933.62*	933.50	0.05	0.12	1.06	925.44	925.30	0.03	0.08	0.97
n-Propylbenzene	937.01	936.82	0.01	0.03	(933.62)*	1035.65	1035.68	0.02	0.06	0.28
3-Ethyl-3-Methylheptane	940.32	940.20	0.03	0.07	1.57	946.53	946.73	0.02	0.05	0.30
1-Ethyl-3-Methylbenzene	944.83*	944.68	0.03	0.08	0.52	1046.12	1046.01	0.02	0.05	0.87
4-Propylheptane	944.91	944.68	0.03	0.08	(944.83)*	937.76	937.30	0.03	0.07	0.16
1,3,5-Trimethylbenzene	952.83	952.76	0.06	0.14	0.77	1051.36	1051.40	0.02	0.05	0.28
4-Methylnonane	954.97	954.77	0.06	0.14	0.18	950.20*	949.90	0.02	0.05	0.91
5-Methylnonane	959.55	959.36	0.07	0.17	0.30	954.84*	954.53	0.02	0.06	0.38
4-Ethyloctane	961.30*	961.15	0.04	0.11	0.91	956.33	956.10	0.02	0.06	0.69
1-Ethyl-2-Methylbenzene	961.45	961.15	0.04	0.11	(961.30)*	1070.46	1070.61	0.03	0.07	0.26
2-Methylnonane	963.97	963.85	0.08	0.21	0.88	957.96	957.83	0.03	0.06	0.68
3-Ethyloctane	966.99	966.64	0.05	0.12	0.30	964.56	964.30	0.02	0.04	0.14
trans-1-Methyl-4-Isopropylcyclohexane	969.7	970.20	0.05	0.13	0.74	992.19	992.10	0.04	0.10	0.29
1,2,4-Trimethylbenzene	976.91	976.70	0.02	0.05	1.06	1080.84	1080.97	0.04	0.09	1.16
3-Ethylnonane	992.53	992.43	0.07	0.18	0.04	1064.57	1064.63	0.05	0.14	0.17
sec-Butylbenzene	995.09	994.72	0.06	0.16	0.28	1090.33	1090.48	0.03	0.09	0.15
1,2,3-Trimethylbenzene	1003.68	1003.51	0.07	0.19	0.47	1120.33	1120.54	0.02	0.04	0.44
1-Methyl-3-Isopropylbenzene	1006.59	1006.38	0.07	0.19	0.17	1103.84	1104.02	0.06	0.15	0.12
p-Cymene	1009.38	1009.34	0.07	0.17	0.09	1104.61	1104.79	0.06	0.15	0.24
n-Butylcyclohexane	1025.65	1025.63	0.04	0.10	0.35	1054.03	1054.05	0.02	0.05	0.40
1-Methyl-3-Propylbenzene	1035.51	1035.41	0.05	0.12	0.26	1134.57	1134.86	0.04	0.11	0.20

NOTE: 95% Confidence Limit for 3 Determinations = $\frac{(\sigma)(4.303)}{(1.732)}$

TABLE 8 (Concluded)

HYDROCARBON NAME	K.I.-101	K.I.-SAMP.	σ	95% C.L.	A%	K.I.-17	K.I.-SAMP.	σ	95% C.L.	A%
1,3-Dimethyl-5-Ethylbenzene	1042.81*	1042.90	0.01	0.04	0.45	1144.78	1145.05	0.07	0.10	0.16
trans-Decalin	1042.88	1042.90	0.01	0.04	(1042.81)*	1102.06	1102.18	0.07	0.18	0.45
Neopentylbenzene	1048.25	1048.11	0.03	0.08	0.07	1135.95	1136.44	0.03	0.08	0.06
1-Methyl-2-Propylbenzene	1049.75	1049.67	0.06	0.14	0.21	1154.98	1155.25	0.00	0.01	0.02
4-Methyldecane	1061.06	1060.93	0.03	0.07	0.38	1056.61	1056.57	0.02	0.05	0.28
1,3-Dimethyl-4-Ethylbenzene	1062.14	1062.06	0.05	0.13	0.10	1168.99	1169.33	0.03	0.08	0.09
2-Methyldecane	1064.77	1064.79	0.03	0.08	0.35	1059.14	1059.06	0.05	0.13	0.37
1,2-Dimethyl-4-Ethylbenzene	1068.04	1068.07	0.06	0.14	0.20	1176.59*	1176.98	0.06	0.14	0.10
tert-Pentylbenzene	1076.00	1076.44	0.06	0.15	0.02	1176.49	1176.98	0.06	0.14	(1176.59)*
cis-Decalin	1084.51	1084.54	0.06	0.16	0.09	1158.23	1158.40	0.04	0.10	0.08
2,6-Dimethyldecane	1119.35	1119.32	0.05	0.13	0.10	1109.50	1109.55	0.07	0.17	0.09
Butane					0.38					0.39
Pentane					1.43					1.43
Hexane					2.30					2.24
Heptane					3.23					3.34
Octane					4.55					3.71
Nonane					4.66					4.92
Decane					3.46					4.27
Undecane					1.86					1.85
Dodecane					0.24					0.25
Tridecane					0.03					0.04
TOTAL					62.70					64.49

TABLE 9

SHALE DERIVED JP-4 FUEL 15B-792009

	OV-101					OV-17				
HYDROCARBON NAME	K.I.-101	K.I. SAMP.	σ	95% C.L.	A%	K.I.-17	K.I. SAMP.	σ	95% C.L.	A%
2-Methylbutane	464.94	464.98	0.24	0.59	0.52	462.44	462.15	0.77	1.92	0.50
Benzene	642.11	642.08	0.13	0.32	0.14	739.24	739.18	0.06	0.16	(739.15)*
Cyclohexane	650.27	650.22	0.00	0.00	0.51	687.73	687.99	0.26	0.64	0.51
2-Methylhexane	659.24	659.19	0.00	0.00	0.45	638.62	639.08	0.53	1.32	0.44
3-Methylhexane	669.11	669.06	0.00	0.00	1.02	655.49	655.84	0.39	0.96	1.03
3-Ethylpentane	681.54	681.39	0.00	0.00	0.06	678.53	678.85	0.26	0.64	0.05
Methylcyclohexane	715.63	715.63	0.04	0.11	1.90	739.15*	739.18	0.06	0.16	2.00
Ethylcyclopentane	725.43	725.50	0.05	0.12	0.23	749.43	749.35	0.05	0.13	0.35
2,5-Dimethylhexane	726.53	726.51	0.03	0.07	0.06	717.57	717.54	0.12	0.30	0.07
2,4-Dimethylhexane	728.30	728.28	0.07	0.17	0.21	720.98	720.99	0.08	0.20	0.43
Methylbenzene	747.63	747.58	0.06	0.14	1.26	845.42	845.70	0.02	0.05	0.86
2,3-Dimethylhexane	754.03	754.07	0.04	0.10	0.28	751.82	751.66	0.05	0.12	0.22
2-Methylheptane	760.60	760.48	0.09	0.23	1.03	753.77	753.63	0.05	0.12	1.11
4-Methylheptane	762.04	762.05	0.05	0.13	0.45	757.35	757.25	0.13	0.32	0.49
3-Methylheptane	768.75	768.65	0.02	0.06	0.55	765.12	765.04	0.04	0.09	0.79
3-Ethylhexane	769.84	770.10	0.03	0.06	(769.96)*	768.08	767.90	0.03	0.08	0.45
cis-1,3-Dimethylcyclohexane	769.96*	770.10	0.03	0.06	1.26	794.50	794.59	0.21	0.52	1.24
cis-1,2-Dimethylcyclohexane	820.39	820.45	0.04	0.10	0.44	851.27	851.31	0.03	0.07	0.34
cis,cis,cis-1,3,5-Trimethylcyclohexane	825.38	825.26	0.02	0.06	0.91	838.47	838.38	0.01	0.02	0.08
2,6-Dimethylheptane	827.06	827.04	0.02	0.05	0.61	816.99	816.94	0.03	0.07	0.61
1,1,3-Trimethylcyclohexane	830.35	830.32	0.02	0.05	0.86	846.55	846.53	0.02	0.06	1.39
3,3-Dimethylheptane	834.68	834.14	0.06	0.16	0.07	830.23	830.03	0.01	0.01	0.03
Ethylbenzene	843.07	843.11	0.01	0.02	0.41	944.10	944.16	0.08	0.19	0.17
cis,trans,trans-1,2,4-Trimethylcyclohexane	844.82	844.83	0.00	0.01	0.51	861.39	861.34	0.11	0.27	0.49
cis,cis,trans-1,3,5-Trimethylcyclohexane	848.69	848.66	0.05	0.12	0.11	868.09	868.01	0.11	0.26	0.08
m-Xylene	851.82	851.67	0.05	0.12	0.87	950.03*	950.16	0.04	0.11	2.10
p-Xylene	852.80	852.95	0.00	0.01	0.57	948.44	948.68	0.08	0.19	0.08
2-Methyloctane	862.66	862.52	0.04	0.09	0.32	856.17	856.22	0.07	0.18	0.76
cis,trans,cis-1,2-3-Trimethylcyclohexane	867.35	867.39	0.02	0.04	0.37	892.49	892.41	0.11	0.26	0.34
cis,trans,cis-1,2,4-Trimethylcyclohexane	869.09	869.30	0.04	0.10	(869.43)*	894.23	894.06	0.11	0.27	0.42
3-Methyloctane	869.43*	869.30	0.04	0.10	0.92	865.52	865.33	0.00	0.01	1.24
o-Xylene	874.53	874.44	0.02	0.06	0.67	981.56	981.81	0.04	0.11	0.60
cis-1-Ethyl-3-Methylcyclohexane	881.29	881.30	0.02	0.04	0.53	906.01	905.98	0.04	0.11	1.55
trans-1-Ethyl-2-Methylcyclohexane	901.06	901.23	0.00	0.00	0.50	927.63	927.41	0.04	0.11	1.03
cis-1-Ethyl-4-Methylcyclohexane	903.98	903.97	0.00	0.01	0.17	930.25	930.12	0.04	0.11	0.12
Cumene	908.92	908.76	0.01	0.01	0.06	1006.00	1005.74	0.04	0.10	0.08
Isopropylcyclohexane	912.85	912.79	0.01	0.02	0.25	943.24	943.10	0.00	0.00	0.19
cis-1-Ethyl-2-Methylcyclohexane	920.98	920.95	0.05	0.13	0.17	954.58	954.53	0.04	0.11	0.36
2,7-Dimethyloctane	929.14	929.53	0.02	0.06	0.20	919.33	919.27	0.04	0.11	0.08
2,6-Dimethyloctane	933.62	933.61	0.02	0.06	0.98	925.44	925.42	0.09	0.22	1.09
3-Ethyl-3-Methylheptane	940.32	940.20	0.02	0.05	0.55	946.53	946.82	0.09	0.22	0.02
1-Ethyl-3-Methylbenzene	944.83	944.71	0.02	0.05	0.45	1046.12	1046.02	0.06	0.14	1.34
1,3,5-Trimethylbenzene	952.83	952.76	0.02	0.05	0.51	1051.36	1051.63	0.02	0.05	0.07
4-Methylnonane	954.97	954.83	0.02	0.05	0.25	950.20	950.16	0.04	0.11	(950.03)*
4-Ethyloctane	961.30*	961.24	0.02	0.05	0.69	956.33	956.19	0.04	0.11	0.65
1-Ethyl-2-Methylbenzene	961.45	961.24	0.02	0.05	(961.30)*	1070.46	1070.72	0.01	0.03	0.10
2-Methylnonane	963.97	963.86	0.02	0.05	0.36	957.96	957.80	0.00	0.00	0.83
3-Ethyloctane	966.99	966.74	0.02	0.06	0.17	964.56	964.33	0.04	0.11	0.05
3-Methylnonane	970.32	970.18	0.02	0.05	0.55	966.96	966.84	0.00	0.00	1.09
1,2,4-Trimethylbenzene	976.91	976.72	0.03	0.07	0.67	1080.84	1081.01	0.07	0.17	1.37
cis-1-Methyl-4-Isopropylcyclohexane	983.78	983.77	0.03	0.08	0.21	1012.55	1012.37	0.04	0.11	0.12
3-Ethylnonane	992.53	992.43	0.04	0.11	0.08	1064.57	1064.49	0.01	0.03	0.44
1,2,3-Trimethylbenzene	1003.68	1003.48	0.04	0.10	0.36	1120.33	1120.49	0.07	0.17	0.35
p-Cymene	1009.38	1009.32	0.00	0.01	0.18	1104.61	1104.64	0.03	0.08	0.53
Indan	1013.44	1013.29	0.01	0.01	0.14	1147.39	1147.63	0.04	0.09	0.03
n-Butylcyclohexane	1025.65	1025.59	0.03	0.07	0.49	1054.03	1053.98	0.06	0.15	0.54
1-Methyl-3-Propylbenzene	1035.51	1035.43	0.02	0.06	0.38	1134.57	1134.66	0.01	0.03	0.42
trans-Decalin	1042.88*	1042.88	0.07	0.17	1.00	1102.07	1102.01	0.00	0.00	0.83
1,3-Dimethyl-5-Ethylbenzene	1042.81	1042.88	0.07	0.17	(1042.88)*	1144.78	1144.87	0.04	0.10	0.05
1,4-Dimethyl-2-Ethylbenzene	1060.58	1060.88	0.09	0.22	0.54	1166.50	1166.52	0.05	0.12	0.06
1,3-Dimethyl-4-Ethylbenzene	1062.14	1062.01	0.01	0.04	0.13	1168.99	1169.09	0.01	0.04	0.05
1,2-Dimethyl-4-Ethylbenzene	1068.04	1067.96	0.03	0.06	0.23	1176.59*	1176.70	0.02	0.04	0.05
tert-Pentylbenzene	1076.00	1076.37	0.03	0.07	0.08	1176.49	1176.70	0.02	0.04	(1176.59)*
cis-Decalin	1084.51	1084.49	0.01	0.01	0.41	1158.23	1158.11	0.04	0.11	0.36
1-Undecene	1088.37	1088.14	0.00	0.01	0.33	1106.67	1106.86	0.01	0.01	0.03

NOTE: 95% Confidence Limit for 3 Determinations = $\frac{(\sigma)\ (4.303)}{(1.732)}$

TABLE 9 (Concluded)

HYDROCARBON NAME	K.I.-101	K.I. SAMP.	σ	95% C.L.	A%	K.I.-17	K.I. SAMP.	σ	95% C.L.	A%
1,2,3,5-Tetramethylbenzene	1102.85	1102.65	0.04	0.09	0.07	1216.82	1217.15	0.04	0.10	0.24
2,6-Dimethyldecane	1119.35	1119.17	0.08	0.20	0.28	1109.50	1109.40	0.07	0.17	0.35
Tetralin	1136.43	1136.37	0.06	0.14	0.60	1288.39	1288.71	0.00	0.00	0.29
n-Pentylbenzene	1141.13	1140.86	0.04	0.10	0.29	1242.74	1243.07	0.04	0.10	0.14
2-Methylundecane	1164.88	1164.79	0.03	0.08	0.31	1159.30	1159.25	0.01	0.02	0.59
1-tert-Butyl-4-Ethylbenzene	1165.62	1166.13	0.07	0.17	0.06	1266.63	1266.76	0.04	0.10	0.06
Butane					0.94					0.94
Pentane					0.91					0.88
Hexane					1.22					1.34
Heptane					1.58					1.75
Octane					2.50					1.71
Nonane					2.42					2.87
Decane					3.76					4.32
Undecane					5.55					4.71
Dodecane					3.84					4.12
Tridecane					2.03					2.13
Tetradecane					0.81					0.84
Pentadecane					0.32					0.37
Hexadecane					0.15					0.14
Heptadecane					0.07					0.06
Octadecene					0.03					0.03
TOTAL					56.93					61.03

TABLE 10

SYNCRUDE JP-4

HYDROCARBON NAME	K.I.-101	K.I. SAMP	σ	95% C.L.	A%	K.I.-17	K.I. SAMP.	σ	95% C.L.	A%
2-Methylbutane	464.94	464.98	0.24	0.59	0.66	462.44	462.60	0.77	1.92	0.61
Methylcyclopentane	620.07	619.96	0.08	0.19	0.38	623.49	623.82	0.14	0.35	0.40
Cyclohexane	650.27	650.11	0.00	0.00	0.13	687.73	687.67	0.26	0.65	0.13
2,3-Dimethylpentane	661.36	661.13	0.10	0.25	0.32	649.08	649.49	0.00	0.01	0.33
3-Methylhexane	669.11	668.95	0.08	0.20	1.58	655.49	655.74	0.28	0.69	1.67
1-cis-2-Dimethylcyclopentane	714.85	714.77	0.04	0.11	0.27	737.03	736.89	0.10	0.25	0.36
Methylcyclohexane	715.63	715.53	0.03	0.07	1.52	739.15	738.96	0.10	0.25	2.03
Ethylcyclopentane	725.43	725.28	0.05	0.12	0.76	749.43	749.02	0.00	0.00	1.13
2,5-Dimethylhexane	726.53	726.28	0.05	0.11	0.07	717.57	717.47	0.21	0.51	0.09
2,4-Dimethylhexane	728.30	728.05	0.05	0.13	0.15	720.98	720.78	0.00	0.00	0.14
2,3,3-Trimethylpentane	747.10	747.31	0.09	0.22	(747.63)*	751.82*	751.45	0.21	0.51	0.04
Methylbenzene	747.63*	747.31	0.09	0.22	1.51	845.42	845.23	0.09	0.21	1.13
2,3-Dimethylhexane	754.03	754.13	0.04	0.10	0.32	751.82	751.45	0.21	0.51	(751.82)*
2-Methylheptane	760.60	760.39	0.05	0.13	2.64	753.77	753.46	0.00	0.00	2.96
4-Methylheptane	762.04	761.84	0.05	0.13	0.65	757.35	757.02	0.00	0.00	0.75
3,4-Dimethylhexane	763.74	763.28	0.06	0.14	0.07	765.11	764.71	0.10	0.25	(765.12)*
3-Methylheptane	768.75	768.34	0.06	0.16	0.82	765.12*	764.71	0.10	0.25	0.96
cis-1,3-Dimethylcyclohexane	769.96	769.78	0.07	0.17	0.84	794.50	794.20	0.21	0.51	0.65
1,1-Dimethylcyclohexane	778.06	777.97	0.08	0.20	0.13	806.05	806.34	0.05	0.12	0.74
cis-1,2-Dimethylcyclohexane	820.39	820.22	0.06	0.15	0.17	851.27	850.86	0.11	0.26	0.05
2,4-Dimethylheptane	821.03	821.20	0.06	0.16	0.08	812.35	812.11	0.04	0.09	0.18
2,6-Dimethylheptane	827.06	826.82	0.02	0.05	1.24	816.99	816.70	0.14	0.34	1.36
1,1,3-Trimethylcyclohexane	830.35	830.14	0.03	0.07	1.22	846.55	846.16	0.02	0.06	(846.25)*
1,1,4-Trimethylcyclohexane	832.51	832.84	0.03	0.07	(833.18)*	846.25*	846.16	0.02	0.06	1.81
2,5-Dimethylheptane	833.18*	832.84	0.03	0.07	0.28	825.03	824.62	0.07	0.19	0.20
Ethylbenzene	843.07	842.74	0.02	0.06	0.71	944.10	943.66	0.02	0.06	0.53
m-Xylene	851.82	851.46	0.02	0.06	1.65	950.03	949.66	0.04	0.09	2.23
p-Xylene	852.81	852.52	0.02	0.06	0.72	948.44	948.20	0.02	0.05	0.39
4-Ethylheptane	858.32	858.52	0.02	0.06	0.12	853.31	853.57	0.04	0.09	0.82
cis,trans,lis-1,2,3-Trimethylcyclohexane	867.35	867.29	0.03	0.07	0.21	892.49	892.08	0.01	0.04	0.18
o-Xylene	874.53	874.11	0.05	0.13	0.93	981.56	981.32	0.01	0.02	1.18
cis-1-Ethyl-3-Methylcyclohexane	881.29	881.06	0.05	0.12	0.24	906.01	905.72	0.00	0.01	0.12
1-Ethyl-1-Methylcyclohexane	903.14	902.83	0.04	0.10	0.02	933.95	933.37	0.06	0.16	0.08
cis-1-Ethyl-4-Methylcyclohexane	903.98	903.76	0.00	0.01	0.04	930.25	929.80	0.03	0.08	0.04
2,2-Dimethyloctane	917.78	917.80	0.04	0.10	0.07	908.18	907.81	0.04	0.10	0.06
cis-1-Ethyl-2-Methylcyclohexane	920.98	920.72	0.02	0.05	0.06	954.58	954.23	0.02	0.06	0.19
2,7-Dimethyloctane	929.14	928.99	0.05	0.13	0.20	919.33	918.91	0.01	0.02	0.14
2,6-Dimethyloctane	933.62	933.36	0.05	0.13	1.55	925.44	925.11	0.04	0.10	1.36
n-Propylbenzene	937.01	936.67	0.05	0.12	0.26	1035.65	1035.46	0.07	0.18	0.29
1-Ethyl-3-Methylbenzene	944.83	944.51	0.05	0.12	0.10	1046.12	1045.68	0.02	0.05	1.17
1,3,5-Trimethylbenzene	952.83	952.44	0.05	0.14	0.47	1051.36	1051.18	0.02	0.05	0.36
1-Ethyl-2-Methylbenzene	961.45	961.01	0.07	0.17	(961.30)*	1070.46	1070.31	0.05	0.11	0.35
4-Ethyloctane	961.30*	961.01	0.07	0.17	1.03	956.33	955.84	0.04	0.09	0.71
2-Methylnonane	963.97	963.61	0.03	0.07	0.68	957.96	957.49	0.04	0.09	0.50
3-Methylnonane	970.32	970.01	0.06	0.15	0.47	966.96	966.53	0.04	0.10	0.43
1,2,4-Trimethylbenzene	976.91	976.46	0.03	0.07	1.15	1080.84	1080.74	0.08	0.20	1.22
cis-1-Methyl-4-Isopropylcyclohexane	983.78	983.30	0.03	0.07	0.13	1012.55	1012.51	0.03	0.08	0.05
3-Ethylnonane	992.53	992.16	0.07	0.18	0.03	1064.57	1064.23	0.03	0.08	0.11
1,2,3-Trimethylbenzene	1003.68	1003.32	0.00	0.01	0.85	1120.33	1120.29	0.03	0.07	1.13
p-Cymene	1009.38	1009.13	0.01	0.01	0.20	1104.61	1104.44	0.04	0.09	0.33
Indan	1013.44	1013.12	0.07	0.17	0.26	1147.39	1147.59	0.02	0.05	0.21
n-Butylcyclohexane	1025.65	1025.40	0.02	0.06	0.19	1054.03	1053.64	0.02	0.04	0.19
1-Methyl-3-Propylbenzene	1035.51	1035.18	0.02	0.05	0.41	1134.57	1134.59	0.02	0.05	0.30
1,3-Dimethyl-5-Ethylbenzene	1042.81*	1042.50	0.03	0.07	0.32	1144.78	1144.86	0.05	0.13	0.25
trans-Decalin	1042.88	1042.50	0.03	0.07	(1042.81)*	1102.06	1101.62	0.00	0.00	0.05
1-Methyl-2-Propylbenzene	1049.75	1049.48	0.03	0.08	0.26	1154.98	1155.04	0.03	0.07	0.14
1,4-Dimethyl-2-Ethylbenzene	1060.58	1060.54	0.05	0.11	0.43	1166.50	1166.71	0.02	0.05	0.13
1,3-Dimethyl-4-Ethylbenzene	1062.14	1061.80	0.04	0.10	0.26	1168.99	1169.14	0.04	0.11	0.28
2-Methyldecane	1064.77	1064.62	0.02	0.05	0.60	1059.14	1058.68	0.02	0.04	0.37
1,2-Dimethyl-4-Ethylbenzene	1068.04	1067.77	0.02	0.05	0.25	1176.59*	1176.74	0.05	0.12	0.22
1,3-Dimethyl-2-Ethylbenzene	1073.15	1072.86	0.02	0.06	0.07	1187.93	1188.17	0.06	0.14	0.06
t-Pentylbenzene	1076.00	1076.23	0.04	0.10	0.03	1176.49	1176.74	0.05	0.12	(1176.59)*
cis-Decalin	1084.51	1084.20	0.03	0.07	0.06	1158.23	1158.07	0.05	0.12	0.08
1,2,3,5-Tetramethylbenzene	1102.85	1102.51	0.07	0.17	0.25	1216.82	1217.14	0.06	0.14	0.16
2,6-Dimethyldecane	1119.35	1119.10	0.05	0.12	0.18	1109.50	1109.21	0.07	0.17	0.27
1,2,3,4-Tetramethylbenzene	1132.90	1132.59	0.04	0.11	0.15	1257.40*	1257.85	0.08	0.20	0.22
1,4-Diisopropylbenzene	1157.71	1157.82	0.03	0.07	0.08	1257.77	1257.85	0.08	0.20	(1257.40)*
2-Methylundecane	1164.88	1164.75	0.02	0.06	0.22	1159.30	1159.26	0.04	0.10	0.37
1-Docecene	1188.62	1188.62	0.15	0.38	0.04	1206.80	1206.82	0.04	0.10	0.20
2-Methylpentylbenzene	1190.88	1191.33	0.03	0.08	0.06	1285.14	1285.49	0.08	0.19	0.18

NOTE: 95% Confidence Limit for 3 Determinations = $\frac{(\sigma)\ (4.303)}{(1.732)}$

TABLE 10 (Concluded)

HYDROCARBON NAME	K.I.-101	K.I. SAMP	σ	95% C.L.	A%	K.I.-17	K.I. SAMP.	σ	95% C.L.	A%
Butane					0.43					0.42
Pentane					0.69					0.75
Hexane					0.73					0.74
Heptane					7.58					8.78
Octane					7.72					7.66
Nonane					7.59					8.16
Decane					7.15					8.38
Undecane					6.14					6.79
Dodecane					2.71					2.70
Tridecane					0.08					0.11
Tetradecane					0.05					0.07
Pentadecane					0.03					0.11
TOTAL					72.72					79.89

Area percent is not intended to quantitatively determine the component but is used merely as a comparison tool to aid in the qualitative identification of peaks. For example, in shale derived JP-4 fuel 15-B (see Table 9), the area percent of the peak thought to be 2-Methylhexane is 0.45% on the OV-101 column and 0.44% on the OV-17 column. This comparative relationship lends additional credibility to the Kovats Index matching process.

The asterisks in the "K.I.-101," "K.I.-17", and "A%" columns indicate compounds that appear to have coeluted. The asterisked number in the "A%" column is actually the library index (i.e. "K.I.-101" or "K.I.-17") of the other compound with which that compound has appeared to coelute. For example, benzene and methylcyclohexane coelute on the OV-17 column. Furthermore, their OV-17 library indices, 739.24 and 739.15 respectively, both fall within the $\pm$ 0.5 assurance limit for the sample peak in petroleum derived JP-4 fuel 1B-792009 (see Table 6) having an index 739.18.

To clarify this situation, the area percents of the fuel 1B suspect constituents, benzene and methylcyclohexane, on the OV-101 were added and compared to the area percent of the OV-17 peak suspected to be coeluting benzene and methylcyclohexane. The resulting 1.48 A% on the OV-101 compared to the 1.44 A% on the OV-17 once again indicating the usefulness of area percent when matching peaks by Kovats Indices.

It must be pointed out, however, that these area percent relationships become increasingly difficult to observe in the middle of the distillation range of any given fuel sample. This is due primarily to the increased number of isomeric compounds existing in that boiling range and the present inability of the $(GC)^2$ system to resolve all of these compounds.

Figures 2 through 11 are chromatograms from both the OV-101 and OV-17 columns for the five fuels selected for analysis in this report. The three petroleum derived JP-4 fuels (1B-792009, 1B-49B-792009 and 1B-62B-792009) chosen for analysis in this report illustrate a need for the characterization of jet fuels in addition to those needs mentioned in

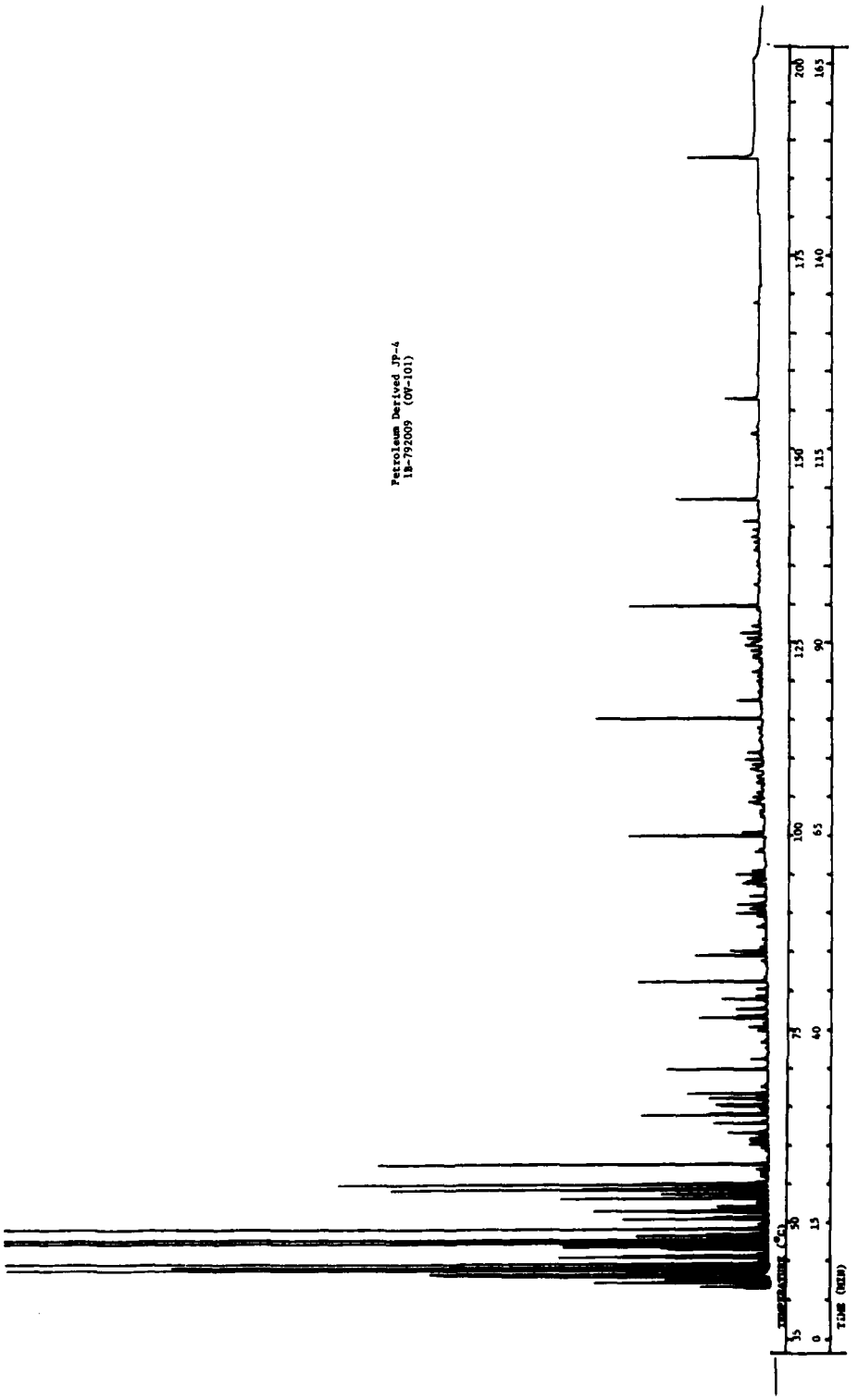

Figure 2. Petroleum Derived JP-4 1B-792009 (OV-101)

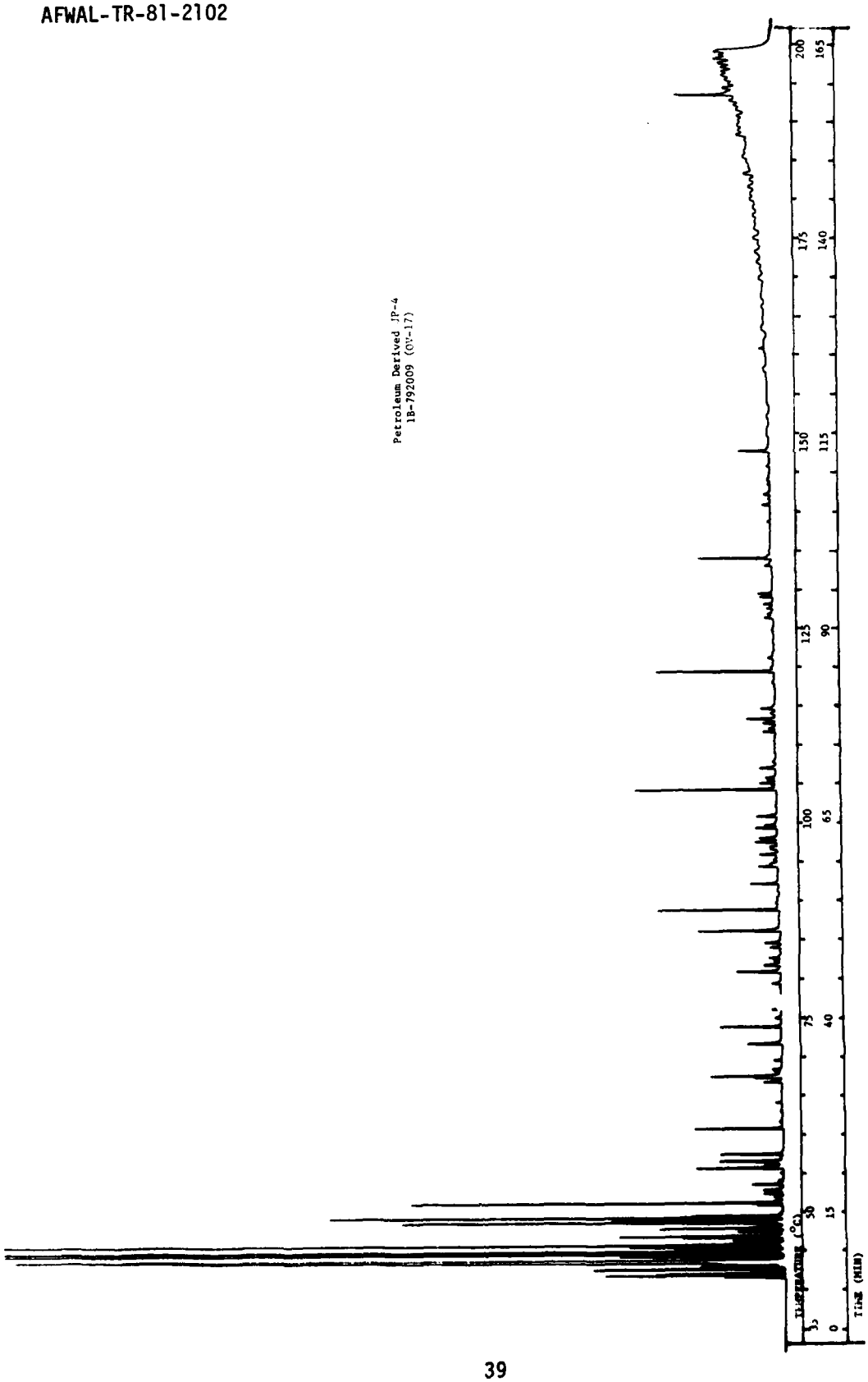

Figure 3. Petroleum Derived JP-4 1B-792009 (OV-17)

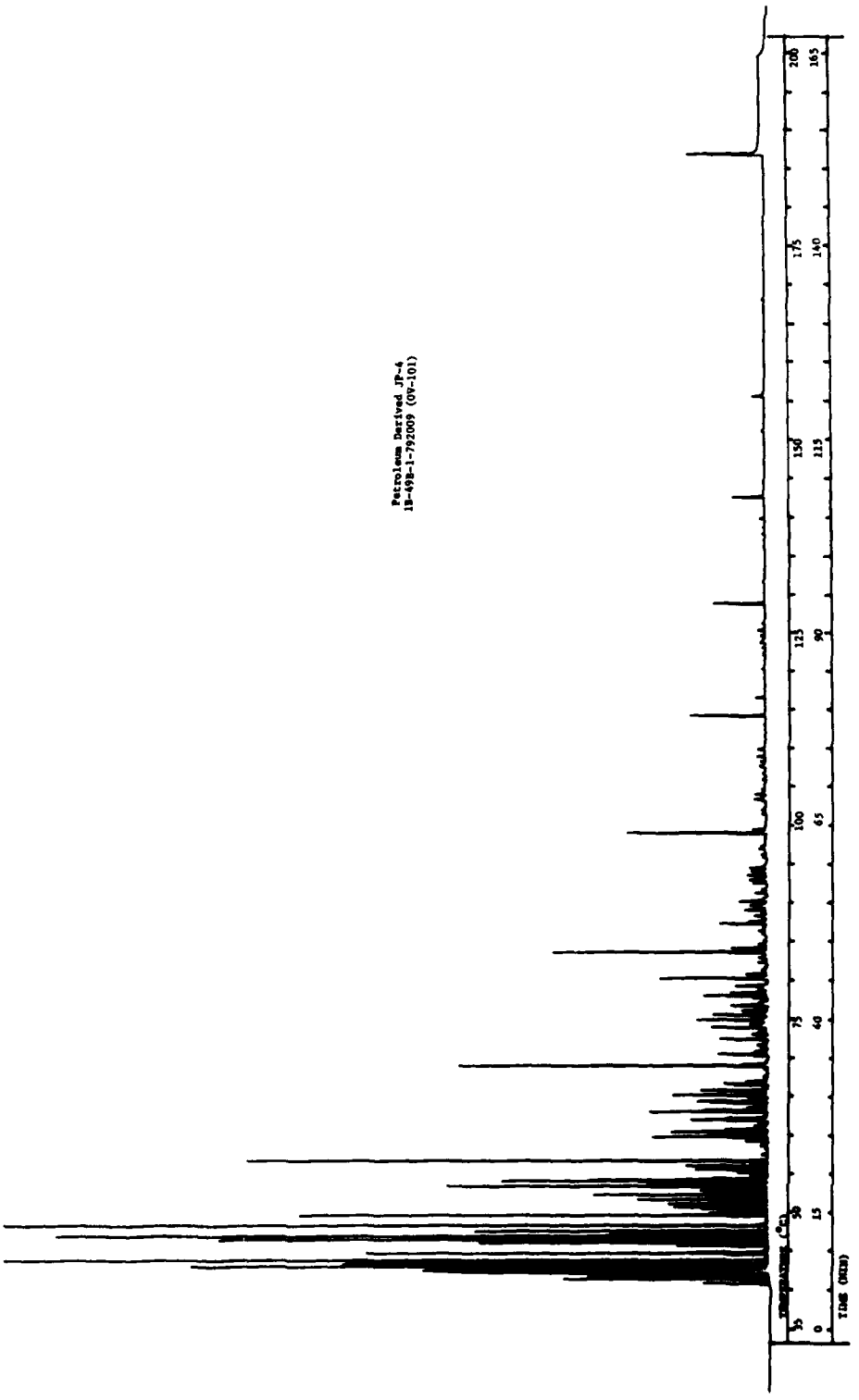

Figure 4. Petroleum Derived JP-4 1B-49B-792009 (OV-101)

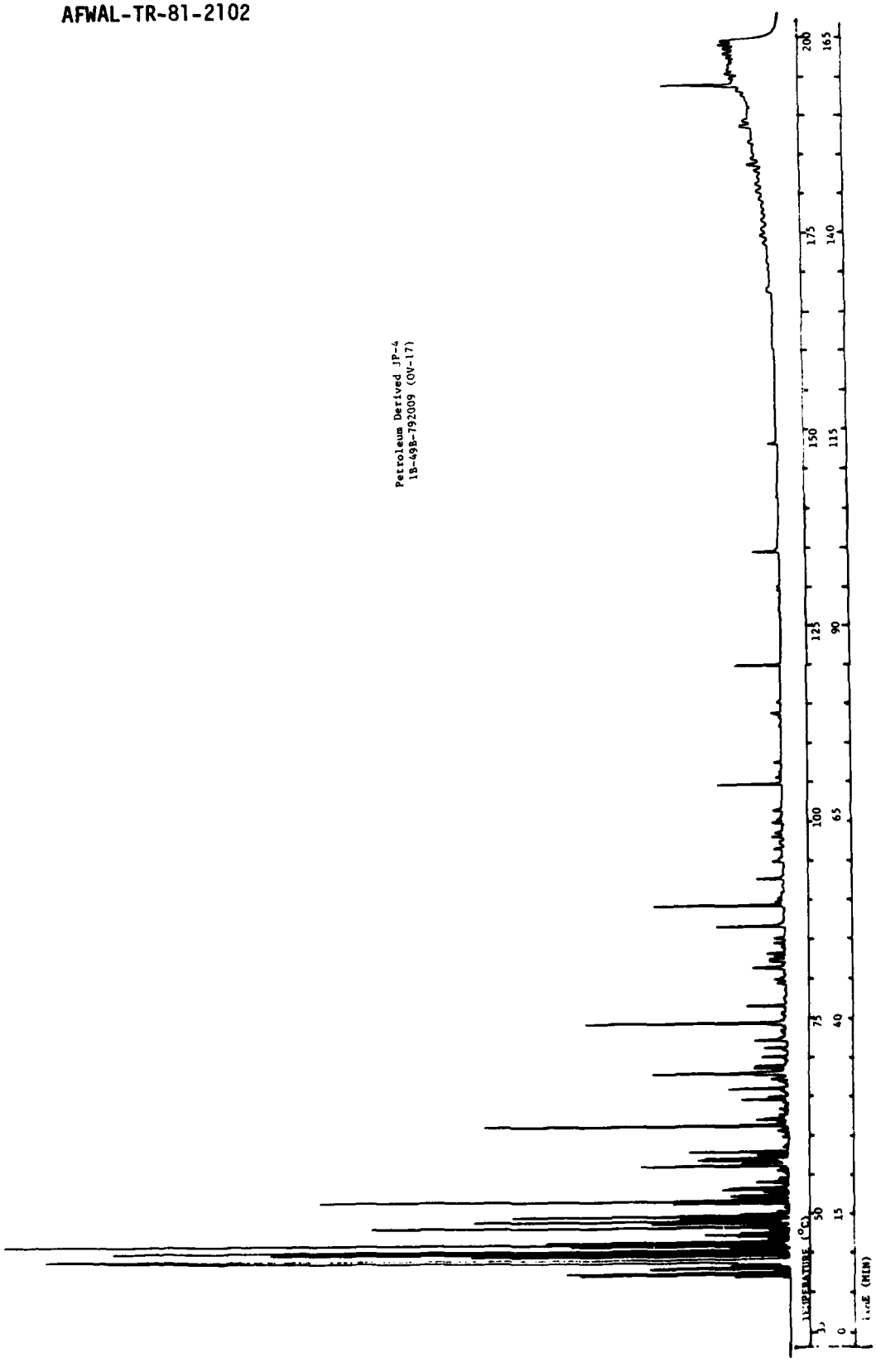

Figure 5. Petroleum Derived JP-4 1B-49B-792009 (OV-17)

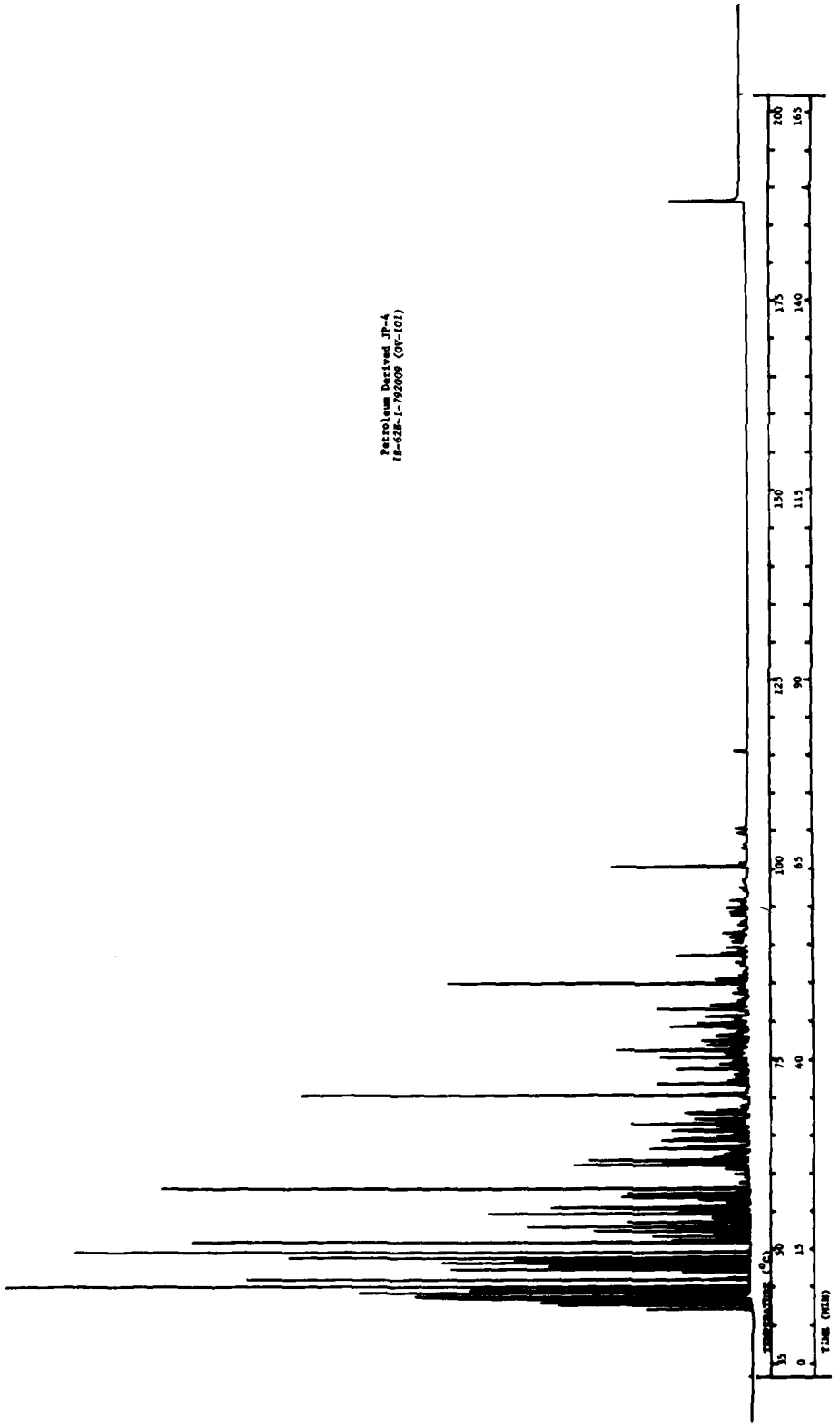

Figure 6. Petroleum Derived JP-4 1B-62B-792009 (OV-101)

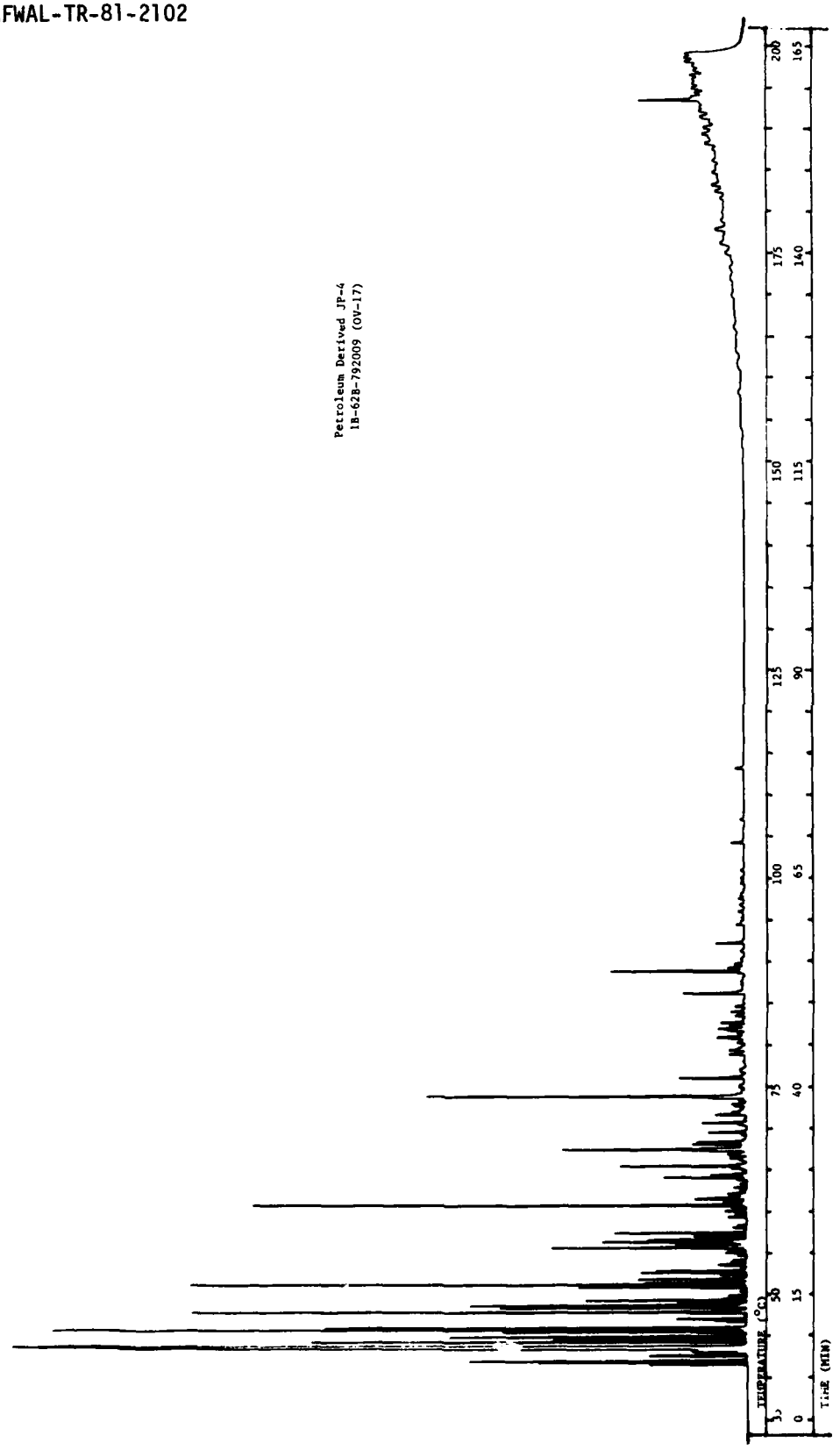

Figure 7. Petroleum Derived JP-4 1B-62B-792009 (OV-17)

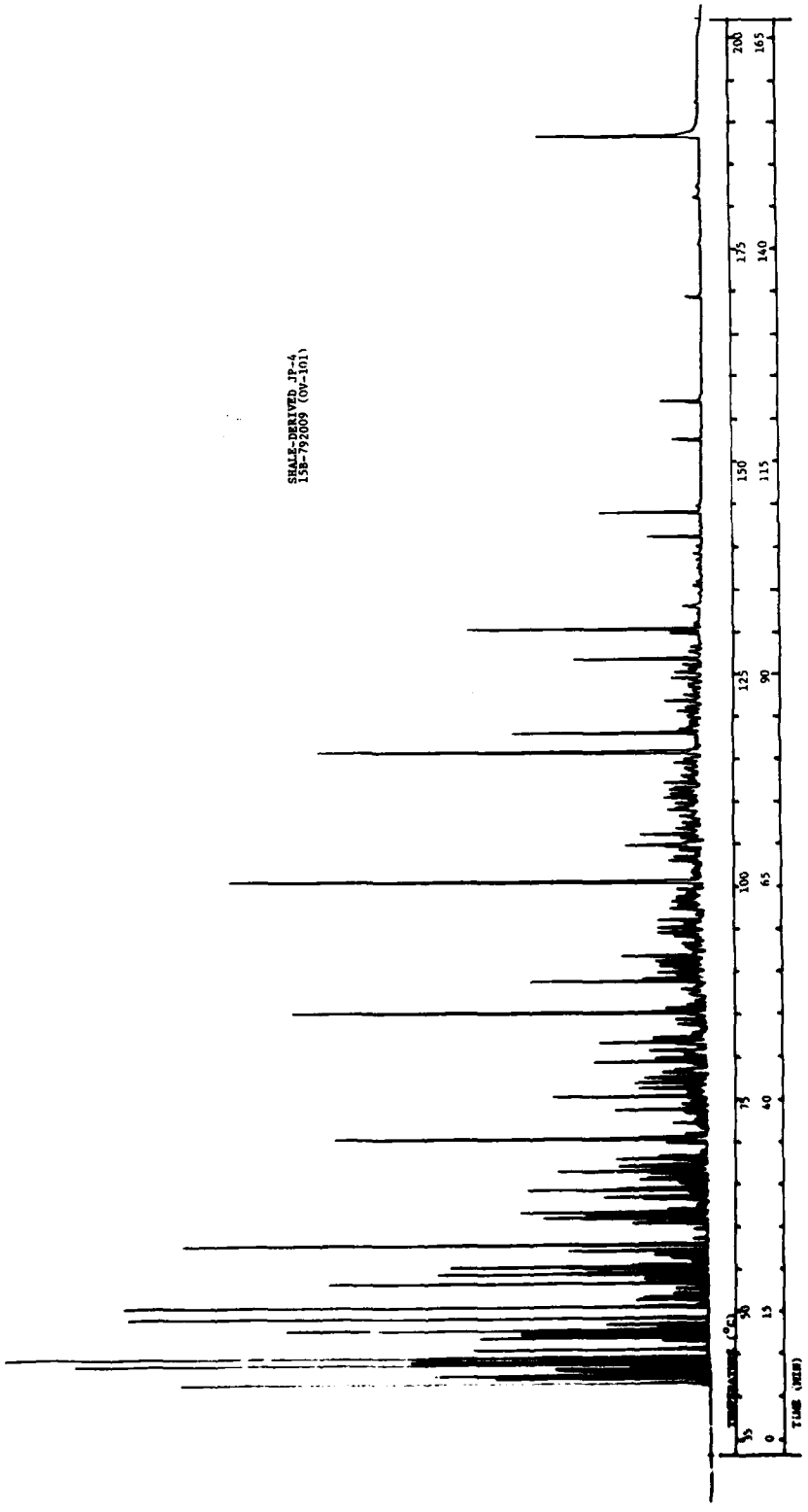

Figure 8. Shale Derived JP-4 15B-792009 (OV-101)

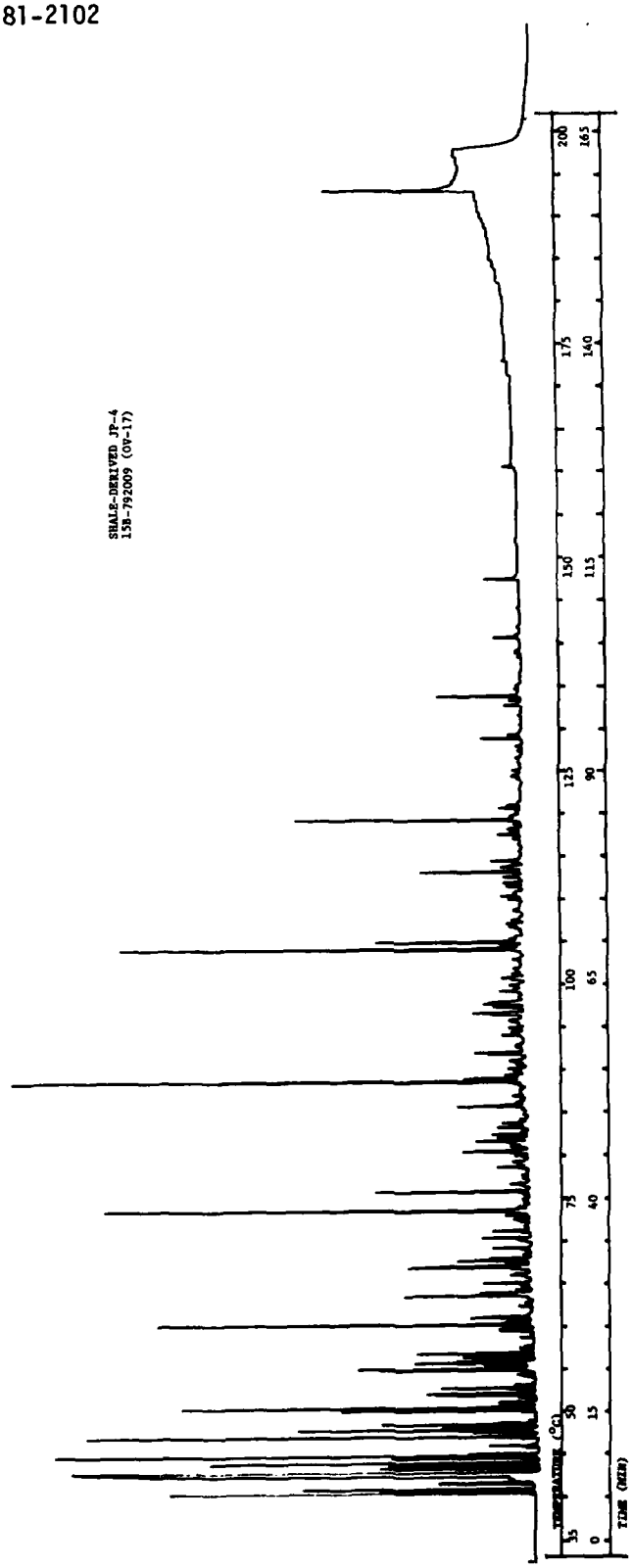

Figure 9. Shale Derived JP-4 15B-792009 (OV-17)

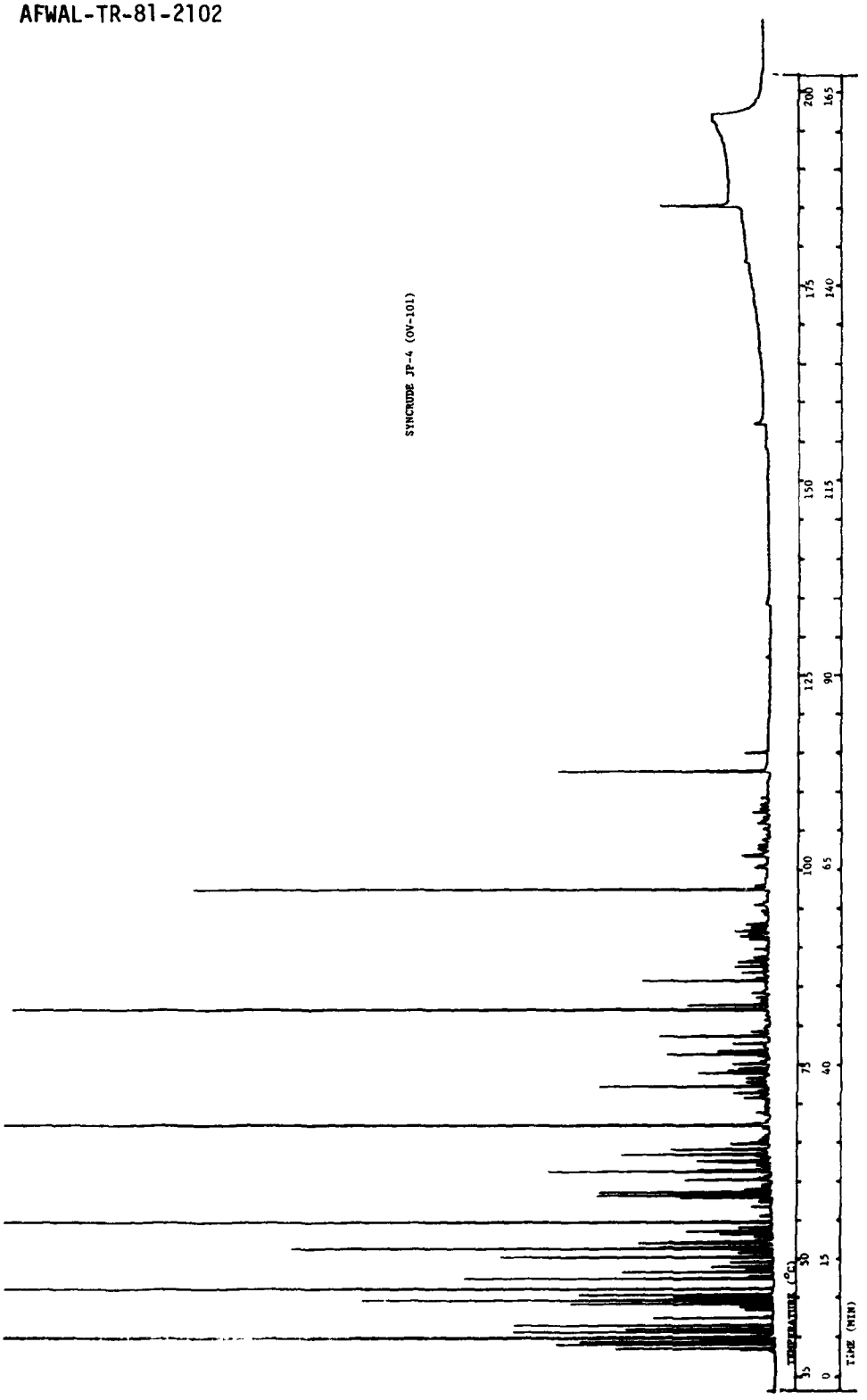

Figure 10. Syncrude JP-4 (OV-101)

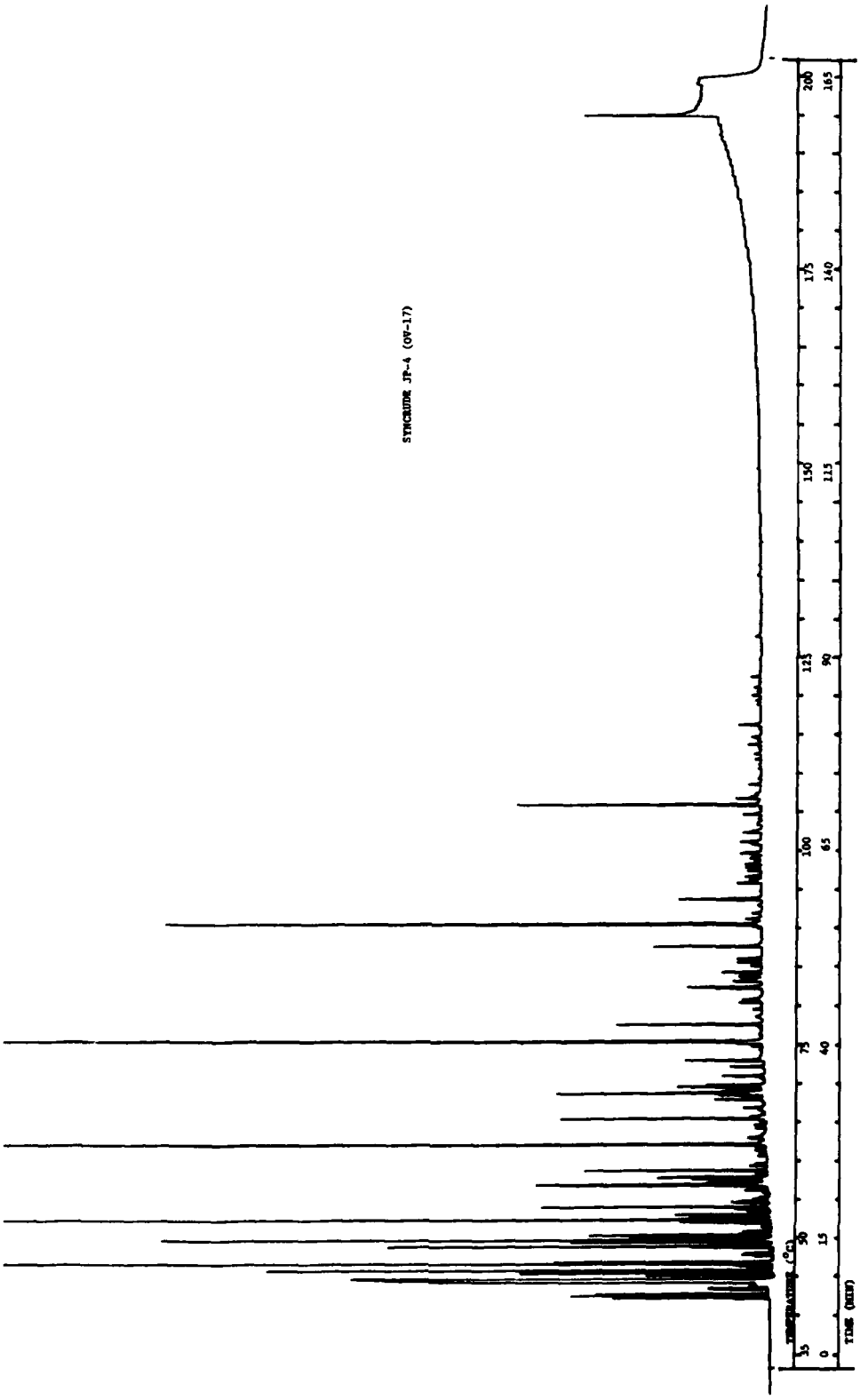

Figure 11. Syncrude JP-4 (OV-17)

section one. These three fuel codes supposedly represented the same fuel only sampled at different points in a fuel handling system. Inspection of the chromatograms readily indicates that the samples are indeed different. A sophisticated Kovats Indices system enables one to tell just how the fuel samples differ.

2. EXTENDING KOVATS DATA

Due to the countless number of compounds existing in a complex hydrocarbon mixture such as jet propulsion fuel, it is necessary to have a method better than random choice to initially select potential compounds for a comprehensive Kovats Indices library.

The initial method used to choose the compounds for the Kovats Indices library in this report was a literature research of other $(GC)^2$ and detailed mass spectroscopy experiments performed on selected JP-4 jet propulsion fuel. However, in an attempt to extend the Kovats Indices library past the limits gained by research of existing literature, several methods utilizing intuition and inference were developed during the course of this study and are being considered for future work.

First, it was noticed while computing the Kovats Indices that members of homologous series generally varied in their Kovats Indices by a set number of units. By generating linear graphs (see Figures 12 through 31) it is easy to estimate the Kovats Index of a member of a homologous series given its carbon number or its boiling point. This method should by no means be used to reliably identify components, but can be used as a valuable tool in helping to choose reference compounds to extend an existing Kovats Indices Library. Table 11 demonstrates the usefulness in extrapolating the linear relationship of a homologous series to predict the presence of a member not among the reference standards. A fuel was selected at random. Indices were calculated from the corresponding carbon number versus Kovats Indices plot and compared with a sample component having nearly the same retention index. In all cases, a peak predicted on the OV-101 column was also successfully predicted on the OV-17 column.

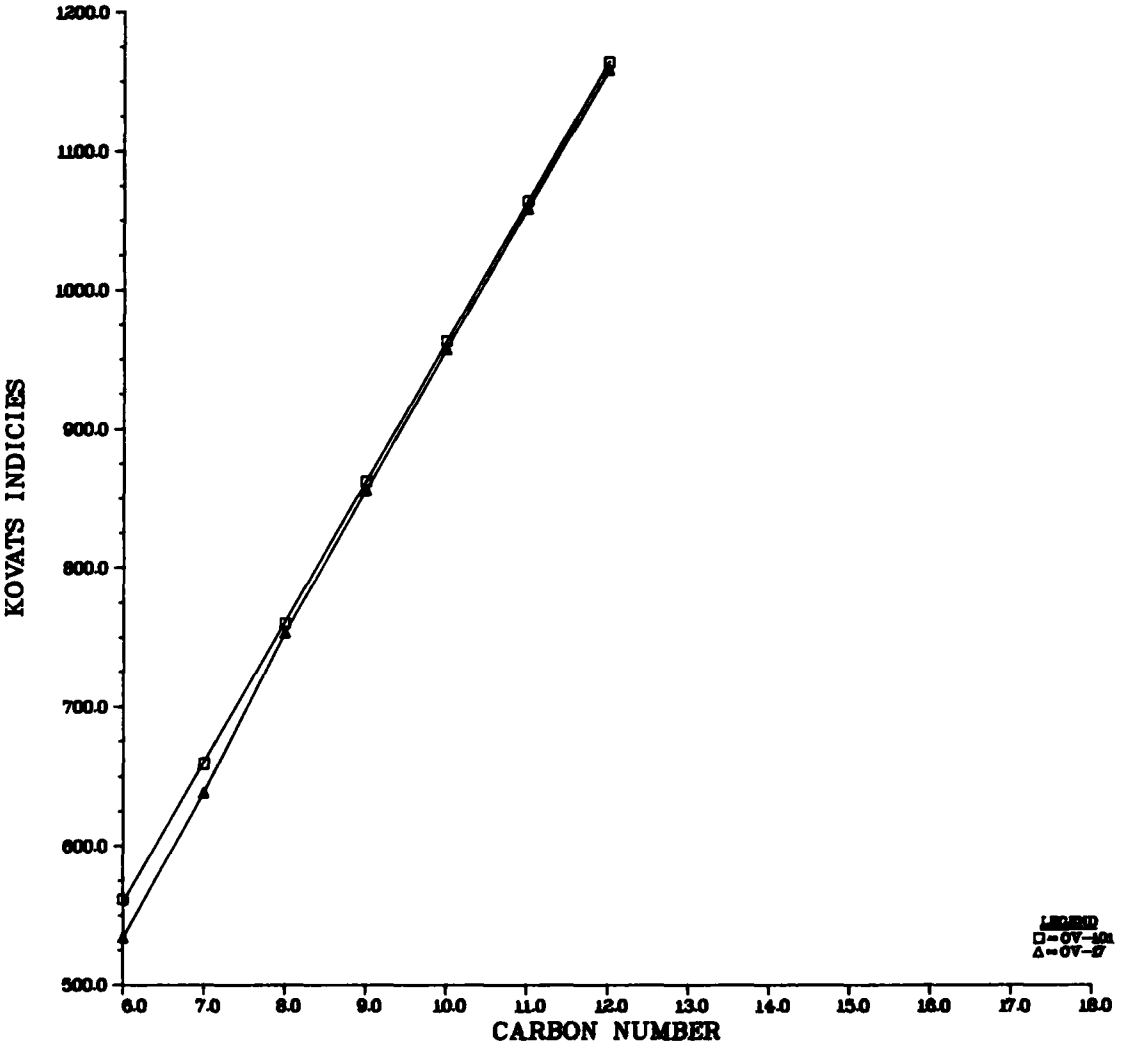

Figure 12. Kovats Indices vs. Carbon Number for 2-Methyl Alkanes on OV-101 and OV-17

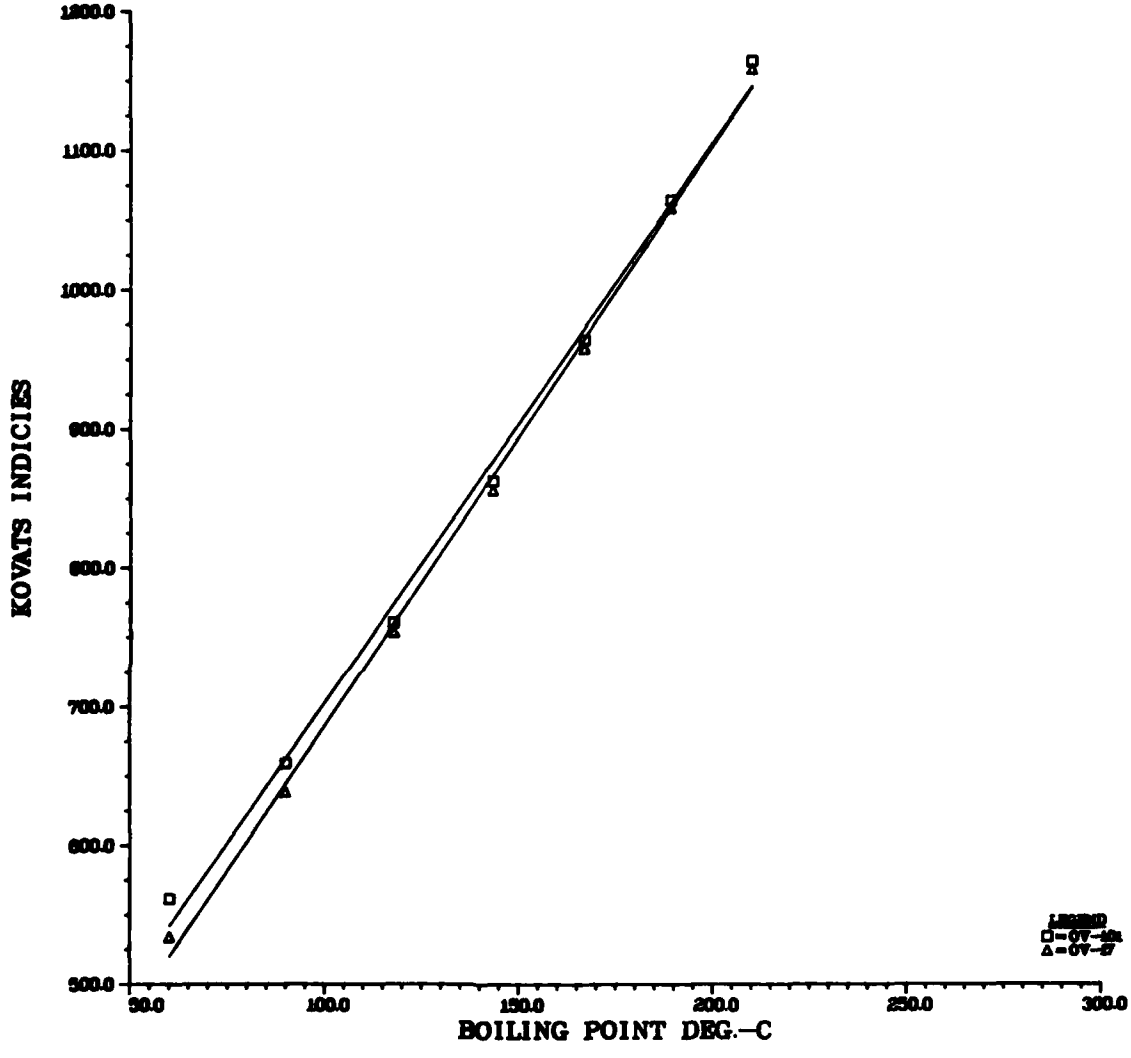

Figure 13. Kovats Indices vs. Boiling Point for 2-Methyl Alkanes on OV-101 and OV-17

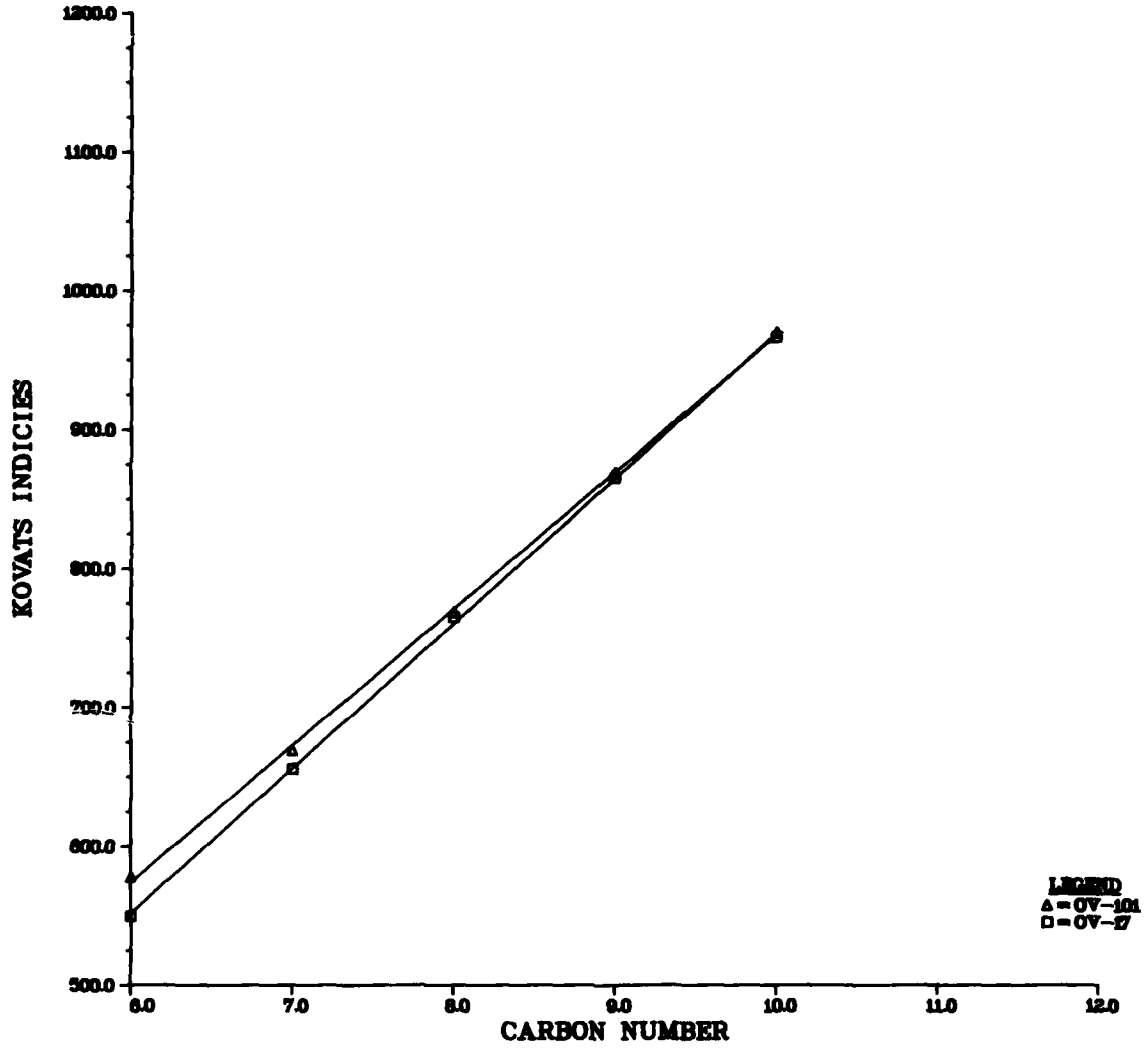

Figure 14. Kovats Indices vs. Carbon Number for 3-Methyl Alkanes on OV-101 and OV-17

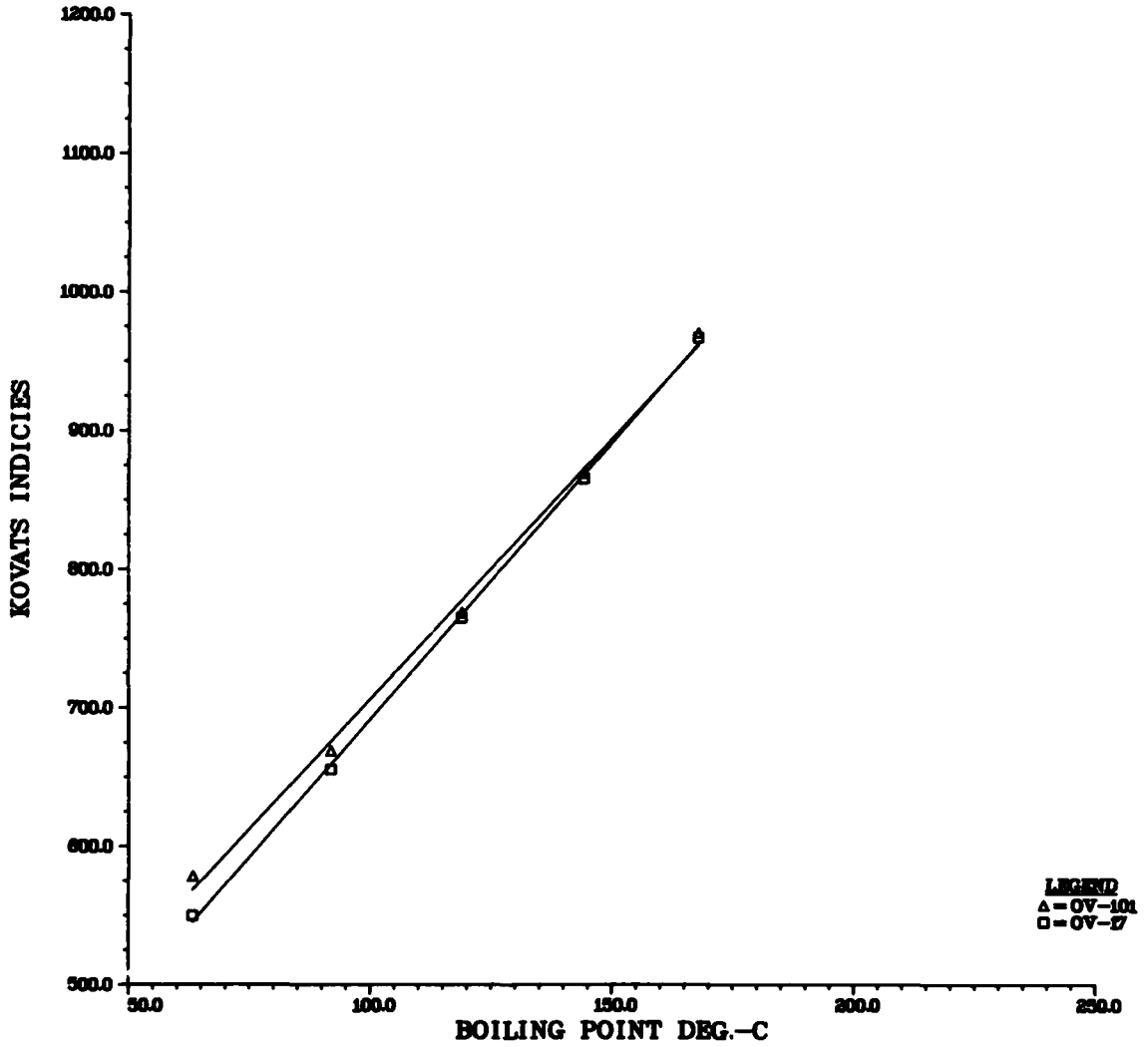

Figure 15. Kovats Indices vs. Boiling Point for 3-Methyl Alkanes on OV-101 and OV-17

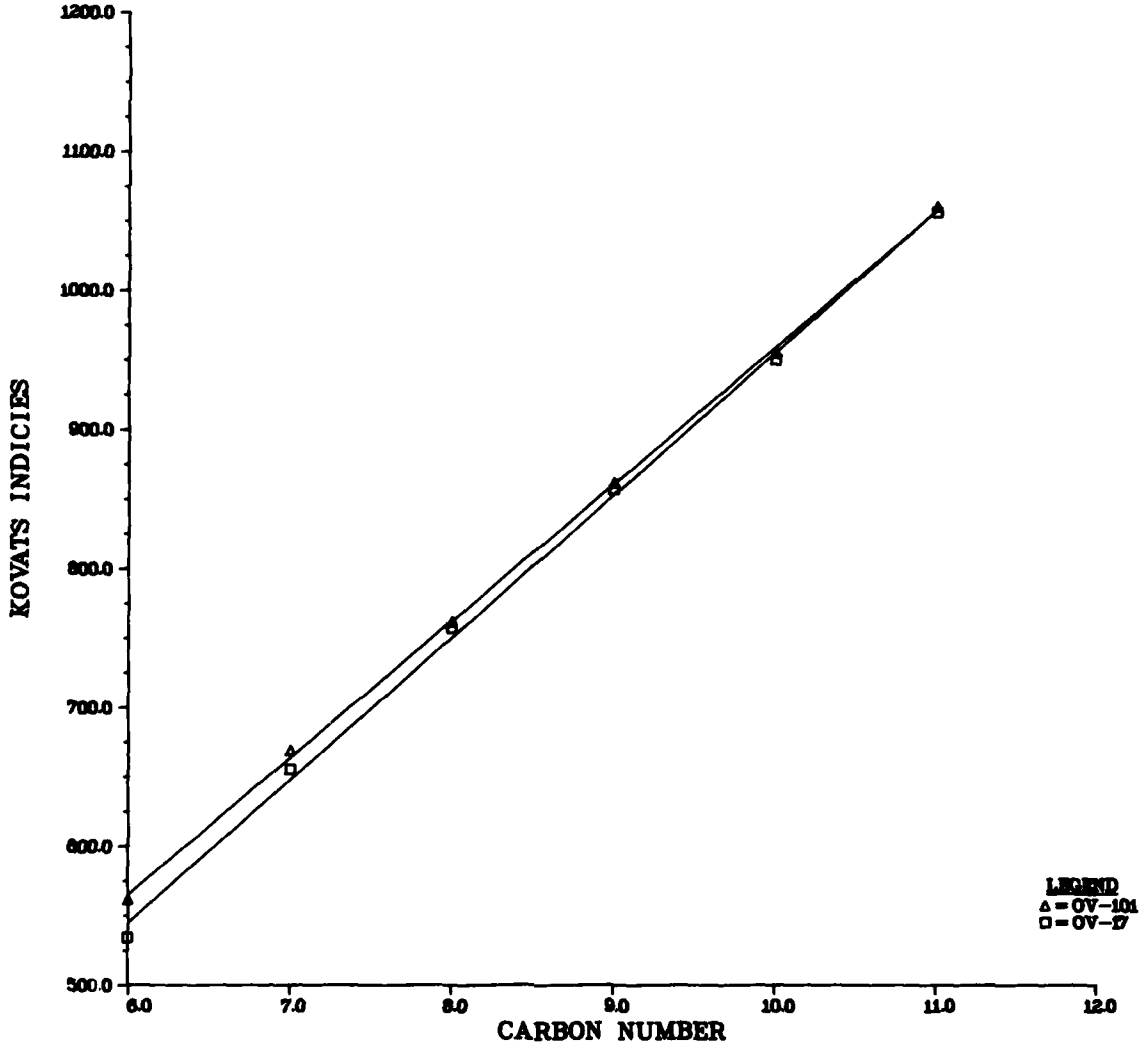

Figure 16. Kovats Indices vs. Carbon Number for 4-Methyl Alkanes on OV-101 and OV-17

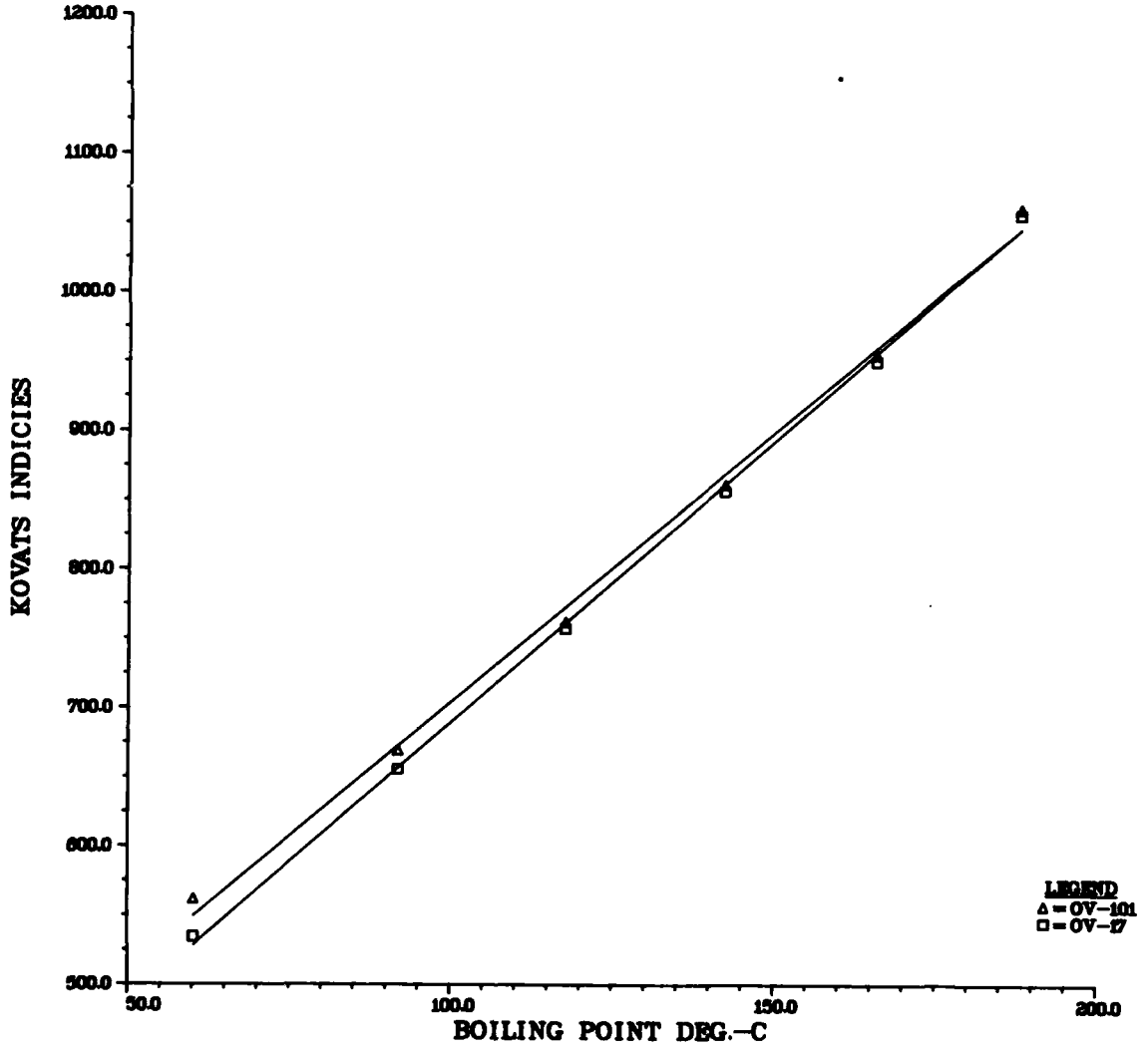

Figure 17. Kovats Indices vs. Boiling Point for 4-Methyl Alkanes on OV-101 and OV-17

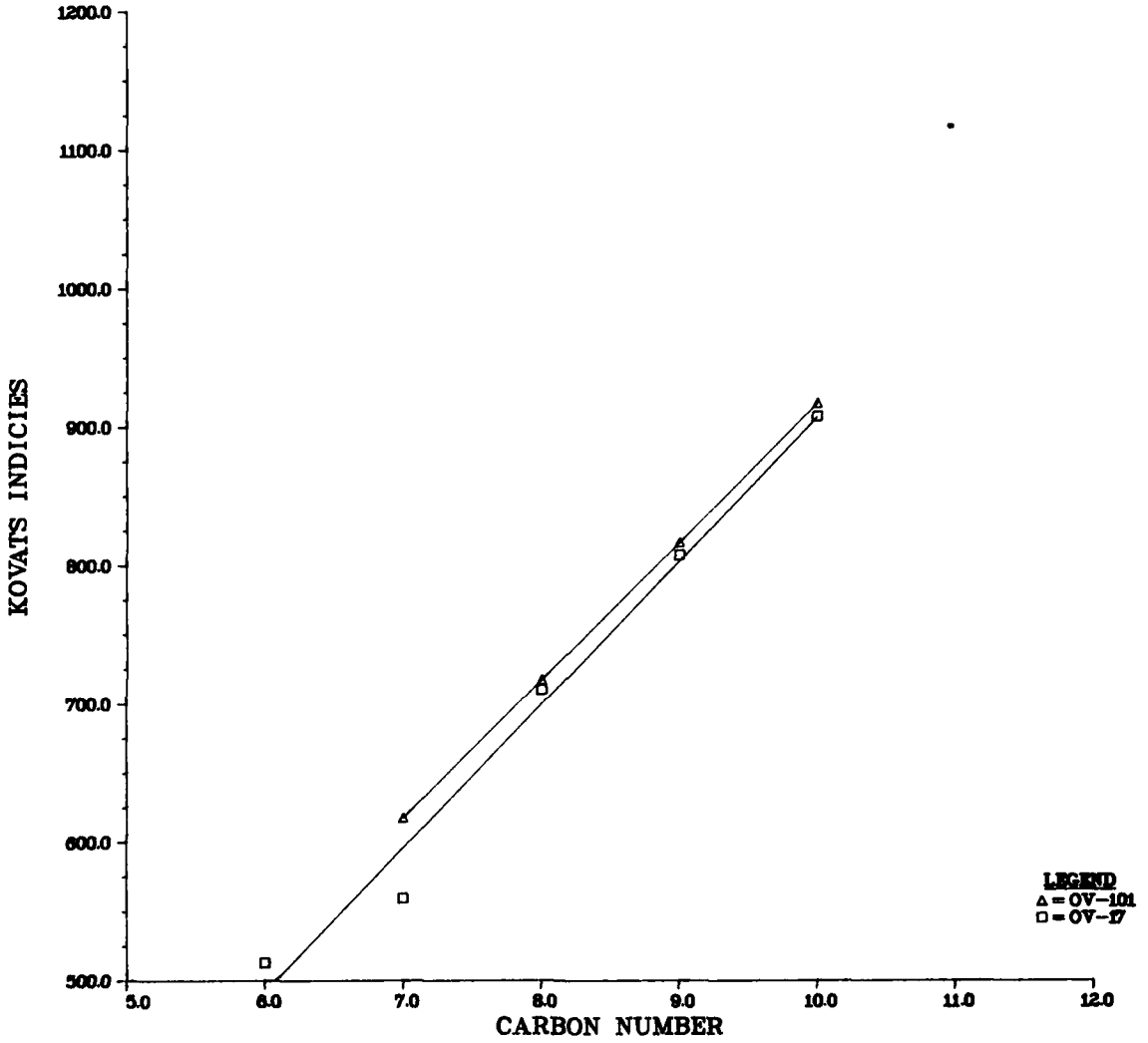

Figure 18. Kovats Indices vs. Carbon Number for 2,2-Dimethyl Alkanes on OV-101 and OV-17.

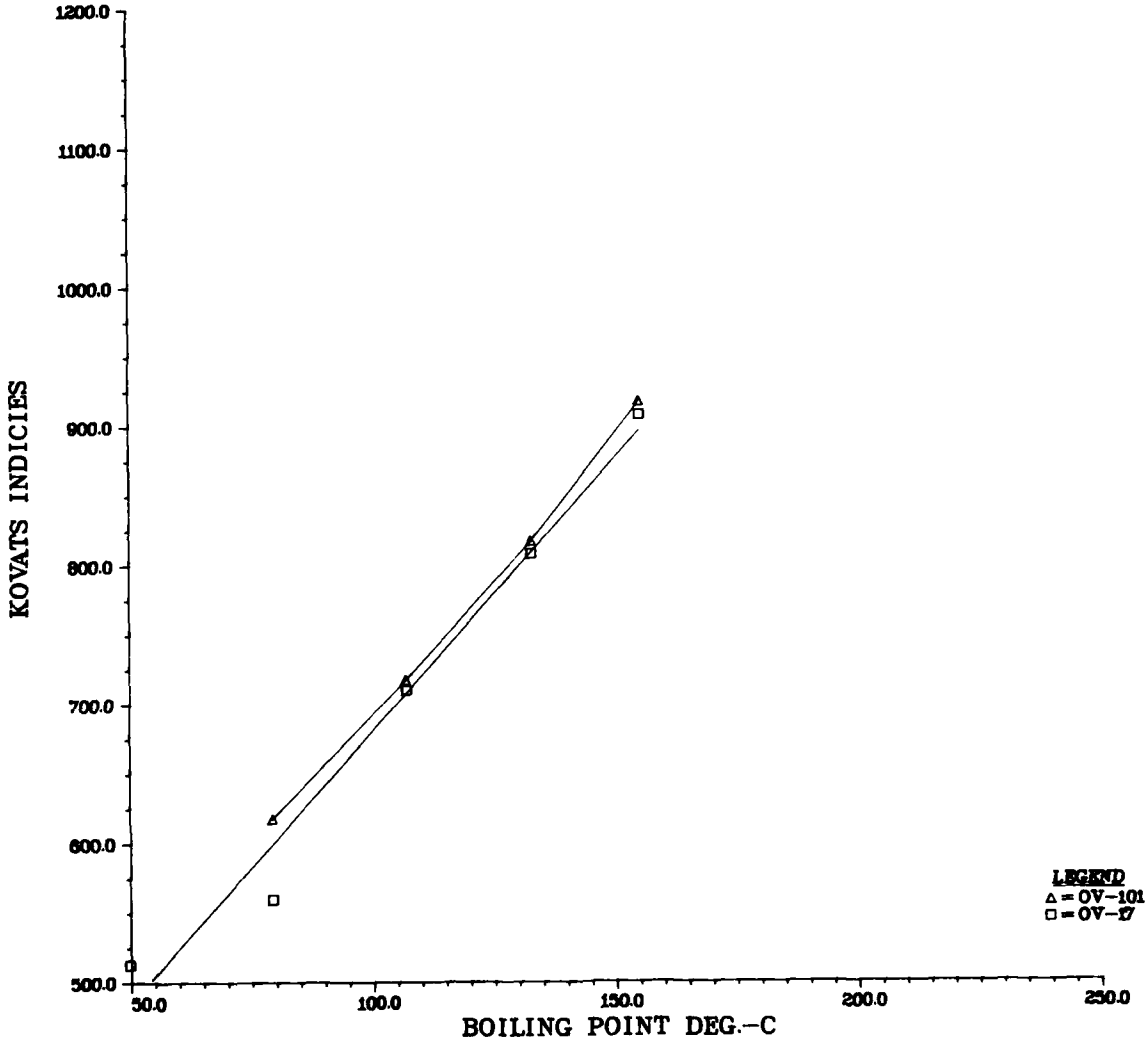

Figure 19. Kovats Indices vs. Boiling Point for 2,2-Dimethyl Alkanes on OV-101 and OV-17

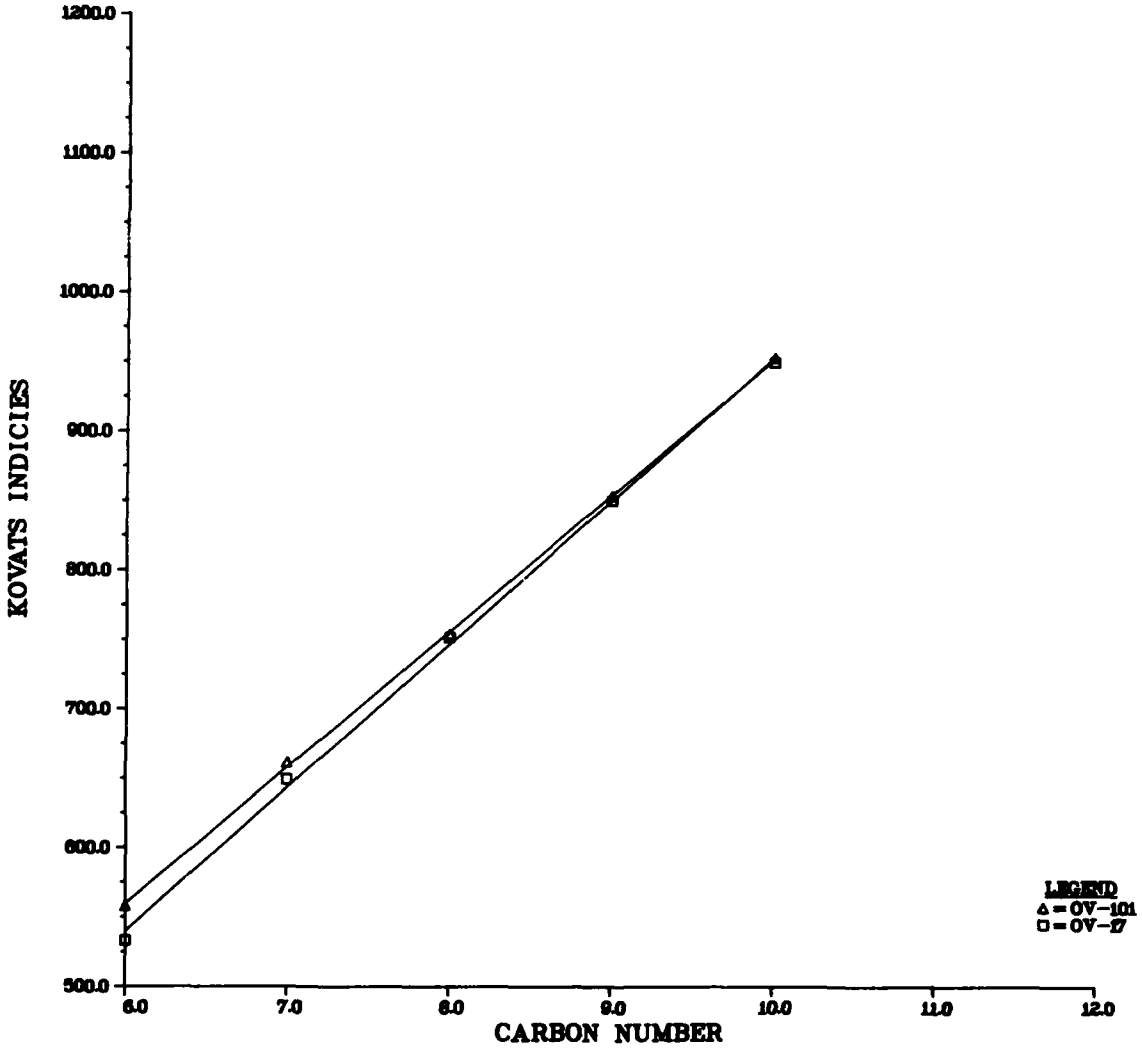

Figure 20. Kovats Indices vs. Carbon Number for 2,3-Dimethyl Alkanes on OV-101 and OV-17

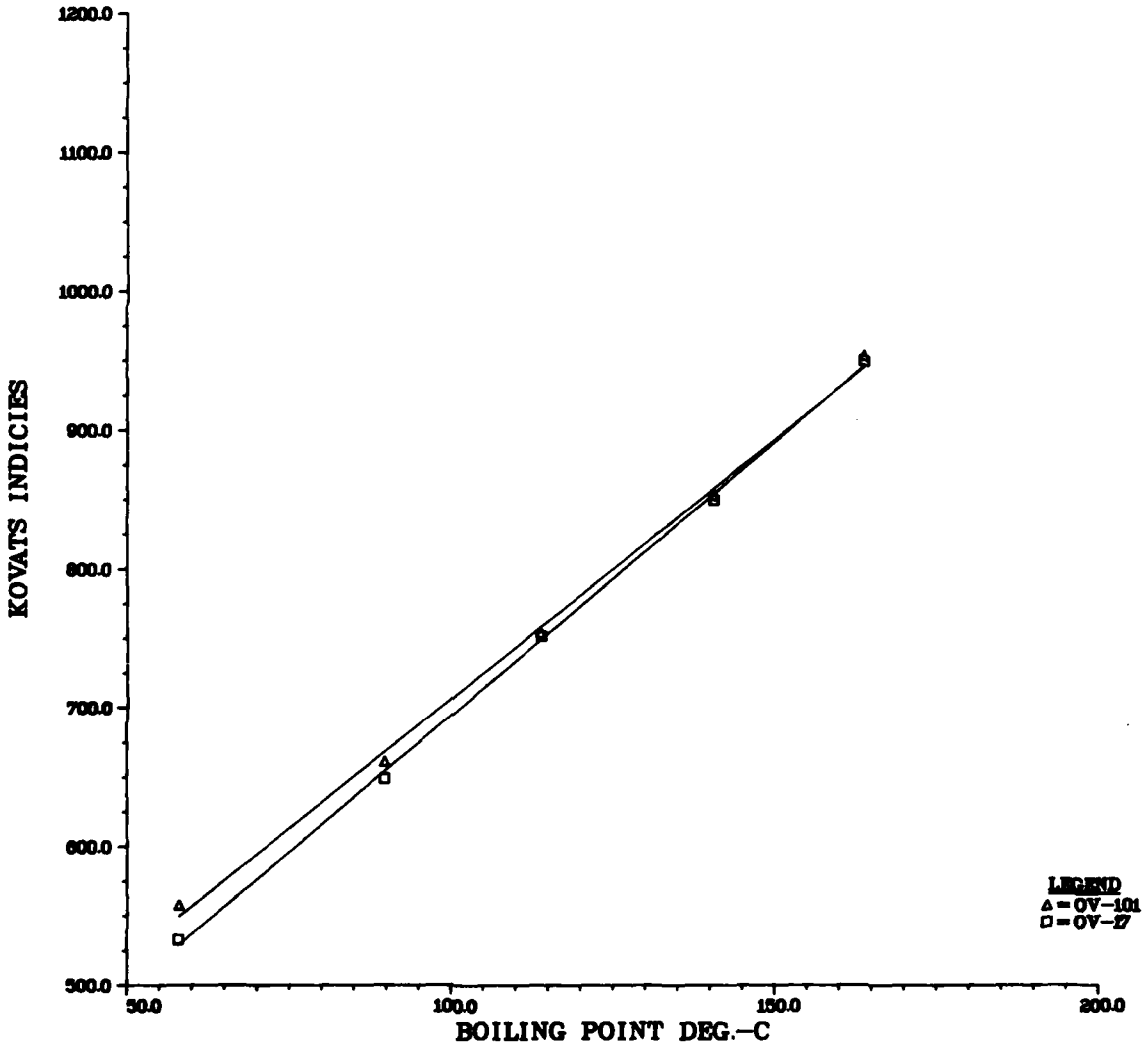

Figure 21. Kovats Indices vs. Boiling Point for 2,3-Dimethyl Alkanes on OV-101 and OV-17

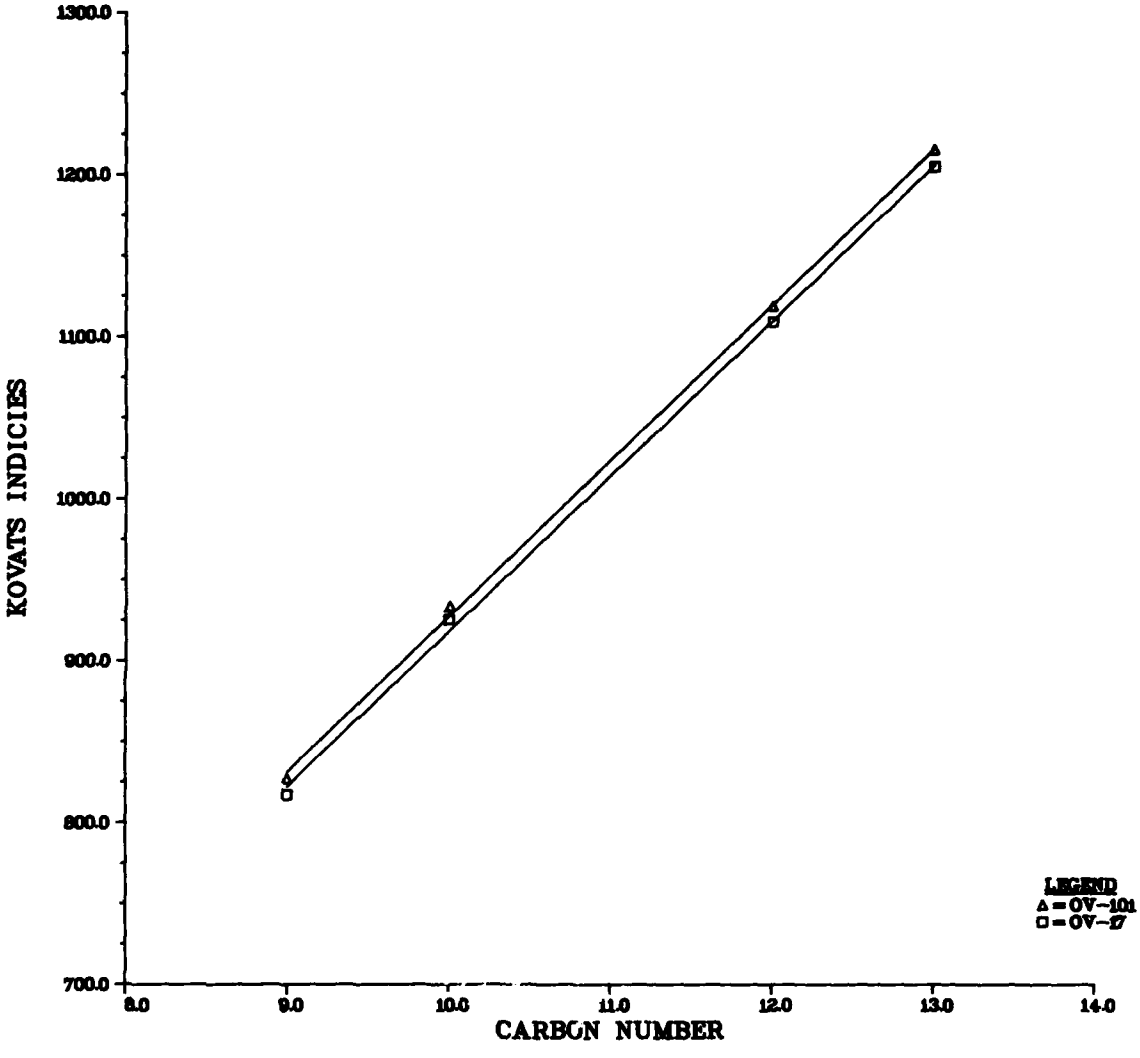

Figure 22. Kovats Indices vs. Carbon Number for 2,6-Dimethyl Alkanes on OV-101 and OV-17

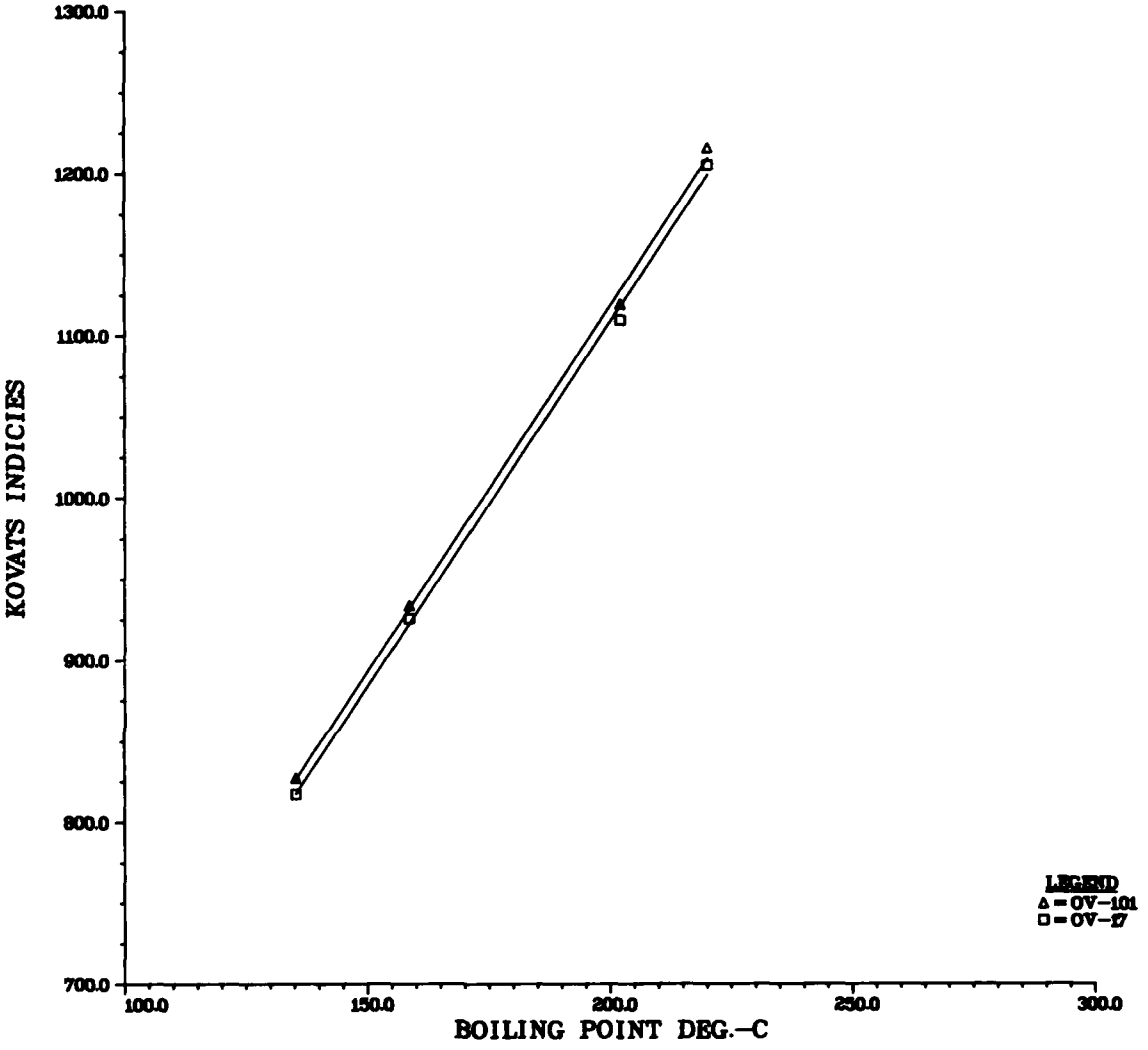

Figure 23. Kovats Indices vs. Boiling Point for 2,6-Dimethyl Alkanes on OV-101 and OV-17

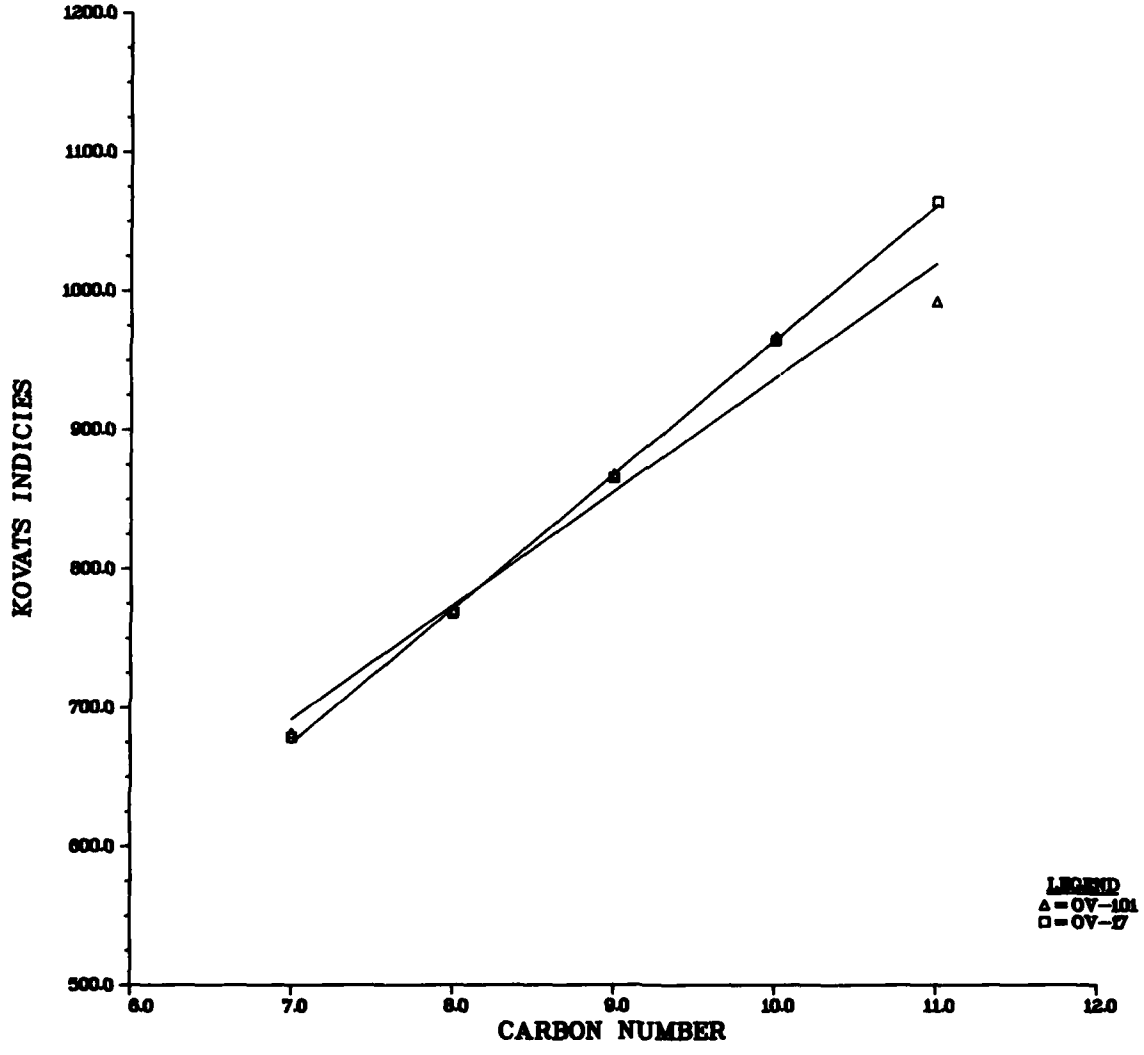

Figure 24. Kovats Indices vs. Carbon Number for 3-Ethyl Alkanes on OV-101 and OV-17

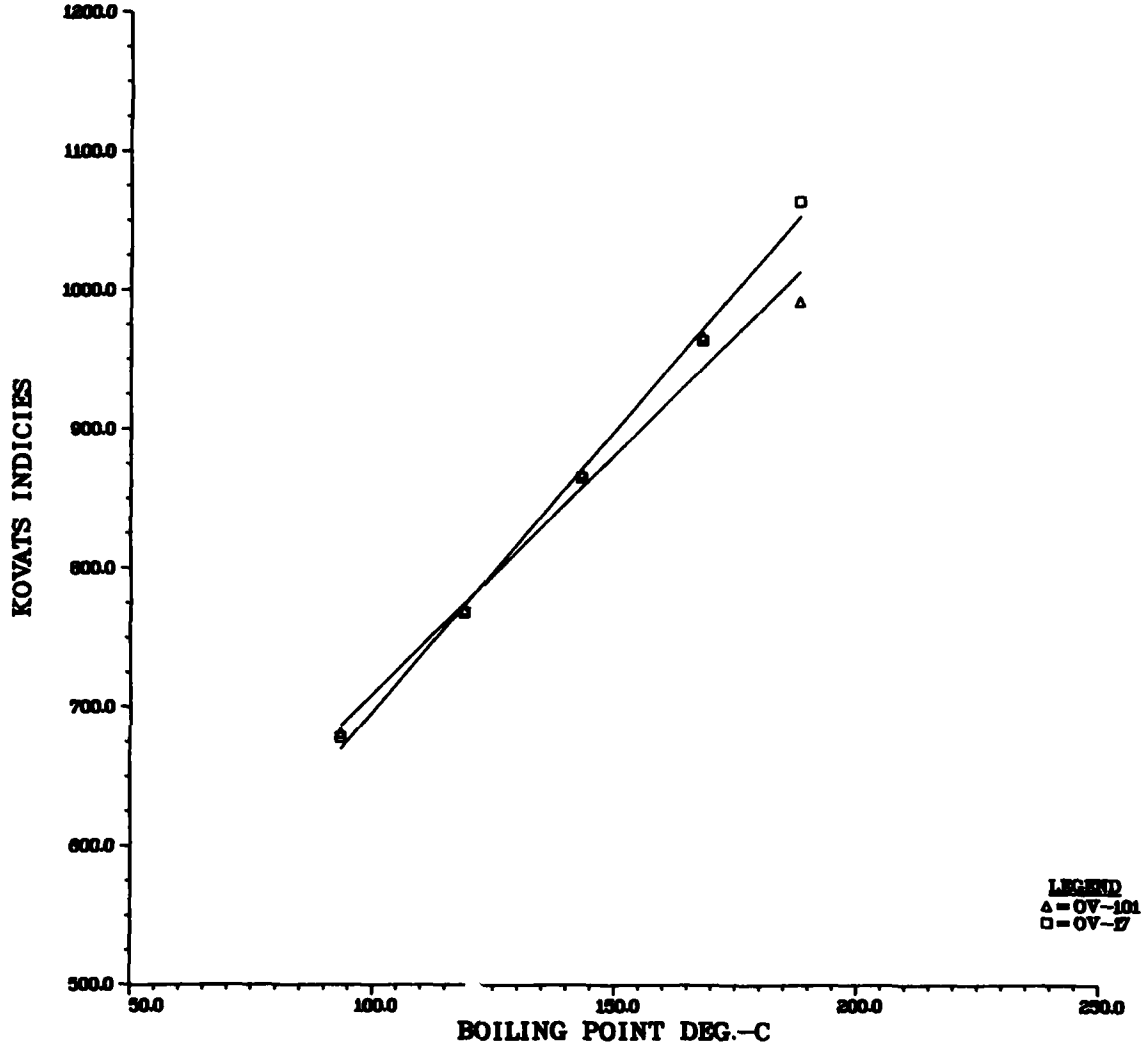

Figure 25. Kovats Indices vs. Boiling Point for 3-Ethyl Alkanes on OV-101 and OV-17

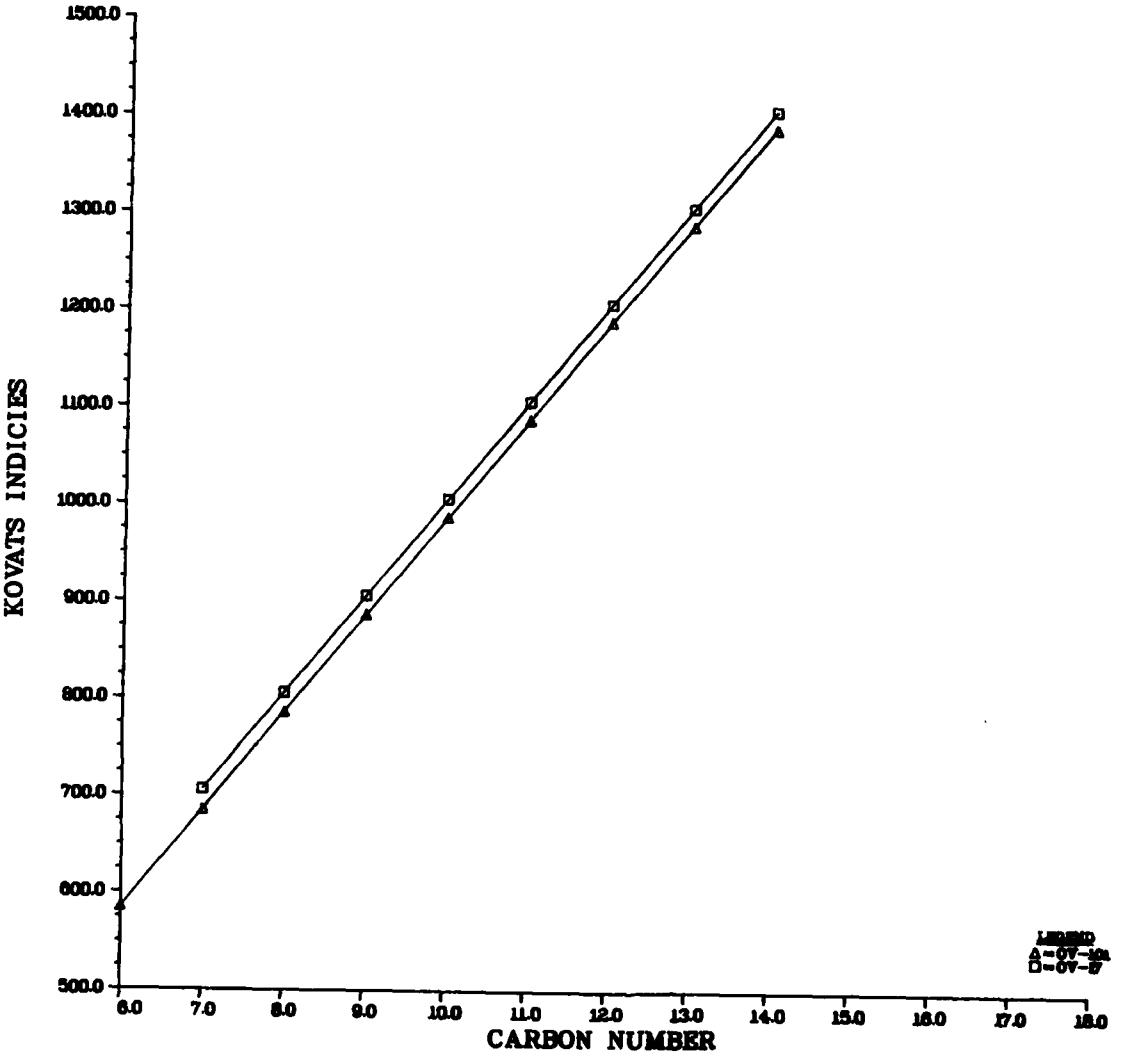

Figure 26. Kovats Indices vs. Carbon Number for 1-Olefins on OV-101 and OV-17

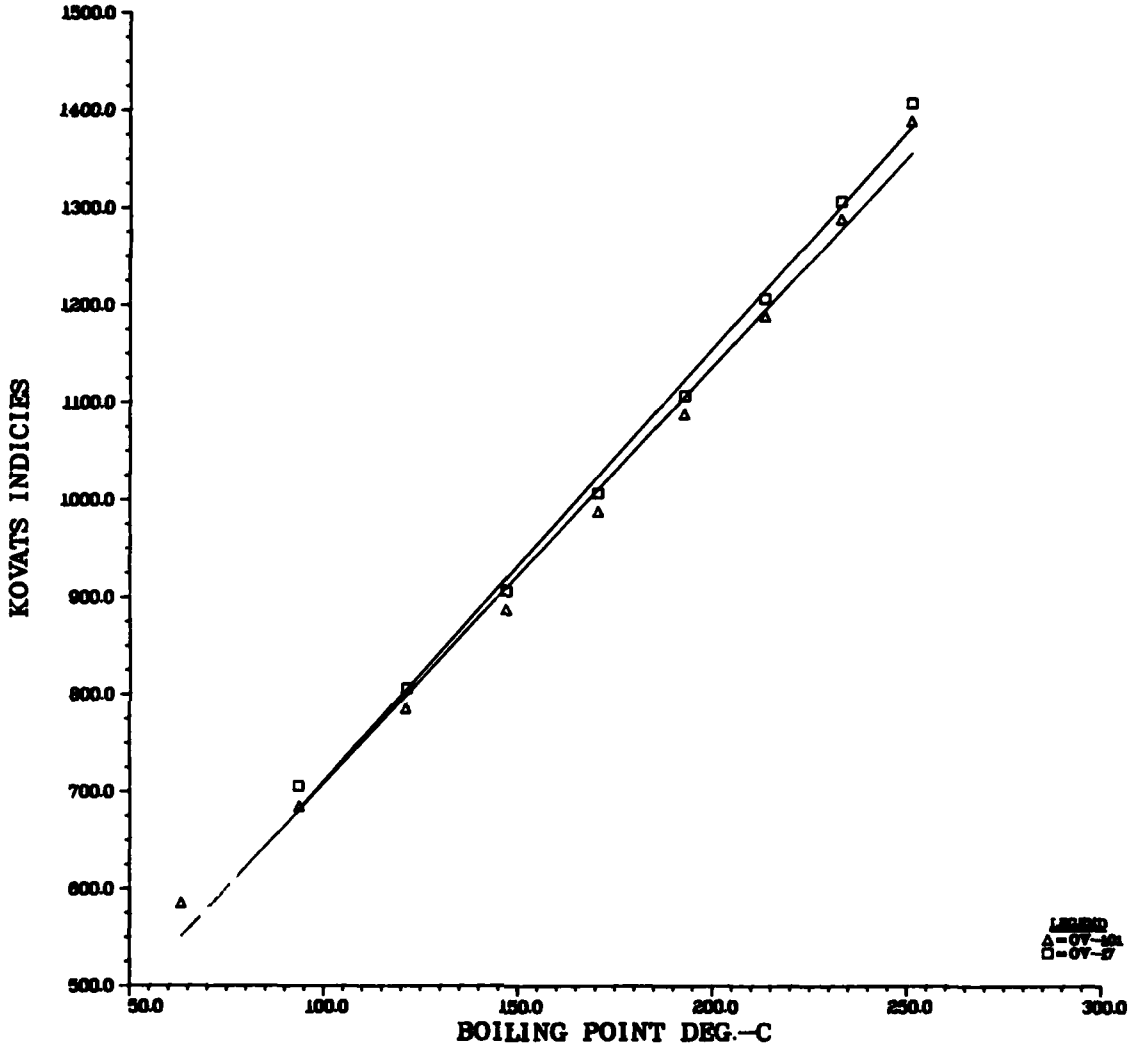

Figure 27. Kovats Indices vs. Boiling Point for 1-Olefins on OV-101 and OV-17

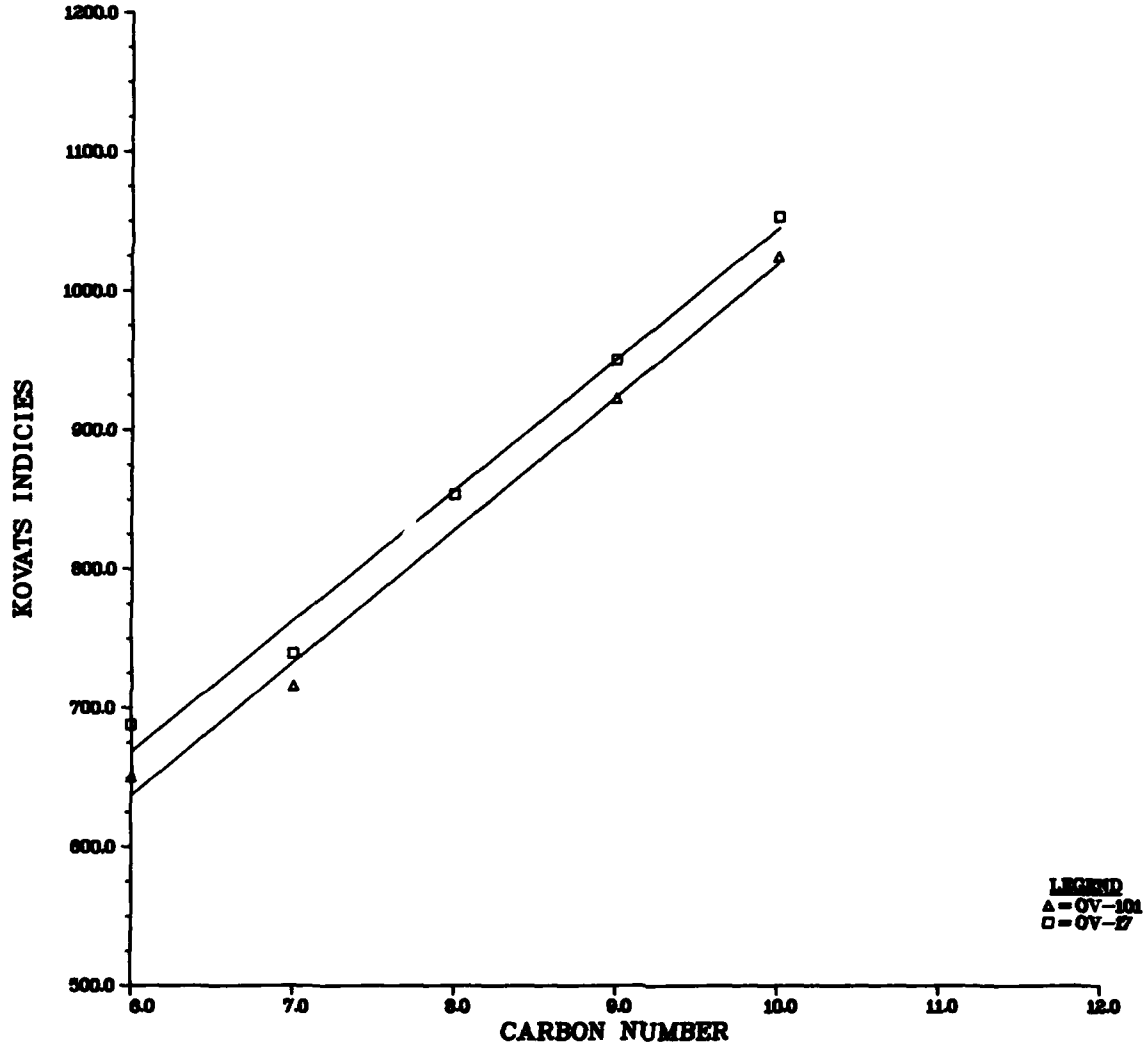

Figure 28. Kovats Indices vs. Carbon Number for Normal Cyclohexanes on OV-101 and OV-17

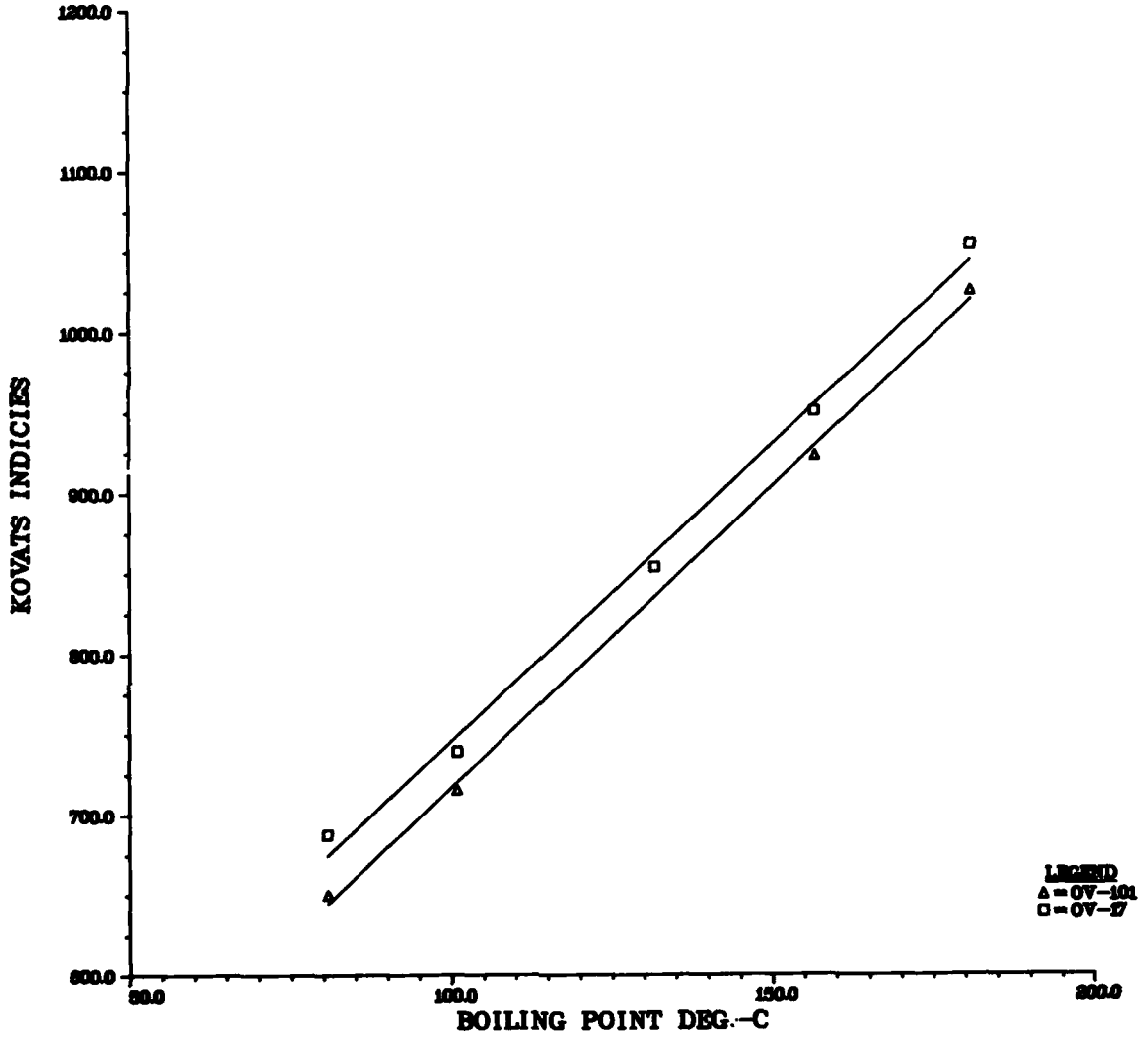

Figure 29. Kovats Indices vs. Boiling Point for Normal Cyclohexanes on OV-101 and OV-17

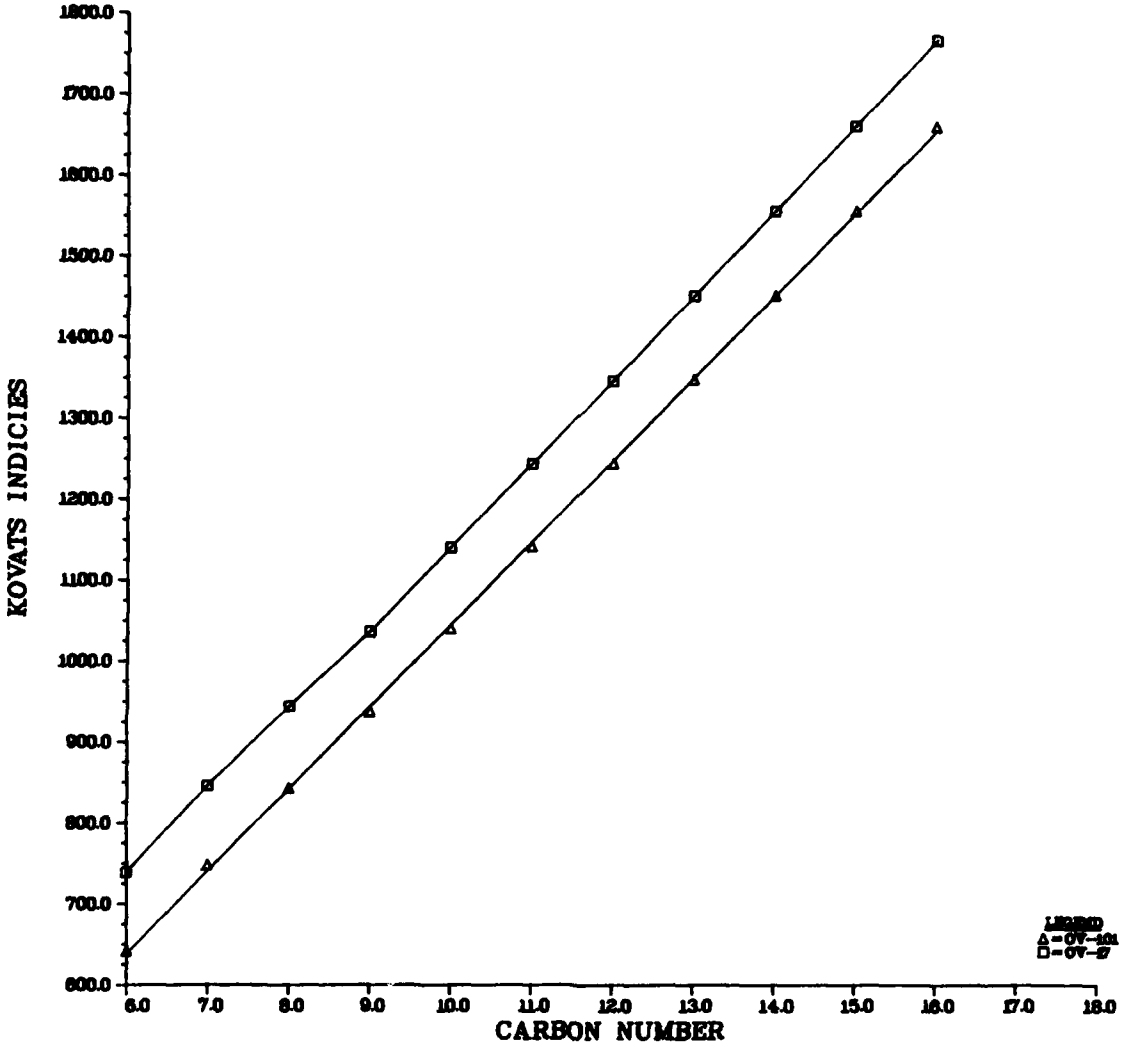

Figure 30. Kovats Indices vs. Carbon Number for Normal Alkyl Benzenes on OV-101 and OV-17

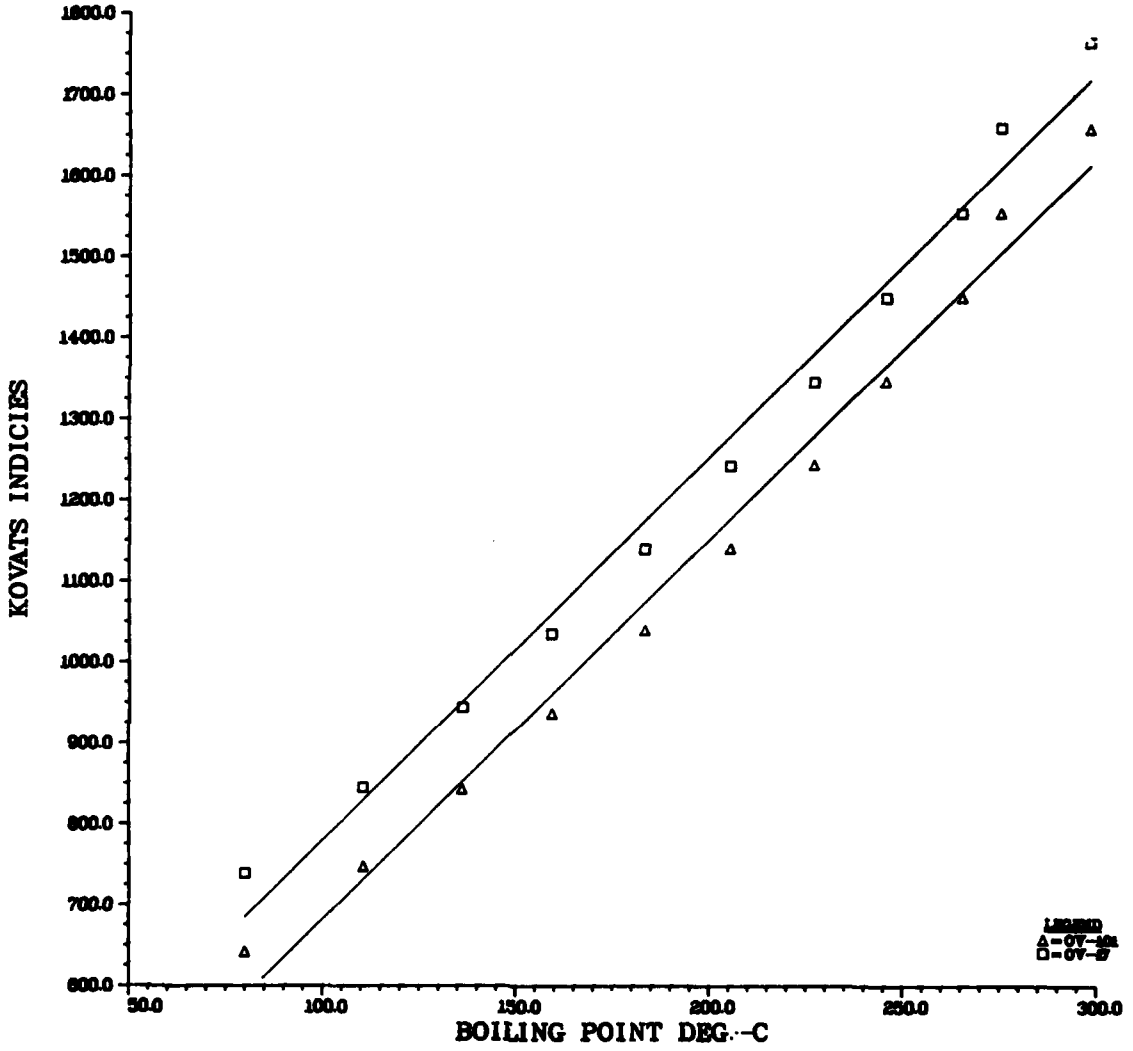

Figure 31. Kovats Indices vs. Boiling Point for Normal Alkyl Benzenes on OV-101 and OV-17

From the existing Kovats libraries it was noted that there were some "gaps" in the tentative identification of components found in the fuel samples. By procuring compounds of classes common to jet propulsion fuel (e.g. branched alkanes, alkyl benzenes, etc.) whose carbon number fall within these "gaps," the likelihood of identifying more compounds in the fuel could also be significantly increased.

While the second method is not as definitive as the first, it can still be a valuable tool for compound selection, especially in areas where there are not sufficient members of a homologous series present in the library to generate a reliable plot.

Another useful feature of these Kovats Libraries on different stationary phases is that an unknown compound, if sufficiently resolved on both columns could be assigned to a general hydrocarbon class by calculating its difference in K.I. values, i.e. delta K.I. In general, branched alkanes demonstrated a rather small negative delta K.I. of about -3 to -10 units with substantial negative values for highly substituted alkanes. Cyclohexanes usually displayed a positive delta K.I. of about +24 units for the standards included in the libraries. The dimethyl cyclohexanes averaged about +26 units while the trimethyls averaged about +18 units. The 1-olefins examined showed a positive delta K.I. of +19 units. The alkyl benzenes studied demonstrated an average positive delta K.I. of 96 units. However, certain substitutions gave delta values in the +110-120 and higher range: 3 or more alkyl groups in the 1,2,3 positions; or 2 alkyl groups in the 1,2 where one group was other than a methyl; or 3 or more alkyl groups in the 1,2,4 positions. It appears that substituents that render the hydrocarbon molecule more spherical or spheroid in shape tend to exhibit higher positive delta K.I. values. The few alkylated naphthalenes investigated showed a positive delta K.I. of almost +201 units.

TABLE 11

EXTRAPOLATED KOVATS INDICES: FUEL 15B-792009

HOMOLOGOUS SERIES	HYDROCARBON NAME	KI-101 extrap	KI-101 sample	KI-17 extrap	KI-17 sample	A% OV-101	A% OV-17
2-methyl alkanes	2-methyl:						
	dodecane	1264.88	1264.92	1259.30	1259.85	0.28	1.18*
	tridecane	1364.88	1364.95	1359.30	1359.47	0.10	0.13
3-methyl alkanes	3-methyl:						
	decane	1071.32	1070.63	1067.96	1067.67	0.37	0.46
	undecane	1171.32	1170.98	1167.96	1167.99	0.27	0.38
	dodecane	1271.32	1271.05	1267.96	1268.24	0.18	0.49
	tridecane	1371.32	1371.29	1367.96	1367.58	0.08	0.29
4-methyl alkanes	4-methyl:						
	undecane	1160.06	1160.36	1156.49	1156.06	0.24	0.41
	dodecane	1260.06	1260.19	1256.49	1255.87	0.28	0.31
3-ethyl alkanes	3-ethyl:						
	nonane	1067.10	1066.69	1064.56	1064.49	0.16	0.43
	decane	1167.10	1167.52	1164.56	1164.11	0.25	0.07
	undecane	1267.10	1267.68	1264.56	1264.28	0.15	0.03
2,2-dimethyl alkanes	2,2-dimethyl:						
	nonane	1017.78	1017.51	1008.18	1008.28	0.28	0.08
	decane	1117.78	1117.70	1108.18	1107.96	0.20	0.08
	undecane	1217.78	1218.15	1208.18	1207.59	0.24	0.08
2,3-dimethyl alkanes	2,3-dimethyl:						
	nonane	1053.33	1053.56	1049.98	1050.27	0.07	0.12
	dodecane	1353.33	1353.15	1349.98	1350.30	0.06	0.11
2,6-dimethyl alkanes	2,6-dimethyl:						
	nonane	1033.62	1033.88	1025.44	1025.27	0.37	0.07
	dodecane	1315.87	1316.06	1305.25	1305.41	0.05	0.10
n-alkyl cyclohexanes	cyclohexane:						
	n-pentyl	1126.65	1127.14	1156.03	1156.06	0.29	0.41

* = relatively large area percent here suggests this component co-eluted with another hydrocarbon

TOTAL Area % (OV-101) = 3.92
TOTAL Area % (OV-17) = 4.07

SECTION V

CONCLUSIONS AND RECOMMENDATIONS

The primary result of the work described in this technical report is that reasonably precise and highly reproducible $(GC)^2$ work can be obtained on complex jet propulsion fuels under temperature programmed conditions.

The inherent precision of the relative retention time method of a Kovats Index system was combined with the expediency of temperature programming to effect precise, definitive characterizations of jet propulsion fuels in a relatively short analysis time.

Through these characterizations both physical and chemical properties of the fuel can eventually be predicted. In addition to this use, profiles of particular fuels can be generated for use in quality control of other fuels testing programs.

Not enough emphasis can be laid on the importance of optimizing resolution in a $(GC)^2$ system used for this type of analysis. One of the major stumbling blocks in peak identification is the coelution of peaks, especially in the middle of the distillation range of jet propulsion fuel. Additional resolution would diminish this problem.

Another problem that can occur during an endeavor of this type is the immense amount of data that must be collected, reduced, and applied. A concise, well planned, computerized data handling system can be a valuable assistance in this area.

SECTION VI

FUTURE WORK

Future work in the area of characterization of jet propulsion fuels will include the quantitation of compounds in the fuels, identification of nitrogen compounds in shale derived fuels and, as mentioned in the previous section, further optimization of the $(GC)^2$ system.

Quantitation will be accomplished by using relative response factors with an internal standard. Calibration solutions and fuel samples will be prepared with weighed amounts of an internal standard. The relative response factors of each compound will be calculated from $(GC)^2$ runs of the calibration solutions. These factors will then be applied to the $(GC)^2$ runs of fuel samples to calculate the amount of each compound identified by the libraries.

Detection of nitrogen compounds will be accomplished by using a thermionic specific detector, and a method of sensing compounds with bound nitrogen using pyro-chemiluminescence.

Additional resolution can only be obtained by preparing a column with more theoretical plates. The operating conditions of any additional columns prepared for future work will be optimized in much the same manner as were the operating conditions of the columns in this technical report.

An alternate to using longer and longer columns to gain resolution for jet fuel analysis is that of prior fractionization. With a system using prior fractionization a fuel sample could be divided into several fractions in a liquid chromatograph. These fractions could then be independently delivered to $(GC)^2$ columns for subsequent characterization. This approach would greatly simplify the present resolution problem.

Future $(GC)^2$ work is expected to be performed on columns made of fused silica. These columns have several advantages over conventional glass capillary columns. The main advantage of fused silica columns is low inherent adsorbtivity. This is of particular interest when analyzing highly polar nitrogen compounds. Fused silica columns also have a much lower bleed rate of the stationary phase than glass columns. This will allow higher temperatures to be used and will also result in longer column life. It should be pointed out at this time that the original intent of this report was to do both qualitative and quantitative characterization of compounds. The large peak at the extreme right of the chromatograms in Figures 2 through 11 is the internal standard added to each fuel sample. Repetitive integration of this peak was not possible due to the unstable baseline caused by high bleed rate. This problem should be greatly diminished by the use of fused silica columns.

The mechanical advantages of fused silica columns are that they are more flexible and smaller in external diameter, which allows optimum positioning of the column in relation to the injector and detector.

Even with greatly increased resolution and use of prior fractionization all qualitative identifications of compounds will be tentative and will require verification by gas chromatography-mass spectrometry.

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