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ortho-Bis(dimethylsilyl)hexamethyldecasilasesquioxane

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(i–C) = 0.005 Å
R factor = 0.070
wR factor = 0.163
Data-to-parameter ratio = 23.7

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

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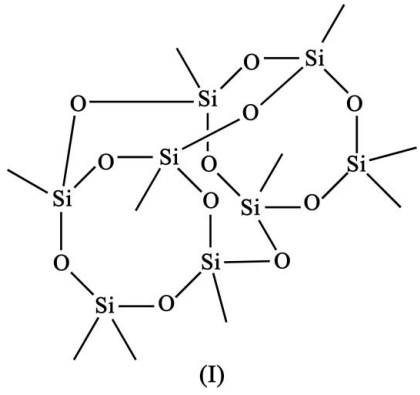
The title compound, $C_{10}H_{30}O_{11}Si_8$, crystallizes with two half-molecules in the asymmetric unit; each molecule is located on a twofold rotation axis. The geometric parameters of the two crystallographically independent molecules are almost identical.

Comment

The title compound, (I), is the product of an insertion reaction (Bassindale *et al.*, 2003). A perspective view of (I) is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 5.27 plus one update; *MOGUL* Version 1.1; Allen, 2002). There are two half-molecules in the asymmetric unit. The complete molecules are generated by twofold rotation axes, one along c and the other along a, respectively. The geometric parameters of the two crystallographically independent molecules are almost identical. A least-squares fit of all non-H atoms (r.m.s. deviation = 0.0142 Å) is shown in Fig. 3.



(I)

Experimental

The title compound was synthesized according to the procedure described by Bassindale *et al.* (2003). Colourless needle-shaped crystals suitable for X-ray diffraction were grown from a 1:1 dichloromethane–acetone solution of (I).

Crystal data

$C_{10}H_{30}O_{11}Si_8$
M_r = 551.06
Orthorhombic, *Pnna*
a = 16.927 (1) Å
b = 36.212 (2) Å
c = 8.5413 (7) Å
V = 5235.5 (6) Å^3
Z = 8
D_x = 1.398 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 510 reflections
θ = 1–25°
μ = 0.45 mm^{-1}
T = 173 (2) K
Needle, colourless
0.52 × 0.18 × 0.15 mm

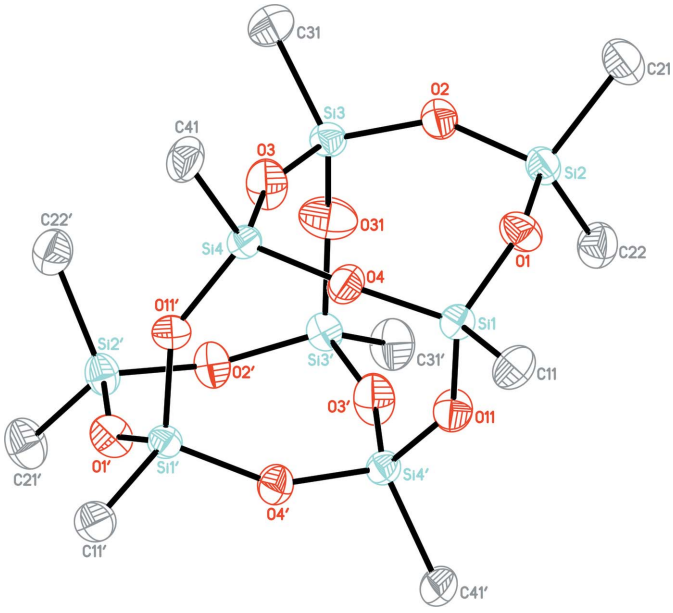


Figure 1
Perspective view of the first crystallographically independent molecule of the title compound with the atom-numbering scheme; displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted for clarity. Primed atoms are generated by the symmetry code $(\frac{1}{2} - x, 1 - y, z)$.

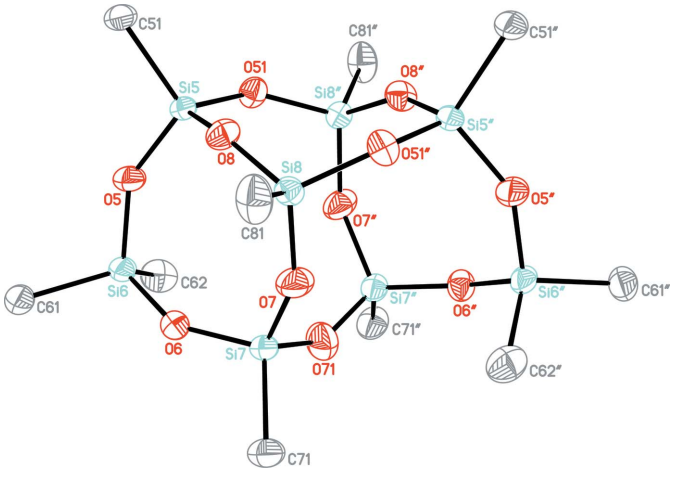


Figure 2
Perspective view of the second crystallographically independent molecule of the title compound with the atom-numbering scheme; displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted for clarity. Doubly primed atoms are generated by the symmetry code $(x, \frac{3}{2} - y, \frac{1}{2} - z)$.

Data collection

Siemens SMART CCD three-circle diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.798, T_{max} = 0.935
85682 measured reflections
6239 independent reflections
4682 reflections with $I > 2\sigma(I)$
R_{int} = 0.096
θ_{max} = 27.9°
$h = -22 \rightarrow 21$
$k = -47 \rightarrow 46$
$l = -11 \rightarrow 11$

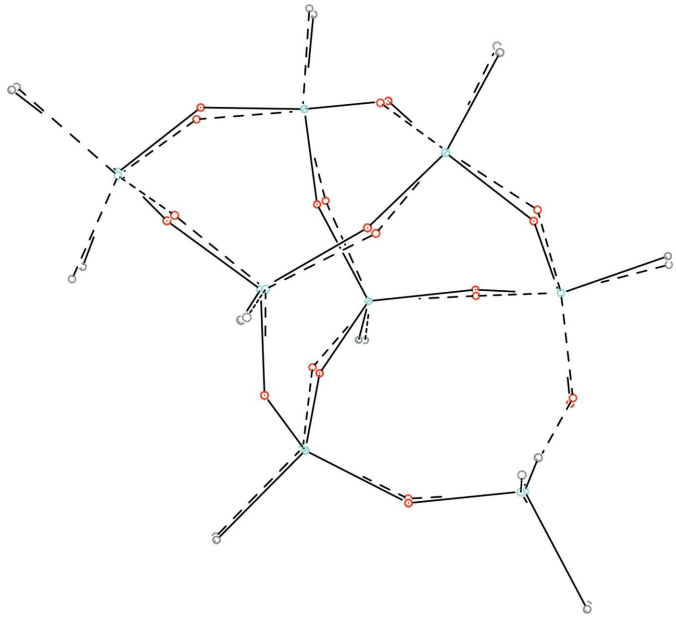


Figure 3
Least-squares fit of the two crystallographically independent molecules.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.163
S = 1.25
6239 reflections
263 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0317P)^2 + 21.419P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

All H atoms were located in a difference map but were positioned with idealized geometry (C—H = 0.98 Å) and refined with fixed individual displacement parameters [U_{iso}(H) = 1.5U_{eq}(C)] using a riding model.

Data collection: *SMART* (Siemens,1995); cell refinement: *SMART*; data reduction: *SAINT* (Siemens,1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

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