Cyclizations by Carbon Monoxide in Friedel–Crafts Reactions. Facile Synthesis of β-Disubstituted α-Indanones[1]

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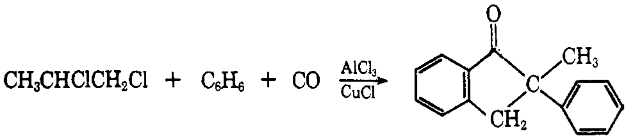
Received April 5, 1967

Carbon monoxide readily condenses with benzene, $AlCl_3$, and certain polyfunctional halides having at least three carbon atoms in an aliphatic chain to give β-disubstituted α-indanones by a new type of cyclization reaction. Thus, 2-methyl-2-phenylindanone-1 can be prepared by reaction of benzene, CO, and $AlCl_3$ with either propylene dichloride, allyl chloride, 1,2,2- or 1,1,2-trichloropropane, 2,3-dichloropropene-1, 1,2-dichloropropene-1, 1-chloropropene-1, or (β-chloropropyl)benzene. Similarly, 2,2-dimethylindanone-1 is obtained from methallyl chloride, isocrotyl chloride, isobutylene dichloride, 2-dichlorobutene-1 and -2, 1,2-, 2,3-, 1,3-, and 2,2-dichlorobutanes, or neophyl chloride. Also prepared by analogous methods were 2,3-dimethyl-2-phenylindanone-1, 2,2,3-trimethylindanone-1, 2,2,3,3-tetramethylindanone-1, and several other β-disubstituted indanones. The reactions occur at room temperature and atmospheric pressure with 1 mole of $AlCl_3$ required per mole of polyfunctional halide employed. Certain polyfunctional halides gave anomalous results: 1,1-dichloro-2-phenylcyclopropane gave 3-phenylindene together with 1,2- and 2,3-diphenylindenes, while 2-chloro-4-methylpentene-1 and -2 gave (1,1-dimethyl-3-indanylene)(1,1,3-trimethylindanyl)methane. From benzene, CO, $AlCl_3$, and 2-chloro-1-methylcyclohexene-1 and -2 there was obtained 10-methyl-1,2,3,4,10,11-hexahydrofluorenone-9.

While investigating the reaction of propylene dichloride with benzene, $AlCl_3$, and carbon monoxide, at room temperature and atmospheric pressure, in an attempt to prepare *p,p'*-dialdehydo-1,2-diphenylpropane (I) by a modified Gattermann–Koch synthesis,[2a] it was noticed that the higher boiling fractions of the complex, liquid aldehydic mixture which was obtained readily crystallized to give a 13–16% yield of pure 2-methyl-2-phenylindanone-1 (II).



II

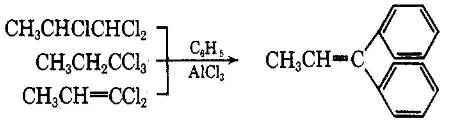
This compound had been prepared previously by Campbell and Ciganek using a five-step synthesis starting with benzyl cyanide, sodium, and benzyl chloride.[2b]

The present study was carried out to improve the yield of II and to determine the scope and usefulness of the reaction when applied to other polyfunctional halides.

The formation of II must involve substitution of a nucleophile for the hydrogen on carbon atom number 2 of the propylene dichloride. It seemed probable, therefore, that by *previously eliminating* this hydrogen atom by the use of $CH_3CCl_2CH_2Cl$, $CH_2{=}CClCH_2Cl$, or $CH_3CCl{=}CHCl$ in place of the $CH_3CHClCH_2Cl$ and by omitting the cuprous chloride cocatalyst which is known to enhance the formation of aldehydes in the Gattermann–Koch reaction, the yield of II might be considerably increased and thus a new and simple method for preparing many hitherto difficultly accessible β-disubstituted α-indanones would be realized. This has proved to be the case.

By using 1 mole of $AlCl_3$ per mole of 3-carbon halide, carbon monoxide, an excess of benzene, and no CuCl, the yield of pure II obtained from 1,2,2-trichloropropane was 58–60%, while 2,3-dichloropropene-1, 1,2-dichloropropene-1, and 1,2-dichloropropane gave II in yields of 41, 30, and 20%, respectively. Yields of 10% II were obtained from 1-chloropropene-1 and 3-chloropropene-1, while 1,1,2-trichloropropane, 1,1,1-trichloropropane, and 1,1-dichloropropene-1 gave II in yields of 19, 2, and 2%, respectively. In the latter three reactions, 1,1-diphenylpropene-1 was obtained as a by-product in yields of 30, 67.5, and 17%, respectively.

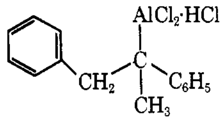
Since the formation of 1,1-diphenylpropene-1 from benzene, $AlCl_3$, and either 1,1,2-trichloropropane, 1,1-dichloropropene-1, or 1,1,1-trichloropropane does not require the use of carbon monoxide, this method furnishes a simple procedure for its preparation, as given by eq 1.



(1)

No indanones could be detected when benzene, CO, and $AlCl_3$ were condensed with 2,2-dichloropropane, 2-chloropropene-1, 1,3-dichloropropene-1,1,2,3-trichloropropene, 1,2,2,3-tetrachloropropane, or 1,1,1,2-tetrachloropropane. The use of ethylene dichloride in place of the above halides did not yield indanone-1, but gave largely 1,2-diphenylethane plus traces of aldehyde. Likewise 1,3-dichloropropane and 1,2,3-trichloropropane gave mixtures of hydrocarbons and aldehydes. It was found that other Friedel–Crafts catalysts, notably $FeCl_3$, $SnCl_4$, and $TiCl_4$, did not give II under the same reaction conditions. Also, small quantities of water (up to about 3% by weight) in the $AlCl_3$ or the other reactants did not appreciably reduce the yields of II.

The formation of II from 1,2-dichloropropane, 3-chloropropene-1, or 1-chloropropene-1 might be in part explained by formation of a common intermediate such



III

as III. Such a formulation has been proposed in the case of analogous complexes of aromatic hydrocarbons,

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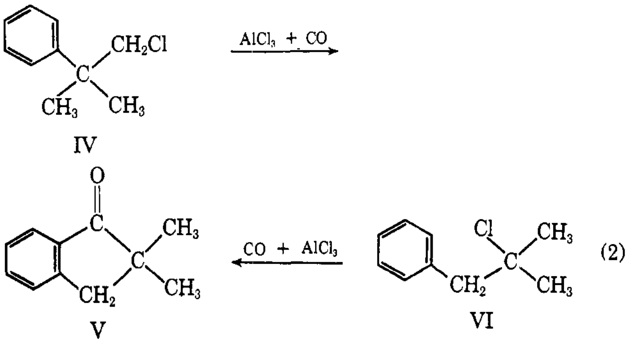
[1] Presented at the 153rd National Meeting of the American Chemical Society, Miami Beach, Fla., April 14, 1967.

[2] (a) W. C. Meuly, U. S. Patent 2,158,518; 2,158,519 (1939); *Chem. Abstr.*, **33**, 6874 (1939). (b) N. Campbell and E. Ciganek, *J. Chem. Soc.*, 3834 (1956).

$AlCl_3$, and HCl by Schroeter.[3] To test this hypothesis, we treated 1,2-diphenylpropane in benzene solution with $AlCl_3$, HCl, and CO under conditions identical with those that gave II and obtained 2-methyl-2-phenylindanone-1 in 11% yield. *This reaction did not take place in the absence of hydrogen chloride.* It consequently seemed probable that any precursor of 1,2-diphenylpropane in the presence of $AlCl_3$, CO, and hydrogen chloride might also yield II. This reaction was therefore applied to benzene with a mixture of the three isomers of β,β′-dichlorodiisopropyl ether which is available commercially from the hypochlorination of propylene and which could undergo ether scission with the formation, *in situ*, of 1,2-diphenylpropane. Actually, a 10% yield of pure II was obtained from this reaction.

Similarly, either $C_6H_5CH_2CHClCH_3$, $C_6H_5CH(CH_3)CH_2Br$, or a mixture of $C_6H_5CH_2CCl_2CH_3$, $C_6H_5CH{=}CClCH_3$, and $C_6H_5CH_2CCl{=}CH_2$ (such as is obtained by treatment of phenylacetone with PCl_5) gave II in 14, 12, and 42% yields, respectively.

These reactions suggested that $C_6H_5C(CH_3)_2CH_2Cl$ (neophyl chloride) (IV) might react in an analogous manner to give 3,3-dimethylindanone-1.[4] However, the condensation gave 2,2-dimethylindanone-1 (V)[5,6] in 81% yield. The same rearrangement took place in the absence of added benzene by using CS_2 as a diluent or solvent for the reaction. By using 2-chloro-2-methyl-3-phenylpropane (VI) in place of neophyl chloride, a 60% yield of pure (V) was obtained (eq 2).



IV
V
VI
(2)

Likewise, upon reacting benzene, CO, and $AlCl_3$ with various possible precursors of IV or VI, notably methallyl chloride, isocrotyl chloride, 1,2-dichloro-2-methylpropane, and the mixed isomers 2-chlorobutene-1 and 2-chlorobutene-2 (obtained from PCl_5 and methyl ethyl ketone), good yields of 2,2-dimethylindanone-1 (V) were obtained.

Unexpectedly, V was also obtained upon reacting benzene, CO, and $AlCl_3$ with 1,2-dichlorobutane, 2,3-dichlorobutane, 2,3-dibromobutane, 1,2-dichlorobutane, and 2,2-dichlorobutane. These yields are shown in Table I.

On the other hand, 1,4-dichlorobutane under the same conditions gave a mixture of hydrocarbons plus a 27.6% yield of 1,2,3,4-tetrahydro-6-naphthaldehyde VII.

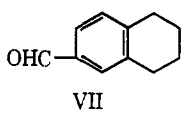

VII

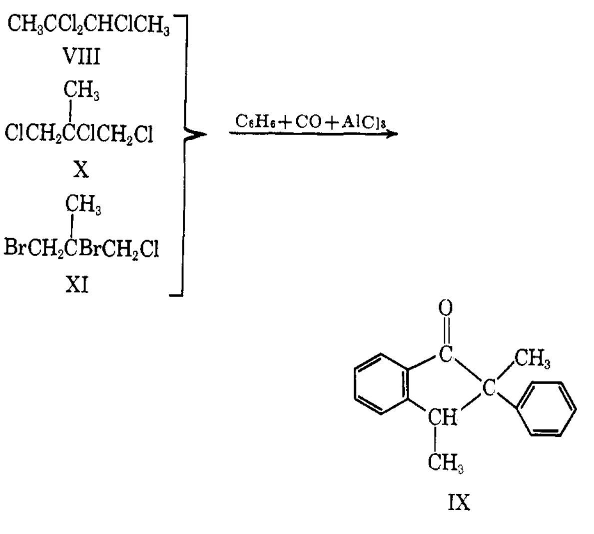
Table I

Aliphatic halide + C_6H_6 + CO + $AlCl_3$	Yield of pure 2,2-dimethylindanone-1, %
$CH_2{=}C(CH_3)CH_2Cl$	46–48.5
$(CH_3)_2C{=}CHCl$	65–68
$(CH_3)_2CClCH_2Cl$	74.5
$CH_2{=}CClCH_2CH_3$ $CH_3CCl{=}CHCH_3$ mixture	48.5
$ClCH_2CHClCH_2CH_3$	61
$CH_3CHClCHClCH_3$	69.5
$CH_3CHBrCHBrCH_3$	55
$ClCH_2CH_2CHClCH_3$	14
$CH_3CCl_2CH_2CH_3$	63.5

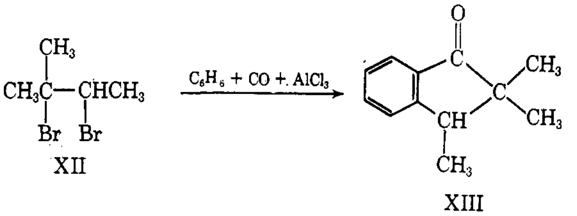
The isomerization of the dihalobutanes other than the 1,4 isomer in the presence of $AlCl_3$ to give 2,2-dimethylindanone under the Friedel–Crafts conditions used is reconcilable with an observation made by Sommer[7] that 1,3-dibromobutane is isomerized at 25° by $AlBr_3$ to form a mixture of 1,2-, 2,3-, 2,2-, 1,1-, and 1,3-dibromobutanes with only traces of 1,4-dibromobutane. Presumably 1,4-dichlorobutane behaves similarly.

It was therefore of interest to determine if 2,2,3-trichlorobutane VIII would react with benzene, CO, and $AlCl_3$ to yield an indanone. This reaction, under the same conditions as those above, gave a 39% yield of a crystalline product, mp 89–90°, which by nmr and mass spectrum analysis proved to be the hitherto unknown 2,3-dimethyl-2-phenylindanone-1 (IX).

Compound IX could also be obtained in 23 and 16% yield, respectively, by a deep-seated rearrangement upon reacting 1,2,3-trichloro-2-methylpropane (X) or 1,2-dibromo-3-chloro-2-methylpropane (XI) with benzene, CO, and $AlCl_3$ as shown in eq 3. In a similar manner, 2,2,3-trimethylindanone-1 (XIII) was obtained in 60% yield by reacting 2,3-dibromo-2-methylbutane (XII) with benzene, CO, and $AlCl_3$ (eq 4). Likewise,



VIII
X
XI
IX
(3)



XII
XIII
(4)

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[3] G. Schroeter, *Ber.*, **57**, 1990 (1924).

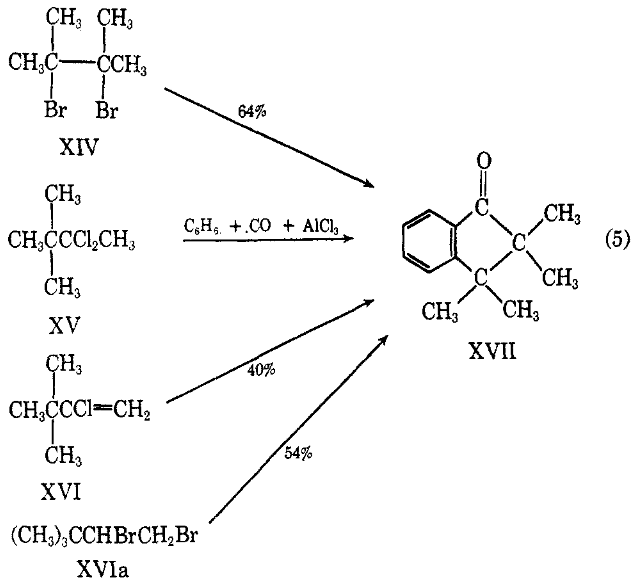
[4] K. von Auwers, *ibid.*, **54**, 994 (1921).

[5] A. Haller and E. Baur, *Ann. Chim.*, **16**, 340 (1921).

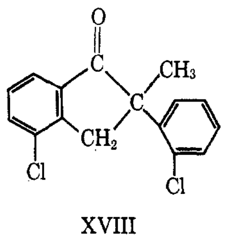
[6] K. von Auwers, *Ann.*, **415**, 161 (1918).

[7] J. M. Sommer, *Bull. Soc. Chim. France*, 1831 (1963); *Chem. Abstr.*, **59**, 15156 (1963).

2,2,3,3-tetramethylindanone-1[8] was obtained in 64% yield by reacting benzene, CO, and $AlCl_3$ with 2,3-dibromo-2,3-dimethylbutane (XIV). The same compound was obtained in 30% yield from 2,2-dichloro-3,3-dimethylbutane (XV), benzene, CO, and $AlCl_3$; in 40% yield in the same way from 2-chloro-3,3-dimethylbutene-1 (XVI), and in 54% yield from 1,2-dibromo-3,3-dimethylbutane (XVIa) by molecular rearrangement as shown in eq 5. By using 1,2-dibromo-2-methylbutane in the reactions in eq 5 with benzene, CO, and $AlCl_3$, there was obtained a 60:40 mixture of 2-methyl-2-ethylindanone-1 and 2,2-dimethyltetralone-1, as determined by nmr and infrared analysis, together with aldehydic by-products.

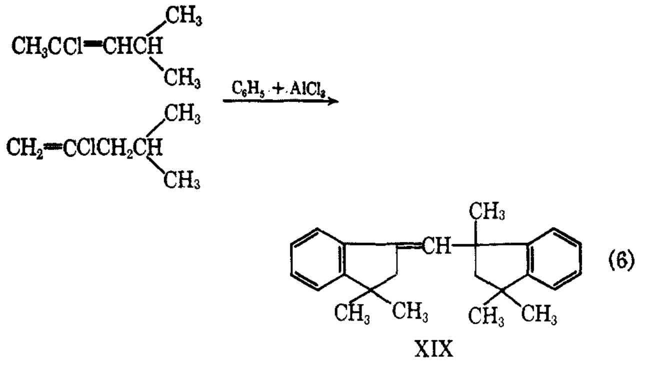


As the chain length of the halogenated alkanes used is increased in length beyond four carbon atoms, the yields of indanones rapidly decrease and there are formed by isomerizations and rearrangements increasing amounts of complex mixtures of hydrocarbons and aldehydes. The same applies in part to reactions in which the benzene is replaced by toluene, the xylenes, and chlorobenzene. These give liquid mixtures of indanones, aldehydes, and hydrocarbons which are difficult to separate by distillation. However, from the condensation of chlorobenzene and 2,3-dichloropropene-1 with CO and $AlCl_3$, a pure, crystalline compound, mp 96°, was isolated in 6.5% yield which, by nmr and infrared analysis, proved to be 2-methyl-2-(*o*-chlorophenyl)-4-chloroindanone-1 (XVIII).

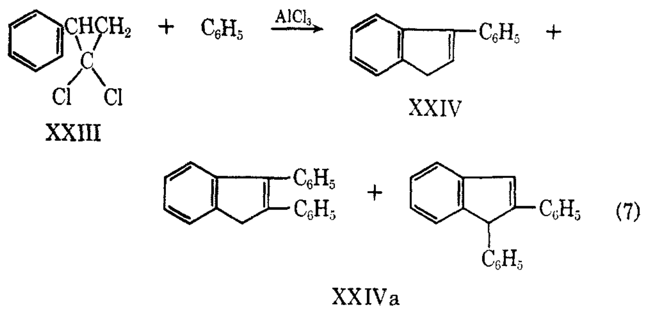


XVIII

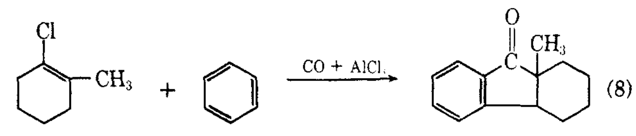
Upon reacting benzene, CO, and $AlCl_3$ with the mixed isomers 2-chloro-4-methylpentene-2 and 2-chloro-4-methylpentene-1 (from PCl_5 plus methyl isobutyl ketone), no indanone formation was detected. Instead a liquid hydrocarbon was isolated having the probable formula of (1,1-dimethyl-3-indanylene)(1,1,3-trimethylindanyl)methane (XIX) (eq 6). The same product was obtained without the use of carbon monoxide.



From the reaction of carbon monoxide, $AlCl_3$, benzene, and 1,1-dichloro-2-phenylcyclopropane[9,10] (XXIII), 3-phenylindene[11] (XXIV), together with a higher boiling by-product consisting of 2,3-diphenylindene and 1,2-diphenylindene (XXIVa), was obtained (eq 7). Obviously, the carbon monoxide did not participate in the reaction and XXIV was obtained in 41% yield without the use of CO by using an excess of benzene and 1 mole of $AlCl_3$ per mole of the 1,1-dichloro-2-phenylcyclopropane. Recently, Buddrus and Nerdel[12] have prepared various indenes by a similar reaction of other dichlorocarbene adducts with benzene and $AlCl_3$.



Finally, it was interesting to determine if a cyclic halide having the $-C(CH_3){=}CCl$ grouping would react with benzene, CO, and $AlCl_3$ to give the corresponding cyclic ketone (XX) as indicated in eq 8. This was found to be the case, thus affording a novel means of introducing an angular methyl group into suitable cyclic structures.



An attempt to introduce two carbonyl groups by reacting carbon monoxide, $AlCl_3$, and 2,5-dimethyl-1,4-bis(β-chloro-*t*-butylbenzene) (XXI) to form XXII failed (eq 9). Instead of XXII, 2,2-dimethylindanone

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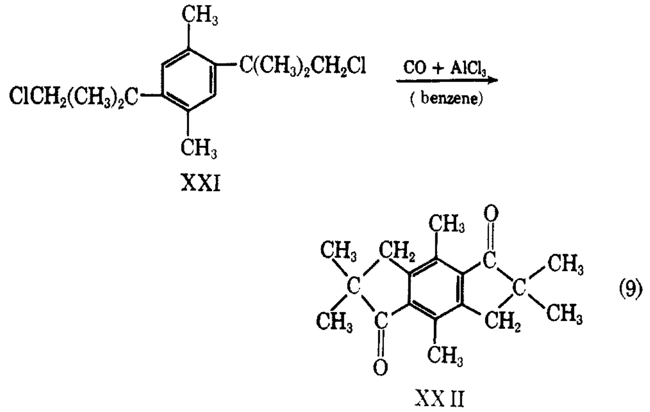
[8] E. Rothstein, *J. Chem. Soc.*, 1461 (1951).

[9] H. A. Bruson and T. P. O'Day, U. S. Patent 3,012,079 (1961).

[10] W. J. Dale and P. E. Schwartzentruber, *J. Org. Chem.*, **24**, 955 (1959).

[11] P. A. Plattner, R. Sandrin, and J. Wyss [*Helv. Chem. Acta*, **29**, 1604 (1946)] named "1-phenylindene." See F. K. Beilstein, "Handbuch der organischen Chemie," Part IV, 2148, for recent correction in nomenclature.

[12] J. Buddrus and F. Nerdel, *Tetrahedron Letters*, **36**, 3197 (1965).



was obtained by cleavage and rearrangement of XXI. An attempt to insert two carbonyl groups by reacting benzene with 2 mole equiv each of methallyl chloride, $AlCl_3$, and CO was unsuccessful, the product being largely tar.

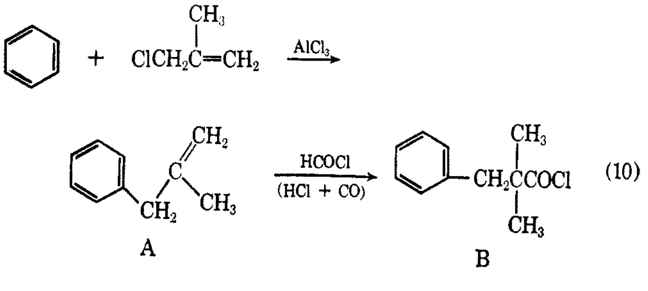
Mechanism of Indanone Formation

The possibility that the organic halides used herein combined with carbon monoxide to form acyl halides by the reaction which is known to occur at higher tem-

$$RX + CO \xrightarrow{\text{HlCl}_3} RCOX$$

peratures and pressures[13] and that such acyl halide intermediates could form indanones was found not to apply in our work, since no carboxylic acid could be found upon hydrolysis of the reaction mixtures produced in our attempts to condense the alkyl halides with CO and HCl in the presence of $AlCl_3$ at room temperature and atmospheric pressure in the absence of benzene.

It seems probable that in the simplest case, the reaction of methallyl chloride, benzene, CO, and $AlCl_3$, for example, the initial step might involve formation of methallyl benzene (A) which then reacts with formyl chloride from the HCl and CO present to give an acid chloride addition product (B) which undergoes ring closure to 2,2-dimethylindanone (eq 10).



Experimental Section

The condensations were carried out in 1000–2000-ml, four-necked, Morton-type, creased flasks, fitted with a high-speed stirrer, reflux condenser, dropping funnel, thermometer, and gas inlet tube (0.25 in. diameter) extending as near to the bottom of the flask as the stirring paddle permitted. (Sintered, porous glass sparger tubes were tried but rapidly plugged.) The carbon monoxide (or hydrogen chloride when employed) was metered in through flow raters. The exit gases were scrubbed free of hydrogen chloride in a water trap, enabling measurement by titration when desired. All work was carried out in a well-ventilated hood.

Carbon monoxide (98% purity) was the "Commercial Grade" supplied in high-pressure cylinders by the Matheson Co., Rutherford, N. J. It was not dried before use. 1-Chloro-2-methylpropene-1, as well as 1,2-dichloroisobutane and 1,2,3-trichloroisobutane, was a commercial product supplied by Chemische Werke Hüls A.G., Marl, Kr. Recklinghausen, West Germany. Most of the other haloalkenes and polyhaloalkanes were supplied by Columbia Organic Chemicals Co., Inc., Columbia, S. C. Others were prepared according to literature references cited herein at the appropriate places.

The benzene (or other aromatic reactant) (4–8 moles) and powdered anhydrous aluminum chloride (1 mole) were placed in the flask which was immersed in a cold water (20–25°) bath. Carbon monoxide was rapidly bubbled into the well-stirred mixture for about 5 min before the dropwise addition of the organic halide was begun. Thereafter CO was continuously bubbled into the stirred mixture during which time a slow dropwise addition was maintained of the organic halide (1 mole). This required from 3 to 5 hr. The reaction mixture was held at 20–25°, preferably at 20°, during the entire operation. After the organic halide had all been added, introduction of CO was allowed to continue for about 30 min longer. The mixture was then added to about 500–700 g of chipped ice and stirred vigorously to decompose the aluminum chloride complex. The organic layer was separated, washed several times with water, dried over Na_2SO_4, and distilled under reduced pressure to remove the excess low boilers. The residual higher boiling material was then fractionally distilled under high vacuum. In some cases, if the organic halide was a solid or if it was desired to lengthen the reaction period, the organic halide was dissolved in a portion of the benzene and this solution was then added dropwise to the balance of the benzene containing the $AlCl_3$ while bubbling in the carbon monoxide.

2-Methyl-2-phenylindanone-1 from 1,2-Dichloropropane.—1,2-Dichloropropane (57 g, 0.5 mole) diluted with 85 g of benzene was added dropwise over a period of 7 hr to a vigorously stirred mixture of 70 g (0.5 mole) of $AlCl_3$ and 149 g of benzene at 25–27° while carbon monoxide was bubbled in continuously at a rate of about 130 cc/min. Work-up and distillation gave a fraction (47.3 g) boiling at 125–170° (0.1 mm) which partially solidified upon cooling and scratching. After washing this material with a little cold petroleum ether (bp 30–60°) and recrystallizing the white solid from about 150 ml of boiling methanol, 19.7 g (18.8%) of 2-methyl-2-phenylindanone-1, mp 110–111°, was obtained. A mixture melting point with an authentic sample kindly supplied by Campbell[2b] at the University of Edinburgh showed no depression. The ultraviolet spectrum of our product agreed with the one published.[14] *Anal.* Calcd for $C_{16}H_{14}O$: C, 86.44; H, 6.35. Found: C, 86.55; H, 6.41.

Its 2,4-dinitrophenylhydrazone melted at 211° (from ethanol). *Anal.* Calcd for $C_{22}H_{18}N_4O_4$: C, 65.64; H, 4.51; N, 13.92. Found: C, 65.88; H, 4.65; N, 14.11.

Its oxime melted at 184–185.5° (from ethanol). *Anal.* Calcd for $C_{16}H_{15}NO$: C, 80.97; H, 6.38; N, 5.90. Found: C, 81.14; H, 6.54; N, 6.00.

2-Methyl-2-phenylindanone-1 from 1,2,2-Trichloropropane.—To a vigorously stirred mixture of 140 g of benzene (1.8 moles) and 42 g of anhydrous $AlCl_3$ (0.3 mole) was added dropwise 1,2,2-trichloropropane (44.5 g, 0.3 mole) during a period of 3 hr at 24–27° while CO was rapidly bubbled in. On work-up the organic layer contained a finely suspended crystalline material which was filtered off and recrystallized from hot ethanol to give 14.5 g of 2-methyl-2-phenylindanone-1, mp 110.5–111°. Distillation of the benzene filtrate gave a crude fraction, bp 125–180° (0.2 mm), which solidified in the receiver. Recrystallization from ethanol gave an additional 24.5 g of 2-methyl-2-phenylindanone-1: mp 111°, total yield, 39 g (58.5%).

1,1-Diphenylpropene-1 from 1,1,1-Trichloropropane.—To a stirred slurry of anhydrous $AlCl_3$ (28 g, 0.2 mole) in 156 g (2.0 moles) of benzene was added 18 g (0.12 mole) of 1,1,1-trichloropropane dropwise over a period of 2 hr at 20–23° while carbon monoxide was rapidly bubbled into the mixture. The reddish oil was hydrolyzed with 300 g of crushed ice and the organic layer distilled under vacuum to give 17.8 g of distillate, bp 95–110° (0.2 mm), which solidified in the receiver. Upon recrystallization from boiling methanol (75 ml), this gave 15.7 g (67.5% yield) of 1,1-diphenylpropene-1, mp 48–49°,[15] identified by its infrared, ultraviolet, and nmr spectrum. *Anal.* Calcd for $C_{15}H_{14}$: C, 92.73; H, 7.27. Found: C, 92.54; H, 7.29.

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[13] I. G. Farben, U. S. Patent 1,891,930 (1932).

[14] H. Christol, C. Martin, and M. Mousseron, *Bull. Soc. Chim. France*, 1696 (1960).

[15] P. Schorigin, *Ber.*, **41**, 2720 (1908).

It reacted with bromine to give 2-bromo-1,1-diphenylpropene-1, mp 48–49°.[16] From the methanolic mother liquor, 0.5 g (2% yield) of 2-methyl-2-phenylindanone-1 was isolated. Similarly, 1,1,2-trichloropropane and 1,1-dichloropropene-1 each reacted with benzene, CO, and $AlCl_3$ to give 1,1-diphenylpropene-1 and 2-methyl-2-phenylindanone.

2-Methyl-2-phenylindanone-1 from β,β'-Dichloroisopropyl Ether.—β,β'-Dichloroisopropyl ether (mixed isomers; $n^{24}D$ 1.4458) (38 g, 0.22 mole) was added dropwise over a period of 2.5 hr to a vigorously stirred suspension of $AlCl_3$ (95 g, 0.7 mole) in 206 g (2.65 moles) of benzene at 22–24°, while carbon monoxide was bubbled continuously through the mixture. After hydrolysis and work-up the oil layer was distilled under reduced pressure. After a small forerun, 22.9 g of crude oily solid was stripped off at 125–170° (0.4 mm). This material was triturated with a few milliliters of low-boiling petroleum ether (bp 30–60°) and filtered to yield 9 g of 2-methyl-2-phenylindanone (10%), mp 109–110°, after recrystallization from 50 ml of methanol.

2-Methyl-2-phenylindanone from 1,2-Diphenylpropane.—A mixture of 1,2-diphenylpropane (49 g, 0.25 mole), 34 g of $AlCl_3$ (0.25 mole), and 150 g of benzene was vigorously stirred at 25–30° while a continuous stream of carbon monoxide and hydrogen chloride (2:1) was bubbled in over a period of 4 hr. The reaction mixture, after hydrolysis and work-up as described above, gave 12.2 g of recovered 1,2-diphenylpropane boiling at 88–120° (0.1 mm) and 16.5 g of crude II boiling at 120–155° (0.1 mm) which, upon scratching and seeding, crystallized. After trituration with cold low-boiling petroleum ether, filtration, and recrystallization from methanol, 6 g (11%) of 2-methyl-2-phenylindanone, mp 109–111°, was obtained.

2-Methyl-2-phenylindanone (II) from Other Polyfunctional Halides. A.—Reacting 78 g of benzene, 20 g of $AlCl_3$, and 17.6 g of 1-phenyl-2-chloropropane[17] with CO at 23–25° gave 3.6 g (14.4%) of pure II.

B.—Reacting 120 g of benzene, 35 g of $AlCl_3$, and 50 g of 1-bromo-2-methyl-2-phenylethane[18] with CO at 20–25° gave 6.7 g (12%) of pure II.

C.—Reacting CO with 188 g of benzene, 55 g of $AlCl_3$, and 61 g of mixed 1-phenyl-2-chloropropenes (bp 65–78° (0.5 mm), $n^{23}D$ 1.5455, made from PCl_5 and phenylacetone) containing 80% 1-phenyl-2-chloropropene-1, 15% 1-phenyl-2-chloropropene-2, and 5% 1-phenyl-2,2-dichloropropane (by vpc analysis) gave 35.5 g (42.3%) of pure II.

2,2-Dimethylindanone-1 (V). A. Neophyl chloride[19] (67.5 g, 0.4 mole) was added dropwise over a period of 3 hr to a vigorously stirred mixture of 54 g (0.4 mole) of $AlCl_3$ in 188 g (2.4 mole) of benzene at 21–22° while CO was rapidly bubbled through the mixture during 4.5 hr. After hydrolysis and work-up by vacuum distillation of the oil layer, 59 g of crude V, boiling at 62–101° (0.1 mm), was obtained. By crystallization from ligroin at −40°, pure V (52 g, 81% yield) was obtained, mp 42–43°. *Anal.* Calcd for $C_{11}H_{12}O$: C, 82.44; H, 7.56. Found: C, 82.19; H, 7.61.

Its 2,4-dinitrophenylhydrazone melted at 186–188°. *Anal.* Calcd for $C_{17}H_{16}N_4O_4$: C, 59.95; H, 4.77; N, 16.46. Found: C, 60.13; H, 5.11; N, 16.30.

Its semicarbazone melted at 196–197°. *Anal.* Calcd for $C_{12}H_{15}N_3O$: C, 66.32; H, 6.96; N, 19.34. Found: C, 60.13; H, 7.13; N, 19.41.

B. 2,2-Dimethylindanone-1 from 1-Phenyl-2-chloro-2-methylpropane.—The 1-phenyl-2-chloro-2-methylpropane used was prepared by refluxing neophyl chloride for 17 hr under an eight-plate column and recovering by distillation a mixture of 1-phenyl-2-methylpropene-1, 1-phenyl-2-methylpropene-2, and 1-phenyl-2-chloro-2-methylpropane.[19] This mixture was then treated with hydrogen chloride gas at 0° which converted the two olefins present into 1-phenyl-2-chloro-2-methylpropane: bp 88° (10 mm); 65%; $n^{23}D$ 1.5155. 1-Phenyl-2-chloro-2-methylpropane (42 g, 0.25 mole) was added dropwise to a vigorously stirred mixture of 35 g (0.25 mole) of $AlCl_3$ in 156 g (2.0 moles) of benzene while a continuous stream of CO was being bubbled through the solution. The temperature was maintained at 23–25° during the 4-hr reaction period. After work-up by hydrolysis, washing, drying over Na_2SO_4, and distillation under reduced pressure, 24.3 g (60%) of pure, recrystallized 2,2-dimethylindanone, mp 44°, was obtained.

C. 2,2-Dimethylindanone-1 from Other Polyfunctional Halides.—From 46 g of methallyl chloride, 105 g of $AlCl_3$, CO, and 234 g of benzene at 24–26°, 35 g (44%) of V, mp 43–44°, was obtained. Other similar runs gave yields of 46–48.5% of theory.

D.—From 45 g of isocrotyl chloride, 67 g of $AlCl_3$, CO, and 234 g of benzene at 21–24°, 54.5 g (68%) of V was obtained.

E.—From 64 g of 1,2-dichloro-2-methylpropane, 70 g of $AlCl_3$, CO, and 234 g of benzene at 24–27°, 59.5 g (74.5%) of V was obtained. In the same manner, 2,2-dichlorobutane, 1,2-dichlorobutane, 2,3-dichlorobutane; 2,3-dibromobutane, 1,3-dichlorobutane, and a mixture of 2-chlorobutene-1 and 2-chlorobutene-2 each reacted with benzene, $AlCl_3$, and CO to give V in the yields shown in Table I.

2,3-Dimethyl-2-phenylindanone (IX) from 2,2,3-Trichlorobutane.—2,2,3-Trichlorobutane (34 g, 0.2 mole) was added dropwise over a period of 2 hr to a vigorously stirred slurry of 28 g (0.2 mole) of $AlCl_3$ in 95 g (1.2 moles) of benzene. Carbon monoxide was rapidly bubbled into the mixture during the addition and for 1 hr thereafter, while maintaining the reaction temperature at 23–25°. After work-up by hydrolysis, washing, and vacuum distillation, 34.8 g of crude product boiling at 120–182° (0.3 mm) was obtained which solidified in the receiver. Upon recrystallization from 100 ml of boiling methanol and chilling to 0°, 2,3-dimethyl-2-phenylindanone (15.2 g, 39% of theory), mp 89–90°, was obtained. *Anal.* Calcd for $C_{17}H_{16}O$: C, 86.37; H, 6.83. Found: C, 86.45; H, 7.04.

Its 2,4-dinitrophenylhydrazone melted at 149–150°. *Anal.* Calcd for $C_{23}H_{20}N_4O_4$: C, 66.32; H, 4.96; N, 13.46. Found: C, 66.57, H, 5.04; N, 13.21.

Its oxime melted at 132.5–133°. *Anal.* Calcd for $C_{17}H_{17}NO$: C, 81.23; H, 6.83; N, 5.57. Found: C, 81.28; H, 6.86; N, 5.50.

2,3-Dimethyl-2-phenylindanone from 1,2,3-Trichloro-2-methylpropane.—1,2,3-Trichloro-2-methylpropane (162 g, 1.0 mole) was added dropwise over a 4.5-hr period to a rapidly stirred slurry of 135 g (1.0 mole) of $AlCl_3$ in 468 g (6.0 moles) of benzene at 20–21°. A rapid stream of carbon monoxide was bubbled through the mixture continuously during the halide addition and for 1 hr thereafter. The dark oil was hydrolyzed with 1000 g of crushed ice; the benzene layer was separated, washed, and distilled, eventually under vacuum, to give 148.1 g of crude distillate, bp 145–210° (0.1 mm), which partially crystallized. Upon recrystallization from ligroin, 55 g (23.3%) of IX, mp 89–90°, was obtained. Its mixed melting point with IX was not depressed. In the same manner, 1,2-dibromo-3-chloro-2-methylpropane[20] with benzene, $AlCl_3$, and CO gave pure IX in 16% yield.

1,2,3,4-Tetrahydro-6-Naphthaldehyde (VII).—1,4-Dichlorobutane (42 g, 0.33 mole) was added dropwise to a vigorously stirred mixture of 46 g (0.33 mole) of $AlCl_3$ in 195 g (2.5 moles) of benzene through which a continuous stream of CO was bubbled (120 ml/min) for a total reaction period of 5.75 hr, while the temperature was maintained at 22–24°. The solution was poured onto 500 g of crushed ice; the benzene layer was separated, washed thoroughly with water, and distilled, first at atmospheric pressure to remove benzene and finally under vacuum. The fraction (29.4 g) boiling at 110–130° (0.2 mm) was redistilled to give a cut (7.8 g), bp 145° (10 mm), $n^{24}D$ 1.5734, the nmr and infrared spectra of which were identical with those of 1,2,3,4-tetrahydro-6-naphthaldehyde. Its semicarbazone melted at 223–224° (lit.[21] mp 221°). *Anal.* Calcd for $C_{12}H_{15}N_3O$: C, 66.32; H, 6.96; N, 19.34. Found: C, 66.76; H, 7.09; N, 19.43.

Its 2,4-dinitrophenylhydrazone melted at 219–220° (lit.[21] 222°).

2,2,3-Trimethylindanone (XIII) from 2,3-Dibromo-2-methylbutane.—The 2,3-dibromo-2-methylbutane, bp 50–53 (11 mm), $n^{22}D$ 1.5099, which was used was prepared by adding 80 g of bromine dropwise to stirred, cooled 2-methylbutene-2 (49 g) in 150 cc of carbon tetrachloride at −10 to −15°. 2,3-Dibromo-2-methylbutane (54 g, 0.23 mole) was added dropwise over a period of 4 hr to a vigorously stirred mixture of 33 g (0.23 mole) of $AlCl_3$ in 110 g (1.4 moles) of benzene maintained at 23–24° while simultaneously bubbling carbon monoxide rapidly through the reaction mixture for a period of 4.75 hr. The solution obtained was poured onto 300 g of crushed ice and the organic layer was

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separated, washed, dried, and distilled. The fraction (31.3 g) boiling at 90–110° (0.4 mm) was redistilled to give 24.3 g (60%) of 2,2,3-trimethylindanone boiling at 87–89° (0.6 mm), n^{22}D 1.5383. *Anal.* Calcd for $C_{12}H_{14}O$: C, 82.70; H, 8.10. Found: C, 83.05; H, 8.10.

Its 2,4-dinitrophenylhydrazone melted at 243–244°. *Anal.* Calcd for $C_{18}H_{18}N_4O_4$: C, 61.00; H, 5.12; N, 15.81. Found: C, 61.15; H, 5.20; N, 15.85.

2,2,3,3-Tetramethylindanone (XVII). A. From 2,3-Dibromo-2,3-dimethylbutane.—The 2,3-dibromo-2,3-dimethylbutane was obtained in 65% yield by reacting 1.0 mole of bromine with 0.58 mole of 2,3-dimethylbutane (from Phillips Petroleum Co.) at room temperature in sunlight.[22] 2,3-Dibromo-2,3-dimethylbutane (61 g, 0.25 mole), as a 35% solution in warm benzene, was added dropwise to a vigorously stirred slurry of 35 g (0.25 mole) of $AlCl_3$ in 100 g (1.25 moles) of benzene while CO was rapidly bubbled through the mixture at 21–22° during a reaction period of 4 hr. After hydrolysis with ice, separation, and washing of the benzene layer, distillation under vacuum gave 34.6 g (73%) of XVII:[8] bp 114–115° (6 mm); n^{20}D 1.5356. *Anal.* Calcd for $C_{13}H_{16}O$: C, 82.92; H, 8.57. Found: C, 83.06; H, 8.33.

Its oxime melted at 142° (lit.[8] mp 143–144°).

B. From 2,2-Dichloro-3,3-dimethylbutane.—2,2-Dichloro-3,3-dimethylbutane[23] (62 g, 0.4 mole), as a 40% solution in warm benzene, was added dropwise to a vigorously stirred slurry of 54 g (0.4 mole) of $AlCl_3$ in 100 g (1.3 moles) of benzene while CO was rapidly bubbled through the mixture at 25–27° during a reaction period of 5 hr. After hydrolysis and work-up as above, 23.1 g (31%) of XVII, bp 118–120° (6.5 mm), n^{25}D 1.5336, was obtained. Its oxime, mp 141–142°, gave no depression when admixed with the oxime obtained in A above.

C. From 2-Chloro-3,3-dimethylbutene-1.—2-Chloro-3,3-dimethylbutene (60 g, 0.5 mole)[23] was added dropwise over a period of 3 hr to a vigorously stirred slurry of 70 g (0.5 mole) of $AlCl_3$ in 234 g (3.0 moles) of benzene maintained at 26–27°, while a rapid stream of CO was continuously bubbled through the mixture during the course of 4 hr. After hydrolysis on ice and work-up as above, 38 g of XVII (40.5% yield), bp 118–120° (6.5 mm), was obtained.

D. From 1,2-Dibromo-3,3-dimethylbutane.—1,2-Dibromo-3,3-dimethylbutane (bp 78–80° (12 mm), n^{22}D 1.5057) (XVIa) was obtained in 93% yield by dropwise addition in the dark of 160 g of bromine to a solution of 84 g of 2,2-dimethylbutene-3 ("neohexene," furnished by Sinclair Petrochemicals, Inc.) in 125 cc of carbon tetrachloride at 0–10°. 1,2-Dibromo-3,3-dimethylbutane (122 g, 0.5 mole) was added dropwise over a period of 2.5 hr to a vigorously stirred slurry of 234 g (3.0 moles) of benzene and 70 g (0.5 mole) of $AlCl_3$ maintained at 19–21°. Carbon monoxide was bubbled continuously into the reaction mixture at such a rate as to be present in excess throughout the addition (24 l. of CO used). The red oil was decomposed on 400 g of crushed ice; the oil layer was separated, washed, dried over Na_2SO_4, and fractionally distilled under vacuum to give 51 g (54% of theory) of XVII.

2-Methyl-2-(*o*-chlorophenyl)-4-chloroindanone-1 (XVIII).—2,3-Dichloropropene-1 (56 g, 0.5 mole) was added dropwise over a period of 4 hr to a vigorously stirred slurry of 70 g (0.5 mole) of $AlCl_3$ in 337.5 g (3.0 moles) of chlorobenzene at 16–24° while a rapid stream of CO was simultaneously and continuously bubbled through the reaction mixture for 5 hr. The product was decomposed with 500 g of crushed ice; the oil layer was separated, washed, dried, and vacuum distilled to give a crude distillate (70.9 g) boiling at 165–205° (0.2 mm). Upon redistillation, the fraction (19 g) boiling at 163–165° (0.15 mm) partly crystallized. Treatment with an equal volume of ice-cold ligroin, filtering, and recrystallization from boiling methanol yielded 5.9 g of white platelets, mp 96–97°. The viscous pot residue from the distillation yielded another 8.1 g of the 96–97° melting product, XVIII. *Anal.* Calcd for $C_{16}H_{12}Cl_2O$: C, 65.95; H, 4.15; Cl, 24.39. Found: C, 66.01; H, 4.04; Cl, 24.40.

Its 2,4-dinitrophenylhydrazone melted at 215–217 dec. *Anal.* Calcd for $C_{22}H_{16}Cl_2N_4O_4$: Cl, 15.07; N, 11.88. Found: Cl, 15.10; N, 12.15.

3-Phenylindene (XXIV) and Diphenylindenes (XXIVa).—1,1-Dichloro-2-phenylcyclopropane (56 g, 0.3 mole)[9,10] was added dropwise to a stirred slurry of 40 g (0.3 mole) of $AlCl_3$ in 118 g (1.5 moles) of benzene at 28–30° during the course of 3 hr. After treatment with 400 g of chipped ice, the organic layer was separated, washed with water, dried over Na_2SO_4, and distilled under vacuum to give 23.7 g (41% yield) of XXIV:[11,24] bp 121–125° (0.1 mm); n^{25}D 1.6333; mp 19°. *Anal.* Calcd for $C_{15}H_{12}$: C, 93.70; H, 6.29; mol wt, 192. Found: C, 93.54; H, 6.45; mol wt, 192 (mass spectrum).

A higher boiling fraction (bp 175–180° (0.1 mm), 3.6 g) solidified in the receiver. After two recrystallizations from methanol it was obtained as colorless crystals melting unsharply at 126–128°. *Anal.* Calcd for $C_{21}H_{16}$: C, 93.98; H, 6.02; mol wt, 384. Found: C, 93.81; H, 6.04; mol wt, 384.

Its nmr spectrum showed the presence of one allylic CH_2 group and 14 aromatic hydrogens. The infrared spectrum was consistent with a phenyl indene. The mass spectrum confirmed the molecular weight and showed fragmentation characteristic of two phenyl groups. The literature describes a 1,2-diphenylindene melting a 177–178°[25,26] and a 2,3-diphenylindene melting at 108–109° obtained from it by alkaline isomerization.[27] That our 126–128° melting compound was a mixture of the 1,2- and 2,3-diphenylindene isomers was shown by boiling it with alcoholic potassium hydroxide[27] and isolating quantitatively the 2,3-diphenylindene, mp 108–109°, in accord with the literature value.

10-Methyl-1,2,3,4,10,11-hexahydrofluorenone-9 (XX).—Phosphorus pentachloride (165 g, 0.8 mole) was added gradually to 90 g (0.8 mole) of 2-methylcyclohexanone while stirring and cooling. The temperature was held at 10–20° during the 40-min addition period. After evolution of HCl ceased, the dark solution was slowly added with cooling to 400 ml of water. The organic layer was separated, dried over anhydrous sodium sulfate, and distilled under reduced pressure. The crude fraction (76.4 g) boiling at 61–135° (22 mm) was redistilled at atmospheric pressure to give 42.6 g (bp 160–162°, n^{22}D 1.4771) and 9.0 g (bp 162–165°, n^{23}D 1.4771–1.4784). These two fractions consisted of a mixture of 2-chloro-1-methylcyclohexene-1 and 2-chloro-1-methylcyclohexene-2 as determined by nmr and vpc. This mixture was reacted with benzene and CO as follows.

2-Chloro-1-methylcyclohexene-1 and -2 (131 g, 1.0 mole) was added dropwise over a period of 4 hr to a vigorously stirred suspension of 135 g (1.0 mole) of $AlCl_3$ in 390 g (5.0 moles) of benzene while carbon monoxide was rapidly bubbled for 5 hr through the reaction mixture maintained at 18–21°. The product was decomposed with 1000 g of chipped ice; the organic layer was separated, washed with water, dried over Na_2SO_4, and distilled under vacuum to give a crude distillate (126.5 g) boiling at 95–180° (0.1 mm) and 27 g of resin in the pot. The crude distillate was carefully redistilled under vacuum to give 32.2 g of product, bp 105–109° (0.1 mm), n^{24}D 1.5600, as a pale yellow thick liquid. *Anal.* Calcd for $C_{14}H_{16}O$: C, 83.95; H, 8.01. Found: C, 84.05; H, 7.98.

Mass spectrograph analysis showed the molecular weight to be 200. Its nmr analysis showed the product to be a mixture of *cis* and *trans* isomers having the angular methyl group on C-10. Its 2,4-dinitrophenylhydrazone melted at 155°. *Anal.* Calcd for $C_{20}H_{20}N_4O_4$: C, 63.13; H, 5.30; N, 14.73. Found: C, 63.42; H, 4.95; N, 14.86.

(1,1-Dimethyl-3-indanylene)(1,1,3-trimethylindanyl)methane (XIX).—2-Chloro-4-methylpentene-1 was prepared by reacting methyl isobutyl ketone with phosphorus pentachloride at 0–10°.[28] The product boiling at 101–104° (760 mm), n^{25}D 1.4215, contained some of the 2-chloro-4-methylpentene-2 isomer and was used as described below.

A.—To a stirred slurry of 70 g of $AlCl_3$ in 240 g of benzene maintained at 23–26° there was added dropwise over a period of 2.5 hr 67 g of 2-chloro-4-methylpentene-1 and -2. The solution was stirred for 2 hr more at this temperature and poured onto 400 g of crushed ice; the oil layer was separated, washed thoroughly with water, dried over Na_2SO_4, and fractionally distilled under vacuum. The fraction (22.5 g, 14% yield) boiling at 132° (0.05 mm), n^{25}D 1.5608, a viscous, faintly yellow liquid, was collected as product XIX. *Anal.* Calcd for $C_{24}H_{28}$: C, 91.08;

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H, 8.92; mol wt, 316. Found: C, 90.77; H, 8.94; mol wt (mass spectrum), 316.

The ^{1}H nmr spectrum showed the presence of 5.4 methyl groups, 2.0 different ring methylene groups, and 1.0 olefinic hydrogen to 8.0 aromatic hydrogens. The fractional methyl is probably an impurity. The compound showed a sharp peak (broad base) by vpc.

B.—2-Chloro-4-methylpentene-1 and -2 (59.3 g) were added dropwise over a period of 2.5 hr to a vigorously stirred mixture of 70 g of $AlCl_3$ in 234 g of benzene while carbon monoxide was rapidly bubbled in at 23–26° during the addition period and for 1.25 hr thereafter. Hydrolysis and work-up of the oil layer by vacuum distillation gave 25.2 g of a fraction, bp 160–180° (0.1 mm), which upon redistillation gave XIX as a heart cut, bp 152–157° (0.1 mm), $n^{23}\text{D}$ 1.5619. No indanones were detected in any of the other fractions.

2,5-Dimethyl-1,4-bis(β-chloro-*t*-butyl)benzene (XXI).—Methallyl chloride (181 g, 2.0 moles) was added dropwise over a period of 5.5 hr to a vigorously stirred mixture of 318 g (3.0 moles) of *p*-xylene and 200 g (2.0 moles) of 96% sulfuric acid while maintaining the temperature at 20–21°. Stirring was continued for 16 hr thereafter at 20–25°. The lower acid layer was then removed and the crystalline solid separated from the oil, then washed, dried, and recrystallized from 350 ml of boiling ethanol to give 66.5 g (11.5% yield) of XXI, mp 117°.[29] No attempt to obtain more XXI from the oil was made.

Reaction of XXI with CO and Benzene.—A solution of 66.5 g of XXI in 300 ml of benzene was added dropwise over a period of 2.5 hr to a stirred slurry of 70 g (0.5 mole) of $AlCl_3$ and 200 ml of benzene at 19–20°. Carbon monoxide was bubbled in continuously and in excess during the halide addition and for 1 hr thereafter. After decomposition with 400 g of ice, the oil layer was separated, washed, dried over Na_2SO_4, and distilled under vacuum to yield (a) 13 g, bp 70–90° (0.1 mm), $n^{24}\text{D}$ 1.5354; (b) 30 g, bp 90–105° (0.1 mm), $n^{24}\text{D}$ 1.5410; and (c) 20.2 g, bp 105–130° (0.1 mm), $n^{24}\text{D}$ 1.5527. Each fraction showed ketone present. The fractions a, b, and c were combined, mixed with 100 ml of low-boiling ligroin, and cooled in a Dry Ice chest overnight. The crystalline product was removed and recrystallized from ligroin at 0° to give 35.7 g of pure 2,2-dimethylindanone (V), mp 41–42°, and showed no melting point depression on admixture with an authentic sample of same.

Registry No.—V, 10489-28-8; V 2,4-dinitrophenylhydrazone, 13864-82-9; V semicarbazone, 13970-33-7; IX, 10474-34-7; IX 2,4-dinitrophenylhydrazone 13864-84-1; IX oxime, 13864-85-2; XIII, 10474-35-8; XIII 2,4-dinitrophenylhydrazone, 10474-73-4; XVII, 10474-33-6; XVIII, 13864-88-5; XVIII 2,4-dinitrophenylhydrazone, 13864-89-6; XIX, 13864-90-9; XX 2,4-dinitrophenylhydrazone, 13864-91-0; XX, 13970-34-8; XXIV, 1961-97-3; XXIVa (2,3-diphenylindene), 5324-00-5; 2-methyl-2-phenylindanone-1, 10474-32-5; its 2,4-dinitrophenylhydrazone, 13864-95-4; its oxime, 13864-96-5; 1,1-diphenylpropene-1, 778-66-5; carbon monoxide, 630-08-0.

Acknowledgment.—We wish to thank Dr. H. Agahigian and his collaborators H. Hoberecht, W. Harple, and G. D. Vickers for carrying out and interpreting the infrared, nmr, and mass spectrum, and other analyses described herein.

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A Method for Manual Generation of Correct von Baeyer Names of Polycyclic Hydrocarbons

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Received December 8, 1966

A general method for naming bridged polycyclic hydrocarbons by the IUPAC 1957 rules (the von Baeyer system) is described in terms of representing the structure of the molecule in terms of a planar graph (a Schlegel diagram). Symmetry elements of the molecule are easily seen by this depiction. The largest possible circuit of the planar graph is determined and the circuit is numbered in such a way as to satisfy IUPAC rule A-32.31. The method, as described, is not limited in scope since it can be applied to the systematic naming of all bridged hydrocarbons. Numerous examples from the current chemical literature of incorrectly named compounds are described and their correct von Baeyer names are given as examples of this system.

Recent advances in the syntheses of regular, three-dimensional, organic solids (polyhedranes[1] and prismanes[2]) and symmetrically bridged hydrocarbons (adamantane,[3] congressane (diamantane),[4] and triamantane[5]) introduce the possibility of an overabundance of trivial names to the nomenclature of bridged hydrocarbons if there is no systematic means for naming them. Although it is possible to name all of the complex polyhedranes synthesized to date by the Definitive Rules for Nomenclature of Organic Chemistry of the International Union of Pure and Applied Chemistry, commonly referred to as the IUPAC 1957 rules,[6] it will eventually be necessary to extend this system.[7]

It is the purpose of this paper to outline and discuss a general method for naming polyhedranes in conformity with the IUPAC nomenclature rules. Numerous examples from the literature of incorrectly named structures will be described in terms of this method, and a number of molecules of potential existence will be named.

It is interesting to note that the nomenclature for bridged hydrocarbons can be entirely independent of esoteric trivial names. Most bridged hydrocarbons capable of existence can be drawn as planar graphs,[8] and it is possible to establish a general method for naming these compounds by first drawing them in two-

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[1] Cubane: P. E. Eaton and T. W. Cole, Jr., *J. Am. Chem. Soc.*, **86**, 962, 3157 (1964).

[2] Hexasubstituted triprismane: H. G. Viehe, R. Merenyi, J. F. M. Oth, J. R. Senders, and P. Valange, *Angew. Chem.*, **76**, 922 (1964).

[3] S. Landa and V. Machacek, *Collection Czech. Chem. Commun.*, **5**, 1 (1933); P. von R. Schleyer, *J. Am. Chem. Soc.*, **79**, 3292 (1957).

[4] C. Cupas, P. von R. Schleyer, and D. J. Trecker, *ibid.*, **87**, 917 (1965).

[5] V. Z. Williams, P. von R. Schleyer, G. J. Gleicher, and L. B. Rodewald, *ibid.*, **88**, 3862 (1966).

[6] "IUPAC Nomenclature of Organic Chemistry, 1957," Butterworth and Co. Ltd., London, 1958; *J. Am. Chem. Soc.*, **82**, 5534 (1960).

[7] Errors in nomenclature of bridged hydrocarbons have already received critical attention: *viz.*, J. Meinwald and J. K. Crandall, *ibid.*, **88**, 1292 (1966); K. Conrow, *J. Chem. Doc.*, **6**, 206 (1966).

[8] A planar graph is a set of points connected by lines in such a way that it is possible to draw a graph on a plane without having any pair of edges intersect. The method described in this paper is also applicable to those compounds which cannot be drawn as planar graphs.