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SYNTHESES AND SOME PROPERTIES OF DIFUNCTIONAL CYCLOSILANES

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Abstract Mixtures of structural isomers of permethylated dichlorocyclohexasilanes and disubstituted cyclopentasilanes can easily be separated after hydrolysis. The syntheses and a crystal structure are discussed.

INTRODUCTION

Difunctional cyclosilanes, which are useful monomers for the syntheses of oligocyclic and cage like silanes, are obtained after chlorination of dodecamethylcyclohexasilane with SbCl_5 in CCl_4 ^{1,2} or with $\text{Me}_3\text{SiCl} / \text{AlCl}_3$ ³, respectively.

SYNTHESES

Figure 1 shows the hydrolysis and subsequent separation of 1,3- and 1,4-dichlorododecamethylcyclohexasilane, which are produced by the SbCl_5 chlorination. The dichloro isomers can easily be regained by chlorination of the products with acetylchloride. Under acidic conditions the hydrolysed products give oligomeric and polymeric structures, which are subject of the ongoing investigations.

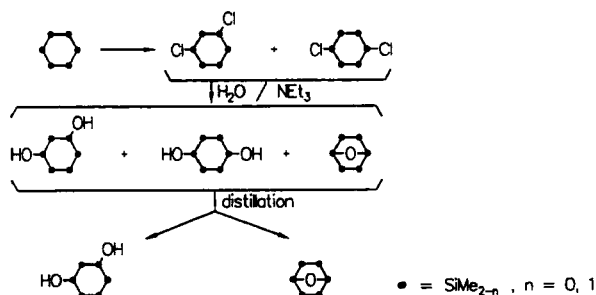


FIGURE 1

The isomeric mixture of 1-chloro-2-(chlorodimethylsilyl)octamethylcyclopentasilane and 1-chloro-3-(chlorodimethylsilyl)octamethylcyclopentasilane, which are formed in the reaction with $\text{Me}_3\text{SiCl} / \text{AlCl}_3$, behaves quite similar. In this case decamethyl-2-oxa-1,3,4,5,6,7-hexasilanorbornane is formed (figure 2).

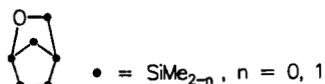


FIGURE 2

X-RAY STRUCTURE

A single crystal containing a mixture of decamethyl-7-oxa-1,2,3,4,5,6-hexasilanorbornane and 1,4-dihydroxydecamethylcyclohexasilane in a 2:1 ratio was used to determine the molecular structure. Some interesting data of decamethyl-7-oxa-1,2,3,4,5,6-hexasilanorbornane are shown in figure 3 and listed in table 1.

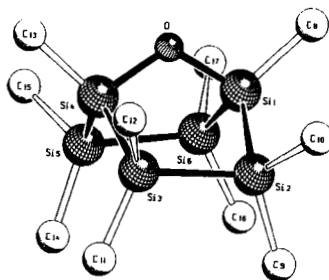


FIGURE 3

TABLE I Characteristic bond lengths and angles of decamethyl-7-oxa-1,2,3,4,5,6-hexasilanorbornane

bonds	angle (deg.)	atoms	distance (nm)
Si2-Si1-Si6	116.81(0.05)	Si1-Si2	237.3(0.1)
Si1-Si2-Si3	96.13(0.05)	Si1-O	169.7(0.2)
Si1-O-Si4	116.38(0.11)	Si1-C8	186.7(0.3)
Si2-Si1-C8	114.15(0.12)	Si2-Si3	235.9(0.2)
C9-Si2-C10	110.12(0.24)	Si2-C9	188.4(0.4)

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