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1-Hydroxy-1,1,3,3,3-pentaphenyldisiloxane, $[Si_2O(OH)(Ph)_5]$, at 150 K

Tatiana R. Amarante,[a] Ana C. Coelho,[a] Jacek Klinowski,[b] Isabel S. Gonçalves[a] and Filipe A. Almeida Paz[a]*

[a]Department of Chemistry, University of Aveiro, CICECO, 3810-193 Aveiro, Portugal, and [b]Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, England
Correspondence e-mail: filipe.paz@ua.pt

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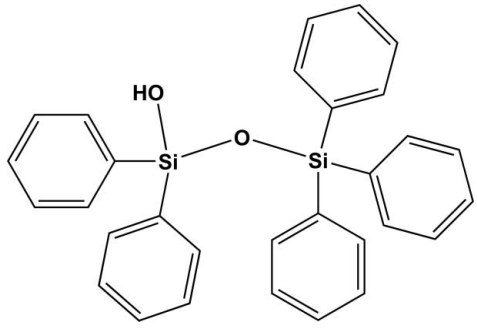
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.009 Å; R factor = 0.079; wR factor = 0.250; data-to-parameter ratio = 14.5.

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 nonlinear Si—O—Si bridge. The asymmetric unit is composed of four $[Si_2O(OH)(Ph)_5]$ molecules. Each pair of adjacent molecules interacts *via* strong and highly directional O—H···O hydrogen bonds connecting neighbouring Si—OH units, and *via* inter-unit O—H···π contacts connecting the second hydroxyl groups with adjacent phenyl groups.

Related literature

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 a crystallographic determination of the title compound at 100 (2) K, see the preceding paper: Coelho *et al.* (2008).



Experimental

Crystal data

$C_{30}H_{26}O_2Si_2$
M_r = 474.69
Triclinic, $P\overline{1}$
a = 15.0113 (12) Å
b = 19.9930 (15) Å
c = 20.1661 (16) Å
α = 65.270 (3)°
β = 71.217 (4)°
γ = 87.173 (4)°
V = 5178.7 (7) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.16 mm^{-1}
T = 150 (2) K
0.30 × 0.22 × 0.12 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
T_{min} = 0.923, T_{max} = 0.981
96391 measured reflections
17802 independent reflections
8243 reflections with $I > 2\sigma(I)$
R_{int} = 0.120

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.079
$wR(F^2)$ = 0.250
S = 1.02
17802 reflections
1229 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O6—H6A···O2	0.84	2.03	2.785 (5)	149
O8—H8A···O4^{i}	0.84	1.94	2.735 (5)	158
O2—H2···Cg(C67–C72)	0.84	2.66	3.355 (5)	142
O4—H4A···Cg(C97–C102)	0.84	2.61	3.249 (5)	134

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

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: TK2229).

References

Brandenburg, K. (2006). *DIAMOND*. Version 3.1e. Crystal Impact GbR, Bonn, Germany.
Bruker (2001). *SHELXTL*. Version 6.12. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2005). *SAINT-Plus*. Version 7.23a. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2006). *APEX2*. Version 2.1-RC13. Bruker AXS, Delft, The Netherlands.
Coelho, A. C., Amarante, T. R., Klinowski, J., Gonçalves, I. S. & Paz, F. A. A. (2008). *Acta Cryst.* E**64**, o237–o238.
Glidewell, C. & Liles, D. C. (1978). *Acta Cryst.* B**34**, 124–128.
Hönle, W., Manríquez, V. & von Schnering, H. G. (1990). *Acta Cryst.* C**46**, 1982–1984.
Morosin, B. & Harrah, L. A. (1981). *Acta Cryst.* B**37**, 579–586.
Sheldrick, G. M. (1998). *SADABS*. Version 2.01. Bruker AXS Inc., Madison, Wisconsin, USA.
Suwińska, K., Palenik, G. J. & Gerdil, R. (1986). *Acta Cryst.* C**42**, 615–620.
Wojnowski, D. W., Becker, B., Peters, K., Peters, E.-M. & von Schnering, H. G. (2004). *Z. Anorg. Allg. Chem.* **563**, 48–52.

supporting information

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1-Hydroxy-1,1,3,3,3-pentaphenyldisiloxane, $[Si_2O(OH)(Ph)_5]$, at 150 K

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S1. Comment

In a separate crystallographic communication we reported the crystal structure of the title compound, (I), at 100 K in the triclinic $P\bar{1}$ space group with two $[Si_2O(OH)(Ph)_5]$ molecular units comprising the asymmetric unit (see Coelho *et al.*, 2008). At 150 K, a decrease in overall long range symmetry, accompanied by an increase in size of the unit cell (by a factor of *ca* 2) and, consequently, in the number of crystallographically independent binuclear $[Si_2O(OH)(Ph)_5]$ molecular units (from two at 100 K to four at 150 K, see Fig. 1. It is important to stress that the reduction of overall symmetry seems to be essentially due to an increase of thermal motion of the coordinated phenyl groups. Indeed, even though the increase in temperature was only of about 50 K, since the intermolecular interactions between adjacent $[Si_2O(OH)(Ph)_5]$ complexes are of rather weak nature (van der Waals interactions alongside with a number of C—H···π contacts between phenyl groups belonging to adjacent complexes), equivalence between adjacent binuclear units is ultimately destroyed by a combined effect of rotation of the phenyl groups around the Si—C bond with in-plane thermal vibration of the carbon atoms (Figure 1). In fact, the average value of U_{eq} for the carbon atoms composing the phenyl groups increases from 0.047 Å^2 (at 100 K) to 0.052 Å^2 (at 150 K).

The intramolecular geometrical features defining the binuclear $[Si_2O(OH)(Ph)_5]$ units in (I) remain relatively unchanged when compared with those at 100 K (Coelho *et al.* (2008), Table 1. For the two Si centres within each unit, $\{SiC_3O\}$ and $\{SiC_2O_2\}$, the Si—C and Si—O bond lengths were found in the 1.842 (5)–1.875 (5) and 1.605 (3)–1.648 (3) Å ranges, respectively, in good agreement with those found in related materials and in our determination at 100 K. Each pair of Si centres is interconnected *via* a μ_2-bridging oxo group, imposing Si···Si internuclear distances ranging from 3.113 (2) Å to 3.216 (2) Å. These distances are shorter than those registered for disiloxanes in which the two Si centres exhibit identical coordination environments (found in the 3.24–3.44 Å range; see Glidewell & Liles, 1978; Hönle *et al.*, 1990; Suwińska *et al.*, 1986). In fact, the presence of distinct coordinating moieties, and the type of intermolecular interactions in which they are involved with neighbouring species, leads to a deformation of the binuclear units through the μ_2-bridge, ultimately imposing shorter Si···Si interatomic distances. The Si—O—Si bond angles for (I) were found in the 145.1 (2)–169.5 (2)° range (Fig. 1 & Table 1) and, as described for the determination of (I) at 100 K, are distributed over two markedly distinct ranges. On the one hand, the high range values are in good agreement with the angle reported by Wojnowski *et al.* (2004) for $[Si_2O(H)(Ph)_5]$ (*ca* 163.3°). On the other, the shorter Si—O—Si angles arise due to O—H···π interactions between the O2 and O4 hydroxyl groups and the neighbouring C57→C72 and C97→C101 phenyl groups, respectively (Fig. 1 and Table 2). In fact, besides the strong and highly directional O—H···O hydrogen bond connecting each pair of adjacent $[Si_2O(OH)(Ph)_5]$ molecular units, these weak O—H···π contacts are the second strongest intermolecular interactions in (I). It is clear from Fig. 1 that the thermal motion of the phenyl groups involved in these interactions is significantly more limited than those of the remaining phenyl groups.

As for the structure at 100 K, at 150 K supramolecular entities formed by the combined effected of the O—H···O hydrogen bonds and O—H···π contacts arrange themselves in an ordely fashion in the *ac* plane of the unit cell forming layers, which close pack along the [010] direction of the unit cell to give the crystal structure of (I), Fig. 2. We also note the presence of a number of C—H···π contacts between phenyl groups (not shown) which help to mediate the crystal packing of individual $[Si_2O(H)(Ph)_5]$ molecular units.

S2. Experimental

Crystals of the title compound were isolated from the same batch as those used for the determination at 100 K of the title compound (see Coelho *et al.*, 2008).

S3. Refinement

A small number of single-crystals of (I) could be indexed at 100 K with the unit-cell parameters summarized in the Experimental Table given in the previous paper (Coelho *et al.*, 2008). Those results led us to infer that the increase of thermal motion, in particular that associated with the coordinated phenyl groups, could, to some extent, reduce overall symmetry. Preliminary measurements for several different crystals at 150 K confirmed the increase of the size of the triclinic unit cell by approximately a factor of 2.

Due to the already well known poor crystal quality of (I) (Coelho *et al.*, 2008), a full data set was collected at 150 K by employing a long exposure time per acquired frame (120 s). Once again, spot shape was seriously compromised by the low quality of the crystals leading to a relatively high value for R_{int}. The structure was solved using direct-methods which allowed the immediate location of almost all non-H atoms comprising the four crystallographically independent $[Si_2O(OH)(Ph)_5]$ molecular units. All remaining non-H atoms were located from difference Fourier maps calculated from successive least-squares refinement cycles. Non-H atoms were 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).

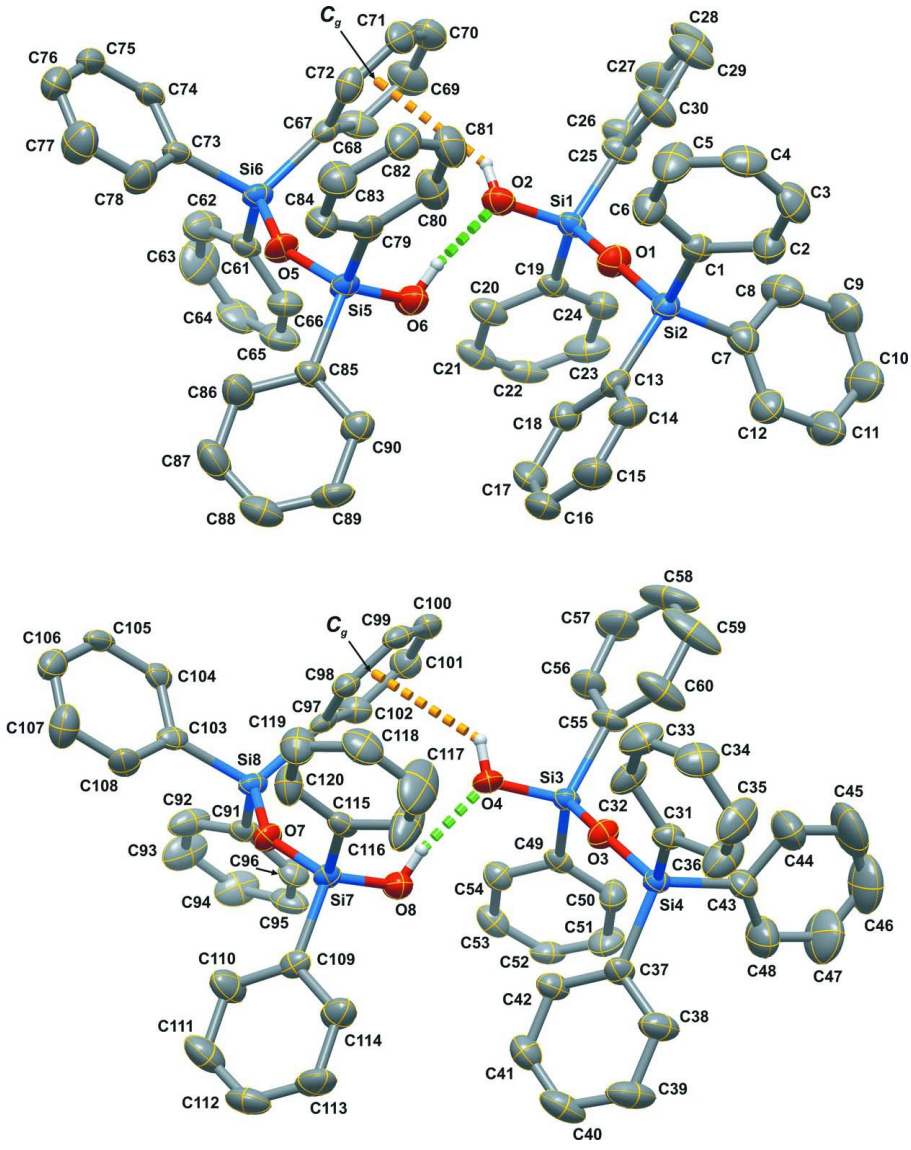

Figure 1

Schematic representation of the four crystallographically independent $[Si_2O(OH)(Ph)_5]$ molecular units composing the asymmetric unit of the title compound 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.

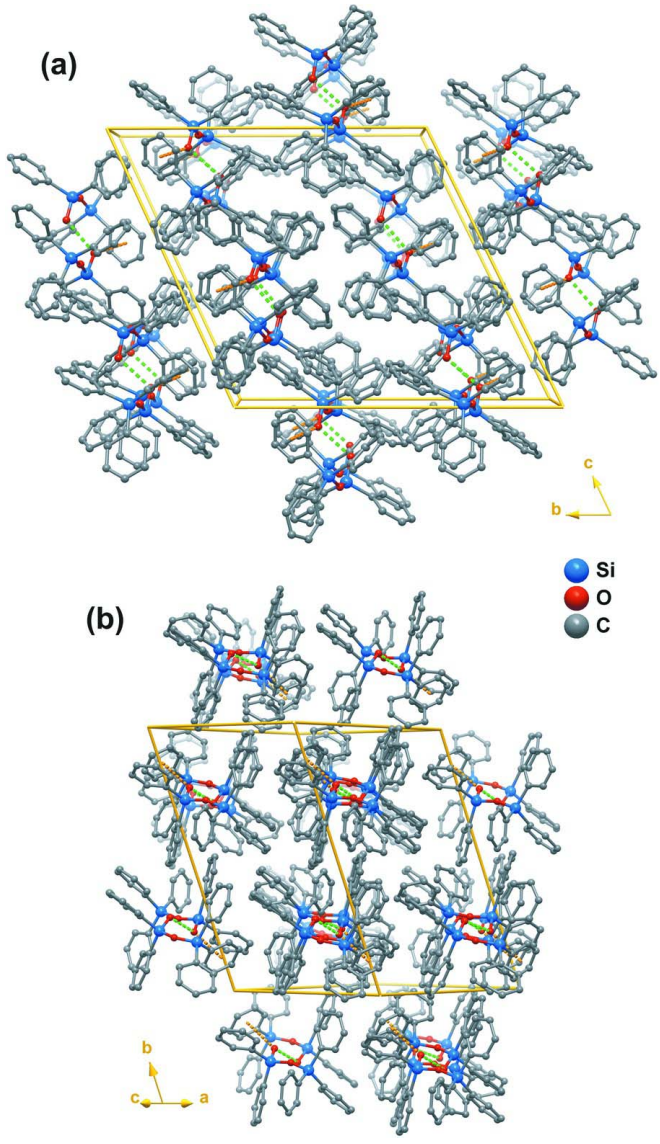

Figure 2

Crystal packing of the title compound viewed in perspective along the (**a**) [010] and (**b**) [101] directions of the unit cell. O—H···O hydrogen bonding interactions and O—H···π contacts are represented as dashed green and orange lines, respectively. 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
$a = 15.0113\ (12)$ Å
$b = 19.9930\ (15)$ Å
$c = 20.1661\ (16)$ Å
$\alpha = 65.270\ (3)°$
$\beta = 71.217\ (4)°$
$\gamma = 87.173\ (4)°$
$V = 5178.7\ (7)$ Å^3
$Z = 8$
$F(000) = 2000$
$D_x = 1.218$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8707 reflections
$\theta = 2.4–22.4°$
$\mu = 0.16$ mm^{-1}

T = 150 K
Prism, colourless
0.30 × 0.22 × 0.12 mm

Data collection

Bruker X8 Kappa CCD APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω/φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
T_{min} = 0.923, T_{max} = 0.981
96391 measured reflections
17802 independent reflections
8243 reflections with $I > 2\sigma(I)$
R_{int} = 0.120
θ_{max} = 25.4°, θ_{min} = 3.5°
h = −18→18
k = −23→23
l = −24→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.079
$wR(F^2)$ = 0.250
S = 1.02
17802 reflections
1229 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1212P)^2 + 1.2286P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 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	0.39433 (9)	0.28703 (8)	0.47224 (8)	0.0318 (4)
Si2	0.17139 (9)	0.30287 (8)	0.52914 (8)	0.0326 (4)
O2	0.4251 (2)	0.2349 (2)	0.54784 (19)	0.0413 (10)
H2	0.4691	0.2105	0.5349	0.062*
O1	0.2822 (2)	0.28788 (19)	0.50744 (19)	0.0419 (10)
C19	0.4559 (3)	0.3818 (3)	0.4276 (3)	0.0329 (13)
C20	0.5076 (4)	0.4029 (3)	0.4637 (3)	0.0420 (14)
H20	0.5103	0.3684	0.5125	0.050*
C21	0.5547 (4)	0.4732 (4)	0.4296 (4)	0.0517 (16)
H21	0.5889	0.4862	0.4555	0.062*
C22	0.5527 (4)	0.5237 (4)	0.3596 (4)	0.0551 (18)
H22	0.5863	0.5713	0.3364	0.066*
C23	0.5022 (5)	0.5059 (4)	0.3225 (4)	0.0595 (19)

H23	0.4995	0.5415	0.2741	0.071*
C24	0.4547 (4)	0.4353 (3)	0.3559 (3)	0.0506 (16)
H24	0.4207	0.4234	0.3293	0.061*
C25	0.4188 (3)	0.2455 (3)	0.4021 (3)	0.0391 (14)
C26	0.4959 (4)	0.2714 (3)	0.3332 (3)	0.0529 (16)
H26	0.5379	0.3120	0.3212	0.063*
C27	0.5125 (5)	0.2385 (4)	0.2814 (4)	0.0619 (19)
H27	0.5651	0.2569	0.2348	0.074*
C28	0.4525 (5)	0.1800 (4)	0.2984 (4)	0.068 (2)
H28	0.4632	0.1578	0.2633	0.082*
C29	0.3777 (5)	0.1534 (4)	0.3649 (4)	0.0649 (19)
H29	0.3374	0.1116	0.3775	0.078*
C30	0.3603 (4)	0.1874 (4)	0.4145 (3)	0.0529 (16)
H30	0.3054	0.1698	0.4593	0.064*
C1	0.0977 (3)	0.2129 (3)	0.5701 (3)	0.0320 (13)
C2	0.0202 (4)	0.2062 (3)	0.5481 (3)	0.0483 (16)
H2A	0.0049	0.2485	0.5103	0.058*
C3	−0.0346 (4)	0.1397 (4)	0.5801 (4)	0.0532 (17)
H3	−0.0859	0.1363	0.5634	0.064*
C4	−0.0148 (4)	0.0791 (3)	0.6355 (3)	0.0495 (16)
H4	−0.0532	0.0336	0.6588	0.059*
C5	0.0602 (4)	0.0842 (3)	0.6574 (4)	0.062 (2)
H5	0.0749	0.0415	0.6951	0.075*
C6	0.1154 (4)	0.1500 (3)	0.6263 (3)	0.0509 (17)
H6	0.1664	0.1522	0.6437	0.061*
C7	0.1419 (4)	0.3688 (3)	0.4433 (3)	0.0447 (15)
C8	0.1661 (4)	0.3559 (4)	0.3769 (3)	0.0603 (18)
H8	0.2024	0.3163	0.3740	0.072*
C9	0.1361 (5)	0.4022 (4)	0.3136 (4)	0.074 (2)
H9	0.1531	0.3947	0.2678	0.088*
C10	0.0810 (5)	0.4589 (4)	0.3203 (4)	0.075 (2)
H10	0.0600	0.4898	0.2787	0.090*
C11	0.0566 (5)	0.4711 (4)	0.3860 (4)	0.068 (2)
H11	0.0202	0.5105	0.3892	0.082*
C12	0.0854 (4)	0.4258 (3)	0.4468 (3)	0.0527 (17)
H12	0.0663	0.4333	0.4927	0.063*
C13	0.1444 (4)	0.3414 (3)	0.6026 (3)	0.0382 (14)
C14	0.0558 (4)	0.3252 (3)	0.6613 (3)	0.0479 (16)
H14	0.0094	0.2916	0.6655	0.057*
C15	0.0346 (4)	0.3568 (4)	0.7130 (3)	0.0562 (18)
H15	−0.0262	0.3456	0.7514	0.067*
C16	0.1008 (5)	0.4044 (3)	0.7096 (4)	0.0553 (17)
H16	0.0864	0.4259	0.7454	0.066*
C17	0.1884 (4)	0.4205 (3)	0.6532 (4)	0.0514 (16)
H17	0.2346	0.4537	0.6498	0.062*
C18	0.2099 (4)	0.3884 (3)	0.6013 (3)	0.0407 (14)
H18	0.2714	0.3991	0.5639	0.049*
Si3	0.10190 (9)	0.72672 (8)	0.00913 (8)	0.0274 (4)

Si4	0.32006 (9)	0.69827 (8)	−0.02096 (8)	0.0272 (4)
O4	0.0753 (2)	0.77425 (19)	−0.07009 (18)	0.0372 (9)
H4A	0.0448	0.8093	−0.0656	0.056*
O3	0.2148 (2)	0.72493 (18)	−0.01884 (18)	0.0353 (9)
C49	0.0418 (3)	0.6318 (3)	0.0516 (3)	0.0295 (12)
C50	0.0627 (4)	0.5732 (3)	0.1106 (3)	0.0466 (15)
H50	0.1078	0.5820	0.1307	0.056*
C51	0.0192 (4)	0.5019 (3)	0.1410 (4)	0.0551 (17)
H51	0.0359	0.4628	0.1808	0.066*
C52	−0.0466 (4)	0.4876 (3)	0.1147 (3)	0.0431 (15)
H52	−0.0772	0.4391	0.1368	0.052*
C53	−0.0690 (4)	0.5435 (3)	0.0559 (3)	0.0437 (15)
H53	−0.1146	0.5338	0.0367	0.052*
C54	−0.0244 (3)	0.6150 (3)	0.0243 (3)	0.0378 (14)
H54	−0.0396	0.6533	−0.0169	0.045*
C55	0.0671 (4)	0.7755 (3)	0.0726 (3)	0.0361 (13)
C56	−0.0278 (4)	0.7820 (3)	0.1058 (3)	0.0539 (17)
H56	−0.0742	0.7595	0.0967	0.065*
C57	−0.0569 (6)	0.8197 (4)	0.1514 (4)	0.071 (2)
H57	−0.1223	0.8230	0.1736	0.085*
C58	0.0105 (7)	0.8530 (4)	0.1643 (4)	0.088 (3)
H58	−0.0083	0.8787	0.1961	0.106*
C59	0.1047 (6)	0.8486 (5)	0.1310 (4)	0.096 (3)
H59	0.1511	0.8711	0.1400	0.115*
C60	0.1320 (5)	0.8115 (4)	0.0844 (4)	0.070 (2)
H60	0.1974	0.8109	0.0598	0.084*
C31	0.4043 (3)	0.7838 (3)	−0.0753 (3)	0.0311 (13)
C32	0.3773 (4)	0.8529 (3)	−0.1120 (3)	0.0436 (15)
H32	0.3144	0.8569	−0.1132	0.052*
C33	0.4385 (4)	0.9165 (3)	−0.1470 (3)	0.0532 (17)
H33	0.4178	0.9632	−0.1723	0.064*
C34	0.5300 (4)	0.9123 (3)	−0.1453 (3)	0.0521 (17)
H34	0.5718	0.9560	−0.1680	0.062*
C35	0.5596 (4)	0.8441 (4)	−0.1104 (4)	0.063 (2)
H35	0.6230	0.8405	−0.1105	0.075*
C36	0.4981 (4)	0.7808 (3)	−0.0752 (4)	0.0579 (19)
H36	0.5195	0.7343	−0.0505	0.070*
C37	0.3436 (3)	0.6322 (3)	−0.0666 (3)	0.0337 (13)
C38	0.4224 (4)	0.5922 (3)	−0.0663 (4)	0.0532 (16)
H38	0.4625	0.5972	−0.0403	0.064*
C39	0.4440 (4)	0.5446 (4)	−0.1034 (4)	0.0636 (19)
H39	0.4990	0.5189	−0.1037	0.076*
C40	0.3843 (4)	0.5355 (4)	−0.1396 (4)	0.0598 (18)
H40	0.3980	0.5041	−0.1654	0.072*
C41	0.3058 (4)	0.5724 (3)	−0.1374 (3)	0.0466 (15)
H41	0.2643	0.5657	−0.1617	0.056*
C42	0.2841 (4)	0.6192 (3)	−0.1014 (3)	0.0372 (14)
H42	0.2276	0.6430	−0.1002	0.045*

C43	0.3256 (3)	0.6524 (3)	0.0794 (3)	0.0378 (14)
C44	0.3382 (5)	0.6943 (5)	0.1155 (4)	0.080 (2)
H44	0.3482	0.7467	0.0880	0.097*
C45	0.3365 (6)	0.6608 (7)	0.1920 (5)	0.112 (3)
H45	0.3440	0.6907	0.2166	0.135*
C46	0.3241 (6)	0.5852 (7)	0.2322 (5)	0.095 (3)
H46	0.3216	0.5627	0.2847	0.114*
C47	0.3155 (6)	0.5438 (5)	0.1971 (4)	0.092 (3)
H47	0.3102	0.4914	0.2236	0.111*
C48	0.3144 (5)	0.5770 (4)	0.1216 (4)	0.068 (2)
H48	0.3054	0.5463	0.0984	0.082*
Si5	0.39510 (9)	0.22194 (8)	0.75524 (8)	0.0318 (4)
Si6	0.60817 (9)	0.19073 (8)	0.70887 (8)	0.0326 (4)
O6	0.3913 (3)	0.2745 (2)	0.67015 (19)	0.0435 (10)
H6A	0.3880	0.2483	0.6473	0.065*
O5	0.5025 (2)	0.2045 (2)	0.75410 (19)	0.0412 (10)
C79	0.3205 (3)	0.1320 (3)	0.7994 (3)	0.0337 (13)
C80	0.2858 (4)	0.1057 (4)	0.7573 (3)	0.0519 (17)
H80	0.3013	0.1343	0.7031	0.062*
C81	0.2295 (4)	0.0394 (4)	0.7919 (4)	0.0602 (18)
H81	0.2068	0.0234	0.7616	0.072*
C82	0.2064 (4)	−0.0033 (3)	0.8702 (4)	0.0523 (17)
H82	0.1667	−0.0484	0.8944	0.063*
C83	0.2413 (4)	0.0200 (3)	0.9129 (3)	0.0512 (16)
H83	0.2270	−0.0096	0.9669	0.061*
C84	0.2973 (4)	0.0864 (3)	0.8774 (3)	0.0455 (15)
H84	0.3208	0.1013	0.9081	0.055*
C85	0.3551 (3)	0.2752 (3)	0.8141 (3)	0.0315 (13)
C86	0.4014 (4)	0.2800 (4)	0.8621 (3)	0.0558 (17)
H86	0.4566	0.2552	0.8651	0.067*
C87	0.3686 (5)	0.3203 (4)	0.9057 (4)	0.0641 (19)
H87	0.4012	0.3223	0.9382	0.077*
C88	0.2898 (4)	0.3569 (3)	0.9019 (3)	0.0538 (17)
H88	0.2675	0.3843	0.9318	0.065*
C89	0.2435 (4)	0.3540 (3)	0.8552 (3)	0.0516 (17)
H89	0.1893	0.3801	0.8519	0.062*
C90	0.2745 (4)	0.3130 (3)	0.8117 (3)	0.0401 (14)
H90	0.2404	0.3108	0.7802	0.048*
C61	0.6837 (3)	0.2802 (3)	0.6537 (3)	0.0361 (13)
C62	0.7812 (4)	0.2860 (4)	0.6360 (4)	0.0569 (18)
H62	0.8115	0.2427	0.6556	0.068*
C63	0.8351 (5)	0.3535 (4)	0.5902 (4)	0.077 (2)
H63	0.9018	0.3555	0.5788	0.092*
C64	0.7950 (5)	0.4176 (4)	0.5610 (4)	0.069 (2)
H64	0.8328	0.4636	0.5295	0.083*
C65	0.6986 (5)	0.4137 (4)	0.5783 (4)	0.0588 (18)
H65	0.6693	0.4577	0.5590	0.071*
C66	0.6438 (4)	0.3472 (3)	0.6231 (3)	0.0422 (14)

H66	0.5773	0.3461	0.6339	0.051*
C67	0.6033 (3)	0.1545 (3)	0.6384 (3)	0.0295 (12)
C68	0.6517 (4)	0.1908 (3)	0.5588 (3)	0.0465 (15)
H68	0.6905	0.2355	0.5393	0.056*
C69	0.6450 (4)	0.1638 (4)	0.5074 (4)	0.0585 (18)
H69	0.6782	0.1903	0.4536	0.070*
C70	0.5910 (4)	0.0994 (4)	0.5339 (4)	0.0547 (17)
H70	0.5872	0.0805	0.4986	0.066*
C71	0.5417 (4)	0.0613 (3)	0.6119 (4)	0.0499 (16)
H71	0.5036	0.0165	0.6304	0.060*
C72	0.5480 (3)	0.0888 (3)	0.6630 (3)	0.0398 (15)
H72	0.5137	0.0622	0.7166	0.048*
C73	0.6498 (3)	0.1209 (3)	0.7858 (3)	0.0327 (13)
C74	0.7274 (4)	0.0825 (3)	0.7694 (3)	0.0399 (14)
H74	0.7623	0.0933	0.7169	0.048*
C75	0.7550 (4)	0.0288 (3)	0.8275 (4)	0.0501 (16)
H75	0.8095	0.0046	0.8144	0.060*
C76	0.7051 (4)	0.0104 (3)	0.9032 (4)	0.0540 (17)
H76	0.7230	−0.0279	0.9428	0.065*
C77	0.6286 (4)	0.0474 (4)	0.9224 (3)	0.0618 (19)
H77	0.5949	0.0357	0.9752	0.074*
C78	0.6005 (4)	0.1019 (3)	0.8645 (3)	0.0516 (17)
H78	0.5470	0.1267	0.8784	0.062*
Si7	−0.10524 (9)	0.23241 (8)	0.26420 (7)	0.0275 (4)
Si8	0.10227 (9)	0.19132 (8)	0.23385 (8)	0.0299 (4)
O8	−0.0967 (2)	0.28293 (19)	0.17544 (18)	0.0388 (9)
H8A	−0.0986	0.2556	0.1536	0.058*
O7	−0.0038 (2)	0.20801 (19)	0.27514 (19)	0.0361 (9)
C109	−0.1486 (3)	0.2906 (3)	0.3164 (3)	0.0297 (13)
C110	−0.1053 (4)	0.3012 (4)	0.3632 (3)	0.0522 (16)
H110	−0.0496	0.2780	0.3684	0.063*
C111	−0.1414 (5)	0.3449 (4)	0.4029 (4)	0.0674 (19)
H111	−0.1098	0.3518	0.4338	0.081*
C112	−0.2219 (4)	0.3774 (3)	0.3969 (3)	0.0548 (17)
H112	−0.2476	0.4058	0.4252	0.066*
C113	−0.2662 (4)	0.3696 (3)	0.3507 (3)	0.0565 (18)
H113	−0.3212	0.3938	0.3453	0.068*
C114	−0.2301 (4)	0.3256 (3)	0.3112 (3)	0.0469 (16)
H114	−0.2621	0.3196	0.2801	0.056*
C115	−0.1853 (3)	0.1465 (3)	0.3054 (3)	0.0303 (12)
C116	−0.2596 (4)	0.1439 (4)	0.2796 (4)	0.075 (2)
H116	−0.2686	0.1866	0.2385	0.090*
C117	−0.3203 (5)	0.0811 (4)	0.3120 (5)	0.092 (3)
H117	−0.3702	0.0808	0.2927	0.110*
C118	−0.3098 (4)	0.0181 (3)	0.3724 (3)	0.0527 (17)
H118	−0.3522	−0.0253	0.3948	0.063*
C119	−0.2387 (4)	0.0193 (3)	0.3990 (3)	0.0482 (16)
H119	−0.2305	−0.0234	0.4405	0.058*

C120	−0.1776 (4)	0.0827 (3)	0.3658 (3)	0.0458 (16)
H120	−0.1280	0.0824	0.3855	0.055*
C91	0.1854 (3)	0.2766 (3)	0.1860 (3)	0.0363 (14)
C92	0.2685 (4)	0.2761 (3)	0.2036 (4)	0.0566 (18)
H92	0.2798	0.2328	0.2428	0.068*
C93	0.3339 (4)	0.3369 (4)	0.1653 (4)	0.070 (2)
H93	0.3893	0.3361	0.1785	0.084*
C94	0.3179 (4)	0.4000 (4)	0.1065 (4)	0.062 (2)
H94	0.3652	0.4408	0.0766	0.075*
C95	0.2345 (5)	0.4033 (3)	0.0916 (3)	0.0529 (17)
H95	0.2221	0.4474	0.0540	0.064*
C96	0.1686 (4)	0.3422 (3)	0.1319 (3)	0.0380 (14)
H96	0.1103	0.3451	0.1223	0.046*
C97	0.1013 (3)	0.1585 (3)	0.1601 (3)	0.0274 (12)
C98	0.0364 (3)	0.1004 (3)	0.1796 (3)	0.0310 (13)
H98	−0.0079	0.0790	0.2306	0.037*
C99	0.0336 (4)	0.0725 (3)	0.1275 (3)	0.0364 (14)
H99	−0.0115	0.0326	0.1431	0.044*
C100	0.0972 (4)	0.1034 (3)	0.0529 (3)	0.0425 (15)
H100	0.0966	0.0849	0.0167	0.051*
C101	0.1616 (4)	0.1617 (3)	0.0319 (3)	0.0424 (15)
H101	0.2050	0.1837	−0.0195	0.051*
C102	0.1639 (4)	0.1884 (3)	0.0843 (3)	0.0386 (14)
H102	0.2095	0.2282	0.0684	0.046*
C103	0.1380 (3)	0.1166 (3)	0.3122 (3)	0.0322 (13)
C104	0.2090 (3)	0.0730 (3)	0.2937 (3)	0.0348 (13)
H104	0.2396	0.0820	0.2411	0.042*
C105	0.2353 (4)	0.0168 (3)	0.3513 (3)	0.0411 (14)
H105	0.2853	−0.0111	0.3379	0.049*
C106	0.1891 (4)	0.0014 (3)	0.4280 (4)	0.0473 (16)
H106	0.2056	−0.0383	0.4675	0.057*
C107	0.1195 (4)	0.0434 (4)	0.4474 (3)	0.0555 (18)
H107	0.0886	0.0336	0.5002	0.067*
C108	0.0940 (4)	0.1001 (3)	0.3901 (3)	0.0416 (15)
H108	0.0453	0.1286	0.4043	0.050*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Si1	0.0271 (8)	0.0377 (9)	0.0358 (8)	0.0028 (6)	−0.0058 (6)	−0.0239 (7)
Si2	0.0295 (8)	0.0308 (9)	0.0385 (8)	0.0042 (6)	−0.0121 (6)	−0.0152 (7)
O2	0.042 (2)	0.044 (2)	0.043 (2)	0.0095 (17)	−0.0107 (17)	−0.0260 (19)
O1	0.027 (2)	0.047 (2)	0.049 (2)	0.0049 (17)	−0.0065 (16)	−0.0224 (19)
C19	0.025 (3)	0.039 (3)	0.041 (3)	0.007 (2)	−0.005 (2)	−0.027 (3)
C20	0.038 (3)	0.046 (4)	0.042 (3)	−0.003 (3)	0.002 (3)	−0.029 (3)
C21	0.038 (3)	0.060 (5)	0.065 (4)	−0.006 (3)	0.000 (3)	−0.046 (4)
C22	0.044 (4)	0.040 (4)	0.077 (5)	−0.002 (3)	0.008 (3)	−0.040 (4)
C23	0.068 (4)	0.035 (4)	0.060 (4)	0.007 (3)	−0.005 (4)	−0.018 (4)

C24	0.059 (4)	0.049 (4)	0.060 (4)	0.018 (3)	−0.028 (3)	−0.034 (4)
C25	0.034 (3)	0.038 (4)	0.045 (3)	−0.004 (3)	−0.004 (3)	−0.024 (3)
C26	0.056 (4)	0.051 (4)	0.059 (4)	0.001 (3)	−0.009 (3)	−0.037 (3)
C27	0.062 (4)	0.071 (5)	0.053 (4)	0.012 (4)	−0.001 (3)	−0.041 (4)
C28	0.076 (5)	0.079 (5)	0.079 (5)	0.004 (4)	−0.019 (4)	−0.067 (4)
C29	0.076 (5)	0.059 (5)	0.071 (5)	−0.014 (4)	−0.013 (4)	−0.044 (4)
C30	0.056 (4)	0.062 (4)	0.046 (4)	−0.013 (3)	−0.005 (3)	−0.034 (3)
C1	0.024 (3)	0.035 (3)	0.037 (3)	0.003 (2)	−0.005 (2)	−0.018 (3)
C2	0.048 (4)	0.043 (4)	0.057 (4)	0.005 (3)	−0.026 (3)	−0.019 (3)
C3	0.042 (4)	0.060 (5)	0.065 (4)	−0.008 (3)	−0.020 (3)	−0.031 (4)
C4	0.051 (4)	0.029 (4)	0.060 (4)	−0.008 (3)	−0.006 (3)	−0.018 (3)
C5	0.065 (4)	0.029 (4)	0.080 (5)	−0.004 (3)	−0.035 (4)	−0.003 (3)
C6	0.049 (4)	0.039 (4)	0.063 (4)	−0.002 (3)	−0.027 (3)	−0.012 (3)
C7	0.051 (4)	0.038 (4)	0.048 (4)	−0.003 (3)	−0.020 (3)	−0.017 (3)
C8	0.082 (5)	0.048 (4)	0.048 (4)	0.008 (3)	−0.016 (3)	−0.023 (3)
C9	0.092 (5)	0.090 (6)	0.060 (4)	0.022 (5)	−0.037 (4)	−0.044 (4)
C10	0.106 (6)	0.070 (5)	0.062 (5)	0.029 (4)	−0.048 (4)	−0.027 (4)
C11	0.103 (6)	0.055 (5)	0.065 (5)	0.023 (4)	−0.044 (4)	−0.032 (4)
C12	0.068 (4)	0.041 (4)	0.052 (4)	0.009 (3)	−0.030 (3)	−0.016 (3)
C13	0.034 (3)	0.036 (3)	0.051 (3)	0.016 (3)	−0.021 (3)	−0.021 (3)
C14	0.044 (4)	0.046 (4)	0.056 (4)	0.013 (3)	−0.014 (3)	−0.025 (3)
C15	0.056 (4)	0.069 (5)	0.059 (4)	0.027 (4)	−0.021 (3)	−0.042 (4)
C16	0.075 (5)	0.055 (4)	0.065 (4)	0.028 (4)	−0.037 (4)	−0.045 (4)
C17	0.059 (4)	0.044 (4)	0.070 (4)	0.008 (3)	−0.031 (4)	−0.034 (4)
C18	0.037 (3)	0.039 (4)	0.052 (4)	0.007 (3)	−0.017 (3)	−0.024 (3)
Si3	0.0244 (7)	0.0293 (8)	0.0327 (8)	0.0060 (6)	−0.0075 (6)	−0.0188 (7)
Si4	0.0231 (7)	0.0279 (8)	0.0348 (8)	0.0050 (6)	−0.0098 (6)	−0.0173 (7)
O4	0.040 (2)	0.034 (2)	0.044 (2)	0.0177 (17)	−0.0180 (17)	−0.0226 (18)
O3	0.0254 (19)	0.036 (2)	0.042 (2)	0.0046 (15)	−0.0100 (15)	−0.0148 (17)
C49	0.023 (3)	0.038 (3)	0.031 (3)	0.003 (2)	−0.002 (2)	−0.024 (3)
C50	0.053 (4)	0.043 (4)	0.054 (4)	0.007 (3)	−0.032 (3)	−0.019 (3)
C51	0.070 (4)	0.028 (4)	0.067 (4)	0.008 (3)	−0.031 (4)	−0.014 (3)
C52	0.044 (3)	0.032 (4)	0.059 (4)	0.007 (3)	−0.013 (3)	−0.028 (3)
C53	0.039 (3)	0.055 (4)	0.043 (3)	−0.005 (3)	−0.007 (3)	−0.030 (3)
C54	0.037 (3)	0.040 (4)	0.036 (3)	0.002 (3)	−0.010 (3)	−0.018 (3)
C55	0.041 (3)	0.032 (3)	0.035 (3)	0.002 (3)	−0.001 (2)	−0.022 (3)
C56	0.057 (4)	0.065 (4)	0.054 (4)	0.023 (3)	−0.019 (3)	−0.041 (4)
C57	0.083 (5)	0.078 (6)	0.069 (5)	0.037 (4)	−0.021 (4)	−0.052 (4)
C58	0.133 (8)	0.055 (5)	0.062 (5)	0.002 (5)	0.012 (5)	−0.045 (4)
C59	0.103 (7)	0.103 (7)	0.088 (6)	−0.048 (5)	0.014 (5)	−0.075 (5)
C60	0.055 (4)	0.092 (6)	0.080 (5)	−0.016 (4)	0.004 (3)	−0.069 (5)
C31	0.027 (3)	0.030 (3)	0.037 (3)	0.002 (2)	−0.007 (2)	−0.017 (3)
C32	0.026 (3)	0.038 (4)	0.055 (4)	0.008 (3)	−0.013 (3)	−0.011 (3)
C33	0.049 (4)	0.032 (4)	0.064 (4)	0.005 (3)	−0.013 (3)	−0.011 (3)
C34	0.045 (4)	0.036 (4)	0.066 (4)	−0.007 (3)	−0.009 (3)	−0.019 (3)
C35	0.032 (3)	0.053 (4)	0.089 (5)	−0.004 (3)	−0.027 (3)	−0.012 (4)
C36	0.040 (4)	0.039 (4)	0.077 (4)	−0.002 (3)	−0.022 (3)	−0.006 (3)
C37	0.025 (3)	0.044 (3)	0.038 (3)	0.008 (2)	−0.008 (2)	−0.025 (3)

C38	0.045 (4)	0.055 (4)	0.078 (4)	0.013 (3)	−0.019 (3)	−0.048 (4)
C39	0.049 (4)	0.059 (4)	0.097 (5)	0.012 (3)	−0.011 (4)	−0.057 (4)
C40	0.060 (4)	0.064 (5)	0.068 (4)	−0.003 (4)	−0.005 (3)	−0.051 (4)
C41	0.052 (4)	0.050 (4)	0.046 (3)	0.001 (3)	−0.019 (3)	−0.026 (3)
C42	0.033 (3)	0.040 (3)	0.048 (3)	0.004 (2)	−0.011 (3)	−0.028 (3)
C43	0.041 (3)	0.033 (4)	0.045 (3)	0.000 (3)	−0.019 (3)	−0.018 (3)
C44	0.123 (6)	0.080 (6)	0.076 (5)	0.027 (5)	−0.061 (5)	−0.049 (5)
C45	0.137 (8)	0.169 (11)	0.084 (7)	0.031 (8)	−0.060 (6)	−0.087 (7)
C46	0.100 (6)	0.134 (9)	0.046 (5)	0.005 (6)	−0.034 (4)	−0.024 (6)
C47	0.113 (7)	0.090 (7)	0.056 (5)	0.004 (5)	−0.038 (5)	−0.005 (5)
C48	0.094 (5)	0.067 (5)	0.054 (4)	0.011 (4)	−0.039 (4)	−0.024 (4)
Si5	0.0277 (8)	0.0379 (9)	0.0314 (8)	0.0137 (7)	−0.0084 (6)	−0.0185 (7)
Si6	0.0244 (8)	0.0336 (9)	0.0439 (9)	0.0089 (6)	−0.0094 (6)	−0.0224 (7)
O6	0.051 (2)	0.044 (2)	0.039 (2)	0.0153 (19)	−0.0158 (18)	−0.0208 (19)
O5	0.0265 (19)	0.053 (2)	0.050 (2)	0.0181 (17)	−0.0104 (16)	−0.030 (2)
C79	0.026 (3)	0.046 (4)	0.038 (3)	0.019 (2)	−0.012 (2)	−0.026 (3)
C80	0.044 (4)	0.073 (5)	0.047 (4)	0.003 (3)	−0.015 (3)	−0.034 (4)
C81	0.056 (4)	0.071 (5)	0.075 (5)	0.006 (4)	−0.035 (4)	−0.041 (4)
C82	0.049 (4)	0.042 (4)	0.071 (5)	0.003 (3)	−0.029 (3)	−0.021 (4)
C83	0.059 (4)	0.043 (4)	0.051 (4)	0.001 (3)	−0.019 (3)	−0.017 (3)
C84	0.058 (4)	0.039 (4)	0.051 (4)	0.009 (3)	−0.028 (3)	−0.023 (3)
C85	0.029 (3)	0.036 (3)	0.031 (3)	0.004 (2)	−0.005 (2)	−0.020 (3)
C86	0.042 (4)	0.083 (5)	0.069 (4)	0.021 (3)	−0.027 (3)	−0.053 (4)
C87	0.068 (5)	0.088 (5)	0.067 (4)	0.010 (4)	−0.033 (4)	−0.053 (4)
C88	0.059 (4)	0.052 (4)	0.057 (4)	0.003 (3)	−0.008 (3)	−0.038 (3)
C89	0.052 (4)	0.047 (4)	0.056 (4)	0.025 (3)	−0.008 (3)	−0.031 (3)
C90	0.037 (3)	0.044 (4)	0.038 (3)	0.009 (3)	−0.010 (2)	−0.018 (3)
C61	0.035 (3)	0.039 (4)	0.046 (3)	0.006 (3)	−0.012 (3)	−0.030 (3)
C62	0.046 (4)	0.048 (4)	0.083 (5)	0.004 (3)	−0.022 (3)	−0.033 (4)
C63	0.050 (4)	0.077 (6)	0.099 (6)	−0.016 (4)	−0.026 (4)	−0.029 (5)
C64	0.090 (6)	0.042 (4)	0.083 (5)	−0.011 (4)	−0.031 (4)	−0.030 (4)
C65	0.077 (5)	0.040 (4)	0.067 (4)	0.007 (4)	−0.022 (4)	−0.032 (4)
C66	0.047 (3)	0.034 (4)	0.048 (3)	0.007 (3)	−0.013 (3)	−0.022 (3)
C67	0.026 (3)	0.022 (3)	0.040 (3)	0.006 (2)	−0.013 (2)	−0.011 (3)
C68	0.044 (3)	0.034 (4)	0.053 (4)	−0.009 (3)	0.001 (3)	−0.022 (3)
C69	0.063 (4)	0.066 (5)	0.048 (4)	0.005 (4)	−0.007 (3)	−0.034 (4)
C70	0.057 (4)	0.064 (5)	0.062 (5)	0.017 (4)	−0.024 (3)	−0.043 (4)
C71	0.043 (4)	0.042 (4)	0.077 (5)	0.004 (3)	−0.032 (3)	−0.029 (4)
C72	0.030 (3)	0.044 (4)	0.039 (3)	0.002 (3)	−0.014 (2)	−0.010 (3)
C73	0.033 (3)	0.034 (3)	0.044 (3)	0.011 (2)	−0.015 (2)	−0.028 (3)
C74	0.044 (3)	0.045 (4)	0.053 (3)	0.015 (3)	−0.023 (3)	−0.037 (3)
C75	0.060 (4)	0.050 (4)	0.076 (5)	0.029 (3)	−0.046 (4)	−0.045 (4)
C76	0.064 (4)	0.050 (4)	0.067 (4)	0.022 (3)	−0.043 (4)	−0.029 (4)
C77	0.064 (4)	0.074 (5)	0.042 (4)	0.016 (4)	−0.018 (3)	−0.021 (4)
C78	0.047 (4)	0.062 (4)	0.053 (4)	0.026 (3)	−0.023 (3)	−0.029 (3)
Si7	0.0222 (7)	0.0313 (9)	0.0310 (8)	0.0079 (6)	−0.0080 (6)	−0.0162 (7)
Si8	0.0242 (8)	0.0279 (9)	0.0442 (9)	0.0078 (6)	−0.0136 (6)	−0.0203 (7)
O8	0.044 (2)	0.037 (2)	0.039 (2)	0.0120 (18)	−0.0152 (17)	−0.0194 (18)

O7	0.0291 (19)	0.041 (2)	0.044 (2)	0.0128 (16)	−0.0168 (16)	−0.0214 (18)
C109	0.025 (3)	0.028 (3)	0.023 (3)	0.003 (2)	0.001 (2)	−0.006 (2)
C110	0.041 (3)	0.068 (5)	0.070 (4)	0.009 (3)	−0.023 (3)	−0.048 (4)
C111	0.079 (5)	0.080 (5)	0.071 (5)	0.004 (4)	−0.025 (4)	−0.056 (4)
C112	0.063 (4)	0.048 (4)	0.054 (4)	0.010 (3)	−0.002 (3)	−0.035 (3)
C113	0.060 (4)	0.058 (4)	0.056 (4)	0.031 (3)	−0.014 (3)	−0.035 (4)
C114	0.047 (4)	0.053 (4)	0.039 (3)	0.018 (3)	−0.010 (3)	−0.022 (3)
C115	0.023 (3)	0.038 (3)	0.040 (3)	0.005 (2)	−0.009 (2)	−0.028 (3)
C116	0.071 (5)	0.048 (4)	0.098 (5)	−0.013 (4)	−0.059 (4)	0.001 (4)
C117	0.089 (6)	0.066 (5)	0.129 (7)	−0.019 (4)	−0.073 (5)	−0.020 (5)
C118	0.053 (4)	0.045 (4)	0.063 (4)	−0.011 (3)	−0.015 (3)	−0.027 (4)
C119	0.053 (4)	0.037 (4)	0.048 (4)	−0.007 (3)	−0.020 (3)	−0.009 (3)
C120	0.044 (3)	0.053 (4)	0.040 (3)	−0.003 (3)	−0.021 (3)	−0.014 (3)
C91	0.029 (3)	0.038 (4)	0.053 (3)	0.012 (2)	−0.013 (3)	−0.031 (3)
C92	0.040 (4)	0.038 (4)	0.097 (5)	0.011 (3)	−0.027 (3)	−0.032 (4)
C93	0.039 (4)	0.055 (5)	0.114 (6)	0.003 (3)	−0.029 (4)	−0.031 (5)
C94	0.039 (4)	0.044 (4)	0.086 (5)	−0.008 (3)	−0.009 (3)	−0.019 (4)
C95	0.082 (5)	0.028 (4)	0.051 (4)	0.002 (3)	−0.017 (3)	−0.021 (3)
C96	0.040 (3)	0.032 (3)	0.045 (3)	−0.004 (3)	−0.015 (3)	−0.018 (3)
C97	0.021 (3)	0.018 (3)	0.042 (3)	0.007 (2)	−0.014 (2)	−0.010 (2)
C98	0.031 (3)	0.024 (3)	0.039 (3)	0.007 (2)	−0.015 (2)	−0.012 (3)
C99	0.036 (3)	0.023 (3)	0.056 (4)	0.010 (2)	−0.023 (3)	−0.018 (3)
C100	0.050 (4)	0.042 (4)	0.050 (4)	0.023 (3)	−0.028 (3)	−0.028 (3)
C101	0.045 (3)	0.043 (4)	0.037 (3)	0.008 (3)	−0.010 (3)	−0.018 (3)
C102	0.038 (3)	0.034 (3)	0.043 (3)	0.004 (3)	−0.009 (3)	−0.019 (3)
C103	0.029 (3)	0.027 (3)	0.050 (3)	0.002 (2)	−0.015 (2)	−0.023 (3)
C104	0.033 (3)	0.043 (3)	0.047 (3)	0.010 (3)	−0.022 (3)	−0.030 (3)
C105	0.044 (3)	0.042 (4)	0.068 (4)	0.023 (3)	−0.033 (3)	−0.042 (3)
C106	0.057 (4)	0.038 (4)	0.061 (4)	0.012 (3)	−0.037 (3)	−0.021 (3)
C107	0.047 (4)	0.069 (5)	0.045 (4)	0.007 (3)	−0.022 (3)	−0.015 (3)
C108	0.034 (3)	0.054 (4)	0.046 (3)	0.021 (3)	−0.015 (3)	−0.032 (3)

Geometric parameters (Å, º)

Si1—O1	1.605 (3)	Si5—O5	1.627 (3)
Si1—O2	1.643 (4)	Si5—O6	1.612 (3)
Si1—C19	1.861 (5)	Si5—C79	1.870 (6)
Si1—C25	1.856 (6)	Si5—C85	1.855 (5)
Si2—O1	1.625 (3)	Si6—O5	1.631 (3)
Si2—C1	1.872 (5)	Si6—C61	1.856 (5)
Si2—C7	1.860 (5)	Si6—C67	1.866 (6)
Si2—C13	1.868 (6)	Si6—C73	1.863 (5)
O2—H2	0.8400	O6—H6A	0.8400
C19—C24	1.398 (7)	C79—C84	1.382 (7)
C19—C20	1.402 (7)	C79—C80	1.399 (8)
C20—C21	1.388 (8)	C80—C81	1.383 (8)
C20—H20	0.9500	C80—H80	0.9500
C21—C22	1.358 (8)	C81—C82	1.375 (8)

C21—H21	0.9500	C81—H81	0.9500
C22—C23	1.370 (9)	C82—C83	1.373 (8)
C22—H22	0.9500	C82—H82	0.9500
C23—C24	1.395 (8)	C83—C84	1.381 (8)
C23—H23	0.9500	C83—H83	0.9500
C24—H24	0.9500	C84—H84	0.9500
C25—C30	1.378 (8)	C85—C86	1.394 (7)
C25—C26	1.400 (7)	C85—C90	1.398 (7)
C26—C27	1.406 (9)	C86—C87	1.394 (9)
C26—H26	0.9500	C86—H86	0.9500
C27—C28	1.367 (9)	C87—C88	1.367 (8)
C27—H27	0.9500	C87—H87	0.9500
C28—C29	1.355 (8)	C88—C89	1.359 (8)
C28—H28	0.9500	C88—H88	0.9500
C29—C30	1.383 (9)	C89—C90	1.398 (8)
C29—H29	0.9500	C89—H89	0.9500
C30—H30	0.9500	C90—H90	0.9500
C1—C6	1.381 (7)	C61—C62	1.389 (7)
C1—C2	1.402 (7)	C61—C66	1.413 (7)
C2—C3	1.381 (8)	C62—C63	1.384 (9)
C2—H2A	0.9500	C62—H62	0.9500
C3—C4	1.360 (8)	C63—C64	1.369 (9)
C3—H3	0.9500	C63—H63	0.9500
C4—C5	1.358 (8)	C64—C65	1.373 (8)
C4—H4	0.9500	C64—H64	0.9500
C5—C6	1.375 (8)	C65—C66	1.373 (8)
C5—H5	0.9500	C65—H65	0.9500
C6—H6	0.9500	C66—H66	0.9500
C7—C12	1.398 (8)	C67—C68	1.399 (7)
C7—C8	1.399 (8)	C67—C72	1.399 (7)
C8—C9	1.424 (8)	C68—C69	1.383 (8)
C8—H8	0.9500	C68—H68	0.9500
C9—C10	1.397 (9)	C69—C70	1.361 (9)
C9—H9	0.9500	C69—H69	0.9500
C10—C11	1.377 (9)	C70—C71	1.381 (8)
C10—H10	0.9500	C70—H70	0.9500
C11—C12	1.372 (8)	C71—C72	1.384 (8)
C11—H11	0.9500	C71—H71	0.9500
C12—H12	0.9500	C72—H72	0.9500
C13—C18	1.380 (7)	C73—C74	1.390 (7)
C13—C14	1.409 (7)	C73—C78	1.407 (7)
C14—C15	1.381 (8)	C74—C75	1.385 (7)
C14—H14	0.9500	C74—H74	0.9500
C15—C16	1.376 (8)	C75—C76	1.360 (8)
C15—H15	0.9500	C75—H75	0.9500
C16—C17	1.378 (8)	C76—C77	1.371 (8)
C16—H16	0.9500	C76—H76	0.9500
C17—C18	1.391 (8)	C77—C78	1.392 (7)

C17—H17	0.9500	C77—H77	0.9500
C18—H18	0.9500	C78—H78	0.9500
Si3—O3	1.608 (3)	Si7—O7	1.631 (3)
Si3—O4	1.648 (3)	Si7—O8	1.610 (3)
Si3—C49	1.860 (5)	Si7—C109	1.842 (5)
Si3—C55	1.851 (5)	Si7—C115	1.859 (5)
Si4—O3	1.636 (3)	Si8—O7	1.632 (3)
Si4—C31	1.864 (5)	Si8—C91	1.859 (5)
Si4—C37	1.866 (6)	Si8—C97	1.865 (5)
Si4—C43	1.868 (5)	Si8—C103	1.873 (5)
O4—H4A	0.8400	O8—H8A	0.8400
C49—C50	1.387 (7)	C109—C110	1.390 (7)
C49—C54	1.393 (7)	C109—C114	1.392 (7)
C50—C51	1.392 (8)	C110—C111	1.399 (9)
C50—H50	0.9500	C110—H110	0.9500
C51—C52	1.354 (8)	C111—C112	1.360 (8)
C51—H51	0.9500	C111—H111	0.9500
C52—C53	1.370 (7)	C112—C113	1.368 (8)
C52—H52	0.9500	C112—H112	0.9500
C53—C54	1.398 (7)	C113—C114	1.399 (8)
C53—H53	0.9500	C113—H113	0.9500
C54—H54	0.9500	C114—H114	0.9500
C55—C60	1.372 (8)	C115—C120	1.378 (7)
C55—C56	1.391 (7)	C115—C116	1.386 (7)
C56—C57	1.376 (9)	C116—C117	1.369 (9)
C56—H56	0.9500	C116—H116	0.9500
C57—C58	1.384 (10)	C117—C118	1.385 (8)
C57—H57	0.9500	C117—H117	0.9500
C58—C59	1.372 (10)	C118—C119	1.345 (8)
C58—H58	0.9500	C118—H118	0.9500
C59—C60	1.380 (10)	C119—C120	1.381 (8)
C59—H59	0.9500	C119—H119	0.9500
C60—H60	0.9500	C120—H120	0.9500
C31—C32	1.380 (7)	C91—C96	1.386 (7)
C31—C36	1.408 (7)	C91—C92	1.400 (7)
C32—C33	1.381 (8)	C92—C93	1.371 (8)
C32—H32	0.9500	C92—H92	0.9500
C33—C34	1.381 (8)	C93—C94	1.399 (8)
C33—H33	0.9500	C93—H93	0.9500
C34—C35	1.377 (8)	C94—C95	1.370 (8)
C34—H34	0.9500	C94—H94	0.9500
C35—C36	1.378 (8)	C95—C96	1.379 (7)
C35—H35	0.9500	C95—H95	0.9500
C36—H36	0.9500	C96—H96	0.9500
C37—C42	1.392 (7)	C97—C98	1.391 (7)
C37—C38	1.394 (7)	C97—C102	1.393 (7)
C38—C39	1.408 (9)	C98—C99	1.392 (7)
C38—H38	0.9500	C98—H98	0.9500

C39—C40	1.383 (9)	C99—C100	1.383 (7)
C39—H39	0.9500	C99—H99	0.9500
C40—C41	1.357 (8)	C100—C101	1.380 (8)
C40—H40	0.9500	C100—H100	0.9500
C41—C42	1.376 (8)	C101—C102	1.379 (8)
C41—H41	0.9500	C101—H101	0.9500
C42—H42	0.9500	C102—H102	0.9500
C43—C44	1.373 (9)	C103—C108	1.390 (7)
C43—C48	1.373 (8)	C103—C104	1.400 (7)
C44—C45	1.394 (10)	C104—C105	1.389 (7)
C44—H44	0.9500	C104—H104	0.9500
C45—C46	1.372 (12)	C105—C106	1.379 (8)
C45—H45	0.9500	C105—H105	0.9500
C46—C47	1.329 (12)	C106—C107	1.370 (8)
C46—H46	0.9500	C106—H106	0.9500
C47—C48	1.387 (9)	C107—C108	1.383 (7)
C47—H47	0.9500	C107—H107	0.9500
C48—H48	0.9500	C108—H108	0.9500

O1—Si1—O2	104.17 (18)	O6—Si5—O5	112.03 (19)
O1—Si1—C25	109.1 (2)	O6—Si5—C85	106.6 (2)
O2—Si1—C25	111.2 (2)	O5—Si5—C85	106.0 (2)
O1—Si1—C19	110.9 (2)	O6—Si5—C79	111.8 (2)
O2—Si1—C19	109.2 (2)	O5—Si5—C79	108.5 (2)
C25—Si1—C19	112.1 (2)	C85—Si5—C79	111.8 (2)
O1—Si2—C7	112.3 (2)	O5—Si6—C61	109.1 (2)
O1—Si2—C13	108.5 (2)	O5—Si6—C73	105.4 (2)
C7—Si2—C13	109.1 (3)	C61—Si6—C73	113.6 (2)
O1—Si2—C1	108.6 (2)	O5—Si6—C67	110.4 (2)
C7—Si2—C1	108.2 (2)	C61—Si6—C67	107.8 (2)
C13—Si2—C1	110.1 (2)	C73—Si6—C67	110.5 (2)
Si1—O2—H2	109.5	Si5—O6—H6A	109.5
Si1—O1—Si2	169.5 (2)	Si5—O5—Si6	149.0 (2)
C24—C19—C20	116.3 (5)	C84—C79—C80	115.5 (5)
C24—C19—Si1	122.2 (4)	C84—C79—Si5	120.8 (4)
C20—C19—Si1	121.5 (4)	C80—C79—Si5	123.7 (4)
C21—C20—C19	121.4 (6)	C81—C80—C79	122.2 (6)
C21—C20—H20	119.3	C81—C80—H80	118.9
C19—C20—H20	119.3	C79—C80—H80	118.9
C22—C21—C20	120.8 (6)	C82—C81—C80	120.1 (6)
C22—C21—H21	119.6	C82—C81—H81	120.0
C20—C21—H21	119.6	C80—C81—H81	120.0
C21—C22—C23	120.0 (6)	C83—C82—C81	119.2 (6)
C21—C22—H22	120.0	C83—C82—H82	120.4
C23—C22—H22	120.0	C81—C82—H82	120.4
C22—C23—C24	119.9 (6)	C82—C83—C84	119.9 (6)
C22—C23—H23	120.1	C82—C83—H83	120.0
C24—C23—H23	120.1	C84—C83—H83	120.0

C23—C24—C19	121.7 (6)	C83—C84—C79	123.0 (6)
C23—C24—H24	119.1	C83—C84—H84	118.5
C19—C24—H24	119.1	C79—C84—H84	118.5
C30—C25—C26	115.7 (5)	C86—C85—C90	116.8 (5)
C30—C25—Si1	121.4 (4)	C86—C85—Si5	123.4 (4)
C26—C25—Si1	122.8 (4)	C90—C85—Si5	119.8 (4)
C25—C26—C27	121.4 (6)	C87—C86—C85	121.5 (5)
C25—C26—H26	119.3	C87—C86—H86	119.3
C27—C26—H26	119.3	C85—C86—H86	119.3
C28—C27—C26	119.6 (6)	C88—C87—C86	120.3 (6)
C28—C27—H27	120.2	C88—C87—H87	119.8
C26—C27—H27	120.2	C86—C87—H87	119.8
C29—C28—C27	120.3 (6)	C89—C88—C87	119.6 (6)
C29—C28—H28	119.8	C89—C88—H88	120.2
C27—C28—H28	119.8	C87—C88—H88	120.2
C28—C29—C30	119.7 (6)	C88—C89—C90	120.9 (5)
C28—C29—H29	120.1	C88—C89—H89	119.5
C30—C29—H29	120.1	C90—C89—H89	119.5
C25—C30—C29	123.2 (6)	C89—C90—C85	120.8 (5)
C25—C30—H30	118.4	C89—C90—H90	119.6
C29—C30—H30	118.4	C85—C90—H90	119.6
C6—C1—C2	116.6 (5)	C62—C61—C66	116.0 (5)
C6—C1—Si2	120.9 (4)	C62—C61—Si6	123.5 (4)
C2—C1—Si2	122.5 (4)	C66—C61—Si6	120.4 (4)
C3—C2—C1	121.6 (5)	C63—C62—C61	121.3 (6)
C3—C2—H2A	119.2	C63—C62—H62	119.4
C1—C2—H2A	119.2	C61—C62—H62	119.4
C4—C3—C2	119.9 (5)	C64—C63—C62	121.7 (6)
C4—C3—H3	120.1	C64—C63—H63	119.2
C2—C3—H3	120.1	C62—C63—H63	119.2
C5—C4—C3	119.5 (5)	C63—C64—C65	118.3 (6)
C5—C4—H4	120.3	C63—C64—H64	120.8
C3—C4—H4	120.3	C65—C64—H64	120.8
C4—C5—C6	121.4 (5)	C64—C65—C66	120.9 (6)
C4—C5—H5	119.3	C64—C65—H65	119.5
C6—C5—H5	119.3	C66—C65—H65	119.5
C5—C6—C1	121.0 (5)	C65—C66—C61	121.8 (5)
C5—C6—H6	119.5	C65—C66—H66	119.1
C1—C6—H6	119.5	C61—C66—H66	119.1
C12—C7—C8	118.6 (5)	C68—C67—C72	115.8 (5)
C12—C7—Si2	121.3 (5)	C68—C67—Si6	123.4 (4)
C8—C7—Si2	119.5 (5)	C72—C67—Si6	120.8 (4)
C7—C8—C9	119.9 (6)	C69—C68—C67	122.3 (5)
C7—C8—H8	120.1	C69—C68—H68	118.8
C9—C8—H8	120.1	C67—C68—H68	118.8
C10—C9—C8	118.6 (7)	C70—C69—C68	120.0 (6)
C10—C9—H9	120.7	C70—C69—H69	120.0
C8—C9—H9	120.7	C68—C69—H69	120.0

C11—C10—C9	121.4 (6)	C69—C70—C71	120.1 (6)
C11—C10—H10	119.3	C69—C70—H70	120.0
C9—C10—H10	119.3	C71—C70—H70	120.0
C12—C11—C10	119.4 (7)	C70—C71—C72	119.7 (6)
C12—C11—H11	120.3	C70—C71—H71	120.2
C10—C11—H11	120.3	C72—C71—H71	120.2
C11—C12—C7	122.0 (6)	C71—C72—C67	122.1 (5)
C11—C12—H12	119.0	C71—C72—H72	118.9
C7—C12—H12	119.0	C67—C72—H72	118.9
C18—C13—C14	116.5 (5)	C74—C73—C78	116.5 (5)
C18—C13—Si2	121.6 (4)	C74—C73—Si6	122.6 (4)
C14—C13—Si2	121.9 (4)	C78—C73—Si6	120.9 (4)
C15—C14—C13	121.6 (6)	C75—C74—C73	121.6 (5)
C15—C14—H14	119.2	C75—C74—H74	119.2
C13—C14—H14	119.2	C73—C74—H74	119.2
C16—C15—C14	120.6 (6)	C76—C75—C74	120.7 (5)
C16—C15—H15	119.7	C76—C75—H75	119.7
C14—C15—H15	119.7	C74—C75—H75	119.7
C15—C16—C17	118.8 (6)	C75—C76—C77	119.9 (5)
C15—C16—H16	120.6	C75—C76—H76	120.1
C17—C16—H16	120.6	C77—C76—H76	120.1
C16—C17—C18	120.6 (6)	C76—C77—C78	120.0 (6)
C16—C17—H17	119.7	C76—C77—H77	120.0
C18—C17—H17	119.7	C78—C77—H77	120.0
C13—C18—C17	121.9 (5)	C77—C78—C73	121.3 (5)
C13—C18—H18	119.1	C77—C78—H78	119.4
C17—C18—H18	119.1	C73—C78—H78	119.4
O3—Si3—O4	105.95 (17)	O8—Si7—O7	113.08 (18)
O3—Si3—C55	109.9 (2)	O8—Si7—C109	106.2 (2)
O4—Si3—C55	109.0 (2)	O7—Si7—C109	106.6 (2)
O3—Si3—C49	110.2 (2)	O8—Si7—C115	111.2 (2)
O4—Si3—C49	106.2 (2)	O7—Si7—C115	107.6 (2)
C55—Si3—C49	115.1 (2)	C109—Si7—C115	112.1 (2)
O3—Si4—C31	106.6 (2)	O7—Si8—C91	110.1 (2)
O3—Si4—C37	108.1 (2)	O7—Si8—C97	110.42 (19)
C31—Si4—C37	113.9 (2)	C91—Si8—C97	109.1 (2)
O3—Si4—C43	110.2 (2)	O7—Si8—C103	106.7 (2)
C31—Si4—C43	107.9 (2)	C91—Si8—C103	111.1 (2)
C37—Si4—C43	110.2 (2)	C97—Si8—C103	109.4 (2)
Si3—O4—H4A	109.5	Si7—O8—H8A	109.5
Si3—O3—Si4	161.2 (2)	Si7—O7—Si8	145.1 (2)
C50—C49—C54	116.3 (5)	C110—C109—C114	116.5 (5)
C50—C49—Si3	121.7 (4)	C110—C109—Si7	123.7 (4)
C54—C49—Si3	122.0 (4)	C114—C109—Si7	119.7 (4)
C49—C50—C51	121.6 (5)	C109—C110—C111	122.0 (6)
C49—C50—H50	119.2	C109—C110—H110	119.0
C51—C50—H50	119.2	C111—C110—H110	119.0
C52—C51—C50	120.8 (5)	C112—C111—C110	119.6 (6)

C52—C51—H51	119.6	C112—C111—H111	120.2
C50—C51—H51	119.6	C110—C111—H111	120.2
C51—C52—C53	119.7 (5)	C111—C112—C113	120.5 (6)
C51—C52—H52	120.1	C111—C112—H112	119.7
C53—C52—H52	120.1	C113—C112—H112	119.7
C52—C53—C54	119.6 (5)	C112—C113—C114	119.7 (6)
C52—C53—H53	120.2	C112—C113—H113	120.2
C54—C53—H53	120.2	C114—C113—H113	120.2
C49—C54—C53	121.9 (5)	C109—C114—C113	121.7 (6)
C49—C54—H54	119.0	C109—C114—H114	119.2
C53—C54—H54	119.0	C113—C114—H114	119.2
C60—C55—C56	116.9 (5)	C120—C115—C116	115.9 (5)
C60—C55—Si3	122.7 (4)	C120—C115—Si7	122.4 (4)
C56—C55—Si3	120.3 (4)	C116—C115—Si7	121.7 (4)
C57—C56—C55	122.5 (7)	C117—C116—C115	121.4 (6)
C57—C56—H56	118.8	C117—C116—H116	119.3
C55—C56—H56	118.8	C115—C116—H116	119.3
C56—C57—C58	118.9 (7)	C116—C117—C118	120.8 (6)
C56—C57—H57	120.6	C116—C117—H117	119.6
C58—C57—H57	120.6	C118—C117—H117	119.6
C59—C58—C57	119.8 (7)	C119—C118—C117	118.9 (6)
C59—C58—H58	120.1	C119—C118—H118	120.5
C57—C58—H58	120.1	C117—C118—H118	120.5
C58—C59—C60	120.0 (7)	C118—C119—C120	119.8 (5)
C58—C59—H59	120.0	C118—C119—H119	120.1
C60—C59—H59	120.0	C120—C119—H119	120.1
C55—C60—C59	121.9 (6)	C115—C120—C119	123.1 (5)
C55—C60—H60	119.1	C115—C120—H120	118.4
C59—C60—H60	119.1	C119—C120—H120	118.4
C32—C31—C36	116.7 (5)	C96—C91—C92	117.7 (5)
C32—C31—Si4	122.8 (4)	C96—C91—Si8	122.0 (4)
C36—C31—Si4	120.3 (4)	C92—C91—Si8	120.3 (4)
C31—C32—C33	122.2 (5)	C93—C92—C91	121.3 (6)
C31—C32—H32	118.9	C93—C92—H92	119.4
C33—C32—H32	118.9	C91—C92—H92	119.4
C32—C33—C34	120.0 (5)	C92—C93—C94	119.2 (6)
C32—C33—H33	120.0	C92—C93—H93	120.4
C34—C33—H33	120.0	C94—C93—H93	120.4
C35—C34—C33	119.2 (5)	C95—C94—C93	120.4 (6)
C35—C34—H34	120.4	C95—C94—H94	119.8
C33—C34—H34	120.4	C93—C94—H94	119.8
C34—C35—C36	120.6 (5)	C94—C95—C96	119.5 (6)
C34—C35—H35	119.7	C94—C95—H95	120.3
C36—C35—H35	119.7	C96—C95—H95	120.3
C35—C36—C31	121.3 (5)	C95—C96—C91	121.6 (5)
C35—C36—H36	119.4	C95—C96—H96	119.2
C31—C36—H36	119.4	C91—C96—H96	119.2
C42—C37—C38	116.6 (5)	C98—C97—C102	116.2 (5)

C42—C37—Si4	122.6 (4)	C98—C97—Si8	120.1 (4)
C38—C37—Si4	120.8 (4)	C102—C97—Si8	123.7 (4)
C37—C38—C39	121.8 (6)	C97—C98—C99	122.7 (5)
C37—C38—H38	119.1	C97—C98—H98	118.6
C39—C38—H38	119.1	C99—C98—H98	118.6
C40—C39—C38	119.3 (6)	C100—C99—C98	119.4 (5)
C40—C39—H39	120.4	C100—C99—H99	120.3
C38—C39—H39	120.4	C98—C99—H99	120.3
C41—C40—C39	118.8 (6)	C101—C100—C99	118.9 (6)
C41—C40—H40	120.6	C101—C100—H100	120.5
C39—C40—H40	120.6	C99—C100—H100	120.5
C40—C41—C42	122.3 (6)	C102—C101—C100	121.0 (5)
C40—C41—H41	118.8	C102—C101—H101	119.5
C42—C41—H41	118.8	C100—C101—H101	119.5
C41—C42—C37	121.0 (5)	C101—C102—C97	121.8 (5)
C41—C42—H42	119.5	C101—C102—H102	119.1
C37—C42—H42	119.5	C97—C102—H102	119.1
C44—C43—C48	116.6 (6)	C108—C103—C104	117.4 (5)
C44—C43—Si4	120.1 (5)	C108—C103—Si8	122.4 (4)
C48—C43—Si4	123.2 (5)	C104—C103—Si8	120.2 (4)
C43—C44—C45	120.7 (8)	C105—C104—C103	120.7 (5)
C43—C44—H44	119.7	C105—C104—H104	119.6
C45—C44—H44	119.7	C103—C104—H104	119.6
C46—C45—C44	120.6 (9)	C106—C105—C104	120.2 (5)
C46—C45—H45	119.7	C106—C105—H105	119.9
C44—C45—H45	119.7	C104—C105—H105	119.9
C47—C46—C45	119.4 (8)	C107—C106—C105	120.0 (5)
C47—C46—H46	120.3	C107—C106—H106	120.0
C45—C46—H46	120.3	C105—C106—H106	120.0
C46—C47—C48	120.2 (8)	C106—C107—C108	120.0 (6)
C46—C47—H47	119.9	C106—C107—H107	120.0
C48—C47—H47	119.9	C108—C107—H107	120.0
C43—C48—C47	122.5 (8)	C107—C108—C103	121.7 (5)
C43—C48—H48	118.8	C107—C108—H108	119.1
C47—C48—H48	118.8	C103—C108—H108	119.1

O2—Si1—O1—Si2	156.0 (15)	O6—Si5—O5—Si6	−33.0 (6)
C25—Si1—O1—Si2	−85.2 (16)	C85—Si5—O5—Si6	−148.9 (5)
C19—Si1—O1—Si2	38.7 (16)	C79—Si5—O5—Si6	90.9 (5)
C7—Si2—O1—Si1	20.3 (16)	C61—Si6—O5—Si5	92.5 (5)
C13—Si2—O1—Si1	−100.4 (16)	C73—Si6—O5—Si5	−145.2 (5)
C1—Si2—O1—Si1	139.9 (15)	C67—Si6—O5—Si5	−25.8 (6)
O1—Si1—C19—C24	−75.4 (4)	O6—Si5—C79—C84	−165.6 (4)
O2—Si1—C19—C24	170.4 (4)	O5—Si5—C79—C84	70.3 (4)
C25—Si1—C19—C24	46.7 (5)	C85—Si5—C79—C84	−46.2 (4)
O1—Si1—C19—C20	105.7 (4)	O6—Si5—C79—C80	15.2 (5)
O2—Si1—C19—C20	−8.5 (5)	O5—Si5—C79—C80	−108.8 (4)
C25—Si1—C19—C20	−132.2 (4)	C85—Si5—C79—C80	134.6 (4)

C24—C19—C20—C21	−0.1 (7)	C84—C79—C80—C81	1.9 (8)
Si1—C19—C20—C21	178.9 (4)	Si5—C79—C80—C81	−178.9 (4)
C19—C20—C21—C22	−0.4 (8)	C79—C80—C81—C82	−0.4 (9)
C20—C21—C22—C23	1.2 (8)	C80—C81—C82—C83	−1.3 (9)
C21—C22—C23—C24	−1.5 (9)	C81—C82—C83—C84	1.4 (9)
C22—C23—C24—C19	0.9 (9)	C82—C83—C84—C79	0.2 (9)
C20—C19—C24—C23	−0.2 (8)	C80—C79—C84—C83	−1.8 (8)
Si1—C19—C24—C23	−179.1 (4)	Si5—C79—C84—C83	179.0 (4)
O1—Si1—C25—C30	−36.8 (5)	O6—Si5—C85—C86	−134.3 (5)
O2—Si1—C25—C30	77.5 (5)	O5—Si5—C85—C86	−14.7 (5)
C19—Si1—C25—C30	−160.0 (5)	C79—Si5—C85—C86	103.3 (5)
O1—Si1—C25—C26	142.1 (5)	O6—Si5—C85—C90	45.9 (4)
O2—Si1—C25—C26	−103.6 (5)	O5—Si5—C85—C90	165.4 (4)
C19—Si1—C25—C26	18.9 (5)	C79—Si5—C85—C90	−76.6 (4)
C30—C25—C26—C27	−1.2 (8)	C90—C85—C86—C87	0.3 (9)
Si1—C25—C26—C27	179.8 (5)	Si5—C85—C86—C87	−179.6 (5)
C25—C26—C27—C28	−0.1 (9)	C85—C86—C87—C88	−0.5 (10)
C26—C27—C28—C29	−0.4 (10)	C86—C87—C88—C89	−0.1 (10)
C27—C28—C29—C30	2.2 (11)	C87—C88—C89—C90	1.0 (9)
C26—C25—C30—C29	3.1 (9)	C88—C89—C90—C85	−1.3 (9)
Si1—C25—C30—C29	−177.9 (5)	C86—C85—C90—C89	0.6 (8)
C28—C29—C30—C25	−3.8 (10)	Si5—C85—C90—C89	−179.5 (4)
O1—Si2—C1—C6	47.1 (5)	O5—Si6—C61—C62	152.4 (5)
C7—Si2—C1—C6	169.3 (4)	C73—Si6—C61—C62	35.1 (6)
C13—Si2—C1—C6	−71.5 (5)	C67—Si6—C61—C62	−87.7 (5)
O1—Si2—C1—C2	−135.5 (4)	O5—Si6—C61—C66	−31.3 (5)
C7—Si2—C1—C2	−13.3 (5)	C73—Si6—C61—C66	−148.6 (4)
C13—Si2—C1—C2	105.9 (5)	C67—Si6—C61—C66	88.6 (5)
C6—C1—C2—C3	−1.1 (9)	C66—C61—C62—C63	−0.8 (9)
Si2—C1—C2—C3	−178.6 (5)	Si6—C61—C62—C63	175.6 (6)
C1—C2—C3—C4	1.4 (9)	C61—C62—C63—C64	0.5 (11)
C2—C3—C4—C5	−1.7 (10)	C62—C63—C64—C65	0.2 (11)
C3—C4—C5—C6	1.8 (11)	C63—C64—C65—C66	−0.7 (10)
C4—C5—C6—C1	−1.6 (11)	C64—C65—C66—C61	0.4 (10)
C2—C1—C6—C5	1.2 (9)	C62—C61—C66—C65	0.4 (8)
Si2—C1—C6—C5	178.8 (5)	Si6—C61—C66—C65	−176.2 (5)
O1—Si2—C7—C12	−135.9 (5)	O5—Si6—C67—C68	120.3 (4)
C13—Si2—C7—C12	−15.6 (6)	C61—Si6—C67—C68	1.2 (5)
C1—Si2—C7—C12	104.3 (5)	C73—Si6—C67—C68	−123.5 (4)
O1—Si2—C7—C8	52.5 (6)	O5—Si6—C67—C72	−58.3 (4)
C13—Si2—C7—C8	172.8 (5)	C61—Si6—C67—C72	−177.4 (4)
C1—Si2—C7—C8	−67.4 (5)	C73—Si6—C67—C72	57.9 (4)
C12—C7—C8—C9	2.3 (9)	C72—C67—C68—C69	0.4 (8)
Si2—C7—C8—C9	174.2 (5)	Si6—C67—C68—C69	−178.3 (4)
C7—C8—C9—C10	−1.3 (10)	C67—C68—C69—C70	−0.9 (9)
C8—C9—C10—C11	0.8 (12)	C68—C69—C70—C71	0.9 (9)
C9—C10—C11—C12	−1.2 (12)	C69—C70—C71—C72	−0.4 (8)
C10—C11—C12—C7	2.3 (10)	C70—C71—C72—C67	−0.1 (8)

C8—C7—C12—C11	−2.9 (9)	C68—C67—C72—C71	0.1 (7)
Si2—C7—C12—C11	−174.6 (5)	Si6—C67—C72—C71	178.8 (4)
O1—Si2—C13—C18	35.2 (5)	O5—Si6—C73—C74	165.2 (4)
C7—Si2—C13—C18	−87.4 (4)	C61—Si6—C73—C74	−75.4 (5)
C1—Si2—C13—C18	153.9 (4)	C67—Si6—C73—C74	45.9 (5)
O1—Si2—C13—C14	−145.8 (4)	O5—Si6—C73—C78	−11.6 (5)
C7—Si2—C13—C14	91.5 (5)	C61—Si6—C73—C78	107.8 (5)
C1—Si2—C13—C14	−27.1 (5)	C67—Si6—C73—C78	−130.9 (5)
C18—C13—C14—C15	2.3 (7)	C78—C73—C74—C75	−0.6 (8)
Si2—C13—C14—C15	−176.7 (4)	Si6—C73—C74—C75	−177.5 (4)
C13—C14—C15—C16	−1.3 (9)	C73—C74—C75—C76	1.9 (9)
C14—C15—C16—C17	0.5 (9)	C74—C75—C76—C77	−2.7 (10)
C15—C16—C17—C18	−0.7 (8)	C75—C76—C77—C78	2.1 (10)
C14—C13—C18—C17	−2.6 (7)	C76—C77—C78—C73	−0.8 (10)
Si2—C13—C18—C17	176.4 (4)	C74—C73—C78—C77	0.0 (9)
C16—C17—C18—C13	1.9 (8)	Si6—C73—C78—C77	177.0 (5)
O4—Si3—O3—Si4	−153.8 (8)	O8—Si7—O7—Si8	−27.5 (5)
C55—Si3—O3—Si4	88.6 (8)	C109—Si7—O7—Si8	−143.8 (4)
C49—Si3—O3—Si4	−39.4 (9)	C115—Si7—O7—Si8	95.7 (4)
C31—Si4—O3—Si3	−151.4 (8)	C91—Si8—O7—Si7	92.4 (4)
C37—Si4—O3—Si3	85.9 (8)	C97—Si8—O7—Si7	−28.2 (5)
C43—Si4—O3—Si3	−34.5 (9)	C103—Si8—O7—Si7	−147.0 (4)
O3—Si3—C49—C50	53.4 (5)	O8—Si7—C109—C110	−128.3 (5)
O4—Si3—C49—C50	167.7 (4)	O7—Si7—C109—C110	−7.4 (5)
C55—Si3—C49—C50	−71.6 (5)	C115—Si7—C109—C110	110.1 (5)
O3—Si3—C49—C54	−124.5 (4)	O8—Si7—C109—C114	53.0 (4)
O4—Si3—C49—C54	−10.2 (5)	O7—Si7—C109—C114	173.9 (4)
C55—Si3—C49—C54	110.5 (4)	C115—Si7—C109—C114	−68.6 (4)
C54—C49—C50—C51	−0.5 (8)	C114—C109—C110—C111	−0.2 (8)
Si3—C49—C50—C51	−178.5 (5)	Si7—C109—C110—C111	−179.0 (5)
C49—C50—C51—C52	−1.2 (9)	C109—C110—C111—C112	1.0 (10)
C50—C51—C52—C53	1.8 (9)	C110—C111—C112—C113	−2.0 (10)
C51—C52—C53—C54	−0.8 (8)	C111—C112—C113—C114	2.2 (10)
C50—C49—C54—C53	1.5 (7)	C110—C109—C114—C113	0.4 (8)
Si3—C49—C54—C53	179.5 (4)	Si7—C109—C114—C113	179.2 (4)
C52—C53—C54—C49	−0.9 (8)	C112—C113—C114—C109	−1.4 (9)
O3—Si3—C55—C60	7.2 (6)	O8—Si7—C115—C120	154.1 (4)
O4—Si3—C55—C60	−108.5 (5)	O7—Si7—C115—C120	29.8 (5)
C49—Si3—C55—C60	132.4 (5)	C109—Si7—C115—C120	−87.2 (5)
O3—Si3—C55—C56	−178.1 (4)	O8—Si7—C115—C116	−29.1 (6)
O4—Si3—C55—C56	66.2 (5)	O7—Si7—C115—C116	−153.5 (5)
C49—Si3—C55—C56	−52.9 (5)	C109—Si7—C115—C116	89.6 (6)
C60—C55—C56—C57	−2.8 (9)	C120—C115—C116—C117	−0.8 (11)
Si3—C55—C56—C57	−177.9 (5)	Si7—C115—C116—C117	−177.8 (7)
C55—C56—C57—C58	0.4 (10)	C115—C116—C117—C118	0.6 (13)
C56—C57—C58—C59	0.8 (11)	C116—C117—C118—C119	−0.1 (12)
C57—C58—C59—C60	0.4 (12)	C117—C118—C119—C120	−0.1 (10)
C56—C55—C60—C59	4.0 (10)	C116—C115—C120—C119	0.6 (9)

Si3—C55—C60—C59	179.0 (6)	Si7—C115—C120—C119	177.5 (5)
C58—C59—C60—C55	−3.0 (12)	C118—C119—C120—C115	−0.1 (10)
O3—Si4—C31—C32	−6.4 (5)	O7—Si8—C91—C96	−55.1 (5)
C37—Si4—C31—C32	112.6 (5)	C97—Si8—C91—C96	66.3 (5)
C43—Si4—C31—C32	−124.7 (5)	C103—Si8—C91—C96	−173.0 (4)
O3—Si4—C31—C36	168.4 (5)	O7—Si8—C91—C92	125.6 (5)
C37—Si4—C31—C36	−72.5 (5)	C97—Si8—C91—C92	−113.1 (5)
C43—Si4—C31—C36	50.1 (5)	C103—Si8—C91—C92	7.6 (6)
C36—C31—C32—C33	−0.1 (9)	C96—C91—C92—C93	−3.8 (9)
Si4—C31—C32—C33	174.9 (5)	Si8—C91—C92—C93	175.5 (5)
C31—C32—C33—C34	−0.8 (10)	C91—C92—C93—C94	−1.4 (11)
C32—C33—C34—C35	1.9 (10)	C92—C93—C94—C95	5.4 (11)
C33—C34—C35—C36	−2.2 (10)	C93—C94—C95—C96	−4.0 (10)
C34—C35—C36—C31	1.3 (11)	C94—C95—C96—C91	−1.4 (9)
C32—C31—C36—C35	−0.2 (9)	C92—C91—C96—C95	5.2 (8)
Si4—C31—C36—C35	−175.3 (5)	Si8—C91—C96—C95	−174.1 (4)
O3—Si4—C37—C42	8.2 (5)	O7—Si8—C97—C98	−51.2 (4)
C31—Si4—C37—C42	−110.0 (4)	C91—Si8—C97—C98	−172.4 (3)
C43—Si4—C37—C42	128.6 (4)	C103—Si8—C97—C98	65.9 (4)
O3—Si4—C37—C38	−170.8 (4)	O7—Si8—C97—C102	129.6 (4)
C31—Si4—C37—C38	71.0 (5)	C91—Si8—C97—C102	8.4 (5)
C43—Si4—C37—C38	−50.4 (5)	C103—Si8—C97—C102	−113.3 (4)
C42—C37—C38—C39	3.9 (8)	C102—C97—C98—C99	0.7 (7)
Si4—C37—C38—C39	−177.0 (5)	Si8—C97—C98—C99	−178.6 (3)
C37—C38—C39—C40	−1.8 (9)	C97—C98—C99—C100	−0.4 (7)
C38—C39—C40—C41	−0.7 (10)	C98—C99—C100—C101	−0.4 (7)
C39—C40—C41—C42	0.8 (9)	C99—C100—C101—C102	0.9 (7)
C40—C41—C42—C37	1.5 (8)	C100—C101—C102—C97	−0.6 (8)
C38—C37—C42—C41	−3.8 (8)	C98—C97—C102—C101	−0.1 (7)
Si4—C37—C42—C41	177.2 (4)	Si8—C97—C102—C101	179.1 (4)
O3—Si4—C43—C44	−80.0 (5)	O7—Si8—C103—C108	−19.1 (5)
C31—Si4—C43—C44	36.0 (6)	C91—Si8—C103—C108	100.9 (5)
C37—Si4—C43—C44	160.9 (5)	C97—Si8—C103—C108	−138.5 (5)
O3—Si4—C43—C48	97.7 (5)	O7—Si8—C103—C104	158.6 (4)
C31—Si4—C43—C48	−146.3 (5)	C91—Si8—C103—C104	−81.4 (5)
C37—Si4—C43—C48	−21.4 (6)	C97—Si8—C103—C104	39.2 (5)
C48—C43—C44—C45	−1.9 (10)	C108—C103—C104—C105	−1.4 (8)
Si4—C43—C44—C45	175.9 (6)	Si8—C103—C104—C105	−179.2 (4)
C43—C44—C45—C46	1.3 (13)	C103—C104—C105—C106	2.4 (8)
C44—C45—C46—C47	1.4 (14)	C104—C105—C106—C107	−2.5 (9)
C45—C46—C47—C48	−3.3 (13)	C105—C106—C107—C108	1.5 (9)
C44—C43—C48—C47	0.0 (10)	C106—C107—C108—C103	−0.5 (9)
Si4—C43—C48—C47	−177.8 (5)	C104—C103—C108—C107	0.4 (8)
C46—C47—C48—C43	2.7 (12)	Si8—C103—C108—C107	178.2 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H6*A*···O2	0.84	2.03	2.785 (5)	149
O8—H8*A*···O4^{i}	0.84	1.94	2.735 (5)	158
O2—H2···*Cg*(C67-C72)	0.84	2.66	3.355 (5)	142
O4—H4*A*···*Cg*(C97-C102)	0.84	2.61	3.249 (5)	134

Symmetry code: (i) −*x*, −*y*+1, −*z*.