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1,5-Dichloro-1,1,2,2,3,3,4,4,5,5-decaphenylpentasilane

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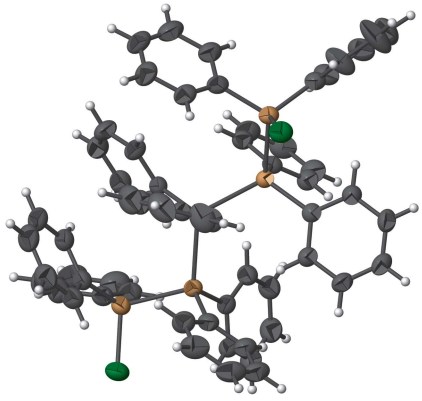
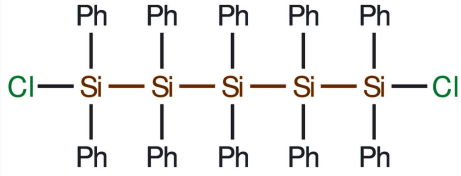
The title compound, $C_{60}H_{50}Cl_2Si_5$, was obtained by a ring-opening reaction of decaphenylcyclopentasilane. The chain of silicon atoms adopts an all *trans* conformation [Si—Si—Si—Si torsion angles = −156.31 (5) and −161.02 (5)°]. One of the Cl atoms is in an *antiperiplanar* conformation with respect to the Si chain [Cl—Si—Si—Si = −156.40 (5)°] while the other Cl substituent adopts a *synclinal* conformation [Si—Si—Si—Cl = 78.82 (6)°].

3D view



Chemical scheme



Structure description

The deposition of silicon from volatile precursors is greatly improved using silanes that already incorporate multiple Si—Si bonds (Chung *et al.*, 2007). The selective synthesis of such oligosilanes typically involves a multi-step synthetic procedure. The oligosilane backbones are formed by basic Wurtz-type coupling of especially dichlorodiphenylsilane to give defined perphenylated silicon-based cycles (Jarvie *et al.*, 1961). Hydrochlorination of these species with catalytic amounts of $AlCl_3$ yields cyclic chlorosilanes (Hengge & Kovar, 1977). These perchlorinated oligosilanes are then excellent precursors for the synthesis of hydrogenated silanes (Hengge & Bauer, 1975). Instead, chlorination reactions with PCl_5 of perphenylated cyclics lead to ring-opening, hence yielding a phenylated silicon chain with terminated Si—Cl functionality. Consequently, *cyclo*-Si_5Ph_{10} was obtained by the reaction of dichlorodiphenylsilane with metallic lithium (Jarvie *et al.*, 1961). Next, treating this cyclic with PCl_5 in 1,1,2,2-tetrachloroethane yielded the title compound (Fig. 1), 1,5-dichlorodecaphenyl-*n*-pentasilane, $C_{60}H_{50}Cl_2Si_5$, (Hengge & Stüger, 1980; Gilman & Chapman, 1967), and the crystal structure is reported herein.

The chain of silicon atoms adopts an all *trans* conformation [torsion angles Si1—Si2—Si3—Si4, −156.31 (5)° and Si2—Si3—Si4—Si5, −161.02 (5)°]. One of the Cl atoms is in an *antiperiplanar* conformation with respect to the Si chain [Cl1—Si1—Si2—Si3,

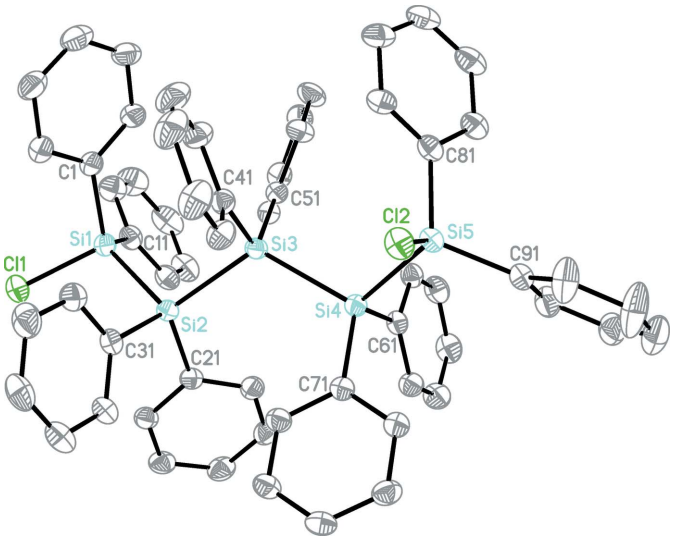


Figure 1
A perspective view of the title compound, with displacement ellipsoids drawn at the 50% probability level. H atoms have been omitted for clarity. Only the pivot atoms of the phenyl rings are labelled.

−156.40 (5)°] while the other Cl substituent adopts a *synclinal* conformation [Si3—Si4—Si5—Cl2, 78.82 (6)°].

The crystal structure of a pseudo-polymorph of the title compound, namely 1,5-dichlorodecaphenylpentasilane benzene solvate, has already been reported (Ovchinnikov *et al.*, 1989). It crystallizes with two 1,5-dichlorodecaphenylpentasilane molecules in the asymmetric unit. One of them displays a similar pattern of torsion angles: Si—Si—Si—Si, 157.5 and 156.9°; Cl—Si—Si—Si, 157.1 and −83.1°. The other one has one Si—Si—Si—Si torsion angle in an *anticlinal* conformation: Si—Si—Si—Si: −172.0 and 109.4°; Cl—Si—Si—Si: 173.6 and −57.0°.

Synthesis and crystallization

1,5-Dichlorodecaphenyl-*n*-pentasilane was synthesized according to published procedures (Hengge & Stüger, 1980; Gilman & Chapman, 1967). *cyclo*-Si_5Ph_{10} (20.30 g, 22.30 mmol) and PCl_5 (5.00 g, 24.00 mmol) were suspended in 1,1,2,2-tetrachloroethane (100 ml) and then heated to 120 °C for 15 minutes. The solvent was removed under vacuum and the oily residue was dissolved in benzene (50 ml). Addition of *n*-pentane (130 ml) led to precipitation of colorless solids, which were dried under vacuum (18.13 g, 18.46 mmol, 88%). ^{1}H NMR (C_6D_6, 500.2 MHz): δ = 7.46 (*d*, $^3J_{H,H}$ = 7.1 Hz, 8 H, 2,4-*o*-Ph*H*), 7.41 (*d*, $^3J_{H,H}$ = 7.1 Hz, 4 H, 3-*o*-Ph*H*), 7.29 (*d*, $^3J_{H,H}$ = 7.3 Hz, 8 H, 1,5-*o*-Ph*H*), 7.12–6.86 (*m*, 30 H, *m*-Ph*H*, *p*-Ph*H*) p.p.m. ^{29}Si NMR (C_6D_6, 99.4 MHz): δ = +2.5 (1,5-*Si*Ph_2Cl), −33.1 (3-*Si*Ph_2), −35.6 (2,4-*Si*Ph_2) p.p.m.

Crystals suitable for single-crystal X-ray crystallography were obtained by vapor diffusion of *n*-pentane into a concentrated solution of 1,5-dichlorodecaphenyl-*n*-pentasilane in toluene.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{60}H_{50}Cl_2Si_5$
M_r	982.35
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	173
a, b, c (Å)	11.6675 (6), 33.682 (2), 13.3653 (7)
β (°)	94.184 (4)
V (Å^3)	5238.4 (5)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.28
Crystal size (mm)	0.29 × 0.28 × 0.28
Data collection	
Diffractometer	Stoe *IPDS* II two-circle
Absorption correction	Multi-scan (*X-AREA*; Stoe & Cie, 2001)
T_{min}, T_{max}	0.673, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	36281, 9222, 8032
R_{int}	0.067
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.070, 0.189, 1.10
No. of reflections	9222
No. of parameters	604
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.65, −0.49

Computer programs: *X-AREA* (Stoe & Cie, 2001), *SHELXS97* (Sheldrick, 2008), *XP* in *SHELXTL-Plus* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *publCIF* (Westrip, 2010).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x161812 [https://doi.org/10.1107/S2414314616018125]

1,5-Dichloro-1,1,2,2,3,3,4,4,5,5-decaphenylpentasilane

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1,5-Dichloro-1,1,2,2,3,3,4,4,5,5-decaphenylpentasilane

Crystal data

$C_{60}H_{50}Cl_2Si_5$
M_r = 982.35
Monoclinic, $P2_1/n$
a = 11.6675 (6) Å
b = 33.682 (2) Å
c = 13.3653 (7) Å
β = 94.184 (4)°
V = 5238.4 (5) Å^3
Z = 4
$F(000)$ = 2056
D_x = 1.246 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 36281 reflections
θ = 1.2–26.1°
μ = 0.28 mm^{-1}
T = 173 K
Block, colourless
0.29 × 0.28 × 0.28 mm

Data collection

Stoe IPDS II two-circle diffractometer
Radiation source: Genix 3D IμS microfocus X-ray source
ω scans
Absorption correction: multi-scan (X-AREA; Stoe & Cie, 2001)
T_{min} = 0.673, T_{max} = 1.000
36281 measured reflections
9222 independent reflections
8032 reflections with $I > 2\sigma(I)$
R_{int} = 0.067
θ_{max} = 25.0°, θ_{min} = 1.2°
h = −13→13
k = −40→40
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.189
S = 1.10
9222 reflections
604 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0998P)^2 + 5.7602P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 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}
Cl1	0.73526 (9)	0.74544 (3)	0.55535 (7)	0.0548 (3)
Cl2	0.99521 (7)	0.51619 (3)	0.17428 (7)	0.0496 (2)
Si1	0.68559 (9)	0.71809 (3)	0.41821 (7)	0.0414 (2)
Si2	0.73273 (8)	0.64983 (3)	0.44527 (6)	0.0368 (2)
Si3	0.75825 (8)	0.61860 (2)	0.28776 (6)	0.0351 (2)
Si4	0.73280 (8)	0.54828 (2)	0.27542 (6)	0.0343 (2)
Si5	0.81971 (8)	0.52103 (3)	0.13595 (7)	0.0378 (2)
C1	0.7733 (3)	0.74134 (10)	0.3218 (3)	0.0463 (8)
C2	0.7319 (4)	0.74204 (11)	0.2205 (3)	0.0507 (9)
H2	0.6569	0.7324	0.2018	0.061*
C3	0.7992 (4)	0.75671 (12)	0.1474 (3)	0.0580 (10)
H3	0.7702	0.7569	0.0791	0.070*
C4	0.9072 (4)	0.77096 (13)	0.1735 (4)	0.0672 (12)
H4	0.9527	0.7811	0.1232	0.081*
C5	0.9504 (4)	0.77076 (13)	0.2722 (4)	0.0641 (11)
H5	1.0252	0.7808	0.2899	0.077*
C6	0.8835 (4)	0.75574 (11)	0.3462 (3)	0.0540 (9)
H6	0.9138	0.7554	0.4141	0.065*
C11	0.5300 (3)	0.73104 (11)	0.3886 (3)	0.0472 (8)
C12	0.5021 (4)	0.76678 (13)	0.3378 (3)	0.0619 (11)
H12	0.5619	0.7846	0.3231	0.074*
C13	0.3893 (5)	0.77648 (16)	0.3088 (4)	0.0785 (14)
H13	0.3721	0.8004	0.2733	0.094*
C14	0.3021 (5)	0.75129 (18)	0.3314 (4)	0.0780 (15)
H14	0.2247	0.7579	0.3115	0.094*
C15	0.3265 (4)	0.71652 (16)	0.3829 (3)	0.0677 (12)
H15	0.2659	0.6993	0.3987	0.081*
C16	0.4405 (4)	0.70664 (12)	0.4119 (3)	0.0531 (9)
H16	0.4567	0.6828	0.4481	0.064*
C21	0.6157 (3)	0.62804 (9)	0.5184 (2)	0.0398 (7)
C22	0.5383 (3)	0.59954 (10)	0.4785 (3)	0.0468 (8)
H22	0.5479	0.5893	0.4134	0.056*
C23	0.4486 (4)	0.58588 (12)	0.5304 (3)	0.0558 (9)
H23	0.3968	0.5667	0.5010	0.067*
C24	0.4341 (4)	0.60016 (12)	0.6255 (3)	0.0584 (10)
H24	0.3725	0.5907	0.6617	0.070*
C25	0.5095 (4)	0.62818 (11)	0.6680 (3)	0.0531 (9)
H25	0.4998	0.6379	0.7335	0.064*
C26	0.5989 (3)	0.64210 (10)	0.6149 (3)	0.0441 (8)
H26	0.6497	0.6615	0.6445	0.053*
C31	0.8735 (3)	0.64869 (10)	0.5259 (3)	0.0433 (8)
C32	0.8859 (3)	0.62656 (11)	0.6141 (3)	0.0472 (8)
H32	0.8223	0.6118	0.6348	0.057*
C33	0.9902 (4)	0.62563 (13)	0.6727 (3)	0.0589 (10)
H33	0.9970	0.6104	0.7326	0.071*

C34	1.0827 (4)	0.64672 (15)	0.6437 (3)	0.0655 (12)
H34	1.1535	0.6461	0.6835	0.079*
C35	1.0726 (4)	0.66877 (15)	0.5567 (4)	0.0667 (12)
H35	1.1366	0.6835	0.5368	0.080*
C36	0.9693 (4)	0.66952 (12)	0.4979 (3)	0.0553 (9)
H36	0.9640	0.6845	0.4375	0.066*
C41	0.9095 (3)	0.63072 (10)	0.2587 (3)	0.0412 (7)
C42	0.9391 (4)	0.66236 (11)	0.1983 (3)	0.0537 (9)
H42	0.8805	0.6796	0.1707	0.064*
C43	1.0520 (4)	0.66926 (14)	0.1777 (4)	0.0727 (13)
H43	1.0699	0.6906	0.1350	0.087*
C44	1.1387 (4)	0.64503 (14)	0.2194 (4)	0.0754 (14)
H44	1.2161	0.6497	0.2051	0.090*
C45	1.1128 (4)	0.61435 (14)	0.2812 (4)	0.0695 (12)
H45	1.1723	0.5979	0.3104	0.083*
C46	0.9994 (3)	0.60743 (11)	0.3009 (3)	0.0504 (9)
H46	0.9824	0.5862	0.3443	0.060*
C51	0.6499 (3)	0.64221 (9)	0.1950 (2)	0.0386 (7)
C52	0.6694 (4)	0.64856 (11)	0.0939 (3)	0.0500 (9)
H52	0.7397	0.6399	0.0695	0.060*
C53	0.5882 (4)	0.66720 (13)	0.0286 (3)	0.0602 (11)
H53	0.6030	0.6710	−0.0398	0.072*
C54	0.4864 (4)	0.68020 (12)	0.0631 (3)	0.0575 (10)
H54	0.4319	0.6937	0.0190	0.069*
C55	0.4634 (3)	0.67378 (11)	0.1611 (3)	0.0513 (9)
H55	0.3928	0.6825	0.1848	0.062*
C56	0.5442 (3)	0.65447 (10)	0.2256 (3)	0.0430 (7)
H56	0.5265	0.6495	0.2927	0.052*
C61	0.5740 (3)	0.53743 (9)	0.2601 (2)	0.0380 (7)
C62	0.5222 (3)	0.51313 (11)	0.3288 (3)	0.0458 (8)
H62	0.5688	0.5013	0.3820	0.055*
C63	0.4052 (3)	0.50578 (13)	0.3215 (3)	0.0560 (9)
H63	0.3722	0.4892	0.3693	0.067*
C64	0.3366 (3)	0.52277 (13)	0.2441 (3)	0.0588 (10)
H64	0.2562	0.5178	0.2387	0.071*
C65	0.3842 (3)	0.54672 (12)	0.1751 (3)	0.0542 (9)
H65	0.3366	0.5584	0.1224	0.065*
C66	0.5013 (3)	0.55387 (10)	0.1822 (3)	0.0442 (8)
H66	0.5332	0.5702	0.1334	0.053*
C71	0.7951 (3)	0.52064 (9)	0.3891 (2)	0.0371 (7)
C72	0.8134 (3)	0.47959 (10)	0.3872 (3)	0.0447 (8)
H72	0.7983	0.4654	0.3262	0.054*
C73	0.8535 (4)	0.45923 (11)	0.4735 (3)	0.0508 (9)
H73	0.8647	0.4313	0.4712	0.061*
C74	0.8770 (3)	0.47950 (11)	0.5621 (3)	0.0478 (8)
H74	0.9046	0.4655	0.6208	0.057*
C75	0.8607 (3)	0.51990 (11)	0.5659 (3)	0.0477 (8)
H75	0.8773	0.5339	0.6269	0.057*

C76	0.8201 (3)	0.54016 (10)	0.4801 (3)	0.0430 (7)
H76	0.8089	0.5681	0.4835	0.052*
C81	0.8055 (3)	0.55343 (10)	0.0225 (3)	0.0438 (8)
C82	0.7140 (4)	0.54849 (12)	−0.0500 (3)	0.0527 (9)
H82	0.6605	0.5276	−0.0434	0.063*
C83	0.7010 (4)	0.57433 (14)	−0.1325 (3)	0.0633 (11)
H83	0.6399	0.5703	−0.1825	0.076*
C84	0.7757 (4)	0.60520 (14)	−0.1415 (3)	0.0614 (11)
H84	0.7644	0.6232	−0.1961	0.074*
C85	0.8674 (4)	0.61026 (13)	−0.0715 (3)	0.0586 (10)
H85	0.9203	0.6313	−0.0788	0.070*
C86	0.8823 (3)	0.58458 (11)	0.0097 (3)	0.0489 (8)
H86	0.9458	0.5882	0.0574	0.059*
C91	0.7683 (3)	0.46900 (10)	0.1078 (3)	0.0426 (7)
C92	0.6537 (4)	0.45762 (12)	0.1105 (3)	0.0557 (9)
H92	0.5981	0.4768	0.1260	0.067*
C93	0.6194 (4)	0.41875 (13)	0.0909 (3)	0.0664 (12)
H93	0.5406	0.4118	0.0916	0.080*
C94	0.6983 (5)	0.39050 (13)	0.0706 (4)	0.0766 (14)
H94	0.6751	0.3637	0.0601	0.092*
C95	0.8108 (5)	0.40094 (15)	0.0654 (6)	0.099 (2)
H95	0.8653	0.3815	0.0487	0.119*
C96	0.8461 (4)	0.44001 (13)	0.0845 (4)	0.0738 (14)
H96	0.9248	0.4468	0.0813	0.089*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0643 (6)	0.0540 (5)	0.0458 (5)	−0.0023 (4)	0.0024 (4)	−0.0125 (4)
Cl2	0.0366 (4)	0.0596 (5)	0.0519 (5)	0.0018 (4)	−0.0013 (4)	−0.0047 (4)
Si1	0.0472 (5)	0.0379 (5)	0.0395 (5)	−0.0010 (4)	0.0053 (4)	−0.0022 (4)
Si2	0.0400 (5)	0.0383 (5)	0.0323 (4)	−0.0015 (3)	0.0048 (4)	−0.0001 (3)
Si3	0.0375 (5)	0.0356 (4)	0.0326 (4)	0.0004 (3)	0.0043 (3)	0.0017 (3)
Si4	0.0342 (5)	0.0359 (4)	0.0327 (4)	0.0002 (3)	0.0017 (3)	0.0009 (3)
Si5	0.0360 (5)	0.0431 (5)	0.0343 (5)	0.0009 (4)	0.0021 (4)	−0.0025 (3)
C1	0.056 (2)	0.0370 (17)	0.046 (2)	−0.0018 (15)	0.0055 (16)	−0.0011 (14)
C2	0.061 (2)	0.0421 (19)	0.049 (2)	−0.0004 (16)	0.0055 (18)	0.0043 (15)
C3	0.073 (3)	0.050 (2)	0.052 (2)	0.0013 (19)	0.015 (2)	0.0110 (17)
C4	0.078 (3)	0.054 (2)	0.073 (3)	−0.005 (2)	0.024 (2)	0.013 (2)
C5	0.063 (3)	0.055 (2)	0.076 (3)	−0.0150 (19)	0.016 (2)	0.002 (2)
C6	0.061 (2)	0.047 (2)	0.054 (2)	−0.0081 (17)	0.0065 (19)	−0.0030 (16)
C11	0.049 (2)	0.0469 (19)	0.046 (2)	0.0066 (15)	0.0026 (16)	−0.0054 (15)
C12	0.068 (3)	0.056 (2)	0.062 (3)	0.013 (2)	0.008 (2)	0.0039 (19)
C13	0.077 (3)	0.078 (3)	0.080 (3)	0.028 (3)	0.002 (3)	0.013 (3)
C14	0.062 (3)	0.110 (4)	0.062 (3)	0.030 (3)	−0.001 (2)	−0.003 (3)
C15	0.049 (2)	0.095 (3)	0.059 (3)	0.006 (2)	0.005 (2)	−0.009 (2)
C16	0.053 (2)	0.061 (2)	0.046 (2)	0.0056 (18)	0.0064 (17)	−0.0052 (17)
C21	0.0423 (19)	0.0395 (17)	0.0377 (17)	0.0020 (13)	0.0048 (14)	0.0032 (13)

C22	0.053 (2)	0.0438 (18)	0.0446 (19)	−0.0016 (15)	0.0100 (16)	−0.0011 (14)
C23	0.057 (2)	0.050 (2)	0.061 (2)	−0.0106 (17)	0.0137 (19)	0.0004 (17)
C24	0.059 (3)	0.057 (2)	0.062 (2)	−0.0045 (18)	0.024 (2)	0.0065 (18)
C25	0.064 (3)	0.053 (2)	0.044 (2)	0.0048 (18)	0.0211 (18)	0.0025 (16)
C26	0.050 (2)	0.0443 (18)	0.0388 (18)	0.0020 (15)	0.0060 (15)	0.0021 (14)
C31	0.047 (2)	0.0444 (18)	0.0382 (17)	−0.0016 (14)	0.0003 (14)	−0.0063 (14)
C32	0.048 (2)	0.055 (2)	0.0379 (18)	0.0023 (16)	−0.0005 (15)	−0.0044 (15)
C33	0.058 (3)	0.075 (3)	0.042 (2)	0.010 (2)	−0.0057 (18)	−0.0060 (18)
C34	0.047 (2)	0.092 (3)	0.055 (2)	0.001 (2)	−0.0093 (19)	−0.017 (2)
C35	0.048 (2)	0.086 (3)	0.066 (3)	−0.017 (2)	0.004 (2)	−0.012 (2)
C36	0.055 (2)	0.060 (2)	0.051 (2)	−0.0090 (18)	−0.0003 (18)	0.0005 (17)
C41	0.0428 (19)	0.0397 (17)	0.0414 (18)	−0.0009 (14)	0.0054 (14)	−0.0041 (13)
C42	0.053 (2)	0.050 (2)	0.061 (2)	−0.0047 (16)	0.0171 (18)	0.0052 (17)
C43	0.069 (3)	0.062 (3)	0.091 (3)	−0.019 (2)	0.035 (3)	0.003 (2)
C44	0.051 (3)	0.068 (3)	0.111 (4)	−0.016 (2)	0.029 (3)	−0.013 (3)
C45	0.040 (2)	0.066 (3)	0.103 (4)	−0.0043 (18)	0.010 (2)	−0.005 (2)
C46	0.0393 (19)	0.048 (2)	0.064 (2)	−0.0026 (15)	0.0056 (17)	0.0011 (17)
C51	0.0443 (18)	0.0348 (15)	0.0366 (16)	0.0000 (13)	0.0032 (14)	0.0007 (12)
C52	0.057 (2)	0.055 (2)	0.0385 (18)	0.0098 (17)	0.0078 (16)	0.0051 (15)
C53	0.080 (3)	0.064 (2)	0.0349 (19)	0.011 (2)	−0.0048 (19)	0.0069 (17)
C54	0.062 (3)	0.054 (2)	0.055 (2)	0.0096 (18)	−0.0127 (19)	0.0048 (17)
C55	0.044 (2)	0.050 (2)	0.059 (2)	0.0036 (15)	−0.0035 (17)	0.0011 (16)
C56	0.0438 (19)	0.0426 (18)	0.0424 (18)	−0.0025 (14)	0.0022 (15)	−0.0003 (14)
C61	0.0365 (17)	0.0395 (16)	0.0380 (17)	0.0003 (13)	0.0028 (13)	−0.0058 (13)
C62	0.0418 (19)	0.0505 (19)	0.0450 (19)	−0.0043 (15)	0.0035 (15)	0.0018 (15)
C63	0.045 (2)	0.069 (2)	0.055 (2)	−0.0096 (18)	0.0110 (18)	0.0005 (18)
C64	0.036 (2)	0.074 (3)	0.065 (3)	−0.0056 (17)	−0.0003 (18)	−0.010 (2)
C65	0.045 (2)	0.065 (2)	0.051 (2)	0.0042 (17)	−0.0090 (17)	−0.0054 (18)
C66	0.0438 (19)	0.0463 (18)	0.0416 (18)	−0.0008 (14)	−0.0025 (15)	−0.0032 (14)
C71	0.0318 (16)	0.0415 (17)	0.0381 (17)	−0.0009 (12)	0.0029 (13)	0.0015 (13)
C72	0.051 (2)	0.0426 (18)	0.0405 (18)	−0.0002 (15)	0.0002 (15)	0.0011 (14)
C73	0.058 (2)	0.0420 (18)	0.052 (2)	0.0072 (16)	0.0044 (17)	0.0103 (15)
C74	0.047 (2)	0.056 (2)	0.0404 (19)	0.0073 (16)	0.0009 (15)	0.0119 (15)
C75	0.052 (2)	0.054 (2)	0.0365 (18)	0.0030 (16)	−0.0025 (15)	0.0035 (15)
C76	0.047 (2)	0.0436 (18)	0.0384 (17)	0.0019 (14)	0.0008 (14)	0.0025 (13)
C81	0.0449 (19)	0.0501 (19)	0.0365 (17)	0.0073 (15)	0.0042 (14)	−0.0047 (14)
C82	0.054 (2)	0.061 (2)	0.042 (2)	0.0032 (17)	−0.0022 (17)	−0.0014 (16)
C83	0.072 (3)	0.080 (3)	0.038 (2)	0.012 (2)	−0.0023 (19)	0.0012 (18)
C84	0.074 (3)	0.074 (3)	0.039 (2)	0.016 (2)	0.0152 (19)	0.0111 (18)
C85	0.063 (3)	0.065 (2)	0.050 (2)	0.0034 (19)	0.0203 (19)	0.0121 (18)
C86	0.047 (2)	0.060 (2)	0.0403 (19)	0.0036 (16)	0.0103 (15)	0.0026 (15)
C91	0.0445 (19)	0.0460 (18)	0.0369 (17)	−0.0003 (14)	0.0009 (14)	−0.0048 (13)
C92	0.052 (2)	0.058 (2)	0.057 (2)	−0.0057 (17)	0.0099 (18)	−0.0137 (18)
C93	0.069 (3)	0.066 (3)	0.065 (3)	−0.024 (2)	0.011 (2)	−0.014 (2)
C94	0.080 (3)	0.048 (2)	0.098 (4)	−0.005 (2)	−0.016 (3)	−0.011 (2)
C95	0.067 (3)	0.054 (3)	0.172 (6)	0.013 (2)	−0.023 (4)	−0.044 (3)
C96	0.048 (2)	0.059 (2)	0.113 (4)	0.0042 (19)	−0.006 (2)	−0.033 (3)

Geometric parameters (Å, º)

Cl1—Si1	2.0950 (13)	C42—H42	0.9500
Cl2—Si5	2.0806 (13)	C43—C44	1.384 (7)
Si1—C1	1.874 (4)	C43—H43	0.9500
Si1—C11	1.880 (4)	C44—C45	1.370 (7)
Si1—Si2	2.3856 (13)	C44—H44	0.9500
Si2—C21	1.885 (4)	C45—C46	1.388 (6)
Si2—C31	1.898 (4)	C45—H45	0.9500
Si2—Si3	2.3912 (12)	C46—H46	0.9500
Si3—C41	1.880 (4)	C51—C56	1.391 (5)
Si3—C51	1.881 (3)	C51—C52	1.403 (5)
Si3—Si4	2.3913 (12)	C52—C53	1.390 (5)
Si4—C71	1.882 (3)	C52—H52	0.9500
Si4—C61	1.884 (3)	C53—C54	1.377 (6)
Si4—Si5	2.3710 (13)	C53—H53	0.9500
Si5—C81	1.866 (4)	C54—C55	1.374 (6)
Si5—C91	1.881 (4)	C54—H54	0.9500
C1—C6	1.391 (6)	C55—C56	1.391 (5)
C1—C2	1.403 (5)	C55—H55	0.9500
C2—C3	1.388 (6)	C56—H56	0.9500
C2—H2	0.9500	C61—C62	1.400 (5)
C3—C4	1.370 (7)	C61—C66	1.409 (5)
C3—H3	0.9500	C62—C63	1.385 (5)
C4—C5	1.377 (7)	C62—H62	0.9500
C4—H4	0.9500	C63—C64	1.385 (6)
C5—C6	1.398 (6)	C63—H63	0.9500
C5—H5	0.9500	C64—C65	1.372 (6)
C6—H6	0.9500	C64—H64	0.9500
C11—C16	1.382 (6)	C65—C66	1.384 (5)
C11—C12	1.409 (6)	C65—H65	0.9500
C12—C13	1.385 (7)	C66—H66	0.9500
C12—H12	0.9500	C71—C76	1.395 (5)
C13—C14	1.375 (8)	C71—C72	1.400 (5)
C13—H13	0.9500	C72—C73	1.393 (5)
C14—C15	1.377 (7)	C72—H72	0.9500
C14—H14	0.9500	C73—C74	1.378 (5)
C15—C16	1.398 (6)	C73—H73	0.9500
C15—H15	0.9500	C74—C75	1.375 (5)
C16—H16	0.9500	C74—H74	0.9500
C21—C22	1.397 (5)	C75—C76	1.387 (5)
C21—C26	1.401 (5)	C75—H75	0.9500
C22—C23	1.377 (5)	C76—H76	0.9500
C22—H22	0.9500	C81—C86	1.398 (5)
C23—C24	1.380 (6)	C81—C82	1.398 (5)
C23—H23	0.9500	C82—C83	1.405 (6)
C24—C25	1.383 (6)	C82—H82	0.9500
C24—H24	0.9500	C83—C84	1.367 (7)

C25—C26	1.385 (5)	C83—H83	0.9500
C25—H25	0.9500	C84—C85	1.380 (6)
C26—H26	0.9500	C84—H84	0.9500
C31—C32	1.393 (5)	C85—C86	1.388 (5)
C31—C36	1.395 (5)	C85—H85	0.9500
C32—C33	1.399 (5)	C86—H86	0.9500
C32—H32	0.9500	C91—C96	1.385 (6)
C33—C34	1.371 (7)	C91—C92	1.394 (5)
C33—H33	0.9500	C92—C93	1.388 (6)
C34—C35	1.377 (7)	C92—H92	0.9500
C34—H34	0.9500	C93—C94	1.365 (7)
C35—C36	1.391 (6)	C93—H93	0.9500
C35—H35	0.9500	C94—C95	1.365 (8)
C36—H36	0.9500	C94—H94	0.9500
C41—C46	1.395 (5)	C95—C96	1.397 (6)
C41—C42	1.395 (5)	C95—H95	0.9500
C42—C43	1.384 (6)	C96—H96	0.9500

C1—Si1—C11	108.98 (17)	C43—C42—C41	121.5 (4)
C1—Si1—Cl1	106.74 (12)	C43—C42—H42	119.3
C11—Si1—Cl1	106.44 (12)	C41—C42—H42	119.3
C1—Si1—Si2	112.06 (12)	C44—C43—C42	119.9 (4)
C11—Si1—Si2	117.63 (12)	C44—C43—H43	120.0
Cl1—Si1—Si2	104.19 (5)	C42—C43—H43	120.0
C21—Si2—C31	109.08 (16)	C45—C44—C43	120.0 (4)
C21—Si2—Si1	106.63 (11)	C45—C44—H44	120.0
C31—Si2—Si1	106.62 (11)	C43—C44—H44	120.0
C21—Si2—Si3	115.27 (11)	C44—C45—C46	119.7 (5)
C31—Si2—Si3	109.45 (11)	C44—C45—H45	120.1
Si1—Si2—Si3	109.43 (5)	C46—C45—H45	120.1
C41—Si3—C51	111.58 (15)	C45—C46—C41	121.9 (4)
C41—Si3—Si2	105.39 (11)	C45—C46—H46	119.1
C51—Si3—Si2	105.88 (11)	C41—C46—H46	119.1
C41—Si3—Si4	108.34 (11)	C56—C51—C52	116.6 (3)
C51—Si3—Si4	107.41 (10)	C56—C51—Si3	120.0 (3)
Si2—Si3—Si4	118.27 (5)	C52—C51—Si3	123.4 (3)
C71—Si4—C61	108.09 (15)	C53—C52—C51	121.5 (4)
C71—Si4—Si5	106.31 (11)	C53—C52—H52	119.2
C61—Si4—Si5	108.24 (10)	C51—C52—H52	119.2
C71—Si4—Si3	113.31 (11)	C54—C53—C52	119.9 (4)
C61—Si4—Si3	108.40 (11)	C54—C53—H53	120.1
Si5—Si4—Si3	112.31 (5)	C52—C53—H53	120.1
C81—Si5—C91	111.99 (16)	C55—C54—C53	120.2 (4)
C81—Si5—Cl2	105.85 (12)	C55—C54—H54	119.9
C91—Si5—Cl2	105.68 (12)	C53—C54—H54	119.9
C81—Si5—Si4	113.25 (11)	C54—C55—C56	119.6 (4)
C91—Si5—Si4	111.67 (12)	C54—C55—H55	120.2
Cl2—Si5—Si4	107.84 (5)	C56—C55—H55	120.2

C6—C1—C2	117.9 (4)	C55—C56—C51	122.1 (3)
C6—C1—Si1	121.7 (3)	C55—C56—H56	118.9
C2—C1—Si1	120.2 (3)	C51—C56—H56	118.9
C3—C2—C1	120.8 (4)	C62—C61—C66	116.7 (3)
C3—C2—H2	119.6	C62—C61—Si4	120.7 (3)
C1—C2—H2	119.6	C66—C61—Si4	122.6 (3)
C4—C3—C2	120.2 (4)	C63—C62—C61	122.0 (3)
C4—C3—H3	119.9	C63—C62—H62	119.0
C2—C3—H3	119.9	C61—C62—H62	119.0
C3—C4—C5	120.5 (4)	C62—C63—C64	119.5 (4)
C3—C4—H4	119.7	C62—C63—H63	120.3
C5—C4—H4	119.7	C64—C63—H63	120.3
C4—C5—C6	119.7 (4)	C65—C64—C63	120.3 (4)
C4—C5—H5	120.2	C65—C64—H64	119.8
C6—C5—H5	120.2	C63—C64—H64	119.8
C1—C6—C5	121.0 (4)	C64—C65—C66	120.1 (4)
C1—C6—H6	119.5	C64—C65—H65	119.9
C5—C6—H6	119.5	C66—C65—H65	119.9
C16—C11—C12	117.7 (4)	C65—C66—C61	121.4 (4)
C16—C11—Si1	123.3 (3)	C65—C66—H66	119.3
C12—C11—Si1	119.0 (3)	C61—C66—H66	119.3
C13—C12—C11	121.2 (5)	C76—C71—C72	117.3 (3)
C13—C12—H12	119.4	C76—C71—Si4	121.0 (2)
C11—C12—H12	119.4	C72—C71—Si4	121.6 (2)
C14—C13—C12	119.8 (5)	C73—C72—C71	120.9 (3)
C14—C13—H13	120.1	C73—C72—H72	119.5
C12—C13—H13	120.1	C71—C72—H72	119.5
C13—C14—C15	120.4 (5)	C74—C73—C72	120.1 (3)
C13—C14—H14	119.8	C74—C73—H73	119.9
C15—C14—H14	119.8	C72—C73—H73	119.9
C14—C15—C16	119.9 (5)	C75—C74—C73	120.1 (3)
C14—C15—H15	120.1	C75—C74—H74	119.9
C16—C15—H15	120.1	C73—C74—H74	119.9
C11—C16—C15	121.0 (4)	C74—C75—C76	119.8 (3)
C11—C16—H16	119.5	C74—C75—H75	120.1
C15—C16—H16	119.5	C76—C75—H75	120.1
C22—C21—C26	117.0 (3)	C75—C76—C71	121.7 (3)
C22—C21—Si2	122.8 (3)	C75—C76—H76	119.1
C26—C21—Si2	120.1 (3)	C71—C76—H76	119.1
C23—C22—C21	122.1 (3)	C86—C81—C82	117.9 (3)
C23—C22—H22	119.0	C86—C81—Si5	121.3 (3)
C21—C22—H22	119.0	C82—C81—Si5	120.8 (3)
C22—C23—C24	119.8 (4)	C81—C82—C83	120.2 (4)
C22—C23—H23	120.1	C81—C82—H82	119.9
C24—C23—H23	120.1	C83—C82—H82	119.9
C23—C24—C25	119.9 (4)	C84—C83—C82	120.5 (4)
C23—C24—H24	120.0	C84—C83—H83	119.8
C25—C24—H24	120.0	C82—C83—H83	119.8

C24—C25—C26	120.1 (4)	C83—C84—C85	120.1 (4)
C24—C25—H25	120.0	C83—C84—H84	119.9
C26—C25—H25	120.0	C85—C84—H84	119.9
C25—C26—C21	121.2 (4)	C84—C85—C86	120.0 (4)
C25—C26—H26	119.4	C84—C85—H85	120.0
C21—C26—H26	119.4	C86—C85—H85	120.0
C32—C31—C36	117.5 (3)	C85—C86—C81	121.2 (4)
C32—C31—Si2	121.6 (3)	C85—C86—H86	119.4
C36—C31—Si2	121.0 (3)	C81—C86—H86	119.4
C31—C32—C33	121.2 (4)	C96—C91—C92	117.2 (4)
C31—C32—H32	119.4	C96—C91—Si5	119.8 (3)
C33—C32—H32	119.4	C92—C91—Si5	122.9 (3)
C34—C33—C32	120.0 (4)	C93—C92—C91	121.3 (4)
C34—C33—H33	120.0	C93—C92—H92	119.4
C32—C33—H33	120.0	C91—C92—H92	119.4
C33—C34—C35	119.9 (4)	C94—C93—C92	120.3 (4)
C33—C34—H34	120.1	C94—C93—H93	119.8
C35—C34—H34	120.1	C92—C93—H93	119.8
C34—C35—C36	120.3 (4)	C95—C94—C93	119.7 (4)
C34—C35—H35	119.9	C95—C94—H94	120.2
C36—C35—H35	119.9	C93—C94—H94	120.2
C35—C36—C31	121.2 (4)	C94—C95—C96	120.4 (5)
C35—C36—H36	119.4	C94—C95—H95	119.8
C31—C36—H36	119.4	C96—C95—H95	119.8
C46—C41—C42	116.9 (3)	C91—C96—C95	121.0 (4)
C46—C41—Si3	118.9 (3)	C91—C96—H96	119.5
C42—C41—Si3	124.1 (3)	C95—C96—H96	119.5

C11—Si1—C1—C6	145.0 (3)	C41—Si3—C51—C56	−147.5 (3)
Cl1—Si1—C1—C6	30.5 (3)	Si2—Si3—C51—C56	−33.3 (3)
Si2—Si1—C1—C6	−83.0 (3)	Si4—Si3—C51—C56	93.9 (3)
C11—Si1—C1—C2	−39.6 (3)	C41—Si3—C51—C52	32.4 (3)
Cl1—Si1—C1—C2	−154.2 (3)	Si2—Si3—C51—C52	146.5 (3)
Si2—Si1—C1—C2	92.3 (3)	Si4—Si3—C51—C52	−86.2 (3)
C6—C1—C2—C3	0.0 (5)	C56—C51—C52—C53	1.8 (5)
Si1—C1—C2—C3	−175.6 (3)	Si3—C51—C52—C53	−178.1 (3)
C1—C2—C3—C4	−0.4 (6)	C51—C52—C53—C54	0.6 (6)
C2—C3—C4—C5	0.3 (7)	C52—C53—C54—C55	−1.9 (7)
C3—C4—C5—C6	0.3 (7)	C53—C54—C55—C56	0.7 (6)
C2—C1—C6—C5	0.6 (6)	C54—C55—C56—C51	1.8 (6)
Si1—C1—C6—C5	176.0 (3)	C52—C51—C56—C55	−3.0 (5)
C4—C5—C6—C1	−0.7 (6)	Si3—C51—C56—C55	176.8 (3)
C1—Si1—C11—C16	149.9 (3)	C71—Si4—C61—C62	1.4 (3)
Cl1—Si1—C11—C16	−95.4 (3)	Si5—Si4—C61—C62	116.1 (3)
Si2—Si1—C11—C16	20.9 (4)	Si3—Si4—C61—C62	−121.8 (3)
C1—Si1—C11—C12	−28.3 (4)	C71—Si4—C61—C66	179.5 (3)
Cl1—Si1—C11—C12	86.5 (3)	Si5—Si4—C61—C66	−65.8 (3)
Si2—Si1—C11—C12	−157.2 (3)	Si3—Si4—C61—C66	56.3 (3)

C16—C11—C12—C13	−2.3 (6)	C66—C61—C62—C63	−0.6 (5)
Si1—C11—C12—C13	175.9 (4)	Si4—C61—C62—C63	177.6 (3)
C11—C12—C13—C14	1.3 (8)	C61—C62—C63—C64	0.2 (6)
C12—C13—C14—C15	0.1 (8)	C62—C63—C64—C65	−0.1 (6)
C13—C14—C15—C16	−0.3 (8)	C63—C64—C65—C66	0.4 (6)
C12—C11—C16—C15	2.0 (6)	C64—C65—C66—C61	−0.8 (6)
Si1—C11—C16—C15	−176.1 (3)	C62—C61—C66—C65	0.9 (5)
C14—C15—C16—C11	−0.8 (7)	Si4—C61—C66—C65	−177.3 (3)
C31—Si2—C21—C22	−132.3 (3)	C61—Si4—C71—C76	−101.8 (3)
Si1—Si2—C21—C22	112.9 (3)	Si5—Si4—C71—C76	142.2 (3)
Si3—Si2—C21—C22	−8.7 (3)	Si3—Si4—C71—C76	18.3 (3)
C31—Si2—C21—C26	51.8 (3)	C61—Si4—C71—C72	75.2 (3)
Si1—Si2—C21—C26	−63.0 (3)	Si5—Si4—C71—C72	−40.8 (3)
Si3—Si2—C21—C26	175.3 (2)	Si3—Si4—C71—C72	−164.6 (3)
C26—C21—C22—C23	0.5 (5)	C76—C71—C72—C73	0.8 (5)
Si2—C21—C22—C23	−175.5 (3)	Si4—C71—C72—C73	−176.3 (3)
C21—C22—C23—C24	−0.7 (6)	C71—C72—C73—C74	−0.7 (6)
C22—C23—C24—C25	0.3 (6)	C72—C73—C74—C75	0.2 (6)
C23—C24—C25—C26	0.4 (6)	C73—C74—C75—C76	0.3 (6)
C24—C25—C26—C21	−0.6 (6)	C74—C75—C76—C71	−0.2 (6)
C22—C21—C26—C25	0.1 (5)	C72—C71—C76—C75	−0.4 (5)
Si2—C21—C26—C25	176.3 (3)	Si4—C71—C76—C75	176.8 (3)
C21—Si2—C31—C32	13.2 (3)	C91—Si5—C81—C86	−148.8 (3)
Si1—Si2—C31—C32	128.0 (3)	Cl2—Si5—C81—C86	−34.1 (3)
Si3—Si2—C31—C32	−113.7 (3)	Si4—Si5—C81—C86	83.8 (3)
C21—Si2—C31—C36	−168.0 (3)	C91—Si5—C81—C82	34.4 (3)
Si1—Si2—C31—C36	−53.2 (3)	Cl2—Si5—C81—C82	149.1 (3)
Si3—Si2—C31—C36	65.1 (3)	Si4—Si5—C81—C82	−92.9 (3)
C36—C31—C32—C33	0.6 (5)	C86—C81—C82—C83	0.0 (6)
Si2—C31—C32—C33	179.5 (3)	Si5—C81—C82—C83	176.8 (3)
C31—C32—C33—C34	0.0 (6)	C81—C82—C83—C84	−1.8 (6)
C32—C33—C34—C35	−0.1 (7)	C82—C83—C84—C85	2.6 (7)
C33—C34—C35—C36	−0.4 (7)	C83—C84—C85—C86	−1.6 (6)
C34—C35—C36—C31	1.1 (7)	C84—C85—C86—C81	−0.2 (6)
C32—C31—C36—C35	−1.1 (6)	C82—C81—C86—C85	1.0 (6)
Si2—C31—C36—C35	180.0 (3)	Si5—C81—C86—C85	−175.8 (3)
C51—Si3—C41—C46	−162.2 (3)	C81—Si5—C91—C96	94.6 (4)
Si2—Si3—C41—C46	83.3 (3)	Cl2—Si5—C91—C96	−20.2 (4)
Si4—Si3—C41—C46	−44.2 (3)	Si4—Si5—C91—C96	−137.2 (3)
C51—Si3—C41—C42	19.0 (4)	C81—Si5—C91—C92	−86.3 (3)
Si2—Si3—C41—C42	−95.5 (3)	Cl2—Si5—C91—C92	158.9 (3)
Si4—Si3—C41—C42	137.0 (3)	Si4—Si5—C91—C92	41.9 (3)
C46—C41—C42—C43	2.7 (6)	C96—C91—C92—C93	0.3 (6)
Si3—C41—C42—C43	−178.5 (3)	Si5—C91—C92—C93	−178.9 (3)
C41—C42—C43—C44	−1.6 (7)	C91—C92—C93—C94	1.4 (7)
C42—C43—C44—C45	−0.2 (8)	C92—C93—C94—C95	−2.8 (9)
C43—C44—C45—C46	0.7 (8)	C93—C94—C95—C96	2.4 (10)
C44—C45—C46—C41	0.6 (7)	C92—C91—C96—C95	−0.6 (8)

C42—C41—C46—C45	−2.2 (6)	Si5—C91—C96—C95	178.6 (5)
Si3—C41—C46—C45	178.9 (3)	C94—C95—C96—C91	−0.7 (10)