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## THE INFRARED ABSORPTION SPECTRA OF SIX C<sub>11</sub> HYDROCARBONS AND THEIR APPLICATION TO THE STUDY OF DIESEL FUELS

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**INTRODUCTION.** Theoretical treatment of simple molecules and correlations of numerous spectra containing a common atomic grouping have shown that functional groups within the molecules often give rise to specific absorption at characteristic regions of the infrared spectrum. The atoms constituting these functional groups can move with characteristic vibrational frequencies which, for the most part, are independent of the remainder of the molecule. The frequency of infrared radiation absorbed corresponds to these vibrational frequencies. If these frequencies are known for various functional groups, it is frequently possible to determine the presence or absence of a particular group in an unknown by a simple observation of its infrared absorption spectrum.

Through the efforts of the American Petroleum Institute and the National Bureau of Standards many relatively pure hydrocarbons are being made available for infrared study, and a library of reference spectrograms is being compiled. This vitally important library is being supported by contributions of data from some 25 laboratories. The University of Oklahoma was one of the earliest contributors.

The ability to distinguish the types of hydrocarbons present in a closely cut petroleum fraction, and further, to gain more quantitative information concerning these hydrocarbons would be of great value in studying the relationship of Diesel fuel composition and its combustion behavior. However, the composition of Diesel fuels is very complex, as the following outline of the hydrocarbons present in straight-run fuel indicates. Cracked stocks would be further complicated by the presence of aliphatic and cyclic olefins.

## HYDROCARBON TYPES

## I. Alkanes

- A. Normal
- B. Branched

## II. Naphthenes (cycloalkanes)

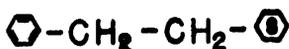
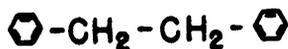
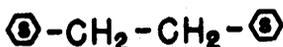
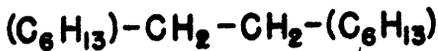
- A. 5-membered rings
  - 1. Monocyclics (alkylated cyclopentanes)
  - 2. Polycyclics (generally only 2 rings in Diesel fuels)
    - a. Fused rings (alkylated bicyclooctane)
    - b. Separate rings
      - (1) Dicyclopentyl alkanes
      - (2) Alkylated dicyclopentyls
- B. 6-membered rings
  - 1. Monocyclics (alkylated cyclohexanes)
  - 2. Polycyclics (generally only 2 rings in Diesel fuels but probably small amounts of tricyclic compounds)
    - a. Fused rings (alkylated decalins)
    - b. Separate rings
      - (1) Dicyclohexyl alkanes
      - (2) Alkylated dicyclohexyls

## III. Aromatics

- A. Monocyclic (as regards aromatic ring)
  - 1. Alkylated benzenes
  - 2. Alkylated tetrahydronaphthalenes
- B. Polycyclic (generally only two but small amounts of three-ring compounds are present)
  - 1. Fused rings
    - a. Alkylated naphthalenes
    - b. Anthracene and other tricyclics
  - 2. Separate rings
    - a. Diphenyl alkanes
    - b. Alkylated diphenyls

One method of attacking such a problem is to study pure compounds in which certain functional groups are changed systematically. Fortunately through the excellent work of the American Petroleum Institute Research Project 43, such a series of compounds in this Diesel fuel boiling range was available. Accordingly, one objective of the research was to determine the spectra of these compounds and evaluate the changes in these spectra caused by the changes of the functional groups. A secondary purpose of the research was to provide American Petroleum Institute Research Project 44 with spectrograms of these compounds.

The six  $C_{11}$  hydrocarbons chosen for study were: *n*-tetradecane; 1-cyclohexyloctane; 1-phenyloctane; 1,2-dicyclohexylethane; 1,2-diphenylethane; and 1-phenyl-2-cyclohexylethane. The interrelation of the compounds in this series is easily seen in the following formulas which are drawn in such a manner as to present each hydrocarbon as a substituted ethane in which the substituent groups are normal  $C_n$ -alkyl, cyclohexyl, and phenyl:



These six hydrocarbons were synthesized and purified at Pennsylvania State College under American Petroleum Institute Research Project 42. No definite information concerning their purity has been made available. However, the advisory committee for this project has specified a minimum purity of 95 mol percent, and the compounds are believed to be considerably higher purity than this.

**PRESENTATION OF DATA.** Spectrograms (per cent transmission vs. wave length) of these six hydrocarbons, throughout the region from 2.5 to 15  $\mu$ , are shown in Figures 1 through 6. Supplementary data are taken from the library of spectrograms of American Petroleum Institute Research Project 44 in an attempt to obtain correlations between absorption bands and functional groups within the molecules of the samples studied.

The approximate positions in microns of bands characteristic of chain, cyclohexyl and phenyl groups are shown in Table I. The approximate intensities of these bands in *n*-tetradecane, 1-cyclohexyloctane and 1-phenyloctane are also included. Based upon measurements with a 0.06 mm cell, a band is designated very weak (VW), weak (W), medium (M), strong (S), or very strong (VS) if its per cent transmission falls between 100 and 80, 80 and 60, 60 and 40, 40 and 20, or 20 and 0, respectively.

Tables II to VII show the wave lengths in microns and the corresponding wave numbers for the absorption maxima, taken from the original records. The accuracy of measurement of the positions of the absorption maxima is  $\pm 0.01 \mu$  at 14  $\mu$  to  $\pm 0.03 \mu$  at 3  $\mu$ . Some weak bands in the region of atmospheric water vapor and carbon dioxide absorption may have escaped detection, or the error in measurement might be slightly larger than the limits given. The accuracy with which these absorption maxima can be located, of course, depends upon the shape of the band and its proximity to others. The spectrometer used has been described by Nielsen, Bruner and Swanson (4).

**ASSIGNMENT OF CERTAIN BANDS TO STRUCTURAL GROUPS.** In a study of the spectra of 14 phenyleicosanes and the analogous cyclohexyleicosanes as reported by Nielsen *et al.*, (4) the absorption bands for these hydrocarbons were classified as arising from one of three functional groups—phenyl, cyclohexyl or chain. These data were supplemented by spectra of other alkyl derivatives of benzene and cyclohexane from the American Petroleum Institute Research Project 44 catalog of infrared spectral data. The six hydrocarbons in the present study contain only these three structural groups, and the data are treated

in a similar manner. It is quite readily seen that several bands repeatedly occur in approximately identical spectral positions and with similar intensities in a group of alkylbenzenes, as in the case of the phenyleicosanes studied by Nielsen *et al.* (4). Some of these bands are not present in the cyclohexyl analogues of these alkylbenzenes and are consequently attributable to vibrations of the benzene ring or atoms connected directly to it. Similarly, a few bands can be assigned to the cyclohexyl ring and others to the alkyl chain. Three of the compounds studied contain a terminal  $-CH_3$  group on the alkyl chain, while the other three do not, which affords a correlation as to which bands are due to vibration within this methyl group.

In Table I are listed the spectral positions of the bands attributed to each of the three main functional groups, along with a rough indication of their respective intensities. Some brief remarks concerning some of these bands follow:

**PARAFFIN CHAIN VIBRATIONS. 13.85  $\mu$ :** This band, characteristic of a paraffin chain, is found in the spectra of *n*-tetradecane, 1-cyclohexyloctane, and 1-phenyloctane (Figures 1, 2, and 3), with its strength decreasing as the per cent of chain decreases. This band position is constant for the normal paraffins above  $C_6$ , shifting to 13.7  $\mu$  for the lower members. The substitution of a phenyl or cyclohexyl group on the normal paraffin chain has little or no effect on the band position, regardless of the position of substitution, in the spectra of the phenyl and cyclohexyl eicosanes reported by Nielsen *et al.* (4). The substitution of a phenyl or cyclohexyl group in a smaller normal chain, such as *n*-octane, would quite likely cause considerable shift of the band position, if the substitution was on the 3rd or 4th carbon atom. No appreciable shift is noted in the 1- or 2-phenyl- or cyclohexyloctane, however. This band has been shown to be present in any molecule containing the group  $-(CH_2)_n-$  in an open chain, where *n* is equal to or greater than 3. It has frequently been assumed to be a skeletal vibration of the carbon atoms in the chain. Recently, however, Sheppard and Sutherland (5) working with fully deuterated long-chain paraffins found that this band had shifted to longer wave lengths by  $\sqrt{2}$ . All of the bands known to be caused by hydrogen vibrations were also shifted by this amount, as predicted from theoretical considerations. This proved conclusively that this 13.8  $\mu$  band arises not from a skeletal vibration but from a vibration involving the hydrogen atom. The most probable explanation is that it is caused by a rocking vibration of the pairs of hydrogen atoms in the methylene ( $CH_2$ ) group.

**11.24  $\mu$ :** This band of weak intensity appears in the normal paraffins above *n*-octane and is seen in the spectrum of *n*-tetradecane (Figure 1). A band in this same position is found in the mono-alkyl-substituted cyclo-hexanes and is discussed further under the classification of cyclohexyl vibrations.

**9.27  $\mu$  and 9.04  $\mu$ :** These positions which were taken from the spectrum of *n*-tetradecane are constant to  $\pm 0.05 \mu$  for *n*-tridecane through *n*-octadecane and probably higher but shift to longer wave lengths in smaller molecules. Both of these bands are present in the  $C_6$  and higher normal paraffins, with the 9.27  $\mu$  band being the more intense in compounds from *n*-octadecane to *n*-dodecane. The 9.04  $\mu$  band becomes more intense in *n*-undecane, is still stronger in decane and nonane and completely obscures the decreasing 9.27  $\mu$  band in *n*-octane. Both bands, however, shift progressively to longer wave lengths with decreasing chain length, until in *n*-octane the 9.04  $\mu$  band has shifted to 9.27  $\mu$ .

**7.24  $\mu$ :** This strong, sharp band which is characteristic of a methyl group (2) is very strong in *n*-tetradecane (Figure 1) with two terminal methyl groups; strong in 1-cyclohexyloctane and 1-phenyloctane (Figures 2 and 3) with only one methyl group; and absent in 1,2-dicyclohexylethane, 1,2-diphenylethane, and 1-phenyl-2-cyclohexylethane (Figures 4, 5, and 6) where no methyl groups are present. The band appears strongly in 1,1-dicyclohexyla-

thane and 1,1-diphenylethane and could be used to identify these 1,1-disubstituted ethanes in the presence of their 1,2-disubstituted isomers.

6.80  $\mu$ : Caused by C-H bending vibrations, this band is common to all hydrocarbons. Its position is quite constant for the paraffins except in some cases of extreme branching of the chain in which it may appear from 6.76 to 6.83  $\mu$ . Phenyl and cyclohexyl substitutions on the *n*-paraffin chain cause it to shift to longer wave lengths, 6.87  $\pm$  0.02  $\mu$ , which is in agreement with the shift reported for the phenyl- and cyclohexyleicosanes by Nielsen *et al* (4).

3.4  $\mu$ : C-H valency vibrations give rise to several strong sharp fundamental bands in this region, which are common to all hydrocarbons. With higher resolution through the use of a lithium fluoride prism, information can be gained from these bands concerning the various types of C-H linkages.

**CYCLOHEXYL VIBRATIONS.** 11.84  $\mu$ : Although a band in this region appears in the spectra of *n*-paraffins, it is broad and of weak intensity. Its intensity is greatly enhanced in the substituted cyclohexanes as seen in the spectra of 1-cyclohexyloctane and 1,2-dicyclohexylethane (Figures 2 and 4) where its intensities are strong and very strong, respectively, compared to the weak intensity in *n*-tetradecane (Figure 1). Its position is approximately constant for 16 mono-alkyl-substituted cyclohexanes (API), at 11.84  $\pm$  0.05  $\mu$  except in the case of 2-cyclohexyl paraffins in which the band appears split into two components at 11.73  $\pm$  0.02  $\mu$  and approximately 11.96  $\mu$ . As the substitution moves toward the center of the chain the band shifts to its 11.84  $\mu$  position.

11.23  $\mu$ : Mono-alkyl-substituted cyclohexanes show a strong sharp band at this position, while the long-chain normal paraffins exhibit only weak absorption as discussed under paraffin vibrations. That a band in this region is caused by the cyclohexyl grouping is indicated by a comparison of the spectra of *n*-tetradecane, 1-cyclohexyloctane, and 1,2-dicyclohexylethane (Figures 1, 2, and 4) in which the carbon content remains constant and the cyclohexyl group increases from none to 1 and 2 with a corresponding decrease in alkyl chain, and the intensity of the band increases from weak to strong and very strong, respectively. The band is very sharp, and of 16 mono-alkyl-substituted cyclohexanes reviewed (API) its position remains constant within  $\pm$  0.02  $\mu$ . It is noted, however, that in the lower *n*-alkyl-substituted cyclohexanes this band apparently splits into two components. This was found in the case of *n*-propyl- and *n*-butylcyclohexane, in which the positions were 11.14-11.34  $\mu$  and 11.18-11.32  $\mu$ , respectively. No such splitting is noted with the longer sidechains as in 1-cyclohexyloctane, or 1-cyclohexyleicosane.

7.92  $\mu$ . Although only medium in intensity, this is probably the most useful of the bands characteristic of a mono-alkyl-cyclohexyl ring. Its position remains constant within  $\pm$  0.01  $\mu$  for 16 mono-alkyl-substituted cyclohexanes reviewed (API) and for cyclohexane itself. Branching of the chain appears to have little or no effect on the band position, but one additional substitution on the ring appears to result in a shift to longer wave lengths, approximately 8.0  $\mu$ .

**PHENYL VIBRATIONS:** 14.34  $\mu$ : This band, whose position is constant within  $\pm$  0.02  $\mu$  for the series of mono-substituted normal alkyl benzenes (excluding toluene), appears to shift to shorter wave lengths, i. e., 14.30  $\pm$  .02  $\mu$ , as the phenyl ring is moved from its terminal position to an internal carbon in the alkyl chain. This same shift is noted in the one available spectrum, isobutylbenzene (API) in which the chain has an *iso* branching on the end, at least one carbon atom removed from the ring. This might infer that the position 14.30  $\pm$  0.02  $\mu$  is constant for all mono-alkylbenzenes other than the normals. Both 1-phenyl-1-cyclohexylethane and 1-phenyl-2-cyclohexylethane show the band at this latter position indicating that the effect of the cyclohexyl ring on the position of the band is analogous to that of a branched alkyl group. In the spectra of 1,1-diphenylethane and 1,1-diphenylheptane, where two

phenyl groups are attached to the same terminal carbon atom, the band is again found at 14.30  $\mu$ . However, for 1,2-diphenylethane the band has shifted to a still shorter wave length, 14.26  $\mu$ .

13.4-13.6  $\mu$ : Mono-alkyl-substituted benzenes show a very strong band in this region, if the ring is adjoined to a primary carbon atom. If the substituent alkyl group is normal, the position appears quite constant at 13.40  $\mu$ , but shifts to longer wave lengths with branching of the chain beyond the first carbon atom. It is found shifted to  $13.15 \pm .05 \mu$  for molecules in which the ring is attached to a secondary or tertiary carbon atom of an alkyl group, as in the case of sec- and tert- butylbenzene. The effect of the introduction of a cyclohexyl ring on the alkyl chain appears to be the same as that of adding a corresponding *n*-alkyl group as seen in a comparison of the spectra of 1-phenyloctane and 2-phenyloctane with 1-phenyl-2-cyclohexylethane and 1-phenyl-1-cyclohexylethane (API) respectively. The 13.40  $\mu$  position of the band in 1-phenyloctane is not altered in 1-phenyl-2-cyclohexylethane where a C<sub>8</sub> portion of the octane chain is replaced by a cyclohexyl ring, the phenyl ring being connected to a primary carbon atom in each case. The 13.15  $\mu$  position of the band in 2-phenyloctane is not appreciably altered (13.18  $\mu$ ) in 1-phenyl-1-cyclohexylethane, in which the C<sub>8</sub> portion of the octane chain is again replaced by a cyclohexyl ring, the phenyl ring being attached in both cases to a secondary carbon atom.

11.00-11.10  $\mu$ : This band appears to be quite characteristic of monosubstituted alkylbenzenes, and its position is little affected by the structure of the substituent group, whether the ring is joined to a primary, secondary, or tertiary carbon atom.

9.70  $\mu$ : For the three phenyl compounds studied in this problem this position was constant: 1-phenyloctane, 9.69  $\mu$ ; 1,2-diphenylethane, 9.70  $\mu$ ; and 1-phenyl-2-cyclohexylethane, 9.70  $\mu$ .

6.67 and 6.23  $\mu$ : These two bands, very strong and strong, respectively, are sharp and constant in position. They are very useful for identification of a benzene nucleus in petroleum fractions because of their strength and occurrence in a region of low absorption for other functional groups common to straight-run petroleum distillates.

5.72, 5.55, 5.33, and 5.13  $\mu$ : The value 5.55  $\mu$ , recorded here, is in agreement with Nielsen *et al* (4) but does not agree with the positions observed in 1-phenyloctane and 1,2-diphenylethane (Figures 3 and 5), where it appeared at 5.48  $\mu$ . Because of the weak intensity with the cells used, and their occurrence in the atmospheric water vapor region, the possible error in wave length measurement could be 0.04  $\mu$ . With 1-phenyl-2-cyclohexylethane (Figure 6) however, the position was in agreement, 5.55  $\mu$ . This group of four bands provides a very useful and reliable pattern for the identification of mono-alkyl-substituted benzenes regardless of the degree of branching of the alkyl chain.

3.27  $\mu$ : This band position is constant to  $\pm .01 \mu$  for each of the three phenyl compounds studied—1-phenyloctane, 3.27  $\mu$ ; 1,2-diphenylethane, 3.28  $\mu$ ; and 1-phenyl-2-cyclohexylethane, 3.28  $\mu$ .

TABLE I

*Positions of Bands Characteristic of Functional Groups*

CHAIN		CYCLOHEXYL		PHENYL	
13.85	VS	11.84	M	14.34	VS
11.24	W	11.23	S	13.40	VS
9.27	VW	7.92	M	11.05	M
9.04	VW	7.40	M	9.70	S
7.24	VS			6.67	VS
6.80	VS			6.49	W
				6.23	S
				5.72	W
				5.63	W
				5.55	W
				5.33	W
				5.13	M
				3.27	S

TABLE II

*Absorption Maxima of n-tetradecane*

WAVE LENGTH IN MICRONS	WAVE NUMBER IN CM <sup>-1</sup>
13.85	722
11.25	889
9.27	1080
9.04	1105
8.82	1135
7.64	1310
7.36	1380
7.23	1385
6.80	1470
3.71	2695
3.38	2960
2.30	4345

TABLE III

*Absorption Maxima of 1-cyclohexyl-octane*

WAVE LENGTH IN MICRONS	WAVE NUMBER IN CM <sup>-1</sup>
13.86	723
13.20	758
12.89	776
11.86	843
11.25	889
10.41	961
9.68	1035
9.26	1080
9.11	1100
8.94	1120
7.92	1265
7.68	1300
7.39	1355
7.24	1380
6.88	1455
4.91	2035
4.22	2370
3.74	2675
3.39	2950
2.33	4290

TABLE IV  
Absorption Maxima of 1-phenyl-  
octane

WAVE LENGTH IN MICRONS	WAVE NUMBER IN CM <sup>-1</sup>
14.34	697
13.83	723
13.40	746
11.07	903
10.22	978
9.69	1030
9.32	1075
8.97	1115
8.64	1155
8.48	1180
8.30	1205
8.02	1245
7.66	1305
7.22	1385
6.84	1460
6.67	1500
6.47	1546
6.22	1610
5.70	1755
5.32	1880
5.14	1945
3.36	2975
3.27	3060
2.30	4350

TABLE V  
Absorption Maxima of  
1,2-dicyclohexylethane

WAVE LENGTH IN MICRONS	WAVE NUMBER IN CM <sup>-1</sup>
13.54	739
12.67	789
12.27	887
11.83	845
11.57	864
11.24	890
10.96	912
10.80	926
10.36	965
10.05	995
9.69	1030
9.47	1055
9.30	1075
9.23	1085
9.07	1105
8.58	1166
8.50	1178
8.41	1190
8.24	1215
8.11	1235
7.92	1262
7.75	1290
7.38	1355
6.88	1455
3.75	2666
3.39	2960
2.38	4200

TABLE VI  
Absorption Maxima of  
1,2-diphenylethane

WAVE LENGTH IN MICRONS	WAVE NUMBER IN CM <sup>-1</sup>
14.72	679
14.26	701
13.27	754
13.02	768
11.85	844
11.74	852
11.04	906
10.66	938
10.37	964
10.18	982
9.97	1005
9.70	1030
9.35	1070
9.26	1080
9.04	1105
8.64	1155
8.46	1180
8.34	1200
8.21	1220
8.00	1260
7.41	1350
7.19	1390
6.85	1460
6.66	1500
6.47	1545
6.23	1605
6.00	1665
5.72	1750
5.48	1825
5.33	1875
5.13	1950
3.48	2875
3.39	2960
3.26	3065

TABLE VII

*Absorption Maxima of 1-phenyl 2-cyclohexylethane*

WAVE LENGTH IN MICRONS	WAVE NUMBER IN $\text{CM}^{-1}$	WAVE LENGTH IN MICRONS	WAVE NUMBER IN $\text{CM}^{-1}$
14.31	699	8.65	1155
13.40	748	8.55	1170
12.87	777	8.48	1180
12.72	786	7.92	1265
12.14	824	7.38	1355
11.98	835	6.86	1460
11.84	845	6.66	1500
11.33	883	6.48	1545
11.24	890	6.29	1590
11.08	903	6.23	1605
10.69	935	5.55	1800
10.37	964	5.35	1870
10.28	973	5.14	1945
10.00	1000	3.75	2665
9.70	1030	3.48	2875
9.51	1050	3.39	2950
9.36	1070	3.28	3050
9.23	1085	2.42	4130
8.89	1125		

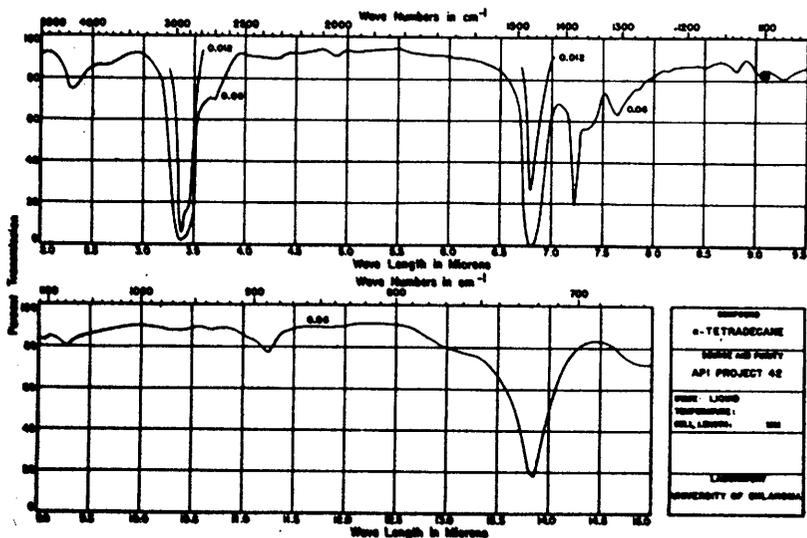


FIGURE 1

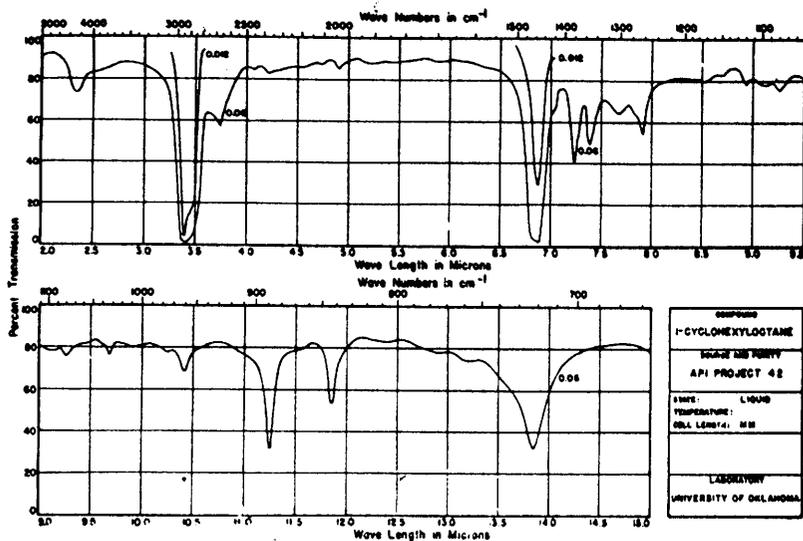


FIGURE 2

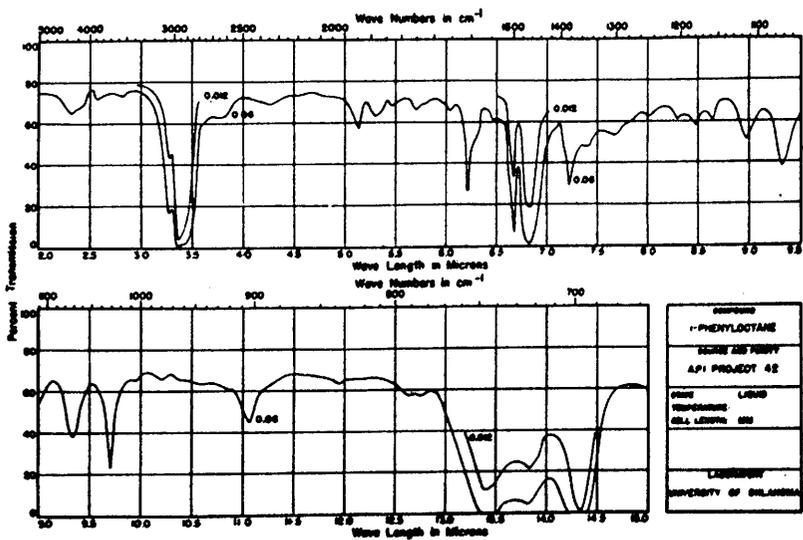


FIGURE 3

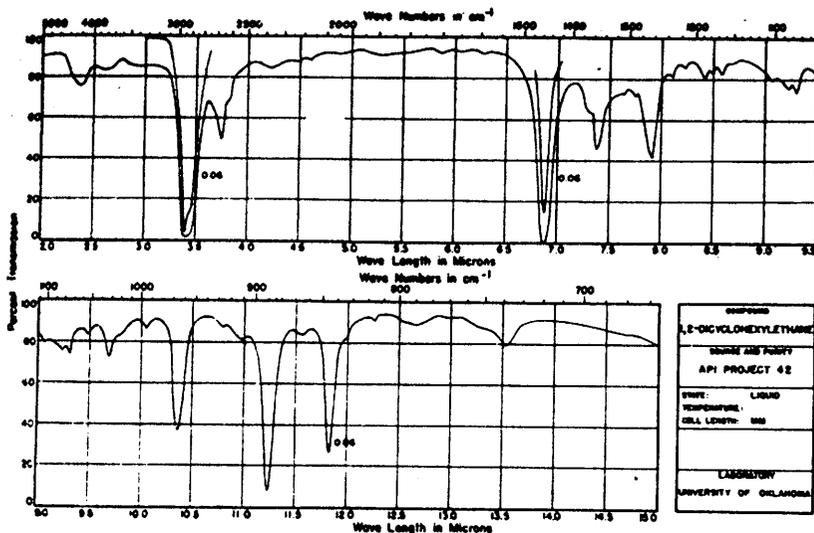


FIGURE 4

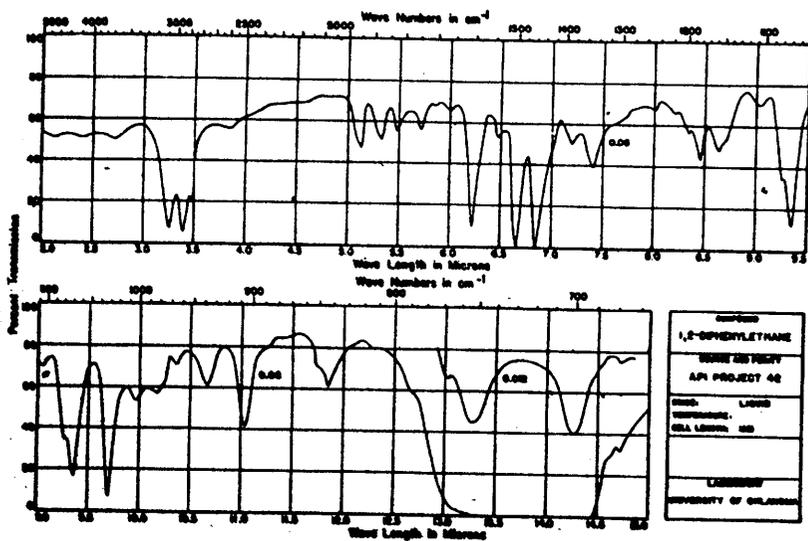


FIGURE 5

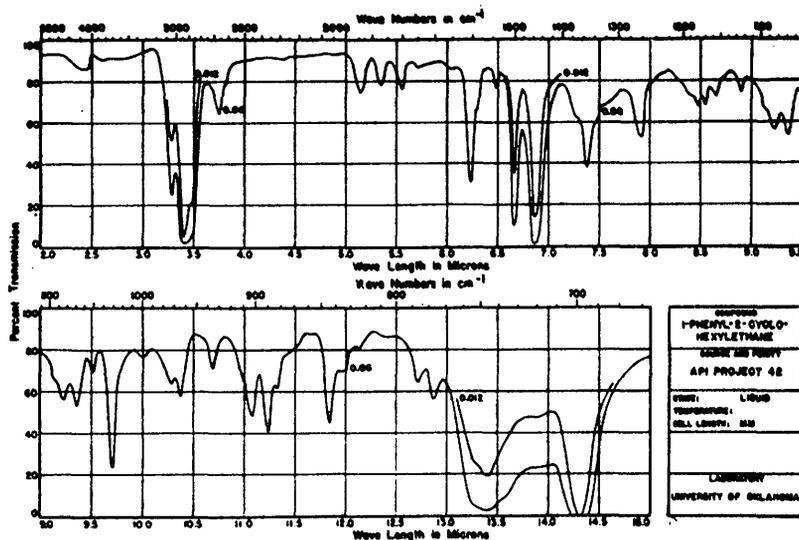


FIGURE 6

## CONCLUSIONS

Frequently, in applying spectra to the identification of various functional groups present within a mixture, bands of other atomic groupings will interfere. If a band is found in a region characteristic of a cyclohexyl ring, for example, it is not proof, but only an indication, that this particular grouping is present. The absence of a band in this region, however, is almost certain proof of the absence of the particular grouping. Atomic groups, for which there are several characteristic bands, such as the phenyl ring, can be identified with a high degree of certainty.

In general, the spectrum of a mixture will be approximately the same, with respect to the characteristic bands, as the spectrum of a complex molecule containing the same functional groups as that mixture. This is clearly seen in the spectrum of 1-phenyl-2-cyclohexylethane (Figure 6) which appears as a composite of the spectra of 1-cyclohexyloctane and 1-phenyloctane, the major differences being due to the  $-CH_2$  groups and the higher ratio of chain to ring in the latter two hydrocarbons.

In the study of the composition of Diesel fuels various methods utilizing the differences in physical and chemical properties are effectively employed to separate the different hydrocarbon types. When these methods are combined with fractional distillation, a high degree of subdivision can be obtained. The results of the present research can be readily adapted to detection of small quantities of one type of hydrocarbon in these subfractions which are predominantly of a second type. For example, through the use of the band positions outlined above one could readily detect, if present, alkylated benzenes as contaminant in the paraffin-naphthene portion from an adsorptive separation of aromatic materials by the use of silica gel (3). Conversely, the mono-alkylated cyclohexanes could be detected as contaminants in the aromatic concentrate, if they were present in appreciable amounts.

The correlations here outlined for mono-alkyl cyclohexanes and benzenes can be very usefully applied in following the course of dehydrogenation re-

actions converting these cyclohexanes to their benzene analogues. This could be done by measuring the intensity of the 11.84, 11.23, and 7.92-micron cyclohexyl bands at periodic intervals during the dehydrogenation process.

A more useful application of infrared spectra in conjunction with the dehydrogenation of naphthenes to the corresponding aromatics would be in the identification of individual naphthenes present in Diesel fuels. The identification of an aromatic hydrocarbon can usually be accomplished easier than the identification of the analogous cyclohexyl compound, for several reasons. In addition to their greater chemical reactivity, useful in the preparation of derivatives, they are easier to identify through their infrared spectra. A greater number of useful bands are present in the spectra of the aromatic hydrocarbons and consequently more correlation work has been reported for this class of hydrocarbons.

Several very useful summaries of these functional-group correlations have recently appeared in the literature. Possibly two of the most comprehensive are those by Barnes and coworkers (2), and by Thompson (6). Many of the assignments are tentative and subject to qualification, for this application is relatively new and requires considerable extension and corroboration.

In the field of hydrocarbon analysis, the available spectra are quite comprehensive for the low molecular weight members of the various types, that is, up to and including  $C_{10}$  hydrocarbons. Correlations for the larger molecules are of necessity based upon a few scattered spectra of these larger molecules supported by correlations developed for those of lower molecular weight. This method cannot be applied in all instances, and there consequently exists a serious void of correlations and spectra for compounds of the condensed dicyclic type, e. g. substituted naphthalenes, tetralines, and decalins. Current studies of the composition of Diesel fuels show the presence of these dicyclic hydrocarbons, and the need is being felt for more spectral data for compounds of this type.

#### LITERATURE CITED

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