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# 2,7-Dimethyl-4,5-bis(trimethylsilyl)octa-2,3,5,6-tetraene

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**Key indicators**

Single-crystal X-ray study
$T$ = 178 K
Mean $\sigma$(C–C) = 0.003 Å
$R$ factor = 0.042
$wR$ factor = 0.115
Data-to-parameter ratio = 24.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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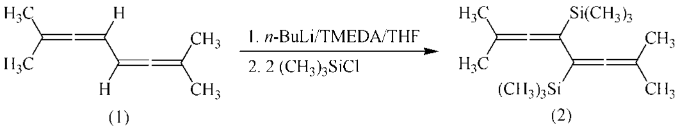
The title compound, $C_{16}H_{30}Si_2$, possesses crystallographic inversion symmetry. The allenic bond lengths are 1.309 (2) and 1.314 (2) Å.

## Comment

As the cumulogues of conjugated dienes, conjugated bis-allenes are of interest for preparative (*e.g.* as partners in cycloaddion reactions; Sankararaman *et al.*, 2000) and structural reasons. The structure of the parent system 1,2,4,5-hexatetraene in solution and in the gas phase has been described (Christensen *et al.*, 1973; Traetteberg *et al.*, 1973). Since structural data for this class of hydrocarbon are still scarce, we decided to prepare 2,7-dimethyl-4,5-bis(trimethylsilyl)octa-2,3,5,6-tetraene, (2), a fully substituted bis-allene, and investigate it by X-ray structural analysis. As a precursor we used 2,7-dimethylocta-2,4,5,6-tetraene, (1), whose solid-state structure we have reported recently (Jones *et al.*, 2002).



The structure of (2) is shown in Fig. 1. The molecule possesses a crystallographic inversion centre at the midpoint of the C4—C4$^i$ bond [symmetry code: (i) $1 - x$, $-y$, $1 - z$]. Bond lengths and angles [*e.g.* the allenic bond lengths of 1.309 (2) and 1.314 (2) Å] may be considered normal [*cf.* 1.3067 (16) and 1.3126 (16) Å in (1); Jones *et al.*, 2002]. The planes C1/2/3/5 and Si/C3/4/4$^i$ are mutually perpendicular [interplanar angle 88.49 (8)°].

The packing (Fig. 2) is unexceptional. The shortest H···H contacts are H6*A*···H8*A*($1 - x$, $1 - y$, $-z$) = 2.53 Å and H7*B*···H8*C*($1 + x$, $y$, $z$) = 2.52 Å.

## Experimental

Compound (1) was metallated with $n$-butyllithium in thf in the presence of tetramethylethylenediamine, and the resulting dianion was then quenched with trimethylsilylchloride (Stamm, 1992). Recrystallization of (2) from pentane afforded single crystals.

*Crystal data*

$C_{16}H_{30}Si_2$
$M_r$ = 278.58
Triclinic, $P\bar{1}$
$a$ = 6.363 (2) Å
$b$ = 8.963 (2) Å
$c$ = 9.157 (3) Å
$\alpha$ = 70.76 (2)°
$\beta$ = 72.13 (2)°
$\gamma$ = 83.41 (2)°
$V$ = 469.2 (2) Å$^3$
$Z$ = 1
$D_x$ = 0.986 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 50 reflections
$\theta$ = 10–11.5°
$\mu$ = 0.18 mm$^{-1}$
$T$ = 178 (2) K
Prism, colourless
0.70 × 0.25 × 0.15 mm

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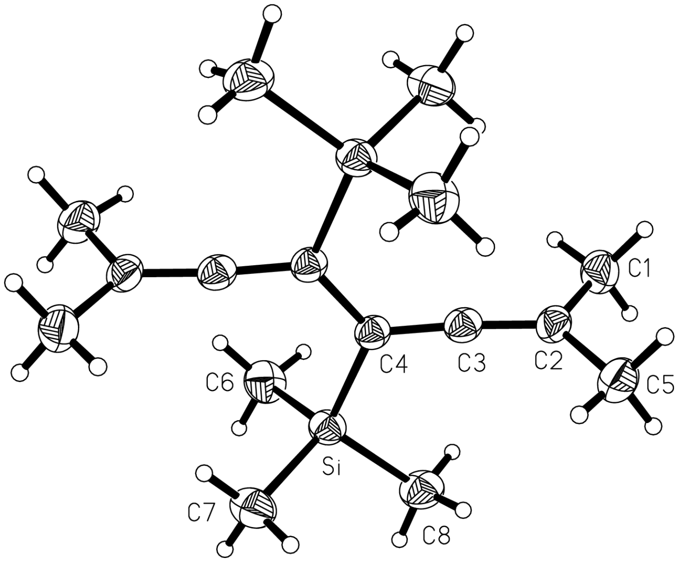

**Figure 1**
The molecule of compound (2) in the crystal. Ellipsoids are drawn at the 50% probability level. H-atom radii are arbitrary.

*Data collection*

Nicolet *R*3 diffractometer
$\omega$ scans
2355 measured reflections
2162 independent reflections
1613 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.015$
$\theta_{\max} = 27.6°$
$h = 0 \rightarrow 8$
$k = -11 \rightarrow 11$
$l = -11 \rightarrow 11$
3 standard reflections
every 147 reflections
intensity decay: none

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.115$
$S = 1.02$
2162 reflections
87 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.056P)^2 + 0.1101P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.29$ e Å$^{-3}$
$\Delta\rho_{\min} = -0.21$ e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| C2—C3 | 1.309 (2) | C4—C4$^{\rm i}$ | 1.501 (3) |
| C3—C4 | 1.314 (2) | | |
| C2—C3—C4 | 174.86 (18) | C3—C4—Si | 116.38 (13) |
| C3—C4—C4$^{\rm i}$ | 121.56 (19) | C4$^{\rm i}$—C4—Si | 122.06 (16) |

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

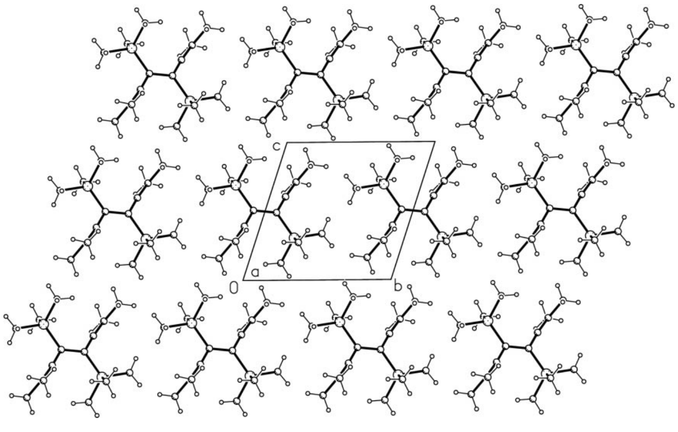

**Figure 2**
The packing of compound (2), projected parallel to the *a* axis. Radii are arbitrary.

Methyl H atoms were identified in difference syntheses, idealized and then refined using rigid methyl groups (C—H = 0.98 Å and H—C—H = 109.5°), allowed to rotate but not tip.

Data collection: *P*3 (Nicolet, 1987); cell refinement: *P*3; data reduction: *XDISK* (Nicolet, 1987); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1994); software used to prepare material for publication: *SHELXL*97.

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