DETERMINATION OF AROMATICITY
OF FUELS AND LUBRICANT BASESTOCKS
BY ULTRAVIOLET SPECTROSCOPY
LEVEL
INTERIM REPORT
AFLRL No. 103
by
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San Antonio, Texas
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## ABSTRACT

A rapid and inexpensive ultraviolet spectroscopic method for determining the aromaticity of turbine and diesel fuels and of lubricant basestocks has been developed. The method employs fixed cells of 0.010, 0.10, and 1.00 cm pathlength in which a sample spectrum is obtained in the 190 to 350 nm region. Absorbance values at several wavelengths and simple matrix calculations yield weight percent ring carbon in substituted benzenes.
20. ABSTRACT (Cont'd)

naphthalenes, and phenanthrenes/anthracenes. The precision and accuracy of the method are good for both standards and fuel blends. The method is currently in use for correlation work in both turbine combustors and diesel engines. A large number of virgin and re-refined lubricant basestocks have been analyzed and the results compared to those from other methods. The UV data are more detailed and are believed to be more reliable and accurate.
FOREWORD

The work reported herein was conducted at the U.S. Army Fuels and Lubricants Research Laboratory (AFLRL), Southwest Research Institute, San Antonio, Texas, under Contracts DAAK70-78-C-0001 and DAAK70-80-C-0001. The work was funded by the U.S. Army Mobility Equipment Research and Development Command (MERADCOM), Ft. Belvoir, VA. Contracting Officer's representative was Mr. F.W. Schaekel, Fuels and Lubricants Division, Energy and Water Resources Laboratory (DRDME-GL).

The authors acknowledge the assistance provided by AFLRL staff members. Special recognition is given to Ms. Tanu'e F. White for her close attention to detail in the method refinement phase of the program.
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Typical Ultraviolet Absorption Spectra for Substituted Benzenes, Naphthalenes, and Anthracenes

Typical Ultraviolet Spectrophotometer Recorder Tracing

Comparison of Aromaticity Data From Several Methods

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Aromaticity for Lubricating Oils
I. INTRODUCTION

Many approaches and methods have been applied to determine the aromatic content of fuels and lubricants. Correlations of data from the various methods have been made to some of the physical properties of fuels and lubricants, but more importantly, to the performance in engines. Some such methods and properties are aniline point, smoke point, index of refraction, density, aromatics by fluorescent indicator analysis, mass spectrometry, nuclear magnetic resonance (NMR), infrared spectroscopy, specific dispersion, and heat of combustion. Relationships exist between a sample's aromaticity, that is, the amount of aromatic ring carbon, and its physical property or the results of the analytical technique applied. However, the correlations are not clear in many cases and are subject to many interferences or, in some cases, are very arbitrary. The lack of a direct method for the determination of aromaticity has demanded a new look at the need and the really significant areas of interest.

Aromaticity is the primary factor that alters the carbon-hydrogen ratio of a fuel and, as a result, the air-fuel ratio required to obtain stoichiometric combustion for maximum engine efficiency. Aromaticity is the major factor that influences the production of smoke in turbine engine exhaust. The soot particles produced cause radiation overheating of critical engine components, reducing engine life. Increased aromaticity can produce increased unburned hydrocarbons in engine exhaust, thus polluting the atmosphere. Recent work indicates polynuclear aromatic hydrocarbons and particulates in diesel engine exhaust may be directly related to diesel fuel aromaticity.

Aromaticity in lubricant basestocks has been correlated to sludge and varnish formation. There has also been considerable interest in correlating aromaticity of lubricants to polynuclear aromatic hydrocarbons in engine exhaust.

Most of the current methods for aromatics are troubled by interferences or by other molecular structures being measured as well. For example, liquid chromatography can accurately determine the aromatic content of a fuel or lubricant, but in so doing, determines the total amount of molecules that include any aromaticity. In order to correlate aromaticity to fuel and lubricant performance, only the aromatic portion of the sample molecules must be
determined. Other methods which give more specific data about the aromaticity of fuels or lubricants are subject to interferences and errors, or require expensive and not always available instrumentation. Such methods, mass and NMR spectroscopy, are capable of measuring either the aromatic ring structure or the amount of hydrogen bound to the aromatic ring. However, both methods require specially trained personnel and very expensive instruments. Gas chromatography (GC) has been used successfully by Starvinoha and Newman\(^1\)* to determine aromatic compounds in gasoline but is limited to compounds boiling below 250\(^\circ\)C. Higher boiling aromatic compounds found in diesel fuels and lubricant base stocks are not candidates for this method. Capillary GC methods are not adequate for the higher boiling ranges because of complexity of composition and lack of adequate standards. Some special applications of GC to the analysis of polynuclear aromatics\(^2\) are specific for certain unique compounds but such methods are limited and not capable of defining the many compounds present in middle distillates and lubricant basestocks. Mengenhauser\(^3\), in his work on a NMR method, has prepared an excellent review and summary of the available methods for aromatics, and has indicated the strengths and weaknesses of each. In his review of ASTM Method D 1017, an ultraviolet method, he points out the boiling range limitation of the method. Since only the 245 to 275 nanometer (nm) region of the ultraviolet spectrum is used, this method is limited in its application. The method described in this report utilizes the 190 to 350 nm range and will be shown to be broad in scope and application.

II. APPROACH

Ultraviolet (UV) spectroscopy was selected as a candidate method to determine aromaticity since absorption in the ultraviolet region of the spectrum is relatively free from alkyl substituent effects, it can be selective as to the number of fused rings and is rapidly performed on readily available equipment. Also, aromaticity can be determined in the UV region without having to determine the molecular weight of the sample or any of its components.

* Superscript numbers in parentheses refer to the list of references at the end of this report.
The unique advantage of ultraviolet absorption spectroscopy in analyzing for aromaticity is that substituted benzenes, naphthalenes, and anthracenes each have absorption maxima at different wavelengths. The absorption maximum for substituted benzenes occurs at 195nm ± 5nm, substituted naphthalenes at 225nm ± 5nm, and anthracenes at 255nm ± 5nm. Figure 1 shows typical absorption spectra of these three types of compounds. To take advantage of these unique absorption properties and analyze for the three types of components simultaneously, it is necessary to determine response factors from the absorption coefficients of pure samples of each type of aromatic compound at each of the three wavelengths, and establish matrix inversion procedures to solve three equations in three unknowns.

From Figure 1, one can see that for the substituted benzenes, the k band absorption at 195nm is approximately two orders of magnitude greater than the b band absorption at 255nm. A sample concentration in solvent producing an optimum absorbance of 0.2-0.7 for the b bands will be totally opaque for the k bands. From the Beer-Lambert equation,

\[ A = abc \]

where

- \( A \) = absorbance at the wavelength in question
- \( a \) = absorptivity constant at that wavelength
- \( b \) = optical pathlength
- \( c \) = concentration of absorbing component,

it is apparent that the only means to reduce absorbance at a given wavelength is either to reduce the concentration by dilution, or to shorten the optical pathlength. Sample dilution is time consuming and introduces errors. Retaining long pathlengths allows trace solvent impurities to increase solvent absorption at wavelengths below 210nm until severe energy limitations occur.

Based on these considerations, it is advantageous to reduce the optical pathlength as the absorbance increases at shorter wavelengths. Thus dilution is avoided and standard spectroscopic grade paraffinic or cycloparaffinic solvents may be used without further purification because proper sample concentration will require pathlengths of 0.010cm near 200nm and such solvents have minimal absorbance at such pathlengths.
FIGURE 1. TYPICAL ULTRAVIOLET ABSORPTION SPECTRA FOR SUBSTITUTED BENZENES, NAPHTHALENES, AND ANTHRACENES
Earlier work employed variable pathlength micrometer cells for incrementally reducing pathlength as sample absorbance increased at the shorter wavelengths. This approach was effective and used for some time, but the precision of the technique was greater than 5% and improvement was desirable for most applications. Matched pairs of fixed pathlength cells of 0.010cm and 0.10cm were obtained. They are accurate in pathlength and meet the requirements of the method.

III. EXPERIMENTAL

When an appropriate concentration of sample is prepared in spectrograde cyclohexane, placed in the 1.00, 0.10, and 0.010cm path sample cells with cyclohexane in the matching reference cells, the spectrum from 350 to 190nm may be recorded without further dilution if the pathlength is reduced by changing cells at appropriate points. A practical sample concentration has been found to be in the range of 8 to 10mg/25ml cyclohexane. In the case of heavy fuels or lubricant basestocks, the sample may be weighed into the volumetric dilution flask. In the case of more volatile fuels, 10.0 microliters of fuel are added to the dilution solvent in the flask with a 10 microliter syringe and the specific gravity of the fuel, determined separately, is used to calculate the sample weight. A typical UV spectrophotometer recorder tracing is shown in Figure 2. As the spectrum is scanned toward lower wavelengths, the absorptivity of the aromatics increases to such a point that the absorbance of the solution will, at some point, exceed 1.0. The scan is stopped at this point, wherever it may occur, and the 1.00cm cells in both the sample and reference beam are replaced by the 0.10cm cells. This procedure reduces the absorbance to 0.1, and the scan is continued. This process is repeated when the absorbance reaches 1.0 again by replacing the 0.10cm cells with the 0.010cm cells. Usually, pathlengths of 0.010cm are short enough to obtain the full spectrum to 190nm without dilution of the sample. The short pathlengths of solvent in both the reference and the sample beams allow scanning to low wavelengths such as 190nm without purification of solvents or operation under limited energy conditions. The absorbance values at maxima near 195, 225, and 255nm are read from the spectrum tracing, factor corrected for the pathlength, and inserted into a matrix inversion calculation to determine the concentration of mono-, di-, and tri-aromatic ring carbon in the sample.
FIGURE 2. TYPICAL UV SPECTROPHOTOMETER RECORDER TRACING
IV. STANDARDIZATION

Determination of absorptivity coefficients was determined by recording the absorption spectra of numerous pure compounds. The previously described procedure was followed in each case. The cells must be carefully cleaned and matched so that no errors are introduced by the cells themselves. Cleanliness must be rigorously maintained, and blank and standard runs must be performed regularly to assure continued quality and accuracy. Average absorptivity for each type of ring carbon at 195, 225, and 255nm was calculated. These average values are employed in the matrix calculation for weight percent of one-, two-, and three-ring carbon.

V. APPLICATION

More than 30 lubricant basestock samples were analyzed by this technique. The samples were both virgin basestocks and re-refined basestocks from a wide variety of sources. The data obtained appeared to be reasonable, but no standard of comparison was available. The method was also applied to middle distillate fuels where good correlation was obtained to smoke point and combustion data.\(^4\) However, some comparison was needed for the lubricants.

Methods which have been used for the determination of aromaticity by other workers are the specific dispersion method\(^5\) and the infrared method of Brandes.\(^6\) The specific dispersion method involves measuring the refractive index of the sample at two different wavelengths in the visible light spectrum and determining the sample's specific gravity. The specific dispersion is calculated as follows:

\[
S.D. = \frac{(n_{\lambda_1} - n_{\lambda_2})}{d} x 10^4
\]

where

- \(n_{\lambda_1}\) = index of refraction of sample at first wavelength, \(\lambda_1\)
- \(n_{\lambda_2}\) = index of refraction of sample at second wavelength, \(\lambda_2\)
- \(d\) = specific gravity of the sample
Correlation of specific dispersion values to lubricant performance has been shown. However, specific dispersion is only a relative value and cannot be employed to determine true aromatic content.

The infrared method by Brandes involves the measurement of the infrared absorbance of a sample at the 1610 cm$^{-1}$ produced by the conjugated carbon-carbon double bonds. The Brandes method is designed to produce correlating data to the ndm method which is based on index of refraction, density, and molecular weight data. In order to obtain correlation, the calculation contains certain terms which gives a positive value for weight % aromatic carbon even when the IR absorbance at 1610 cm$^{-1}$ is zero. This obvious error cannot be accepted for a modern analytical method.

As an alternative, a series of known aromatic compounds were used to recalibrate the basically sound approach of an infrared method. Classical methodology was employed to obtain absorptivity coefficients for weight % ring carbon at 1610 cm$^{-1}$. All lubricant samples were then recalculated using these coefficients.

VI. DISCUSSION

All lube oil data obtained are shown in Table 1. For clarity and simplicity, summarized data are illustrated in Figure 3, entitled "Comparison of Aromaticity Data From Several Methods."

All data are plotted and compared to the sum of the one-, two-, and three-ring weight % carbon found by UV. Thus, the better the agreement between the compared method data and the UV data, the closer the data points approach the line. Since the specific dispersion data form an arbitrary scale and do not directly correlate numerically, they are not expected to coincide with any of the other data. However, the trend of the specific dispersion data is indicative of the general merit of each of the methods. Only a limited number of samples could be analyzed by this method because the method is not applicable to samples which are highly colored. The majority of the re-refined oil samples were too highly colored to measure refractive index.
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1 = Brandes method.
2 = Recalibrated IR method.

The Brandes method data are consistently high as expected since the equation has a 1.2 weight % ring carbon intercept term. The slope of the curve appears to be slightly greater than it should be.

The recalibrated IR data are somewhat closer to the expected values, although generally low. Some of these data actually agree well with the UV data. The disagreement of the IR data can be expected since substitution on the ring, geometry, and symmetry will all affect the IR absorptivity of the ring struc-
FIGURE 3. COMPARISON OF AROMATICITY DATA FROM SEVERAL METHODS
ture. The surprisingly good agreement is an indication of the validity of the UV method.

It should be pointed out that, for the sake of clarity, all data points have not been plotted. Many other data points occur among those which are illustrated.

VII. CONCLUSIONS

It may be concluded from the data shown and the experience gained in obtaining these data, that a very powerful and meaningful method has been developed and applied. The UV method not only gives weight % ring carbon, but also gives the configuration of the rings. These data are being correlated to practical performance data and should form a base for a better understanding of fuel and lubricant technology.

VIII. REFERENCES


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