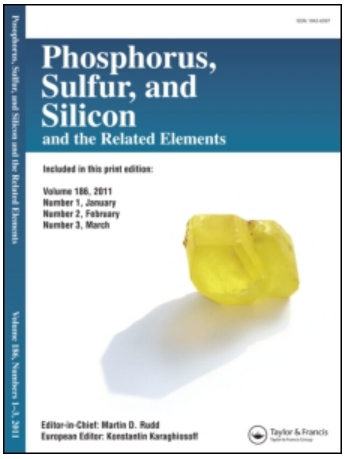

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1,4-Di(undecamethylcyclohexasilanyl)Benzene; Synthesis and Spectroscopic Properties

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1,4-DI(UNDECAMETHYLCYCLOHEXASILANYL)BENZENE; SYNTHESIS AND SPECTROSCOPIC PROPERTIES

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Abstract 1,4-Di(undecamethylcyclohexasilanyl)benzene has been synthezised and its X-ray structure determined.

INTRODUCTION

Methylated polycyclic Si-ring systems, bearing phenyl substituents, in particular 1,4-di(cylosilanyl)benzenes, should be able to form stable radical anions. This offers the possibility to investigate the expected electron acceptor effects of the Si-rings by ESR. Now we are able to report on the synthesis of the first representative of this new class of compounds.

SYNTHESIS

'One-pot *in situ*' Grignard reaction[1] of monohalocyclosilanes (*cyclo*-$Me_{11}Si_6$)-X (X = F,Cl,Br) with *p*-dibromobenzene and Mg affords 1,4-di(undecamethyl-cyclohexasilanyl)benzene in very poor yields depending on X. Bi(undecamethycyclohexasilanyl), the separation of which requires chromatographic methods, is formed as the main product by transmetallation of the halosilane. Formation of the title compound in suitable yields without any transmetallation products therefore is achieved by treating chloroundecamethylcyclohexasilane with BrMg-C_6H_4-MgBr in THF under sonication[2] (Figure 1).

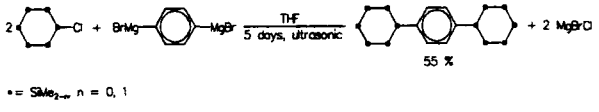

FIGURE 1 Synthesis of 1,4-di(undecamethylcyclohexasilanyl)benzene

X-RAY STRUCTURE OF 1,4-DI(UNDECAMETHYLCYCLOHEXASILANYL)-BENZENE

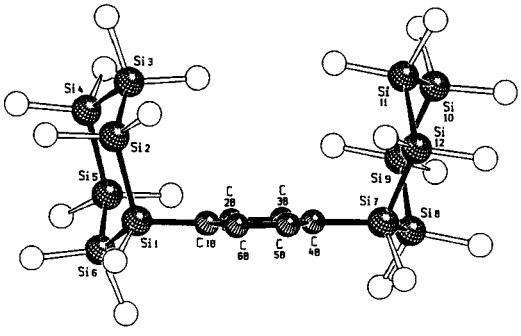

FIGURE 2 X-ray structure of 1,4-Di(undecamethylcyclohexasilanyl)benzene

The X-ray study revealed a triclinic unit cell containing three molecules. The benzene ring occupies the axial sites of the two cyclohexasilane chairs, whereas the two phenyl rings in 1,4-diphenyldecamethylcyclohexasilane are in equatorial positions[3]. Si-Si distances exhibit rather usual values between 2.350 (0.006) and 2.330 (0.006) Å. Interesting distances and angles are given in Table I.

TABLE I Interatomic distances (Å) and angles (deg)

Atoms	Distance	Bonds	Angle
Si(3)-Si(11)	7.390 (0.006)		
Si(5)-Si(9)	7.914 (0.006)	Si(6)-Si(1)-CB(1)	111.26 (0.43)
Si(1)-CB(1)	1.874 (0.011)	Si(8)-Si(7)-CB(4)	110.98 (0.40)
Si(7)-CB(4)	1.876 (0.011)	Si(2)-Si(1)-Si(7)-Si(12)	17.20 (0.23)
CB(1)-CB(2)	1.371 (0.015)	CB(6)-CB(1)-CB(2)	115.27 (1.01)
CB(2)-CB(3)	1.371 (0.014)	CB(1)-CB(2)-CB(3)	122.94 (1.06)
CB(3)-CB(4)	1.404 (0.014)	CB(2)-CB(3)-CB(4)	122.08 (1.02)
CB(4)-CB(5)	1.387 (0.015)	CB(3)-CB(4)-CB(5)	114.43 (0.97)
CB(5)-CB(6)	1.371 (0.014)	CB(4)-CB(5)-CB(6)	122.51 (1.04)
CB(6)-CB(1)	1.380 (0.015)	CB(5)-CB(6)-CB(1)	122.73 (1.06)

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