REPORT 1003

CORRELATION OF PHYSICAL PROPERTIES WITH MOLECULAR STRUCTURE FOR SOME DICYCLIC HYDROCARBONS HAVING HIGH THERMAL-ENERGY RELEASE PER UNIT VOLUME[1]

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SUMMARY

As part of a program to study the correlation between molecular structure and physical properties of high-density hydrocarbons, the net heats of combustion, melting points, boiling points, densities, and kinematic viscosities of some hydrocarbons in the 2-n-alkylbiphenyl, 1,1-diphenylalkane, α, ω-diphenylalkane, 1,1-dicyclohexylalkane, and α,ω-dicyclohexylalkane series are presented. Comparisons are made on the following three bases:

1. As members of an homologous series in which the compounds have similar structures and differ in molecular weight

2. As isomers with the same molecular weight and molecular formula but different molecular structure

3. As compounds with the same carbon skeleton but different molecular formulas due to hydrogenation of the aromatic rings

The three series of aromatic hydrocarbons, 2-n-alkylbiphenyl, 1,1-diphenylalkane, and α,ω-diphenylalkane, did not show great differences in heat of combustion per unit volume. These series averaged 20 percent higher than typical aircraft fuels of AN–F–58 specification with respect to this property. The two series of dicyclohexyl hydrocarbons, 1,1-dicyclohexylalkane and α,ω-dicyclohexylalkane, had somewhat lower heats of combustion, but still averaged about 13 percent higher than AN–F–58 fuel.

Each series followed its own characteristic pattern in the relation of melting point and structure. The general trend was toward lower melting points by addition of a side chain to the parent hydrocarbon. With two exceptions, the dicyclohexyl compounds melted at lower temperatures than the analogous aromatic hydrocarbons.

The molecular weight had a greater influence on boiling point than the molecular structure. The α,ω-diphenylalkane series, however, showed a more rapid rate of increase in boiling point with increasing molecular weight than the other series of aromatic hydrocarbons.

In these three closely related homologous series of aromatic hydrocarbons, the molecular weight had a greater effect on viscosity than the molecular structure when the substituent groups were all normal alkyl in type. The cyclohexyl derivatives had viscosities 40 to 200 percent higher than the analogous aromatic hydrocarbons.

INTRODUCTION

High-speed aircraft are volume-limited because of the design requirements of thin wings and small fuselages; the fuel-storage space is therefore restricted. In evaluating fuels for such aircraft, one of the important properties is the heat of combustion per unit volume. Fuels with high heat of combustion per unit volume would be valuable in providing increased flight range.

A survey of the literature pertaining to properties of hydrocarbons was therefore made at the NACA Lewis laboratory with particular emphasis on the heat of combustion per unit volume. The hydrocarbons were compared as homologous series to determine which features of molecular structure might be expected to be associated with high heat of combustion per unit volume. The net heats of combustion of the normal paraffin, normal alkylcyclohexane, and normal alkylbenzene hydrocarbons of seven to fourteen carbon atoms vary from 824,000 to 977,000 Btu per cubic foot. For an equivalent number of carbon atoms, the comparison of net heat of combustion is: *n*-alkylbenzene>*n*-alkylcyclohexane>*n*-paraffin. It is evident that a ring structure increases the heat of combustion per unit volume and that the unsaturated ring in benzene has an advantage over the saturated cyclohexane ring. These values of net heat of combustion were calculated from data obtained in references 1 and 2.

Compounds from these three homologous series are principal constituents of the aircraft fuels AN–F–48, AN–F–32a, and AN–F–58, which are currently used and are described by the specifications in references 3, 4, and 5, respectively. Fuels that were purchased under these specifications and used at the Lewis laboratory were found to have the following values of net heat of combustion: AN–F–48, 823,000; AN–F–32a, 960,000; and AN–F–58, 894,000 Btu per cubic foot. These values vary depending upon the source of supply; they have been arbitrarily chosen, however, as a standard for comparing the hydrocarbons discussed herein.

The advantage of an aromatic ring in a molecule led to the investigation of the properties of biphenyl, diphenylmethane, and naphthalene. Each of these compounds has two aromatic rings per molecule, and the net heats of com-

[1] Supersedes NACA TN 2081, "Correlation of Physical Properties with Molecular Structure for Dicyclic Hydrocarbons. I—2-*n*-Alkylbiphenyl, 1,1-Diphenylalkane, α,ω-Diphenylalkane, 1,1-Dicyclohexylalkane, and α,ω-Dicyclohexylalkane, Series," by P. H. Wise, K. T. Serijan, and I. A. Goodman, 1950.

bustion (references 1 and 2) are 1,096,000; 1,110,000; and 1,210,000 Btu per cubic foot, respectively. These values represent an average increase of 30 percent over AN–F–48, 15 percent over AN–F–32a, and 20 percent over AN–F–58. On the basis of heat of combustion, these three hydrocarbons would be desirable fuels; however, they have relatively high melting points and are unsuitable for use as liquid fuels. If the introduction of various alkyl groups into these hydrocarbons would sufficiently lower the melting points without reducing the heat of combustion per unit volume, a superior fuel would be obtained. The data on many of these alkyl derivatives are incomplete and in some cases inaccurate; consequently, they cannot be used as a basis for a reliable analysis of the usefulness of these high-energy hydrocarbons as aircraft-engine fuels.

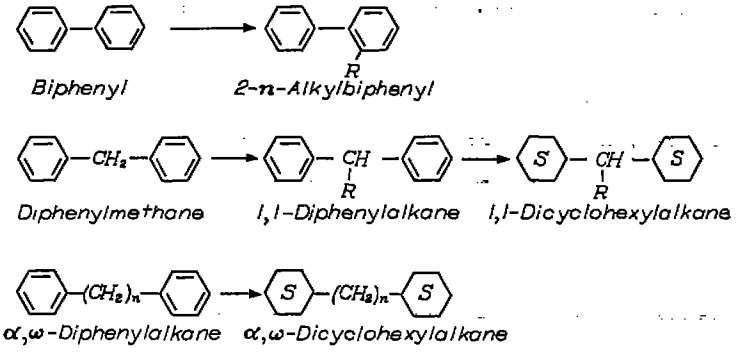


FIGURE 1.—Structure of hydrocarbons.

An investigation was therefore undertaken at the Lewis laboratory during 1945 to determine the effects of systematic alteration in structure of dicyclic-aromatic-type molecules on the following important properties of the fuel: net heat of combustion per unit volume, heat of combustion per unit weight, melting point, boiling point, and viscosity.

Comparisons are made on the following three bases:

1. As members of an homologous series in which the compounds have similar structures and differ in molecular weight

2. As isomers with the same molecular weight and molecular formula but different molecular structure

3. As compounds with the same carbon skeleton but different molecular formulas due to hydrogenation of the aromatic rings

METHOD AND APPARATUS

The compounds discussed represent five homologous series of hydrocarbons; namely, the 2-*n*-alkylbiphenyl; 1,1-diphenylalkane; 1,1-dicyclohexylalkane; α,ω-diphenylalkane; and α,ω-dicyclohexylalkane series. The structures of these hydrocarbons are illustrated in figure 1. The normal alkyl groups illustrated at the bottom of the figure were selected to study the effect of increasing the chain length of these substituent groups when they are attached to the parent hydrocarbons, biphenyl and diphenylmethane. From diphenylmethane two series are developed, the 1,1-diphenylalkane series by adding the alkyl group as a side chain attached to the carbon atom between the phenyl groups and the α,ω-diphenylalkane series by lengthening the chain of carbon atoms between the two rings.

The saturated, or cyclohexyl, derivatives corresponding to the aromatic compounds are also illustrated. They are prepared by hydrogenation of the pure aromatic compounds. It is known that the saturated compounds generally have lower melting points and burn with less carbon formation than the corresponding aromatic hydrocarbons. On the other hand, saturated hydrocarbons have higher viscosities and lower net heats of combustion per unit volume than their aromatic counterparts. Inasmuch as many properties must be considered in selecting a fuel, it seemed advisable to study the saturated compounds to determine accurately the extent of the changes produced by hydrogenation.

With the exceptions noted in the tables of properties, the compounds were synthesized and purified, or purified from commercial stocks, at the Lewis laboratory; the properties were then determined. Before final measurement of the properties was made, precautions were taken to ascertain that the high purity essential for the accurate study of properties was attained.

The time-temperature melting curves were determined with a platinum resistance thermometer and a G–2 Mueller bridge with accessory equipment and by methods described in reference 6, and the melting points were determined from the curves according to the graphical method described in reference 7. Densities were determined by use of a gravimetric balance according to the method of reference 8, and the refractive indices were measured with a Bausch & Lomb precision oil-model five-place instrument. The boiling points were determined by the use of a platinum resistance thermometer in an apparatus modified from that described in reference 9. The system was pressurized with dry air from a surge tank and held at constant pressure by adjusting a continuous bleed. The kinematic viscosities were determined in viscosimeters that had been calibrated with National Bureau of Standards standard viscosity samples H–5, H–7, D–7, or L–17. The A.S.T.M. procedure of reference 10 was followed. The net heats of combustion were determined according to reference 11 in an oxygen bomb calorimeter that had been calibrated on Bureau of Standards benzoic acid.

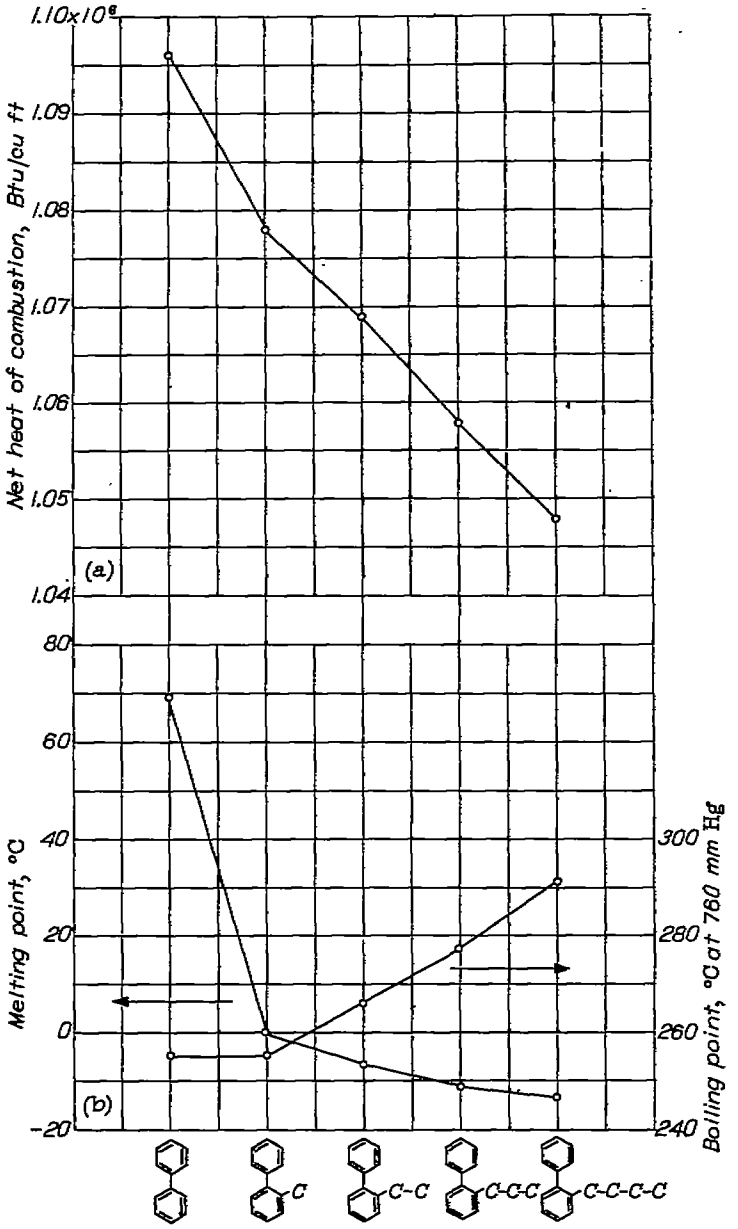
The magnitude of the uncertainties is estimated as follows: melting point, 0.02° C; density, 0.00005 gram per milliliter; refractive index, 0.0002; boiling point, 0.1° C; kinematic viscosity, 0.5 percent of determined value relative to 1.007 centistokes for water at 20° C; and net heat of combustion, ±100 Btu per pound, which is equivalent to 10 to 15 kilogram-calories per mole for these compounds.

The precision of measurements is: freezing point, ±0.003° C; density, ±0.00002 to ±0.00003 gram per milliliter; refractive index, ±0.0001; boiling point, ±0.04° C; kinematic viscosity, 0.2 percent of determined value; and net heat of combustion, ±60 Btu per pound.

DISCUSSION OF RESULTS

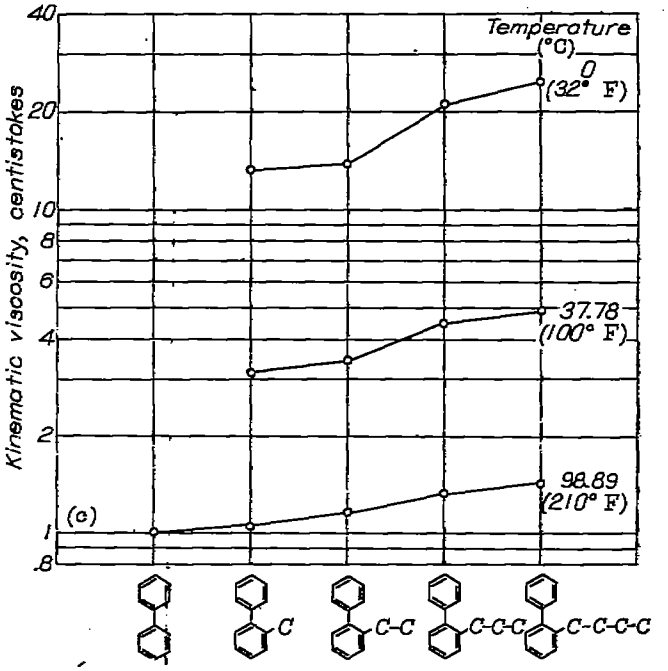
2-*n*-ALKYLBIPHENYL HYDROCARBONS

The physical properties of the 2-*n*-alkylbiphenyl hydrocarbons are presented in table I (a) and the heat-of-combustion data are given in table I (b). The data are plotted in figure 2. The comparison of molecular structure with net heat of combustion in Btu per cubic foot for the 2-*n*-alkylbiphenyl hydrocarbons is shown in figure 2 (a). The parent hydrocarbon, biphenyl, has the highest value, 1,096,000 Btu per cubic foot. The first member of the series, 2-methylbiphenyl, is slightly lower at 1,078,000 Btu per cubic foot. Each carbon atom that is subsequently added to lengthen the side chain causes some decrease in



(a) Net heat of combustion.
(b) Melting and boiling points.

FIGURE 2.—Variation of properties with structure of 2-*n*-alkylbiphenyl hydrocarbons.



(c) Kinematic viscosity at various temperatures.

FIGURE 2.—Concluded. Variation of properties with structure of 2-*n*-alkylbiphenyl hydrocarbons.

the net heat of combustion per unit volume, and 2-*n*-butylbiphenyl with four carbon atoms in the side chain has a value of 1,048,000 Btu per cubic foot, which is a loss of 4.3 percent from biphenyl. This value is, however, still 17 percent higher than a typical AN–F–58 aircraft fuel.

The melting- and boiling-point comparisons of this series of hydrocarbons are shown in figure 2 (b). Biphenyl melts at 69.2° C, and each member of the series has a lower melting point as the molecular weight and side-chain length are increased. The fourth member of the series, 2-*n*-butylbiphenyl, melts at −13.71° C, a decrease of 83° C from the value for biphenyl.

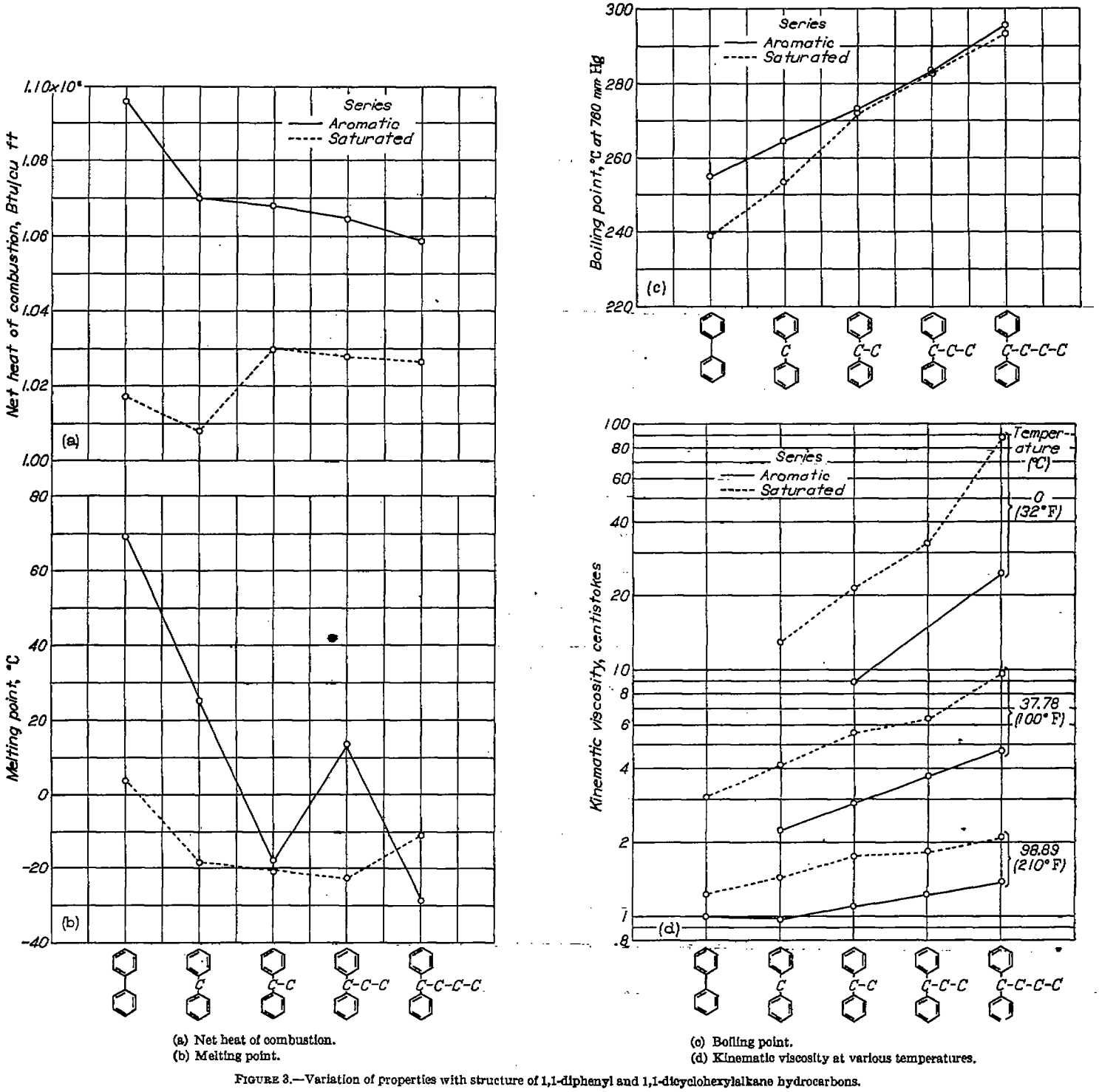
The boiling-point curve shows the reverse trend, increasing from 255.0° to 291.20° C in the transition from the parent hydrocarbon to 2-*n*-butylbiphenyl.

The viscosities of these hydrocarbons at three temperatures are compared in figure 2 (c). The trend is the same as for the boiling point; an increase in molecular weight by lengthening the side chain is accompanied by an increase in viscosity. At 0° C (32° F), where the viscosity of biphenyl cannot be determined because the compound is a solid, there is an increase of 85 percent from 2-methylbiphenyl to 2-*n*-butylbiphenyl. The effect of temperature is even more pronounced. The average increase in viscosity for the individual members of the series is 200 percent when the temperature is lowered from 98.89° C (210° F) to 37.78° C (100° F) and about 1300 percent when the temperature is 0° C (32° F) compared with 98.89° C (210° F). No data were obtained below 0° C (32° F) because most of these compounds are crystalline solids at temperatures only a few degrees below this temperature.

1,1-DIPHENYLALKANE AND 1,1-DICYCLOHEXYLALKANE HYDROCARBONS

The properties of these two series of hydrocarbons are shown in table II and plotted in figure 3. By using data from these two series, it is possible to compare compounds that have like arrangement of the carbon skeleton and different hydrogen-carbon ratios. The data for the two series are therefore plotted in the same figures, with solid lines representing the aromatic series and dashed lines, the saturated series.

The net heat of combustion in Btu per cubic foot is compared with the molecular structure in figure 3 (a). Biphenyl is considered to be the parent hydrocarbon and is compared with the other members of this series, as was the case with



(a) Net heat of combustion.
(b) Melting point.
(c) Boiling point.
(d) Kinematic viscosity at various temperatures.

FIGURE 3.—Variation of properties with structure of 1,1-diphenyl and 1,1-dicyclohexylalkane hydrocarbons.

the 2-*n*-alkylbiphenyl hydrocarbons. The carbon atom added between the two rings in diphenylmethane results in a 2-percent loss in Btu per cubic foot. A small decrease in net heat of combustion per cubic foot is observed with each carbon atom that is added to the side chain. The over-all loss from biphenyl to 1,1-diphenylbutane is, however, only 3.3 percent.

In plotting the dicyclohexyl derivatives, each point indicates the value for the hydrogenated compound with the carbon skeleton corresponding to that of the aromatic compound immediately below the point on the figure. The average decrease in net heat of combustion per unit volume is 5 percent when each saturated compound is compared with its aromatic counterpart. This decrease is due to the lower density of the hydrogenated derivatives in comparison with the aromatic hydrocarbons.

The melting points of these two series of hydrocarbons are shown in figure 3 (b). The aromatic series shows a consistent decrease from biphenyl (melting point, 69.2° C) to 1,1-diphenylbutane (melting point, —28.4° C) except for one member, 1,1-diphenylpropane, which melts at 13.3° C. This melting point is higher than that of the compound preceding or following it in the series.

The saturated compounds melt at lower temperatures than the corresponding aromatic hydrocarbons except in the comparison of the butane derivatives where the saturated compound has a higher melting point than the diphenyl derivative.

The boiling points of the two series (fig. 3 (c)) show a regular increase with lengthening of the carbon chain. The difference between analogous members of the two series decreases with increasing chain length. The first members of the two series differ about 16° C; the last three pairs differ 1° to 3° C. The diphenyl compounds have consistently higher boiling points than the saturated derivatives.

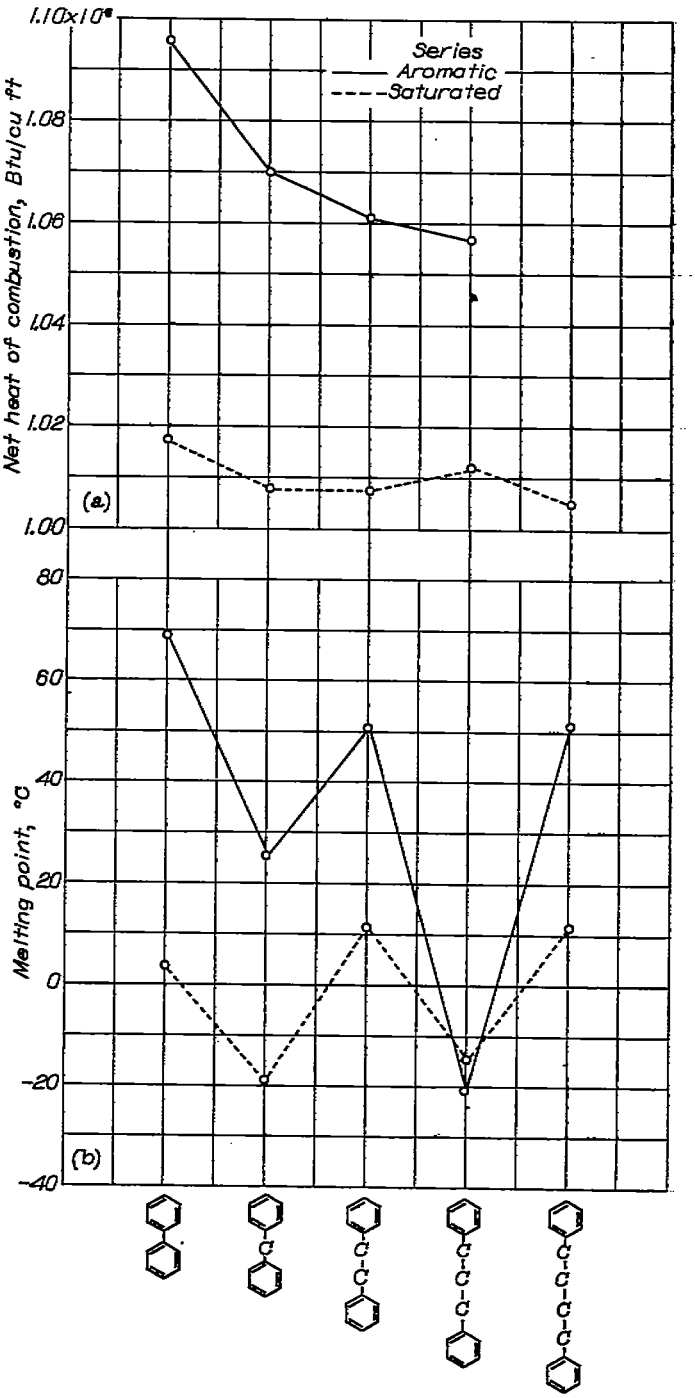
The increase in viscosity due to hydrogenation of the aromatic nuclei to saturated rings is observed by comparing the viscosities of these two series in figure 3 (d). The saturated derivatives average 48 percent higher at 98.89° C (210° F) and 200 percent higher at 0° C (32° F). Both series show consistent increases in viscosity with increase in chain length.

α,ω-DIPHENYLALKANE AND α,ω-DICYCLOHEXYLALKANE HYDROCARBONS

The properties of the two series of α,ω-dicyclicalkanes are tabulated in table III and plotted in figure 4. With the two α,ω-dicyclicalkane hydrocarbon series of compounds, it is again possible to compare the aromatic and the saturated derivatives. The data for net heat of combustion are shown in figure 4 (a). In the aromatic series, a decrease of 3.5 percent in Btu per cubic foot is observed as the carbon chain between the two rings is lengthened. The values for the saturated series are quite uniform and average about 5 percent lower than the aromatic hydrocarbons. The saturated compounds, however, average about 12 percent higher than an AN–F–58 aircraft fuel on the basis of heat of combustion per unit volume.

The two series follow similar patterns in melting-point behavior as the length of the carbon chain is increased (fig. 4 (b)). The melting points of the saturated compounds are consistently lower than those of the corresponding aromatic hydrocarbons except for the 1,3-dicyclic compounds, in which case the aromatic derivative is slightly lower.

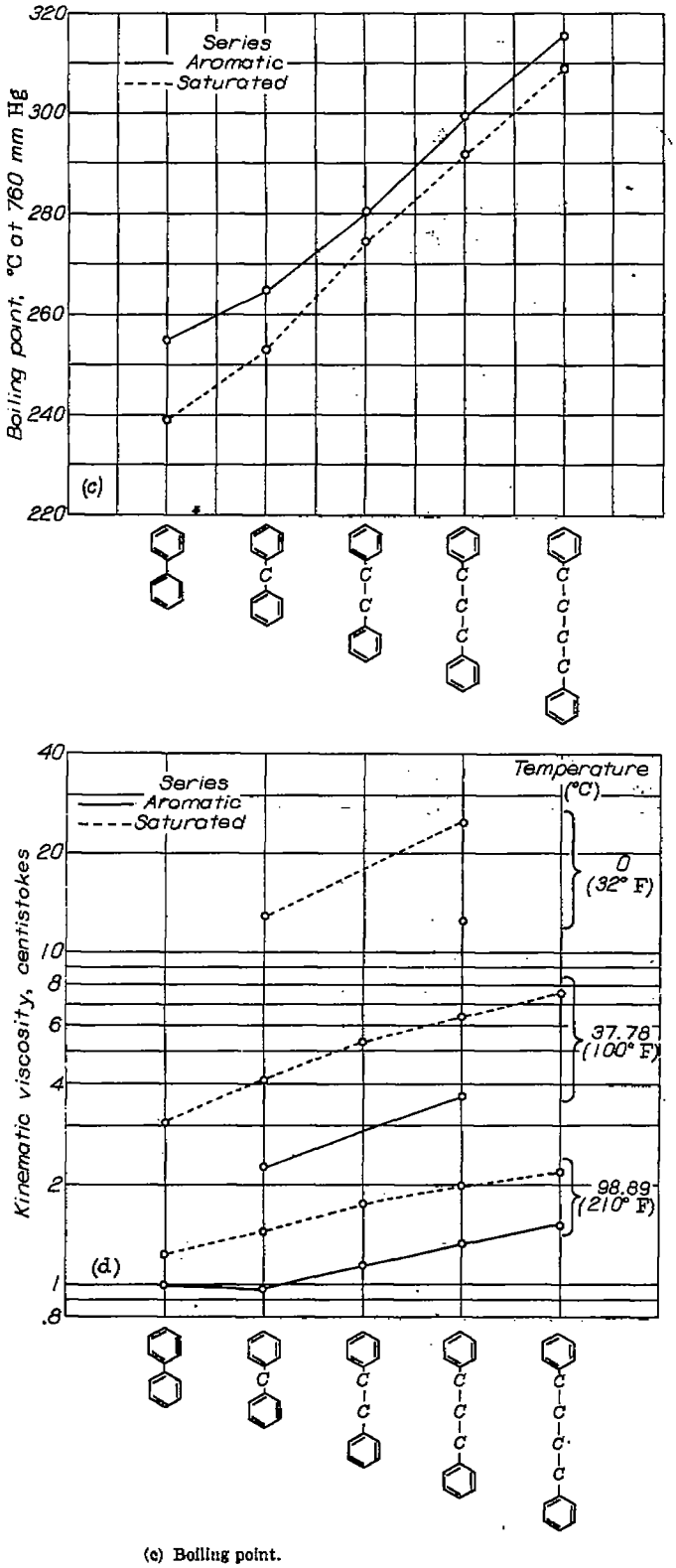
The boiling-point data for these compounds, shown in figure 4 (c), indicate uniform increases in both series as the carbon chain between the rings is lengthened. The boiling points of the aromatic compounds are consistently higher than those of the saturated derivatives with the corresponding carbon skeleton.



(a) Net heat of combustion.
(b) Melting point.

FIGURE 4.—Variation of properties with structure of α,ω-diphenylalkane and α,ω-dicyclohexylalkane hydrocarbons.

Comparison of viscosities in these series, plotted in figure 4 (d), is necessarily incomplete because the aromatic compounds have relatively high melting points and are solids at several of the temperatures of measurement. The aromatic compounds are liquids at 98.89° C (210° F), and the viscosity increases slowly with increasing chain length. At this temperature, the viscosity values of the saturated compounds average 43 percent higher than the corresponding aromatic compounds. At the lower temperatures some data points are missing, but the trends are the same.



(c) Boiling point.
(d) Kinematic viscosity at various temperatures.

FIGURE 4.—Concluded. Variation of properties with structure of α,ω-diphenylalkane and α,ω-dicyclohexylalkane hydrocarbons.

COMPARISON OF THREE AROMATIC SERIES

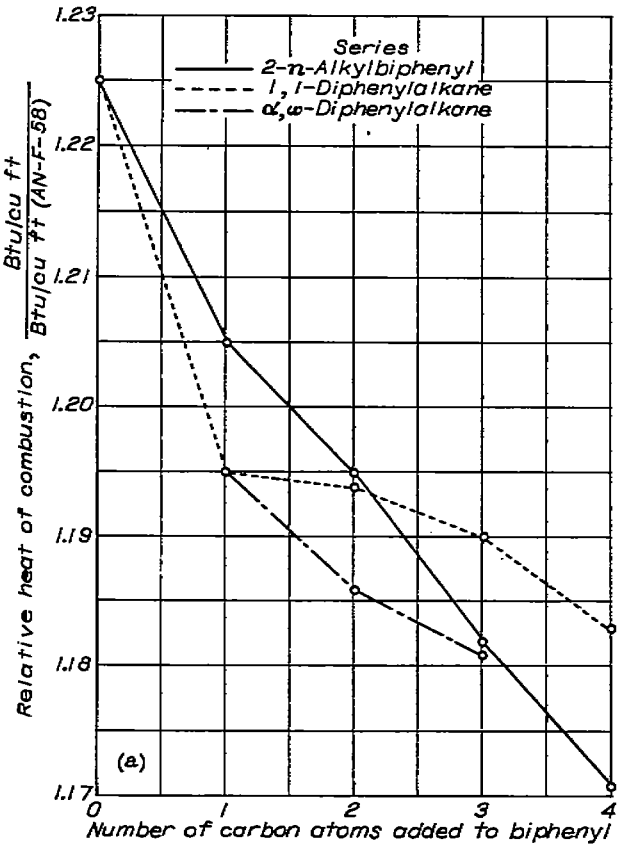
The comparisons that have been presented were made on the basis of homologous series in which the molecular structure of the individual members of a series differed only by the length of the aliphatic carbon chain in the molecule. Each series started from the common parent hydrocarbon, biphenyl. A comparison of the effect of structure on the properties can also be made by studying the properties of the hydrocarbons, one from each series, that have a common molecular formula. An example would be those with the formula $C_{14}H_{14}$, that is, 2-ethylbiphenyl, 1,1-diphenylethane, and 1,2-diphenylethane. In order to make this comparison, the properties of each series have been plotted in figure 5. The properties are plotted as the ordinates and the number of carbon atoms added to the parent hydrocarbon is plotted as the abscissa.

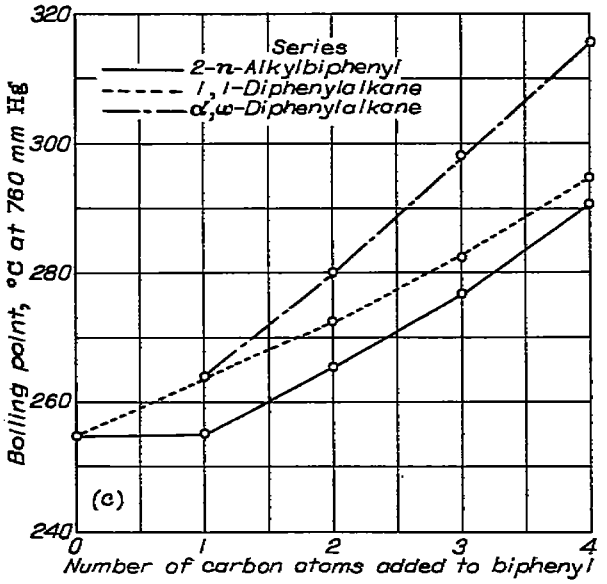
The effect of structure on heat of combustion per unit volume is shown in figure 5 (a). The ratio of Btu per cubic foot to the corresponding value for a typical AN–F–58 aircraft fuel (table I, footnote d) is used as the ordinate rather than the absolute value determined for the compounds. This ratio is a measure of the advantage to be gained in heat of combustion per unit volume by using fuels of this type. The 1,1-diphenylalkane series decreased less rapidly in heat of combustion per unit volume than the other two series as the carbon chain was lengthened. None of these series, however, decreased more than 6 percent from the parent hydrocarbon, and they are all about 20 percent higher than AN–F–58 with respect to this property.

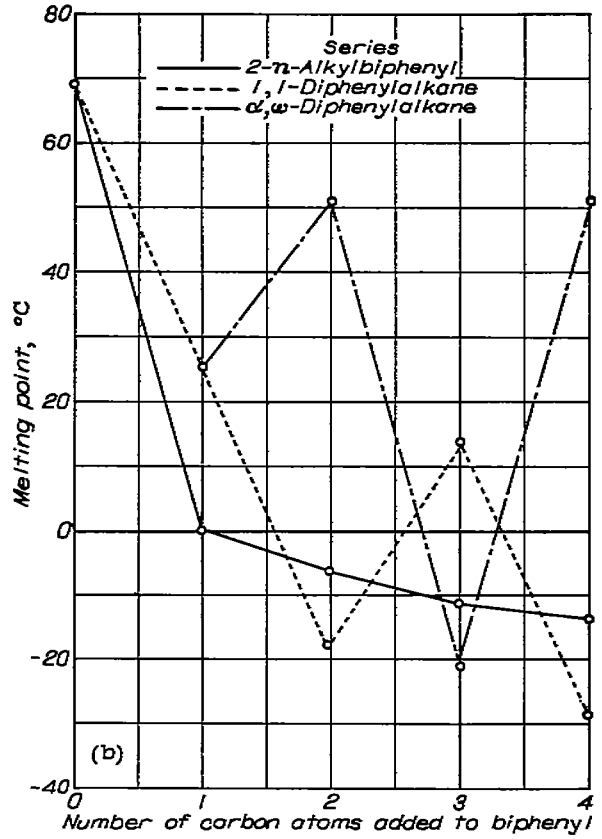
The divergent behavior of these three series with respect to their melting points is illustrated in figure 5 (b). The 2-*n*-alkylbiphenyl series has increasingly lower melting points as the side chain is increased in length. The other series are characterized by alternate lower and higher melting points as the series are extended.

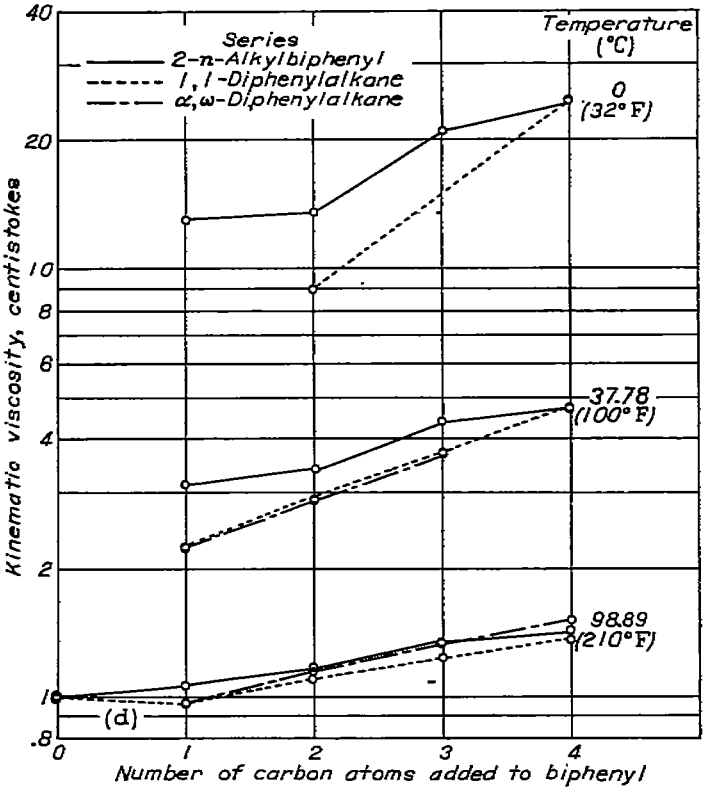
The curves of figure 5 (c) show that the molecular weight has more influence on boiling point than the structure, because the boiling points are quite closely grouped. The α,ω-diphenylalkane series does show, however, a more rapid rate of increase in boiling point with increase in chain length than the other two series. The boiling point of 1,3-diphenylpropane is higher than those of 1,1-diphenylbutane and 2-*n*-butylbiphenyl, which have one more carbon atom per molecule.

The viscosities of the three series of hydrocarbons at the three temperatures of measurement are plotted in figure 5 (d). The viscosities depend more upon the molecular weight than upon the molecular structure in these closely related series. As the molecular weight increases, the differences between the viscosity values of the isomers in the three series diminish.









(a) Net heat of combustion.
(b) Melting point.
(c) Boiling point.
(d) Kinematic viscosity at various temperatures.

FIGURE 5.—Comparison of properties and structural changes of three homologous series of hydrocarbons related to biphenyl.

SUMMARY OF RESULTS

A study of the variation of properties with change in molecular structure in the homologous series—2-*n*-alkylbiphenyl; 1,1-diphenylalkane; α,ω-diphenylalkane; 1,1-dicyclohexylalkane; and α,ω-dicyclohexylalkane—indicated the following trends:

1. The net heat of combustion per unit volume decreased an average of about 5 percent as the molecular weight was increased from the parent hydrocarbon, biphenyl, to 1,3-diphenylpropane and to the $C_{16}H_{18}$ isomers in the 2-*n*-alkylbiphenyl and 1,1-diphenylalkane hydrocarbon series. All three series averaged about 20 percent higher than an AN–F–58 aircraft fuel with respect to this property.

2. In the two series of hydrogenated compounds, 1,1-dicyclohexylalkane and α,ω-dicyclohexylalkane, the values of net heat of combustion per unit volume were somewhat lower than the analogous aromatic compounds and did not vary greatly throughout the series. The series averaged about 13 percent higher than an AN–F–58 fuel.

3. Each of the aromatic series followed a characteristic pattern of melting-point variation as the molecular weight was increased. The general trend was toward lower melting points as the size of the alkyl substituent was increased, but exceptions to this general statement were observed in the α,ω-diphenylalkane series and the 1,1-diphenylalkane series.

4. Hydrogenation of the aromatic nuclei to saturated rings lowered the melting point in all of the cases except two.

5. The boiling points of the investigated hydrocarbons were influenced more by their molecular weight than by molecular structure. The α,ω-diphenylalkane series, however, did show a more rapid rate of increase of boiling point with increase in molecular weight than the 1,1-diphenylalkane and 2-*n*-alkylbiphenyl series. The saturated derivatives had boiling points slightly lower than those of the corresponding diphenyl compounds.

6. In the three aromatic series, the viscosity increased uniformly with increase in molecular weight. The viscosity values of the isomers were nearly equal in many cases; it was therefore concluded that with the types of molecule studied the molecular weight influenced viscosity to a greater extent than did molecular structure. The saturated hydrocarbons had much higher viscosities than the corresponding diphenyl compounds, with the increases ranging from approximately 40 to 200 percent.

7. Of the compounds investigated, 1,1-diphenylbutane had the lowest melting point, −28.4° C. This compound had a net heat of combustion of 1,059,000 Btu per cubic foot, which is 18 percent greater than the AN–F–58 fuel selected for comparison.

LEWIS FLIGHT PROPULSION LABORATORY,
NATIONAL ADVISORY COMMITTEE FOR AERONAUTICS,
CLEVELAND, OHIO, *June 20, 1949.*

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TABLE I—PROPERTIES OF 2-*n*-ALKYLBIPHENYL HYDROCARBONS

(a) Physical properties.

[S designates solid at indicated temperature.]

Hydrocarbon	Melting point		Boiling point at 760 mm		Density at 20° C (g/ml)	Kinematic viscosity (centistokes)			Refractive index n_D^{20}
	°C	°F	°C	°F		98.89° C (210° F)	37.78° C (100° F)	0° C (32° F)	
Biphenyl	69.2	156.6	255.0	491.0	1.041 [a]	0.992	S	S	S
2-Methylbiphenyl	−.20	31.64	255.30	491.54	1.01134	1.06	3.18	13.3	1.5914
2-Ethylbiphenyl	−6.13	20.97	255.97	510.75	.99671	1.17	3.44	13.8	1.5905
2-*n*-Propylbiphenyl	−11.26	11.73	277.22	531.00	.98018	1.33	4.44	22.4	1.5896
2-*n*-Butylbiphenyl	−13.71 [b] −9.65 [b]	7.32 [b] 14.63 [b]	291.20	556.16	.96763	1.43	4.87	24.7	1.5804

(b) Heats of combustion.

Hydrocarbon	Net heat of combustion			Ratio to AN-F-58	
	kcal/mole	Btu/lb	Btu/cu ft	Weight basis [c]	Volume basis [d]
Biphenyl	1443.5	16,850 [a]	1.096×10^6	0.905	1.225
2-Methylbiphenyl	1598.2	17,100	1.078	.918	1.205
2-Ethylbiphenyl	1739.0	17,175	1.069	.922	1.195
2-*n*-Propylbiphenyl	1886.5	17,300	1.058	.929	1.182
2-*n*-Butylbiphenyl	2030.0	17,375	1.048	.933	1.171

[a] Reference 2.
[b] Two different crystalline modifications.
[c] Based on experimentally determined value of 18,625 Btu/lb for fuel used at Lewis laboratory.
[d] The value of 894,000 Btu/cu ft for AN-F-58 was calculated from the value in footnote c using the experimentally determined value of 0.769^{60}_{60} for the specific gravity of the fuel.

TABLE II—PROPERTIES OF 1,1-DICYCLICALKANE HYDROCARBONS

(a) Physical properties.

[S designates solid at indicated temperature.]

Hydrocarbon	Melting point		Boiling point at 760 mm		Density at 20° C (g/ml)	Kinematic viscosity (centistokes)			Refractive index n_D^{20}
	°C	°F	°C	°F		98.89° C (210° F)	37.78° C (100° F)	0° C (32° F)	
Diphenylalkanes									
Biphenyl	69.2	156.6	255.0	491.0	1.041 [a]	0.992	S	S	S
Diphenylmethane	25.20	77.36	264.27	507.69	1.00593	.965	2.22	S	1.5776
1,1-Diphenylethane	−18.01	−.42	272.63	522.73	.99961	1.10	2.90	8.92	1.5725
1,1-Diphenylpropane	13.29	55.92	283.22	541.80	.98663	1.23	3.72	S	1.5643
1,1-Diphenylbutane	−23.38 [b] −25.2 [b]	−19.08 −13.4	294.29	561.72	.97498	1.38	4.70	24.8	1.5568
Dicyclohexylalkanes									
Bicyclohexyl	3.50	38.30	238.87	461.97	0.88604	1.23	3.07	S	1.4796
Dicyclohexylmethane	−13.69	−1.64	252.77	486.99	.87646	1.43	4.10	13.0	1.4763
1,1-Dicyclohexylethane	−20.98	−5.76	271.17	520.11	.89309	1.76	5.59	21.3	1.4845
1,1-Dicyclohexylpropane	−23.46	−10.23	282.31	540.16	.89299	1.83	6.41	32.9	1.4848
1,1-Dicyclohexylbutane	−10.46	13.17	292.97	559.35	.89021	2.10	9.64	88.3	1.4843

(b) Heats of combustion.

Hydrocarbon	Net heat of combustion			Ratio to AN-F-58	
	kcal/mole	Btu/lb	Btu/cu ft	Weight basis [c]	Volume basis [d]
Diphenylalkanes					
Biphenyl	1443.5	16,850 [a]	1.096×10^6	0.905	1.225
Diphenylmethane	1593.5	17,050	1.070	.916	1.196
1,1-Diphenylethane	1733.8	17,125	1.068	.920	1.194
1,1-Diphenylpropane	1886.5	17,300	1.065	.929	1.190
1,1-Diphenylbutane	2032.9	17,400	1.059	.934	1.183
Dicyclohexylalkanes					
Bicyclohexyl	1700.0	18,400	1.017×10^6	0.988	1.137
Dicyclohexylmethane	1845.9	18,425	1.008	.989	1.127
1,1-Dicyclohexylethane	1997.5	18,500	1.030	.993	1.150
1,1-Dicyclohexylpropane	2138.8	18,475	1.028	.992	1.149
1,1-Dicyclohexylbutane	2285.8	18,500	1.027	.993	1.148

[a] Reference 2.
[b] Two different crystalline modifications.
[c] Based on experimentally determined value of 18,625 Btu/lb for fuel used at Lewis laboratory.
[d] The value of 894,000 Btu/cu ft for AN-F-58 was calculated from the value in footnote c using the experimentally determined value of 0.769^{60}_{60} for the specific gravity of the fuel.

TABLE III—PROPERTIES OF α,ω-DICYCLICALKANE HYDROCARBONS

(a) Physical properties.

[S designates solid at indicated temperature.]

Hydrocarbon	Melting point		Boiling point at 760 mm		Density at 20° C (g/ml)	Kinematic viscosity (centistokes)			Refractive index n_D^{20}
	°C	°F	°C	°F		98.89° C (210° F)	37.78° C (100° F)	0° C (32° F)	
Diphenylalkanes									
Biphenyl	69.2	156.6	255.0	491.0	1.041 [a]	0.992	S	S	S
Diphenylmethane	25.20	77.36	264.27	507.69	1.00592	.965	2.22	S	1.5776
1,2-Diphenylethane	51.16	124.09	280.49	536.88	S	1.14	S	S	S
					.9890 [b]				
1,3-Diphenylpropane	−20.78	−5.40	298 [c]	568 [c]	.97972	1.31	3.64	12.38	1.5594
1,4-Diphenylbutane	52.27	126.29	315.91	600.64	S	1.49	S	S	S
Dicyclohexylalkanes									
Bicyclohexyl	3.50	38.30	238.87	461.97	0.88604	1.23	3.07	S	1.4796
Dicyclohexylmethane	−18.69	−1.64	252.77	486.99	.87645	1.42	4.10	13.0	1.4768
1,2-Dicyclohexylethane	11.44	52.59	274.38	525.88	.87380	1.72	5.38	S	1.4759
1,3-Dicyclohexylpropane	−14.80	5.36	291.69	557.04	.87128	1.96	6.39	24.9	1.4752
1,4-Dicyclohexylbutane	11.62	52.92	309.0	568.2	.87027	2.19	7.58	S	1.4751

(b) Heats of combustion.

Hydrocarbon	Net heat of combustion			Ratio to AN-F-58	
	kcal/mole	Btu/lb	Btu/cu ft	Weight basis [e]	Volume basis [f]
Diphenylalkanes					
Biphenyl	1443.5	16,850 [a]	1.096×10^6	0.905	1.225
Diphenylmethane	1593.5	17,050	1.070	.916	1.196
1,2-Diphenylethane	1741.5	17,200	1.061	.923	1.186
1,3-Diphenylpropane	1886.5	17,300	1.057	.929	1.181
1,4-Diphenylbutane	2032.9	17,400	(d)	.929	-----
Dicyclohexylalkanes					
Bicyclohexyl	1700.0	18,400	1.017×10^6	0.988	1.137
Dicyclohexylmethane	1845.9	18,425	1.008	.989	1.127
1,2-Dicyclohexylethane	1997.5	18,500	1.008	.993	1.127
1,3-Dicyclohexylpropane	2156.2	18,625	1.012	1.000	1.131
1,4-Dicyclohexylbutane	2285.7	18,500	1.005	.993	1.123

[a] Reference 2.

[b] Extrapolated value from reference 12.

[c] Slight decomposition at this pressure.

[d] 1,4-Diphenylbutane is a solid at temperature (20° C) at which density measurements were made. No value is available in the literature, as in the case of biphenyl and 1,2-diphenyl ethane.

[e] Based on experimentally determined value of 18,625 Btu/lb for fuel used at Lewis laboratory.

[f] The value of 894,000 Btu/cu ft for AN-F-58 was calculated from the value in footnote c of table I using the experimentally determined value of 0.769^{60}_{60} for the specific gravity of the fuel.