Crystal structure of di-*tert*-butylbis(3-trimethylsilylethinyl)silane, $(C_4H_9)_2Si[C_2Si(CH_3)_3]_2$

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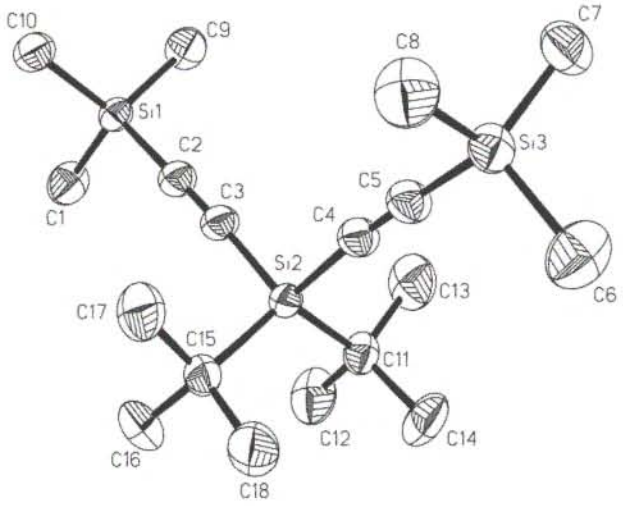

Abstract

$C_{18}H_{36}Si_3$, monoclinic, $C12/c1$ (No. 15), $a = 27.284(2)$ Å, $b = 8.769(1)$ Å, $c = 20.467(2)$ Å, $\beta = 99.75(1)°$, $V = 4826.1$ Å^3, $Z = 8$, $R_{gt}(F) = 0.059$, $wR(F) = 0.057$, T = 293 K.

Source of material

Photolysis of hexa-*tert*-butylcyclotrisilane or 1,1-di-*tert*-butyl-*trans*-2,3-dimethylsilirane in the presence of 1,4-bis(trimethylsilyl)buta-1,3-diyne furnishes the title compound [1].

Discussion

The crystal structure analysis reveals a distorted tetrahedral environment of the middle silicon atom. The most conspicuous features are the short Si–C bond lengths to the acetylenic carbon atoms of 184.4(2) pm and 185.2(3) pm and the considerable widened C–Si–C bond angle of 119.7(1)° within the $^tBu_2Si$ moiety [2].

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Table 1. Data collection and handling.

Crystal:	colourless plate, size 1.2 × 1.0 × 0.3 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	1.90 cm^{-1}
Diffractometer, scan mode:	Bruker AXS P4, ω
$2\theta_{max}$:	55°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	6035, 5546
Criterion for F_{obs}, $N(hkl)_{gt}$:	$F_{obs} > 3\,\sigma(F_{obs})$, 3924
$N(param)_{refined}$:	190
Program:	SHELXTL-plus [3]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(1A)	8*f*	–0.0708(1)	–0.3171(4)	0.6489(2)	0.08
H(1B)	8*f*	–0.0486(1)	–0.1820(4)	0.6947(2)	0.08
H(1C)	8*f*	–0.0144(1)	–0.3178(4)	0.6809(2)	0.08
H(6A)	8*f*	0.2563(1)	0.6265(4)	0.5253(2)	0.08
H(6B)	8*f*	0.2658(1)	0.4751(4)	0.5662(2)	0.08
H(6C)	8*f*	0.2356(1)	0.6081(4)	0.5918(2)	0.08
H(7A)	8*f*	0.2088(1)	0.4401(4)	0.4038(2)	0.08
H(7B)	8*f*	0.1654(1)	0.3273(4)	0.4107(2)	0.08
H(7C)	8*f*	0.2197(1)	0.2916(4)	0.4464(2)	0.08
H(8A)	8*f*	0.1497(1)	0.6963(4)	0.4538(2)	0.08
H(8B)	8*f*	0.1312(1)	0.6774(4)	0.5219(2)	0.08
H(8C)	8*f*	0.1073(1)	0.5797(4)	0.4606(2)	0.08
H(9A)	8*f*	–0.0399(1)	–0.3518(3)	0.5113(2)	0.08
H(9B)	8*f*	0.0159(1)	–0.3528(3)	0.5465(2)	0.08
H(9C)	8*f*	–0.0021(1)	–0.2345(3)	0.4901(2)	0.08
H(10A)	8*f*	–0.1076(1)	–0.0851(3)	0.5381(1)	0.08
H(10B)	8*f*	–0.0693(1)	0.0297(3)	0.5164(1)	0.08
H(10C)	8*f*	–0.0852(1)	0.0459(3)	0.5862(1)	0.08
H(12A)	8*f*	0.1514(1)	–0.0189(4)	0.7942(2)	0.08
H(12B)	8*f*	0.1832(1)	–0.1532(4)	0.7730(2)	0.08
H(12C)	8*f*	0.1271(1)	–0.1367(4)	0.7408(2)	0.08
H(13A)	8*f*	0.1897(1)	–0.0229(4)	0.6120(2)	0.08
H(13B)	8*f*	0.1504(1)	–0.1394(4)	0.6298(2)	0.08
H(13C)	8*f*	0.2065(1)	–0.1559(4)	0.6620(2)	0.08
H(14A)	8*f*	0.2156(1)	0.1638(4)	0.7667(2)	0.08
H(14B)	8*f*	0.2302(1)	0.1594(4)	0.6958(2)	0.08
H(14C)	8*f*	0.2457(1)	0.0251(4)	0.7456(2)	0.08
H(16A)	8*f*	0.1057(1)	0.1742(4)	0.8097(2)	0.08
H(16B)	8*f*	0.0524(1)	0.1691(4)	0.7668(2)	0.08
H(16C)	8*f*	0.0693(1)	0.3122(4)	0.8108(2)	0.08
H(17A)	8*f*	0.0326(1)	0.3347(4)	0.6674(2)	0.08
H(17B)	8*f*	0.0724(1)	0.4494(4)	0.6497(2)	0.08
H(17C)	8*f*	0.0483(1)	0.4761(4)	0.7131(2)	0.08
H(18A)	8*f*	0.1692(1)	0.3557(4)	0.7795(2)	0.08
H(18B)	8*f*	0.1314(1)	0.4895(4)	0.7811(2)	0.08
H(18C)	8*f*	0.1555(1)	0.4628(4)	0.7178(2)	0.08

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Si(1)	8*f*	–0.02664(2)	–0.15231(8)	0.58919(3)	0.0481(4)	0.0539(4)	0.0582(4)	–0.0054(3)	0.0031(3)	–0.0029(3)
Si(2)	8*f*	0.12083(2)	0.15682(8)	0.66944(3)	0.0419(3)	0.0546(4)	0.0468(4)	–0.0053(3)	0.0075(3)	0.0001(3)
Si(3)	8*f*	0.18411(3)	0.47532(9)	0.50689(4)	0.0707(5)	0.0676(5)	0.0695(5)	–0.0014(4)	0.0171(4)	0.0195(4)
C(1)	8*f*	–0.0420(1)	–0.2546(4)	0.6622(2)	0.074(2)	0.100(2)	0.093(2)	–0.005(2)	0.013(2)	0.025(2)
C(2)	8*f*	0.0292(1)	–0.0337(3)	0.6178(1)	0.057(1)	0.066(2)	0.058(1)	–0.006(1)	0.007(1)	–0.002(1)
C(3)	8*f*	0.06531(9)	0.0434(3)	0.6361(1)	0.054(1)	0.066(2)	0.053(1)	–0.008(1)	0.005(1)	–0.002(1)
C(4)	8*f*	0.14303(9)	0.2619(3)	0.6016(1)	0.062(2)	0.067(2)	0.055(1)	–0.010(1)	0.009(1)	0.002(1)
C(5)	8*f*	0.1593(1)	0.3408(3)	0.5629(1)	0.071(2)	0.070(2)	0.059(2)	–0.008(1)	0.014(1)	0.004(1)
C(6)	8*f*	0.2425(1)	0.5560(4)	0.5531(2)	0.106(3)	0.092(3)	0.140(3)	–0.025(2)	0.005(2)	0.024(2)
C(7)	8*f*	0.1959(1)	0.3711(4)	0.4331(2)	0.101(3)	0.138(3)	0.078(2)	0.017(2)	0.031(2)	0.022(2)
C(8)	8*f*	0.1375(1)	0.6251(4)	0.4829(2)	0.117(3)	0.095(3)	0.129(3)	0.020(2)	0.024(3)	0.028(2)
C(9)	8*f*	–0.0113(1)	–0.2894(3)	0.5268(2)	0.080(2)	0.071(2)	0.094(2)	–0.000(2)	0.007(2)	–0.018(2)
C(10)	8*f*	–0.0784(1)	–0.0251(3)	0.5531(1)	0.069(2)	0.075(2)	0.073(2)	0.004(2)	–0.000(1)	–0.006(2)
C(11)	8*f*	0.17158(9)	0.0171(3)	0.7039(1)	0.056(2)	0.070(2)	0.075(2)	0.007(1)	0.013(1)	0.009(1)
C(12)	8*f*	0.1570(1)	–0.0820(4)	0.7579(2)	0.095(3)	0.111(3)	0.128(3)	0.031(2)	0.022(2)	0.050(3)
C(13)	8*f*	0.1803(1)	–0.0847(4)	0.6466(2)	0.103(3)	0.097(3)	0.141(3)	0.037(2)	0.026(2)	–0.007(3)
C(14)	8*f*	0.2203(1)	0.0989(4)	0.7305(2)	0.055(2)	0.125(3)	0.136(3)	0.015(2)	–0.010(2)	–0.001(3)
C(15)	8*f*	0.10035(9)	0.3069(3)	0.7257(1)	0.055(1)	0.069(2)	0.067(2)	0.001(1)	0.014(1)	–0.015(1)
C(16)	8*f*	0.0800(1)	0.2338(4)	0.7837(2)	0.110(3)	0.122(3)	0.079(2)	0.008(2)	0.043(2)	–0.014(2)
C(17)	8*f*	0.0597(1)	0.4003(4)	0.6853(2)	0.095(2)	0.094(2)	0.120(3)	0.031(2)	0.023(2)	–0.011(2)
C(18)	8*f*	0.1431(1)	0.4137(4)	0.7536(2)	0.096(3)	0.109(3)	0.132(3)	–0.016(2)	0.028(2)	–0.062(3)

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