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A new pseudopolymorph of perchlorinated neopentasilane: the benzene monosolvate $Si(SiCl_3)_4{\cdot}C_6H_6$

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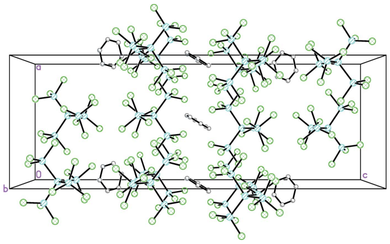
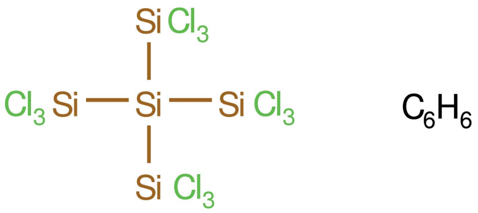
A new pseudopolymorph of dodecachloropentasilane, namely a benzene monosolvate, $Si_5Cl_{12}{\cdot}C_6H_6$, is described. There are two half molecules of each kind in the asymmetric unit. Both Si_5Cl_{12} molecules are completed by crystallographic twofold symmetry. One of the benzene molecules is located on a twofold rotation axis with two C—H groups located on this rotation axis. The second benzene molecule has all atoms on a general position: it is disordered over two equally occupied orientations. No directional interactions beyond normal van der Waals contacts occur in the crystal.



1. Chemical context

Since the 1980s, silicon hydrides, such as $Si(SiH_3)_4$, have attracted considerable attention as precursors for the liquid phase deposition (LPD) of silicon thin films (Nishimura *et al.*, 1985). In this context it should be noted that the perchlorinated neopentasilane $Si(SiCl_3)_4$ (Si_5Cl_{12}) is easily accessible in large amounts by the amine-induced disproportionation (Meyer-Wegner *et al.*, 2011; Tillmann *et al.*, 2012) of perchloropolysilanes, *e.g.* Si_2Cl_6 or Si_3Cl_8 (Meyer-Wegner *et al.*, 2011; Urry, 1970). Subsequent hydrogenation of $Si(SiCl_3)_4$ (I) then yields the neopentasilane $Si(SiH_3)_4$, which can be used as an LPD agent (Cannady & Zhou, 2008) (see Fig. 1).



In this paper we describe the structure of a new pseudopolymorph of perchlorinated neopentasilane (I), namely the benzene monosolvate $Si(SiCl_3)_4{\cdot}C_6H_6$, and make a comparison of its structure with those of $Si(SiCl_3)_4$ (Meyer-Wegner *et al.*, 2011) and $Si(SiCl_3)_4{\cdot}SiCl_4$ (Fleming, 1972).

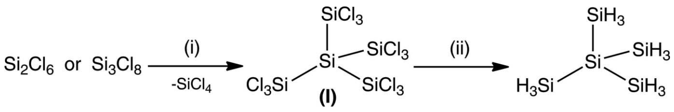


Figure 1
Amine-induced disproportionation of Si_2Cl_6 and Si_3Cl_8: (i) + NMe_3, or NMe_2Et, or NEt_3 in benzene at room temperature; (ii) + $LiAlH_4$ in diethyl ether at room temperature

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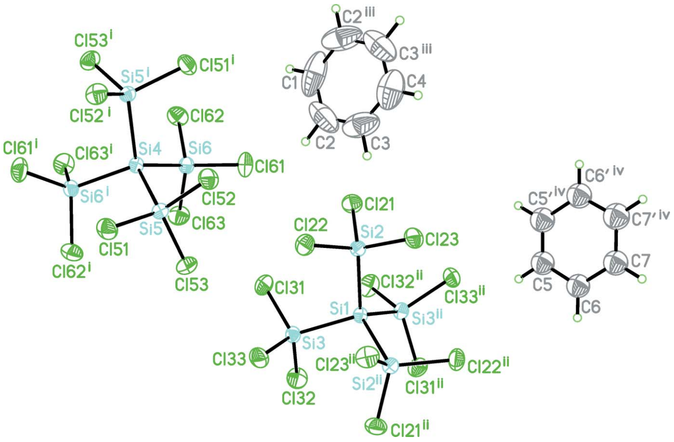

Figure 2
A perspective view of the title compound. Displacement ellipsoids are drawn at the 50% probability level. Symmetry codes: (i) $-y, -x, -z + \frac{1}{4}$; (ii) $1 - y, 1 - x, -z + \frac{1}{4}$; (iii) $-x, y, -z$; (iv) $1 - x, y, -z$.

2. Structural commentary

There are two half molecules of each kind in the asymmetric unit of (I). Both Si_5Cl_{12} molecules are completed by crystallographic twofold symmetry, with the rotation axes orientated in the [110] and [$\bar{1}$10] directions and the central Si atom located on the axis (Fig. 2). One of the benzene molecules is located on a twofold rotation axis propagating along the *a* or *b* axes with two C—H groups located on this rotation axis. The second benzene molecule has all atoms on general positions: it is disordered over two equally occupied orientations about a twofold rotation axis running in the [100] and [010] directions.

3. Supramolecular features

A view of the molecular packing of (I) (Fig. 3) reveals that the benzene molecules fill the voids between the dodecachloropentasilane molecules. There are no identified directional intermolecular interactions.

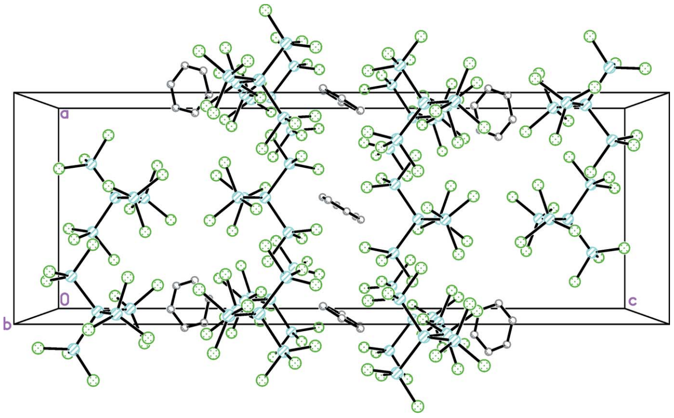

Figure 3
Packing diagram of the title compound viewed down [010].

Table 1
Bond lengths (Å) in the different structures containing Si_5Cl_{12} molecules.

For (I), mean values of the two molecules are given. For (II), mean values of the non-disordered molecule are given. Because of the high symmetry of (III), there is only one value for each bond length.

	Si—Si	Si—Cl
(I)	2.324	2.019
(II)	2.340	2.026
(III)	2.332 (9)	1.994 (7)

4. Database survey

There are two already known structures of dodecachloropentasilane: first, there is pure Si_5Cl_{12} (Meyer-Wegner *et al.*, 2011; CCDC deposition number 793308) and second, a co-crystal with silicon tetrachloride (Fleming, 1972; CCDC deposition number 1592571). In each of these structures, the Si_5Cl_{12} molecule is located on a special position. As noted above, in (I), both molecules in the asymmetric unit are found on a twofold rotation axis. Compound (II) also crystallizes with two molecules in the asymmetric unit. One of them is located on a threefold rotation axis and the other is disordered about a special position of site symmetry $\bar{3}$. In the second molecule, it is noteworthy that only the Si atoms carrying the Cl atoms are disordered: the central Si atom and the Cl atoms

Table 2
Experimental details.

Crystal data	
Chemical formula	$Cl_{12}Si_5 \cdot C_6H_6$
M_r	643.96
Crystal system, space group	Tetragonal, $P4_122$
Temperature (K)	173
a, *c* (Å)	11.9633 (4), 33.7848 (16)
V (Å^3)	4835.3 (4)
Z	8
Radiation type	Mo *Kα*
μ (mm^{-1})	1.62
Crystal size (mm)	0.28 × 0.18 × 0.16
Data collection	
Diffractometer	Stoe *IPDS* II two-circle
Absorption correction	Multi-scan (*X-AREA*; Stoe & Cie, 2001)
T_{min}, T_{max}	0.803, 1.0
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	39180, 5189, 4790
R_{int}	0.047
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.642
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.027, 0.075, 1.08
No. of reflections	5189
No. of parameters	207
No. of restraints	5
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.39, −0.42
Absolute structure	Flack *x* determined using 1905 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.48 (5)

Computer programs: *X-AREA* (Stoe & Cie, 2001), *SHELXS97* (Sheldrick, 2008), *XP* in *SHELXTL-Plus* (Sheldrick, 2008), *SHELXL2018* (Sheldrick, 2015) and *publCIF* (Westrip, 2010).

themselves are not disordered. In (III), the Si_5Cl_{12} molecule is located on a special position of site symmetry 23. The central Si atom is located at the intersection of the twofold and the threefold rotation axes (the twofold rotation axis coincides with a $\overline{4}$ axis). The Si—Si and Si—Cl bond lengths in all three structures agree well (Table 1).

5. Synthesis and crystallization

The perchlorinated neopentasilane (I) was synthesized according to a literature procedure (Kaczmarczyk & Urry, 1960). Single crystals of $Si(SiCl_3)_4 \cdot C_6H_6$ were grown from a solution of $Si(SiCl_3)_4$ in benzene after one week at room temperature.

$Si(SiCl_3)_4$ (**I**). $^{29}Si\{^1H\}$NMR (C_6D_6, external TMS): δ = −80.9 [$Si(SiCl_3)_4$], δ = 3.5 [$Si(SiCl_3)_4$].

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The H atoms were refined using a riding model with C—H = 0.95 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$. One of the benzene molecules is disordered over two equally occupied orientations: its carbon atoms were isotropically refined. The C—C distances in the non-disordered benzene molecule were restrained to 1.390 (2) Å. The crystal chosen for data collection was found to crystallize as a racemic twin.

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Computing details

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA* (Stoe & Cie, 2001); data reduction: *X-AREA* (Stoe & Cie, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL2018* (Sheldrick, 2015) and *publCIF* (Westrip, 2010).

Dodecachloropentasilane benzene monosolvate

Crystal data

$Cl_{12}Si_5{\cdot}C_6H_6$
$M_r = 643.96$
Tetragonal, $P4_122$
$a = 11.9633$ (4) Å
$c = 33.7848$ (16) Å
$V = 4835.3$ (4) Å^3
$Z = 8$
$F(000) = 2528$
$D_x = 1.769$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 62511 reflections
$\theta = 1.9$–27.6°
$\mu = 1.62$ mm^{-1}
$T = 173$ K
Block, colourless
0.28 × 0.18 × 0.16 mm

Data collection

Stoe IPDS II two-circle diffractometer
ω scans
Absorption correction: multi-scan (X-AREA; Stoe & Cie, 2001)
$T_{min} = 0.803$, $T_{max} = 1.0$
39180 measured reflections
5189 independent reflections
4790 reflections with $I > 2\sigma(I)$
$R_{int} = 0.047$
$\theta_{max} = 27.1°$, $\theta_{min} = 1.8°$
$h = -14 \rightarrow 15$
$k = -15 \rightarrow 15$
$l = -43 \rightarrow 43$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.075$
$S = 1.08$
5189 reflections
207 parameters
5 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0375P)^2 + 2.8317P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.39$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ e Å^{-3}
Absolute structure: Flack x determined using 1905 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.48 (5)

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	$U_{\rm iso}$*/$U_{\rm eq}$	Occ. (<1)
Si1	0.54973 (7)	0.45027 (7)	0.125000	0.0222 (3)	
Si2	0.38834 (7)	0.45056 (7)	0.08678 (2)	0.02447 (19)	
Si3	0.54972 (8)	0.29277 (8)	0.16530 (3)	0.0264 (2)	
Cl21	0.40377 (8)	0.34525 (8)	0.04060 (2)	0.0400 (2)	
Cl22	0.25695 (7)	0.39988 (8)	0.11990 (3)	0.0387 (2)	
Cl23	0.35776 (8)	0.60671 (7)	0.06658 (3)	0.0384 (2)	
Cl31	0.49743 (8)	0.15929 (7)	0.13366 (3)	0.0408 (2)	
Cl32	0.70602 (8)	0.26452 (9)	0.18579 (3)	0.0453 (2)	
Cl33	0.44514 (8)	0.31660 (9)	0.21128 (3)	0.0412 (2)	
Si4	0.04988 (7)	−0.04988 (7)	0.125000	0.0225 (3)	
Si5	0.05165 (7)	0.11311 (7)	0.16232 (2)	0.02420 (19)	
Si6	0.20502 (8)	−0.05209 (8)	0.08356 (3)	0.0263 (2)	
Cl51	−0.05058 (7)	0.09833 (8)	0.20938 (2)	0.0382 (2)	
Cl52	−0.00287 (8)	0.24225 (7)	0.12875 (3)	0.0367 (2)	
Cl53	0.20867 (7)	0.14553 (8)	0.18124 (3)	0.0379 (2)	
Cl61	0.23134 (9)	0.10282 (8)	0.06166 (3)	0.0449 (2)	
Cl62	0.17856 (9)	−0.15973 (8)	0.03862 (2)	0.0414 (2)	
Cl63	0.34091 (8)	−0.10198 (9)	0.11430 (3)	0.0424 (2)	
C1	0.000000	0.3434 (6)	0.000000	0.100 (4)	
H1	0.000000	0.263981	0.000000	0.120*	
C2	0.0511 (5)	0.4024 (4)	0.03030 (13)	0.094 (2)	
H2	0.087169	0.363505	0.051231	0.113*	
C3	0.0495 (5)	0.5176 (4)	0.03001 (14)	0.090 (2)	
H3	0.083717	0.556596	0.051284	0.107*	
C4	0.000000	0.5786 (7)	0.000000	0.087 (3)	
H4	0.000000	0.657984	0.000000	0.104*	
C5	0.5409 (8)	0.8628 (10)	0.0236 (3)	0.051 (2)*	0.5
H5	0.570943	0.806236	0.040196	0.062*	0.5
C6	0.5561 (8)	0.9738 (11)	0.0335 (3)	0.050 (2)*	0.5
H6	0.594385	0.992910	0.057205	0.059*	0.5
C7	0.5158 (9)	1.0566 (8)	0.0092 (3)	0.054 (3)*	0.5
H7	0.527035	1.132987	0.015732	0.065*	0.5
C5′	0.5145 (10)	0.8339 (8)	0.0086 (3)	0.057 (3)*	0.5
H5′	0.526088	0.757264	0.014687	0.068*	0.5
C6′	0.5559 (9)	0.9177 (12)	0.0335 (3)	0.058 (2)*	0.5
H6′	0.594991	0.897299	0.056942	0.069*	0.5
C7′	0.5410 (10)	1.0290 (11)	0.0247 (4)	0.062 (3)*	0.5
H7′	0.569534	1.085379	0.041783	0.074*	0.5

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Si1	0.0213 (4)	0.0213 (4)	0.0241 (6)	0.0004 (5)	0.0008 (3)	0.0008 (3)
Si2	0.0245 (4)	0.0238 (4)	0.0251 (4)	0.0000 (3)	−0.0010 (3)	0.0009 (3)
Si3	0.0252 (4)	0.0247 (4)	0.0294 (4)	0.0001 (4)	−0.0007 (3)	0.0046 (3)
Cl21	0.0521 (5)	0.0364 (5)	0.0316 (4)	−0.0014 (4)	0.0003 (4)	−0.0084 (3)
Cl22	0.0269 (4)	0.0476 (5)	0.0418 (4)	−0.0054 (4)	0.0051 (3)	0.0042 (4)
Cl23	0.0464 (5)	0.0278 (4)	0.0411 (4)	0.0058 (4)	−0.0079 (4)	0.0060 (3)
Cl31	0.0452 (5)	0.0268 (4)	0.0503 (5)	−0.0048 (4)	−0.0003 (4)	−0.0032 (4)
Cl32	0.0317 (4)	0.0461 (5)	0.0579 (5)	0.0068 (4)	−0.0113 (4)	0.0116 (4)
Cl33	0.0406 (5)	0.0529 (6)	0.0302 (4)	−0.0059 (4)	0.0065 (4)	0.0031 (4)
Si4	0.0214 (4)	0.0214 (4)	0.0245 (6)	0.0000 (5)	0.0006 (3)	0.0006 (3)
Si5	0.0236 (4)	0.0242 (4)	0.0248 (4)	−0.0008 (3)	−0.0010 (3)	−0.0011 (3)
Si6	0.0248 (4)	0.0259 (4)	0.0282 (4)	0.0001 (4)	0.0038 (3)	0.0010 (3)
Cl51	0.0366 (5)	0.0486 (5)	0.0295 (4)	0.0010 (4)	0.0072 (3)	−0.0013 (4)
Cl52	0.0436 (5)	0.0268 (4)	0.0398 (4)	0.0039 (4)	−0.0050 (4)	0.0042 (3)
Cl53	0.0282 (4)	0.0428 (5)	0.0429 (4)	−0.0063 (4)	−0.0069 (3)	−0.0033 (4)
Cl61	0.0489 (5)	0.0325 (4)	0.0533 (5)	−0.0063 (4)	0.0126 (4)	0.0108 (4)
Cl62	0.0520 (5)	0.0404 (5)	0.0317 (4)	0.0053 (4)	0.0022 (4)	−0.0084 (4)
Cl63	0.0274 (4)	0.0505 (5)	0.0494 (5)	0.0067 (4)	−0.0039 (4)	0.0003 (4)
C1	0.074 (6)	0.043 (4)	0.184 (11)	0.000	0.056 (7)	0.000
C2	0.068 (4)	0.147 (7)	0.067 (4)	0.011 (4)	0.001 (3)	0.055 (4)
C3	0.070 (4)	0.138 (6)	0.060 (3)	−0.026 (4)	0.006 (3)	−0.037 (4)
C4	0.067 (5)	0.068 (5)	0.125 (8)	0.000	0.040 (5)	0.000

Geometric parameters (Å, º)

Si1—Si2	2.3227 (11)	Si6—Cl61	2.0202 (13)
Si1—Si2^{i}	2.3228 (11)	C1—C2	1.3855 (18)
Si1—Si3^{i}	2.3246 (11)	C1—C2^{iii}	1.3855 (18)
Si1—Si3	2.3247 (11)	C1—H1	0.9500
Si2—Cl21	2.0138 (12)	C2—C3	1.378 (3)
Si2—Cl23	2.0221 (12)	C2—H2	0.9500
Si2—Cl22	2.0225 (12)	C3—C4	1.3824 (18)
Si3—Cl33	2.0150 (13)	C3—H3	0.9500
Si3—Cl31	2.0209 (13)	C4—H4	0.9500
Si3—Cl32	2.0223 (13)	C5—C6	1.382 (15)
Si4—Si5	2.3221 (11)	C5—H5	0.9500
Si4—Si5^{ii}	2.3222 (11)	C6—C7	1.375 (14)
Si4—Si6	2.3250 (11)	C6—H6	0.9500
Si4—Si6^{ii}	2.3251 (11)	C7—H7	0.9500
Si5—Cl51	2.0138 (12)	C5′—C6′	1.399 (15)
Si5—Cl53	2.0218 (12)	C5′—H5′	0.9501
Si5—Cl52	2.0243 (12)	C6′—C7′	1.376 (15)
Si6—Cl62	2.0158 (13)	C6′—H6′	0.9500
Si6—Cl63	2.0194 (13)	C7′—H7′	0.9500

Si2—Si1—Si2^{i}	107.85 (6)	C2—C1—C2^{iii}	118.8 (7)
Si2—Si1—Si3^{i}	110.38 (3)	C2—C1—H1	120.6
Si2^{i}—Si1—Si3^{i}	109.07 (3)	C2^{iii}—C1—H1	120.6
Si2—Si1—Si3	109.07 (3)	C3—C2—C1	119.9 (6)
Si2^{i}—Si1—Si3	110.37 (3)	C3—C2—H2	120.1
Si3^{i}—Si1—Si3	110.06 (7)	C1—C2—H2	120.1
Cl21—Si2—Cl23	109.46 (5)	C2—C3—C4	122.6 (6)
Cl21—Si2—Cl22	108.20 (6)	C2—C3—H3	118.7
Cl23—Si2—Cl22	108.85 (6)	C4—C3—H3	118.7
Cl21—Si2—Si1	110.71 (5)	C3^{iii}—C4—C3	116.3 (7)
Cl23—Si2—Si1	109.84 (5)	C3^{iii}—C4—H4	121.9
Cl22—Si2—Si1	109.75 (4)	C3—C4—H4	121.9
Cl33—Si3—Cl31	109.11 (6)	C6—C5—C5^{iv}	106.0 (6)
Cl33—Si3—Cl32	109.50 (6)	C6—C5—H5	119.4
Cl31—Si3—Cl32	109.58 (6)	C5^{iv}—C5—H5	134.6
Cl33—Si3—Si1	109.69 (5)	C5—C6—C7	120.0 (9)
Cl31—Si3—Si1	109.31 (5)	C5—C6—C7^{iv}	104.5 (8)
Cl32—Si3—Si1	109.63 (5)	C5—C6—H6	120.0
Si5—Si4—Si5^{ii}	108.07 (6)	C7—C6—H6	120.0
Si5—Si4—Si6	109.22 (3)	C7^{iv}—C6—H6	135.5
Si5^{ii}—Si4—Si6	110.07 (3)	C7^{iv}—C7—C6	133.9 (6)
Si5—Si4—Si6^{ii}	110.08 (3)	C6—C7—C6^{iv}	103.4 (9)
Si5^{ii}—Si4—Si6^{ii}	109.22 (3)	C7^{iv}—C7—H7	105.9
Si6—Si4—Si6^{ii}	110.15 (7)	C6—C7—H7	120.2
Cl51—Si5—Cl53	109.35 (5)	C6^{iv}—C7—H7	136.4
Cl51—Si5—Cl52	108.28 (6)	C5′^{iv}—C5′—C6′	134.3 (6)
Cl53—Si5—Cl52	109.28 (6)	C5′^{iv}—C5′—H5′	105.1
Cl51—Si5—Si4	110.45 (5)	C6′—C5′—H5′	120.6
Cl53—Si5—Si4	109.95 (5)	C6′^{iv}—C5′—H5′	136.3
Cl52—Si5—Si4	109.50 (5)	C7′—C6′—C5′	121.1 (10)
Cl62—Si6—Cl63	108.97 (6)	C7′—C6′—H6′	119.4
Cl62—Si6—Cl61	109.56 (6)	C5′—C6′—H6′	119.4
Cl63—Si6—Cl61	109.51 (6)	C5′^{iv}—C6′—H6′	134.0
Cl62—Si6—Si4	109.60 (5)	C6′—C7′—C7′^{iv}	104.6 (7)
Cl63—Si6—Si4	109.65 (5)	C6′—C7′—H7′	120.6
Cl61—Si6—Si4	109.54 (5)	C7′^{iv}—C7′—H7′	134.8

C2^{iii}—C1—C2—C3	0.6 (4)	C7^{iv}—C6—C7—C6^{iv}	−1 (2)
C1—C2—C3—C4	−1.2 (9)	C5′^{iv}—C5′—C6′—C7′	0 (4)
C2—C3—C4—C3^{iii}	0.6 (4)	C6′^{iv}—C5′—C6′—C7′	0.0 (10)
C5^{iv}—C5—C6—C7	−1.7 (13)	C6′^{iv}—C5′—C6′—C5′^{iv}	0 (3)
C5^{iv}—C5—C6—C7^{iv}	−1.2 (10)	C5′—C6′—C7′—C7′^{iv}	−0.1 (14)
C5—C6—C7—C7^{iv}	2 (3)	C5′^{iv}—C6′—C7′—C7′^{iv}	−0.2 (11)
C5—C6—C7—C6^{iv}	1.0 (9)		

Symmetry codes: (i) −*y*+1, −*x*+1, −*z*+1/4; (ii) −*y*, −*x*, −*z*+1/4; (iii) −*x*, *y*, −*z*; (iv) −*x*+1, *y*, −*z*.