Crystal structure of bis(3,3-dimethylbut-1-ynyl)di-*tert*-butylsilane, $(C_4H_9C_2)_2Si(C_4H_9)_2$

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Abstract

$C_{20}H_{36}Si$, monoclinic, $P12_1/c1$ (No. 14), $a = 11.2100(7)$ Å, $b = 11.2574(7)$ Å, $c = 17.874(2)$ Å, $\beta = 99.213(6)^\circ$, $V = 2226.5$ Å³, $Z = 4$, $R_g(F) = 0.082$, $wR(F) = 0.080$, $T = 293$ K.

Source of material

Photolysis of 1,1-di-*tert*-butyl-*trans*-2,3-dimethylsilirane in the presence of 2,2,7,7-tetramethylocta-3,5-diene or the light-induced rearrangement of 1,1,2-tri-*tert*-butyl-3-(3,3-dimethylbut-1-ynyl)-1*H*-silirene furnishes the title compound.

Discussion

The crystal structure analysis reveals a distorted tetrahedral environment of the central silicon atom. The most conspicuous features are the short Si—C bond lengths to the acetylenic carbon atoms of 182.1(3) pm and 182.6(3) pm (normal bond length 189 pm [1]) and the appreciably widened C—Si—C bond angle of $119.3(2)^\circ$ within the *tert*-Bu₂Si moiety.

Table 1. Data collection and handling.

Crystal:	colourless prism, size $0.55 \times 0.75 \times 0.95$ mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ :	1.00 cm^{-1}
Diffractometer, scan mode:	Bruker AXS P4, ω
$2\theta_{\max}$:	55°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	5610, 5083
Criterion for F_{obs} , $N(hkl)_{\text{gt}}$:	$F_{\text{obs}} > 3 \sigma(F_{\text{obs}})$, 3954
$N(\text{param})_{\text{refined}}$:	190
Program:	SHELXTL-plus [2]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(31A)	4e	0.2999(4)	0.1546(4)	0.1459(2)	0.08
H(31B)	4e	0.2634(4)	0.0880(4)	0.2158(2)	0.08
H(31C)	4e	0.3543(4)	0.0291(4)	0.1689(2)	0.08
H(32A)	4e	0.5344(4)	0.1096(4)	0.3400(2)	0.08
H(32B)	4e	0.4917(4)	0.0050(4)	0.2842(2)	0.08
H(32C)	4e	0.4007(4)	0.0639(4)	0.3312(2)	0.08
H(33A)	4e	0.4411(4)	0.3140(3)	0.3041(2)	0.08
H(33B)	4e	0.3141(4)	0.2532(3)	0.2983(2)	0.08
H(33C)	4e	0.3481(4)	0.3229(3)	0.2288(2)	0.08
H(61A)	4e	0.7542(3)	0.4858(4)	−0.0945(2)	0.08
H(61B)	4e	0.8866(3)	0.5091(4)	−0.0537(2)	0.08
H(61C)	4e	0.8110(3)	0.6128(4)	−0.0964(2)	0.08
H(62A)	4e	0.8185(4)	0.6847(3)	0.0969(2)	0.08
H(62B)	4e	0.8500(4)	0.7320(3)	0.0199(2)	0.08
H(62C)	4e	0.9257(4)	0.6282(3)	0.0626(2)	0.08
H(63A)	4e	0.6395(3)	0.7022(3)	−0.0409(2)	0.08
H(63B)	4e	0.6104(3)	0.6507(3)	0.0356(2)	0.08
H(63C)	4e	0.5812(3)	0.5759(3)	−0.0391(2)	0.08
H(71A)	4e	0.7885(4)	0.3025(4)	0.2875(2)	0.08
H(71B)	4e	0.8610(4)	0.3896(4)	0.2432(2)	0.08
H(71C)	4e	0.9296(4)	0.3092(4)	0.3077(2)	0.08
H(72A)	4e	0.8962(4)	0.0392(4)	0.2111(3)	0.08
H(72B)	4e	0.8170(4)	0.0875(4)	0.2692(3)	0.08
H(72C)	4e	0.9582(4)	0.0978(4)	0.2870(3)	0.08
H(73A)	4e	1.0200(3)	0.1938(5)	0.1464(3)	0.08
H(73B)	4e	1.0605(3)	0.2463(5)	0.2278(3)	0.08
H(73C)	4e	0.9918(3)	0.3267(5)	0.1632(3)	0.08
H(81A)	4e	0.7992(4)	−0.0302(3)	0.1104(3)	0.08
H(81B)	4e	0.7245(4)	−0.0612(3)	0.0310(3)	0.08
H(81C)	4e	0.6586(4)	−0.0133(3)	0.0959(3)	0.08
H(82A)	4e	0.9252(4)	0.1053(4)	0.0439(3)	0.08
H(82B)	4e	0.8638(4)	0.2035(4)	−0.0115(3)	0.08
H(82C)	4e	0.8424(4)	0.0688(4)	−0.0318(3)	0.08
H(83A)	4e	0.5617(4)	0.1478(4)	0.0143(2)	0.08
H(83B)	4e	0.6231(4)	0.0903(4)	−0.0498(2)	0.08
H(83C)	4e	0.6445(4)	0.2249(4)	−0.0295(2)	0.08

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Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
Si(1)	4e	0.75049(7)	0.22898(7)	0.12828(4)	0.0561(4)	0.0529(4)	0.0716(5)	0.0082(4)	0.0252(4)	0.0144(4)
C(1)	4e	0.6129(3)	0.2098(3)	0.1696(2)	0.062(2)	0.068(2)	0.074(2)	0.004(1)	0.021(1)	0.012(1)
C(2)	4e	0.5291(3)	0.1893(3)	0.2015(2)	0.061(2)	0.069(2)	0.070(2)	0.002(1)	0.017(1)	0.008(1)
C(3)	4e	0.4280(3)	0.1614(3)	0.2415(2)	0.064(2)	0.072(2)	0.072(2)	−0.001(1)	0.028(1)	0.008(2)
C(4)	4e	0.7513(3)	0.3755(3)	0.0853(2)	0.069(2)	0.062(2)	0.072(2)	0.012(1)	0.025(1)	0.012(1)
C(5)	4e	0.7562(3)	0.4661(3)	0.0508(2)	0.065(2)	0.057(2)	0.066(2)	0.009(1)	0.020(1)	0.005(1)
C(6)	4e	0.7619(3)	0.5750(3)	0.0065(2)	0.067(2)	0.057(2)	0.065(2)	0.007(1)	0.019(1)	0.015(1)
C(7)	4e	0.8813(3)	0.2217(3)	0.2095(2)	0.068(2)	0.088(2)	0.088(2)	0.009(2)	0.016(2)	0.020(2)
C(8)	4e	0.7429(3)	0.1190(3)	0.0479(2)	0.087(2)	0.070(2)	0.093(3)	0.008(2)	0.032(2)	−0.000(2)
C(31)	4e	0.3279(4)	0.1029(4)	0.1877(2)	0.105(3)	0.159(5)	0.130(4)	−0.038(3)	0.050(3)	−0.015(3)
C(32)	4e	0.4679(4)	0.0782(4)	0.3051(2)	0.125(4)	0.137(4)	0.132(4)	0.024(3)	0.067(3)	0.052(3)
C(33)	4e	0.3786(4)	0.2729(3)	0.2710(2)	0.112(3)	0.093(3)	0.148(4)	0.003(2)	0.075(3)	−0.001(3)
C(61)	4e	0.8073(3)	0.5427(4)	−0.0663(2)	0.120(3)	0.104(3)	0.092(3)	0.020(2)	0.048(2)	0.028(2)
C(62)	4e	0.8465(4)	0.6627(3)	0.0508(2)	0.112(3)	0.077(2)	0.134(4)	−0.009(2)	0.008(3)	0.012(2)
C(63)	4e	0.6367(3)	0.6313(3)	−0.0114(2)	0.087(2)	0.100(3)	0.106(3)	0.027(2)	0.032(2)	0.045(2)
C(71)	4e	0.8621(4)	0.3134(4)	0.2673(2)	0.097(3)	0.157(5)	0.108(3)	−0.003(3)	−0.006(3)	−0.016(3)
C(72)	4e	0.8891(4)	0.1002(4)	0.2476(3)	0.144(4)	0.125(4)	0.127(4)	0.010(3)	−0.024(3)	0.051(3)
C(73)	4e	0.9988(3)	0.2477(5)	0.1838(3)	0.063(2)	0.201(5)	0.140(4)	0.012(3)	0.009(2)	0.025(4)
C(81)	4e	0.7308(4)	−0.0083(3)	0.0735(3)	0.195(5)	0.069(3)	0.149(4)	0.005(3)	0.042(4)	−0.012(3)
C(82)	4e	0.8542(4)	0.1257(4)	0.0088(3)	0.145(4)	0.148(4)	0.137(4)	0.006(3)	0.074(3)	−0.039(3)
C(83)	4e	0.6328(4)	0.1474(4)	−0.0094(2)	0.153(4)	0.131(4)	0.102(3)	0.005(3)	0.014(3)	−0.036(3)

References

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