Journal of Organometallic Chemistry, 228 (1982) C83—C85
Elsevier Sequoia S.A., Lausanne — Printed in The Netherlands

Corrigendum

A CORRECTION TO THE MOLECULAR STRUCTURE OF [DIMETHYL(PHENYL)SILYL]TRIS(TRIMETHYLSILYL)METHANE

PETER B. HITCHCOCK

School of Chemistry and Molecular Sciences, University of Sussex, Brighton BN1 9QJ (Great Britain)

(Received January 18th, 1982)

Summary

In a recently published structure of $(Me_3Si)_3C(SiMe_2Ph)$ the hydrogen atoms were inadvertently misplaced. The hydrogen atom positions have been redetermined and the structure refinement repeated. There is no significant change in the averaged values for chemically equivalent bond lengths and angles from those previously reported, and the previous conclusions stand.

Introduction

During the previously reported [1] structure determination of $(Me_3Si)_3C(SiMe_2Ph)$ a systematic numbering error when transferring the coordinates of hydrogen atom peaks from a connectivity file to an atom parameter file resulted in the hydrogen atoms being assigned coordinates of either Si or C atoms*. Since the H atoms were not refined and bonds and angles involving H atoms were not recalculated the incorrect H atom coordinates were carried through the structures determination unnoticed. The H atom coordinates have now been redetermined and the least squares refinement repeated.

Experimental

The observed structure factor amplitudes were taken from the structure factor listing and assigned unit weights. Possible positions for all H atoms were taken from a difference map based on the Si and C atoms. A full matrix least squares refinement of Si and C with anisotropic temperature factors and H atoms with isotropic temperature factors was carried out. The majority of the

*I am grateful to Dr B. Beagley for drawing attention to the error.

0022-328X/82/0000—0000/$02.75

H atoms refined satisfactorily though one or two have high temperature factors and a poor geometry. The final R values were $R = 0.072$, $R' = 0.087$. The calculations were done on a PDP 11/34 computer using the Enraf-Nonius Structure Determination Package. Final atom coordinates are listed in Table 1A and 1B, and bond lengths and angles in Table 2.

TABLE 1A

FRACTIONAL ATOMIC COORDINATES ($\times 10^4$) WITH ESTIMATED STANDARD DEVIATIONS IN PARENTHESES

	x	y	z
Si(1)	1352(2)	2870(2)	5166(3)
Si(2)	825(2)	2191(2)	1963(3)
Si(3)	1108(2)	4066(2)	2474(4)
Si(4)	2655(2)	2868(2)	2613(4)
C(1)	1480(6)	2987(6)	3060(10)
C(2)	2188(9)	3407(8)	6305(13)
C(3)	323(8)	3293(8)	5805(13)
C(4)	1378(7)	1781(7)	5926(11)
C(5)	2103(9)	1444(8)	6626(14)
C(6)	2102(10)	682(10)	7270(18)
C(7)	1404(10)	224(8)	7292(17)
C(8)	662(10)	542(8)	6655(18)
C(9)	647(9)	1297(8)	5993(15)
C(10)	1320(9)	1140(8)	2061(14)
C(11)	−296(8)	2077(9)	2554(15)
C(12)	675(9)	2419(10)	−65(14)
C(13)	−78(8)	4171(9)	2218(16)
C(14)	1429(9)	4886(7)	3870(16)
C(15)	1554(10)	4397(9)	662(14)
C(16)	3309(8)	3818(9)	3075(14)
C(17)	3212(7)	2004(8)	3648(14)
C(18)	2812(8)	2673(11)	621(15)

TABLE 1B

HYDROGEN ATOM COORDINATES ($\times 10^3$) WITH ESTIMATED STANDARD DEVIATIONS IN PARENTHESES

	x	y	z
H(2A)	215(6)	357(6)	729(11)
H(2B)	267(6)	298(7)	607(11)
H(2C)	225(9)	389(9)	597(16)
H(3A)	31(5)	314(5)	688(8)
H(3B)	49(9)	369(9)	581(16)
H(3C)	−3(5)	317(5)	521(8)
H(5)	250(6)	180(6)	686(10)
H(6)	247(8)	60(7)	757(13)
H(7)	145(8)	−29(8)	807(14)
H(8)	17(8)	29(8)	633(14)
H(9)	13(6)	157(6)	560(10)
H(10A)	188(5)	127(5)	145(9)
H(10B)	97(6)	76(7)	128(11)
H(10C)	121(8)	84(6)	288(10)
H(11A)	−70(7)	255(7)	227(12)
H(11B)	−42(6)	198(6)	345(9)
H(11C)	−27(12)	182(12)	255(21)
H(12A)	112(6)	233(6)	−44(10)
H(12B)	42(5)	281(5)	−21(8)
H(12C)	56(10)	210(11)	−65(18)
H(13A)	−29(7)	376(7)	115(11)
H(13B)	−19(6)	462(6)	193(11)
H(13C)	−50(6)	393(6)	303(10)
H(14A)	198(5)	482(5)	380(8)
H(14B)	113(6)	502(7)	475(11)
H(14C)	125(6)	525(6)	346(10)
H(15A)	139(6)	484(6)	30(10)
H(15B)	113(8)	411(9)	−12(14)
H(15C)	210(7)	457(7)	103(12)
H(16A)	388(7)	369(6)	263(11)
H(16B)	342(6)	387(6)	426(11)
H(16C)	325(6)	391(7)	229(11)
H(17A)	364(6)	187(6)	305(10)
H(17B)	342(6)	225(6)	460(10)
H(17C)	293(5)	154(5)	363(9)
H(18A)	331(4)	265(4)	61(7)
H(18B)	265(5)	221(6)	32(9)
H(18C)	261(10)	311(10)	−28(17)

TABLE 2

INTRAMOLECULAR DISTANCES(Å) AND ANGLES(°) WITH ESTIMATED STANDARD DEVIATIONS IN PARENTHESES

(a) Bonds			
Si(1)—C(1)	1.920(6)	Si(1)—C(2)	1.852(9)
Si(1)—C(3)	1.873(10)	Si(1)—C(4)	1.903(7)
Si(2)—C(1)	1.905(6)	Si(2)—C(10)	1.884(9)
Si(2)—C(11)	1.874(11)	Si(2)—C(12)	1.884(12)
Si(3)—C(1)	1.921(6)	Si(3)—C(13)	1.880(9)
Si(3)—C(14)	1.886(10)	Si(3)—C(15)	1.879(10)
Si(4)—C(1)	1.919(6)	Si(4)—C(16)	1.896(10)
Si(4)—C(17)	1.883(9)	Si(4)—C(18)	1.844(11)
C(4)—C(5)	1.39(1)	C(4)—C(9)	1.40(1)
C(5)—C(6)	1.37(1)	C(6)—C(7)	1.33(2)
C(7)—C(8)	1.38(1)	C(8)—C(9)	1.37(1)
(b) Angles			
C(1)—Si(1)—C(2)	113.2(4)	C(1)—Si(1)—C(3)	113.3(4)
C(1)—Si(1)—C(4)	116.4(3)	C(2)—Si(1)—C(3)	105.1(5)
C(2)—Si(1)—C(4)	103.9(4)	C(3)—Si(1)—C(4)	103.8(5)
C(1)—Si(2)—C(10)	112.4(4)	C(1)—Si(2)—C(11)	114.6(5)
C(1)—Si(2)—C(12)	114.3(5)	C(10)—Si(2)—C(11)	106.8(6)
C(10)—Si(2)—C(12)	105.1(5)	C(11)—Si(2)—C(12)	102.5(6)
C(1)—Si(3)—C(13)	113.9(4)	C(1)—Si(3)—C(14)	113.5(4)
C(1)—Si(3)—C(15)	112.3(4)	C(13)—Si(3)—C(14)	104.6(5)
C(13)—Si(3)—C(15)	105.9(5)	C(14)—Si(3)—C(15)	105.8(6)
C(1)—Si(4)—C(16)	113.0(4)	C(1)—Si(4)—C(17)	113.9(4)
C(1)—Si(4)—C(18)	113.1(4)	C(16)—Si(4)—C(17)	105.5(5)
C(16)—Si(4)—C(18)	105.0(6)	C(17)—Si(4)—C(18)	105.6(5)
Si(1)—C(1)—Si(2)	111.3(3)	Si(1)—C(1)—Si(3)	108.4(3)
Si(1)—C(1)—Si(4)	109.9(3)	Si(2)—C(1)—Si(3)	109.3(3)
Si(2)—C(1)—Si(4)	109.2(3)	Si(3)—C(1)—Si(4)	108.7(3)
Si(1)—C(4)—C(5)	122.3(6)	Si(1)—C(4)—C(9)	122.5(6)
C(5)—C(4)—C(9)	114.7(7)	C(4)—C(5)—C(6)	122(1)
C(5)—C(6)—C(7)	122(1)	C(6)—C(7)—C(8)	118.0(9)
C(7)—C(8)—C(9)	121(1)	C(4)—C(9)—C(8)	121.9(9)

Discussion

The average dimensions in the molecule with r.m.s. deviations are Si—C(1) 1.916(7) Å, other Si—C 1.877(16) Å, Si—C(1)—Si 109.5(9)°, C(1)—Si—C 113.7(11)°, and other C—Si—C 105.0(11)°. These values are essentially the same as those previously reported. This confirms that the steric strain mainly manifests itself in a closing up of the angles within the $SiMe_3$ and $SiMe_2Ph$ groups and a lengthening of the bonds from silicon to the central carbon atom C(1).

Reference

1 C. Eaborn, P.B. Hitchcock and P.D. Lickiss, J. Organometal. Chem., 221 (1981) 13.