

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

tert-Butyldimethylsilanol hemihydrateSarah M. Barry,^a Helge Mueller-Bunz^b and Peter J. Rutledge^{c*}^aCentre for Synthesis and Chemical Biology, University College Dublin, Belfield, Dublin 4, Ireland, ^bSchool of Chemistry and Chemical Biology, University College Dublin, Belfield, Dublin 4, Ireland, and ^cSchool of Chemistry F11, University of Sydney, NSW 2006, Australia

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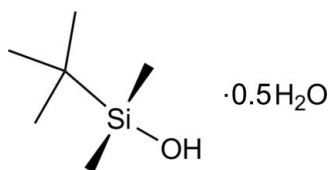
Received 21 February 2008; accepted 22 May 2008

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.056; wR factor = 0.149; data-to-parameter ratio = 22.6.

The crystal structure of the title compound, $\text{C}_6\text{H}_{16}\text{OSi}\cdot 0.5\text{H}_2\text{O}$, reveals an asymmetric unit containing two molecules of the silanol and a single water molecule. There is evidence of hydrogen bonding between the three molecules in the asymmetric unit. The H atoms of the silanol OH groups and the water H atoms are each disordered equally over two positions.

Related literature

For related literature, see: Krall *et al.* (2005); Lickiss *et al.* (1995); Mansfeld, Schürmann & Mehring (2005); Mansfeld, Mehring & Schürmann (2005); McGeary *et al.* (1991); Veith *et al.* (2006); Barry & Rutledge (2008); Görbitz (1999).



Experimental

Crystal data

$\text{C}_6\text{H}_{16}\text{OSi}\cdot 0.5\text{H}_2\text{O}$
 $M_r = 141.29$
 Monoclinic, $P2_1/c$
 $a = 7.7078$ (18) Å
 $b = 22.119$ (5) Å
 $c = 11.058$ (3) Å
 $\beta = 90.307$ (4)°

$V = 1885.2$ (8) Å³
 $Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 0.19$ mm⁻¹
 $T = 100$ (2) K
 $1.00 \times 1.00 \times 0.80$ mm

Data collection

Bruker SMART APEX detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 2000)
 $T_{\min} = 0.519$, $T_{\max} = 0.865$

15971 measured reflections
 4093 independent reflections
 3529 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.054$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.055$
 $wR(F^2) = 0.149$
 $S = 1.05$
 4093 reflections
 181 parameters
 6 restraints

H atoms treated by a mixture of independent and constrained refinement

$\Delta\rho_{\text{max}} = 0.55$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.49$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1}-\text{H1O1}\cdots\text{O3}^{\text{i}}$	0.84	2.09	2.717 (3)	131
$\text{O1}-\text{H2O1}\cdots\text{O3}$	0.84	1.96	2.706 (3)	147
$\text{O2}-\text{H1O2}\cdots\text{O3}^{\text{ii}}$	0.84	2.04	2.718 (3)	138
$\text{O2}-\text{H2O2}\cdots\text{O3}$	0.84	2.05	2.707 (3)	135
$\text{O3}-\text{H1O3}\cdots\text{O1}$	0.824 (19)	1.91 (3)	2.706 (3)	163 (6)
$\text{O3}-\text{H4O3}\cdots\text{O1}^{\text{i}}$	0.815 (19)	1.92 (2)	2.717 (3)	164 (6)
$\text{O3}-\text{H2O3}\cdots\text{O2}$	0.82 (2)	1.89 (2)	2.707 (3)	173 (6)
$\text{O3}-\text{H3O3}\cdots\text{O2}^{\text{ii}}$	0.822 (19)	1.92 (2)	2.718 (3)	164 (6)

Symmetry codes: (i) $-x, -y + 1, -z + 2$; (ii) $-x + 1, -y + 1, -z + 2$.

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

The authors thank the Irish Research Council for Science, Engineering and Technology for an Embark Award post-graduate scholarship to SMB, the Centre for Synthesis & Chemical Biology (CSCB) funded by the Irish Higher Education Authority (HEA) through the Programme for Research in Third-Level Institutions (PRTLII) for financial support, and Professor Cameron Kepert for helpful advice.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KJ2088).

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supporting information

Acta Cryst. (2008). E64, o1174 [doi:10.1107/S1600536808015444]

***tert*-Butyldimethylsilanol hemihydrate**

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S1. Comment

The structure of the title compound *tert*-butyldimethylsilanol hemihydrate is shown below (Fig. 1, 2); dimensions are available in the archived CIF. This compound has previously been characterized by gas-phase electron diffraction of both the free silanol and its hemihydrate (Lickiss *et al.*, 1995). It has also been structurally characterized within lanthanoid complexes (McGeary *et al.*, 1991) and in recent structures of complexes with several main group and transition metals (for examples see Mansfeld, Mehring & Schürmann, 2005; Mansfeld, Schürmann & Mehring, 2005, Veith *et al.*, 2006). However direct crystallographic characterization of the silanol has hitherto remained elusive.

tert-Butyldimethylsilanol hemihydrate was isolated in crystalline form during the synthesis of biomimetic ligands for iron-mediated hydrocarbon oxidation (Krall *et al.*, 2005, Barry & Rutledge, 2008). The title compound was obtained as the side product of reactions to prepare a compound incorporating the *tert*-butyldimethylsilyl ether as a protecting group (2-(bromomethyl)-6-((*tert*-butyldimethylsilyloxy)methyl)pyridine).

The asymmetric unit contains two molecules of the silanol and one water molecule, linked by hydrogen bonding. The hydrogen atoms of the water molecule and the silanol O—H groups are disordered between two alternative occupancies (Fig. 2).

S2. Experimental

The title compound crystallized serendipitously as colourless needles from a sample of the silyl ether 2-(bromomethyl)-6-((*tert*-butyldimethylsilyloxy)methyl)pyridine (isolated as an oil from a pentane:ether solvent mixture), upon standing at room temperature for several weeks.

Large crystals of the silanol were obtained (1.00 × 1.00 × 0.80 mm) and data was collected from a crystal at the upper size limit of the beam used. Moreover, the crystals of *tert*-butyldimethylsilanol hemihydrate that have been isolated exhibit remarkably low density (0.996 g cm⁻³), a property that may be linked to the high volatility of this compound.

S3. Refinement

A full sphere of the reciprocal space was scanned by φ - ω scans. Hydrogen atoms of the silanol molecules were added at calculated positions and refined using a riding model. C—H distances were assumed to be 0.98 Å, O—H distances to be 0.84 Å. The water protons were located in the difference Fourier map. The distance of these protons to the oxygen atom was restrained to be 0.84 Å using the *DFIX* command. In the same way the H—O—H angles were restrained to be 114°, the value to which a preliminary refinement of one component converged. $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{carrier})$ for all H atoms.

The site occupation factor of the disordered hydrogen atoms was fixed to 0.5. Attempts to refine the occupation factors were unsuccessful. However, electron densities in the difference Fourier map suggest a fairly even distribution between the two disordered parts.

Discrepancies between the expected and reported values of the maximum and minimum transmission (T_{\max}/T_{\min}) are thought to have arisen from the large size of the crystal relative to the beam, and because the crystal mount has given rise to some absorption during data collection. However this is not thought to impact significantly on the dataset given that there is an almost fourfold redundancy with the collection of a full sphere, and the capacity of *SADABS* to handle data collected from large crystals (Görlitz, 1999, Sheldrick, 2000).

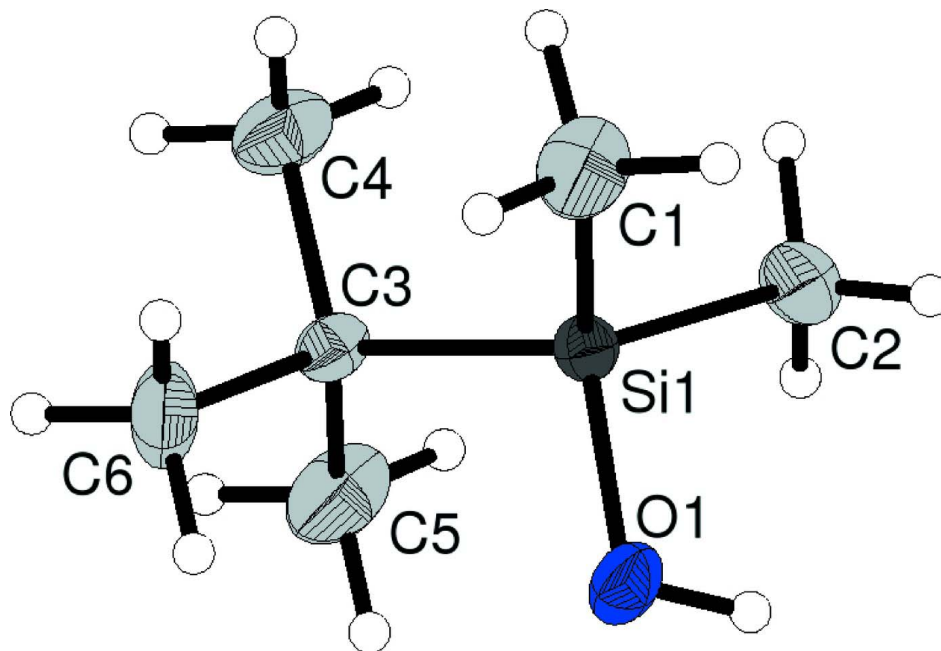


Figure 1

The molecular structure of the title compound with atom labels and thermal ellipsoids drawn on the 50% probability level. Carbon atoms are shown in grey, the silicon in black and the oxygen in blue.

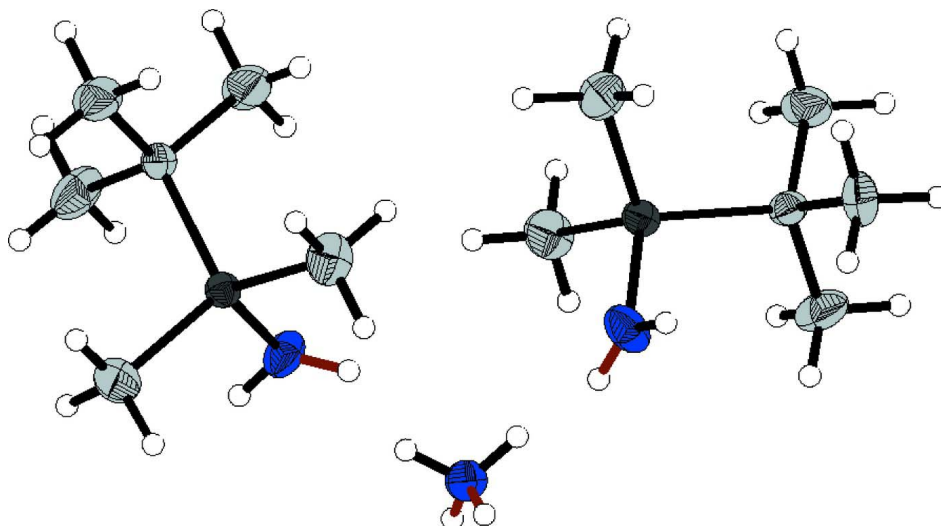


Figure 2

View of two adjacent silanols and a bridging water showing the disorder that is present (Part 1 black bonds, Part 2 brown bonds); thermal ellipsoids are drawn on the 50% probability level.

tert-Butyldimethylsilanol hemihydrate*Crystal data*C₆H₁₆OSi·0.5H₂O $M_r = 141.29$ Monoclinic, $P2_1/c$ $a = 7.7078$ (18) Å $b = 22.119$ (5) Å $c = 11.058$ (3) Å $\beta = 90.307$ (4)° $V = 1885.2$ (8) Å³ $Z = 8$ $F(000) = 632$ $D_x = 0.996$ Mg m⁻³Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 5333 reflections

 $\theta = 2.6$ – 29.4 ° $\mu = 0.19$ mm⁻¹ $T = 100$ K

Block, colourless

 $1.00 \times 1.00 \times 0.80$ mm*Data collection*Bruker SMART APEX detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 φ and ω scansAbsorption correction: multi-scan
(*SADABS*; Sheldrick, 2000) $T_{\min} = 0.519$, $T_{\max} = 0.865$

15971 measured reflections

4093 independent reflections

3529 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.054$ $\theta_{\max} = 27.0$ °, $\theta_{\min} = 0.9$ ° $h = -9 \rightarrow 9$ $k = -28 \rightarrow 28$ $l = -14 \rightarrow 14$ *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.055$ $wR(F^2) = 0.149$ $S = 1.05$

4093 reflections

181 parameters

6 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sitesH atoms treated by a mixture of independent
and constrained refinement $w = 1/[\sigma^2(F_o^2) + (0.0859P)^2 + 1.0972P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.040$ $\Delta\rho_{\max} = 0.55$ e Å⁻³ $\Delta\rho_{\min} = -0.49$ e Å⁻³*Special details*

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Si1	0.08637 (10)	0.59717 (3)	1.24126 (7)	0.01975 (18)	
O1	0.0393 (3)	0.56062 (9)	1.1151 (2)	0.0313 (5)	
H1O1	-0.0509	0.5399	1.1251	0.047*	0.50
H2O1	0.1314	0.5488	1.0825	0.047*	0.50

C1	0.0225 (5)	0.55098 (15)	1.3734 (3)	0.0408 (8)	
H1A	-0.1001	0.5398	1.3660	0.061*	
H1B	0.0400	0.5744	1.4477	0.061*	
H1C	0.0937	0.5143	1.3766	0.061*	
C2	0.3243 (4)	0.60908 (15)	1.2437 (3)	0.0350 (7)	
H2A	0.3834	0.5699	1.2401	0.052*	
H2B	0.3575	0.6301	1.3184	0.052*	
H2C	0.3580	0.6336	1.1738	0.052*	
C3	-0.0367 (4)	0.67096 (12)	1.2379 (2)	0.0227 (5)	
C4	-0.0021 (5)	0.70679 (15)	1.3542 (3)	0.0385 (8)	
H4A	0.1224	0.7151	1.3616	0.058*	
H4B	-0.0405	0.6831	1.4240	0.058*	
H4C	-0.0661	0.7451	1.3512	0.058*	
C5	0.0191 (6)	0.70852 (15)	1.1297 (3)	0.0471 (10)	
H5A	-0.0453	0.7467	1.1288	0.071*	
H5B	-0.0051	0.6861	1.0550	0.071*	
H5C	0.1437	0.7169	1.1355	0.071*	
C6	-0.2315 (4)	0.65768 (16)	1.2285 (3)	0.0425 (8)	
H6A	-0.2677	0.6336	1.2984	0.064*	
H6B	-0.2553	0.6351	1.1541	0.064*	
H6C	-0.2961	0.6958	1.2271	0.064*	
Si2	0.41635 (10)	0.62186 (3)	0.80713 (7)	0.02124 (19)	
O2	0.4716 (3)	0.56071 (10)	0.8832 (2)	0.0345 (5)	
H1O2	0.5780	0.5619	0.8996	0.052*	0.50
H2O2	0.3931	0.5346	0.8761	0.052*	0.50
C7	0.4726 (5)	0.68968 (15)	0.8981 (3)	0.0402 (8)	
H7A	0.3994	0.6911	0.9703	0.060*	
H7B	0.4531	0.7261	0.8496	0.060*	
H7C	0.5948	0.6876	0.9225	0.060*	
C8	0.1783 (4)	0.61756 (15)	0.7803 (3)	0.0381 (8)	
H8A	0.1509	0.5805	0.7356	0.057*	
H8B	0.1407	0.6528	0.7332	0.057*	
H8C	0.1179	0.6172	0.8581	0.057*	
C9	0.5397 (4)	0.62185 (11)	0.6618 (2)	0.0226 (6)	
C10	0.4979 (5)	0.56497 (14)	0.5889 (3)	0.0379 (8)	
H10A	0.5657	0.5650	0.5142	0.057*	
H10B	0.3739	0.5643	0.5690	0.057*	
H10C	0.5274	0.5291	0.6369	0.057*	
C11	0.7347 (4)	0.62329 (15)	0.6898 (3)	0.0375 (8)	
H11A	0.7654	0.5886	0.7407	0.056*	
H11B	0.7634	0.6608	0.7325	0.056*	
H11C	0.7998	0.6214	0.6140	0.056*	
C12	0.4920 (5)	0.67741 (14)	0.5854 (3)	0.0364 (7)	
H12A	0.5209	0.7143	0.6303	0.055*	
H12B	0.3673	0.6769	0.5674	0.055*	
H12C	0.5572	0.6766	0.5096	0.055*	
O3	0.2501 (2)	0.48396 (9)	0.99424 (19)	0.0261 (4)	
H1O3	0.190 (7)	0.503 (2)	1.043 (5)	0.039*	0.50

H2O3	0.316 (7)	0.506 (2)	0.956 (5)	0.039*	0.50
H3O3	0.327 (6)	0.464 (2)	1.026 (6)	0.039*	0.50
H4O3	0.172 (6)	0.464 (2)	0.963 (6)	0.039*	0.50

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Si1	0.0189 (3)	0.0196 (3)	0.0207 (3)	−0.0005 (3)	−0.0001 (3)	0.0000 (3)
O1	0.0248 (11)	0.0336 (12)	0.0354 (11)	−0.0016 (8)	0.0018 (9)	−0.0151 (9)
C1	0.050 (2)	0.0316 (17)	0.0408 (18)	0.0045 (14)	0.0121 (16)	0.0115 (14)
C2	0.0251 (16)	0.0441 (18)	0.0357 (17)	0.0006 (13)	−0.0040 (13)	−0.0035 (14)
C3	0.0275 (14)	0.0209 (13)	0.0198 (12)	−0.0004 (10)	0.0043 (10)	−0.0001 (10)
C4	0.055 (2)	0.0293 (16)	0.0317 (16)	−0.0003 (14)	0.0047 (15)	−0.0066 (13)
C5	0.077 (3)	0.0299 (17)	0.0342 (17)	0.0152 (17)	0.0179 (18)	0.0108 (14)
C6	0.0287 (17)	0.0419 (18)	0.057 (2)	0.0116 (14)	−0.0020 (15)	−0.0126 (16)
Si2	0.0187 (4)	0.0208 (3)	0.0242 (4)	−0.0002 (3)	−0.0008 (3)	0.0022 (3)
O2	0.0254 (11)	0.0366 (12)	0.0415 (12)	0.0014 (9)	0.0020 (10)	0.0170 (10)
C7	0.053 (2)	0.0360 (17)	0.0315 (16)	−0.0072 (15)	0.0082 (15)	−0.0135 (14)
C8	0.0212 (15)	0.0394 (18)	0.054 (2)	0.0025 (12)	−0.0009 (14)	0.0073 (15)
C9	0.0282 (14)	0.0184 (12)	0.0211 (13)	0.0008 (10)	0.0008 (11)	−0.0017 (10)
C10	0.053 (2)	0.0259 (16)	0.0349 (17)	0.0045 (14)	−0.0021 (15)	−0.0099 (13)
C11	0.0272 (16)	0.0475 (19)	0.0379 (17)	−0.0007 (13)	0.0123 (14)	0.0009 (14)
C12	0.055 (2)	0.0263 (15)	0.0279 (15)	0.0023 (14)	0.0011 (15)	0.0053 (12)
O3	0.0188 (11)	0.0259 (10)	0.0334 (11)	0.0004 (8)	−0.0024 (9)	−0.0003 (9)

Geometric parameters (Å, °)

Si1—O1	1.651 (2)	Si2—C8	1.859 (3)
Si1—C1	1.852 (3)	Si2—C9	1.871 (3)
Si1—C2	1.853 (3)	O2—H1O2	0.8400
Si1—C3	1.888 (3)	O2—H2O2	0.8400
O1—H1O1	0.8400	C7—H7A	0.9800
O1—H2O1	0.8400	C7—H7B	0.9800
C1—H1A	0.9800	C7—H7C	0.9800
C1—H1B	0.9800	C8—H8A	0.9800
C1—H1C	0.9800	C8—H8B	0.9800
C2—H2A	0.9800	C8—H8C	0.9800
C2—H2B	0.9800	C9—C10	1.528 (4)
C2—H2C	0.9800	C9—C11	1.533 (4)
C3—C5	1.521 (4)	C9—C12	1.535 (4)
C3—C4	1.532 (4)	C10—H10A	0.9800
C3—C6	1.533 (4)	C10—H10B	0.9800
C4—H4A	0.9800	C10—H10C	0.9800
C4—H4B	0.9800	C11—H11A	0.9800
C4—H4C	0.9800	C11—H11B	0.9800
C5—H5A	0.9800	C11—H11C	0.9800
C5—H5B	0.9800	C12—H12A	0.9800
C5—H5C	0.9800	C12—H12B	0.9800

C6—H6A	0.9800	C12—H12C	0.9800
C6—H6B	0.9800	O3—H1O3	0.824 (19)
C6—H6C	0.9800	O3—H2O3	0.82 (2)
Si2—O2	1.648 (2)	O3—H3O3	0.822 (19)
Si2—C7	1.856 (3)	O3—H4O3	0.815 (19)
O1—Si1—C1	109.79 (15)	O2—Si2—C9	107.90 (12)
O1—Si1—C2	107.15 (13)	C7—Si2—C9	110.33 (14)
C1—Si1—C2	109.53 (17)	C8—Si2—C9	111.62 (16)
O1—Si1—C3	107.38 (12)	Si2—O2—H1O2	109.5
C1—Si1—C3	110.88 (14)	Si2—O2—H2O2	109.5
C2—Si1—C3	112.00 (14)	Si2—C7—H7A	109.5
Si1—O1—H1O1	109.5	Si2—C7—H7B	109.5
Si1—O1—H2O1	109.5	H7A—C7—H7B	109.5
Si1—C1—H1A	109.5	Si2—C7—H7C	109.5
Si1—C1—H1B	109.5	H7A—C7—H7C	109.5
H1A—C1—H1B	109.5	H7B—C7—H7C	109.5
Si1—C1—H1C	109.5	Si2—C8—H8A	109.5
H1A—C1—H1C	109.5	Si2—C8—H8B	109.5
H1B—C1—H1C	109.5	H8A—C8—H8B	109.5
Si1—C2—H2A	109.5	Si2—C8—H8C	109.5
Si1—C2—H2B	109.5	H8A—C8—H8C	109.5
H2A—C2—H2B	109.5	H8B—C8—H8C	109.5
Si1—C2—H2C	109.5	C10—C9—C11	109.1 (3)
H2A—C2—H2C	109.5	C10—C9—C12	108.6 (3)
H2B—C2—H2C	109.5	C11—C9—C12	109.0 (3)
C5—C3—C4	109.2 (2)	C10—C9—Si2	110.3 (2)
C5—C3—C6	109.4 (3)	C11—C9—Si2	109.2 (2)
C4—C3—C6	108.8 (3)	C12—C9—Si2	110.6 (2)
C5—C3—Si1	110.1 (2)	C9—C10—H10A	109.5
C4—C3—Si1	110.2 (2)	C9—C10—H10B	109.5
C6—C3—Si1	109.13 (19)	H10A—C10—H10B	109.5
C3—C4—H4A	109.5	C9—C10—H10C	109.5
C3—C4—H4B	109.5	H10A—C10—H10C	109.5
H4A—C4—H4B	109.5	H10B—C10—H10C	109.5
C3—C4—H4C	109.5	C9—C11—H11A	109.5
H4A—C4—H4C	109.5	C9—C11—H11B	109.5
H4B—C4—H4C	109.5	H11A—C11—H11B	109.5
C3—C5—H5A	109.5	C9—C11—H11C	109.5
C3—C5—H5B	109.5	H11A—C11—H11C	109.5
H5A—C5—H5B	109.5	H11B—C11—H11C	109.5
C3—C5—H5C	109.5	C9—C12—H12A	109.5
H5A—C5—H5C	109.5	C9—C12—H12B	109.5
H5B—C5—H5C	109.5	H12A—C12—H12B	109.5
C3—C6—H6A	109.5	C9—C12—H12C	109.5
C3—C6—H6B	109.5	H12A—C12—H12C	109.5
H6A—C6—H6B	109.5	H12B—C12—H12C	109.5
C3—C6—H6C	109.5	H1O3—O3—H2O3	113 (4)

H6A—C6—H6C	109.5	H1O3—O3—H3O3	113 (7)
H6B—C6—H6C	109.5	H2O3—O3—H3O3	95 (6)
O2—Si2—C7	109.13 (16)	H1O3—O3—H4O3	98 (7)
O2—Si2—C8	106.94 (13)	H2O3—O3—H4O3	123 (7)
C7—Si2—C8	110.79 (16)	H3O3—O3—H4O3	115 (4)
O1—Si1—C3—C5	-60.8 (2)	O2—Si2—C9—C10	59.0 (2)
C1—Si1—C3—C5	179.3 (2)	C7—Si2—C9—C10	178.1 (2)
C2—Si1—C3—C5	56.6 (3)	C8—Si2—C9—C10	-58.3 (2)
O1—Si1—C3—C4	178.8 (2)	O2—Si2—C9—C11	-60.9 (2)
C1—Si1—C3—C4	58.8 (3)	C7—Si2—C9—C11	58.3 (2)
C2—Si1—C3—C4	-63.9 (2)	C8—Si2—C9—C11	-178.1 (2)
O1—Si1—C3—C6	59.4 (2)	O2—Si2—C9—C12	179.1 (2)
C1—Si1—C3—C6	-60.6 (3)	C7—Si2—C9—C12	-61.7 (3)
C2—Si1—C3—C6	176.7 (2)	C8—Si2—C9—C12	61.9 (2)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1—H1O1...O3 ⁱ	0.84	2.09	2.717 (3)	131
O1—H2O1...O3	0.84	1.96	2.706 (3)	147
O2—H1O2...O3 ⁱⁱ	0.84	2.04	2.718 (3)	138
O2—H2O2...O3	0.84	2.05	2.707 (3)	135
O3—H1O3...O1	0.82 (2)	1.91 (3)	2.706 (3)	163 (6)
O3—H4O3...O1 ⁱ	0.82 (2)	1.92 (2)	2.717 (3)	164 (6)
O3—H2O3...O2	0.82 (2)	1.89 (2)	2.707 (3)	173 (6)
O3—H3O3...O2 ⁱⁱ	0.82 (2)	1.92 (2)	2.718 (3)	164 (6)

Symmetry codes: (i) $-x, -y+1, -z+2$; (ii) $-x+1, -y+1, -z+2$.