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5-Butyl-5-(2-methyl-1*H*-inden-1-yl)-5*H*-dibenzo-[*b*,*d*]silole

Michael G. Medvedev,[a]* Vyatcheslav V. Izmer,[b] Dmitry S. Kononovich,[b] Dmitry V. Uborsky[b] and Alexander Z. Voskoboynikov[b]

[a]X-ray Structural Laboratory, A.N. Nesmeyanov Institute of Organoelement Compounds, Vavilova St. 28, GSP-1, Moscow 119991, V-334, Russian Federation, and [b]Department of Chemistry, Lomonosov Moscow State University, 1/3 Leninskie Gory, GSP-1, Moscow 119991, Russian Federation. *Correspondence e-mail: medvedev.m.g@gmail.com

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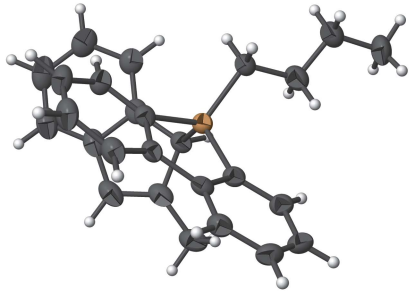
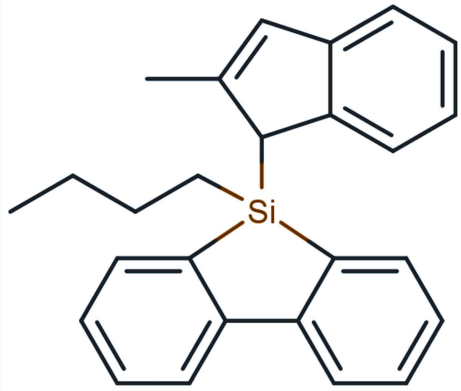
Structural data: full structural data are available from iucrdata.iucr.org

The structure of the title compound [systematic name: 8-butyl-8-(2-methyl-1*H*-inden-1-yl)-8-silatricyclo[7.4.0.0^{2,3}]trideca-1(13),2,4,6,9,11-hexaene], $C_{26}H_{26}Si$, at 110 K has orthorhombic (*Pbca*) symmetry. In the molecule, the butyl group displays an extended conformation with the C—C—C—C torsion angle of 176.8 (2)°. The dihedral angle between the biphenyl group and the indole group is 60.04 (2)°. The structure exhibits a weak intramolecular C—H···π interaction.

3D view



Chemical scheme



Structure description

Benzannulated siloles are distinguish from their all-carbon analogues by their unique electronic structure (Yamaguchi & Tamao, 2005), and so are valuable building blocks for π-conjugated polymers. In the title molecule (Fig. 1), the butyl group displays an extended conformation with the C23—C24—C25—C26 torsion angle of 176.8 (2)°. All bond lengths are normal. The structure contains an intramolecular C—H···π interaction (Table 1).

Synthesis and crystallization

This compound was obtained *via* treatment of 5,5-dichloro-5*H*-dibenzo[*b*,*d*]silole (Liu *et al.*, 2002) with 1 equivalent of lithium salt of 2-methyl-1*H*-indene in THF followed by 1 equivalent of 2.5 *M* butyllithium in hexanes. Single crystals suitable for X-ray crystal structure analysis were grown from an *n*-hexane solution at 243 K.

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

*Cg*1 is the centroid of the C16–C21 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···*Cg*1	0.95	2.78	3.446 (3)	128

Refinement

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

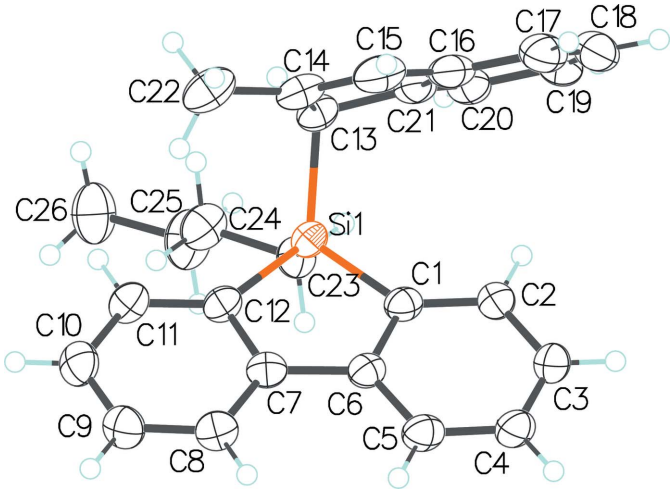


Figure 1
The molecular structure with displacement ellipsoids shown at the 50% probability level.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{26}H_{26}Si$
M_r	366.56
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	110
a, *b*, *c* (Å)	7.490 (2), 18.968 (6), 28.635 (9)
V (Å^3)	4068 (2)
Z	8
Radiation type	Mo *Kα*
μ (mm^{-1})	0.12
Crystal size (mm)	0.2 × 0.2 × 0.1
Data collection	
Diffractometer	Bruker SMART 1000 CCD
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	25428, 5934, 2858
R_{int}	0.075
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.704
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.057, 0.148, 0.86
No. of reflections	5934
No. of parameters	246
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.52, −0.24

Computer programs: *SMART* and *SAINT* (Bruker, 2007), *SHELXS* (Sheldrick, 2008), *SHELXL* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

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full crystallographic data

IUCrData (2016). **1**, x161151 [https://doi.org/10.1107/S2414314616011512]

5-Butyl-5-(2-methyl-1*H*-inden-1-yl)-5*H*-dibenzo[*b*,*d*]silole

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8-Butyl-8-(2-methyl-1*H*-inden-1-yl)-8-silatricyclo[7.4.0.0^{2,3}]trideca-1(13),2,4,6,9,11-hexaene

Crystal data

$C_{26}H_{26}Si$
M_r = 366.56
Orthorhombic, *Pbca*
a = 7.490 (2) Å
b = 18.968 (6) Å
c = 28.635 (9) Å
V = 4068 (2) Å^3
Z = 8
F(000) = 1568
D_x = 1.197 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 879 reflections
θ = 3–60°
μ = 0.12 mm^{-1}
T = 110 K
Block, clear light yellow
0.2 × 0.2 × 0.1 mm

Data collection

Bruker SMART 1000 CCD diffractometer
phi and ω scans
25428 measured reflections
5934 independent reflections
2858 reflections with $I > 2\sigma(I)$
R_{int} = 0.075
θ_{max} = 30.0°, θ_{min} = 2.2°
h = −10→7
k = −23→26
l = −40→36

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.148
S = 0.86
5934 reflections
246 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0757P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Si1	0.79777 (7)	0.42501 (3)	0.11255 (2)	0.02993 (15)

C1	0.8311 (2)	0.49615 (10)	0.15680 (6)	0.0309 (4)
C2	0.8055 (3)	0.56845 (10)	0.15463 (7)	0.0356 (5)
H2	0.7520	0.5887	0.1277	0.043*
C3	0.8574 (3)	0.61143 (12)	0.19140 (7)	0.0418 (5)
H3	0.8412	0.6610	0.1894	0.050*
C4	0.9330 (3)	0.58188 (12)	0.23114 (7)	0.0421 (5)
H4	0.9678	0.6115	0.2563	0.050*
C5	0.9581 (3)	0.51005 (11)	0.23455 (6)	0.0370 (5)
H5	1.0097	0.4902	0.2619	0.044*
C6	0.9068 (2)	0.46663 (10)	0.19746 (6)	0.0298 (4)
C7	0.9323 (2)	0.38906 (11)	0.19620 (6)	0.0306 (4)
C8	1.0081 (3)	0.34974 (11)	0.23220 (6)	0.0363 (5)
H8	1.0422	0.3722	0.2605	0.044*
C9	1.0334 (3)	0.27829 (11)	0.22679 (7)	0.0401 (5)
H9	1.0844	0.2516	0.2515	0.048*
C10	0.9851 (3)	0.24487 (12)	0.18556 (7)	0.0402 (5)
H10	1.0039	0.1957	0.1819	0.048*
C11	0.9089 (3)	0.28411 (11)	0.14960 (7)	0.0364 (5)
H11	0.8759	0.2611	0.1214	0.044*
C12	0.8803 (3)	0.35598 (10)	0.15409 (6)	0.0312 (4)
C13	0.5556 (3)	0.41772 (11)	0.09236 (6)	0.0339 (5)
H13	0.5437	0.3888	0.0633	0.041*
C14	0.4367 (3)	0.39131 (12)	0.13116 (7)	0.0398 (5)
C15	0.3431 (3)	0.44517 (13)	0.14891 (7)	0.0450 (6)
H15	0.2677	0.4422	0.1755	0.054*
C16	0.3726 (3)	0.50819 (13)	0.12209 (7)	0.0426 (5)
C17	0.3022 (3)	0.57576 (14)	0.12600 (9)	0.0520 (6)
H17	0.2229	0.5873	0.1507	0.062*
C18	0.3497 (3)	0.62550 (15)	0.09335 (9)	0.0579 (7)
H18	0.3032	0.6719	0.0959	0.069*
C19	0.4644 (3)	0.60938 (13)	0.05667 (8)	0.0510 (6)
H19	0.4931	0.6444	0.0342	0.061*
C20	0.5374 (3)	0.54217 (12)	0.05272 (7)	0.0425 (5)
H20	0.6170	0.5311	0.0280	0.051*
C21	0.4918 (3)	0.49199 (11)	0.08540 (7)	0.0361 (5)
C22	0.4270 (3)	0.31583 (12)	0.14542 (7)	0.0498 (6)
H22A	0.3819	0.2876	0.1193	0.075*
H22B	0.3462	0.3110	0.1722	0.075*
H22C	0.5463	0.2993	0.1542	0.075*
C23	0.9444 (3)	0.43149 (11)	0.05995 (6)	0.0356 (5)
H23A	0.8986	0.4692	0.0392	0.043*
H23B	1.0663	0.4449	0.0699	0.043*
C24	0.9537 (3)	0.36211 (12)	0.03241 (7)	0.0468 (6)
H24A	0.9976	0.3247	0.0536	0.056*
H24B	0.8312	0.3491	0.0228	0.056*
C25	1.0688 (4)	0.36308 (13)	−0.00973 (8)	0.0585 (7)
H25A	1.1902	0.3784	−0.0006	0.070*
H25B	1.0210	0.3983	−0.0320	0.070*

C26	1.0816 (4)	0.29247 (13)	−0.03404 (8)	0.0625 (7)
H26A	1.1471	0.2979	−0.0634	0.094*
H26B	0.9612	0.2747	−0.0406	0.094*
H26C	1.1447	0.2590	−0.0139	0.094*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Si1	0.0326 (3)	0.0299 (3)	0.0273 (3)	−0.0030 (2)	0.0000 (2)	−0.0030 (2)
C1	0.0260 (10)	0.0348 (11)	0.0319 (9)	−0.0018 (8)	0.0007 (8)	−0.0039 (8)
C2	0.0360 (11)	0.0341 (12)	0.0367 (10)	0.0027 (9)	−0.0051 (9)	−0.0040 (9)
C3	0.0390 (12)	0.0347 (12)	0.0516 (13)	0.0048 (10)	−0.0053 (10)	−0.0128 (10)
C4	0.0395 (13)	0.0438 (14)	0.0429 (11)	0.0043 (10)	−0.0079 (9)	−0.0177 (10)
C5	0.0347 (12)	0.0444 (13)	0.0319 (10)	0.0002 (10)	−0.0025 (8)	−0.0076 (9)
C6	0.0250 (10)	0.0340 (11)	0.0303 (9)	−0.0013 (8)	0.0032 (8)	−0.0042 (8)
C7	0.0253 (10)	0.0369 (12)	0.0297 (9)	−0.0035 (8)	0.0049 (8)	0.0019 (8)
C8	0.0378 (12)	0.0413 (13)	0.0297 (10)	−0.0023 (10)	0.0011 (8)	0.0010 (9)
C9	0.0429 (13)	0.0394 (13)	0.0381 (11)	−0.0019 (10)	0.0005 (9)	0.0110 (9)
C10	0.0435 (13)	0.0328 (12)	0.0443 (11)	−0.0045 (10)	0.0042 (10)	0.0072 (9)
C11	0.0417 (12)	0.0347 (12)	0.0328 (10)	−0.0063 (10)	0.0009 (9)	−0.0007 (9)
C12	0.0312 (10)	0.0332 (11)	0.0292 (9)	−0.0053 (9)	0.0010 (8)	−0.0008 (8)
C13	0.0337 (11)	0.0389 (13)	0.0289 (9)	−0.0053 (9)	0.0006 (8)	−0.0060 (8)
C14	0.0331 (12)	0.0532 (15)	0.0330 (10)	−0.0131 (10)	−0.0005 (9)	−0.0085 (10)
C15	0.0321 (12)	0.0651 (17)	0.0377 (11)	−0.0076 (11)	0.0023 (9)	−0.0134 (11)
C16	0.0283 (11)	0.0563 (16)	0.0433 (12)	0.0005 (10)	−0.0070 (9)	−0.0152 (11)
C17	0.0349 (13)	0.0624 (17)	0.0587 (14)	0.0091 (12)	−0.0070 (11)	−0.0187 (13)
C18	0.0480 (15)	0.0590 (18)	0.0667 (16)	0.0178 (13)	−0.0199 (13)	−0.0181 (14)
C19	0.0517 (15)	0.0484 (15)	0.0530 (14)	0.0066 (12)	−0.0206 (11)	−0.0010 (12)
C20	0.0424 (13)	0.0475 (14)	0.0378 (11)	0.0022 (11)	−0.0115 (9)	−0.0048 (10)
C21	0.0303 (11)	0.0433 (13)	0.0346 (10)	−0.0007 (9)	−0.0115 (8)	−0.0083 (9)
C22	0.0504 (15)	0.0581 (16)	0.0407 (11)	−0.0217 (12)	0.0057 (10)	−0.0055 (11)
C23	0.0357 (11)	0.0363 (12)	0.0347 (10)	0.0014 (9)	0.0053 (8)	−0.0013 (9)
C24	0.0470 (13)	0.0502 (15)	0.0431 (12)	−0.0055 (11)	0.0074 (10)	−0.0081 (10)
C25	0.0693 (18)	0.0516 (16)	0.0545 (14)	0.0009 (13)	0.0223 (13)	−0.0068 (12)
C26	0.0764 (19)	0.0528 (16)	0.0582 (15)	0.0133 (14)	0.0165 (14)	−0.0154 (13)

Geometric parameters (Å, º)

Si1—C1	1.8678 (19)	C14—C22	1.491 (3)
Si1—C12	1.874 (2)	C15—H15	0.9500
Si1—C13	1.909 (2)	C15—C16	1.438 (3)
Si1—C23	1.8680 (19)	C16—C17	1.390 (3)
C1—C2	1.386 (3)	C16—C21	1.413 (3)
C1—C6	1.411 (3)	C17—H17	0.9500
C2—H2	0.9500	C17—C18	1.375 (3)
C2—C3	1.387 (3)	C18—H18	0.9500
C3—H3	0.9500	C18—C19	1.391 (3)
C3—C4	1.389 (3)	C19—H19	0.9500

C4—H4	0.9500	C19—C20	1.392 (3)
C4—C5	1.379 (3)	C20—H20	0.9500
C5—H5	0.9500	C20—C21	1.378 (3)
C5—C6	1.398 (2)	C22—H22A	0.9800
C6—C7	1.484 (3)	C22—H22B	0.9800
C7—C8	1.393 (3)	C22—H22C	0.9800
C7—C12	1.414 (2)	C23—H23A	0.9900
C8—H8	0.9500	C23—H23B	0.9900
C8—C9	1.377 (3)	C23—C24	1.536 (3)
C9—H9	0.9500	C24—H24A	0.9900
C9—C10	1.388 (3)	C24—H24B	0.9900
C10—H10	0.9500	C24—C25	1.483 (3)
C10—C11	1.393 (3)	C25—H25A	0.9900
C11—H11	0.9500	C25—H25B	0.9900
C11—C12	1.386 (3)	C25—C26	1.512 (3)
C13—H13	1.0000	C26—H26A	0.9800
C13—C14	1.510 (3)	C26—H26B	0.9800
C13—C21	1.501 (3)	C26—H26C	0.9800
C14—C15	1.339 (3)		

C1—Si1—C12	91.72 (9)	C14—C15—H15	124.7
C1—Si1—C13	112.64 (8)	C14—C15—C16	110.56 (19)
C1—Si1—C23	114.88 (9)	C16—C15—H15	124.7
C12—Si1—C13	117.07 (9)	C17—C16—C15	131.7 (2)
C23—Si1—C12	111.33 (9)	C17—C16—C21	120.0 (2)
C23—Si1—C13	108.62 (9)	C21—C16—C15	108.3 (2)
C2—C1—Si1	131.75 (15)	C16—C17—H17	120.7
C2—C1—C6	119.02 (17)	C18—C17—C16	118.7 (2)
C6—C1—Si1	109.08 (14)	C18—C17—H17	120.7
C1—C2—H2	119.7	C17—C18—H18	119.3
C1—C2—C3	120.58 (19)	C17—C18—C19	121.5 (2)
C3—C2—H2	119.7	C19—C18—H18	119.3
C2—C3—H3	120.0	C18—C19—H19	119.8
C2—C3—C4	119.9 (2)	C18—C19—C20	120.4 (2)
C4—C3—H3	120.0	C20—C19—H19	119.8
C3—C4—H4	119.6	C19—C20—H20	120.6
C5—C4—C3	120.81 (19)	C21—C20—C19	118.7 (2)
C5—C4—H4	119.6	C21—C20—H20	120.6
C4—C5—H5	120.3	C16—C21—C13	107.86 (18)
C4—C5—C6	119.42 (19)	C20—C21—C13	131.28 (19)
C6—C5—H5	120.3	C20—C21—C16	120.8 (2)
C1—C6—C7	115.15 (16)	C14—C22—H22A	109.5
C5—C6—C1	120.24 (19)	C14—C22—H22B	109.5
C5—C6—C7	124.57 (18)	C14—C22—H22C	109.5
C8—C7—C6	124.41 (17)	H22A—C22—H22B	109.5
C8—C7—C12	120.37 (19)	H22A—C22—H22C	109.5
C12—C7—C6	115.17 (17)	H22B—C22—H22C	109.5
C7—C8—H8	120.0	Si1—C23—H23A	109.1

C9—C8—C7	119.99 (19)	Si1—C23—H23B	109.1
C9—C8—H8	120.0	H23A—C23—H23B	107.8
C8—C9—H9	119.7	C24—C23—Si1	112.61 (14)
C8—C9—C10	120.60 (19)	C24—C23—H23A	109.1
C10—C9—H9	119.7	C24—C23—H23B	109.1
C9—C10—H10	120.3	C23—C24—H24A	108.4
C9—C10—C11	119.4 (2)	C23—C24—H24B	108.4
C11—C10—H10	120.3	H24A—C24—H24B	107.4
C10—C11—H11	119.3	C25—C24—C23	115.71 (19)
C12—C11—C10	121.36 (19)	C25—C24—H24A	108.4
C12—C11—H11	119.3	C25—C24—H24B	108.4
C7—C12—Si1	108.79 (14)	C24—C25—H25A	108.8
C11—C12—Si1	132.81 (14)	C24—C25—H25B	108.8
C11—C12—C7	118.22 (18)	C24—C25—C26	113.6 (2)
Si1—C13—H13	112.1	H25A—C25—H25B	107.7
C14—C13—Si1	111.22 (13)	C26—C25—H25A	108.8
C14—C13—H13	112.1	C26—C25—H25B	108.8
C21—C13—Si1	105.95 (13)	C25—C26—H26A	109.5
C21—C13—H13	112.1	C25—C26—H26B	109.5
C21—C13—C14	102.78 (17)	C25—C26—H26C	109.5
C15—C14—C13	109.6 (2)	H26A—C26—H26B	109.5
C15—C14—C22	127.1 (2)	H26A—C26—H26C	109.5
C22—C14—C13	123.30 (19)	H26B—C26—H26C	109.5

Si1—C1—C2—C3	−173.53 (16)	C12—Si1—C1—C2	178.22 (19)
Si1—C1—C6—C5	174.92 (14)	C12—Si1—C1—C6	2.78 (14)
Si1—C1—C6—C7	−2.8 (2)	C12—Si1—C23—C24	60.18 (17)
Si1—C13—C14—C15	103.56 (18)	C12—C7—C8—C9	0.3 (3)
Si1—C13—C14—C22	−77.7 (2)	C13—Si1—C1—C2	−61.4 (2)
Si1—C13—C21—C16	−107.51 (15)	C13—Si1—C1—C6	123.17 (13)
Si1—C13—C21—C20	68.8 (2)	C13—Si1—C12—C7	−118.75 (13)
Si1—C23—C24—C25	−179.64 (18)	C13—Si1—C12—C11	66.4 (2)
C1—Si1—C12—C7	−2.15 (14)	C13—Si1—C23—C24	−70.15 (17)
C1—Si1—C12—C11	−177.0 (2)	C13—C14—C15—C16	6.1 (2)
C1—Si1—C23—C24	162.69 (14)	C14—C13—C21—C16	9.3 (2)
C1—C2—C3—C4	−1.1 (3)	C14—C13—C21—C20	−174.4 (2)
C1—C6—C7—C8	178.61 (17)	C14—C15—C16—C17	177.9 (2)
C1—C6—C7—C12	1.2 (2)	C14—C15—C16—C21	0.1 (2)
C2—C1—C6—C5	−1.2 (3)	C15—C16—C17—C18	−176.9 (2)
C2—C1—C6—C7	−178.87 (16)	C15—C16—C21—C13	−6.3 (2)
C2—C3—C4—C5	0.3 (3)	C15—C16—C21—C20	176.95 (17)
C3—C4—C5—C6	0.1 (3)	C16—C17—C18—C19	0.6 (3)
C4—C5—C6—C1	0.4 (3)	C17—C16—C21—C13	175.67 (18)
C4—C5—C6—C7	177.83 (18)	C17—C16—C21—C20	−1.1 (3)
C5—C6—C7—C8	1.0 (3)	C17—C18—C19—C20	−1.4 (3)
C5—C6—C7—C12	−176.39 (18)	C18—C19—C20—C21	0.9 (3)
C6—C1—C2—C3	1.5 (3)	C19—C20—C21—C13	−175.58 (19)
C6—C7—C8—C9	−177.02 (18)	C19—C20—C21—C16	0.4 (3)

C6—C7—C12—Si1	1.0 (2)	C21—C13—C14—C15	−9.4 (2)
C6—C7—C12—C11	176.75 (17)	C21—C13—C14—C22	169.30 (18)
C7—C8—C9—C10	0.4 (3)	C21—C16—C17—C18	0.6 (3)
C8—C7—C12—Si1	−176.51 (14)	C22—C14—C15—C16	−172.57 (19)
C8—C7—C12—C11	−0.8 (3)	C23—Si1—C1—C2	63.7 (2)
C8—C9—C10—C11	−0.6 (3)	C23—Si1—C1—C6	−111.74 (14)
C9—C10—C11—C12	0.0 (3)	C23—Si1—C12—C7	115.47 (14)
C10—C11—C12—Si1	175.10 (16)	C23—Si1—C12—C11	−59.4 (2)
C10—C11—C12—C7	0.6 (3)	C23—C24—C25—C26	176.8 (2)

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C16–C21 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···*Cg*1	0.95	2.78	3.446 (3)	128