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1-Hydroxy-1,1,3,3,3-pentaphenyldisiloxane, $[Si_2O(OH)(Ph)_5]$, at 100 K

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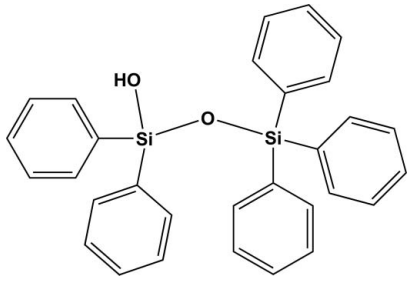
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.008 Å; R factor = 0.072; wR factor = 0.185; data-to-parameter ratio = 14.9.

In the crystal structure of the title compound, $C_{30}H_{26}O_2Si_2$, one $Si(Ph)_3$ residue is bound to another $Si(OH)(Ph)_2$ residue *via* a non-linear Si—O—Si bridge. The asymmetric unit is composed of two such molecules which interact, on the one hand, *via* a strong and highly directional O—H···O hydrogen bond involving the two neighbouring Si—OH units and, on the other, *via* an O—H···π contact connecting the second hydroxyl group with an adjacent phenyl group.

Related literature

For the structure of the title compound at 150 (2) K, see the next paper: Amarante *et al.* (2008). For related structures of disiloxane compounds, see: Glidewell & Liles (1978); Hönle *et al.* (1990); Morosin & Harrah (1981); Suwińska *et al.* (1986); Wojnowski *et al.* (2004). For literature relevant to this communication and published by our group, see: Abrantes *et al.* (2002); Bruno *et al.* (2006, 2007); Nunes *et al.* (2003). For the Cambridge Structural Database (Version 5.28 with three updates, August 2007), see: Allen (2002).



Experimental

Crystal data

$C_{30}H_{26}O_2Si_2$
M_r = 474.69
Triclinic, $P\overline{1}$
a = 10.3611 (6) Å
b = 14.2844 (8) Å
c = 18.4367 (9) Å
α = 99.421 (4)°
β = 98.492 (4)°
γ = 107.415 (4)°
V = 2511.8 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.17 mm^{-1}
T = 100 (2) K
0.14 × 0.08 × 0.08 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
T_{min} = 0.977, T_{max} = 0.987
33504 measured reflections
9155 independent reflections
4059 reflections with $I > 2\sigma(I)$
R_{int} = 0.140

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.072
$wR(F^2)$ = 0.185
S = 0.98
9155 reflections
615 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···O2	0.84	1.94	2.742 (4)	160
O2—H2···Cg(C55–C60)	0.84	2.44	3.181 (2)	147

Data collection: *APEX2* (Bruker, 2006); cell refinement: *APEX2*; data reduction: *SAINT-Plus* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Bruker 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2228).

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supporting information

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1-Hydroxy-1,1,3,3,3-pentaphenyldisiloxane, $[Si_2O(OH)(Ph)_5]$, at 100 K

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S1. Comment

Even though derivatives of triphenylsilane, $SiH(Ph)_3$, have been widely used in organometallic chemistry and chemistry in general for many years, disiloxanes (*i.e.*, compounds having two Si centres bridged *via* an oxo group) in which one Si centre is bound to a hydroxyl group are unknown as revealed by a search of the literature in conjunction with another of the Cambridge Structural Database (CSD, Version 5.28 with three updates - August 2007; Allen, 2002). Moreover, disiloxanes having one of the two Si centres bound to three phenyl groups are scarce, with only a handful of compounds being available in the literature (Glidewell & Liles, 1978; Hönle *et al.*, 1990; Morosin & Harrah, 1981; Suwińska *et al.*, 1986; Wojnowski *et al.*, 2004). Following our on-going research toward the synthesis, structural characterization and catalytic application of novel triphenylsiloxy derivatives (Abrantes *et al.*, 2002; Bruno *et al.*, 2006, 2007; Nunes *et al.*, 2003), we have recently isolated the unprecedented $[Si_2O(OH)(Ph)_5]$ disiloxane, in which one $Si(Ph)_3$ residue is bound to another $Si(OH)(Ph)_2$ residue *via* a non-linear Si—O—Si bridge.

The crystal structure of the title compound, (I), at the low temperature of 100 K is fully described in the triclinic $P\bar{1}$ space group with the asymmetric unit being composed of two crystallographically independent $[Si_2O(OH)(Ph)_5]$ molecular units, Fig. 1 & Table 1. Within each binuclear unit, the two Si centres exhibit distinct coordination environments, even though the μ_2-bridging oxo group is common to the two Si centres. While one Si is coordinated to three phenyl groups, $\{SiC_3O\}$, the other is bound to two phenyl groups plus a hydroxyl moiety, $\{SiC_2O_2\}$. For the two independent molecular units, the Si—C and Si—O bond lengths were found in the 1.841 (5)–1.861 (5) and 1.605 (3)–1.637 (3) Å ranges, respectively, in good agreement with those found in related materials.

It is of considerable importance to note that while for the disiloxanes which have identical coordination environments for the Si centres the internal Si—O—Si bridge is almost linear, such as for the compounds reported by Glidewell & Liles (1978), Hönle *et al.* (1990) and Suwińska *et al.* (1986), the presence of distinct coordinating chemical moieties and their interaction with adjacent species in (I) induces a kink in this μ_2-bridge. Indeed, the Si—O—Si bond angles for (I) range from 147.7 (2)° to 166.0 (2)°, values which are consistent with that reported by Wojnowski *et al.* (2004) for $[Si_2O(H)(Ph)_5]$ (*ca* 163°). We also note the markedly distinct nature of the bridging angles for the two molecular units, a structural feature which can be rationalized taking into consideration the strongest intermolecular interactions present. Indeed, besides the very strong and linear O—H···O hydrogen bonding interaction connecting adjacent $[Si_2O(OH)(Ph)_5]$ units, the O2-hydroxyl group is further engaged in a O—H···π interaction with the neighbouring C55→C60 phenyl group, Table 2. Consequently, in order to maximize these two interactions the Si3—O3—Si4 angle decreases, while the Si1—O1—Si2 approaches linearity so to minimize steric hindrance between coordinating moieties.

The two interactions described above (O—H···O and O—H···π) create a supramolecular entity (Fig. 1) which packs in a parallel fashion in the *ab* plane of the unit cell forming layers (Fig. 2). Adjacent layers alternate along the [001] direction

of the unit cell with a number of C—H···π contacts mediating the interactions between adjacent phenyl groups (not shown).

S2. Experimental

The title compound was isolated as a secondary product during our synthetic attempts to isolate organometallic vanadium(V) oxides from $AgVO_3$ and triphenylchlorosilane (Ph_3SiCl, 97.0%, Fluka). Standard Schlenk line techniques were employed.

$AgVO_3$ was obtained in our laboratories by adding a solution (*ca* 10 ml) of silver nitrate ($AgNO_3$, 0.77 g; 99.0%, Sigma-Aldrich) to another of ammonium metavanadate (NH_4VO_3, 0.51 g; 99%, Sigma-Aldrich) in *ca* 100 ml of distilled water. A yellow precipitate ($AgVO_3$) was immediately isolated by vacuum filtering and in-vacuo drying.

To a solution of $AgVO_3$ (0.31 g) in dried 1,2-dichloroethane, another solution of Ph_3SiCl (0.44 g) was added dropwise, and the resulting mixture was allowed to react over a period of 87 h under reflux in an oil bath at 263 K. After reacting, the obtained precipitate was separated from the yellow mother liquor by using dried Celite 545 (Aldrich). The isolated solution was then concentrated to an oil by slowly evaporating 1,2-dichloroethane in a water bath, under vacuum for 5 h. The title compound (a secondary product) was separated from the desired synthesized product by washing with *ca* 10 ml of *n*-hexane (HPLC grade, 95%, Aldrich). Well formed prismatic colourless crystals of $[Si_2O(OH)(Ph)_5]$ were thus obtained from the total evaporation of the *n*-hexane in open air for about 24 h.

S3. Refinement

Crystals of the title compound were manually harvested from the crystallization vial and mounted on CryoLoops purchased from Hampton Research using FOMBLIN Y perfluoropolyether vacuum oil (LVAC 25/6) purchased from Aldrich, with the help of a Stemi 2000 stereomicroscope equipped with Carl Zeiss lenses. Different crystals from the same batch systematically diffracted very weakly at high angle. A full data set was collected at the low temperature of 100 (2) K with a long exposure time per frame, revealing the existence of a poorly defined spot shape which ultimately had a strong influence in the high value of R_{int}. Nevertheless, the structure was readily solved using Patterson synthesis which allowed the immediate location of the four crystallographically unique Si centres. All remaining non-H atoms were located from difference Fourier maps calculated from successive least-squares refinements cycles. Non-H atoms were successfully refined using anisotropic displacement parameters. H atoms bound to C and the terminal Si—OH groups were located at their idealized positions and allowed to ride on their parent atoms with C—H = 0.95Å and O—H = 0.84 Å, and with U_{iso} = 1.2 or 1.5×U_{eq} of the parent atoms (C and O, respectively).

It is of considerable importance to emphasize that a minor amount of the isolated crystals was instead indexed with a larger triclinic unit cell, with this being particularly apparent when the temperature of the data collection was increased to 150 (2) K. This procedure increases the thermal motion associated with the phenyl groups, reducing overall symmetry and increasing the number of crystallographically independent $[Si_2O(OH)(Ph)_5]$ molecular units. The structure of the title compound at 150 (2) K will be the subject of a different crystallographic communication (Amarante *et al.*, 2008).

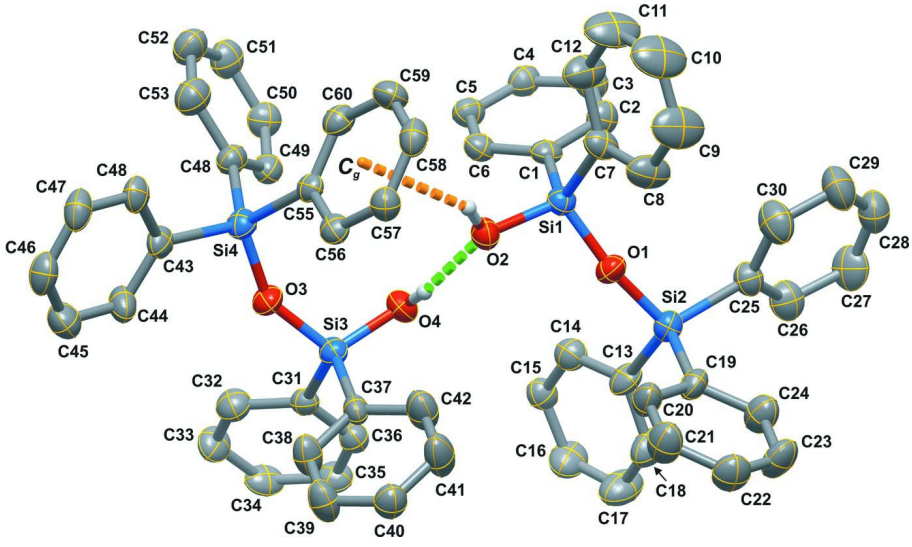

Figure 1

Schematic representation of the two crystallographically independent $[Si_2O(OH)(Ph)_5]$ molecular units comprising the asymmetric unit of (I) showing the labelling scheme for all non-H atoms. Displacement ellipsoids are drawn at the 50% probability level and H atoms associated with the hydroxyl groups are represented as small spheres with arbitrary radii. All H-atoms bound to carbon were omitted for clarity. The O—H···O hydrogen bond and O—H···π contact connecting neighbouring binuclear units are represented as green and orange dashed lines, respectively.

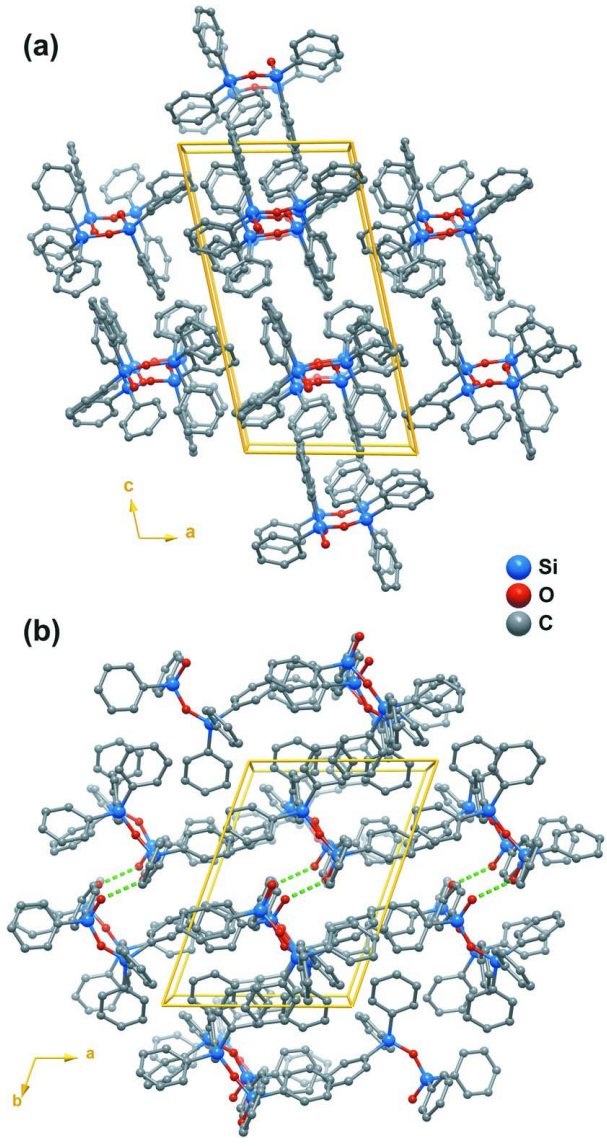

Figure 2

Crystal packing of (I) viewed along the (**a**) [010] and (**c**) [001] directions of the unit cell. The O—H···O hydrogen bonding interactions are represented as dashed green lines and all H atoms have been omitted for clarity.

1-hydroxy-1,1,3,3,3-pentaphenyldisiloxane

Crystal data

$C_{30}H_{26}O_2Si_2$
$M_r = 474.69$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 10.3611\ (6)$ Å
$b = 14.2844\ (8)$ Å
$c = 18.4367\ (9)$ Å
$\alpha = 99.421\ (4)°$
$\beta = 98.492\ (4)°$
$\gamma = 107.415\ (4)°$
$V = 2511.8\ (3)$ Å^3
$Z = 4$
$F(000) = 1000$
$D_x = 1.255$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1283 reflections
$\theta = 2.8–17.4°$
$\mu = 0.17$ mm^{-1}

T = 100 K
Prism, colourless

0.14 × 0.08 × 0.08 mm

Data collection

Bruker X8 KappaCCD APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω/φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
T_{min} = 0.977, T_{max} = 0.987

33504 measured reflections
9155 independent reflections
4059 reflections with $I > 2\sigma(I)$
R_{int} = 0.140
θ_{max} = 25.4°, θ_{min} = 3.6°
h = −12→12
k = −17→17
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.072
$wR(F^2)$ = 0.185
S = 0.98
9155 reflections
615 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0681P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Special details

Experimental. See dedicated section in the main paper

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_{iso}*/U_{eq}
Si1	0.65378 (14)	0.38772 (10)	0.22723 (7)	0.0325 (4)
Si2	0.37645 (15)	0.20240 (10)	0.20581 (7)	0.0349 (4)
O1	0.5137 (3)	0.3003 (2)	0.22680 (16)	0.0353 (8)
O2	0.6412 (3)	0.4896 (2)	0.27676 (17)	0.0373 (8)
H2	0.7188	0.5246	0.3040	0.056*
C1	0.6626 (5)	0.4060 (4)	0.1306 (3)	0.0321 (12)
C2	0.6737 (5)	0.3310 (4)	0.0760 (3)	0.0404 (14)
H2A	0.6778	0.2699	0.0885	0.049*
C3	0.6790 (5)	0.3443 (4)	0.0033 (3)	0.0447 (14)
H3	0.6880	0.2929	−0.0334	0.054*
C4	0.6711 (5)	0.4324 (4)	−0.0152 (3)	0.0380 (13)
H4A	0.6722	0.4407	−0.0652	0.046*
C5	0.6617 (5)	0.5071 (4)	0.0371 (3)	0.0388 (13)

H5	0.6570	0.5677	0.0240	0.047*
C6	0.6591 (5)	0.4946 (4)	0.1097 (3)	0.0355 (12)
H6	0.6547	0.5481	0.1464	0.043*
C7	0.8033 (5)	0.3584 (4)	0.2723 (3)	0.0380 (13)
C8	0.7915 (6)	0.2950 (4)	0.3225 (3)	0.0559 (16)
H8	0.7044	0.2661	0.3347	0.067*
C9	0.9063 (7)	0.2736 (5)	0.3551 (3)	0.074 (2)
H9	0.8971	0.2285	0.3881	0.089*
C10	1.0333 (7)	0.3181 (6)	0.3394 (4)	0.083 (2)
H10	1.1125	0.3053	0.3627	0.100*
C11	1.0457 (6)	0.3805 (5)	0.2903 (3)	0.076 (2)
H11	1.1337	0.4108	0.2796	0.091*
C12	0.9337 (6)	0.4001 (4)	0.2563 (3)	0.0573 (17)
H12	0.9442	0.4425	0.2214	0.069*
C13	0.2320 (5)	0.2360 (4)	0.1589 (3)	0.0391 (13)
C14	0.2492 (5)	0.3110 (4)	0.1194 (3)	0.0403 (13)
H14	0.3403	0.3501	0.1178	0.048*
C15	0.1392 (5)	0.3315 (4)	0.0820 (3)	0.0382 (13)
H15	0.1547	0.3835	0.0549	0.046*
C16	0.0087 (6)	0.2768 (4)	0.0841 (3)	0.0556 (16)
H16	−0.0677	0.2893	0.0572	0.067*
C18	0.0978 (6)	0.1848 (4)	0.1625 (3)	0.0569 (17)
H18	0.0816	0.1351	0.1917	0.068*
C17	−0.0138 (6)	0.2042 (4)	0.1247 (3)	0.0649 (18)
H17	−0.1054	0.1670	0.1270	0.078*
C19	0.3412 (5)	0.1655 (4)	0.2950 (3)	0.0367 (13)
C20	0.3761 (5)	0.2357 (4)	0.3611 (3)	0.0446 (14)
H20	0.4199	0.3044	0.3613	0.054*
C21	0.3497 (6)	0.2096 (4)	0.4268 (3)	0.0567 (16)
H21	0.3762	0.2600	0.4718	0.068*
C22	0.2853 (6)	0.1111 (4)	0.4281 (3)	0.0539 (16)
H22	0.2653	0.0934	0.4737	0.065*
C23	0.2503 (6)	0.0392 (4)	0.3640 (3)	0.0548 (16)
H23	0.2061	−0.0293	0.3645	0.066*
C24	0.2791 (5)	0.0656 (4)	0.2979 (3)	0.0500 (15)
H24	0.2560	0.0145	0.2535	0.060*
C25	0.4074 (5)	0.0972 (4)	0.1459 (3)	0.0381 (13)
C26	0.3073 (6)	0.0290 (4)	0.0873 (3)	0.0505 (15)
H26	0.2212	0.0393	0.0742	0.061*
C27	0.3288 (7)	−0.0545 (4)	0.0470 (3)	0.0582 (17)
H27	0.2580	−0.1018	0.0079	0.070*
C28	0.4551 (7)	−0.0662 (4)	0.0655 (3)	0.0577 (16)
H28	0.4715	−0.1222	0.0378	0.069*
C29	0.5557 (7)	−0.0022 (4)	0.1208 (3)	0.0612 (17)
H29	0.6425	−0.0123	0.1319	0.073*
C30	0.5324 (6)	0.0794 (4)	0.1623 (3)	0.0567 (16)
H30	0.6033	0.1240	0.2027	0.068*
Si3	0.41436 (14)	0.65882 (10)	0.26844 (7)	0.0326 (4)

Si4	0.70163 (14)	0.82551 (10)	0.29771 (7)	0.0350 (4)
O3	0.5376 (3)	0.7660 (2)	0.28621 (16)	0.0375 (9)
O4	0.4511 (3)	0.5704 (2)	0.21842 (16)	0.0371 (8)
H4	0.5029	0.5495	0.2462	0.056*
C31	0.2633 (5)	0.6726 (3)	0.2105 (2)	0.0300 (12)
C32	0.2548 (5)	0.7665 (4)	0.2015 (3)	0.0448 (14)
H32	0.3300	0.8259	0.2255	0.054*
C33	0.1395 (5)	0.7738 (4)	0.1585 (3)	0.0456 (14)
H33	0.1355	0.8380	0.1534	0.055*
C34	0.0307 (5)	0.6891 (4)	0.1231 (3)	0.0443 (14)
H34	−0.0493	0.6949	0.0941	0.053*
C35	0.0364 (5)	0.5960 (4)	0.1291 (3)	0.0416 (14)
H35	−0.0385	0.5371	0.1037	0.050*
C36	0.1517 (5)	0.5887 (4)	0.1722 (2)	0.0350 (12)
H36	0.1550	0.5238	0.1758	0.042*
C37	0.3804 (5)	0.6264 (3)	0.3589 (3)	0.0324 (12)
C38	0.3412 (6)	0.6867 (4)	0.4095 (3)	0.0473 (15)
H38	0.3341	0.7479	0.3987	0.057*
C39	0.3109 (6)	0.6628 (4)	0.4766 (3)	0.0507 (15)
H39	0.2846	0.7076	0.5108	0.061*
C40	0.3191 (5)	0.5752 (4)	0.4931 (3)	0.0447 (14)
H40	0.2953	0.5569	0.5379	0.054*
C41	0.3619 (6)	0.5143 (4)	0.4449 (3)	0.0608 (17)
H41	0.3723	0.4545	0.4569	0.073*
C42	0.3904 (6)	0.5393 (4)	0.3776 (3)	0.0549 (16)
H42	0.4177	0.4948	0.3437	0.066*
C43	0.7384 (5)	0.9429 (3)	0.3686 (3)	0.0349 (12)
C44	0.6351 (6)	0.9785 (4)	0.3864 (3)	0.0467 (14)
H44	0.5431	0.9449	0.3587	0.056*
C45	0.6613 (6)	1.0623 (4)	0.4440 (3)	0.0555 (16)
H45	0.5880	1.0853	0.4553	0.067*
C46	0.7932 (6)	1.1110 (4)	0.4839 (3)	0.0496 (15)
H46	0.8111	1.1670	0.5243	0.060*
C47	0.8996 (6)	1.0802 (4)	0.4665 (3)	0.0473 (15)
H47	0.9917	1.1159	0.4934	0.057*
C48	0.8725 (5)	0.9964 (3)	0.4094 (3)	0.0378 (13)
H48	0.9468	0.9749	0.3978	0.045*
C49	0.7447 (5)	0.8425 (4)	0.2052 (3)	0.0358 (13)
C50	0.6623 (5)	0.7799 (4)	0.1391 (3)	0.0387 (13)
H50	0.5792	0.7298	0.1410	0.046*
C51	0.6962 (6)	0.7872 (4)	0.0707 (3)	0.0437 (14)
H51	0.6351	0.7443	0.0260	0.052*
C52	0.8162 (6)	0.8554 (4)	0.0663 (3)	0.0497 (15)
H52	0.8405	0.8586	0.0189	0.060*
C53	0.9022 (6)	0.9195 (4)	0.1298 (3)	0.0523 (15)
H53	0.9856	0.9682	0.1268	0.063*
C54	0.8669 (6)	0.9130 (4)	0.1991 (3)	0.0501 (15)
H54	0.9274	0.9576	0.2433	0.060*

C55	0.8023 (5)	0.7503 (3)	0.3357 (2)	0.0300 (12)
C56	0.7791 (5)	0.7161 (3)	0.4014 (3)	0.0356 (12)
H56	0.7115	0.7321	0.4259	0.043*
C57	0.8516 (5)	0.6599 (4)	0.4314 (3)	0.0396 (13)
H57	0.8341	0.6381	0.4761	0.048*
C58	0.9489 (5)	0.6354 (4)	0.3967 (3)	0.0426 (14)
H58	0.9981	0.5958	0.4169	0.051*
C59	0.9754 (5)	0.6686 (4)	0.3325 (3)	0.0460 (14)
H59	1.0432	0.6521	0.3084	0.055*
C60	0.9029 (5)	0.7258 (3)	0.3031 (3)	0.0384 (13)
H60	0.9231	0.7490	0.2592	0.046*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Si1	0.0309 (9)	0.0326 (8)	0.0341 (8)	0.0114 (7)	0.0055 (6)	0.0069 (6)
Si2	0.0357 (9)	0.0306 (8)	0.0364 (8)	0.0085 (7)	0.0069 (7)	0.0074 (6)
O1	0.032 (2)	0.0321 (19)	0.0375 (19)	0.0036 (16)	0.0082 (15)	0.0070 (15)
O2	0.038 (2)	0.0311 (19)	0.041 (2)	0.0124 (17)	0.0058 (16)	0.0031 (16)
C1	0.023 (3)	0.040 (3)	0.037 (3)	0.013 (2)	0.008 (2)	0.011 (3)
C2	0.047 (4)	0.039 (3)	0.037 (3)	0.014 (3)	0.007 (3)	0.014 (3)
C3	0.046 (4)	0.044 (3)	0.040 (3)	0.013 (3)	0.010 (3)	−0.001 (3)
C4	0.036 (3)	0.040 (3)	0.040 (3)	0.012 (3)	0.008 (2)	0.015 (3)
C5	0.037 (3)	0.043 (3)	0.042 (3)	0.015 (3)	0.014 (3)	0.017 (3)
C6	0.033 (3)	0.038 (3)	0.039 (3)	0.016 (3)	0.009 (2)	0.008 (2)
C7	0.037 (3)	0.049 (3)	0.036 (3)	0.023 (3)	0.008 (2)	0.016 (3)
C8	0.053 (4)	0.079 (4)	0.053 (4)	0.032 (4)	0.020 (3)	0.034 (3)
C9	0.069 (5)	0.115 (6)	0.067 (4)	0.049 (5)	0.015 (4)	0.059 (4)
C10	0.064 (5)	0.129 (6)	0.083 (5)	0.059 (5)	0.010 (4)	0.054 (5)
C11	0.040 (4)	0.127 (6)	0.082 (5)	0.043 (4)	0.008 (3)	0.053 (5)
C12	0.043 (4)	0.075 (4)	0.067 (4)	0.024 (3)	0.014 (3)	0.042 (3)
C13	0.029 (3)	0.036 (3)	0.041 (3)	0.000 (3)	−0.001 (2)	0.007 (3)
C14	0.037 (3)	0.041 (3)	0.040 (3)	0.011 (3)	0.005 (3)	0.005 (3)
C15	0.041 (4)	0.039 (3)	0.037 (3)	0.017 (3)	0.009 (3)	0.011 (2)
C16	0.036 (4)	0.058 (4)	0.072 (4)	0.016 (3)	−0.001 (3)	0.021 (3)
C18	0.043 (4)	0.050 (4)	0.076 (4)	0.010 (3)	0.001 (3)	0.030 (3)
C17	0.035 (4)	0.072 (4)	0.087 (5)	0.012 (3)	0.004 (3)	0.034 (4)
C19	0.031 (3)	0.029 (3)	0.045 (3)	0.003 (2)	0.004 (2)	0.011 (3)
C20	0.055 (4)	0.031 (3)	0.047 (3)	0.009 (3)	0.020 (3)	0.007 (3)
C21	0.076 (5)	0.046 (4)	0.043 (3)	0.014 (3)	0.018 (3)	0.004 (3)
C22	0.063 (4)	0.056 (4)	0.046 (4)	0.017 (3)	0.021 (3)	0.017 (3)
C23	0.064 (4)	0.045 (4)	0.049 (4)	0.001 (3)	0.020 (3)	0.018 (3)
C24	0.058 (4)	0.043 (3)	0.041 (3)	0.007 (3)	0.012 (3)	0.004 (3)
C25	0.042 (3)	0.037 (3)	0.036 (3)	0.017 (3)	0.006 (3)	0.009 (2)
C26	0.059 (4)	0.050 (4)	0.045 (3)	0.023 (3)	0.007 (3)	0.013 (3)
C27	0.070 (5)	0.051 (4)	0.041 (3)	0.015 (4)	0.000 (3)	−0.005 (3)
C28	0.072 (5)	0.039 (4)	0.063 (4)	0.022 (4)	0.014 (4)	0.009 (3)
C29	0.070 (5)	0.049 (4)	0.067 (4)	0.031 (4)	0.007 (4)	0.003 (3)

C30	0.059 (4)	0.051 (4)	0.053 (4)	0.023 (3)	−0.004 (3)	−0.002 (3)
Si3	0.0279 (8)	0.0310 (8)	0.0360 (8)	0.0087 (7)	0.0040 (6)	0.0033 (6)
Si4	0.0293 (9)	0.0328 (8)	0.0387 (8)	0.0071 (7)	0.0017 (7)	0.0072 (7)
O3	0.028 (2)	0.0314 (19)	0.044 (2)	0.0030 (16)	0.0026 (16)	0.0028 (15)
O4	0.038 (2)	0.040 (2)	0.0366 (19)	0.0191 (17)	0.0068 (16)	0.0061 (16)
C31	0.027 (3)	0.031 (3)	0.030 (3)	0.009 (2)	0.006 (2)	0.004 (2)
C32	0.034 (3)	0.043 (3)	0.050 (3)	0.007 (3)	0.002 (3)	0.005 (3)
C33	0.038 (4)	0.044 (3)	0.057 (4)	0.019 (3)	0.000 (3)	0.018 (3)
C34	0.032 (3)	0.063 (4)	0.046 (3)	0.024 (3)	0.004 (3)	0.023 (3)
C35	0.030 (3)	0.048 (3)	0.041 (3)	0.010 (3)	−0.001 (2)	0.005 (3)
C36	0.036 (3)	0.034 (3)	0.036 (3)	0.014 (3)	0.009 (2)	0.007 (2)
C37	0.029 (3)	0.025 (3)	0.041 (3)	0.011 (2)	0.002 (2)	0.001 (2)
C38	0.071 (4)	0.038 (3)	0.039 (3)	0.026 (3)	0.012 (3)	0.011 (3)
C39	0.072 (4)	0.046 (4)	0.042 (3)	0.032 (3)	0.013 (3)	0.006 (3)
C40	0.053 (4)	0.041 (3)	0.042 (3)	0.014 (3)	0.015 (3)	0.010 (3)
C41	0.094 (5)	0.044 (4)	0.064 (4)	0.036 (4)	0.035 (4)	0.023 (3)
C42	0.077 (5)	0.046 (4)	0.053 (4)	0.030 (3)	0.025 (3)	0.010 (3)
C43	0.033 (3)	0.029 (3)	0.044 (3)	0.012 (3)	0.002 (3)	0.014 (2)
C44	0.037 (4)	0.029 (3)	0.066 (4)	0.011 (3)	−0.001 (3)	−0.001 (3)
C45	0.053 (4)	0.047 (4)	0.072 (4)	0.025 (3)	0.015 (3)	0.009 (3)
C46	0.062 (4)	0.030 (3)	0.046 (3)	0.009 (3)	0.001 (3)	0.003 (3)
C47	0.049 (4)	0.029 (3)	0.055 (4)	0.010 (3)	−0.009 (3)	0.010 (3)
C48	0.044 (3)	0.028 (3)	0.041 (3)	0.014 (3)	0.001 (3)	0.011 (2)
C49	0.034 (3)	0.036 (3)	0.039 (3)	0.010 (3)	0.008 (3)	0.014 (2)
C50	0.033 (3)	0.034 (3)	0.049 (3)	0.012 (3)	0.008 (3)	0.008 (3)
C51	0.047 (4)	0.045 (3)	0.040 (3)	0.016 (3)	0.007 (3)	0.012 (3)
C52	0.057 (4)	0.046 (3)	0.052 (4)	0.021 (3)	0.011 (3)	0.019 (3)
C53	0.057 (4)	0.043 (3)	0.056 (4)	0.010 (3)	0.019 (3)	0.016 (3)
C54	0.050 (4)	0.049 (4)	0.051 (4)	0.014 (3)	0.008 (3)	0.018 (3)
C55	0.027 (3)	0.025 (3)	0.031 (3)	0.003 (2)	0.002 (2)	−0.001 (2)
C56	0.029 (3)	0.032 (3)	0.039 (3)	0.007 (3)	0.000 (2)	0.001 (2)
C57	0.045 (4)	0.034 (3)	0.039 (3)	0.014 (3)	0.008 (3)	0.008 (2)
C58	0.041 (4)	0.030 (3)	0.050 (3)	0.011 (3)	−0.005 (3)	0.008 (3)
C59	0.041 (4)	0.050 (4)	0.053 (4)	0.020 (3)	0.019 (3)	0.009 (3)
C60	0.030 (3)	0.038 (3)	0.041 (3)	0.005 (3)	0.002 (3)	0.010 (3)

Geometric parameters (Å, º)

Si1—O1	1.605 (3)	Si3—O4	1.612 (3)
Si1—O2	1.637 (3)	Si3—O3	1.620 (3)
Si1—C7	1.841 (5)	Si3—C31	1.841 (5)
Si1—C1	1.854 (5)	Si3—C37	1.858 (5)
Si2—O1	1.612 (3)	Si4—O3	1.620 (3)
Si2—C13	1.844 (5)	Si4—C43	1.848 (5)
Si2—C25	1.852 (5)	Si4—C55	1.854 (5)
Si2—C19	1.861 (5)	Si4—C49	1.861 (5)
O2—H2	0.8400	O4—H4	0.8400
C1—C2	1.389 (6)	C31—C36	1.387 (6)

C1—C6	1.390 (6)	C31—C32	1.405 (6)
C2—C3	1.391 (6)	C32—C33	1.374 (6)
C2—H2A	0.9500	C32—H32	0.9500
C3—C4	1.379 (6)	C33—C34	1.367 (6)
C3—H3	0.9500	C33—H33	0.9500
C4—C5	1.353 (6)	C34—C35	1.371 (6)
C4—H4A	0.9500	C34—H34	0.9500
C5—C6	1.382 (6)	C35—C36	1.375 (6)
C5—H5	0.9500	C35—H35	0.9500
C6—H6	0.9500	C36—H36	0.9500
C7—C8	1.391 (6)	C37—C38	1.355 (6)
C7—C12	1.400 (7)	C37—C42	1.372 (6)
C8—C9	1.391 (7)	C38—C39	1.390 (6)
C8—H8	0.9500	C38—H38	0.9500
C9—C10	1.375 (8)	C39—C40	1.359 (6)
C9—H9	0.9500	C39—H39	0.9500
C10—C11	1.365 (8)	C40—C41	1.356 (7)
C10—H10	0.9500	C40—H40	0.9500
C11—C12	1.361 (7)	C41—C42	1.394 (7)
C11—H11	0.9500	C41—H41	0.9500
C12—H12	0.9500	C42—H42	0.9500
C13—C14	1.375 (6)	C43—C44	1.374 (7)
C13—C18	1.381 (7)	C43—C48	1.396 (6)
C14—C15	1.376 (6)	C44—C45	1.391 (7)
C14—H14	0.9500	C44—H44	0.9500
C15—C16	1.354 (6)	C45—C46	1.364 (7)
C15—H15	0.9500	C45—H45	0.9500
C16—C17	1.360 (7)	C46—C47	1.365 (7)
C16—H16	0.9500	C46—H46	0.9500
C18—C17	1.384 (7)	C47—C48	1.385 (7)
C18—H18	0.9500	C47—H47	0.9500
C17—H17	0.9500	C48—H48	0.9500
C19—C20	1.369 (6)	C49—C50	1.376 (6)
C19—C24	1.393 (6)	C49—C54	1.395 (6)
C20—C21	1.365 (6)	C50—C51	1.371 (6)
C20—H20	0.9500	C50—H50	0.9500
C21—C22	1.371 (7)	C51—C52	1.353 (7)
C21—H21	0.9500	C51—H51	0.9500
C22—C23	1.356 (7)	C52—C53	1.362 (7)
C22—H22	0.9500	C52—H52	0.9500
C23—C24	1.380 (6)	C53—C54	1.388 (7)
C23—H23	0.9500	C53—H53	0.9500
C24—H24	0.9500	C54—H54	0.9500
C25—C26	1.382 (6)	C55—C60	1.380 (6)
C25—C30	1.393 (7)	C55—C56	1.404 (6)
C26—C27	1.393 (7)	C56—C57	1.377 (6)
C26—H26	0.9500	C56—H56	0.9500
C27—C28	1.369 (8)	C57—C58	1.369 (7)

C27—H27	0.9500	C57—H57	0.9500
C28—C29	1.332 (7)	C58—C59	1.380 (6)
C28—H28	0.9500	C58—H58	0.9500
C29—C30	1.391 (7)	C59—C60	1.386 (6)
C29—H29	0.9500	C59—H59	0.9500
C30—H30	0.9500	C60—H60	0.9500
O1—Si1—O2	104.71 (18)	O4—Si3—O3	112.18 (18)
O1—Si1—C7	109.5 (2)	O4—Si3—C31	105.99 (19)
O2—Si1—C7	110.8 (2)	O3—Si3—C31	107.02 (19)
O1—Si1—C1	110.52 (19)	O4—Si3—C37	110.2 (2)
O2—Si1—C1	108.2 (2)	O3—Si3—C37	108.71 (19)
C7—Si1—C1	112.7 (2)	C31—Si3—C37	112.7 (2)
O1—Si2—C13	108.3 (2)	O3—Si4—C43	105.9 (2)
O1—Si2—C25	109.7 (2)	O3—Si4—C55	109.85 (19)
C13—Si2—C25	112.2 (2)	C43—Si4—C55	108.6 (2)
O1—Si2—C19	107.69 (19)	O3—Si4—C49	109.6 (2)
C13—Si2—C19	110.5 (2)	C43—Si4—C49	115.4 (2)
C25—Si2—C19	108.3 (2)	C55—Si4—C49	107.5 (2)
Si1—O1—Si2	166.0 (2)	Si3—O3—Si4	147.7 (2)
Si1—O2—H2	109.5	Si3—O4—H4	109.5
C2—C1—C6	117.3 (4)	C36—C31—C32	116.5 (4)
C2—C1—Si1	120.8 (4)	C36—C31—Si3	120.7 (4)
C6—C1—Si1	121.9 (4)	C32—C31—Si3	122.8 (4)
C1—C2—C3	120.9 (5)	C33—C32—C31	121.1 (5)
C1—C2—H2A	119.6	C33—C32—H32	119.5
C3—C2—H2A	119.6	C31—C32—H32	119.5
C4—C3—C2	119.6 (5)	C34—C33—C32	120.4 (5)
C4—C3—H3	120.2	C34—C33—H33	119.8
C2—C3—H3	120.2	C32—C33—H33	119.8
C5—C4—C3	120.7 (5)	C33—C34—C35	120.3 (5)
C5—C4—H4A	119.6	C33—C34—H34	119.8
C3—C4—H4A	119.6	C35—C34—H34	119.8
C4—C5—C6	119.6 (5)	C34—C35—C36	119.3 (5)
C4—C5—H5	120.2	C34—C35—H35	120.3
C6—C5—H5	120.2	C36—C35—H35	120.3
C5—C6—C1	121.8 (5)	C35—C36—C31	122.4 (5)
C5—C6—H6	119.1	C35—C36—H36	118.8
C1—C6—H6	119.1	C31—C36—H36	118.8
C8—C7—C12	117.9 (5)	C38—C37—C42	116.3 (5)
C8—C7—Si1	121.9 (4)	C38—C37—Si3	121.6 (4)
C12—C7—Si1	120.2 (4)	C42—C37—Si3	122.1 (4)
C7—C8—C9	120.5 (5)	C37—C38—C39	122.9 (5)
C7—C8—H8	119.7	C37—C38—H38	118.6
C9—C8—H8	119.7	C39—C38—H38	118.6
C10—C9—C8	119.7 (5)	C40—C39—C38	119.7 (5)
C10—C9—H9	120.1	C40—C39—H39	120.1
C8—C9—H9	120.1	C38—C39—H39	120.1

C11—C10—C9	120.0 (6)	C41—C40—C39	119.1 (5)
C11—C10—H10	120.0	C41—C40—H40	120.5
C9—C10—H10	120.0	C39—C40—H40	120.5
C12—C11—C10	121.0 (6)	C40—C41—C42	120.2 (5)
C12—C11—H11	119.5	C40—C41—H41	119.9
C10—C11—H11	119.5	C42—C41—H41	119.9
C11—C12—C7	120.8 (5)	C37—C42—C41	121.8 (5)
C11—C12—H12	119.6	C37—C42—H42	119.1
C7—C12—H12	119.6	C41—C42—H42	119.1
C14—C13—C18	116.4 (5)	C44—C43—C48	116.9 (5)
C14—C13—Si2	123.6 (4)	C44—C43—Si4	121.9 (4)
C18—C13—Si2	120.0 (4)	C48—C43—Si4	121.0 (4)
C13—C14—C15	122.4 (5)	C43—C44—C45	122.0 (5)
C13—C14—H14	118.8	C43—C44—H44	119.0
C15—C14—H14	118.8	C45—C44—H44	119.0
C16—C15—C14	119.5 (5)	C46—C45—C44	119.4 (6)
C16—C15—H15	120.3	C46—C45—H45	120.3
C14—C15—H15	120.3	C44—C45—H45	120.3
C15—C16—C17	120.4 (5)	C45—C46—C47	120.6 (5)
C15—C16—H16	119.8	C45—C46—H46	119.7
C17—C16—H16	119.8	C47—C46—H46	119.7
C13—C18—C17	121.6 (5)	C46—C47—C48	119.6 (5)
C13—C18—H18	119.2	C46—C47—H47	120.2
C17—C18—H18	119.2	C48—C47—H47	120.2
C16—C17—C18	119.5 (5)	C47—C48—C43	121.5 (5)
C16—C17—H17	120.2	C47—C48—H48	119.3
C18—C17—H17	120.2	C43—C48—H48	119.3
C20—C19—C24	116.9 (5)	C50—C49—C54	116.3 (5)
C20—C19—Si2	121.3 (4)	C50—C49—Si4	121.2 (4)
C24—C19—Si2	121.8 (4)	C54—C49—Si4	122.3 (4)
C21—C20—C19	121.8 (5)	C51—C50—C49	122.2 (5)
C21—C20—H20	119.1	C51—C50—H50	118.9
C19—C20—H20	119.1	C49—C50—H50	118.9
C20—C21—C22	120.4 (5)	C52—C51—C50	120.3 (5)
C20—C21—H21	119.8	C52—C51—H51	119.8
C22—C21—H21	119.8	C50—C51—H51	119.8
C23—C22—C21	119.5 (5)	C51—C52—C53	120.2 (5)
C23—C22—H22	120.2	C51—C52—H52	119.9
C21—C22—H22	120.2	C53—C52—H52	119.9
C22—C23—C24	119.9 (5)	C52—C53—C54	119.5 (5)
C22—C23—H23	120.0	C52—C53—H53	120.2
C24—C23—H23	120.0	C54—C53—H53	120.2
C23—C24—C19	121.4 (5)	C53—C54—C49	121.5 (5)
C23—C24—H24	119.3	C53—C54—H54	119.3
C19—C24—H24	119.3	C49—C54—H54	119.3
C26—C25—C30	116.8 (5)	C60—C55—C56	116.6 (4)
C26—C25—Si2	122.9 (4)	C60—C55—Si4	123.3 (4)
C30—C25—Si2	120.1 (4)	C56—C55—Si4	120.1 (4)

C25—C26—C27	122.0 (5)	C57—C56—C55	121.9 (5)
C25—C26—H26	119.0	C57—C56—H56	119.1
C27—C26—H26	119.0	C55—C56—H56	119.1
C28—C27—C26	118.0 (6)	C58—C57—C56	120.0 (5)
C28—C27—H27	121.0	C58—C57—H57	120.0
C26—C27—H27	121.0	C56—C57—H57	120.0
C29—C28—C27	122.5 (6)	C57—C58—C59	119.8 (5)
C29—C28—H28	118.7	C57—C58—H58	120.1
C27—C28—H28	118.7	C59—C58—H58	120.1
C28—C29—C30	119.3 (6)	C58—C59—C60	119.9 (5)
C28—C29—H29	120.4	C58—C59—H59	120.0
C30—C29—H29	120.4	C60—C59—H59	120.0
C29—C30—C25	121.4 (5)	C55—C60—C59	121.8 (5)
C29—C30—H30	119.3	C55—C60—H60	119.1
C25—C30—H30	119.3	C59—C60—H60	119.1

O2—Si1—O1—Si2	144.4 (9)	O4—Si3—O3—Si4	−27.6 (4)
C7—Si1—O1—Si2	−96.7 (9)	C31—Si3—O3—Si4	−143.4 (4)
C1—Si1—O1—Si2	28.1 (10)	C37—Si3—O3—Si4	94.6 (4)
C13—Si2—O1—Si1	−87.0 (9)	C43—Si4—O3—Si3	−146.9 (4)
C25—Si2—O1—Si1	35.8 (10)	C55—Si4—O3—Si3	−29.8 (5)
C19—Si2—O1—Si1	153.5 (9)	C49—Si4—O3—Si3	88.1 (4)
O1—Si1—C1—C2	−65.9 (4)	O4—Si3—C31—C36	45.6 (4)
O2—Si1—C1—C2	180.0 (4)	O3—Si3—C31—C36	165.5 (3)
C7—Si1—C1—C2	57.0 (5)	C37—Si3—C31—C36	−75.1 (4)
O1—Si1—C1—C6	114.5 (4)	O4—Si3—C31—C32	−133.3 (4)
O2—Si1—C1—C6	0.3 (4)	O3—Si3—C31—C32	−13.4 (5)
C7—Si1—C1—C6	−122.6 (4)	C37—Si3—C31—C32	106.1 (4)
C6—C1—C2—C3	−0.9 (7)	C36—C31—C32—C33	1.9 (7)
Si1—C1—C2—C3	179.4 (4)	Si3—C31—C32—C33	−179.2 (4)
C1—C2—C3—C4	−0.9 (7)	C31—C32—C33—C34	−0.5 (8)
C2—C3—C4—C5	1.7 (7)	C32—C33—C34—C35	−1.1 (8)
C3—C4—C5—C6	−0.5 (7)	C33—C34—C35—C36	1.1 (8)
C4—C5—C6—C1	−1.5 (7)	C34—C35—C36—C31	0.3 (7)
C2—C1—C6—C5	2.2 (7)	C32—C31—C36—C35	−1.8 (7)
Si1—C1—C6—C5	−178.2 (4)	Si3—C31—C36—C35	179.3 (4)
O1—Si1—C7—C8	−23.1 (5)	O4—Si3—C37—C38	−177.1 (4)
O2—Si1—C7—C8	91.9 (5)	O3—Si3—C37—C38	59.6 (5)
C1—Si1—C7—C8	−146.6 (4)	C31—Si3—C37—C38	−58.9 (5)
O1—Si1—C7—C12	156.8 (4)	O4—Si3—C37—C42	1.5 (5)
O2—Si1—C7—C12	−88.2 (5)	O3—Si3—C37—C42	−121.8 (4)
C1—Si1—C7—C12	33.3 (5)	C31—Si3—C37—C42	119.7 (4)
C12—C7—C8—C9	−0.5 (8)	C42—C37—C38—C39	−0.7 (8)
Si1—C7—C8—C9	179.4 (5)	Si3—C37—C38—C39	178.0 (4)
C7—C8—C9—C10	2.1 (10)	C37—C38—C39—C40	−0.5 (8)
C8—C9—C10—C11	−1.9 (11)	C38—C39—C40—C41	2.4 (8)
C9—C10—C11—C12	0.1 (11)	C39—C40—C41—C42	−3.0 (8)
C10—C11—C12—C7	1.5 (10)	C38—C37—C42—C41	0.0 (8)

C8—C7—C12—C11	−1.3 (9)	Si3—C37—C42—C41	−178.6 (4)
Si1—C7—C12—C11	178.8 (5)	C40—C41—C42—C37	1.8 (9)
O1—Si2—C13—C14	26.6 (5)	O3—Si4—C43—C44	−17.0 (4)
C25—Si2—C13—C14	−94.7 (5)	C55—Si4—C43—C44	−134.9 (4)
C19—Si2—C13—C14	144.3 (4)	C49—Si4—C43—C44	104.4 (4)
O1—Si2—C13—C18	−153.2 (4)	O3—Si4—C43—C48	159.4 (3)
C25—Si2—C13—C18	85.5 (5)	C55—Si4—C43—C48	41.5 (4)
C19—Si2—C13—C18	−35.5 (5)	C49—Si4—C43—C48	−79.2 (4)
C18—C13—C14—C15	−3.2 (8)	C48—C43—C44—C45	−1.8 (7)
Si2—C13—C14—C15	177.0 (4)	Si4—C43—C44—C45	174.7 (4)
C13—C14—C15—C16	0.5 (8)	C43—C44—C45—C46	0.1 (8)
C14—C15—C16—C17	1.9 (8)	C44—C45—C46—C47	1.9 (8)
C14—C13—C18—C17	3.7 (8)	C45—C46—C47—C48	−2.3 (8)
Si2—C13—C18—C17	−176.5 (5)	C46—C47—C48—C43	0.6 (7)
C15—C16—C17—C18	−1.4 (9)	C44—C43—C48—C47	1.4 (7)
C13—C18—C17—C16	−1.5 (10)	Si4—C43—C48—C47	−175.1 (4)
O1—Si2—C19—C20	31.0 (5)	O3—Si4—C49—C50	−23.3 (5)
C13—Si2—C19—C20	−87.1 (5)	C43—Si4—C49—C50	−142.7 (4)
C25—Si2—C19—C20	149.6 (4)	C55—Si4—C49—C50	96.0 (4)
O1—Si2—C19—C24	−148.6 (4)	O3—Si4—C49—C54	162.3 (4)
C13—Si2—C19—C24	93.3 (5)	C43—Si4—C49—C54	42.9 (5)
C25—Si2—C19—C24	−30.0 (5)	C55—Si4—C49—C54	−78.4 (4)
C24—C19—C20—C21	−0.9 (8)	C54—C49—C50—C51	−1.4 (7)
Si2—C19—C20—C21	179.5 (4)	Si4—C49—C50—C51	−176.1 (4)
C19—C20—C21—C22	−0.7 (9)	C49—C50—C51—C52	2.3 (8)
C20—C21—C22—C23	1.4 (9)	C50—C51—C52—C53	−2.1 (8)
C21—C22—C23—C24	−0.3 (9)	C51—C52—C53—C54	1.2 (8)
C22—C23—C24—C19	−1.4 (9)	C52—C53—C54—C49	−0.3 (8)
C20—C19—C24—C23	2.0 (8)	C50—C49—C54—C53	0.4 (7)
Si2—C19—C24—C23	−178.4 (4)	Si4—C49—C54—C53	175.1 (4)
O1—Si2—C25—C26	−142.9 (4)	O3—Si4—C55—C60	126.9 (4)
C13—Si2—C25—C26	−22.4 (5)	C43—Si4—C55—C60	−117.7 (4)
C19—Si2—C25—C26	99.8 (4)	C49—Si4—C55—C60	7.8 (4)
O1—Si2—C25—C30	42.0 (5)	O3—Si4—C55—C56	−53.8 (4)
C13—Si2—C25—C30	162.5 (4)	C43—Si4—C55—C56	61.6 (4)
C19—Si2—C25—C30	−75.3 (5)	C49—Si4—C55—C56	−172.9 (3)
C30—C25—C26—C27	0.8 (7)	C60—C55—C56—C57	−0.8 (6)
Si2—C25—C26—C27	−174.4 (4)	Si4—C55—C56—C57	179.9 (3)
C25—C26—C27—C28	−1.9 (8)	C55—C56—C57—C58	−0.4 (7)
C26—C27—C28—C29	1.2 (9)	C56—C57—C58—C59	1.0 (7)
C27—C28—C29—C30	0.6 (9)	C57—C58—C59—C60	−0.4 (7)
C28—C29—C30—C25	−1.8 (9)	C56—C55—C60—C59	1.4 (7)
C26—C25—C30—C29	1.0 (8)	Si4—C55—C60—C59	−179.3 (4)
Si2—C25—C30—C29	176.4 (4)	C58—C59—C60—C55	−0.9 (7)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4···O2	0.84	1.94	2.742 (4)	160
O2—H2···*Cg*(C55–C60)	0.84	2.44	3.181 (2)	147