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Heats, Equilibrium Constants, and Free Energies of Formation of the Alkylcyclopentanes and Alkylcyclohexanes*[1]

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For cyclopentane, cyclohexane, the seven dimethylcyclohexanes, and the normal alkylcyclopentanes and alkylcyclohexanes, values are presented for the following thermodynamic properties to 1,000° or 1,500°K: The heat of formation from the elements; the free energy of formation from the elements; and the logarithm of the equilibrium constant of formation from the elements. For cyclopentane, cyclohexane, and the normal alkylcyclopentanes and alkylcyclohexanes, values are also given to 1,500°K, for the following properties: The heat-content function; the free-energy function; the entropy; the heat content; and the heat capacity.

Equilibrium constants and concentrations are given in tabular and graphical form for some reactions of isomerization, hydrogenation, and cyclization.

I. Introduction

As a part of the work of the American Petroleum Institute Research Project 44 at the National Bureau of Standards and the University of California, values have been calculated for the heat-content function, free-energy function, entropy, heat content and heat capacity of the normal alkylcyclopentanes and the normal alkylcyclohexanes above ethylcyclohexane, in the gaseous state to 1,500° K. These data, together with previously published data on cyclopentane, cyclohexane, methylcyclohexane, and ethylcyclohexane, have been combined with values of the heats of formation at 25° C to calculate values of the heats, free energies, and equilibrium constants of formation of 17 alkylcyclopentanes and 24 alkylcyclohexanes. The free energies and equilibrium constants of a number of reactions involving these compounds have been calculated.

II. Fundamental Constants

The unit of energy, atomic weights, and values of the fundamental constants used in this report are the same as those previously used [5, 13][6].

III. Heat-Content Function, Free-Energy Function, Entropy, Heat Content, and Heat Capacity

1. Method and Data Used in the Calculations

For cyclopentane, cyclohexane, methylcyclohexane, ethylcyclohexane, and the seven dimethylcyclohexanes, the values were taken from references [1, 2].

For methylcyclopentane, the thermodynamic functions were calculated by means of the following relation:

$$[\text{methylcyclopentane}] = [\text{cyclopentane}] + [\text{methyl}] + [\text{restricted rotation of ring puckering}] + (R \ln 10). \quad (1)$$

The terms written in brackets represent a given thermodynamic function of the indicated sub-

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[6] Figures in brackets indicate the literature references at the end of the paper.

stance. In eq 1, the term [methyl] represents the contribution (vibration and restricted rotation) of the methyl group and was calculated by the following relation:

$$[\text{methyl}]=[\text{methylcyclohexane}]-[\text{steric factor}]-[\text{cyclohexane}]-(R \ln 6). \quad (2)$$

In eq 2, the term [steric factor] is the contribution of the equatorial-polar tautomerism of methylcyclohexane to its thermodynamic functions. The term [methyl] is therefore the difference between the functions of methylcyclohexane and cyclohexane, without the inclusion of the effects of tautomerism and of symmetry number. The symmetry number corrections, which are written in parentheses, are to be used for the negative of the free-energy function, $-(F-H_0^\circ)/T$, and for the entropy, S°, but not for the other functions.

The term [restricted rotation of ring puckering] is the contribution arising from a restricting barrier of 750 cal/mole from the asymmetry induced by the presence of the methyl group on the ring. See reference [1] for details. A classical partition function was used.

The thermodynamic functions of ethylcyclopentane were calculated from the following relation:

$$[\text{ethylcyclopentane}]=[\text{methylcyclopentane}]+[\text{2-methylbutane}]-[\text{2-methylpropane}]-(R \ln 3). \quad (3)$$

For normal propylcyclopentane and each of the higher normal alkylcyclopentanes, the following relation, with the appropriate number of CH_2 groups, was used to calculate the thermodynamic functions:

$$[\text{normal alkylcyclopentane}]=[\text{ethylcyclopentane}]+n\ [CH_2]. \quad (4)$$

The thermodynamic functions of normal propylcyclohexane were calculated from the following relation:

$$[\text{normal propylcyclohexane}]=[\text{ethylcyclohexane}]+[\text{2-methylpentane}]-[\text{2-methylbutane}]. \quad (5)$$

In the case of normal butylcyclohexane and the higher normal alkylcyclohexanes, a relation similar to eq 4 was used:

$$[\text{normal alkylcyclohexane}]=[\text{normal propylcyclohexane}]+n\ [CH_2]. \quad (6)$$

The thermodynamic functions of the paraffin hydrocarbons and of the CH_2 increment that are used in eq 3 to 6 are taken from reference [14].

2. Results

The resulting values of the thermodynamic properties for the normal alkylcyclopentanes and alkylcyclohexanes are presented in tables 1 to 10, which give values of the following properties: Heat-content function, $(H^\circ-H_0^\circ)/T$; free-energy function, $(F^\circ-H_0^\circ)/T$; entropy, S°; heat content, $H^\circ-H_0^\circ$; and heat capacity, C_p°.

TABLE 1.—*Values of the heat content function, for the ideal gaseous state, to 1,500° K, for the normal alkylcyclopentanes*

Compound (gas)	Formula	Temperature in °K														
		0	298.16	300	400	500	600	700	800	900	1,000	1,100	1,200	1,300	1,400	1,500
		Heat content function $(H°-H°_0)/T$, in cal/deg mole														
Cyclopentane	C_5H_{10}	0	12.07	12.12	15.12	18.52	21.98	25.29	28.40	31.29	33.97	36.46	38.75	40.87	42.83	44.65
Methylcyclopentane	C_6H_{12}	0	16.01	16.09	19.88	24.03	28.17	32.09	35.75	39.15	42.28	45.18	47.87	50.34	52.62	54.74
Ethylcyclopentane	C_7H_{14}	0	18.91	19.01	23.70	28.66	33.55	38.16	42.43	46.38	50.00	53.36	56.47	59.32	61.96	64.40
n-Propylcyclopentane	C_8H_{16}	0	22.34	22.46	27.9	33.6	39.1	44.4	49.2	53.7	57.8	61.6	65.1	68.3	71.3	74.1
n-Butylcyclopentane	C_9H_{18}	0	25.77	25.90	32.1	38.5	44.7	50.6	56.0	61.0	65.6	69.8	73.7	77.3	80.6	83.7
n-Pentylcyclopentane	$C_{10}H_{20}$	0	29.20	29.35	36.3	43.4	50.3	56.8	62.8	68.3	73.3	78.0	82.3	86.3	90.0	93.4
n-Hexylcyclopentane	$C_{11}H_{22}$	0	32.63	32.80	40.5	48.3	55.9	63.0	69.5	75.6	81.1	86.2	91.0	95.3	99.4	103.0
n-Heptylcyclopentane	$C_{12}H_{24}$	0	36.06	36.24	44.8	53.2	61.5	69.2	76.3	82.8	88.9	94.4	99.6	104.3	108.7	112.7
n-Octylcyclopentane	$C_{13}H_{26}$	0	39.49	39.69	49.0	58.2	67.1	75.4	83.1	90.1	96.6	102.6	108.2	113.3	118.0	122.4
n-Nonylcyclopentane	$C_{14}H_{28}$	0	42.92	43.14	53.2	63.1	72.7	81.6	89.9	97.4	104.4	110.8	116.8	122.3	127.4	132.0
n-Decylcyclopentane	$C_{15}H_{30}$	0	46.35	46.59	57.4	68.0	78.2	87.9	96.6	104.7	112.2	119.1	125.4	131.3	136.7	141.7
n-Undecylcyclopentane	$C_{16}H_{32}$	0	49.78	50.03	61.6	72.9	83.8	94.1	103.4	112.0	120.0	127.3	134.0	140.3	146.1	151.3
n-Dodecylcyclopentane	$C_{17}H_{34}$	0	53.21	53.48	65.8	77.8	89.4	100.3	110.2	119.3	127.7	135.5	142.7	149.3	155.4	161.0
n-Tridecylcyclopentane	$C_{18}H_{36}$	0	56.64	56.93	70.0	82.8	95.0	106.5	117.0	126.6	135.5	143.7	151.3	158.3	164.8	170.7
n-Tetradecylcyclopentane	$C_{19}H_{38}$	0	60.07	60.37	74.2	87.7	100.6	112.7	123.8	133.9	143.3	151.9	159.9	167.3	174.1	180.3
n-Pentadecylcyclopentane	$C_{20}H_{40}$	0	63.50	63.82	78.4	92.6	106.2	118.9	130.5	141.2	151.0	160.1	168.5	176.3	183.5	190.0
n-Hexadecylcyclopentane	$C_{21}H_{42}$	0	66.93	67.27	82.6	97.5	111.8	125.1	137.3	148.5	158.8	168.3	177.2	185.3	192.8	199.6
Increment per CH_2 group		0	3.430	3.447	4.21	4.92	5.59	6.21	6.78	7.29	7.77	8.21	8.62	9.00	9.35	9.66

TABLE 2.—*Values of the heat content function, for the ideal gaseous state, to 1,500° K, for the normal alkylcyclohexanes*

Compound (gas)	For mula	Temperature in °K														
		0	298.16	300	400	500	600	700	800	900	1,000	1,100	1,200	1,300	1,400	1,500
		Heat content function $(H°-H°_0)/T$, in cal/deg mole														
Cyclohexane	C_6H_{12}	0	14.21	14.28	18.38	22.85	27.34	31.64	35.67	39.40	42.85	46.0	48.9	51.6	54.0	56.3
Methylcyclohexane	C_7H_{14}	0	17.55	17.66	22.84	28.26	33.53	38.53	43.16	47.42	51.33	54.9	58.2	61.2	64.0	66.5
Ethylcyclohexane	C_8H_{16}	0	20.45	20.58	26.7	32.9	38.9	44.6	49.9	54.7	59.1	63.1	66.8	70.2	73.3	76.2
n-Propylcyclohexane	C_9H_{18}	0	23.66	23.81	30.6	37.7	44.3	50.6	56.4	61.8	66.7	71.3	75.4	79.2	82.6	85.9
n-Butylcyclohexane	$C_{10}H_{20}$	0	27.09	27.26	34.8	42.6	50.0	56.8	63.2	69.1	74.5	79.5	84.0	88.2	92.0	95.5
n-Pentylcyclohexane	$C_{11}H_{22}$	0	30.52	30.70	39.0	47.5	55.5	63.0	70.0	76.4	82.2	87.7	92.7	97.2	101.3	105.2
n-Hexylcyclohexane	$C_{12}H_{24}$	0	33.95	34.15	43.2	52.5	61.1	69.2	76.7	83.7	90.0	96.0	101.3	106.2	110.7	114.8
n-Heptylcyclohexane	$C_{13}H_{26}$	0	37.38	37.60	47.4	57.4	66.6	75.5	83.5	91.0	97.8	104.2	109.9	115.2	120.0	124.5
n-Octylcyclohexane	$C_{14}H_{28}$	0	40.81	41.05	51.6	62.3	72.2	81.7	90.3	98.3	105.6	112.4	118.5	124.2	129.4	134.2
n-Nonylcyclohexane	$C_{15}H_{30}$	0	44.24	44.49	55.9	67.2	77.8	87.9	97.1	105.6	113.3	120.6	127.1	133.2	138.7	143.8
n-Decylcyclohexane	$C_{16}H_{32}$	0	47.67	47.94	60.1	72.1	83.4	94.1	103.8	112.9	121.1	128.8	135.8	142.2	148.1	153.5
n-Undecylcyclohexane	$C_{17}H_{34}$	0	51.10	51.39	64.3	77.0	89.0	100.3	110.6	120.1	128.9	137.0	144.4	151.2	157.4	163.1
n-Dodecylcyclohexane	$C_{18}H_{36}$	0	54.53	54.83	68.5	82.0	94.6	106.5	117.4	127.4	136.7	145.2	153.0	160.2	166.8	172.8
n-Tridecylcyclohexane	$C_{19}H_{38}$	0	57.96	58.28	72.7	86.9	100.2	112.7	124.2	134.7	144.4	153.4	161.6	169.2	176.1	182.5
n-Tetradecylcyclohexane	$C_{20}H_{40}$	0	61.39	61.73	76.9	91.8	105.8	118.9	130.9	142.0	152.2	161.7	170.2	178.2	185.5	192.1
n-Pentadecylcyclohexane	$C_{21}H_{42}$	0	64.82	65.17	81.1	96.7	111.3	125.2	137.7	149.3	160.0	169.9	178.9	187.2	194.8	201.8
n-Hexadecylcyclohexane	$C_{22}H_{44}$	0	68.25	68.62	85.3	101.6	116.9	131.4	144.5	156.6	167.7	178.1	187.5	196.2	204.2	211.4
Increment per CH_2 group		0	3.430	3.447	4.21	4.92	5.59	6.21	6.78	7.29	7.77	8.21	8.62	9.00	9.35	9.66

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TABLE 3.—*Values of the free energy function, for the ideal gaseous state, to 1,500° K, for the normal alkylcyclopentanes*

Compound (gas)	Formula	Temperature in ° K														
		0	298.16	300	400	500	600	700	800	900	1,000	1,100	1,200	1,300	1,400	1,500
		Free energy function $(F°-H°_0)/T$, in cal/deg mole														
Cyclopentane	C_5H_{10}	0	−57.93	−58.00	−61.88	−65.62	−69.30	−72.95	−76.52	−80.04	−83.48	−86.84	−90.13	−93.31	−96.40	−99.42
Methylcyclopentane	C_6H_{12}	0	−65.23	−65.33	−70.45	−75.33	−80.07	−84.72	−89.26	−93.68	−97.97	−102.13	−106.18	−110.08	−113.89	−117.63
Ethylcyclopentane	C_7H_{14}	0	−71.71	−71.83	−77.90	−83.72	−89.34	−94.89	−100.30	−105.53	−110.62	−115.54	−120.32	−124.97	−129.41	−133.79
n-Propylcyclopentane	C_8H_{16}	0	−77.46	−77.61	−84.8	−91.6	−98.2	−104.6	−110.9	−117.0	−122.9	−128.6	−134.1	−139.4	−144.5	−149.6
n-Butylcyclopentane	C_9H_{18}	0	−83.22	−83.38	−91.6	−99.5	−107.0	−114.4	−121.6	−128.4	−135.1	−141.6	−147.8	−153.9	−159.7	−165.3
n-Pentylcyclopentane	$C_{10}H_{20}$	0	−88.97	−89.16	−98.5	−107.4	−115.9	−124.2	−132.2	−139.9	−147.4	−154.6	−161.6	−168.4	−174.8	−181.1
n-Hexylcyclopentane	$C_{11}H_{22}$	0	−94.72	−94.94	−105.4	−115.3	−124.7	−133.9	−142.8	−151.4	−159.6	−167.6	−175.4	−182.8	−189.9	−196.9
n-Heptylcyclopentane	$C_{12}H_{24}$	0	−100.48	−100.72	−112.2	−123.2	−133.6	−143.7	−153.4	−162.8	−171.9	−180.7	−189.1	−197.3	−205.1	−212.6
n-Octylcyclopentane	$C_{13}H_{26}$	0	−106.23	−106.49	−119.1	−131.0	−142.4	−153.4	−164.1	−174.3	−184.2	−193.7	−202.9	−211.8	−220.2	−228.4
n-Nonylcyclopentane	$C_{14}H_{28}$	0	−111.98	−112.27	−126.0	−138.9	−151.2	−163.2	−174.7	−185.8	−196.4	−206.7	−216.6	−226.2	−235.3	−244.2
n-Decylcyclopentane	$C_{15}H_{30}$	0	−117.73	−118.05	−132.8	−146.8	−160.1	−172.9	−185.3	−197.2	−208.7	−219.7	−230.4	−240.7	−250.5	−259.9
n-Undecylcyclopentane	$C_{16}H_{32}$	0	−123.49	−123.82	−139.7	−154.7	−168.9	−182.7	−195.9	−208.7	−220.9	−232.8	−244.2	−255.1	−265.6	−275.7
n-Dodecylcyclopentane	$C_{17}H_{34}$	0	−129.24	−129.60	−146.6	−162.6	−177.8	−192.4	−206.6	−220.1	−233.2	−245.8	−257.9	−269.6	−280.7	−291.5
n-Tridecylcyclopentane	$C_{18}H_{36}$	0	−134.99	−135.38	−153.4	−170.5	−186.6	−202.2	−217.2	−231.6	−245.4	−258.8	−271.7	−284.1	−295.9	−307.2
n-Tetradecylcyclopentane	$C_{19}H_{38}$	0	−140.75	−141.15	−160.3	−178.4	−195.5	−211.9	−227.8	−243.0	−257.7	−271.8	−285.4	−298.5	−311.0	−323.0
n-Pentadecycyclopentane	$C_{20}H_{40}$	0	−146.50	−146.93	−167.2	−186.2	−204.3	−221.7	−238.4	−254.5	−270.0	−284.8	−299.2	−313.0	−326.1	−338.8
n-Hexadecylcyclopentane	$C_{21}H_{42}$	0	−152.25	−152.71	−174.0	−194.1	−213.1	−231.4	−249.1	−266.0	−282.2	−297.9	−313.0	−327.4	−341.3	−354.5
Increment per CH_2 group		0	−5.753	−5.777	−6.87	−7.89	−8.84	−9.75	−10.63	−11.46	−12.26	−13.02	−13.76	−14.46	−15.13	−15.77

TABLE 4.—*Values of the free energy function, for the ideal gaseous state, to 1,500° K, for the normal alkylcyclohexanes*

Compound (gas)	Formula	Temperature in ° K														
		0	298.16	300	400	500	600	700	800	900	1,000	1,100	1,200	1,300	1,400	1,500
		Free energy function $(F°-H°_0)/T$, in cal/deg mole														
Cyclohexane	C_6H_{12}	0	−57.07	−57.16	−61.80	−66.39	−70.96	−75.50	−79.98	−84.40	−88.74	−93.0	−97.1	−101.1	−105.0	−108.8
Methylcylohexane	C_7H_{14}	0	−64.51	−64.62	−70.38	−76.06	−81.68	−87.24	−92.70	−98.04	−103.24	−108.3	−113.2	−118.0	−122.6	−127.1
Ethylcyclohexane	C_8H_{16}	0	−70.99	−71.12	−77.8	−84.5	−91.0	−97.4	−103.7	−109.9	−115.9	−121.7	−127.3	−132.8	−138.1	−143.3
n-Propylcyclohexane	C_9H_{18}	0	−76.45	−76.62	−84.4	−91.9	−99.4	−106.7	−113.9	−120.9	−127.7	−134.2	−140.5	−146.8	−152.7	−158.5
n-Butylcyclohexane	$C_{10}H_{20}$	0	−82.20	−82.40	−91.3	−99.8	−108.2	−116.5	−124.5	−132.4	−140.0	−147.2	−154.3	−161.3	−167.8	−174.3
n-Pentylcyclohexane	$C_{11}H_{22}$	0	−87.96	−88.17	−98.1	−107.7	−117.1	−126.2	−135.2	−143.8	−152.2	−160.2	−168.0	−175.7	−183.0	−190.0
n-Hexylcyclohexane	$C_{12}H_{24}$	0	−93.71	−93.95	−105.0	−115.6	−125.9	−136.0	−145.8	−155.3	−164.5	−173.3	−181.8	−190.2	−198.1	−205.8
n-Heptylcyclohexane	$C_{13}H_{26}$	0	−99.46	−99.73	−111.9	−123.4	−134.8	−145.7	−156.4	−166.7	−176.7	−186.3	−195.5	−204.7	−213.2	−221.6
n-Octylcyclohexane	$C_{14}H_{28}$	0	−105.22	−105.51	−118.7	−131.3	−143.6	−155.5	−167.0	−178.2	−189.0	−199.3	−209.3	−219.1	−228.4	−237.3
n-Nonylcyclohexane	$C_{15}H_{30}$	0	−110.97	−111.28	−125.6	−139.2	−152.5	−165.2	−177.7	−189.7	−201.2	−212.3	−223.1	−233.6	−243.5	−253.1
n-Decylcyclohexane	$C_{16}H_{32}$	0	−116.72	−117.06	−132.5	−147.1	−161.3	−175.0	−188.3	−201.1	−213.5	−225.4	−236.8	−248.0	−258.6	−268.9
n-Undecylcyclohexane	$C_{17}H_{34}$	0	−122.47	−122.84	−139.3	−155.0	−170.1	−184.7	−198.9	−212.6	−225.8	−238.4	−250.6	−262.5	−273.8	−284.6
n-Dodecylcyclohexane	$C_{18}H_{36}$	0	−128.23	−128.61	−146.2	−162.9	−179.0	−194.5	−209.5	−224.0	−238.0	−251.4	−264.3	−277.0	−288.9	−300.4
n-Tridecylcyclohexane	$C_{19}H_{38}$	0	−133.98	−134.39	−153.1	−170.8	−187.8	−204.2	−220.2	−235.5	−250.3	−264.4	−278.1	−291.4	−304.0	−316.2
n-Tetradecylcyclohexane	$C_{20}H_{40}$	0	−139.73	−140.17	−159.9	−178.7	−196.7	−214.0	−230.8	−247.0	−262.5	−277.5	−291.8	−305.9	−319.2	−331.9
n-Pentadecylcyclohexane	$C_{21}H_{42}$	0	−145.49	−145.94	−166.8	−186.5	−205.5	−223.7	−241.4	−258.4	−274.8	−290.5	−305.6	−320.4	−334.3	−347.7
n-Hexadecylcyclohexane	$C_{22}H_{44}$	0	−151.24	−151.72	−173.7	−194.4	−214.4	−233.5	−252.1	−269.9	−287.0	−303.5	−319.4	−334.8	−349.4	−363.5
Increment per CH_2 group		0	−5.753	−5.777	−6.87	−7.89	−8.84	−9.75	−10.63	−11.46	−12.26	−13.02	−13.76	−14.46	−15.13	−15.77

TABLE 5.—*Values of the entropy, for the ideal gaseous state, to 1,500° K, for the normal alkylcyclopentanes*

Compound (gas)	Formula	Temperature in ° K														
		0	298.16	300	400	500	600	700	800	900	1,000	1,100	1,200	1,300	1,400	1,500
		Entropy, $S°$, in cal/deg mole														
Cyclopentane	C_5H_{10}	0	70.00	70.12	77.00	84.14	91.28	98.24	104.92	111.33	117.45	123.30	128.88	134.18	139.23	144.07
Methylcyclopentane	C_6H_{12}	0	81.24	81.42	90.33	99.36	108.24	116.81	125.01	132.83	140.25	147.31	154.05	160.42	166.51	172.37
Ethylcyclopentane	C_7H_{14}	0	90.62	90.84	101.60	112.38	122.89	133.05	142.73	151.91	160.62	168.90	176.79	184.29	191.37	198.19
n-Propylcyclopentane	C_8H_{16}	0	99.80	100.06	112.7	125.2	137.3	149.0	160.1	170.7	180.6	190.1	199.2	207.8	215.8	223.6
n-Butylcyclopentane	C_9H_{18}	0	108.99	109.29	123.8	138.0	151.8	165.0	177.5	189.4	200.7	211.4	221.6	231.2	240.3	249.0
n-Pentylcyclopentane	$C_{10}H_{20}$	0	118.17	118.51	134.8	150.8	166.2	181.0	194.9	208.2	220.7	232.6	243.9	254.7	264.8	274.5
n-Hexylcyclopentane	$C_{11}H_{22}$	0	127.35	127.74	145.9	163.6	180.6	196.9	212.4	226.9	240.7	253.8	266.3	278.1	289.3	299.9
n-Heptylcyclopentane	$C_{12}H_{24}$	0	136.54	136.96	157.0	176.4	195.0	212.9	229.8	245.7	260.8	275.1	288.7	301.6	313.8	325.3
n-Octylcyclopentane	$C_{13}H_{26}$	0	145.72	146.18	168.1	189.2	209.5	228.8	247.2	264.4	280.8	296.3	311.1	325.0	338.2	350.8
n-Nonylcyclopentane	$C_{14}H_{28}$	0	154.90	155.41	179.1	202.0	223.9	244.8	264.6	283.2	300.8	317.6	333.4	348.5	362.7	376.2
n-Decylcyclopentane	$C_{15}H_{30}$	0	164.08	164.63	190.2	214.8	238.3	260.8	282.0	301.9	320.9	338.8	355.8	372.0	387.2	401.6
n-Undecylcyclopentane	$C_{16}H_{32}$	0	173.27	173.86	201.3	227.6	252.8	276.7	299.4	320.7	340.9	360.0	378.2	395.4	411.7	427.0
n-Dodecylcyclopentane	$C_{17}H_{34}$	0	182.45	183.08	212.4	240.4	267.2	292.7	316.8	339.4	360.9	381.3	400.6	418.9	436.2	452.5
n-Tridecylcyclopentane	$C_{18}H_{36}$	0	191.63	192.30	223.4	253.2	281.6	308.7	334.2	358.2	381.0	402.5	423.0	442.4	460.6	477.9
n-Tetradecylcyclopentane	$C_{19}H_{38}$	0	200.82	201.53	234.5	266.0	296.0	324.6	351.6	377.0	401.0	423.7	445.3	465.8	485.1	503.3
n-Pentadecylcyclopentane	$C_{20}H_{40}$	0	210.00	210.75	245.6	278.8	310.5	340.6	369.0	395.7	421.0	445.0	467.7	489.3	509.6	528.7
n-Hexadecylcyclopentane	$C_{21}H_{42}$	0	219.18	219.98	256.7	291.6	324.9	356.6	386.4	414.4	441.0	466.2	490.1	512.7	534.1	554.2
Increment per CH_2 group		0	9.183	9.224	11.08	12.80	14.43	15.97	17.40	18.75	20.03	21.24	22.38	23.46	24.48	25.43

TABLE 6.—*Values of the entropy, for the ideal gaseous state, to, 1500° K, for the normal alkylcyclohexanes*

Compound (gas)	Formula	Temperature in ° K														
		0	298.16	300	400	500	600	700	800	900	1,000	1,100	1,200	1,300	1,400	1,500
		Entropy, $S°$, in cal/deg mole														
Cyclohexane	C_6H_{12}	0	71.28	71.44	80.18	89.24	98.30	107.14	115.65	123.80	131.59	139.0	146.0	152.7	159.0	165.1
Methylcyclohexane	C_7H_{14}	0	82.06	82.28	93.22	104.32	115.21	125.77	135.86	145.46	154.57	163.2	171.4	179.2	186.6	193.7
Ethylcyclohexane	C_8H_{16}	0	91.44	91.70	104.5	117.3	129.9	142.0	153.6	164.5	174.9	184.8	194.2	203.0	211.4	219.5
n-Propylcyclohexane	C_9H_{18}	0	100.11	100.43	115.0	129.6	143.7	157.3	170.4	182.7	194.3	205.5	215.9	226.0	235.3	244.4
n-Butylcyclohexane	$C_{10}H_{20}$	0	109.29	109.66	126.1	142.4	158.1	173.3	187.8	201.5	214.3	226.7	238.3	249.5	259.8	269.8
n-Pentylcyclohexane	$C_{11}H_{22}$	0	118.48	118.87	137.2	155.2	172.6	189.2	205.2	220.2	234.4	248.0	260.7	272.9	284.3	295.3
n-Hexylcyclohexane	$C_{12}H_{24}$	0	127.66	128.10	148.2	168.0	187.0	205.2	222.6	239.0	254.4	269.2	283.0	296.4	308.7	320.7
n-Heptylcyclohexane	$C_{13}H_{26}$	0	136.84	137.33	159.3	180.8	201.4	221.2	240.0	257.7	274.4	290.4	305.4	319.8	333.2	346.1
n-Octylcyclohexane	$C_{14}H_{28}$	0	146.03	146.56	170.4	193.6	215.8	237.1	257.4	276.5	294.4	311.7	327.8	343.3	357.7	371.5
n-Nonylcyclohexane	$C_{15}H_{30}$	0	155.21	155.77	181.5	206.4	230.3	253.1	274.8	295.2	314.5	332.9	350.2	366.8	382.2	397.0
n-Decylcyclohexane	$C_{16}H_{32}$	0	164.39	165.00	192.5	219.2	244.7	269.1	292.2	314.0	334.5	354.2	372.6	390.2	406.7	422.4
n-Undecylcyclohexane	$C_{17}H_{34}$	0	173.57	174.23	203.6	232.0	259.1	285.0	309.6	332.7	354.5	375.4	394.9	413.7	431.1	447.8
n-Dodecylcyclohexane	$C_{18}H_{36}$	0	182.76	183.44	214.7	244.8	273.6	301.0	327.0	351.5	374.6	396.6	417.3	437.1	455.6	473.2
n-Tridecylcyclohexane	$C_{19}H_{38}$	0	191.94	192.67	225.8	257.6	288.0	317.0	344.4	370.2	394.6	417.9	439.7	460.6	480.1	498.7
n-Tetradecylcyclohexane	$C_{20}H_{40}$	0	201.12	201.90	236.8	270.4	302.4	332.9	361.8	389.0	414.6	439.1	462.1	484.1	504.6	524.1
n-Pentadecylcyclohexane	$C_{21}H_{42}$	0	210.31	211.11	247.9	283.2	316.9	348.9	379.2	407.7	434.7	460.3	484.4	507.5	529.1	549.5
n-Hexadecylcyclohexane	$C_{22}H_{44}$	0	219.49	220.34	259.0	296.1	331.3	364.9	396.7	426.5	454.7	481.6	506.8	531.0	553.5	575.0
Increment per CH_2 group		0	9.183	9.224	11.08	12.80	14.43	15.97	17.40	18.75	20.03	21.24	22.38	23.46	24.48	25.43

TABLE 7.—*Values of the heat content, for the ideal gaseous state, to 1,500° K, for the normal alkylcyclopentanes*

Compound (gas)	Formula	Temperature in ° K														
		0	298.16	300	400	500	600	700	800	900	1,000	1,100	1,200	1,300	1,400	1,500
		Heat content ($H°-H°_0$), in cal/mole														
Cyclopentane	C_5H_{10}	0	3,599	3,636	6,048	9,260	13,188	17,703	22,720	28,161	33,970	40,110	46,500	53,130	59,960	66,980
Methylcyclopentane	C_6H_{12}	0	4,774	4,827	7,952	12,015	16,902	22,463	28,600	35,235	42,280	49,700	57,440	65,440	73,670	82,110
Ethylcyclopentane	C_7H_{14}	0	5,638	5,703	9,480	14,330	20,100	26,700	33,900	41,700	50,000	58,700	67,800	77,100	86,700	96,600
n-Propylcyclopentane	C_8H_{16}	0	6,661	6,737	11,160	16,790	23,500	31,100	39,400	48,300	57,800	67,700	78,100	88,800	99,800	111,100
n-Butylcyclopentane	C_9H_{18}	0	7,683	7,771	12,850	19,250	26,800	35,400	44,800	54,900	65,500	76,800	88,400	100,500	112,900	125,600
n-Pentylcyclopentane	$C_{10}H_{20}$	0	8,706	8,805	14,530	21,710	30,200	39,800	50,200	61,400	73,300	85,800	98,800	112,200	126,000	140,100
n-Hexylcyclopentane	$C_{11}H_{22}$	0	9,729	9,839	16,220	24,160	33,500	44,100	55,600	68,000	81,100	94,800	109,100	123,900	139,100	154,600
n-Heptylcyclopentane	$C_{12}H_{24}$	0	10,752	10,874	17,900	26,620	36,900	48,500	61,100	74,600	88,900	103,800	119,500	135,600	152,200	169,000
n-Octylcyclopentane	$C_{13}H_{26}$	0	11,774	11,908	19,580	29,080	40,200	52,800	66,500	81,100	96,600	112,900	129,800	147,300	165,300	183,500
n-Nonylcyclopentane	$C_{14}H_{28}$	0	12,797	12,942	21,270	31,540	43,600	57,200	71,900	87,700	104,400	121,900	140,100	159,000	178,400	198,000
n-Decylcyclopentane	$C_{15}H_{30}$	0	13,820	13,976	22,950	34,000	46,900	61,500	77,300	94,300	112,200	130,900	150,500	170,700	191,500	212,500
n-Undecylcyclopentane	$C_{16}H_{32}$	0	14,842	15,010	24,640	36,460	50,300	65,900	82,700	100,800	120,000	140,000	160,800	182,400	204,600	227,000
n-Dodecylcyclopentane	$C_{17}H_{34}$	0	15,865	16,044	26,320	38,920	53,600	70,200	88,200	107,400	127,700	149,000	171,200	194,100	217,600	241,500
n-Tridecylcyclopentane	$C_{18}H_{36}$	0	16,888	17,078	28,000	41,370	57,000	74,600	93,600	113,900	135,500	158,000	181,500	205,800	230,700	256,000
n-Tetradecylcyclopentane	$C_{19}H_{38}$	0	17,910	18,112	29,690	43,830	60,400	78,900	99,000	120,500	143,300	167,000	191,800	217,500	243,800	270,500
n-Pentadecylcyclopentane	$C_{20}H_{40}$	0	18,933	19,146	31,370	46,290	63,700	83,200	104,400	127,100	151,000	176,100	202,200	229,200	256,900	285,000
n-Hexadecylcyclopentane	$C_{21}H_{42}$	0	19,956	20,180	33,060	48,750	67,100	87,600	109,900	133,600	158,800	185,100	212,500	240,900	270,000	299,500
Increment per CH_2 group		0	1,022.7	1,034.1	1,684	2,458	3,350	4,350	5,420	6,560	7,770	9,030	10,340	11,700	13,090	14,490

TABLE 8.—*Values of the heat content, for the ideal gaseous state, to 1,500° K, for the normal alkylcyclohexanes*

Compound (gas)	Formula	Temperature in ° K														
		0	298.16	300	400	500	600	700	800	900	1,000	1,100	1,200	1,300	1,400	1,500
		Heat content ($H°-H°_0$), in cal/mole														
Cyclohexane	C_6H_{12}	0	4,237	4,284	7,352	11,435	16,404	22,148	28,536	35,460	42,850	50,600	58,680	67,080	75,600	84,450
Methylcyclohexane	C_7H_{14}	0	5,233	5,298	9,136	14,130	20,118	26,971	34,528	42,678	51,330	60,390	69,840	79,560	89,600	99,750
Ethylcyclohexane	C_8H_{16}	0	6,097	6,174	10,680	16,450	23,300	31,200	39,900	49,200	59,100	69,400	80,200	91,300	102,600	114,300
n-Propylcyclohexane	C_9H_{18}	0	7,054	7,143	12,240	18,850	26,600	35,400	45,100	55,600	66,700	78,400	90,500	103,000	115,700	128,800
n-Butylcyclohexane	$C_{10}H_{20}$	0	8,077	8,177	13,920	21,310	29,900	39,800	50,500	62,200	74,500	87,500	100,800	114,700	128,800	143,300
n-Pentylcyclohexane	$C_{11}H_{22}$	0	9,100	9,211	15,610	23,770	33,300	44,100	56,000	68,700	82,200	96,500	111,200	126,400	141,900	157,800
n-Hexylcyclohexane	$C_{12}H_{24}$	0	10,123	10,245	17,290	26,230	36,600	48,500	61,400	75,300	90,000	105,500	121,500	138,100	155,000	172,300
n-Heptylcyclohexane	$C_{13}H_{26}$	0	11,145	11,279	18,980	28,680	40,000	52,800	66,800	81,900	97,800	114,600	131,900	149,800	168,100	186,800
n-Octylcyclohexane	$C_{14}H_{28}$	0	12,168	12,313	20,660	31,140	43,300	57,200	72,200	88,400	105,600	123,600	142,200	161,500	181,200	201,200
n-Nonylcyclohexane	$C_{15}H_{30}$	0	13,191	13,348	22,340	33,600	46,700	61,500	77,700	95,000	113,300	132,600	152,500	173,200	194,200	215,700
n-Decylcyclohexane	$C_{16}H_{32}$	0	14,213	14,382	24,030	36,060	50,000	65,900	83,100	101,600	121,100	141,600	162,900	184,900	207,300	230,200
n-Undecylcyclohexane	$C_{17}H_{34}$	0	15,236	15,416	25,710	38,520	53,400	70,200	88,500	108,100	128,900	150,700	173,200	196,600	220,400	244,700
n-Dodecylcyclohexane	$C_{18}H_{36}$	0	16,259	16,450	27,400	40,980	56,700	74,600	93,900	114,700	136,700	159,700	183,600	208,300	233,500	259,200
n-Tridecylcyclohexane	$C_{19}H_{38}$	0	17,282	17,484	29,080	43,440	60,100	78,900	99,300	121,300	144,400	168,700	193,900	220,000	246,600	273,700
n-Tetradecylcyclohexane	$C_{20}H_{40}$	0	18,304	18,518	30,760	45,890	63,500	83,300	104,800	127,800	152,200	177,800	204,200	231,700	259,700	288,200
n-Pentadecylcyclohexane	$C_{21}H_{42}$	0	19,327	19,552	32,450	48,350	66,800	87,600	110,200	134,400	160,000	186,800	214,600	243,400	272,800	302,700
n-Hexadecylcyclohexane	$C_{22}H_{44}$	0	20,350	20,586	34,130	50,810	70,200	92,000	115,600	141,000	167,700	195,800	224,900	255,100	285,900	317,200
Increment per CH_2 group		0	1,022.7	1,034.1	1,684	2,458	3,350	4,350	5,420	6,560	7,770	9,030	10,340	11,700	13,090	14,490

TABLE 9.—*Values of the heat capacity, for the ideal gaseous state, to 1,500° K, for the normal alkylcyclopentanes*

Compound (gas)	Formula	Temperature in ° K														
		0	298.16	300	400	500	600	700	800	900	1,000	1,100	1,200	1,300	1,400	1,500
		Heat capacity, C_p°, in cal/deg mole														
Cyclopentane	C_5H_{10}	0	19.82	19.98	28.24	35.86	42.36	47.81	52.44	56.37	59.75	62.68	65.18	67.36	69.24	70.89
Methylcyclopentane	C_6H_{12}	0	26.24	26.46	36.11	44.94	52.43	58.68	64.00	68.53	72.44	75.82	78.72	81.24	83.43	85.35
Ethylcyclopentane	C_7H_{14}	0	31.93	32.18	43.39	53.55	62.09	69.24	75.31	80.48	84.94	88.81	92.12	95.00	97.51	99.69
n-Propylcyclopentane	C_8H_{16}	0	37.69	37.99	50.5	62.0	71.6	79.6	86.4	92.3	97.3	101.7	105.4	108.7	111.5	113.9
n-Butylcyclopentane	C_9H_{18}	0	43.45	43.80	57.7	70.4	81.0	90.0	97.6	104.1	109.7	114.5	118.7	122.3	125.5	128.2
n-Pentylcyclopentane	$C_{10}H_{20}$	0	49.21	49.61	64.8	78.9	90.5	100.3	108.7	115.9	122.0	127.4	132.0	136.0	139.5	142.4
n-Hexylcyclopentane	$C_{11}H_{22}$	0	54.97	55.42	71.9	87.3	100.0	110.7	119.9	127.6	134.4	140.2	145.3	149.7	153.5	156.7
n-Heptylcyclopentane	$C_{12}H_{24}$	0	60.73	61.23	79.1	95.7	109.4	121.1	131.0	139.4	146.8	153.1	158.6	163.4	167.4	171.0
n-Octylcyclopentane	$C_{13}H_{26}$	0	66.49	67.04	86.2	104.2	118.9	131.4	142.2	151.2	159.2	166.0	171.9	177.0	181.4	185.2
n-Nonylcyclopentane	$C_{14}H_{28}$	0	72.25	72.85	93.3	112.6	128.4	141.8	153.3	163.0	171.5	178.8	185.2	190.7	195.4	199.5
n-Decylcyclopentane	$C_{15}H_{30}$	0	78.01	78.66	100.4	121.0	137.8	152.2	164.4	174.8	183.9	191.7	198.4	204.4	209.4	213.7
n-Undecylcyclopentane	$C_{16}H_{32}$	0	83.77	84.47	107.6	129.5	147.3	162.5	175.6	186.6	196.3	204.6	211.7	218.0	223.4	228.0
n-Dodecylcyclopentane	$C_{17}H_{34}$	0	89.53	90.28	114.7	137.9	156.8	172.9	186.7	198.4	208.6	217.4	225.0	231.7	237.4	242.2
n-Tridecylcyclopentane	$C_{18}H_{36}$	0	95.29	96.09	121.8	146.4	166.2	183.3	197.8	210.2	221.0	230.3	238.3	245.4	251.4	256.5
n-Tetradecylcyclopentane	$C_{19}H_{38}$	0	101.05	101.90	129.0	154.8	175.7	193.6	209.0	222.0	233.4	243.1	251.6	259.0	265.4	270.7
n-Pentadecylcyclopentane	$C_{20}H_{40}$	0	106.81	107.71	136.1	163.2	185.2	204.0	220.1	233.8	245.8	256.0	264.9	272.7	279.3	285.0
n-Hexadecylcyclopentane	$C_{21}H_{42}$	0	112.57	113.52	143.2	171.7	194.6	214.4	231.3	245.6	258.1	268.8	278.2	286.4	293.3	299.2
Increment per CH_2 group		0	5.760	5.810	7.13	8.44	9.47	10.37	11.14	11.79	12.37	12.86	13.29	13.67	13.99	14.25

TABLE 10.—*Values of the heat capacity, for the ideal gaseous state to 1,500° K, for the normal alkylcyclohexanes*

Compound (gas)	Formula	Temperature in ° K														
		0	298.16	300	400	500	600	700	800	900	1,000	1,100	1,200	1,300	1,400	1,500
		Heat capacity, C_p°, in cal/deg mole														
Cyclohexane	C_6H_{12}	0	25.40	25.58	35.82	45.47	53.83	60.87	66.76	71.68	75.80	79.3	82.2	84.7	86.8	88.6
Methylcyclohexane	C_7H_{14}	0	32.27	32.51	44.35	55.21	64.46	72.23	78.74	84.20	88.79	92.7	96.0	98.8	101.2	103.2
Ethylcyclohexane	C_8H_{16}	0	37.96	38.23	51.6	63.8	74.1	82.8	90.1	96.2	101.3	105.7	109.4	112.5	115.3	117.6
n-Propylcyclohexane	C_9H_{18}	0	43.59	43.89	58.6	72.1	83.5	93.1	101.1	107.9	113.6	118.6	122.7	126.2	129.3	131.9
n-Butylcyclohexane	$C_{10}H_{20}$	0	49.35	49.70	65.7	80.5	93.0	103.5	112.2	119.7	126.0	131.4	136.0	139.8	143.3	146.1
n-Pentylcyclohexane	$C_{11}H_{22}$	0	55.11	55.51	72.9	89.0	102.4	113.8	123.4	131.5	138.3	144.3	149.3	153.5	157.3	160.4
n-Hexylcyclohexane	$C_{12}H_{24}$	0	60.87	61.32	80.0	97.4	111.9	124.2	134.5	143.3	150.7	157.1	162.6	167.2	171.2	174.6
n-Heptylcyclohexane	$C_{13}H_{26}$	0	66.63	67.13	87.1	105.8	121.4	134.6	145.7	155.1	163.1	170.0	175.8	180.8	185.2	188.9
n-Octylcyclohexane	$C_{14}H_{28}$	0	72.39	72.94	94.3	114.3	130.8	144.9	156.8	166.9	175.4	182.9	189.1	194.5	199.2	203.1
n-Nonylcyclohexane	$C_{15}H_{30}$	0	78.15	78.75	101.4	122.7	140.3	155.3	167.9	178.7	187.8	195.7	202.4	208.2	213.2	217.4
n-Decylcyclohexane	$C_{16}H_{32}$	0	83.91	84.56	108.5	131.2	149.8	165.7	179.1	190.5	200.2	208.6	215.7	221.9	227.2	231.6
n-Undecylcyclohexane	$C_{17}H_{34}$	0	89.67	90.37	115.7	139.6	159.2	176.0	190.2	202.2	212.6	221.4	229.0	235.5	241.2	245.9
n-Dodecylcyclohexane	$C_{18}H_{36}$	0	95.43	96.18	122.8	148.0	168.7	186.4	201.4	214.0	224.9	234.3	242.3	249.2	255.2	260.1
n-Tridecylcyclohexane	$C_{19}H_{38}$	0	101.19	101.99	129.9	156.5	178.2	196.8	212.5	225.8	237.3	247.2	255.6	262.9	269.2	274.4
n-Tetradecylcyclohexane	$C_{20}H_{40}$	0	106.95	107.80	137.1	164.9	187.6	207.1	223.6	237.6	249.7	260.0	268.9	276.5	283.1	288.6
n-Pentadecylcyclohexane	$C_{21}H_{42}$	0	112.71	113.61	144.2	173.3	197.1	217.5	234.8	249.4	262.0	272.9	282.2	290.2	297.1	302.9
n-Hexadecylcyclohexane	$C_{22}H_{44}$	0	118.47	119.42	151.3	181.8	206.6	227.9	245.9	261.2	274.4	285.7	295.5	303.9	311.1	317.1
Increment per CH_2 group		0	5.760	5.810	7.13	8.44	9.47	10.37	11.14	11.79	12.37	12.86	13.29	13.67	13.99	14.25

IV. Heat of Formation, Free Energy of Formation, and Equilibrium Constant of Formation

1. Method and Data Used in the Calculations

The same method of calculation was used as described in section IV, 1 of reference [5].

For the heats of formation at 25° C of the cyclopentane and cyclohexane derivatives treated in this report, the values given in references [3, 4] were used.

2. Results

The resulting values of the thermodynamic properties for the formation of cyclopentane, cyclohexane, the seven dimethylcyclohexanes and the normal alkylcyclopentanes and alkylcyclohexanes, in the gaseous state, from the elements carbon (solid, graphite) and hydrogen (gaseous), are presented in tables 11 to 19, which give values of the following properties, to 1,000° K or 1,500° K: heat of formation, $\Delta Hf°$; free energy of formation, $\Delta Ff°$; and the logarithm of the equilibrium constant of formation, $\log_{10}Kf$.

TABLE 11.—*Values of the heat of formation, for the ideal gaseous state, to 1,500° K, for the normal alkylcyclopentanes*

Compound (gas)	Formula	Temperature in ° K														
		0	298.16	300	400	500	600	700	800	900	1,000	1,100	1,200	1,300	1,400	1,500
		Heat of formation, $\Delta Hf°$, in kcal/mole														
Cyclopentane	C_5H_{10}	−10.68	−18.46	−18.50	−20.80	−22.67	−24.12	−25.25	−26.06	−26.61	−26.91	−27.01	−26.97	−26.81	−26.57	−26.25
Methylcyclopentane	C_6H_{12}	−16.62	−25.50	−25.54	−28.07	−30.11	−31.68	−32.88	−33.74	−34.29	−34.58	−34.65	−34.52	−34.30	−33.97	−33.56
Ethylcyclopentane	C_7H_{14}	−20.80	−30.37	−30.42	−33.24	−35.50	−37.24	−38.54	−39.47	−40.06	−40.36	−40.40	−40.22	−39.94	−39.53	−39.04
n-Propylcyclopentane	C_8H_{16}	−23.85	−35.39	−35.44	−38.6	−41.1	−43.0	−44.4	−45.4	−46.1	−46.4	−46.4	−46.2	−45.9	−45.4	−44.8
n-Butylcyclopentane	C_9H_{18}	−27.43	−40.22	−40.28	−43.7	−46.4	−48.5	−50.1	−51.2	−51.9	−52.2	−52.2	−52.0	−51.6	−51.0	−50.4
n-Pentylcyclopentane	$C_{10}H_{20}$	−31.10	−45.15	−45.21	−48.9	−51.9	−54.2	−55.9	−57.1	−57.8	−58.2	−58.2	−57.9	−57.4	−56.8	−56.1
n-Hexylcyclopentane	$C_{11}H_{22}$	−34.77	−50.07	−50.14	−54.1	−57.4	−59.8	−61.6	−63.0	−63.8	−64.1	−64.1	−63.8	−63.3	−62.6	−61.8
n-Heptylcyclopentane	$C_{12}H_{24}$	−38.44	−55.00	−55.08	−59.4	−62.8	−65.5	−67.4	−68.8	−69.7	−70.1	−70.0	−69.6	−69.1	−68.3	−67.5
n-Octylcyclopentane	$C_{13}H_{26}$	−42.12	−59.92	−60.01	−64.6	−68.3	−71.1	−73.2	−74.7	−75.6	−76.0	−76.0	−75.5	−74.9	−74.1	−73.2
n-Nonylcyclopentane	$C_{14}H_{28}$	−45.79	−64.85	−64.94	−69.8	−73.8	−76.8	−79.0	−80.6	−81.6	−82.0	−81.9	−81.4	−80.8	−79.8	−78.9
n-Decylcyclopentane	$C_{15}H_{30}$	−49.46	−69.78	−69.87	−75.0	−79.2	−82.4	−84.8	−86.4	−87.5	−87.9	−87.8	−87.3	−86.6	−85.6	−84.6
n-Undecylcyclopentane	$C_{16}H_{32}$	−53.14	−74.70	−74.80	−80.2	−84.7	−88.1	−90.5	−92.3	−93.4	−93.8	−93.7	−93.2	−92.4	−91.4	−90.3
n-Dodecylcyclopentane	$C_{17}H_{34}$	−56.81	−79.63	−79.73	−85.5	−90.2	−93.7	−96.3	−98.2	−99.3	−99.8	−99.7	−99.1	−98.2	−97.1	−96.0
n-Tridecylcyclopentane	$C_{18}H_{36}$	−60.48	−84.55	−84.66	−90.7	−95.6	−99.4	−102.1	−104.0	−105.3	−105.7	−105.6	−105.0	−104.1	−102.9	−101.6
n-Tetradecylcyclopentane	$C_{19}H_{38}$	−64.16	−89.48	−89.59	−95.9	−101.1	−105.0	−107.9	−109.9	−111.2	−111.6	−111.5	−110.8	−109.9	−108.6	−107.3
n-Pentadecylcyclopentane	$C_{20}H_{40}$	−67.83	−94.41	−94.52	−101.1	−106.5	−110.7	−113.6	−115.8	−117.1	−117.6	−117.4	−116.7	−115.7	−114.4	−113.0
n-Hexadecylcyclopentane	$C_{21}H_{42}$	−71.50	−99.33	−99.45	−106.4	−112.0	−116.3	−119.4	−121.6	−123.0	−123.5	−123.4	−122.6	−121.6	−120.1	−118.7
Increment per CH_2 group		−3.673	−4.926	−4.931	−5.22	−5.46	−5.65	−5.78	−5.87	−5.93	−5.94	−5.93	−5.89	−5.83	−5.76	−5.69

TABLE 12.—*Values of the heat of formation, for the ideal gaseous state, to 1,500° K, for the normal alkylcyclohexanes*

Compound (gas)	Formula	Temperature in ° K														
		0	298.16	300	400	500	600	700	800	900	1,000	1,100	1,200	1,300	1,400	1,500
		Heat of formation, $\Delta Hf°$, in kcal/mole														
Cyclohexane	C_6H_{12}	−20.01	−29.43	−29.48	−31.70	−34.08	−35.57	−36.59	−37.19	−37.46	−37.41	−37.14	−36.68	−36.05	−35.44	−34.61
Methylcyclohexane	C_7H_{14}	−26.30	−36.99	−37.04	−39.79	−41.92	−43.46	−44.50	−45.10	−45.34	−45.25	−44.92	−44.36	−43.71	−42.89	−42.10
Ethylcyclohexane	C_8H_{16}	−28.94	−41.05	−41.10	−44.13	−46.50	−48.22	−49.35	−49.98	−50.25	−50.17	−49.84	−49.25	−48.51	−47.69	−46.71
n-Propylcyclohexane	C_9H_{18}	−32.79	−46.20	−46.27	−49.6	−52.2	−54.2	−55.4	−56.2	−56.5	−56.4	−56.0	−55.3	−54.5	−53.7	−52.5
n-Butylcyclohexane	$C_{10}H_{20}$	−36.29	−50.95	−51.02	−54.7	−57.5	−59.6	−61.0	−61.9	−62.3	−62.2	−61.7	−61.0	−60.2	−59.3	−58.0
n-Pentylcyclohexane	$C_{11}H_{22}$	−39.96	−55.88	−55.95	−59.9	−62.9	−65.3	−66.8	−67.8	−68.2	−68.2	−67.6	−66.9	−66.0	−65.0	−63.7
n-Hexylcyclohexane	$C_{12}H_{24}$	−43.64	−60.80	−60.88	−65.2	−68.4	−70.9	−72.6	−73.7	−74.1	−74.1	−73.6	−72.8	−71.8	−70.8	−69.4
n-Heptylcyclohexane	$C_{13}H_{26}$	−47.31	−65.73	−65.81	−70.4	−73.9	−76.6	−78.4	−79.6	−80.1	−80.0	−79.5	−78.7	−77.6	−76.5	−75.1
n-Octylcyclohexane	$C_{14}H_{28}$	−50.98	−70.65	−70.74	−75.6	−79.3	−82.2	−84.2	−85.4	−86.0	−86.0	−85.4	−84.6	−83.5	−82.3	−80.8
n-Nonylcyclohexane	$C_{15}H_{30}$	−54.66	−75.58	−75.68	−80.8	−84.8	−87.9	−89.9	−91.3	−91.9	−91.9	−91.3	−90.5	−89.3	−88.0	−86.5
n-Decylcyclohexane	$C_{16}H_{32}$	−58.33	−80.51	−80.61	−86.0	−90.3	−93.5	−95.7	−97.2	−97.8	−97.9	−97.3	−96.4	−95.1	−93.8	−92.2
n-Undecylcyclohexane	$C_{17}H_{34}$	−62.00	−85.43	−85.54	−91.3	−95.7	−99.2	−101.5	−103.0	−103.8	−103.8	−103.2	−102.2	−101.0	−99.6	−97.9
n-Dodecylcyclohexane	$C_{18}H_{36}$	−65.67	−90.36	−90.47	−96.5	−101.2	−104.8	−107.3	−108.9	−109.7	−109.8	−109.1	−108.1	−106.8	−105.3	−103.6
n-Tridecylcyclohexane	$C_{19}H_{38}$	−69.35	−95.28	−95.40	−101.7	−106.7	−110.4	−113.0	−114.8	−115.6	−115.7	−115.0	−114.0	−112.6	−111.1	−109.3
n-Tetradecylcyclohexane	$C_{20}H_{40}$	−73.02	−100.21	−100.33	−106.9	−112.1	−116.1	−118.8	−120.6	−121.6	−121.6	−121.0	−119.9	−118.5	−116.8	−115.0
*n*Pentadecylcyclohexane	$C_{21}H_{42}$	−76.69	−105.14	−105.26	−112.2	−117.6	−121.8	−124.6	−126.5	−127.5	−127.6	−126.9	−125.8	−124.3	−122.6	−120.6
n-Hexadecylcyclohexane	$C_{22}H_{44}$	−80.37	−110.06	−110.19	−117.4	−123.1	−127.4	−130.4	−132.4	−133.4	−133.5	−132.8	−131.7	−130.1	−128.4	−126.3
Increment per CH_2 group		−3.673	−4.926	−4.931	−5.22	−5.46	−5.65	−5.78	−5.87	−5.93	−5.94	−5.93	−5.89	−5.83	−5.76	−5.69

TABLE 13.—*Values of the heat of formation, for the ideal gaseous state, to 1,500° K, for the 7 dimethylcyclohexanes*

Compound (gas)	Formula	Temperature in ° K														
		0	298.16	300	400	500	600	700	800	900	1,000	1,100	1,200	1,300	1,400	1,500
		Heat of formation, $\triangle Hf°$, in kcal/mole														
1,1-Dimethylcyclohexane	C_8H_{16}	−30.93	−43.26	−43.31	−46.4	−48.9	−50.6	−51.8	−52.4	−52.5	−52.4	−51.9	−51.2	−50.4	−49.4	−48.4
cis-1,2-Dimethylcyclohexane	C_8H_{16}	−28.95	−41.15	−41.20	−44.3	−46.7	−48.4	−49.6	−50.2	−50.5	−50.4	−50.0	−49.4	−48.6	−47.4	−46.9
trans-1,2-Dimethylcyclohexane	C_8H_{16}	−30.91	−43.02	−43.07	−46.1	−48.4	−50.1	−51.2	−51.9	−52.0	−51.9	−51.5	−50.9	−50.1	−49.2	−48.2
cis-1,3-Dimethylcyclohexane[a]	C_8H_{16}	−32.02	−44.16	−44.21	−47.3	−49.7	−51.4	−52.5	−53.1	−53.3	−53.2	−52.8	−52.1	−51.2	−50.4	−49.3
trans-1,3-Dimethylcyclohexane[a]	C_8H_{16}	−30.06	−42.20	−42.25	−45.3	−47.7	−49.5	−50.7	−51.3	−51.6	−51.6	−51.2	−50.6	−49.9	−49.1	−48.1
cis-1,4-Dimethylcyclohexane	C_8H_{16}	−30.08	−42.22	−42.27	−45.4	−47.7	−49.5	−50.7	−51.4	−51.7	−51.6	−51.2	−50.6	−49.9	−49.1	−48.2
trans-1,4-Dimethylcyclohexane	C_8H_{16}	−31.99	−44.12	−44.17	−47.2	−49.6	−51.3	−52.3	−53.0	−53.2	−53.0	−52.6	−51.9	−51.2	−50.3	−49.3

[a] See footnotes a and b of table 22.

TABLE 14.—*Values of the free energy of formation, for the ideal gaseous state, to 1,500° K, for the normal alkylcyclopentanes*

Compound (gas)	Formula	Temperature in ° K														
		0	298.16	300	400	500	600	700	800	900	1,000	1,100	1,200	1,300	1,400	1,500
		Free energy of formation, $\Delta Ff°$, in kcal/mole														
Cyclopentane	C_5H_{10}	−10.68	+9.23	9.40	19.06	29.25	39.78	50.52	61.40	72.37	83.38	94.41	105.43	116.47	127.48	138.47
Methylcyclopentane	C_6H_{12}	−16.62	+8.55	8.76	20.59	33.00	45.78	58.79	71.93	85.17	98.46	111.77	125.08	138.41	151.68	164.87
Ethylcyclopentane	C_7H_{14}	−20.08	+10.59	10.84	25.05	39.90	55.17	70.66	86.29	102.06	117.86	133.68	149.50	165.29	181.11	196.83
n-Propylcyclopentane	C_8H_{16}	−23.85	+12.54	12.84	29.4	46.7	64.5	82.5	100.7	119.0	137.4	155.7	174.1	192.4	210.8	229.1
n-Butylcyclopentane	C_9H_{18}	−27.43	+14.69	15.02	34.0	53.8	74.0	94.6	115.3	136.1	157.0	177.9	198.8	219.7	240.6	261.5
n-Pentylcyclopentane	$C_{10}H_{20}$	−31.10	+16.73	17.11	38.5	60.7	83.4	106.5	129.7	153.2	176.6	200.0	223.5	246.9	270.4	293.8
n-Hexylcyclopentane	$C_{11}H_{22}$	−34.77	+18.78	19.20	43.0	67.6	92.9	118.5	144.2	170.2	196.2	222.2	248.2	274.2	300.2	326.2
n-Heptylcyclopentane	$C_{12}H_{24}$	−38.44	+20.83	21.29	47.4	74.6	102.3	130.4	158.7	187.2	215.8	244.3	272.8	301.4	329.9	358.5
n-Octylcyclopentane	$C_{13}H_{26}$	−42.12	+22.88	23.38	51.9	81.5	111.7	142.4	173.2	204.2	235.3	266.4	297.5	328.6	359.7	390.8
n-Nonylcyclopentane	$C_{14}H_{28}$	−45.79	+24.93	25.47	56.4	88.4	121.2	154.3	187.7	221.3	254.9	288.6	322.2	355.8	389.5	423.2
n-Decylcyclopentane	$C_{15}H_{30}$	−49.46	+26.97	27.56	60.9	95.4	130.6	166.3	202.2	238.3	274.5	310.7	346.8	383.0	419.2	455.5
n-Undecylcyclopentane	$C_{16}H_{32}$	−53.14	+29.02	29.65	65.4	102.3	140.0	178.2	216.6	255.3	294.1	332.8	371.5	410.2	449.0	487.8
n-Dodecylcyclopentane	$C_{17}H_{34}$	−56.81	+31.07	31.74	69.8	109.2	149.4	190.2	231.1	272.4	313.6	354.9	396.2	437.4	478.8	520.1
n-Tridecylcyclopentane	$C_{18}H_{36}$	−60.48	+33.12	33.83	74.3	116.1	158.9	202.1	245.6	289.4	333.2	377.0	420.8	464.7	508.5	552.5
n-Tetradecylcyclopentane	$C_{19}H_{38}$	−64.16	+35.17	35.92	78.8	123.1	168.3	214.1	260.1	306.4	352.8	399.2	445.5	491.9	538.3	584.8
n-Pentadecylcyclopentane	$C_{20}H_{40}$	−67.83	+37.21	38.01	83.3	130.0	177.7	226.0	274.6	323.4	372.4	421.3	470.2	519.1	568.0	617.1
n-Hexadecylcyclopentane	$C_{21}H_{42}$	−71.50	+39.26	40.10	87.8	136.9	187.2	238.0	289.1	340.5	392.0	443.4	494.8	546.3	597.8	649.5
Increment per CH_2 group	------	−3.673	+2.048	2.090	4.48	6.93	9.43	11.95	14.48	17.03	19.58	22.12	24.67	27.22	29.76	32.33

TABLE 15.—*Values of the free energy of formation, for the ideal gaseous state, to 1,500° K, for the normal alkylcyclohexanes*

Compound (gas)	Formula	Temperature in ° K														
		0	298.16	300	400	500	600	700	800	900	1,000	1,100	1,200	1,300	1,400	1,500
		Free energy of formation, $\Delta Ff°$, in kcal/mole														
Cyclohexane	C_6H_{12}	−20.01	+7.59	7.81	20.66	34.07	47.86	61.85	75.96	90.13	104.30	118.42	132.58	146.69	160.73	174.72
Methylcyclohexane	C_7H_{14}	−26.30	+6.52	6.79	21.84	37.51	53.55	69.80	86.16	102.59	119.03	135.43	151.83	168.13	184.43	200.65
Ethylcyclohexane	C_8H_{16}	−28.94	+9.38	9.69	27.12	45.19	63.72	82.50	101.37	120.28	139.23	158.17	177.11	195.93	214.71	233.36
n-Propylcyclohexane	C_9H_{18}	−32.79	+11.33	11.70	31.5	52.2	73.2	94.6	116.0	137.6	159.1	180.7	202.3	223.6	245.0	266.4
n-Butylcyclohexane	$C_{10}H_{20}$	−36.29	+13.55	13.97	36.2	59.3	82.8	106.7	130.7	154.8	178.8	203.0	227.1	251.0	275.0	298.9
n-Pentylcyclohexane	$C_{11}H_{22}$	−39.96	+15.60	16.06	40.7	66.2	92.3	118.7	145.2	171.8	198.4	225.1	251.8	278.2	304.8	331.2
n-Hexylcyclohexane	$C_{12}H_{24}$	−43.64	+17.65	18.15	45.2	73.2	101.7	130.6	159.6	188.8	218.0	247.2	276.5	305.4	334.5	363.5
n-Heptylcyclohexane	$C_{13}H_{26}$	−47.31	+19.69	20.24	49.6	80.1	111.1	142.6	174.1	205.8	237.6	269.4	301.1	332.6	364.3	395.9
n-Octylcyclohexane	$C_{14}H_{28}$	−50.98	+21.74	22.33	54.1	87.0	120.6	154.5	188.6	222.9	257.2	291.5	325.8	359.8	394.0	428.2
n-Nonylcyclohexane	$C_{15}H_{30}$	−54.66	+23.79	24.42	58.6	94.0	130.0	166.5	203.1	239.9	276.7	313.6	350.5	387.0	423.8	460.5
n-Decylcyclohexane	$C_{16}H_{32}$	−58.33	+25.84	26.51	63.1	100.9	139.4	178.4	217.6	256.9	296.3	335.7	375.1	414.3	453.6	492.9
n-Undecylcyclohexane	$C_{17}H_{34}$	−62.00	+27.89	28.60	67.6	107.8	148.8	190.4	232.1	274.0	315.9	357.9	399.8	441.5	483.3	525.2
n-Dodecylcyclohexane	$C_{18}H_{36}$	−65.67	+29.93	30.69	72.0	114.8	158.3	202.3	246.6	291.0	335.5	380.0	424.5	468.7	513.1	557.5
n-Tridecylcyclohexane	$C_{19}H_{38}$	−69.35	+31.98	32.78	76.5	121.7	167.7	214.3	261.0	308.0	355.0	402.1	449.1	495.9	542.9	589.9
n-Tetradecylcyclohexane	$C_{20}H_{40}$	−73.02	+34.03	34.87	81.0	128.6	177.1	226.2	275.5	325.0	374.6	424.2	473.8	523.1	572.6	622.2
n-Pentadecylcyclohexane	$C_{21}H_{42}$	−76.69	+36.08	36.96	85.5	135.5	186.6	238.2	290.0	342.1	394.2	446.4	498.5	550.3	602.4	654.5
n-Hexadecylcyclohexane	$C_{22}H_{44}$	−80.37	+38.13	39.05	90.0	142.5	196.0	250.1	304.5	359.1	413.8	468.5	523.1	577.6	632.2	686.8
Increment per CH_2 group		−3.673	+2.048	2.090	4.48	6.93	9.43	11.95	14.48	17.03	19.58	22.12	24.67	27.22	29.76	32.33

TABLE 16.—*Values of the free energy of formation, for the ideal gaseous state, to 1,500° K, for the seven dimethylcyclohexanes*

Compound (gas)	Formula	Temperature in ° K														
		0	298.16	300	400	500	600	700	800	900	1,000	1,100	1,200	1,300	1,400	1,500
		Free energy of formation, $\Delta Ff°$, in kcal/mole														
1,1-Dimethylcyclohexane	C_8H_{16}	−30.93	+8.42	8.74	26.6	45.2	64.1	83.4	102.7	122.1	141.4	160.8	180.2	199.5	218.4	237.1
cis-1,2-Dimethylcyclohexane	C_8H_{16}	−28.95	+9.85	10.17	27.8	46.1	64.8	83.8	102.9	122.1	141.2	160.4	179.5	198.6	217.4	236.0
trans-1,2-Dimethylcyclohexane	C_8H_{16}	−30.91	+8.24	8.55	26.2	44.6	63.4	82.4	101.5	120.6	139.9	159.1	178.1	197.3	216.1	234.9
cis-1,3-Dimethylcyclohexane [a]	C_8H_{16}	−32.02	+7.13	7.44	25.2	43.6	62.4	81.4	100.6	119.8	139.0	158.3	177.5	196.6	215.6	234.5
trans-1,3-Dimethylcyclohexane [a]	C_8H_{16}	−30.06	+8.68	8.99	26.6	44.8	63.6	82.5	101.5	120.6	139.8	158.9	178.0	197.2	216.0	234.7
cis-1,4-Dimethylcyclohexane	C_8H_{16}	−30.08	+9.07	9.38	27.1	45.5	64.3	83.4	102.6	121.8	141.2	160.4	179.7	190.0	217.8	236.5
trans-1,4-Dimethycyclohexane	C_8H_{16}	−31.99	+7.58	7.89	25.8	44.3	63.2	82.4	101.6	121.0	140.3	159.6	179.0	198.2	217.2	235.9

[a] See footnotes *a* and *b* of table 22.

TABLE 17.—*Values of the logarithm of the equilibrium constant of formation, for the ideal gaseous state, to 1,500° K, for the normal alkylcyclopentanes*

Compound (gas)	Formula	Temperature in ° K													
		0	298.16	300	400	500	600	700	800	900	1,000	1,100	1,200	1,300	1,400	1,500
		Logarithm of equilibrium constant of formation, $\log_{10} Kf$														
Cyclopentane	C_5H_{10}	Infinite	−6.7643	−6.8490	−10.4144	−12.7851	−14.4897	−15.7722	−16.7736	−17.5731	−18.2228	−18.7571	−19.2005	−19.5796	−19.9002	−20.1753
Methylcyclopentane	C_6H_{12}	do	−6.2649	−6.3801	−11.2501	−14.4250	−16.6770	−18.3549	−19.6492	−20.6813	−21.5189	−22.2067	−22.7795	−23.2694	−23.6775	−24.0218
Ethylcyclopentane	C_7H_{14}	do	−7.7632	−7.8999	−13.6861	−17.4379	−20.0959	−22.0620	−23.5741	−24.7831	−25.7585	−26.5600	−27.2278	−27.7871	−28.2725	−28.6778
n-Propylcyclopentane	C_8H_{16}	do	−9.195	−9.351	−16.082	−20.429	−23.495	−25.763	−27.504	−28.896	−30.016	−30.936	−31.703	−32.347	−32.904	−33.375
n-Butylcyclopentane	C_9H_{18}	do	−10.768	−10.942	−18.582	−23.498	−26.965	−29.523	−31.487	−33.054	−34.316	−35.351	−36.213	−36.938	−37.565	−38.099
n-Pentylcyclopentane	$C_{10}H_{26}$	do	−12.269	−12.465	−21.029	−26.528	−30.399	−33.254	−35.444	−37.189	−38.595	−39.746	−40.706	−41.513	−42.212	−42.809
n-Hexylcyclopentane	$C_{11}H_{22}$	do	−13.770	−13.987	−23.476	−29.557	−33.833	−36.985	−39.401	−41.325	−42.874	−44.140	−45.199	−46.088	−46.858	−47.520
n-Heptylcyclopentane	$C_{12}H_{24}$	do	−15.271	−15.510	−25.924	−32.587	−37.268	−40.716	−43.358	−45.460	−47.153	−48.534	−49.691	−50.664	−51.504	−52.231
n-Octylcyclopentane	$C_{13}H_{26}$	do	−16.772	−17.032	−28.371	−35.616	−40.702	−44.448	−47.314	−49.595	−51.432	−52.929	−54.184	−55.239	−56.150	−56.941
n-Nonylcyclopentane	$C_{14}H_{28}$	do	−18.274	−18.555	−30.818	−38.646	−44.136	−48.179	−51.271	−53.730	−55.711	−57.323	−58.676	−59.814	−60.797	−61.652
n-Decylcyclopentane	$C_{15}H_{30}$	do	−19.775	−20.078	−33.265	−41.675	−47.570	−51.910	−55.228	−57.865	−59.990	−61.718	−63.169	−64.389	−65.443	−66.362
n-Undecylcyclopentane	$C_{16}H_{32}$	do	−21.276	−21.600	−35.712	−44.705	−51.004	−55.641	−59.185	−62.001	−64.269	−66.112	−67.662	−68.964	−70.089	−71.073
n-Dodecylcyclopentane	$C_{17}H_{34}$	do	−22.777	−23.123	−38.160	−47.734	−54.438	−59.372	−63.142	−66.136	−68.548	−70.506	−72.154	−73.540	−74.736	−75.784
n-Tridecylcyclopentane	$C_{18}H_{36}$	do	−24.278	−24.645	−40.607	−50.764	−57.872	−63.104	−67.098	−70.271	−72.827	−74.901	−76.647	−78.115	−79.382	−80.494
n-Tetradecylcyclopentane	$C_{19}H_{38}$	do	−25.780	−26.168	−43.054	−53.793	−61.306	−66.835	−71.055	−74.406	−77.106	−79.295	−81.139	−82.690	−84.028	−85.205
n-Pentadecylcyclopentane	$C_{20}H_{40}$	do	−27.281	−27.691	−45.501	−56.823	−64.740	−70.566	−75.012	−78.541	−81.385	−83.690	−85.632	−87.265	−88.675	−89.915
n-Hexadecylcyclopentane	$C_{21}H_{42}$	do	−28.782	−29.213	−47.948	−59.852	−68.174	−74.297	−78.969	−82.677	−85.664	−88.084	−90.125	−91.840	−93.321	−94.626
Increment per CH_2 group		do	−1.5012	−1.5226	−2.4472	−3.0295	−3.4341	−3.7312	−3.9568	−4.1352	−4.2790	−4.3944	−4.4926	−4.5752	−4.6463	−4.7106

TABLE 18.—*Values of the logarithm of the equilibrium constant of formation, for the ideal gaseous state, to 1,500° K, for the normal alkylcyclohexanes*

Compound (gas)	Formula	Temperature in ° K														
		0	298.16	300	400	500	600	700	800	900	1,000	1,100	1,200	1,300	1,400	1,500
		Logarithm of equilibrium constant of formation, $\log_{10} Kf$														
Cyclohexane	C_6H_{12}	Infinite	−5.5605	−5.6931	−11.2861	−14.8932	−17.4318	−19.3103	−20.7501	−21.8852	−22.7943	−23.5277	−24.1458	−24.6613	−25.0905	−25.4571
Methylcyclohexane	C_7H_{14}	do	−4.7819	−4.9487	−11.9344	−16.3959	−19.5065	−21.7937	−23.5374	−24.9110	−26.0133	−26.9077	−27.6521	−28.2657	−28.7908	−29.2345
Ethylcyclohexane	C_8H_{16}	do	−6.8744	−7.0592	−14.8200	−19.7522	−23.2097	−25.7561	−27.6926	−29.2075	−30.4279	−31.4243	−32.2567	−32.9394	−33.5168	−33.9999
n-Propylcyclohexane	C_9H_{18}	do	−8.304	−8.522	−17.232	−22.814	−26.679	−29.534	−31.696	−33.402	−34.770	−35.900	−36.841	−37.587	−38.253	−38.810
n-Butylcyclohexane	$C_{10}H_{20}$	do	−9.935	−10.174	−19.776	−25.918	−30.176	−33.318	−35.700	−37.579	−39.086	−40.330	−41.365	−42.192	−42.928	−43.546
n-Pentylcyclohexane	$C_{11}H_{22}$	do	−11.436	−11.697	−22.223	−28.948	−33.610	−37.050	−39.657	−41.715	−43.365	−44.724	−45.857	−46.767	−47.574	−48.257
n-Hexylcyclohexane	$C_{12}H_{24}$	do	−12.937	−13.219	−24.670	−31.978	−37.044	−40.781	−43.613	−45.850	−47.644	−49.119	−50.350	−51.342	−52.220	−52.967
n-Heptylcyclohexane	$C_{13}H_{26}$	do	−14.438	−14.742	−27.118	−35.007	−40.478	−44.512	−47.570	−49.985	−51.923	−53.513	−54.842	−55.917	−56.866	−57.678
n-Octylcyclohexane	$C_{14}H_{28}$	do	−15.940	−16.264	−29.565	−38.036	−43.912	−48.243	−51.527	−54.120	−56.202	−57.908	−59.335	−60.492	−61.513	−62.388
n-Nonylcyclohexane	$C_{15}H_{30}$	do	−17.441	−17.787	−32.012	−41.066	−47.346	−51.974	−55.484	−58.255	−60.481	−62.302	−63.828	−65.068	−66.159	−67.099
n-Decylcyclohexane	$C_{16}H_{32}$	do	−18.942	−19.310	−34.459	−44.096	−50.780	−55.706	−59.441	−62.391	−64.760	−66.696	−68.320	−69.643	−70.805	−71.810
n-Undecylcyclohexane	$C_{17}H_{34}$	do	−20.443	−20.852	−36.906	−47.125	−54.214	−59.437	−63.397	−66.526	−69.039	−71.091	−72.813	−74.218	−75.452	−76.520
n-Dodecylcyclohexane	$C_{18}H_{36}$	do	−21.944	−22.355	−39.354	−50.154	−57.648	−63.168	−67.354	−70.661	−73.318	−75.485	−77.305	−78.793	−80.098	−81.231
n-Tridecylcyclohexane	$C_{19}H_{38}$	do	−23.446	−23.878	−41.801	−53.184	−61.083	−66.899	−71.311	−74.796	−77.597	−79.880	−81.798	−83.368	−84.744	−85.941
n-Tetradecylcyclohexane	$C_{20}H_{40}$	do	−24.947	−25.400	−44.248	−56.214	−64.517	−70.630	−75.268	−78.931	−81.876	−84.274	−86.291	−87.944	−89.390	−90.652
n-Pentadecylcyclohexane	$C_{21}H_{42}$	do	−26.448	−26.923	−46.695	−59.243	−67.951	−74.362	−79.225	−83.067	−86.155	−88.668	−90.783	−92.519	−94.037	−95.363
n-Hexadecylcyclohexane	$C_{22}H_{44}$	do	−27.949	−28.445	−49.142	−62.272	−71.385	−78.093	−83.181	−87.202	−90.434	−93.063	−95.276	−97.094	−98.683	−100.073
Increment per CH_2 group	.....	do	−1.5012	−1.5226	−2.4472	−3.0295	−3.4341	−3.7312	−3.9568	−4.1352	−4.2790	−4.3944	−4.4926	−4.5752	−4.6463	−4.7106

TABLE 19.—*Values of the logarithm of the equilibrium constant of formation, for the ideal gaseous state, to 1,500° K, for the 7 dimethylcyclohexanes*

Compound (gas)	Formula	Temperature in ° K														
		0	298.16	300	400	500	600	700	800	900	1,000	1,100	1,200	1,300	1,400	1,500
		Logarithm of equilibrium constant of formation, $\log^{10} Kf$														
1,1-Dimethylcyclohexane	C_8H_{16}	Infinite	−6.174	−6.363	−14.541	−19.735	−23.359	−26.031	−28.045	−29.642	−30.911	−31.947	−32.813	−33.544	−34.146	−34.628
cis-1,2-Dimethylcyclohexane	C_8H_{16}	do	−7.225	−7.408	−15.186	−20.163	−23.622	−26.168	−28.105	−29.642	−30.863	−31.859	−32.692	−33.396	−33.974	−34.435
trans-1,2-Dimethylcyclohexane	C_8H_{16}	do	−6.038	−6.227	−14.334	−19.503	−23.083	−25.731	−27.723	−29.298	−30.566	−31.601	−32.445	−33.176	−33.755	−34.259
cis-1,3-Dimethylcyclohexane [a]	C_8H_{16}	do	−5.228	−5.423	−13.749	−19.040	−22.722	−25.428	−27.485	−29.094	−30.389	−31.446	−32.330	−33.055	−33.670	−34.185
trans-1,3-Dimethylcyclohexane [a]	C_8H_{16}	do	−6.363	−6.549	−14.510	−19.590	−23.152	−25.756	−27.737	−29.286	−30.555	−31.573	−32.425	−33.144	−33.736	−34.230
cis-1,4-Dimethylcyclohexane	C_8H_{16}	do	−6.650	−6.836	−14.831	−19.887	−23.429	−26.034	−27.994	−29.586	−30.856	−31.875	−32.727	−33.447	−34.038	−34.533
trans-1,4-Dimethylcyclohexane	C_8H_{16}	do	−5.552	−5.746	−14.071	−19.359	−23.039	−25.722	−27.756	−29.384	−30.657	−31.714	−32.597	−33.322	−33.937	−34.430

[a] See footnotes a and b of table 22.

Figures 1 and 2 show the thermodynamic stability of the normal alkylcyclopentanes and alkylcyclohexanes in the gaseous state as a function of the temperature, in the form of a plot of the standard free energy of formation, per carbon atom, divided by the absolute temperature $(\Delta Ff°/n)/T$.

V. Free Energies and Equilibria of Some Reactions of Isomerization, Cyclization, and Hydrogenation Involving Alkylcyclopentanes and Alkylcyclohexanes

In figures 3 and 4 are plotted, as a function of temperature, values of the logarithm of the equilibrium constant for the reaction of cyclization of a given normal paraffin to a normal alkylcyclopentane or a normal alkylcyclohexane.

In figure 5 are plotted, as a function of temperature, values of the logarithm of the equilibrium constant for the reaction of isomerization of a given normal alkylcyclohexane to a normal alkylcyclopentane.

Values of the logarithm of the equilibrium constant for the reactions of hydrogenation of the normal alkylbenzenes [17] to normal alkylcyclopentanes and alkylcyclohexanes, as a function of temperatures, are plotted in figures 6 and 7.

Figures 8 and 9 show the logarithms of the equilibrium constants of the reactions of cyclization of normal l-alkenes [18] to normal alkylcyclopentanes and alkylcyclohexanes, as a function of the temperature.

In figure 10 are plotted, as a function of the temperature, the values of $\Delta F°/T$ for the isomerization of ethylcyclohexane into each of the seven dimethylcyclohexanes. The corresponding numerical values are given in table 20.

In figure 11 are plotted, as a function of the temperature, for the C_8H_{16} alkylcyclohexanes, the amounts, in mole fraction, of each of the isomers present at equilibrium with its other isomers in the gas phase. The corresponding numerical values are given in table 21.

TABLE 20.—*Free energies and equilibrium constants for the isomerization of ethylcyclohexane to the isomeric dimethylcyclohexanes in the ideal gaseous state to 1,500° K*

Temperature	Ethylcyclohexane=1,1-dimethylcyclohexane		Ethylcyclohexane=*cis*-1,2-dimethylcyclohexane		Ethylcyclohexane=*trans*-1,2-dimethylcyclohexane	
°K	$\Delta F°/T$	K	$\Delta F°/T$	K	$\Delta F°/T$	K
200	6.65	28.4	−1.55	0.46	7.05	34.8
298.16	3.20	5.01	−1.61	.446	3.83	6.85
300	3.18	4.97	−1.60	.446	3.81	6.79
400	1.28	1.90	−1.68	.431	2.23	3.06
500	0.08	1.04	−1.88	.388	1.14	1.77
600	−.68	0.710	−1.88	.388	0.58	1.34
700	−1.26	.531	−1.89	.388	.11	1.06
800	−1.61	.445	−1.89	.388	−.14	0.933
900	−1.99	.367	−1.99	.367	−.41	.813
1,000	−2.21	.329	−1.99	.367	−.63	.728
1,100	−2.39	.300	−1.99	.367	−.81	.665
1,200	−2.54	.278	−1.99	.367	−.86	.649
1,300	−2.77	.248	−2.09	.349	−1.09	.579
1,400	−2.88	.235	−2.09	.349	−1.09	.579
1,500	−2.87	.236	−1.99	.307	−1.19	.551

	Ethylcyclohexane=*cis*-1,3-dimethylcyclohexane [a]		Ethylcyclohexane=*trans*-1,3-dimethylcyclohexane [a]		Ethylcyclohexane=*cis*-1,4-dimethylcyclohexane		Ethylcyclohexane=*trans*-1,4-dimethylcyclohexane	
	$\Delta F°/T$	K	$\Delta F°/T$	K	$\Delta F°/T$	K	$\Delta F°/T$	K
200	12.60	568.	4.2	8.28	2.9	4.31	11.15	274.
298.16	7.53	44.3	2.34	3.24	1.02	1.68	6.05	21.0
300	7.49	43.2	2.33	3.24	1.02	1.67	6.01	20.6
400	4.90	11.8	1.40	2.04	−0.05	0.975	3.43	5.61
500	3.26	5.15	0.74	1.45	−.62	.733	1.80	2.47
600	2.23	3.08	.27	1.14	−1.00	.604	0.78	1.48
700	1.50	2.13	.00	1.00	−1.27	.527	.16	1.08
800	0.95	1.61	−.20	0.904	−1.47	.500	−.29	0.865
900	.52	1.30	−.36	.836	−1.73	.418	−.81	.665
1,000	.18	1.09	−.58	.747	−1.96	.373	−1.05	.590
1,100	−.10	0.951	−.68	.710	−2.06	.354	−1.33	.513
1,200	−.33	.845	−.77	.679	−2.15	.339	−1.56	.457
1,300	−.53	.766	−.94	.624	−2.32	.310	−1.75	.414
1,400	−.70	.703	−1.00	.604	−2.39	.301	−1.92	.380
1,500	−.85	.653	−1.05	.589	−2.44	.293	−1.97	.372

[a] See footnotes a and b of table 22.

TABLE 21.—*Equilibrium concentrations of the C_8H_{16} alkylcyclohexanes in the ideal gaseous state to 1,500°K.*

Temperature	Composition, in mole fraction, of equilibrium mixture of isomers							
	Ethylcyclohexane	Dimethylcyclohexanes [a]						
		1,1	*cis*-1,2	*trans*-1,2	*cis*-1,3	*trans*-1,3	*cis*-1,4	*trans*-1,4
°K								
200	0.0011	0.0309	0.0005	0.0379	0.6179	0.0090	0.0047	0.2981
298.16	.0120	.0600	.0053	.0820	.5304	.0388	.0201	.2514
300	.0122	.0607	.0055	.0829	.5273	.0396	.0204	.2515
400	.0373	.0709	.0161	.1141	.4400	.0761	.0364	.2092
500	.0719	.0743	.0277	.1264	.3678	.1036	.0524	.1764
600	.1027	.0729	.0397	.1376	.3162	.1170	.0620	.1519
700	.1296	.0688	.0502	.1374	.2761	.1296	.0683	.1400
800	.1505	.0670	.0582	.1404	.2423	.1361	.0753	.1302
900	.1734	.0636	.0636	.1410	.2255	.1450	.0725	.1153
1,000	.1914	.0630	.0703	.1394	.2087	.1430	.0714	.1129
1,100	.2058	.0617	.0755	.1368	.1957	.1461	.0728	.1056
1,200	.2167	.0603	.0795	.1407	.1831	.1472	.0735	.0990
1,300	.2331	.0578	.0814	.1350	.1786	.1455	.0723	.0965
1,400	.2410	.0566	.0841	.1393	.1694	.1455	.0725	.0916
1,500	.2462	.0581	.0904	.1357	.1608	.1450	.0721	.0916

[a] See footnotes a and b of table 22.

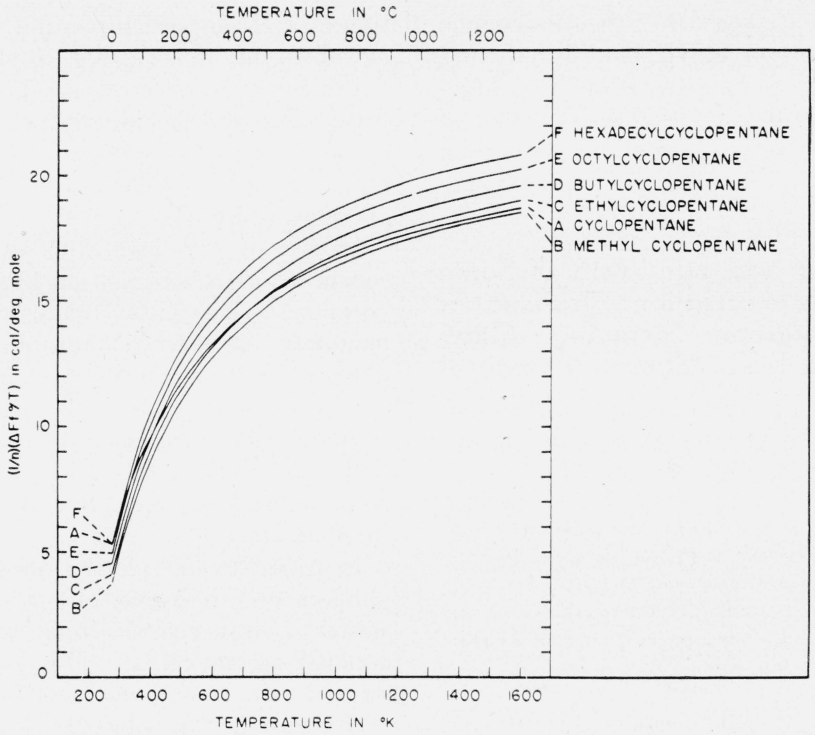

FIGURE 1.—*Thermodynamic stability of the n-alkylcyclopentanes in gaseous state as of a function of the temperature.*

The scale of ordinates gives the value of $(1/n)$ $(\Delta Ff°/T)$ in calories per degree mole, where n is the number of carbon atoms per molecule, T is the absolute temperature in degrees Kelvin, and $\Delta Ff°$ is the standard free energy of formation of the hydrocarbon from the elements, solid carbon (graphite) and gaseous hydrogen, all at the given temperature. The scale of abscissas gives the temperature in degrees Kelvin.

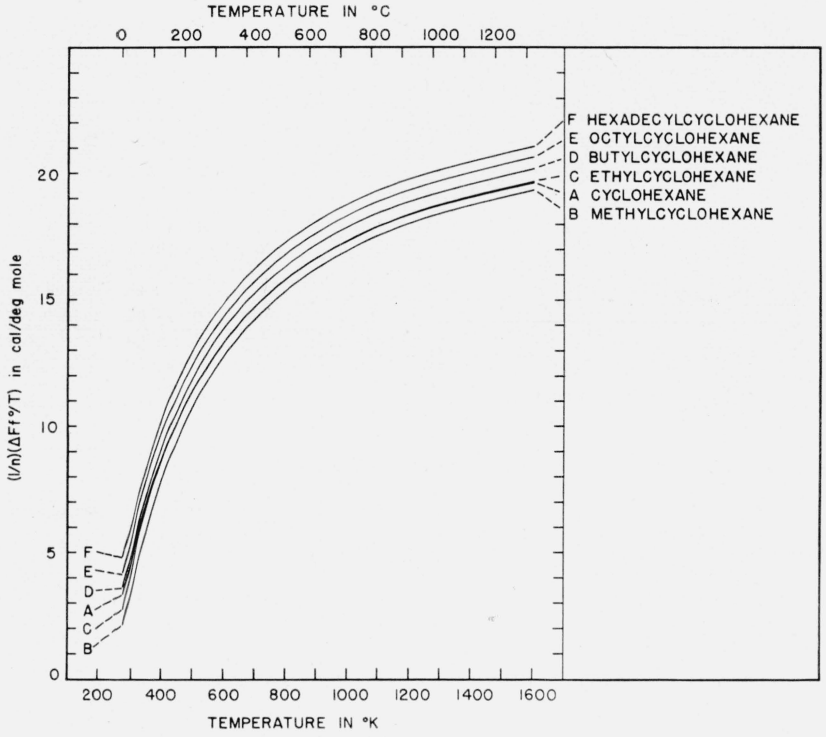

FIGURE 2.—*Thermodynamic stability of the n-alkylcyclohexanes in the gaseous state as a function of the temperature.*

The scale of ordinates gives the value of $(1/n)$ $(\Delta Ff°/T)$ in calories per degree mole, where n is the number of carbon atoms per molecule, T is the absolute temperature in degrees Kelvin, and $\Delta Ff°$ is the standard free energy of formation of the hydrocarbon from the elements, solid carbon (graphite) and gaseous hydrogen, all at the given temperature. The scale of abscissas gives the temperature in degrees Kelvin.

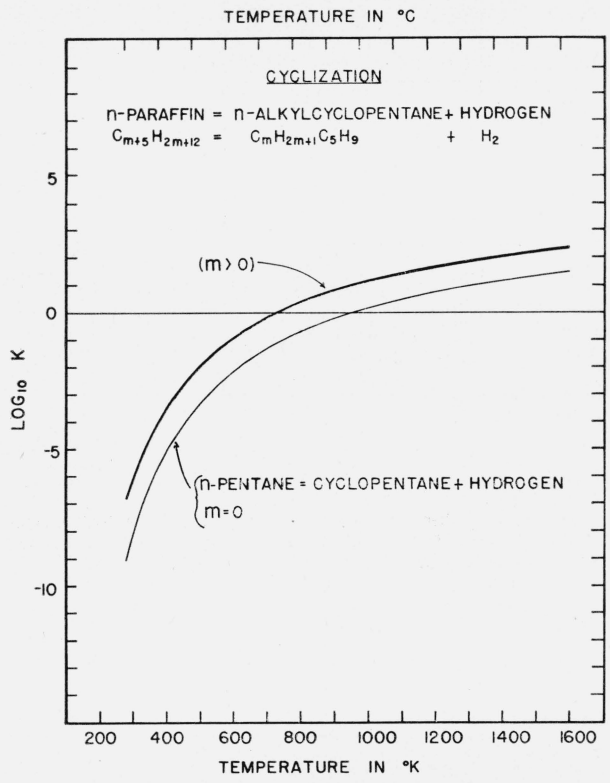

FIGURE 3.—*Logarithm of the equilibrium constant for the reaction of cyclization of n-paraffins to n-alkylcyclopentanes.*

The scale of ordinates gives the value of the logarithm (to the base 10) of the equilibrium constant for the reaction of cyclization of a given *n*-paraffin to the corresponding *n*-alkylcyclopentane, in the gaseous state. The scale of abscissas gives the temperature in degrees Kelvin. The values calculated for methylcyclopentane, ethylcyclopentane, and the higher *n*-alkylcyclopentanes all fall within the width of the heavy line indicated.

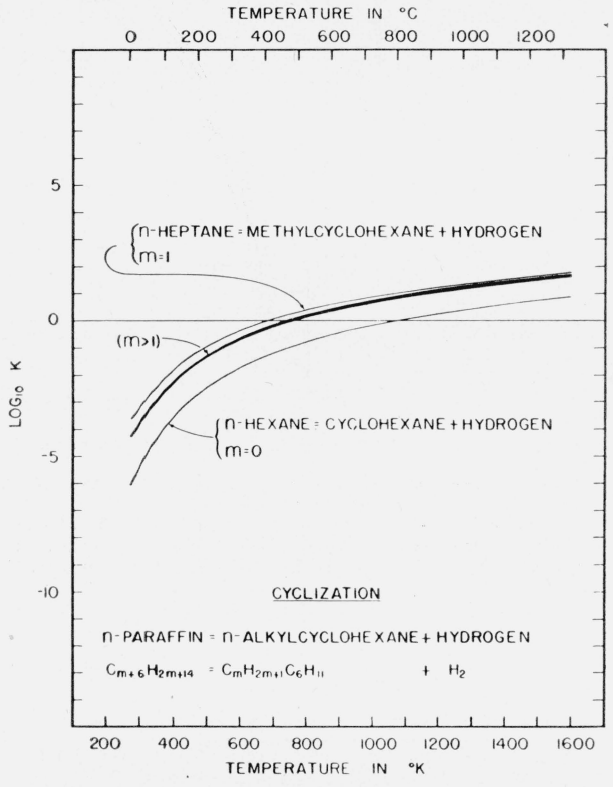

FIGURE 4.—*Logarithm of the equilibrium constant for the reaction of cyclization of n-paraffins to n-alkylcyclohexanes.*

The scale of ordinates gives the value of the logarithm (to the base 10) of the equilibrium constant for the reaction of cyclization of a given *n*-paraffin to the corresponding *n*-alkylcyclohexane, in the gaseous state. The scale of abscissas gives the temperature in degrees Kelvin. The values calculated for ethylcyclohexane, *n*-propylcyclohexane, and the higher *n*-alkylcyclohexanes all fall within the width of the heavy line indicated.

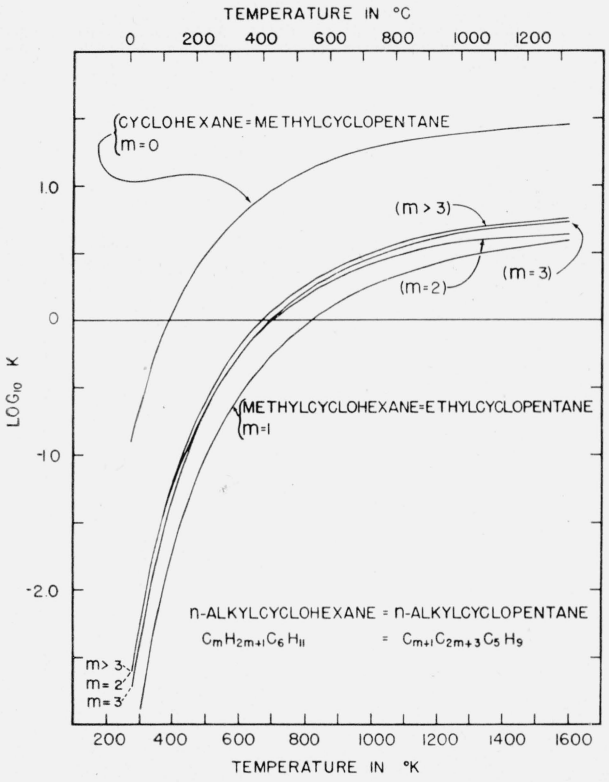

FIGURE 5.—*Logarithm of the equilibrium constant for the reaction of conversion of n-alkylcyclohexanes to n-alkylcyclopentanes.*

The scale of ordinates gives the value of the logarithm (to the base 10) of the equilibrium constant for the reaction of conversion of a given *n*-alkylcyclohexane to the corresponding *n*-alkylcyclopentane, in the gaseous state. The scale of abscissas gives the temperature in degrees Kelvin.

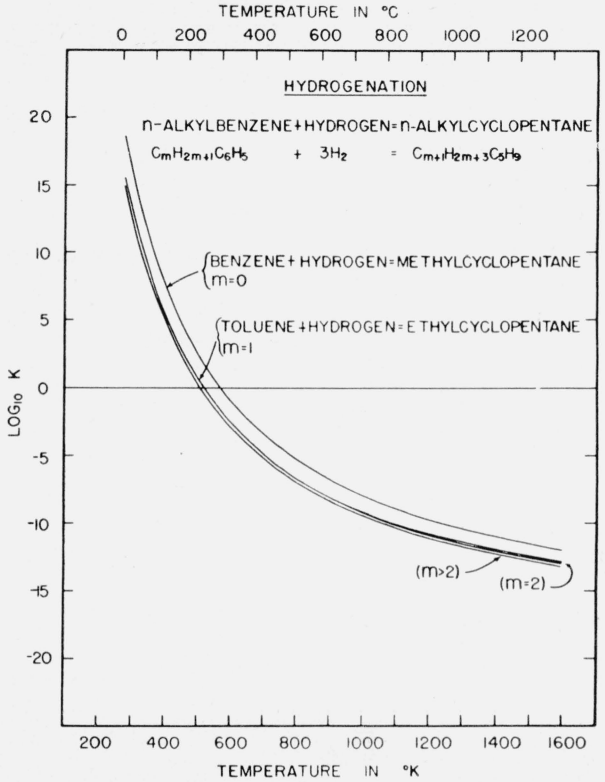

FIGURE 6.—*Logarithm of the equilibrium constant for the reaction of hydrogenation of n-alkylbenzenes to n-alkylcyclopentanes.*

The scale of ordinates gives the value of the logarithm (to the base 10) of the equilibrium constant for the reaction of hydrogenation of a given *n*-alkylbenzene to the corresponding *n*-alkylcyclopentane, in the gaseous state The scale of abscissas gives the temperature in degrees Kelvin.

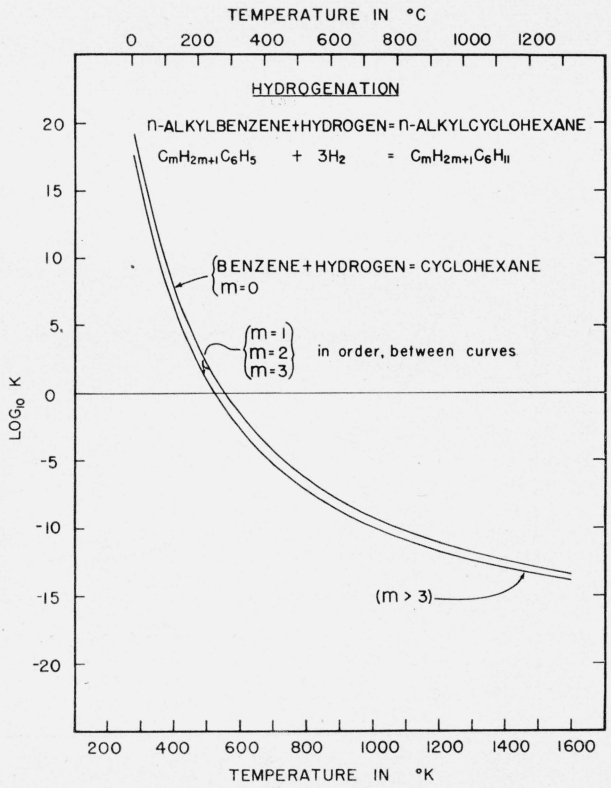

FIGURE 7.—*Logarithm of the equilibrium constant for the reaction of hydrogenation of n-alkylbenzenes to n-alkylcyclohexanes.*

The scale of ordinates gives the value of the logarithm (to the base 10) of the equilibrium constant for the reaction of hydrogenation of a given *n*-alkylbenzene to the corresponding *n*-alkylcyclohexane, in the gaseous state. The scale of abscissas gives the temperature in degrees Kelvin. The upper curve is that for the hydrogenation of benzene and the lower curve is for the hydrogenation of butylbenzene, *n*-pentylbenzene and the higher *n*-alkylbenzenes. The curves for toluene, ethylbenzene, and *n*-propylbenzene lie, in order, between the two curves.

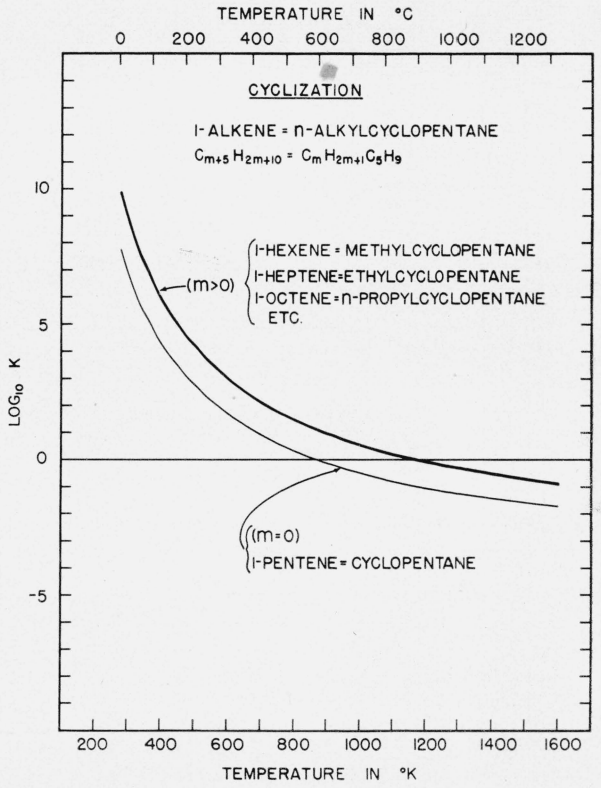

FIGURE 8.—*Logarithm of the equilibrium constant for the reaction of cyclization of 1-olefins to n-alkylcyclopentanes.*

The scale of ordinates gives the value of the logarithm (to the base 10) of the equilibrium constant for the reaction of cyclization of a given 1-olefin to the corresponding *n*-alkylcyclopentane, in the gaseous state. The scale of abscissas gives the temperature in degrees Kelvin. The values for the formation of methylcyclopentane, ethylcyclopentane, and higher *n*-alkylcyclopentanes all fall within the width of the heavy line indicated.

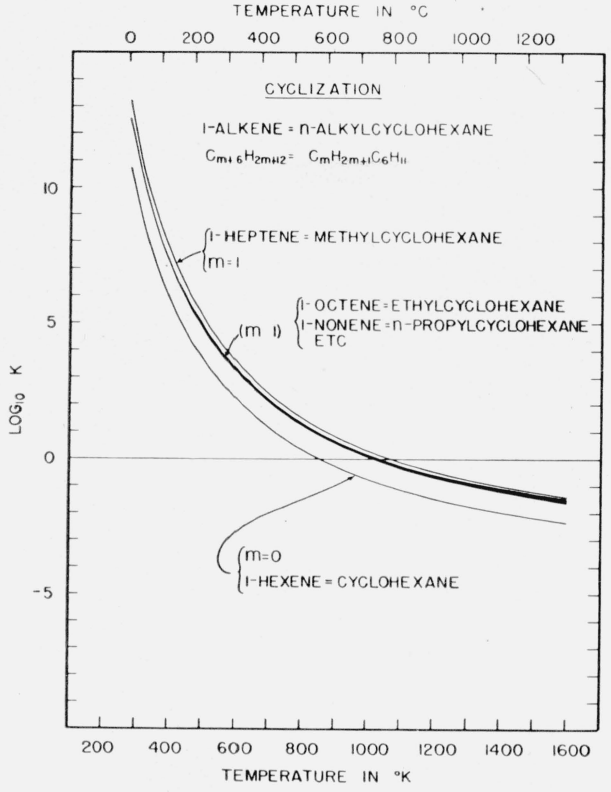

FIGURE 9.—*Logarithms of the equilibrium constant for the reaction of cyclization of 1-olefins to n-alkylcyclohexanes.*

The scale of ordinates gives the value of the logarithm (to the base 10) of the equilibrium constant for the reaction of cyclization of a given 1-olefin to the corresponding *n*-alkylcyclohexane, in the gaseous state. The scale of abscissas gives the temperature in degrees Kelvin. The values calculated for ethylcyclohexane, propylcyclohexane and the higher *n*-alkylcyclohexanes all fall within the width of the heavy line indicated.

Figure 12 shows, for the equilibrium between cyclohexane and methylcyclopentane, a comparison of the values derived from this report with values reported experimentally by Schuit, Hoog, and Verheus [9], Glasebrook and Lovell [10], Shell Development Co. [11], and Mizusima, Morino, and Fujisiro [12].

Table 22 gives, for the relative amounts of the *cis* and *trans* isomers of 1,2-dimethylcyclohexane, 1,3-dimethylcyclohexane, and 1,4-dimethylcyclohexane, a comparison of the values derived from this report with experimental values reported by Boord, Greenlee, et al. [15].

TABLE 22.—*Comparison of the calculated and experimental values for the relative amounts at equilibrium of some pairs of isomeric (cis and trans) dimethylcyclohexanes*

Compounds	Temperature	Relative amounts at equilibrium	
		Calculated (liquid)	Experimental [c] (liquid)
	°C		
cis-1,2-Dimethylcyclohexane	250	21	35
trans-1,2-Dimethylcyclohexane		79	65
cis-1,3-Dimethylcyclohexane [a]	225	77	78
trans-1,3-Dimethylcyclohexane [b]		23	22
cis-1,4-Dimethylcyclohexane	200	22	37
trans-1,4-Dimethylcyclohexane		78	63

[a] This isomer, formerly labeled "*trans*", has the following properties [16]: Boiling point at 1 atm, 120.09° C; refractive index, n_D at 25° C, 1.4206; density at 25° C, 07620 g/ml.

[b] This isomer, formerly labeled "*cis*", has the following properties [16]: Boiling point at 1 atm, 124.45° C; refractive index, n_D at 25° C, 1.4284; density, at 25° C, 0.7806 g/ml.

[c] From reference [15].

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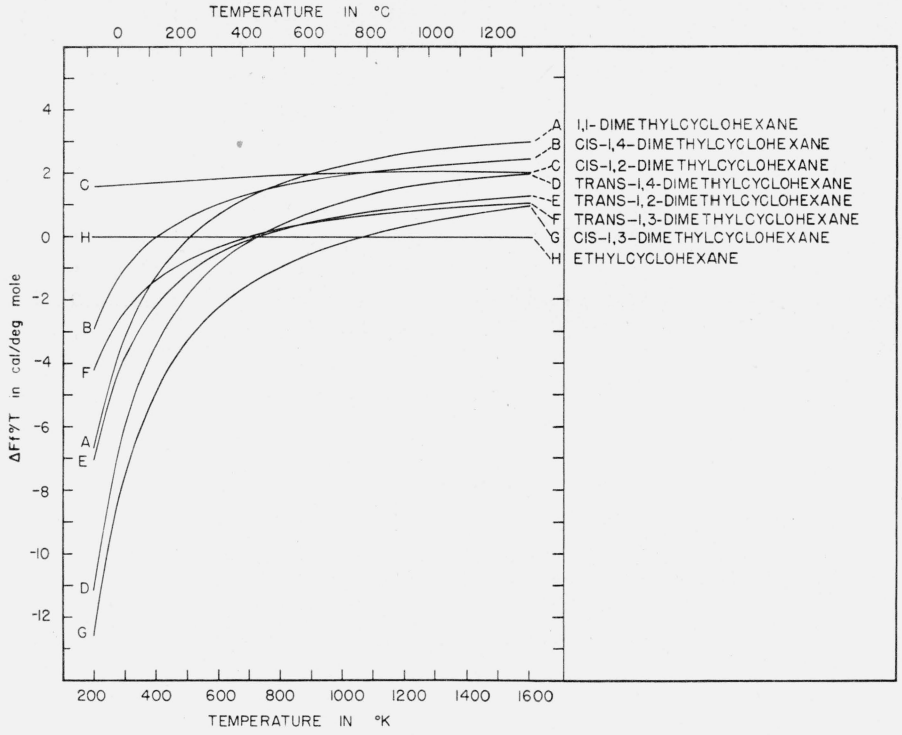

FIGURE 10.—*Free energy of isomerization of the eight* C_8H_{16} *alkylcyclohexanes.*

The scale of ordinates gives the value of $\Delta F^\circ/T$, in calories per degree mole, for the isomerization of ethylcyclohexane into the other isomers, in the gaseous state, as indicated. The scale of abscissas gives the temperature in degrees Kelvin. See reference [16] for identification of the dimethylcyclohexanes.

VI. References

[1] J. E. Kilpatrick, K. S. Pitzer, and R. Spitzer, J. Am. Chem. Soc. **69**, 2488 (1947)

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[13] American Petroleum Institute Research Project 44 at the National Bureau of Standards. Selected Values of Properties of Hydrocarbons. Table $_\alpha$. Values of constants.

[14] American Petroleum Institute Research Project 44 at the National Bureau of Standards. Selected Values of Properties of Hydrocarbons. Tables 1, 2, 5, 20, and 24, r, s, and v. Heat-content function, Free-energy function, and Heat capacity.

[15] C. E. Boord, K. W. Greenlee, et al., American Petroleum Institute Research Project 45. Ohio State University. Unpublished data.

[16] American Petroleum Institute Research Project 44 at the National Bureau of Standards. Selected Values of Properties of Hydrocarbons. Table 7a. Boiling point, refractive index, density, and freezing point.

[17] W. J. Taylor, D. D. Wagman, M. G. Williams, K. S. Pitzer, and F. D. Rossini, J. Research NBS **37,** 95 (1946) RP1732.

[18] J. E. Kilpatrick, E. J. Prosen, K. S. Pitzer, and F. D. Rossini, J. Research NBS **36,** 559 (1946) RP1722.

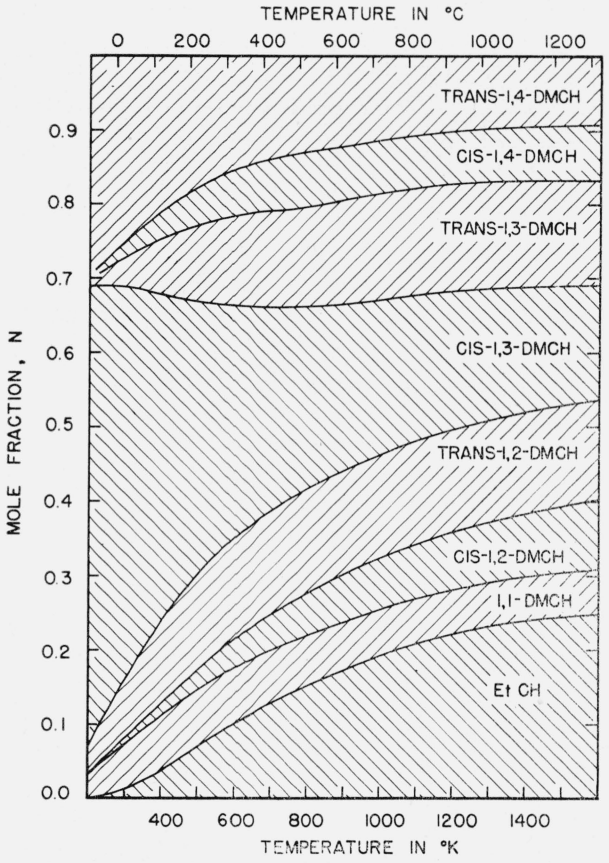

FIGURE 11.—*Equilibrium concentrations of the eight* C_8H_{16} *alkylcyclohexanes.*

The scale of ordinates measures the amount in mole fraction, and the scale of abscissas gives the temperature in degrees Kelvin and degrees centigrade. The vertical width of a band at a given temperature measures the mole fraction of the given isomer present when at equilibrium with all of its other isomers, in the gas phase. See reference [16] for identification of the dimethylcyclohexanes.

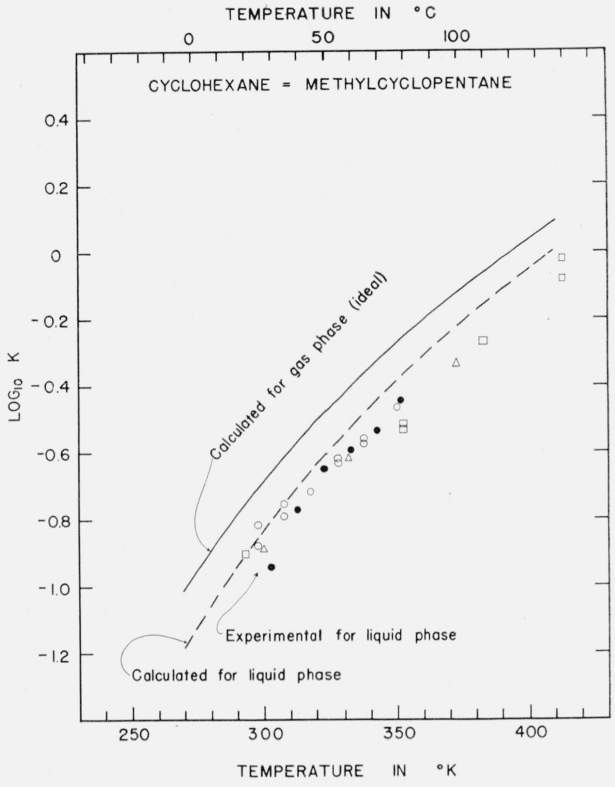

FIGURE 12.—*Comparison of calculated and experimental data on the equilibrium between cyclohexane and methylcyclopentane.*

The scale of ordinates gives the value of the logarithm (to the base 10) of the equilibrium constant for the reaction of isomerization of cyclohexane to methylcyclopentane. The scale of abscissas gives the temperature in degrees Kelvin. The solid line refers to the reaction with both components in the liquid phase. The experimental data refer to the liquid phase and are from the following investigations: □, Schuit, Hoog, and Verheus [9]; ○, Glasebrook and Lovell [10]; △, Shell Development Company [11]; ●, Mizusima, Morino and Fujisiro [12]. The dotted line refers to the reaction with both components in the ideal gaseous phase.

WASHINGTON, July 18, 1947.