

# The crystal structure of 2-[(*tert*-butyldiphenylsilyl)-oxy]-1,2-diphenylethan-1-one

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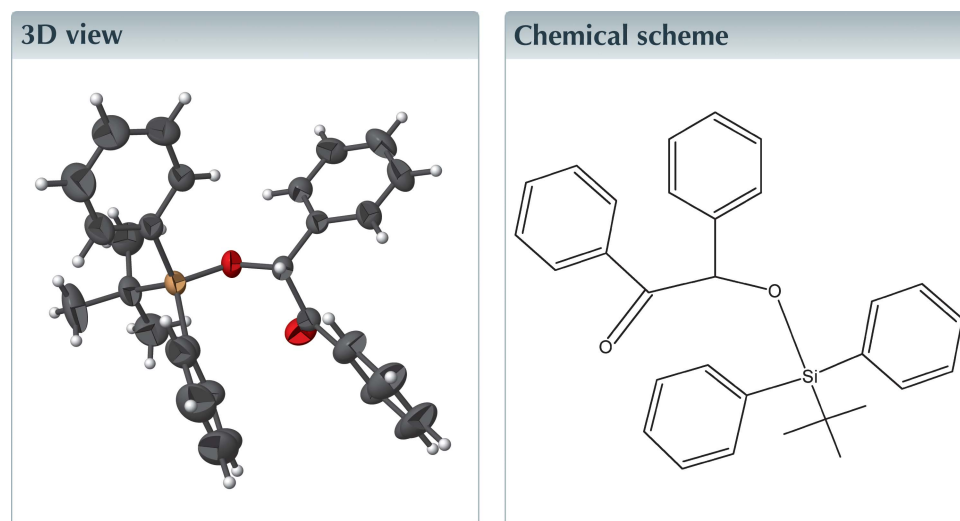
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Keywords: crystal structure; benzoin; silyl derivative; bulky group; conformation.

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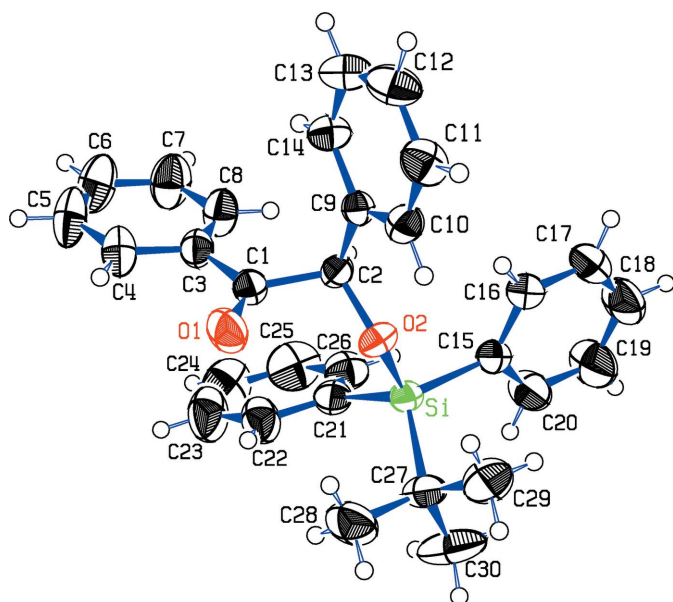
Structural data: full structural data are available from iucrdata.iucr.org

The title compound,  $C_{30}H_{30}O_2Si$ , was synthesized and structurally characterized in order to determine the influence of the bulky silyl protecting group on the conformation of the benzoin moiety, with a view to directing the stereochemistry of the borohydride reduction of the benzoin. The crystal structure shows a benzoin  $O-C-C-O$  torsion angle of  $38.34(1)^\circ$ , not greatly different from that found in benzoin itself. In the crystal, a weak  $C-H \cdots O$  hydrogen bond between the carbonyl group and a phenyl H atom of a symmetry-related molecule forms chains along  $[100]$ .



## Structure description

As part of a program designed to alter the stereoselectivity of the reduction of benzoin derivatives, the oxysilyl benzoin derivative named in the title was synthesized in an attempt to explore the stereochemical effect of the large hydroxyl-protecting silyl group. The stereochemistry of this reduction can be explained by the Felkin–Anh or the Cram chelation model (Rowland, 1983). Given the need for a method that would afford the alternate racemic diols, the bulky silyl protecting group *tert*-butyldiphenylsilyl (TBDPS) was introduced with the expectation that this large substituent would allow for the production of the alternate diastereoisomer (as a racemic mixture). In the crystal structure reported here (Fig. 1), however, the conformation is close to that of benzoin itself (Haisa *et al.*, 1980; Fajardo *et al.*, 1984; Solé *et al.*, 1998) in spite of the presence of the TBDPS group and the differing crystalline environments of the two molecules. The  $O1-C1-C2-O2$  torsion angle of  $38.34(16)^\circ$  and the torsion angle  $C3-C1-C2-C9$  between the ethane phenyl groups of  $96.20(13)^\circ$  in the present structure are similar to the corresponding values of  $26.4$  and  $85.5^\circ$  given for benzoin. The phenyl ring on C1 in the present structure is almost co-planar with the  $sp^2$  plane at C1, with an angle of  $12.68(5)^\circ$  between the plane through the phenyl group and the best plane through C1/

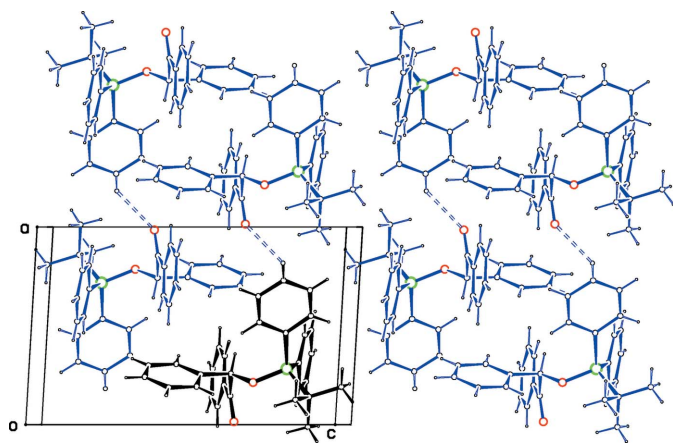


**Figure 1**

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. Displacement parameters for the H atoms are arbitrary.

O1/C2/O9. This leads to the short intramolecular contact H2  $\cdots$  H8 = 2.04 Å. In benzoin this phenyl group is twisted 11.6° from the  $sp^2$  C1 plane, with an H  $\cdots$  H distance of 2.36 Å. The phenyl group bonded to C2 in the present structure is oriented so as to almost eclipse the C2–O2 bond, with torsion angle O2–C2–C9–C10 =  $-9.07$  (16)°, which brings the H10  $\cdots$  O2 distance to 2.40 Å. This orientation is not however seen in the benzoin structure, where the corresponding torsion angle is  $-48.4^\circ$ .

Formation of the silyloxy derivative prohibits the strong O–H  $\cdots$  O hydrogen bonding expected in benzoin and its other derivatives, but a C=O  $\cdots$  H–C intermolecular interaction is seen (Table 1 and Fig. 2), linking the molecules in chains along the *a*-axis direction. Only three intermolecular H



**Figure 2**

Projection along the *b* axis for the title compound, tilted by 4° for clarity. The reference molecule is in black. Silicon atoms are green, oxygen atoms red.

**Table 1**

Hydrogen-bond geometry (Å, °).

<i>D</i> –H $\cdots$ <i>A</i>	<i>D</i> –H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> –H $\cdots$ <i>A</i>
C18–H18 $\cdots$ O1 <sup>i</sup>	0.93	2.49	3.211 (2)	135

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

**Table 2**

Experimental details.

Crystal data	
Chemical formula	C <sub>30</sub> H <sub>30</sub> O <sub>2</sub> Si
<i>M<sub>r</sub></i>	450.63
Crystal system, space group	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	300
<i>a</i> , <i>b</i> , <i>c</i> (Å)	10.3403 (3), 10.3926 (3), 14.1442 (3)
$\alpha$ , $\beta$ , $\gamma$ (°)	78.9928 (14), 83.6739 (15), 60.2736 (11)
<i>V</i> (Å <sup>3</sup> )	1295.45 (6)
<i>Z</i>	2
Radiation type	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	0.11
Crystal size (mm)	0.5 $\times$ 0.4 $\times$ 0.2
Data collection	
Diffractometer	Enraf–Nonius KappaCCD
Absorption correction	–
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	6102, 6102, 5246
<i>R</i> <sub>int</sub>	0.032
( $\sin \theta/\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.655
Refinement	
$R[F^2 > 2\sigma(F^2)]$ , $wR(F^2)$ , <i>S</i>	0.043, 0.123, 1.04
No. of reflections	6102
No. of parameters	301
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$ , $\Delta\rho_{\min}$ (e Å <sup>-3</sup> )	0.27, $-0.18$

Computer programs: *KappaCCD Server Software* (Nonius, 1997), *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997), *SHELXT* (Sheldrick, 2015a), *SHELXL2017* (Sheldrick, 2015b), *ORTEP3* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 2012) and *publCIF* (Westrip, 2010).

$\cdots$  H contacts are closer than 2.6 Å, with the shortest contact H4  $\cdots$  H12(*x*,1 + *y*,*z*) at 2.48 Å.

The stereochemical outcome of the reduction of the title compound will be reported elsewhere.

## Synthesis and crystallization

The title compound was easily prepared in high yield (*t*-butyldiphenylsilyl chloride (TBDPS-Cl), imidazole, ( $\pm$ )-benzoin, DMF, RT) from ( $\pm$ )-benzoin and was isolated after column chromatography as a low-melting, crystalline solid. Suitable crystals were obtained by recrystallization from hexanes (m.p. 346–345 K).

<sup>1</sup>H (400 MHz) NMR spectra were recorded on a Bruker Avance 400 spectrometer in CDCl<sub>3</sub> with tetramethylsilane (TMS) as the internal standard, and chemical shifts are reported in parts per million (p.p.m.,  $\delta$ ): 7.57–7.69 ppm, 2H, *m*; 7.51–7.55 ppm, 4H, *m*; 7.23–7.47 ppm, 14H, *m*; 5.82 ppm, 1H, *s*; 1.08 ppm, 9H, *s*. An infrared spectrum obtained with a Nicolet iS50 FT–IR machine showed  $\mu(\text{C}=\text{O})$  at 1694 cm<sup>-1</sup>.

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

## Acknowledgements

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## full crystallographic data

*IUCrData* (2019). 4, x190478 [https://doi.org/10.1107/S2414314619004784]

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2-[(*tert*-Butyldiphenylsilyl)oxy]-1,2-diphenylethan-1-one*Crystal data*

$C_{30}H_{30}O_2Si$	$Z = 2$
$M_r = 450.63$	$F(000) = 480$
Triclinic, $P\bar{1}$	$D_x = 1.155 \text{ Mg m}^{-3}$
$a = 10.3403 (3) \text{ \AA}$	Mo $K\alpha$ radiation, $\lambda = 0.71070 \text{ \AA}$
$b = 10.3926 (3) \text{ \AA}$	Cell parameters from 4557 reflections
$c = 14.1442 (3) \text{ \AA}$	$\theta = 1.0\text{--}25.0^\circ$
$\alpha = 78.9928 (14)^\circ$	$\mu = 0.11 \text{ mm}^{-1}$
$\beta = 83.6739 (15)^\circ$	$T = 300 \text{ K}$
$\gamma = 60.2736 (11)^\circ$	Block, colorless
$V = 1295.45 (6) \text{ \AA}^3$	$0.5 \times 0.4 \times 0.2 \text{ mm}$

*Data collection*

Enraf–Nonius KappaCCD diffractometer	6102 independent reflections
Radiation source: fine-focus sealed tube	5246 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{\text{int}} = 0.032$
Detector resolution: 9 pixels $\text{mm}^{-1}$	$\theta_{\text{max}} = 27.7^\circ$ , $\theta_{\text{min}} = 2.3^\circ$
combination of $\omega$ and $\varphi$ scans	$h = 0 \rightarrow 13$
6102 measured reflections	$k = -11 \rightarrow 13$
	$l = -18 \rightarrow 18$

*Refinement*

Refinement on $F^2$	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.043$	H-atom parameters constrained
$wR(F^2) = 0.123$	$w = 1/[\sigma^2(F_o^2) + (0.060P)^2 + 0.290P]$
$S = 1.04$	where $P = (F_o^2 + 2F_c^2)/3$
6102 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
301 parameters	$\Delta\rho_{\text{max}} = 0.27 \text{ e \AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.18 \text{ e \AA}^{-3}$

*Special details*

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

**Refinement.** H atoms were placed at ideal positions and refined riding on their parent C atoms, with C—H distances of 0.93 Å for the phenyl H atoms, 0.96 Å for the methyl H atoms and 0.98 Å for the methine H atom H2.  $U_{\text{iso}}$  values of the H atoms were set at  $1.2xU_{\text{eq}}(\text{C})$  or  $1.5xU_{\text{eq}}(\text{C}_{\text{methyl}})$  of the bonded atoms.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Si1	0.28262 (4)	0.65987 (4)	0.79919 (2)	0.03862 (11)
O1	0.01496 (12)	0.63949 (13)	0.63925 (9)	0.0617 (3)
O2	0.21373 (11)	0.71114 (10)	0.68988 (6)	0.0429 (2)
C1	0.14561 (15)	0.55370 (15)	0.62691 (9)	0.0412 (3)
C2	0.25752 (14)	0.61237 (14)	0.62185 (9)	0.0362 (3)
H2	0.357881	0.528187	0.635855	0.043*
C3	0.19912 (16)	0.39651 (15)	0.61292 (10)	0.0436 (3)
C4	0.0932 (2)	0.35680 (19)	0.59831 (13)	0.0591 (4)
H4	-0.007416	0.427740	0.597544	0.071*
C5	0.1373 (3)	0.2125 (2)	0.58496 (16)	0.0779 (6)
H5	0.066449	0.187090	0.573793	0.093*
C6	0.2845 (3)	0.1068 (2)	0.58808 (17)	0.0820 (6)
H6	0.313308	0.009475	0.579652	0.098*
C7	0.3901 (2)	0.1432 (2)	0.60358 (17)	0.0760 (5)
H7	0.490202	0.070587	0.606047	0.091*
C8	0.34815 (19)	0.28761 (17)	0.61550 (13)	0.0588 (4)
H8	0.420262	0.312108	0.625342	0.071*
C9	0.25367 (13)	0.69454 (14)	0.52002 (9)	0.0364 (3)
C10	0.19247 (16)	0.84890 (16)	0.50123 (10)	0.0462 (3)
H10	0.154230	0.904214	0.551675	0.055*
C11	0.18776 (19)	0.92173 (18)	0.40766 (12)	0.0591 (4)
H11	0.148554	1.025326	0.395693	0.071*
C12	0.24112 (19)	0.8407 (2)	0.33231 (11)	0.0636 (4)
H12	0.237759	0.889559	0.269512	0.076*
C13	0.29938 (19)	0.6874 (2)	0.35035 (11)	0.0606 (4)
H13	0.333830	0.632934	0.299448	0.073*
C14	0.30696 (16)	0.61416 (17)	0.44335 (10)	0.0487 (3)
H14	0.347958	0.510344	0.454959	0.058*
C15	0.46458 (15)	0.65965 (16)	0.78902 (10)	0.0435 (3)
C16	0.51811 (16)	0.69987 (16)	0.69988 (10)	0.0476 (3)
H16	0.463805	0.723616	0.644968	0.057*
C17	0.6500 (2)	0.7053 (2)	0.69108 (13)	0.0650 (4)
H17	0.684405	0.730468	0.630669	0.078*
C18	0.7301 (2)	0.6735 (3)	0.77164 (16)	0.0814 (6)
H18	0.817611	0.679282	0.765984	0.098*
C19	0.6807 (2)	0.6332 (3)	0.86067 (15)	0.0875 (7)
H19	0.734885	0.611584	0.915286	0.105*
C20	0.5509 (2)	0.6250 (2)	0.86883 (12)	0.0670 (5)
H20	0.519897	0.595383	0.929264	0.080*
C21	0.31257 (17)	0.46557 (17)	0.84700 (9)	0.0477 (3)
C22	0.1945 (2)	0.4339 (2)	0.85593 (13)	0.0671 (5)
H22	0.098158	0.512169	0.843669	0.081*
C23	0.2182 (3)	0.2883 (3)	0.88267 (16)	0.0908 (7)
H23	0.138077	0.270004	0.888059	0.109*
C24	0.3597 (4)	0.1713 (3)	0.90119 (17)	0.1016 (8)

H24	0.375578	0.073612	0.918301	0.122*
C25	0.4775 (3)	0.1987 (2)	0.89439 (16)	0.0878 (7)
H25	0.573134	0.119791	0.907816	0.105*
C26	0.4540 (2)	0.34389 (19)	0.86758 (11)	0.0610 (4)
H26	0.535038	0.360655	0.863168	0.073*
C27	0.14080 (17)	0.81037 (18)	0.86866 (10)	0.0522 (3)
C28	-0.0120 (2)	0.8198 (2)	0.86986 (16)	0.0762 (5)
H28A	-0.007814	0.730819	0.907911	0.114*
H28B	-0.038814	0.828291	0.805212	0.114*
H28C	-0.085088	0.906099	0.897227	0.114*
C29	0.1260 (2)	0.9610 (2)	0.81732 (16)	0.0788 (6)
H29A	0.220344	0.958032	0.816822	0.118*
H29B	0.053143	1.040075	0.850727	0.118*
H29C	0.095176	0.979230	0.752289	0.118*
C30	0.1904 (3)	0.7799 (3)	0.97251 (14)	0.0974 (8)
H30A	0.281746	0.782916	0.972241	0.146*
H30B	0.205707	0.682618	1.002855	0.146*
H30C	0.114895	0.854971	1.007482	0.146*

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Si1	0.03999 (19)	0.0469 (2)	0.03221 (17)	-0.02263 (16)	0.00197 (13)	-0.01050 (14)
O1	0.0417 (6)	0.0639 (7)	0.0825 (8)	-0.0269 (5)	0.0105 (5)	-0.0214 (6)
O2	0.0513 (5)	0.0426 (5)	0.0349 (4)	-0.0207 (4)	-0.0033 (4)	-0.0114 (4)
C1	0.0410 (7)	0.0477 (7)	0.0397 (6)	-0.0252 (6)	0.0001 (5)	-0.0069 (5)
C2	0.0381 (6)	0.0373 (6)	0.0359 (6)	-0.0189 (5)	-0.0015 (5)	-0.0096 (5)
C3	0.0509 (7)	0.0466 (7)	0.0418 (7)	-0.0307 (6)	-0.0044 (5)	-0.0031 (5)
C4	0.0608 (9)	0.0594 (9)	0.0695 (10)	-0.0399 (8)	-0.0159 (8)	0.0021 (8)
C5	0.0936 (14)	0.0661 (11)	0.1005 (15)	-0.0584 (11)	-0.0289 (11)	0.0014 (10)
C6	0.1014 (16)	0.0496 (9)	0.1096 (16)	-0.0451 (11)	-0.0234 (13)	-0.0081 (10)
C7	0.0701 (12)	0.0462 (9)	0.1123 (16)	-0.0259 (8)	-0.0117 (11)	-0.0152 (9)
C8	0.0550 (9)	0.0470 (8)	0.0814 (11)	-0.0279 (7)	-0.0079 (8)	-0.0128 (7)
C9	0.0323 (6)	0.0424 (6)	0.0372 (6)	-0.0198 (5)	-0.0006 (4)	-0.0079 (5)
C10	0.0507 (8)	0.0439 (7)	0.0462 (7)	-0.0240 (6)	0.0011 (6)	-0.0102 (6)
C11	0.0625 (10)	0.0473 (8)	0.0590 (9)	-0.0242 (7)	-0.0005 (7)	0.0027 (7)
C12	0.0610 (10)	0.0707 (11)	0.0418 (8)	-0.0241 (8)	0.0020 (7)	0.0042 (7)
C13	0.0613 (9)	0.0672 (10)	0.0407 (7)	-0.0217 (8)	0.0083 (6)	-0.0141 (7)
C14	0.0498 (8)	0.0476 (7)	0.0437 (7)	-0.0191 (6)	0.0046 (6)	-0.0128 (6)
C15	0.0424 (7)	0.0507 (7)	0.0408 (7)	-0.0243 (6)	0.0030 (5)	-0.0121 (6)
C16	0.0498 (8)	0.0517 (8)	0.0435 (7)	-0.0262 (6)	0.0040 (6)	-0.0106 (6)
C17	0.0603 (10)	0.0818 (12)	0.0615 (10)	-0.0437 (9)	0.0153 (8)	-0.0130 (8)
C18	0.0597 (11)	0.1225 (18)	0.0823 (13)	-0.0603 (12)	0.0062 (9)	-0.0188 (12)
C19	0.0668 (12)	0.149 (2)	0.0667 (11)	-0.0673 (14)	-0.0089 (9)	-0.0136 (12)
C20	0.0596 (10)	0.1078 (15)	0.0454 (8)	-0.0507 (10)	-0.0025 (7)	-0.0078 (9)
C21	0.0597 (8)	0.0558 (8)	0.0322 (6)	-0.0328 (7)	-0.0008 (5)	-0.0035 (5)
C22	0.0788 (12)	0.0796 (12)	0.0576 (9)	-0.0536 (10)	-0.0062 (8)	0.0037 (8)
C23	0.132 (2)	0.1018 (17)	0.0746 (13)	-0.0906 (17)	-0.0119 (13)	0.0104 (12)

C24	0.163 (3)	0.0748 (14)	0.0804 (15)	-0.0748 (18)	-0.0191 (16)	0.0176 (11)
C25	0.1129 (18)	0.0577 (11)	0.0726 (13)	-0.0308 (12)	-0.0133 (12)	0.0099 (9)
C26	0.0708 (10)	0.0601 (9)	0.0458 (8)	-0.0297 (8)	-0.0022 (7)	-0.0002 (7)
C27	0.0490 (8)	0.0610 (9)	0.0424 (7)	-0.0209 (7)	0.0063 (6)	-0.0205 (6)
C28	0.0490 (9)	0.0847 (13)	0.0845 (13)	-0.0246 (9)	0.0164 (9)	-0.0235 (10)
C29	0.0812 (13)	0.0592 (10)	0.0931 (14)	-0.0285 (10)	0.0175 (11)	-0.0334 (10)
C30	0.0848 (14)	0.1205 (19)	0.0525 (10)	-0.0135 (13)	-0.0004 (9)	-0.0453 (11)

*Geometric parameters (Å, °)*

Si1—O2	1.6534 (9)	C15—C20	1.396 (2)
Si1—C15	1.8701 (14)	C16—C17	1.384 (2)
Si1—C21	1.8802 (15)	C16—H16	0.9300
Si1—C27	1.8860 (14)	C17—C18	1.373 (3)
O1—C1	1.2097 (17)	C17—H17	0.9300
O2—C2	1.4158 (14)	C18—C19	1.375 (3)
C1—C3	1.4888 (19)	C18—H18	0.9300
C1—C2	1.5430 (17)	C19—C20	1.378 (2)
C2—C9	1.5213 (17)	C19—H19	0.9300
C2—H2	0.9800	C20—H20	0.9300
C3—C8	1.387 (2)	C21—C26	1.394 (2)
C3—C4	1.3940 (19)	C21—C22	1.401 (2)
C4—C5	1.380 (3)	C22—C23	1.388 (3)
C4—H4	0.9300	C22—H22	0.9300
C5—C6	1.365 (3)	C23—C24	1.373 (4)
C5—H5	0.9300	C23—H23	0.9300
C6—C7	1.371 (3)	C24—C25	1.372 (4)
C6—H6	0.9300	C24—H24	0.9300
C7—C8	1.379 (2)	C25—C26	1.385 (3)
C7—H7	0.9300	C25—H25	0.9300
C8—H8	0.9300	C26—H26	0.9300
C9—C10	1.3828 (19)	C27—C28	1.532 (2)
C9—C14	1.3911 (18)	C27—C29	1.535 (3)
C10—C11	1.386 (2)	C27—C30	1.532 (2)
C10—H10	0.9300	C28—H28A	0.9600
C11—C12	1.379 (2)	C28—H28B	0.9600
C11—H11	0.9300	C28—H28C	0.9600
C12—C13	1.376 (2)	C29—H29A	0.9600
C12—H12	0.9300	C29—H29B	0.9600
C13—C14	1.377 (2)	C29—H29C	0.9600
C13—H13	0.9300	C30—H30A	0.9600
C14—H14	0.9300	C30—H30B	0.9600
C15—C16	1.3947 (19)	C30—H30C	0.9600
O2—Si1—C15	107.79 (6)	C17—C16—H16	119.2
O2—Si1—C21	108.53 (6)	C15—C16—H16	119.2
C15—Si1—C21	110.02 (7)	C16—C17—C18	119.94 (16)
O2—Si1—C27	104.30 (6)	C16—C17—H17	120.0

C15—Si1—C27	110.93 (7)	C18—C17—H17	120.0
C21—Si1—C27	114.88 (7)	C17—C18—C19	119.95 (17)
C2—O2—Si1	123.85 (8)	C17—C18—H18	120.0
O1—C1—C3	121.75 (12)	C19—C18—H18	120.0
O1—C1—C2	118.40 (12)	C20—C19—C18	119.89 (18)
C3—C1—C2	119.81 (11)	C20—C19—H19	120.1
O2—C2—C9	110.69 (10)	C18—C19—H19	120.1
O2—C2—C1	108.95 (10)	C19—C20—C15	121.91 (16)
C9—C2—C1	107.17 (10)	C19—C20—H20	119.0
O2—C2—H2	110.0	C15—C20—H20	119.0
C9—C2—H2	110.0	C26—C21—C22	116.57 (16)
C1—C2—H2	110.0	C26—C21—Si1	121.98 (12)
C8—C3—C4	118.63 (14)	C22—C21—Si1	121.23 (13)
C8—C3—C1	123.36 (12)	C23—C22—C21	121.5 (2)
C4—C3—C1	118.00 (13)	C23—C22—H22	119.3
C5—C4—C3	120.15 (17)	C21—C22—H22	119.3
C5—C4—H4	119.9	C22—C23—C24	120.1 (2)
C3—C4—H4	119.9	C22—C23—H23	119.9
C4—C5—C6	120.32 (17)	C24—C23—H23	119.9
C4—C5—H5	119.8	C25—C24—C23	119.8 (2)
C6—C5—H5	119.8	C25—C24—H24	120.1
C7—C6—C5	120.36 (17)	C23—C24—H24	120.1
C7—C6—H6	119.8	C24—C25—C26	120.1 (2)
C5—C6—H6	119.8	C24—C25—H25	120.0
C6—C7—C8	120.06 (18)	C26—C25—H25	120.0
C6—C7—H7	120.0	C21—C26—C25	121.90 (19)
C8—C7—H7	120.0	C21—C26—H26	119.1
C3—C8—C7	120.47 (15)	C25—C26—H26	119.1
C3—C8—H8	119.8	C28—C27—C29	108.18 (15)
C7—C8—H8	119.8	C28—C27—C30	109.19 (16)
C10—C9—C14	118.92 (12)	C29—C27—C30	109.94 (17)
C10—C9—C2	121.38 (11)	C28—C27—Si1	111.09 (12)
C14—C9—C2	119.64 (12)	C29—C27—Si1	107.71 (11)
C9—C10—C11	120.41 (13)	C30—C27—Si1	110.68 (12)
C9—C10—H10	119.8	C27—C28—H28A	109.5
C11—C10—H10	119.8	C27—C28—H28B	109.5
C12—C11—C10	120.08 (15)	H28A—C28—H28B	109.5
C12—C11—H11	120.0	C27—C28—H28C	109.5
C10—C11—H11	120.0	H28A—C28—H28C	109.5
C13—C12—C11	119.78 (14)	H28B—C28—H28C	109.5
C13—C12—H12	120.1	C27—C29—H29A	109.5
C11—C12—H12	120.1	C27—C29—H29B	109.5
C12—C13—C14	120.38 (15)	H29A—C29—H29B	109.5
C12—C13—H13	119.8	C27—C29—H29C	109.5
C14—C13—H13	119.8	H29A—C29—H29C	109.5
C13—C14—C9	120.40 (14)	H29B—C29—H29C	109.5
C13—C14—H14	119.8	C27—C30—H30A	109.5
C9—C14—H14	119.8	C27—C30—H30B	109.5



C16—C15—C20	116.62 (14)	H30A—C30—H30B	109.5
C16—C15—Si1	120.66 (11)	C27—C30—H30C	109.5
C20—C15—Si1	122.69 (11)	H30A—C30—H30C	109.5
C17—C16—C15	121.65 (14)	H30B—C30—H30C	109.5
C15—Si1—O2—C2	81.57 (10)	C27—Si1—C15—C16	-113.04 (12)
C21—Si1—O2—C2	-37.55 (11)	O2—Si1—C15—C20	178.38 (14)
C27—Si1—O2—C2	-160.47 (10)	C21—Si1—C15—C20	-63.45 (15)
Si1—O2—C2—C9	-146.22 (9)	C27—Si1—C15—C20	64.77 (16)
Si1—O2—C2—C1	96.18 (11)	C20—C15—C16—C17	-0.1 (2)
O1—C1—C2—O2	38.34 (16)	Si1—C15—C16—C17	177.83 (13)
C3—C1—C2—O2	-143.99 (11)	C15—C16—C17—C18	-1.3 (3)
O1—C1—C2—C9	-81.47 (15)	C16—C17—C18—C19	1.4 (3)
C3—C1—C2—C9	96.20 (13)	C17—C18—C19—C20	-0.1 (4)
O1—C1—C3—C8	-168.27 (15)	C18—C19—C20—C15	-1.4 (4)
C2—C1—C3—C8	14.1 (2)	C16—C15—C20—C19	1.5 (3)
O1—C1—C3—C4	10.5 (2)	Si1—C15—C20—C19	-176.41 (18)
C2—C1—C3—C4	-167.10 (13)	O2—Si1—C21—C26	116.05 (12)
C8—C3—C4—C5	-1.2 (2)	C15—Si1—C21—C26	-1.66 (14)
C1—C3—C4—C5	179.98 (16)	C27—Si1—C21—C26	-127.68 (13)
C3—C4—C5—C6	1.4 (3)	O2—Si1—C21—C22	-58.46 (14)
C4—C5—C6—C7	-0.6 (4)	C15—Si1—C21—C22	-176.18 (12)
C5—C6—C7—C8	-0.4 (4)	C27—Si1—C21—C22	57.80 (15)
C4—C3—C8—C7	0.2 (3)	C26—C21—C22—C23	-0.8 (3)
C1—C3—C8—C7	178.91 (17)	Si1—C21—C22—C23	173.96 (15)
C6—C7—C8—C3	0.7 (3)	C21—C22—C23—C24	0.1 (3)
O2—C2—C9—C10	-9.07 (16)	C22—C23—C24—C25	0.8 (4)
C1—C2—C9—C10	109.62 (13)	C23—C24—C25—C26	-0.9 (4)
O2—C2—C9—C14	173.66 (11)	C22—C21—C26—C25	0.7 (2)
C1—C2—C9—C14	-67.66 (15)	Si1—C21—C26—C25	-174.02 (14)
C14—C9—C10—C11	-1.6 (2)	C24—C25—C26—C21	0.1 (3)
C2—C9—C10—C11	-178.85 (13)	O2—Si1—C27—C28	59.42 (13)
C9—C10—C11—C12	1.5 (2)	C15—Si1—C27—C28	175.21 (12)
C10—C11—C12—C13	-0.2 (3)	C21—Si1—C27—C28	-59.24 (14)
C11—C12—C13—C14	-1.1 (3)	O2—Si1—C27—C29	-58.89 (13)
C12—C13—C14—C9	1.0 (3)	C15—Si1—C27—C29	56.90 (14)
C10—C9—C14—C13	0.3 (2)	C21—Si1—C27—C29	-177.55 (12)
C2—C9—C14—C13	177.65 (13)	O2—Si1—C27—C30	-179.10 (15)
O2—Si1—C15—C16	0.57 (13)	C15—Si1—C27—C30	-63.31 (17)
C21—Si1—C15—C16	118.74 (12)	C21—Si1—C27—C30	62.24 (17)

## 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>
C18—H18...O1 <sup>i</sup>	0.93	2.49	3.211 (2)	135

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