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INFRARED-SPECTROPHOTOMETRIC ANALYSIS OF BINARY AND

TERNARY MIXTURES OF LIQUID HYDROCARBONS

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NATIONAL ADVISORY COMMITTEE FOR AERONAUTICS

ADVANCE RESTRICTED REPORT

INFRARED-SPECTROPHOTOMETRIC ANALYSIS OF BINARY AND

TERNARY MIXTURES OF LIQUID HYDROCARBONS

By Alden P. Cleaves and Mildred E. Sherrick

SUMMARY

An investigation was conducted to determine the suitability and precision of a modified, routine-model, infrared spectrophotometer for analyzing binary and ternary mixtures of aircraft-fuel components. Analyses by means of infrared measurements are described for the following hydrocarbon mixtures: 12 known mixtures of 2,2,3-trimethylbutane (triptane) and cyclohexane, 4 known mixtures of triptane and benzene, and 4 known mixtures of triptane, cyclohexane, and benzene.

The effects of certain factors on the accuracy of the analyses are considered and the precision attained is reported. Computed differences between weighed and spectrophotometric percentages are regarded as uncertainties of the analyses. Five repeated spectrophotometric measurements on the groups of four known mixtures make possible the estimation of the reproducibility for these cases. Imperfect reproducibility and minor deviations of the measurements from a linear relation between extinction and concentration are important sources of uncertainty.

The results indicate that rapid and reliable analyses of binary and ternary mixtures of the three types of liquid hydrocarbon represented by 2,2,3-trimethylbutane (triptane), cyclohexane, and benzene are feasible by use of a routine-model infrared spectrophotometer with an average uncertainty (relative to compounds regarded as pure) of approximately ±1 percent. The improved reliability that results from determining the mean of five extinctions indicates the desirability of repeating extinction measurements when a small increase of time required for analysis is unimportant.

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INTRODUCTION

Simple, rapid, and reliable methods of analysis for individual hydrocarbons facilitate scientific control of the production of high-antiknock components for aircraft fuels. Extensive production of fuels for military aircraft by new methods of petroleum processing and fuel synthesis has increased the need for such analytical methods. As the antiknock characteristics of new hydrocarbons become known, analyses of synthetic fuel components provide a guide for the rational modification of processes and the scientific blending of the products into high-performance aircraft fuels that meet predetermined specifications. Chemical methods are generally either too slow or too restricted in scope to serve adequately these purposes.

Prior to about 1940 much knowledge concerning the composition of hydrocarbon mixtures similar to the gasoline fraction of petroleum was acquired from measurements of the physical properties of narrow-boiling fractions obtained by distillation. These techniques. perfected in the investigations of reference 1, have been amplified by adsorption techniques (reference 2) and freezing-point measurements (reference 3) into physical methods for quantitative analysis that are effective but often tedious. Usually these physical methods can be based on accurate values of the properties of pure hydrocarbons, such as compiled in reference 4. Infrared analysis, another physical method that has recently been developed (references 5 to 8), is reliable, relatively rapid, and often adequate for the analysis of fractions containing about six components. This method, supplemented by distillation, may therefore expedite the analysis of complex fuel components. Inherent differences in infrared spectrophotometers make it essential that surples of pure hydrocarbons be available for the calibrations on which infrared analyses are based.

Information received from the Spectrographic Subcommittee of the British Technical Advisory Committee indicates that researchtype infrared spectrophotometers having high dispersion have been used to analyze liquid hydrocarbon fractions with boiling ranges loss than 5° C and boiling temperatures below 100° C. Some progress has also been made by British and American scientists with hydrocarbon mixtures in the boiling range above this temperature.

In connection with a general program to evaluate and compare hydrocarbon products of high antiknock value, an investigation was conducted at the NACA Cleveland laboratory during

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the spring and summer of 1944 to determine the suitability of a modified, routine-model, infrared spectrophotometer for analyzing synthetic liquid hydrocarbon mixtures. This instrument was reported in reference 7 to be adequate for vapor mixtures. The investigation consisted in analyses of synthetic binary and ternary mixtures of liquid paraffinic, naphthenic, and aromatic hydrocarbons and also included a study of some factors affecting accuracy of the results. Some details of the analytical methods employed have been omitted from this report owing to the extensiveness of the available literature on the subject.

CONSTITUENTS OF THE MIXTURES

The difficulty of spectrophotometric analysis is affected by the number of components, their molecular structure, and their boiling points. As boiling points increase, temperature intervals between adjacent-boiling compounds and the wavelength intervals between bands in the infrared spectrum of each compound tend to decrease. Separation by distillation and analysis based on the spectra for mixtures that contain compounds with boiling points above approximately 100° C are difficult, and resulting analytical errors may sometimes amount to more than 1 percent of the total sample. Progress may nevertheless be expected in the successful application of infrared methods.

<u>Choice of hydrocarbons.</u> - Components that form mixtures of medium analytical difficulty were selected for trial analyses. The compounds chosen for the present investigation were 2,2,3-trimethylbutane (triptane), benzene, and cyclohexane. These hydrocarbons represent typical paraffinic, aromatic, and naphthenic components, respectively, of an aviation-fuel cut that boils at approximately 80° C. The boiling point of the triptane is 80.9° C and the boiling points of the other two hydrocarbons are within 1° of this temperature.

<u>Purity of the samples</u>. - Because all analyses presented herein are in terms of the actual hydrocarbon samples (which were regarded as pure), the accuracy of these analyses relative to absolutely pure compounds is affected by the purity of the samples used. All samples were dehydrated, and a description of additional treatment to reduce errors caused by the presence of impurities is given in the following paragraphs.

The sample of triptane was a middle fraction obtained by distillation with a still of 40 theoretical plates from part of a batch supplied by the General Motors Corporation. The batch was 97 percent pure or better according to information from the supplier. Refractive indices of cuts in the distillation ranged from 1.3891 to 1.3895. The variation in indices of the cuts is probably evidence of some selective fractionation favorable to improved purity. The index 1.3895 is that of the sample used in this investigation and is identical with the value for pure triptane given in reference 4 (p. 2).

The cyclohoxane sample was also a middle fraction distilled from about 2 liters of the compound supplied by the Phillips Petroleum Company. Refractive indices of the consecutive cuts decreased from 1.42644 to 1.42619, and the index of the center cut used was 1.42621, which agrees with the value for pure cyclohexane given in reference 4 (p. 116).

The benzene sample, obtained from The Barrett Division of Allied Chemical & Dye Corporation, was extensively treated by the Fuels Synthesis Section at the Cleveland laboratory to improve its purity. The agreement of values representing its physical properties as obtained by the Fuel Synthesis Section with values given in reference 4 (p. 75) is shown in the following tabulation and is evidence of the high purity of the sample.

Sample	Source	Refrac- tive index, 20 D	Freezing point (^O C)	Boiling point (°C)	Specific gravity, d ²⁰ 4
Benzene	Cleveland laboratory	1.5011	5.49	80.1	0.8789
	Reference 4 (p.75)	1.5012	5.51	80.09	.87893

APPARATUS

Routine-model infrared spectrophotometer. - The routinemodel infrared spectrophotometer, described in detail in reforences 5 to 7, has a 60° rock-salt prism with 4- by C-centimeter faces and slits of 1-centimeter length, which are adjustable with a precision of about 0.01 millimeter in the range of widths from 0.01 to 2 millimeters. The spectrophotometer is equipped with 17 individually adjustable stops for making reproducible wavelength settings in the range from 3 μ to 15 μ . The effect of temperature change on the refractive index of the prism is compensated by a differential-expansion mechanism that controls the exact position of the parabolic collimating mirror.

The spectrophotometer was modified for the present tests by installing a micrometer screw (0.001 in. per graduated division) that made possible continuous adjustment of wavelength. A support for liquid-absorption cells was mounted between the water-cooled shutter and the entrance window of the spectrophotometer. The output of the compensated thermopile was registered by a D'Arsonval galvanometer having a sensitivity of 0.045 microvolt per millimeter at 1 meter. The slit widths used (0.3 to 0.5 mm) corresponded to an effective slit width of about 50 cm⁻¹ (1 cm⁻¹ = $1/\lambda$ (cm), where λ is wavelength). Galvanometer deflections when no liquid cell was in the light path were maintained greater than 100 millimeters.

Liquid absorption cells. - Ideas from the literature (for example, reference 9) were used for the design and the construction of liquid cells with polystyrene-coated, rock-salt windows about 3/16 inch thick separated by metal-foil spacers either 0.002 or 0.013 inch thick. The details and assembly of a liquid cell are shown in the sketches of figure 1. A mercury-amalgam coating on the foil sealed the liquid space. Center-drilled, brass machine screws with heads removed were forced into tapered, tapped holes in one of the rock-salt windows to provide filling and emptying orifices that could be closed with tapped metal caps. Hollow, cylindrical steel attachments, tapped at one end, replaced the caps during filling and cleaning operations. The cells slid horizontally on ways so mounted that a cell could be moved at will into or out of the entrant radiation.

DISCUSSION OF FACTORS AFFECTING PRECISION

Effective slit width. - References 10 and 11 present compilations of the infrared spectra of pure hydrocarbons. The infrared spectra of triptane, cyclohexane, and benzeno measured with a high-dispersion infrared spectrophotometer by the British Spectrographic Subcommittee (reference 10) are reproduced in figure 2. The effective slit widths of the spectrophotometer are indicated on the graph. The triptane spectrum for the region from 8 μ to 9.5 μ , obtained at the Cleveland laboratory with the routine-model spectrophotometer used for the present tests, is presented as a superposed dashed curve in figure 2 to demonstrate the relative resolving power (effective slit width) of the spectrophotometer. The bands in the triptane spectrum at approximately 9.07 μ and 9.26 μ (separation, 22 cm⁻¹) are not resolved in the dashed curve but are merged into an asymmetrical peak, whereas the bands at 8.3 μ and 8.7 μ (separation, 58 cm⁻¹) are resolved almost equally well by both instruments. This evidence indicates that the effective slit width of the routine-model spectrophotometer in this region is about 50 cm⁻¹.

Accuracy may be decreased if an enalysis based on bands separated by less than 50 cm⁻¹ is attempted. This source of error was obviated as far as possible in the present analyses by the selection of favorable wavelengths. Deviation from Beer's law may be expected if the width of a band used is considerably less than 50 cm⁻¹. Correction for this deviation was considered unnecessary because other random errors were of the same order of magnitude.

Choice of wavelengths for analysis. - When two or more compounds in a multicomponent mixture absorb radiation at the same wavelength, their absorptions are said to "interfere." For the sake of accuracy, this interference should be as small as possible at the wavelengths chosen for analysis. A survey of the spectra in figure 2 to find a suitable intense absorption band that is characteristic of each compound indicates the following possibilities:

Compound	Wavelength of absorption band (µ)		
2,2,3-Trimethylbutane (triptane)	8.3, 8.7, 9.3		
Cyclohexane	7.9, 11.6		
Beuzane	8.5 9.7		

Final choice of one or two wavelengths for analysis of binary and ternary mixtures is influenced by consideration of which two hydrocarbons are in the binary mixtures or of whether any one of the three hydrocarbons is known to be a principal component of the ternary mixtures. For example: When only benzene absorption is considered, the intense band at 9.7 μ would be preferable to the weaker band at 8.5 μ for analyzing triptane-benzene mixtures because of interference by the triptane bands at 8.3 μ and 8.7 μ . For analysis of cyclohexanebenzene mixtures, the benzene band at 8.5 μ would probably be better because of absorption by cyclohexane near 9.7 μ . For ternary mixtures, choice between these two bands should apparently be determined by the concentration of triptane or cyclohexane, estimated by preliminary analysis. The benzene band

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Absorption by cell windows. - For the present investigation each extinction E was computed as the logerithm of the ratio of the galvanometer deflection at a given wavelength when no cell was in the light path to the deflection at the same wavelength when a cell filled with liquid was in the light path. Hence, each measured extinction is the sum of the extinctions of the liquid and of the cell windows. If the absorption by cell windows does not change during a series of measurements, these measured extinctions are a reliable basis for analysis. If fogging of either the inside or the outside surfaces of the windows occurs, the measured extinction will necessarily increase a definite amount and this increase will be present in subsequent measurements. In order that corrections for such changes may be applied, extinctions of the pure liquid components measured at several wavelengths and regarded as constant standards may be made daily during a series of analyses. Necessary corrections indicated by changes in these standard extinctions can then be applied to subsequent measurements. If a value for the window absorption is required, the extinction measured with a liquid of negligible absorption in the coll may be used. This general problem and solutions for it are discussed in reference 8.

Instrumental variables. - The undesirable effects of background radiation or stray light arising from scattering and reflection of radiation at wavelengths shorter than the wavelength being measured were minimized by the optical design of the spectrometer, by baffles, by light-absorbent paint, and by the use of an appropriate filter or shutter. Magnesium oxide served as the filter for the region from 3μ to 10μ and lithium fluoride as the shutter for the rogion from 10μ to 15μ .

A constant-voltage transformor stabilized the power supply, and reliance was placed on the design of the spectrometer for constancy of source intensity and reproducibility of slit-width settings. The continuously adjustable screw (described under APPARATUS) did not afford as good reproducibility as the turret stops but was more convenient for the wavelength settings. The galvanometer was set at zero prior to each deflection by manual adjustment of the sliding translucent scale.

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A single cell was used for each series of analyses and its thickness was not accurately determined; cell thickness was assumed constant and no correction was made for any increase of thickness owing to solution of salt from the inside window surfaces by the dehydrated hydrocarbons. Effects on precision of gradual variations of source intensity or thermopile or galvanemeter sensitivity were minimized by determining consecutively two deflections for calculating each extinction in as brief an interval as possible, about 40 seconds for the average case.

PROCEDURE AND RESULTS

Twenty mixtures of the pure liquid hydrocarbons were quantitatively prepared by weighing, and extinctions to be used for analyses were measured in a 0.002-inch cell at the wavelengths designated in the following tabulation. The last two columns designate the table and the figure in which the results of measurements and analyses are shown.

Number of mixtures	Type of mixture	Hydrocarbons in mixture	Wavelengths used for measuring extinctions (µ)	Figure	Table
12	Binary	Triptane, cyclo- hexane	8.3 and 11.6	3	I
4	Binary	Triptane, benzene	9.7	4	II
4	Ternary	Triptane, benzene, and cyclohexane	8.3 and 9.7	5	III

Exploratory investigations were essential as aids in the choice of wavelengths for the analyses. The precision of preliminary analyses based on various wavelengths was compared. In many cases, choice of wavelength had only a small effect on precision, but it was found that use of a wavelength of 8.3 μ resulted in errors about one-third as large as those resulting from the use of a wavelength of 11.5 μ for analysis of the same group of triptane-cyclchexane mixtures. (See table I.) The larger error was probably due to interference by the triptane band at 12 μ . These preliminary tests also indicated the desirability of analyzing binary mixtures by using the most suitable single wavelength to determine one component and by calculating the amount of the other component by subtraction from 100 percent. Similarly, two wavelengths were found to be adequate for

analyzing ternary mixtures. Wavelengths of 8.3 μ and 9.7 μ , characteristic of triptane and benzene, respectively, were chosen as the probable best pair for analysis of the ternary mixtures prepared for this investigation.

<u>Binary mixtures.</u> - For the binary mixtures of triptane and cyclohexane, two independent graphical analyses were made by using the data for the pure compounds and for mixtures 2, 5, 8, and 11 in table I to establish the straight lines shown in figure 3. Representative straight lines were drawn and the eight other mixtures were independently analyzed relative to the lines for wavelengths of 8.3μ and 11.6μ . The 12 mixtures were also analyzed by means of the data at 8.3μ by a simple mathematical technique based on the slope and the intercepts of the representative line. In all these analyses, the concentrations for the unreported component may be determined by subtraction from 100 percent. Results of the analyses, expressed as volume percentages and as differences between analytical and weighed values, are presented in table I.

Five measurements of extinction at 9.7 μ were made for each of the four binary mixtures of triptane and benzene. The data were treated by the following two methods that are similar in principle: (a) analysis on the basis of these five extinctions by using a straight line through the mean extinctions at 9.7 μ for the pure compounds, as shown in figure 4; and (b) analysis on the basis of the same individual extinctions by means of equation (6) in reference 7, adapted for binary mixtures. Arithmetic means of the resulting concentrations together with the average differences of individual values from the mean of five measurements, computed in percentage by volume, are presented in table II.

<u>Ternary mixtures</u>. - The four ternary mixtures containing triptane, cyclohexane, and benzene were analyzed by using equation (6) of reference 7 for each pair of the five repeated measurements of extinction at wavelengths of 8.3μ and 9.7μ . The results together with the differences, the mean values, the differences between weighed and mean values, and the mean of means are presented in table III. The compositions of the ternary mixtures, plotted on the trilinear chart in figure 5 show that triptane was present in the greatest concentrations and that only a portion of the possible range of composition was investigated. The method of analysis, however, did not involve any adjustment of the data and should give results of uniform accuracy for the complete range of composition.

DISCUSSION OF RESULTS

All analyses are reported in percentages by volume of the liquid hydrocarbon samples blended in the mixtures. Tables I and II present the most accurate sets of values selected from exploratory tests at various wavelengths.

With one exception all of the points for mixtures 3 to 10 of table I are above the straight line for 8.3 μ in figure 3; whereas all points for mixtures 1, 11, 12, and the pure hydrocarbons are below this line. This distribution of the points indicates that a slight curvature (convex upward) in the line used for analysis would have decreased the average error of the analyses. Unpublished calculations based on a parabola gave about 0.1-percent improvement. The data taken at 8.3 μ (fig. 3) seem to indicate a little deviation from Beer's law. Measurements at 8.3 μ were also used to analyze the ternary mixtures; hence it is possible that the uncertainties reported in table III might have been slightly reduced by todious corrections for deviations from Beer's law according to the method described in reference 7.

The data presented in tables II and III indicate that the average absolute difference of five individual triptane determinations from the mean values or from the weighed values was in nearly all of the cases larger than the difference between weighed and mean analytical values of the concentration. Nonreproducibility of measurements is evidently an important source of uncertainty. The actual time for making measurements is but a fraction of the total time per analysis because data for a repeated evaluation of extinction can be readily obtained in less than 1 minute. An analysis based on a mean of five measurements, therefore, requires additional time of less than 4 minutes for the cases reported in table II and less than 8 minutes for the ternary analyses in table III. This increase, which is about one-fifth of the average time for each analysis, decreased the uncertainty of the results in tables II and III by about one-half and one-fifth, respectively. In many cases the increased reliability of the analyses would more than compensate for the additional time required.

In addition to lack of reproducibility in measurements, interference and small deviations from Beer's law (which may have been due to the large effective slit widths of the routinemodel infrared spectrometer) were important sources of uncertainty. The better precision of the binary-mixture analyses as

compared with the analyses of ternary mixtures probably resulted from more successful elimination of these factors. In all cases, however, the precision attained is satisfactory for many applications of a rapid infrared-analysis technique.

CONCLUSIONS

From analyses of 16 binary and 4 ternary mixtures of liquid hydrocarbons with a modified routine-model infrared spectrophotometer, the following conclusions were drawn:

1. Rapid and reliable analyses of binary and ternary mixtures of the three types of liquid hydrocarbon represented by 2,2,3-trimethylbutane (triptane), cyclohexane, and benzene are feasible by use of a routine-model infrared spectrophotometer with an average uncertainty, relative to compounds regarded as pure, of about ±1 percent.

2. Exploratory measurements on synthetic mixtures and pure compounds are essential to determine the validity of Beer's law and to establish the best method of analysis for each group of compounds.

3. The improved reliability of analyses that results from using the means of five extinctions indicates the desirability of repeating extinction measurements when a small increase of time required for analysis is unimportant.

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TABLE I

INFRARED ANALYSES OF BINARY MIXTURES OF 2,2,3-TRIMETHYLBUTANE

(TRIPTANE) AND CYCLOHEXANE

[Spectrophotometric values based on graphical analysis using mixtures 2, 5, 8, and 11 as standards]

Mix- turo	2,2 (1	2,5-Trimethy] in mixtur porcent by vo	Magnitude of differ- once between weighed and spectrophoto- metric values			
	Weighed	Spectroph	otometric	(percent by volume)		
		λ = 8.3 μ	$\lambda = 8.3 \mu$	$\lambda = 11.6 \mu$		
1	3.2	3.2 2.7		0.5	0.8	
2	10.0	! <i>→</i> + -			3.2	
- 3	20.0	20.5	16.8	.5		
4	28.7	24.3	29.0	.6	•3	
5	41.0		*******			
6	49.(50.7	50.0	1.0	.3	
7	50.0	49.8	50.5	.2	.5	
8	59.9					
9	74.7	75.8	19.8	1.1	5.1	
10	80.0	80.0	81,8	.0	1.8	
11	92.2					
12	. 95.5	95.3	99.2	.6	3.3	
Mean			0.6	1.9		

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TABLE II

INFRARED ANALYSES OF BINARY MIXTURES OF 2,2,3-TRIMETHYLBUTANE

(TRIPTANE) AND BENZENE

Spectrophotometric measurements at wavelength λ of 9.7 μ]

Mix- ture	2,:	2,3-Trimethy (porcont	Magnitude of differ- once between weighed values and spectro- photometric means (percent by volume)			
1	Weighed	Spe				
		Mean of five graph- ical dotor- minations	Moan of fivo calcu- latud deter- minations	Avcrage differ- ence (a)	Graphical	Calculatod
1 2 3 4	20.2 30.9 63.9 85.3	20.2 31.7 64.5 84.5	19.6 31.1 64.2 84.3	1.5 1.0 1.0 .4	0 .8 .8 .8	0.6 .2 .3 1.0
Mean				1.0	0.5	0.5

^eValues represent average of magnitudes of differences in individual determinations from the given mean values.

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TABLE III - INFRARED ANALYSES OF TERNARY MIXTURES OF 2,2,3-TRIMETHYLBUTANE

(TRIPTANE), BENZENE, AND CYCLOHEXANE

[Spectrophotometric analyses calculated on the basis of measurements at 8.3μ and 9.7μ .]

Mix- ture	Deter- mina-	2,2,3-Trimethylbutane (percent by volume)			Benzene (percent by volume)		Cyclohexane (percent by volume)			
	tion	Weighed	Spectro- photo- metric	Differ- ence	Weighed	Spectro- photo- metric	Differ- ence	Weighed	Spectro- photo- metric	Differ- ence
1	8	40.6	42.6	2.0	50.2	51.1	0.9	9.2	6.3	-2.9
	Ъ		39.5	-1.1		50.1	1		10.4	1.2
	c		40.4	2		49.3	9		10.3	1.1
	d		38.6	-2.0		52.0	1.8		9.4	.2
	θ		38.6	-2.0		50.3	.1		11.1	1.9
Mean			39.9	-0.7		50.6	0.4		9.5	0.3
2	8	63.6	63.7	0.1	26.1	29.6	3.5	10.3	6.7	-3.6
	b		62.1	-1.5		28.7	2.6		9.2	-1.1
	c		63.9	.3		29.0	2.9		7.1	-3.2
	d		63.0	6	*******	29.4	3.3		7.6	-2.7
	e		60.9	-2.7		27.7	1.6		11.4	1.1
Nean			62.7	-0.9		28.9	2.8		8.4	-1.9
3	8.	64.2	66.2	2.0	9,8	8.7	-1.1	26.0	25.1	-0.9
	Ъ		64.9	.7		9.5	3		25.6	4
	C		66.5	2.3		9,9	.1		23.6	-2.4
	d		65.8	1.6		9.1	7		25.1	9
	0		66.9	2.7		10.9	1.1		22.2	-3.8
Nean	~~~~~~		66.1	1.9		9.6	-0.2	*******	24.3	-1.7
4	a	87.4	89.0	1.6	8.2	7.4	-0.8	4.4	3.6	-0.8
	Ъ		88.3	.9		7.5	7		4.2	2
	C		88.9	1.5		7.1	-1.1		4.0	4
	đ		90.6	3.2		7.1	-1.1		2.3	-2.1
	8		88.2	.8		6.7	-1.5	********	5.1	.7
Mean		*******	89.0	1.6		7.2	-1.0		3.8	-0.6
ilean c	f means			±1.3			±1.1		********	±1.2

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Fig. 1





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Fig. 2



Figure 2. - Infrared spectra of 2,2,3-trimethylbutane (triptane), cyclohexane, and benzene. Reproduced from reference 11. Superposed dashed curve for triptane (from 8 to 9.5 μ) obtained at the Cleveland laboratory with a routine-model infrared spectrometer. Arrows indicate absorption bands chosen for analysis.



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Fig. 3



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Triptane, percent by volume



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Fig. 4





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