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Hexakis(trimethylsiloxymethyl)benzene methanol disolvate

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In the structure of the centrosymmetric title compound, $C_{30}H_{66}O_6Si_6\cdot 2CH_3OH$, $OSiMe_3$ groups are located above and below the plane defined by the central benzene ring in an alternating fashion.

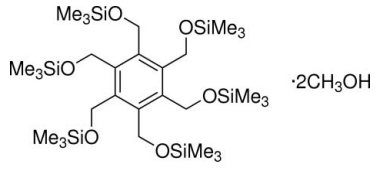
Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.004 Å
Disorder in main residue
R factor = 0.057
wR factor = 0.213
Data-to-parameter ratio = 22.4

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

Comment

The molecular stucture of $C_{32}H_{74}O_8Si_6$, (I), is shown in Fig. 1. The benzene ring is located on an inversion centre. Atom O1 is disordered over two positions (1:1). One methanol solvent molecule is disordered over two positions (3:1).



(I)

Experimental

The title compound was prepared according to a published procedure and recrystallized from methanol (Alphonse *et al.*, 1988).

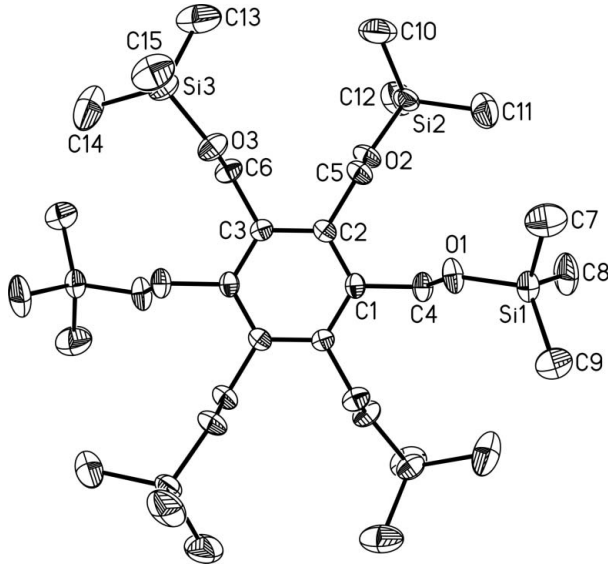


Figure 1
The molecular structure of (I) (displacement ellipsoids are drawn at the 50% probability level). H atoms are drawn as spheres of arbitrary radius. Only one disordered component is shown; methanol solvent molecules have been omitted for clarity. Unlabelled atoms are related to labelled atoms by $(1-x, 1-y, 1-z)$.

Crystal data

$C_{30}H_{66}O_6Si_6 \cdot 2CH_4O$
$M_r = 755.45$
Triclinic, $P\overline{1}$
$a = 9.7075$ (19) Å
$b = 10.153$ (2) Å
$c = 12.227$ (2) Å
$\alpha = 101.34$ (3)°
$\beta = 97.61$ (4)°
$\gamma = 96.04$ (3)°
$V = 1160.4$ (4) Å^3
$Z = 1$
Mo $K\alpha$ radiation
$\mu = 0.22$ mm^{-1}
$T = 173$ (2) K
0.30 × 0.30 × 0.20 mm

Data collection

Stoe Stadi-4 diffractometer
Absorption correction: none
9084 measured reflections
5117 independent reflections
3168 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.213$
$S = 1.07$
5117 reflections
228 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max} = 0.77$ e Å^{-3}
$\Delta\rho_{min} = -1.06$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O4′—H4′···O1	0.84	2.41	2.981 (15)	126
O4′—H4′···O1′	0.84	2.73	3.382 (15)	135
O4—H4···O3	0.84	2.59	2.863 (6)	101

H atoms were treated as riding, with C—H = 0.98–0.99 Å, O—H = 0.84 Å, and U_{iso}(H) values set at 1.2 or 1.5 times U_{eq}(C) and 1.5 times U_{eq}(O). The methanol solvent molecule was refined using isotropic displacement parameters and one restraint to fix a C—O bond distance. The methanol molecule is disordered over two positions. One CH_2—O group of the main molecule is disordered equally over two positions.

Data collection: *STADI4* (Stoe & Cie, 1995); cell refinement: *STADI4*; data reduction: *STADI4*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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