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Bis(trimethylsilyl)acetylene

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Abstract

The structure of the title compound, $C_8H_{18}Si_2$, at 102 K, is characterized by a centre of inversion located on the central triple bond, which is 1.208 (3) Å long.

Comment

Most transition metals form polynuclear complexes containing bridging acetylenic ligands (Varga, Mach, Schmid & Thewalt, 1994). The metal used for complexation is crucial for the strength of coordination, which is reflected, among other ways, in the elongation of the acetylenic C—C bond (Hiller *et al.*, 1996). Some of these complexes are of interest as postulated intermediates in catalytic reactions (Bonrath, Pörschke, Wilke, Angermund & Krüger, 1988) and as models for the chemisorption of unsaturated hydrocarbons to metallic surfaces of heterogeneous catalysts (Beck, Niemer & Wieser, 1993). The title compound, (I), is frequently used as a ligand in such complexation studies; therefore its molecular structure is of interest.

(I)

A crystal of (I) (m.p. 293 K) was grown using *in situ* techniques as described previously (Brodalla, Mootz, Boese & Osswald, 1985). The crystal structure analysis reveals (I) to be located on a centre of inversion. As a consequence, both trimethylsilyl groups are in staggered positions (Fig. 1). The C1—C1^i [symmetry code: (i) $-x, -y, 1 - z$] length [1.208 (3) Å] is typical for C≡C bonds. The C_{sp}—Si bond length is somewhat shorter than the C_{sp^3}—Si bonds (Table 2). Intramolecular steric strain between the methyl groups results in C_{sp^3}—Si—C_{sp^3} angles [110.35 (8)–111.16 (8)°] being widened by about 2–3° compared with the C_{sp}—Si—C_{sp^3} angles [107.83 (6)–108.49 (6)°]. The slight deviation of the Si—C1—C1^i angle [179.1 (2)°] from the idealized 180° may be due to intermolecular interactions.

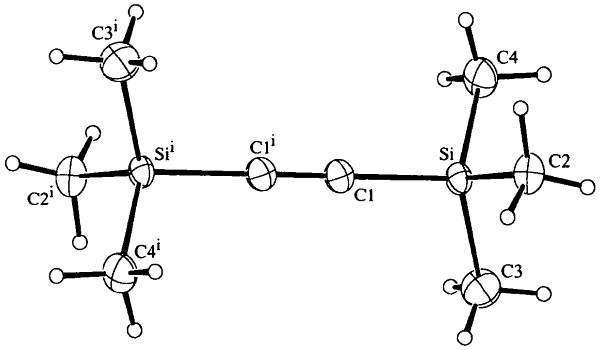

Fig. 1. A view (*ORTEP*II; Johnson, 1976) of the title molecule showing the labelling of the non-H atoms. Displacement ellipsoids are drawn at the 50% probability level.

Experimental

The crystal was grown by zone-melting techniques in a glass capillary with a focused halogen lamp as heat source (Brodalla, Mootz, Boese & Osswald, 1985) at 292 K.

Crystal data

$C_8H_{18}Si_2$
$M_r = 170.40$
Monoclinic
$P2_1/c$
$a = 6.025\,(1)$ Å
$b = 10.519\,(1)$ Å
$c = 9.584\,(1)$ Å
$\beta = 105.91\,(1)°$
$V = 584.1\,(1)$ Å^3
$Z = 2$
$D_x = 0.969$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 25 reflections
$\theta = 9.1–25.6°$
$\mu = 0.248$ mm^{-1}
$T = 102$ K
Cylindrical
$0.35 \times 0.30 \times 0.25$ mm
Colourless

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega–2\theta$ scan
Absorption correction: none
1491 measured reflections
1337 independent reflections
1229 reflections with $I > 2\sigma(I)$

$R_{int} = 0.010$
$\theta_{max} = 27.45°$
$h = -7 \rightarrow 7$
$k = 0 \rightarrow 13$
$l = 0 \rightarrow 12$
3 standard reflections
frequency: 30 min
intensity decay: 6.2%

Refinement

Refinement on F^2
$R(F) = 0.045$
$wR(F^2) = 0.124$
$S = 1.117$
1337 reflections
82 parameters
All H atoms refined
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.527$ e Å^{-3}
$\Delta\rho_{min} = -0.587$ e Å^{-3}
Extinction correction: none
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)*

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U^{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Si	0.12554 (6)	0.11021 (3)	0.30972 (3)	0.0187 (2)
C1	0.0320 (2)	0.02729 (12)	0.45355 (14)	0.0224 (3)
C2	−0.1365 (2)	0.1508 (2)	0.1626 (2)	0.0274 (3)
C3	0.2819 (3)	0.2570 (2)	0.3881 (2)	0.0348 (4)
C4	0.3183 (3)	0.00263 (15)	0.2430 (2)	0.0297 (4)

Table 2. *Selected geometric parameters (Å, °)*

Si—C1	1.844 (1)	Si—C3	1.857 (2)
Si—C2	1.855 (2)	C1—C1^{i}	1.208 (3)
Si—C4	1.855 (1)		
C1—Si—C2	107.83 (6)	C2—Si—C3	110.35 (8)
C1—Si—C4	108.49 (6)	C4—Si—C3	110.51 (8)
C2—Si—C4	111.16 (8)	C1^{i}—C1—Si	179.1 (2)
C1—Si—C3	108.40 (7)		

Symmetry code: (i) $-x, -y, 1 - z$.

The structure was solved by direct methods (Sheldrick, 1990) and refined by full-matrix least squares (Sheldrick, 1993). The H atoms were refined isotropically.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989). Cell refinement: *CAD*-4 *Software*. Data reduction: *DATAP* (Coppens, Leiserowitz & Rabinovich, 1965). Molecular graphics: *ORTEP*II (Johnson, 1976).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: JZ1194). Services for accessing these data are described at the back of the journal.

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Pyrrole and a Co-crystal of 1*H*- and 2*H*-1,2,3-Triazole

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Abstract

The crystal structures of solid pyrrole, C_4H_5N, and 1,2,3-triazole, $C_2H_3N_3$, are described. Pyrrole shows an N—H···π interaction between neighbouring molecules, whereas 1,2,3-triazole is found to crystallize as a 1:1 molecular complex of its two possible tautomers, 1*H*-1,2,3-triazole and 2*H*-1,2,3-triazole, linked by an N—H···N hydrogen bond.

Comment

In all, there are six thermally stable aza derivatives of pyrrole resulting from progressive substitution of

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