Physical Properties of Twelve Isomeric Alkyl-Substituted Naphthalenes, Tetrahydronaphthalenes and Decahydronaphthalenes

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AS A PORTION of a continuing study of hydrocarbon structure and physical properties (*1*, *4*), 12 polyalkylnaphthalenes, -tetrahydronaphthalenes, and decahydronaphthalenes have been prepared and studied. The hydrocarbons were synthesized (*3*, *5*) utilizing classical organic reactions and were carefully purified by means of high efficiency fractional distillation and chromatography. The purities of hydrocarbons were estimated from gas liquid partition chromatograms (6-foot column, SE-30 on Gas Chrom Z obtained from Applied Science Laboratories, Inc., State College, Pa.) to be in excess of 99 mole %. The decahydronaphthalene derivatives are mixtures of the *cis*- and *trans*-isomers obtained upon hydrogenation of the corresponding tetrahydronaphthalenes.

The physical properties of the new hydrocarbons are listed in Tables I and II. Dixon and Clark noted previously

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Table I. Physical Properties of Alkylnaphthalenes, Tetrahydronaphthalenes

Hydrocarbon	Viscosity, (Cp)., at ° C. 0.0°	20.0°	37.8°	60.0°	98.9°	KVI[a]
2-Butyl-3-hexylnaphthalene	81.31	24.89	11.49	5.506	2.271	70
7-Butyl-1-hexylnaphthalene	65.32	22.03	10.54	5.257	2.227	90
1,4-Dimethyl-5-octylnaphthalene	114.8	31.42	13.71	6.303	2.580	75
2,6-Dimethyl-3-octylnaphthalene	[b]	[b]	13.46	6.189	2.488	65
1,2,3,4-Tetrahydro-6-butyl-7-hexylnaphthalene	92.05	29.21	13.30	6.287	2.500	79
1,2,3,4-Tetrahydro-7-butyl-1-hexylnaphthalene	61.43	20.81	10.08	5.017	2.158	94
1,2,3,4-Tetrahydro-5,8-dimethyl-1-octylnaphthalene	2.022 (115°)	34.36	14.68	6.701	2.688	80
1,2,3,4-Tetrahydro-2,6-dimethyl-7-octylnaphthalene	[b]	25.42	11.64	5.593	2.333	87
2-Butyl-3-hexyldecahydronaphthalene[c]	111.7	30.76	13.17	5.977	2.346	56
7-Butyl-1-hexyldecahydronaphthalene[c]	74.55	24.03	11.24	5.491	2.283	93
1,4-Dimethyl-5-octyldecahydronaphthalene[c]	55.23	19.03	9.496	4.881	2.184	119
2,6-Dimethyl-3-octyldecahydronaphthalene[c]	[b]	20.78	10.07	5.080	2.213	110

[a] Kinematic viscosity index (*2*). [b] Solid at this temperature. [c] Mixtures of *cis-trans* isomers obtained by hydrogenation over a supported nickel catalyst of the corresponding tetrahydronaphthalene derivative.

Table II. Physical Properties of Alkylnaphthalenes, Tetrahydronaphthalenes and Decahydronaphthalenes

Hydrocarbon	Boiling Point, (° C.), at Mm. of Hg					ΔH_v^a	Refractive Index (n_D) at ° C.			Molecular Refraction	
	0.50 Mm.	1.00 Mm.	2.00 Mm.	5.00 Mm.	10.00 Mm.	(Cal./ G.)	20°	30°	40°	Exptl.	Theor.
2-Butyl-3-hexylnaphthalene	148.5	161.5	175.5	195.5	212.0	72	1.5471	1.5430	1.5388	91.7	87.9
7-Butyl-1-hexylnaphthalene	144.5	157.5	171.5	191.5	207.5	71	1.5514	1.5472	1.5431	91.8	87.9
1,4-Dimethyl-5-octylnaphthalene	159.0	172.0	186.5	207.0	223.5	73	1.5589	1.5550	...	91.1	87.9
2,6-Dimethyl-3-octylnaphthalene	157.0	170.5	184.5	205.0	221.0	74	[b]	1.5506	...	[b]	87.9
1,2,3,4-Tetrahydro-6-butyl-7-hexylnaphthalene	139.5	152.5	166.5	186.0	202.0	69	1.5075	1.5037	1.4998	89.8	88.8
1,2,3,4-Tetrahydro-7-butyl-1-hexylnaphthalene	136.0	149.0	162.5	182.0	197.5	69	1.5127	1.5090	1.5051	90.1	88.8
1,2,3,4-Tetrahydro-5,8-dimethyl-1-octylnaphthalene	146.0	159.0	173.0	193.0	209.0	70	1.5162	1.5126	1.5091	89.3	88.8
1,2,3,4-Tetrahydro-2,6-dimethyl-7-octylnaphthalene	144.5	157.5	171.0	191.0	207.0	70	1.5087	1.5051	...	90.0	88.8
2-Butyl-3-hexyldecahydronaphthalene[c]	134.0	146.0	159.5	179.0	194.5	67	1.4763	1.4730	1.4690	90.2	90.2
7-Butyl-1-hexyldecahydronaphthalene[c]	133.5	146.0	159.5	178.5	194.0	67	1.4785	1.4748	1.4713	90.1	90.2
1,4-Dimethyl-5-octyldecahydronaphthalene[c]	131.0	144.0	157.5	177.5	193.0	65	1.4781	1.4745	1.4712	90.1	90.2
2,6-Dimethyl-3-octyldecahydronaphthalene[c]	133.0	146.1	159.8	179.5	195.8	65	1.4759	1.4724	1.4690	90.3	90.2

[a] Calcd. from boiling points at 0.5 and 10 mm. of Hg using Clausium-Clapeyron equation. [b] Solid at this temperature. [c] Mixtures of *cis-trans* isomers obtained by hydrogenation over a supported nickel catalyst of the corresponding tetrahydronaphthalene derivative. [d] Calculated molecular refraction using 2.420 and 1.100 for carbon and hydrogen, respectively.

and Decahydronaphthalenes

Density, (Gram/Ml.), at ° C.				
0.0°	20.0°	37.8°	60.0°	98.9°
0.9470	0.9330	0.9209	0.9058	0.8796
0.9424	0.9284	0.9164	0.9014	0.8748
0.9639	0.9507	0.9389	0.9243	0.8991
[b]	[b]	0.9231	0.9079	0.8815
0.9222	0.9086	0.8967	0.8818	0.8555
0.9173	0.9039	0.8916	0.8766	0.8500
[b]	0.9217	0.9098	0.8951	0.8695
[b]	0.9035	0.8916	0.8770	0.8514
0.8888	0.8755	0.8639	0.8494	0.8239
0.8843	0.8713	0.8595	0.8451	0.8196
0.8884	0.8755	0.8641	0.8499	0.8250
[b]	0.8697	0.8582	0.8439	0.8186

(*1*) that methyl substitution on benzene derivatives resulted in somewhat anamalous changes in viscosity and change of viscosity with temperature. It may be seen from Table I that similar effects are observed with the naphthalene system.

The viscosities and densities at five temperatures, refractive indices at three temperatures, and boiling points at five pressures are reported for 2-butyl-3-hexylnaphthalene, 7-butyl-1-hexylnaphthalene, 1,4-dimethyl-5-octylnaphthalene, 2,6-dimethyl-3-octylnaphthalene, 1,2,3,4-tetrahydro-6-butyl-7-hexylnaphthalene, 1,2,3,4-tetrahydro-7-butyl-1-hexylnaphthalene, 1,2,3,4-tetrahydro-5,8-dimethyl-1-octylnaphthalene, 1,2,3,4-tetrahydro-2,6-dimethyl-7-octylnaphthalene, 2-butyl-3-hexyldecahydronaphthalene, 7-butyl-1-hexyl-decahydronaphthalene, 1,4-dimethyl-5-octyldecahydronaphthalene, 2,6-dimethyl-3-octyldecahydronaphthalene.

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