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Dodecaallylhexasilacyclohexane

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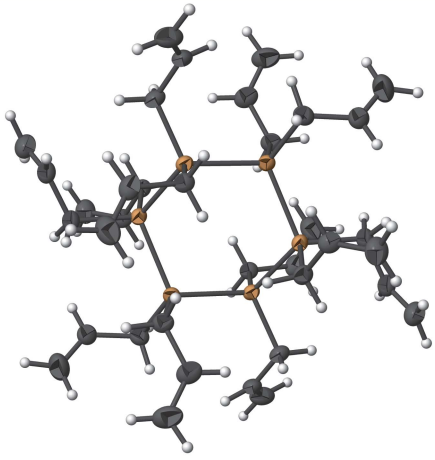
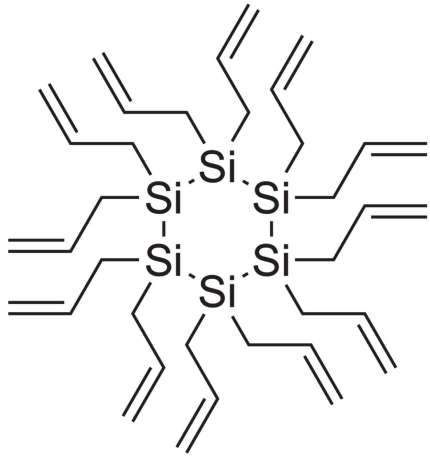
The molecule of the title compound, $C_{36}H_{60}Si_6$, exhibits point group symmetry C_i, with the centre of inversion located at the centre of the Si_6 ring. The Si_6 ring has a chair conformation. In the crystal, molecules are linked *via* C—H$\cdots\pi$(allyl) interactions.

3D view



Chemical scheme



Structure description

Hexasilacyclohexane derivatives, *i.e.* six-membered cyclic oligosilanes, are of interest from the viewpoint of their unique structures and properties. However, it is challenging to prepare such cyclic oligosilanes because of synthetic difficulties, low yields and long purification times. While a number of crystal structures for hexasilacyclohexane derivatives have been reported, those for derivatives with twelve identical carbon subsitituents are limited to dodecamethyl (Carrell & Donohue, 1972) and dodecaphenyl (M'hirsi & Brini, 1968; Dräger & Walter, 1981) as well as to a hexa(1,1-silole) derivative (Yamaguchi *et al.*, 1999). Herein, we describe the synthesis and structural characterization of dodecaallylhexasilacyclohexane by utilizing an effective synthesis method, *viz*. the reaction of $[pedeta{\cdot}SiH_2Cl]_2Si_6Cl_{14}$ (pedeta = *N*,*N*,*N*′,*N*′,*N*″-pentaethyldiethylenetriamine; Choi *et al.*, 2001) with allylmagnesium bromide.

The crystal structure comprises one molecule of the title compound per unit cell (Fig. 1). The molecule exhibits point group symmetry C_i, with the centre of inversion at the centre of the Si_6 ring. The latter has a chair conformation with typical bond lengths in the range of 2.3500 (6)–2.3598 (5) Å. The average value of the Si—Si bond lengths (2.354 Å) lies between those for the dodecamethyl (2.338 Å) and dodecaphenyl derivatives (2.394 Å). The Si—Si—Si angles are almost the same and range from 110.35 (2)–110.46 (2)°; the average Si—Si—Si angle (110.4°) is smaller than that of Si_6Me_{12} (111.9°) and of Si_6Ph_{12} (113.8°). In the crystal structure, molecules are linked by several C—H$\cdots\pi$(allyl) interactions into a three-dimensional network (Table 1, Fig. 2).

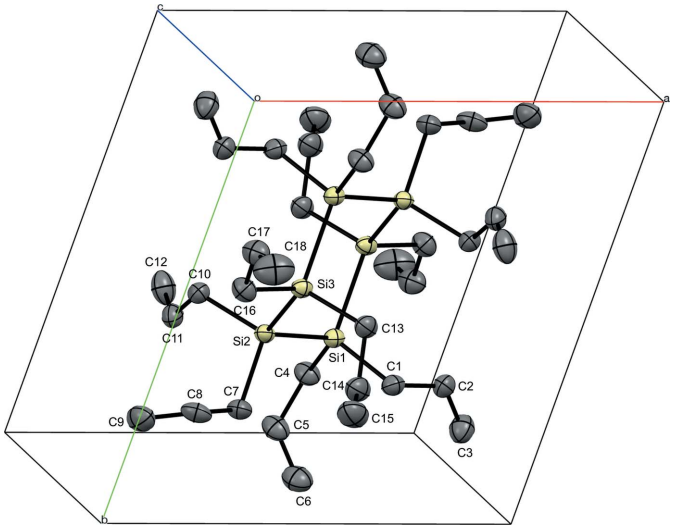


Figure 1
The molecular structure of the title compound, showing displacement ellipsoids at the 50% probability level. H atoms have been omitted for clarity. Unlabelled atoms are related by labelled atoms by the symmetry code ($-x+1, -y+1, -z+1$).

Synthesis and crystallization

To a THF solution of $[pedeta{\cdot}SiH_2Cl]_2Si_6Cl_{14}$ (1.20 g, 0.936 mmol) was slowly added a 1.0 *M* solution of allylmagnesium bromide in diethyl ether (15 ml, 15 mmol) at 293 K. After stirring for 48 h at 363 K, the mixture was treated with a saturated aqueous NH_4Cl solution and extracted with diethyl ether. The combined organic layer was dried over Na_2SO_4 and concentrated under vacuum. The crude material was then purified by column chromatography on silica gel (eluting with hexane) to give the title compound (275 mg, 0.416 mmol, 44%). Single crystals were obtained by recrystallization from a hexane solution.

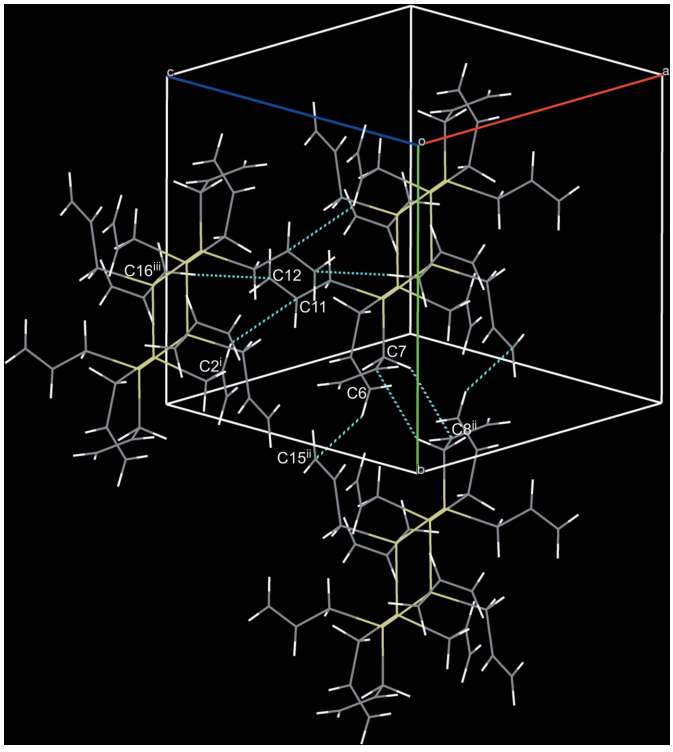


Figure 2
Parts of the crystal packing of the title compound, emphasizing intermolecular C—H$\cdots\pi$(allyl) interactions (light-blue dotted lines). [Symmetry codes: (i) $x-1, y, z$; (ii) $-x+1, -y+2, -z+1$; (iii) $-x, -y+1, -z+1$.]

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C2^{i}—H2$^{i}\cdots$C11	0.95	2.84	3.622 (3)	140
C7—H7$A\cdots$C8^{ii}	0.99	2.82	3.669 (2)	145
C6—H6$A\cdots$C15^{ii}	0.95	2.88	3.678 (4)	142
C16^{iii}—H16$^{iii}\cdots$C12	0.99	2.75	3.684 (3)	159

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+1, -y+2, -z+1$; (iii) $-x, -y+1, -z+1$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{36}H_{60}Si_6$
M_r	661.38
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	103
a, b, c (Å)	9.6036 (2), 10.8060 (3), 11.4686 (3)
α, β, γ (°)	108.617 (2), 100.558 (2), 109.4774 (12)
V (Å^3)	1005.90 (5)
Z	1
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.23
Crystal size (mm)	0.25 × 0.20 × 0.20
Data collection	
Diffractometer	Rigaku Saturn
Absorption correction	Multi-scan (*MULABS*; Blessing, 1995)
T_{min}, T_{max}	0.902, 0.953
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13675, 3630, 3398
R_{int}	0.035
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.600
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.032, 0.089, 1.04
No. of reflections	3630
No. of parameters	190
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.45, −0.18

Computer programs: *CrystalClear* (Rigaku, 1999), *HKL-2000* (Otwinowski & Minor, 1997), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2016* (Sheldrick, 2015*b*), *Yadokari-XG* (Wakita, 2001; Kabuto *et al.*, 2009), *Mercury* (Macrae *et al.*, 2008), *CrystalMaker* (Palmer, 2007) and *publCIF* (Westrip, 2010).

Refinement

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

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References

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Carrell, H. L. & Donohue, J. (1972). *Acta Cryst.* B**28**, 1566–1571.
Choi, S.-B., Kim, B.-K., Boudjouk, P. & Grier, D. G. (2001). *J. Am. Chem. Soc.* **123**, 8117–8118.
Dräger, M. & Walter, K. G. (1981). *Z. Anorg. Allg. Chem.* **479**, 65–74.
Kabuto, C., Akine, S., Nemoto, T. & Kwon, E. (2009). *J. Crystallogr. Soc. Japan*, **51**, 218–224.
Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
M'hirsi, M. & Brini, M. (1968). *Bull. Soc. Chim. Fr.* p. 1509.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Palmer, D. (2007). *CrystalMaker*. CrystalMaker, Bicester, England.
Rigaku (1999). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Wakita, K. (2001). *Yadokari-XG*. Software for Crystal Structure Analyses.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
Yamaguchi, S., Jin, R. & Tamao, K. (1999). *J. Am. Chem. Soc.* **121**, 2937–2938.

full crystallographic data

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Dodecaallylhexasilacyclohexane

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1,1,2,2,3,3,4,4,5,5,6,6-Dodecaallylhexasilinane

Crystal data

$C_{36}H_{60}Si_6$
M_r = 661.38
Triclinic, $P\overline{1}$
a = 9.6036 (2) Å
b = 10.8060 (3) Å
c = 11.4686 (3) Å
α = 108.617 (2)°
β = 100.558 (2)°
γ = 109.4774 (12)°
V = 1005.90 (5) Å^3
Z = 1
$F(000)$ = 360
D_x = 1.092 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71075 Å
Cell parameters from 13675 reflections
θ = 2.2–25.3°
μ = 0.23 mm^{-1}
T = 103 K
Prism, colorless
0.25 × 0.20 × 0.20 mm

Data collection

Rigaku Saturn diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 28.5714 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*MULABS*; Blessing, 1995)
T_{min} = 0.902, T_{max} = 0.953
13675 measured reflections
3630 independent reflections
3398 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 25.3°, θ_{min} = 2.2°
h = −11→11
k = −12→12
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.089
S = 1.04
3630 reflections
190 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0439P)^2 + 0.4743P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Si1	0.62028 (5)	0.70739 (4)	0.68222 (4)	0.02374 (12)
Si2	0.39667 (5)	0.66287 (4)	0.52192 (4)	0.02298 (12)
Si3	0.38195 (5)	0.51111 (4)	0.31623 (4)	0.02389 (12)
C1	0.79247 (18)	0.80929 (17)	0.63994 (16)	0.0298 (3)
H1	0.777913	0.756251	0.547308	0.036*
H1A	0.795241	0.904968	0.651480	0.036*
C2	0.94384 (19)	0.82874 (18)	0.72153 (16)	0.0328 (4)
H2	0.962604	0.744968	0.706635	0.039*
C3	1.0536 (2)	0.9493 (2)	0.81160 (18)	0.0437 (4)
H3	1.040539	1.036134	0.830237	0.052*
H3A	1.146668	0.950252	0.858559	0.052*
C4	0.6406 (2)	0.82817 (18)	0.85323 (15)	0.0340 (4)
H4	0.564939	0.771180	0.884893	0.041*
H4A	0.746680	0.858916	0.911725	0.041*
C5	0.6143 (2)	0.95884 (18)	0.86206 (16)	0.0385 (4)
H5	0.509679	0.948784	0.846449	0.046*
C6	0.7207 (2)	1.0850 (2)	0.88904 (19)	0.0476 (5)
H6	0.827075	1.100392	0.905397	0.057*
H6A	0.692275	1.161954	0.892422	0.057*
C7	0.40334 (19)	0.84318 (16)	0.52689 (16)	0.0321 (4)
H7	0.405292	0.901263	0.614148	0.038*
H7A	0.501467	0.895855	0.514069	0.038*
C8	0.2692 (2)	0.82944 (17)	0.42707 (17)	0.0369 (4)
H8	0.272856	0.804777	0.340775	0.044*
C9	0.1460 (2)	0.8484 (2)	0.4476 (2)	0.0471 (5)
H9	0.137296	0.873155	0.532377	0.057*
H9A	0.065728	0.837287	0.377657	0.057*
C10	0.20865 (18)	0.57289 (16)	0.55145 (15)	0.0283 (3)
H10	0.119715	0.562799	0.484119	0.034*
H10A	0.194912	0.475100	0.542961	0.034*
C11	0.20665 (19)	0.65531 (18)	0.68227 (17)	0.0346 (4)
H11	0.220179	0.751764	0.702115	0.041*
C12	0.1882 (2)	0.6082 (2)	0.77254 (18)	0.0476 (5)
H12	0.174187	0.512519	0.757449	0.057*
H12A	0.188669	0.669719	0.853299	0.057*
C13	0.55616 (19)	0.59051 (17)	0.26470 (16)	0.0321 (4)
H13	0.648570	0.589225	0.318371	0.039*
H13A	0.535167	0.527929	0.173060	0.039*
C14	0.5950 (2)	0.7412 (2)	0.2765 (2)	0.0416 (4)
H14	0.638415	0.815402	0.361902	0.050*
C15	0.5749 (3)	0.7797 (2)	0.1812 (2)	0.0544 (5)
H15	0.531764	0.709246	0.093991	0.065*
H15A	0.603140	0.878307	0.198303	0.065*
C16	0.2031 (2)	0.48798 (18)	0.19265 (16)	0.0345 (4)
H16	0.114083	0.466976	0.226362	0.041*

H16A	0.223758	0.579997	0.183665	0.041*
C17	0.1580 (2)	0.37190 (19)	0.06203 (17)	0.0397 (4)
H17	0.105052	0.275635	0.051906	0.048*
C18	0.1842 (3)	0.3903 (3)	−0.0389 (2)	0.0637 (6)
H18	0.236804	0.484745	−0.033199	0.076*
H18A	0.151028	0.309423	−0.118898	0.076*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Si1	0.0259 (2)	0.0202 (2)	0.0237 (2)	0.00853 (16)	0.00824 (16)	0.00849 (16)
Si2	0.0256 (2)	0.0194 (2)	0.0252 (2)	0.00936 (16)	0.00987 (17)	0.00997 (16)
Si3	0.0279 (2)	0.0223 (2)	0.0239 (2)	0.01044 (17)	0.01077 (17)	0.01121 (17)
C1	0.0302 (8)	0.0251 (8)	0.0317 (8)	0.0087 (6)	0.0105 (7)	0.0117 (6)
C2	0.0299 (8)	0.0325 (8)	0.0394 (9)	0.0129 (7)	0.0151 (7)	0.0169 (7)
C3	0.0344 (9)	0.0455 (11)	0.0412 (10)	0.0133 (8)	0.0100 (8)	0.0104 (8)
C4	0.0406 (9)	0.0321 (8)	0.0265 (8)	0.0171 (7)	0.0090 (7)	0.0078 (7)
C5	0.0460 (10)	0.0358 (9)	0.0295 (9)	0.0205 (8)	0.0081 (7)	0.0070 (7)
C6	0.0543 (12)	0.0375 (10)	0.0427 (11)	0.0194 (9)	0.0101 (9)	0.0093 (8)
C7	0.0360 (9)	0.0238 (8)	0.0388 (9)	0.0134 (7)	0.0128 (7)	0.0144 (7)
C8	0.0546 (11)	0.0264 (8)	0.0330 (9)	0.0196 (8)	0.0113 (8)	0.0150 (7)
C9	0.0438 (10)	0.0429 (10)	0.0576 (12)	0.0192 (9)	0.0082 (9)	0.0278 (9)
C10	0.0264 (8)	0.0276 (8)	0.0319 (8)	0.0105 (6)	0.0108 (6)	0.0135 (7)
C11	0.0293 (8)	0.0324 (9)	0.0398 (9)	0.0129 (7)	0.0155 (7)	0.0097 (7)
C12	0.0481 (11)	0.0658 (13)	0.0377 (10)	0.0340 (10)	0.0197 (9)	0.0182 (9)
C13	0.0365 (9)	0.0326 (8)	0.0359 (9)	0.0161 (7)	0.0196 (7)	0.0186 (7)
C14	0.0468 (10)	0.0387 (10)	0.0523 (11)	0.0202 (8)	0.0303 (9)	0.0242 (9)
C15	0.0679 (14)	0.0512 (12)	0.0698 (14)	0.0315 (11)	0.0393 (12)	0.0396 (11)
C16	0.0388 (9)	0.0373 (9)	0.0311 (9)	0.0195 (8)	0.0104 (7)	0.0156 (7)
C17	0.0420 (10)	0.0356 (9)	0.0348 (9)	0.0158 (8)	0.0038 (8)	0.0117 (8)
C18	0.0889 (18)	0.0539 (13)	0.0342 (11)	0.0196 (12)	0.0166 (11)	0.0138 (10)

Geometric parameters (Å, º)

Si1—C1	1.8980 (16)	C8—C9	1.315 (3)
Si1—C4	1.9089 (16)	C8—H8	0.9500
Si1—Si2	2.3500 (6)	C9—H9	0.9500
Si1—Si3^{i}	2.3598 (6)	C9—H9A	0.9500
Si2—C10	1.8931 (15)	C10—C11	1.488 (2)
Si2—C7	1.9100 (16)	C10—H10	0.9900
Si2—Si3	2.3511 (6)	C10—H10A	0.9900
Si3—C13	1.9009 (16)	C11—C12	1.306 (3)
Si3—C16	1.9015 (17)	C11—H11	0.9500
C1—C2	1.485 (2)	C12—H12	0.9500
C1—H1	0.9900	C12—H12A	0.9500
C1—H1A	0.9900	C13—C14	1.499 (2)
C2—C3	1.304 (2)	C13—H13	0.9900
C2—H2	0.9500	C13—H13A	0.9900

C3—H3	0.9500	C14—C15	1.292 (3)
C3—H3A	0.9500	C14—H14	0.9500
C4—C5	1.491 (2)	C15—H15	0.9500
C4—H4	0.9900	C15—H15A	0.9500
C4—H4A	0.9900	C16—C17	1.485 (2)
C5—C6	1.298 (3)	C16—H16	0.9900
C5—H5	0.9500	C16—H16A	0.9900
C6—H6	0.9500	C17—C18	1.290 (3)
C6—H6A	0.9500	C17—H17	0.9500
C7—C8	1.489 (2)	C18—H18	0.9500
C7—H7	0.9900	C18—H18A	0.9500
C7—H7A	0.9900		

C1—Si1—C4	106.79 (8)	C8—C7—H7A	108.8
C1—Si1—Si2	105.58 (5)	Si2—C7—H7A	108.8
C4—Si1—Si2	113.40 (6)	H7—C7—H7A	107.7
C1—Si1—Si3^{i}	112.49 (5)	C9—C8—C7	125.87 (17)
C4—Si1—Si3^{i}	108.24 (5)	C9—C8—H8	117.1
Si2—Si1—Si3^{i}	110.35 (2)	C7—C8—H8	117.1
C10—Si2—C7	105.65 (7)	C8—C9—H9	120.0
C10—Si2—Si1	113.07 (5)	C8—C9—H9A	120.0
C7—Si2—Si1	108.47 (5)	H9—C9—H9A	120.0
C10—Si2—Si3	107.10 (5)	C11—C10—Si2	112.41 (11)
C7—Si2—Si3	112.04 (5)	C11—C10—H10	109.1
Si1—Si2—Si3	110.46 (2)	Si2—C10—H10	109.1
C13—Si3—C16	106.55 (8)	C11—C10—H10A	109.1
C13—Si3—Si2	113.06 (5)	Si2—C10—H10A	109.1
C16—Si3—Si2	107.39 (5)	H10—C10—H10A	107.9
C13—Si3—Si1^{i}	105.61 (5)	C12—C11—C10	126.47 (17)
C16—Si3—Si1^{i}	113.91 (6)	C12—C11—H11	116.8
Si2—Si3—Si1^{i}	110.38 (2)	C10—C11—H11	116.8
C2—C1—Si1	112.56 (11)	C11—C12—H12	120.0
C2—C1—H1	109.1	C11—C12—H12A	120.0
Si1—C1—H1	109.1	H12—C12—H12A	120.0
C2—C1—H1A	109.1	C14—C13—Si3	114.81 (11)
Si1—C1—H1A	109.1	C14—C13—H13	108.6
H1—C1—H1A	107.8	Si3—C13—H13	108.6
C3—C2—C1	126.54 (16)	C14—C13—H13A	108.6
C3—C2—H2	116.7	Si3—C13—H13A	108.6
C1—C2—H2	116.7	H13—C13—H13A	107.5
C2—C3—H3	120.0	C15—C14—C13	126.06 (19)
C2—C3—H3A	120.0	C15—C14—H14	117.0
H3—C3—H3A	120.0	C13—C14—H14	117.0
C5—C4—Si1	114.30 (12)	C14—C15—H15	120.0
C5—C4—H4	108.7	C14—C15—H15A	120.0
Si1—C4—H4	108.7	H15—C15—H15A	120.0
C5—C4—H4A	108.7	C17—C16—Si3	114.17 (12)
Si1—C4—H4A	108.7	C17—C16—H16	108.7

H4—C4—H4A	107.6	Si3—C16—H16	108.7
C6—C5—C4	126.23 (18)	C17—C16—H16A	108.7
C6—C5—H5	116.9	Si3—C16—H16A	108.7
C4—C5—H5	116.9	H16—C16—H16A	107.6
C5—C6—H6	120.0	C18—C17—C16	125.72 (19)
C5—C6—H6A	120.0	C18—C17—H17	117.1
H6—C6—H6A	120.0	C16—C17—H17	117.1
C8—C7—Si2	113.75 (11)	C17—C18—H18	120.0
C8—C7—H7	108.8	C17—C18—H18A	120.0
Si2—C7—H7	108.8	H18—C18—H18A	120.0
C4—Si1—C1—C2	66.90 (13)	C7—Si2—C10—C11	−63.26 (13)
Si2—Si1—C1—C2	−172.12 (10)	Si1—Si2—C10—C11	55.23 (12)
Si3^{i}—Si1—C1—C2	−51.71 (12)	Si3—Si2—C10—C11	177.14 (10)
Si1—C1—C2—C3	−109.91 (18)	Si2—C10—C11—C12	−121.92 (18)
Si1—C4—C5—C6	−92.8 (2)	Si3—C13—C14—C15	−109.0 (2)
Si2—C7—C8—C9	101.37 (18)	Si3—C16—C17—C18	−102.9 (2)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2^{ii}—H2^{ii}···C11	0.95	2.84	3.622 (3)	140
C7—H7*A*···C8^{iii}	0.99	2.82	3.669 (2)	145
C6—H6*A*···C15^{iii}	0.95	2.88	3.678 (4)	142
C16^{iv}—H16^{iv}···C12	0.99	2.75	3.684 (3)	159

Symmetry codes: (ii) *x*−1, *y*, *z*; (iii) −*x*+1, −*y*+2, −*z*+1; (iv) −*x*, −*y*+1, −*z*+1.