pyrimidine gave 5-acetyl-4-bromomethyl-2-phenylpyrimidine as one of the bromination products. Its structure was established by oxidation to 4-bromomethyl-2-phenyl-5-pyrimidine-carboxylic acid and 2-phenyl-4-,5-pyrimidinedicarboxylic acid.

By the coupling of 5-acetyl-4-bromomethyl-2-phenylpyrimidine with various secondary amines (dimethylamine, diethylamine, morpholine) followed by catalytic reduction, compounds of the type 4-dialkylaminomethyl-5-(1-hydroxyethyl)-2-phenylpyrimidine have been prepared.

RECEIVED AUGUST 26, 1947

[CONTRIBUTION FROM KEDZIE CHEMICAL LABORATORY, MICHIGAN STATE COLLEGE]

Condensation of Some Tertiary Octyl Alcohols with Benzene

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Previous communications[2] from this Laboratory have reported the condensation of eight of the seventeen possible tertiary octyl alcohols with benzene in the presence of aluminum chloride. The purpose of this investigation was to condense the remaining tertiary octyl alcohols with benzene and to determine the boiling points, refractive indices and surface tensions of the resulting octylbenzenes. To this end, the alcohols shown in Table I were prepared.[3] Of these, 3,4-dimethyl-3-hexanol has not been reported previously. This alcohol was synthesized successfully from 3-methyl-2-pentanone and ethyl Grignard reagent and from 3-methyl-4-hexanone and methyl Grignard reagent. Attempts to prepare it from butanone and secondary butyl Grignard reagent failed, the product being contaminated with large amounts of homomesityl oxide, which boils at approximately the same temperature as the desired alcohol.[4]

In general the condensations of the alcohols with benzene were carried out as described previously.[2c,5] The products were distilled under diminished pressure, traces of octyl chloride were removed from the octylbenzene fraction by refluxing with alcoholic potassium hydroxide or alcoholic silver nitrate, and the octylbenzene fraction was carefully distilled through a Fenske-type column.

TABLE I

TERTIARY OCTYL ALCOHOLS

	Carbonyl cpd.	Grignard	B. p., °C. (mm.)	n^{20}_D
3-Methyl-3-heptanol	MeCOEt	BuMgBr[a]	158 (742) 63–64 (13)	1.4270 (22°)
4-Methyl-4-heptanol	$MeCO_2Et$	PrMgBr[b]	62–63 (12)	1.4258
3-Ethyl-3-hexanol	$PrCO_2H$ PrCOCl	EtMgBr[c] EtMgBr[d]	153–155 (748) 64–65 (14)	1.4326
2,3-Dimethyl-3-hexanol	*i*-PrCOMe	PrMgBr[e]	155.5–157.5 (748) 54–56 (13)	1.4332
2,4-Dimethyl-4-hexanol	MeCOEt *i*-BuCOMe	*i*-BuMgBr[f] EtMgBr[g]	54.5 (13) 60–62 (16)	1.4278
3,4-Dimethyl-3-hexanol	See Experimental		150–152 (740) 58 (11)	1.4350
2-Methyl-3-ethyl-3-pentanol	*i*-$PrCO_2H$ *i*-PrCOCl	EtMgBr[c] EtMgBr[d]	156–157 (748) 53 (10)	1.4372
2,3,4-Trimethyl-3-pentanol	(*i*-$Pr)_2CO$	MeMgBr[h]	146–147 (740) 53–54 (13)	1.4342

[a] Whitmore and Badertscher, THIS JOURNAL, **55**, 1559 (1933). [b] Halse, *J. prakt. Chem.*, **89**, 453 (1914). [c] Ref. 14. [d] E. R. Breining, Master's Thesis, Michigan State College, 1938. [e] Clarke, THIS JOURNAL, **33**, 528 (1911). [f] Meyer and Tuot, *Compt. rend.*, **196**, 1232 (1933). [g] Clarke, THIS JOURNAL, **30**, 1147 (1908). [h] Whitmore and Laughlin, *ibid.*, **54**, 4392 (1932).

Our results agree with previous observations from this Laboratory[2b,5] that branching on the β-carbon atom of the alcohol results in a decreased yield of the octylbenzene (see Table II). The alcohols without branching on the β-carbon atom, namely, 3-methyl-3-heptanol, 4-methyl-4-heptanol, 3-ethyl-3-hexanol and 2,4-dimethyl-4-hexanol gave their respective octylbenzenes in yields of 19 to 31%. These hydrocarbons possess closely related physical properties and the determined molecular refractions are within 0.1 unit of the theoretical value. Because of the large yields of pure hydrocarbons with practically constant boiling points and indices of refraction, the accuracy with which the physical constants of these compounds were determined is greater than for the other four octylbenzenes.

Those alcohols with branching on one β-carbon atom, 2,3-dimethyl-3-hexanol, 3,4-dimethyl-3-hexanol, and 2-methyl-3-ethyl-3-pentanol fall into a second group. The crude octylbenzene fraction obtained from these is more complex than that obtained from the alcohols in the first group. Fractionation gave only a few grams (5 to 9%) of ma-

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(1) Present location: (a) Flint Junior College, Flint, Michigan; (b) Pigments Division, du Pont Company, Newport, Del.; (c) Wyeth, Inc., Mason, Mich.; (d) Ethyl Corporation, Baton Rouge, La.

(2) (a) Huston and Guile, THIS JOURNAL, **61**, 69 (1939); (b) Huston, Guile, Sculati and Watson, *J. Org. Chem.*, **6**, 252 (1941); (c) Huston and Krantz, *ibid.*, **13**, 63 (1948).

(3) The condensation of 2,3,3-trimethyl-2-pentanol is now being reinvestigated along with the condensation of 2,2,3-trimethyl-3-pentanol.

(4) Grignard and Fluchaire, *Ann. chim.*, **9**, 27 (1927), have shown that butanone yields homomesityl oxide when treated with bromo- or iodo-magnesium butoxides. Since appreciable quantities of 2-butanol were recovered in our work, the bromo-magnesium alkoxide of this alcohol was probably responsible for the condensation.

(5) Huston, Fox and Binder, *J. Org. Chem.*, **3**, 251 (1938).

TABLE II[a]

TERTIARY OCTYLBENZENES

	Yield, %	B. p., °C.		n^{20}_D	d^{20}_4	γ_{20}	M^{20}_D	Analyses, %[d]	
		Macro (mm.)	Micro (mm.)[b]					C	H
3-Methyl-3-phenylheptane	19.2	105.2–106.5 (8.5–9)	241.4–241.6 (732)	1.4928	0.8729	29.51	63.35[c]		6.74[e]
4-Methyl-4-phenylheptane[f]	30.6	110 (11)	239.4–239.6 (732)	1.4930	.8736	29.37	63.31	88.34	11.64
3-Ethyl-3-phenylhexane[f]	25.3	106.5–107.5 (10)	240.8 (732)	1.4938	.8752	29.61	63.29	88.17	11.65
2,3-Dimethyl-3-phenylhexane	9.5	109.2–110 (15)	234.6 (754)	1.4860	.8543	28.03	63.96	88.43	11.68
2,4-Dimethyl-4-phenylhexane	23.2	107–107.5 (12)	236.6–236.8 (732)	1.4924	.8722	28.87	63.35		6.67[e]
3,4-Dimethyl-3-phenylhexane	5.5	105–105.6 (12)	232–232.2 (732)	1.4860	.8590	27.8	63.61	81.41[g]	10.57[g]
2-Methyl-3-ethyl-3-phenylpentane	8.2	103.2–105 (10.5)	231.6–231.8 (732)	1.4850	.8573	27.82	63.63	88.13	11.64
2,3,4-Trimethyl-3-phenylpentane	4.3–7.6	104–106 (13)[h]	234–236 (743)[i]	1.4968	.8808	31.76[j]	63.20	88.55	11.51

[a] The provisional values for the physical constants for these hydrocarbons were included in Egloff, "Physical Constants of Hydrocarbons," Vol. III, Reinhold Publishing Corporation, New York, N. Y., 1946. [b] Micro boiling points are corrected (using Anschütz thermometers). [c] Calcd. 63.25. [d] Calcd. for $C_{14}H_{22}$: C, 88.35; H, 11.65. [e] N for *p*-amino-octylbenzenes. Calcd. for $C_{14}H_{23}N$: N, 6.82. [f] Previously reported, ref. *b*, Table I. [g] For 3,4-dimethyl-3-(*p*-hydroxyphenyl)-hexane. Calcd. for $C_{14}H_{22}O$: C, 81.50; H, 10.75. [h] Huston and Awuapara, *J. Org. Chem.*, 9, 405 (1944), report 104–105 (11 mm.). [i] Macro b. p. [j] Determined by du Noüy method.

terial with nearly constant boiling point and index of refraction. Figure 1 shows the weight of hydrocarbon plotted against index of refraction for 3,4-dimethyl-3-phenylhexane and 2-methyl-3-ethyl-3-phenylpentane. The portions with constant index of refraction at 1.4850 and 1.4860 are considered to be hydrocarbons of maximum obtainable purity under the experimental conditions used. Although the 2,3-dimethyl-3-phenylhexane was passed through a spinning band column[6] 80 cm. in length rather than through the Fenske-type column, its constants are almost identical with those of the two hydrocarbons just described. The observed molecular refractions for these three compounds varied from the theoretical by 0.35 to 0.61 unit.

The alcohol with branching on two *β*-carbon atoms, 2,3,4-trimethyl-3-pentanol, gave a low yield of the corresponding octylbenzene. Although the 2,3,4-trimethyl-3-phenylpentane has a high refractive index, the value corresponds quite closely to the 1.4958 reported for 2,3,4-trimethyl-2-phenylpentane.[2c] The observed molecular refraction checks the theoretical very closely.

Each of these eight octylbenzenes was nitrated, reduced, diazotized and hydrolyzed to the corresponding para-tertiary octylphenol.[7] The phenols were identified by the melting points of their derivatives. Nitration was shown to be *para* to the alkyl group by oxidizing the nitro derivatives to *p*-nitrobenzoic acid.

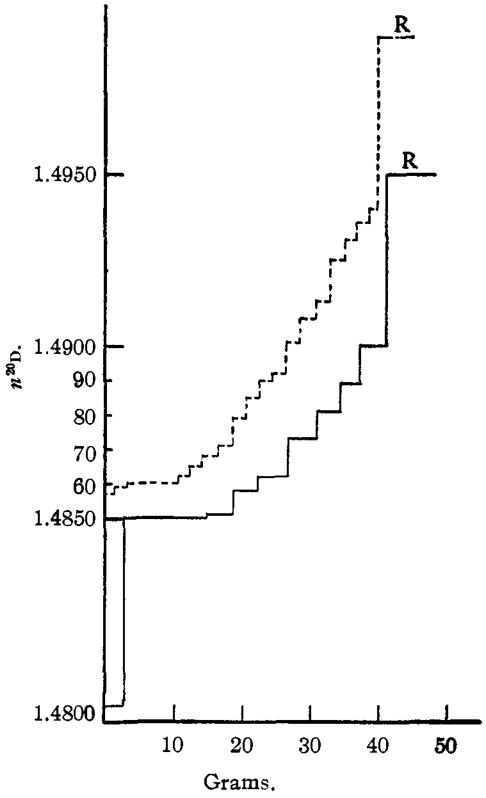

Fig. 1.—Refractive index *vs.* weight for distillation of crude octylbenzene fraction of 2-methyl-3-ethyl-3-phenylpentane — (from 1.25 moles of alcohol) and 3,4-dimethyl-3-phenylhexane - - - - (from 1 mole of alcohol). R is the residue in each distillation.

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[6] Baker, Barkenbus and Roswell, *Ind. Eng. Chem., Anal. Ed.*, 12, 468 (1940). The head was of the type described by Whitmore and Lux, THIS JOURNAL, 54, 3451 (1932).

[7] Huston and Meloy, *ibid.*, 64, 2655 (1942); Huston, Langdon and Snyder, *ibid.*, in press.

Experimental

Boiling points are uncorrected unless otherwise noted.

Preparation of Alcohols.—The alcohols were prepared by the reaction of the appropriate carbonyl compound and Grignard reagent as shown in Table I.

3,4-Dimethyl-3-hexanol. (a) **From 3-Methyl-2-pentanone and Ethylmagnesium Bromide.**—One mole of *s*-butylmagnesium bromide was added dropwise to one mole of acetyl chloride. After standing overnight, the reaction mixture was hydrolyzed, acidified, washed with dilute sodium carbonate solution and dried over anhydrous sodium sulfate. Removal of the ether followed by fractionation gave the ketone distilling at[8] 118°. The ketone was added dropwise to an equimolecular solution of ethylmagnesium bromide. The reaction mixture was worked up as usual and the alcohol fractionated under diminished pressure; b. p. 59–61° (14 mm.); 150–152° (740 mm.); yield, 61% based on the ketone, d^{25} 0.8345. *Anal.* Calcd. for $C_8H_{18}O$: C, 73.78; H, 13.93. Found: C, 73.72; H, 13.67.

(b) **From 3-Methyl-4-hexanone and Methylmagnesium Bromide.**—The ketone was prepared as follows: to 53 g. (2.3 moles) of powdered sodium,[9] suspended in 200 ml. of anhydrous ether in a two-liter, three-neck flask equipped with strrer, condenser and dropping funnel, was added 63 ml. (1.1 moles) of absolute ethyl alcohol. The condenser was replaced by a 60-cm. Fenske-type column packed with 3/32 inch glass helices. Eight hundred fifty grams of ethyl propionate was added portionwise and the reactants maintained at reflux temperature. The ether slowly distilled and was followed by a mixture of ethyl alcohol and ethyl propionate. After four hours, the condensation of the ethyl propionate and the sodium enolate of ethyl α-propionylpropionate[10] was considered to be complete as judged by the boiling point (95°+) and the refractive index (1.3840). To this solution was added 150 ml. of toluene (dried over sodium). In a period of three to four hours, the sodium enolate was alkylated[11] to ethyl α-methyl-α-propionylbutyrate by slowly adding 316 g. of ethyl bromide (65 g. excess). During this addition and for one additional hour, the reaction mixture was maintained at the reflux temperature.

The solid sodium bromide was removed by suction and the liquid layer A saved for fractionation. The sodium bromide was dissolved in water, the solution acidified with acetic acid, the oil separated and the water layer extracted with ether. The liquids were washed with 10% sodium carbonate and, after drying over anhydrous potassium carbonate, were combined with the liquid layer A. Distillation through the Fenske-type column gave 239 g. (1.285 moles) of ethyl α-methyl-α-propionylbutyrate, b. p. 94–95° (11 mm.); n^{20}_{D} 1.4288; reported,[12] b. p. 98–100° (15 mm.); yield, 55.8% based on sodium.

Ketone hydrolysis of the ester[13] required fourteen hours. The reaction mixture was poured onto ice and made alkaline with sodium hydroxide. The oil was separated and the water layer extracted with ether. The combined oil and ether extracts were dried and distilled. The average yield for the hydrolysis of two 250-g. batches of the keto ester was 84%. The 3-methyl-4-hexanone boiled at 76–76.4° (107 mm.); micro b. p. 135.2 (743 mm.) (cor.); n^{20}_{D} 1.4069; d^{20}_{4} 0.8162; reported,[13] (b. p. 135–136 (760 mm.).

To the methylmagnesium bromide prepared from 3.3 moles of magnesium and methyl bromide (Dow Chemical) in 900 ml. of anhydrous ether was added dropwise 262 g. (2.3 moles) of 3-methyl-4-hexanone. After standing overnight, large colorless crystals settled around the sides of the flask and on the stirrer. These were identified by analysis (Mg, 11.1%) as the complex $C_{16}H_{46}O_5Mg_4Br_6$ observed in this Laboratory in the preparation of tertiary alcohols from acids and the Grignard reagent.[14] Five hundred milliliters of ether was distilled from the reaction mixture, 200 ml. of dry benzene was added and the whole refluxed four or five hours at a temperature of 60°. After hydrolysis, and after washing and drying the ethereal solution, distillation gave 261 g. of 3,4-dimethyl-3-hexanol (87% yield based on the ketone).

Condensation of the Alcohols with Benzene.—All but three of the alcohols were condensed according to the method described by Huston, *et al.*,[5] using 0.5 mole of aluminum chloride per mole of alcohol. The technique described by Huston and Krantz[2c] was used for the condensation of 2,3-dimethyl-3-hexanol, 3,4-dimethyl-3-hexanol and 2-methyl-3-ethyl-3-pentanol, using, respectively, 0.33, 0.41 and 0.25 mole of aluminum chloride per mole of alcohol. No gaseous organic compounds were obtained in these reactions. The condensation of 2,3-dimethyl-3-hexanol was varied further in that dry hydrogen chloride gas was bubbled into the reaction flask during the addition of the last 0.7 mole of alcohol.

After standing for two to twelve hours, the reaction mixture was hydrolyzed by adding water. If the aqueous layer did not become clear, a small volume of C. P. hydrochloric acid was added. The benzene layer was removed and the aqueous layer extracted with benzene. The combined benzene extracts were washed with 10% sodium carbonate solution and dried over anhydrous potassium carbonate.

Fractionation of Crude Product.—Distillations were through the Fenske-type column described above except for the products obtained from the condensation of 2,3-dimethyl-3-hexanol (spinning band column[6]) and of 2,3,4-trimethyl-3-pentanol (Vigreux). After removal of the benzene, the following fractions were obtained in each case:

1. **Alkane–Alkene Fraction.**—B. p. 50–60° at 90 to 100 mm.: from alcohols with branching on the β-carbon atom, unsaturated (bromine in carbon tetrachloride), chloride-free liquids were obtained, probably alkenes formed by dehydration of the alcohols. From alcohols without branching on the β-carbon atom, saturated, chloride-free liquids with physical constants approximating alkanes were obtained. Product from 4-methyl-4-heptanol: yield, 24.2%; b. p. 56° (93 mm.); micro b. p. 117.2° (744 mm.) (cor.); n^{20}_{D} 1.3980; d^{20}_{4} 0.7036. These values agree fairly well with the physical constants of 4-methylheptane.[15] These liquids are under further investigation.
2. **Chloride Fraction.**—B. p. 50–55° at 10–12 mm.: these liquids were not identified but were probably the chlorides derived from the respective alcohols since they gave heavy precipitates with alcoholic silver nitrate.
3. **Crude Octylbenzene Fraction.**—B. p. 102–110° at 10–15 mm.: these fractions usually contained an appreciable quantity of chlorides.
4. **Residue.**—B. p. above 110° (11 mm.) and refractive index greater than 1.5000.

Purification and Isolation of Pure Octylbenzenes.—In each case fraction 3 was refluxed for three to six hours with an equal volume of alcoholic potassium hydroxide solution (1 g. potassium hydroxide to 10 ml. 95% ethyl alcohol). (2,3-Dimethyl-3-phenylhexane required additional treatment with alcoholic silver nitrate.) To this solution was added 200 ml. of water, the oil was separated and the aqueous layer extracted with benzene. The combined oil-benzene solution was washed with 10% acetic acid, 10% sodium carbonate and water and dried over anhydrous potassium carbonate.

The dry liquids were fractionated at reduced pressure through the columns described above. The head was maintained at total reflux until equilibrium was reached. A small volume of liquid was then removed and the head

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[8] Ginnings, Plonk and Carter, THIS JOURNAL, **62**, 1923 (1940).

[9] "Organic Syntheses," Coll. Vol. II, John Wiley and Sons, Inc., New York, N. Y., 1943, p. 272.

[10] McElvain, THIS JOURNAL, **51**, 3124 (1929).

[11] Dieckmann and Kron, *Ber.*, **41**, 1269 (1908).

[12] Hudson and Hauser, THIS JOURNAL, **63**, 3159 (1941).

[13] Hudson and Hauser, *ibid.*, **63**, 3163 (1941).

[14] Huston and Bailey, *ibid.*, **68**, 1382 (1946).

[15] Egloff, "Physical Constants of Hydrocarbons," Vol. I, Reinhold Publishing Corporation, New York, N. Y., 1939, p. 51.

returned to total reflux. When equilibrium was again attained, the process was repeated. Individual samples of one to three grams of liquid were taken and the refractive index determined. Samples of nearly constant boiling point and equal refractive index were combined. The yields of the octylbenzenes recorded in Table II are based on the weight of the liquid where the refractive index varies by no more than 0.001 unit (the 2,3,4-trimethyl-3-phenylpentane was repeatedly distilled through a Vigreux column until pure). The physical constants were determined on the largest combined sample of constant refractive index. In Fig. 1, the fractions of constant refractive index were obtained by combining a number of samples of the same refractive index.

Surface tensions were determined by the drop-weight method. The correction factor was calculated according to the "International Critical Tables."[16]

Summary

Eight tertiary octyl alcohols have been condensed with benzene to produce the corresponding tertiary octylbenzenes. The physical constants of the latter have been determined.

3,4-Dimethyl-3-hexanol has been synthesized by two methods.

(16) "I. C. T.," 1928, Vol. IV, p. 435.

EAST LANSING, MICHIGAN RECEIVED AUGUST 25, 1947

[CONTRIBUTION FROM THE DEPARTMENT OF CHEMISTRY, THE UNIVERSITY OF TEXAS]

Allylic Chlorides. IV. Relative Reactivities with Potassium Iodide in Acetone[1]

BY LEWIS F. HATCH, LEON B. GORDON AND JOHN J. RUSS[2]

A number of different reactions has been used to demonstrate marked differences in relative reactivity between various types of organic halides. Of these methods, the most satisfactory bimolecular (S_N2) reaction for alkyl chlorides is the metathetical reaction between the chloride and potassium iodide in dry acetone.[3] This reaction usually proceeds at an easily measured rate for most chlorides, at readily obtainable temperatures, and without side reactions.

Although this reaction has been used to compare the relative reactivities of a large number of alkyl chlorides, it was not until 1941 that the reaction was utilized in a study of the relative reactivities of several allylic chlorides.[4] The reaction proved to be entirely satisfactory for this type of chloride.

Recent work[5] on the cuprous chloride catalyzed acid hydrolysis of the isomeric 1,3-dichloropropenes has shown that geometrical configuration has a marked influence on the rate of reaction. The present investigation was undertaken to reinvestigate the reaction between allylic chlorides and potassium iodide and to determine if the previously noted effect of geometrical configuration on the hydrolysis reaction also applied to a bimolecular metathetical reaction.

Materials

Potassium Iodide.—C. P. potassium iodide was recrystallized from water and dried three hours at 120°. It failed to give a positive test for iodate ion.

Acetone.—The actone used boiled at 56.6° and did not color anhydrous copper sulfate in one hour. It retained a faint pink color of potassium permanganate for thirty minutes and liberated neither iodine nor hydriodic acid from 0.04 molar potassium iodide when kept in the dark.

1-Chloro-1-propene.—A mixture of *cis*- and *trans*-1-chloro-1-propene[6] was distilled to obtain a fraction with a boiling range of 33–34°. This fraction, being intermediate in boiling range between the two isomers (*cis* 32.0–32.2°; *trans* 36.7°), contained both isomers.

Allyl Chloride.—Allyl chloride boiling at 44.9° was obtained by distillation from crude allyl chloride[7] with a boiling range of 44.5–45.1°. It was used without further purification.

2-Bromo-3-chloro-1-propene.—2-Bromo-3-chloro-1-propene, obtained from Halogen Chemicals of Columbia, S. C., was distilled at 150 mm. pressure. The fraction used had the following constants: b. p. 61.6° (150 mm.); n^{25}_D 1.4968; d^{25}_4 1.6290; *MR* (calcd.) 28.22, (obsd.) 27.61.

2,3-Dichloro-1-propene.—2,3-Dichloro-1-propene[6] with a boiling range of 93–94° was distilled at 150 mm. pressure and a fraction boiling at 48.0° was used.

Methallyl Chloride.—Methallyl chloride[7] was redistilled and a fraction boiling at 72.1° was used.

1,3-Dichloropropene.—In the still bottoms remaining from the distillation of crude allyl chloride, prepared by the high temperature substitutive chlorination of propylene, there remains an appreciable quantity of higher boiling material containing a dichloride fraction consisting of approximately 63% 1,3-dichloropropene (*cis* and *trans*), 35% 1,2-dichloropropane and 2% 2,3-dichloro-1-propene. This material[7,8] was separated by distillation into fractions containing the low and high boiling isomers of 1,3-dichloropropene. These fractions were redistilled at 150 mm. pressure and the following data were obtained: low boiling 1,3-dichloropropene, b. p. 57.0°, n^{20}_D 1.4673; high boiling 1,3-dichloropropene, b. p. 64.7°, n^{20}_D 1.4745.

1,3-Dichloro-2-methyl-1-propene.—The isomeric 1,3-dichloro-2-methyl-1-propenes were prepared from methallyl chloride.[9] The methallyl chloride was chlorinated to 1,2,3-trichloro-2-methylpropane using sulfuryl chloride. The trichloride was dehydrochlorinated and hydrolyzed to a mixture of the 3-chloro-2-methyl-2-propen-1-ols which were separated using a Podbielniak Hypercal distillation column. The chloroalcohols were converted to the corresponding dichlorides using concentrated hydrochloric acid.

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(1) Presented in part at the Texas Regional Meeting of the American Chemical Society, Dallas, Texas, December 13, 1946.

(2) Present address: Magnolia Petroleum Company, Dallas, Texas.

(3) (a) Conant and Kirner, THIS JOURNAL, **46**, 232 (1924); (b) Conant and Hussey, *ibid.*, **47**, 476 (1925); (c) Conant, Kirner and Hussey, *ibid.*, **47**, 488 (1925).

(4) Tamele, Ott, Marple and Hearne, *Ind. Eng. Chem.*, **33**, 115 (1941).

(5) Hatch and Roberts, THIS JOURNAL, **68**, 1196 (1946).

(6) Obtained from Research Chemicals, San José, California.

(7) Furnished us for this investigation by Shell Development Co., Emeryville, California.

(8) These isomers are now available from Shell Chemical Co., San Francisco, California.

(9) Hatch, Russ and Gordon, THIS JOURNAL, **69**, 2614 (1947).