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# 1,1,3,3-Tetra-tert-butyl-2,2-diisopropyl-4,4-diphenylcyclotetrasilane

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Key indicators: single-crystal X-ray study; T = 173 K; mean  $\sigma$ (C–C) = 0.004 Å; R factor = 0.048; wR factor = 0.095; data-to-parameter ratio = 16.1.

The molecule in the structure of the title compound,  $C_{34}H_{60}Si_4$ , lies on a twofold rotation axis that passes through the two Si atoms, resulting in a planar cyclotetrasilane ring. The dihedral angle between the cyclotetrasilane ring and the phenyl ring is  $68.20(5)^\circ$ . The Si-Si bonds [2.4404(8) and 2.4576 (8) Å] are longer than a standard Si–Si bond (2.34 Å) and the C-Si-C bond angle [97.07 (14)°] of the phenylsubstituted Si atom is smaller than the tetrahedral bond angle (109.5°). These long bonds and small bond angle are favorable for reducing the steric hindrance among the bulky substituents.

### **Related literature**

For background to and applications of phenyl-substituted oligosilanes, see: Hinch & Krc (1957); Matsumoto & Tanaka (2008). For a related structure of a cyclotetrasilane without phenyl groups, see: Kyushin et al. (1995).



### **Experimental**

#### Crystal data

a	TT <b>A 1 -</b> 1 <b>-</b>
$C_{34}H_{60}S_{14}$	V = 34/4.0 (4) A <sup>3</sup>
$M_r = 581.18$	Z = 4
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
a = 11.9477 (9)  Å	$\mu = 0.19 \text{ mm}^{-1}$
b = 17.6585 (12)  Å	T = 173  K
c = 17.0422 (13) Å	$0.50 \times 0.40 \times 0.20$
$\beta = 104.9394 \ (8)^{\circ}$	

### Data collection

Rigaku R-AXIS IV imaging plate diffractometer Absorption correction: multi-scan (REQAB; Jacobson, 1998)  $T_{\min} = 0.910, \ T_{\max} = 0.963$ 

#### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.048$  $wR(F^2) = 0.095$ S = 1.242917 reflections

8534 measured reflections 2917 independent reflections 2899 reflections with  $I > 2\sigma(I)$  $R_{\rm int} = 0.025$ 

mm

181 parameters H-atom parameters constrained  $\Delta \rho_{\rm max} = 0.24 \text{ e } \text{\AA}^{-3}$  $\Delta \rho_{\rm min} = -0.20$  e Å<sup>-3</sup>

Data collection: CrystalClear (Rigaku, 2003); cell refinement: CrystalClear; data reduction: CrystalClear; program(s) used to solve structure: SIR2004 (Burla et al., 2005); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 2012); software used to prepare material for publication: SHELXL97 and Yadokari-XG 2009 (Kabuto et al., 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5224).

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# supporting information

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# 1,1,3,3-Tetra-tert-butyl-2,2-diisopropyl-4,4-diphenylcyclotetrasilane

# Takayoshi Kuribara and Soichiro Kyushin

## S1. Comment

Birefringent materials have a wide range of optical applications. Single crystals of calcium carbonate and barium borate have been well known as inorganic birefringent materials. Organic single crystals such as urea have also been known to show birefringence. Since birefringence is related to crystal structures, studies on molecular structures and packing in a crystal are important. In 1957, birefringence of tetrakis(4-phenylphenyl)silane was reported (Hinch & Krc, 1957). Recently, birefringence of single crystals of phenyl-substituted linear oligosilanes and their application to polarizers have been reported (Matsumoto & Tanaka, 2008). From these results, crystals of phenyl-substituted silicon compounds seem interesting as potential optical materials. We report herein the synthesis and X-ray crystal analysis of a phenyl-substituted cyclotetrasilane.

The coupling of 1,3-dibromo-1,1,3,3-tetra-*tert*-butyl-2,2-diphenyltrisilane and dichlorodiisopropylsilane with lithium in tetrahydrofuran (THF) gave 1,1,3,3-tetra-*tert*-butyl-2,2-diisopropyl-4,4-diphenylcyclotetrasilane (1) in 21% yield (Fig. 1). The molecular structure of **1** is shown in Fig. 2. Compound **1** has the crystallographic *C*2 symmetry, and therefore the cyclotetrasilane ring has a completely planar structure. The silicon–silicon bonds [2.4404 (8) and 2.4576 (8) Å] are longer than the standard silicon–silicon bond (2.34 Å). The C1–Si1–C1<sup>i</sup> bond angle [97.07 (14)°] is smaller than the tetrahedral bond angle (109.5°), while the C7–Si2–C11 [111.39 (10)°] and C15–Si3–C15<sup>i</sup> [106.97 (15)°] bond angles are within normal values. The long silicon–silicon bonds and the small carbon–silicon–carbon bond angle are favorable for reducing the steric hindrance among bulky substituents.

Packing diagram of 1 is shown in Fig. 3. Four molecules are present in a unit cell. All cyclotetrasilane rings are oriented toward the same direction with the line through the Si1 and Si3 atoms parallel to the *b* axis. There is no intermolecular  $\pi$ - $\pi$  interaction among phenyl groups.

## **S2.** Experimental

A mixture of 1,3-dibromo-1,1,3,3-tetra-*tert*-butyl-2,2-diphenyltrisilane (5.00 g, 7.98 mmol), dichlorodiisopropylsilane (2.24 g, 12.1 mmol) and lithium (0.28 g, 40 mmol) in THF (50 ml) was stirred at room temperature for 1 day. The solvent was removed under reduced pressure. The residue was dissolved in hexane and passed through a short column of silica gel. After the silica gel was washed with hexane, the eluent was changed to diethyl ether. The diethyl ether eluate was evaporated. Recrystallization of the residue from methanol–THF (*ca* 1:1) gave **1** (0.956 g, 21%) as colorless crystals. Single crystals were obtained from methanol–THF (*ca* 1:1) by slow evaporation.

M.p.: 210–211 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  1.21 (s, 36H), 1.46 (d, 12H, J = 7.4 Hz), 1.94 (sept, 2H, J = 7.4 Hz), 7.14–7.18 (m, 6H), 7.68–7.70 (m, 4H). <sup>13</sup>C NMR (76 MHz, CDCl<sub>3</sub>):  $\delta$  17.5, 24.7, 25.4, 32.8, 127.1, 127.4, 138.6, 142.1. <sup>29</sup>Si NMR (119 MHz, CDCl<sub>3</sub>):  $\delta$  -6.2, 14.0, 20.4. IR (KBr): 3050, 2950, 2920, 2850, 1470, 1420, 1390, 1360, 810, 730, 700 cm<sup>-1</sup>. MS (EI, 70 eV): m/z 580 ( $M^+$ , 17), 360 (100).

**S3. Refinement** 

All hydrogen atoms were generated at calculated positions and refined as riding atoms, with C—H = 0.95 (phenyl), 0.98 (methyl) or 1.00 (methine) Å, and with  $U_{iso}(H) = 1.2U_{eq}(phenyl C)$ ,  $1.5U_{eq}(methyl C)$  or  $1.2U_{eq}(methine C)$ .



**Figure 1** Synthesis of 1.





The molecular structure of 1, showing 50% probability displacement ellipsoids. [Symmetry code: (i) -x, y, -z + 3/2.]



F(000) = 1280

 $\theta = 1.2 - 28.3^{\circ}$ 

 $\mu = 0.19 \text{ mm}^{-1}$ 

Prism, colourless

 $0.50 \times 0.40 \times 0.20 \text{ mm}$ 

T = 173 K

 $D_{\rm x} = 1.111 \text{ Mg m}^{-3}$ 

Melting point = 483–484 K

Mo *K* $\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 7676 reflections

## Figure 3

Packing diagram of 1, showing 50% probability displacement ellipsoids.

1,1,3,3-Tetra-tert-butyl-2,2-diisopropyl-4,4-diphenylcyclotetrasilane

Crystal data

C<sub>34</sub>H<sub>60</sub>Si<sub>4</sub>  $M_r = 581.18$ Monoclinic, C2/c Hall symbol: -C 2yc a = 11.9477 (9) Å b = 17.6585 (12) Å c = 17.0422 (13) Å  $\beta = 104.9394$  (8)° V = 3474.0 (4) Å<sup>3</sup> Z = 4

## Data collection

Rigaku R-AXISIV imaging plate	8534 measured reflections
diffractometer	2917 independent reflections
Radiation source: rotating anode	2899 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{\rm int} = 0.025$
Detector resolution: 10.00 pixels mm <sup>-1</sup>	$\theta_{\text{max}} = 25.0^{\circ}, \ \theta_{\text{min}} = 2.1^{\circ}$
$\omega$ scans	$h = -14 \rightarrow 14$
Absorption correction: multi-scan	$k = -18 \rightarrow 20$
(REQAB; Jacobson, 1998)	$l = -20 \rightarrow 20$
$T_{\min} = 0.910, \ T_{\max} = 0.963$	

Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier
Least-squares matrix: full	map
$R[F^2 > 2\sigma(F^2)] = 0.048$	Hydrogen site location: inferred from
$wR(F^2) = 0.095$	neighbouring sites
S = 1.24	H-atom parameters constrained
2917 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0127P)^2 + 7.2943P]$
181 parameters	where $P = (F_{o}^{2} + 2F_{c}^{2})/3$
0 restraints	$(\Delta/\sigma)_{\rm max} = 0.001$
Primary atom site location: structure-invariant	$\Delta  ho_{ m max} = 0.24 \  m e \ { m \AA}^{-3}$
direct methods	$\Delta \rho_{\rm min} = -0.20 \text{ e } \text{\AA}^{-3}$

## Special details

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

**Refinement**. Refinement of  $F^2$  against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on  $F^2$ , conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative  $F^2$ . The threshold expression of  $F^2 > 2\sigma(F^2)$  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  $(A^2)$ 

	x	У	Ζ	$U_{ m iso}$ */ $U_{ m eq}$
Si1	0.0000	0.32355 (5)	0.7500	0.01350 (19)
Si2	0.09403 (5)	0.22594 (3)	0.68813 (3)	0.01324 (15)
Si3	0.0000	0.12695 (5)	0.7500	0.01475 (19)
C1	-0.07934 (19)	0.39557 (13)	0.67052 (13)	0.0179 (5)
C2	-0.0078 (2)	0.45046 (14)	0.64962 (15)	0.0269 (6)
H1	0.0725	0.4498	0.6763	0.032*
C3	-0.0487 (2)	0.50564 (15)	0.59179 (17)	0.0330 (6)
H2	0.0031	0.5416	0.5791	0.040*
C4	-0.1657 (2)	0.50818 (15)	0.55245 (15)	0.0307 (6)
Н3	-0.1947	0.5455	0.5122	0.037*
C5	-0.2392 (2)	0.45599 (15)	0.57252 (16)	0.0313 (6)
H4	-0.3196	0.4576	0.5462	0.038*
C6	-0.1968 (2)	0.40088 (14)	0.63102 (15)	0.0262 (5)
Н5	-0.2494	0.3659	0.6444	0.031*
C7	0.03683 (19)	0.22973 (13)	0.56985 (13)	0.0191 (5)
C8	-0.0961 (2)	0.23931 (15)	0.54491 (14)	0.0259 (5)
H6	-0.1243	0.2356	0.4857	0.039*
H7	-0.1165	0.2890	0.5629	0.039*
H8	-0.1318	0.1994	0.5703	0.039*
C9	0.0639 (2)	0.15671 (16)	0.52878 (15)	0.0331 (6)
H9	0.0373	0.1622	0.4697	0.050*
H10	0.0240	0.1139	0.5462	0.050*
H11	0.1476	0.1476	0.5444	0.050*
C10	0.0887 (2)	0.29704 (15)	0.53389 (15)	0.0307 (6)
H12	0.1716	0.2884	0.5404	0.046*

# supporting information

H13	0.0779	0.3436	0.5623	0.046*
H14	0.0497	0.3020	0.4760	0.046*
C11	0.26218 (18)	0.23095 (14)	0.72206 (14)	0.0204 (5)
C12	0.3017 (2)	0.21501 (14)	0.81400 (14)	0.0253 (5)
H15	0.2866	0.1618	0.8242	0.038*
H16	0.2587	0.2477	0.8425	0.038*
H17	0.3848	0.2254	0.8338	0.038*
C13	0.3052 (2)	0.31047 (16)	0.70706 (17)	0.0347 (6)
H18	0.3880	0.3148	0.7340	0.052*
H19	0.2621	0.3486	0.7291	0.052*
H20	0.2929	0.3186	0.6486	0.052*
C14	0.3208 (2)	0.17278 (18)	0.67839 (17)	0.0379 (7)
H21	0.3064	0.1865	0.6209	0.057*
H22	0.2889	0.1223	0.6830	0.057*
H23	0.4044	0.1724	0.7034	0.057*
C15	0.0992 (2)	0.06194 (13)	0.82929 (15)	0.0241 (5)
H24	0.1364	0.0948	0.8766	0.029*
C16	0.0306 (3)	0.00034 (16)	0.86183 (17)	0.0387 (7)
H25	0.0068	-0.0395	0.8209	0.058*
H26	-0.0382	0.0231	0.8734	0.058*
H27	0.0798	-0.0215	0.9118	0.058*
C17	0.1985 (2)	0.02186 (16)	0.80303 (19)	0.0387 (7)
H28	0.2509	-0.0020	0.8504	0.058*
H29	0.2414	0.0591	0.7796	0.058*
H30	0.1662	-0.0170	0.7624	0.058*

Atomic displacement parameters  $(\mathring{A}^2)$ 

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Si1	0.0139 (4)	0.0121 (4)	0.0151 (4)	0.000	0.0047 (3)	0.000
Si2	0.0127 (3)	0.0149 (3)	0.0133 (3)	-0.0005 (2)	0.0055 (2)	-0.0008(2)
Si3	0.0165 (4)	0.0118 (4)	0.0169 (4)	0.000	0.0061 (4)	0.000
C1	0.0219 (11)	0.0167 (12)	0.0162 (11)	0.0022 (9)	0.0072 (10)	-0.0007 (9)
C2	0.0260 (12)	0.0273 (14)	0.0279 (14)	0.0013 (10)	0.0081 (11)	0.0074 (10)
C3	0.0415 (15)	0.0258 (14)	0.0367 (15)	-0.0008 (11)	0.0189 (13)	0.0106 (11)
C4	0.0465 (16)	0.0230 (14)	0.0230 (13)	0.0109 (11)	0.0101 (12)	0.0100 (10)
C5	0.0273 (13)	0.0336 (15)	0.0298 (14)	0.0095 (11)	0.0012 (12)	0.0062 (11)
C6	0.0227 (12)	0.0271 (14)	0.0276 (13)	0.0002 (10)	0.0044 (11)	0.0060 (10)
C7	0.0236 (12)	0.0209 (12)	0.0143 (11)	0.0012 (9)	0.0078 (10)	-0.0023 (9)
C8	0.0242 (12)	0.0346 (15)	0.0179 (12)	0.0005 (10)	0.0033 (10)	0.0002 (10)
C9	0.0410 (15)	0.0343 (16)	0.0232 (13)	0.0076 (12)	0.0070 (12)	-0.0095 (11)
C10	0.0375 (14)	0.0359 (16)	0.0219 (13)	-0.0041 (11)	0.0135 (12)	0.0068 (11)
C11	0.0144 (10)	0.0271 (13)	0.0210 (12)	-0.0006 (9)	0.0068 (10)	-0.0040 (9)
C12	0.0192 (11)	0.0299 (14)	0.0240 (13)	0.0013 (10)	0.0005 (10)	-0.0042 (10)
C13	0.0288 (13)	0.0431 (17)	0.0327 (15)	-0.0176 (12)	0.0086 (12)	0.0011 (12)
C14	0.0210 (13)	0.058 (2)	0.0355 (16)	0.0079 (12)	0.0092 (12)	-0.0157 (14)
C15	0.0289 (12)	0.0170 (12)	0.0243 (13)	0.0059 (10)	0.0029 (11)	0.0024 (9)
C16	0.0570 (18)	0.0254 (15)	0.0335 (15)	-0.0005 (13)	0.0113 (14)	0.0090 (12)

# supporting information

C17	0.0319 (14)	0.0246 (15)	0.058 (2)	0.0119 (11)	0.0084 (14)	0.0004 (13)	
Geome	Geometric parameters (Å, °)						
Sil—C	21	1.921 (	2)	С9—Н11	0	.9800	
Si1—S	i2	2.4404	(8)	C10—H12	C	.9800	
Si2—C	211	1.944 (	2)	C10—H13	C	.9800	
Si2—C	27	1.956 (	2)	C10—H14	C	.9800	
Si2—S	i3	2.4576	(8)	C11—C14	1	.539 (3)	
Si3—C	215	1.929 (	2)	C11—C13	1	.539 (3)	
C1—C	6	1.394 (	3)	C11—C12	1	.541 (3)	
C1—C	2	1.398 (	3)	C12—H15	C	.9800	
С2—С	3	1.382 (	3)	C12—H16	C	.9800	
С2—Н	1	0.9500		C12—H17	C	.9800	
С3—С	4	1.386 (	4)	C13—H18	C	.9800	
С3—Н	2	0.9500		C13—H19	C	.9800	
С4—С	5	1.376 (	4)	C13—H20	C	.9800	
С4—Н	3	0.9500		C14—H21	C	.9800	
С5—С	6	1.392 (	3)	C14—H22	C	.9800	
С5—Н	4	0.9500		C14—H23	C	.9800	
С6—Н	5	0.9500		C15—C17	1	.543 (3)	
С7—С	10	1.539 (	3)	C15—C16	1	.548 (3)	
С7—С	9	1.541 (	3)	C15—H24	1	.0000	
С7—С	8	1.544 (	3)	C16—H25	C	.9800	
С8—Н	6	0.9800		C16—H26	C	.9800	
С8—Н	7	0.9800		C16—H27	C	.9800	
С8—Н	8	0.9800		C17—H28	C	.9800	
С9—Н	9	0.9800		С17—Н29	C	.9800	
С9—Н	10	0.9800		С17—Н30	C	.9800	
C1 <sup>i</sup> —S	il—Cl	97.07 (	14)	H10—C9—H11	1	09.5	
C1 <sup>i</sup> —S	i1—Si2	125.03	(7)	С7—С10—Н12	1	09.5	
C1—Si	i1—Si2	111.19	(6)	С7—С10—Н13	1	09.5	
Si2 <sup>i</sup> —S	Si1—Si2	90.13 (	4)	H12—C10—H13	1	09.5	
C11—5	Si2—C7	111.39	(10)	С7—С10—Н14	1	09.5	
C11—5	Si2—Si1	113.26	(7)	H12—C10—H14	1	09.5	
C7—Si	2—Si1	110.10	(7)	H13—C10—H14	1	09.5	
C11—5	Si2—Si3	117.16	(8)	C14—C11—C13	1	08.4 (2)	
C7—Si	i2—Si3	112.93	(7)	C14—C11—C12	1	08.2 (2)	
Si1—S	i2—Si3	90.27 (	3)	C13—C11—C12	1	07.92 (19)	
C15 <sup>i</sup> —	Si3—C15	106.97	(15)	C14—C11—Si2	1	12.95 (16)	
C15 <sup>i</sup> —	Si3—Si2	112.89	(7)	C13—C11—Si2	1	10.84 (17)	
C15—5	Si3—Si2	117.23	(7)	C12—C11—Si2	1	08.42 (14)	
Si2 <sup>i</sup> —S	Si3—Si2	89.33 (	4)	С11—С12—Н15	1	09.5	
С6—С	1—C2	115.8 (	2)	С11—С12—Н16	1	09.5	
С6—С	1—Si1	129.59	(18)	Н15—С12—Н16	1	09.5	
С2—С	1—Sil	114.57	(17)	С11—С12—Н17	1	09.5	
С3—С	2—C1	122.9 (	2)	H15—C12—H17	1	09.5	

С3—С2—Н1	118.6	H16—C12—H17	109.5
C1—C2—H1	118.6	C11—C13—H18	109.5
C2—C3—C4	119.7 (2)	C11—C13—H19	109.5
С2—С3—Н2	120.2	H18—C13—H19	109.5
C4—C3—H2	120.2	C11—C13—H20	109.5
C5—C4—C3	119.1 (2)	H18—C13—H20	109.5
С5—С4—Н3	120.4	H19—C13—H20	109.5
C3—C4—H3	120.4	C11—C14—H21	109.5
C4—C5—C6	120.6 (2)	C11—C14—H22	109.5
C4—C5—H4	119.7	$H_{21} - C_{14} + H_{22}$	109.5
C6-C5-H4	119.7	$C_{11} - C_{14} - H_{23}$	109.5
$C_{5}$ $C_{6}$ $C_{1}$	121.9(2)	$H_{21}$ $-C_{14}$ $H_{23}$	109.5
C5 C6 H5	110.1	$H_{22} = C_{14} = H_{23}$	109.5
C1 C6 H5	119.1	1122 - C14 - 1123	109.3 107.4(2)
$C_{1} = C_{0} = 115$	117.1	C17 - C15 - C10	107.4(2)
C10 - C7 - C9	106.16(19) 107.2(2)	C1(-C15-S13)	110.08(18)
C10 - C7 - C8	107.3(2)	C10 - C15 - S15	112.50 (17)
	106.7 (2)	C1/C15H24	106.6
C10-C7-S12	111.55 (16)	С16—С15—Н24	106.6
C9—C7—S12	112.41 (16)	S13—C15—H24	106.6
C8—C7—Si2	110.42 (14)	C15—C16—H25	109.5
С7—С8—Н6	109.5	C15—C16—H26	109.5
С7—С8—Н7	109.5	H25—C16—H26	109.5
Н6—С8—Н7	109.5	C15—C16—H27	109.5
С7—С8—Н8	109.5	H25—C16—H27	109.5
Н6—С8—Н8	109.5	H26—C16—H27	109.5
Н7—С8—Н8	109.5	C15—C17—H28	109.5
С7—С9—Н9	109.5	С15—С17—Н29	109.5
С7—С9—Н10	109.5	H28—C17—H29	109.5
H9—C9—H10	109.5	С15—С17—Н30	109.5
C7—C9—H11	109.5	H28—C17—H30	109.5
H9—C9—H11	109.5	H29—C17—H30	109.5
$C1^{i}$ Si1 Si2 C11	-3.63(12)	$C_{3}-C_{4}-C_{5}-C_{6}$	-0.6(4)
C1 = Si1 = Si2 = C11	112 02 (11)	C4-C5-C6-C1	-0.9(4)
$Si2^{i}$ _Si1_Si2_C11	-110.02(11)	$C_{2}$ $C_{1}$ $C_{6}$ $C_{5}$	20(4)
$C1^{i}$ $S1^{i}$ $S1^{i}$ $S1^{i}$ $C7$	-120.08(11)	$C_2 = C_1 = C_0 = C_3$	-177.0(2)
$C_1 = S_{11} = S_{12} = C_7$	-12.9.06(11)	$C_{11} = C_{11} = C$	-51.24(10)
Sigi Sil Sig C7	13.43(11)	C11 - 512 - C7 - C10	51.24(19)
S12 - S11 - S12 - C/	114.03(8)	S11 - S12 - C7 - C10	73.27(10)
C1 - S11 - S12 - S13	110.29 (8)	S13 - S12 - C7 - C10	1/4.50 (14)
C1 - S11 - S12 - S13	-128.06 (7)	C11 - S12 - C/ - C9	/0.49 (19)
S12 <sup>i</sup> —S11—S12—S13	0.0	$S_{11} = S_{12} = C_{12} = C_{23}$	-163.01 (15)
$C11 - S12 - S13 - C15^{1}$	-124.05 (11)	S13—S12—C7—C9	-63.78 (18)
C7—Si2—Si3—C15 <sup>1</sup>	7.41 (11)	C11—Si2—C7—C8	-170.44 (16)
Si1—Si2—Si3—C15 <sup>i</sup>	119.45 (8)	Si1—Si2—C7—C8	-43.93 (18)
C11—Si2—Si3—C15	0.95 (12)	Si3—Si2—C7—C8	55.30 (18)
C7—Si2—Si3—C15	132.41 (11)	C7—Si2—C11—C14	-51.3 (2)
Si1—Si2—Si3—C15	-115.55 (9)	Si1—Si2—C11—C14	-176.05 (16)
C11—Si2—Si3—Si2 <sup>i</sup>	116.50 (8)	Si3—Si2—C11—C14	80.87 (19)

C7—Si2—Si3—Si2 <sup>i</sup>	-112.04 (8)	C7—Si2—C11—C13	70.59 (18)
Si1—Si2—Si3—Si2 <sup>i</sup>	0.0	Si1—Si2—C11—C13	-54.17 (17)
C1 <sup>i</sup> —Si1—C1—C6	-127.9 (2)	Si3—Si2—C11—C13	-157.25 (14)
Si2 <sup>i</sup> —Si1—C1—C6	-5.8 (3)	C7—Si2—C11—C12	-171.14 (15)
Si2—Si1—C1—C6	100.2 (2)	Si1—Si2—C11—C12	64.11 (17)
C1 <sup>i</sup> —Si1—C1—C2	52.17 (16)	Si3—Si2—C11—C12	-38.97 (18)
Si2 <sup>i</sup> —Si1—C1—C2	174.29 (14)	C15 <sup>i</sup> —Si3—C15—C17	74.54 (19)
Si2—Si1—C1—C2	-79.77 (18)	Si2 <sup>i</sup> —Si3—C15—C17	-155.06 (17)
C6—C1—C2—C3	-1.9 (4)	Si2—Si3—C15—C17	-53.4 (2)
Si1—C1—C2—C3	178.1 (2)	C15 <sup>i</sup> —Si3—C15—C16	-50.24 (16)
C1—C2—C3—C4	0.5 (4)	Si2 <sup>i</sup> —Si3—C15—C16	80.16 (18)
C2—C3—C4—C5	0.7 (4)	Si2—Si3—C15—C16	-178.14 (15)

Symmetry code: (i) -x, y, -z+3/2.