

## **Experimental Procedures and Characterization Data for New Compounds**

### **Synthesis and Properties of the First 1-Silanaphthalene**

Nobuhiro Takeda, Akihiro Shinohara, Norihiro Tokitoh\*

*Institute for Chemical Research, Kyoto University, Gokasho, Uji, Kyoto 611-0011, Japan*

**General Procedure.** All melting points are uncorrected. All solvents used were purified by the reported methods. THF was purified by distillation from sodium diphenylketyl before use. All reactions were carried out under an argon atmosphere, unless otherwise noted. Preparative gel permeation liquid chromatography (GPLC) was performed on an LC-908 instrument with JAI gel 1H+2H columns (Japan Analytical Industry) using chloroform as solvent. Flash column chromatography (FCC) was carried out with Nacalai Tesque Silica Gel 60. Preparative thin-layer chromatography (PTLC) and flash column chromatography (FCC) were performed with Merck Kieselgel 60 PF254 (Art. No. 7747) and Merck Silica Gel 60, respectively. The <sup>1</sup>H NMR (400 or 300 MHz) and <sup>13</sup>C NMR (100 or 75 MHz) spectra were measured in CDCl<sub>3</sub> or C<sub>6</sub>D<sub>6</sub> with a JEOL AL-400 or AL-300 spectrometer using CHCl<sub>3</sub> or C<sub>6</sub>D<sub>5</sub>H as an internal standard. The <sup>29</sup>Si NMR (59 MHz) spectra were measured in CDCl<sub>3</sub> or C<sub>6</sub>D<sub>6</sub> with a JEOL AL-300 spectrometer using tetramethylsilane as an external standard. The electronic spectra were recorded on a JASCO Ubest-50 UV-vis spectrometer. Elemental analyses were performed by the Microanalytical Laboratory of the Institute for Chemical Research, Kyoto University.

**Preparation of 1,4-Dihydro-1-[2,4,6-tris[bis(trimethylsilyl)methyl]phenyl]-1-sila-naphthalene (6).** To a solution of 1-bromo-2-(3-bromo-2-propenyl)benzene **5** (140 mg, 0.511 mmol) in ether (5 ml) was added 2.32 M hexane solution of *t*-butyllithium (0.86 ml, 2.0 mmol) at -78 °C. After the solution was stirred at -78 °C for 1.5 h and at room temperature for 1 h, a solution of [2,4,6-tris[bis(trimethylsilyl)methyl]phenyl]trihydrosilane (357 mg, 0.613 mmol) in ether (4 ml) was added at room temperature. After further stirring for 1 h, the reaction mixture was quenched with an aqueous solution of NH<sub>4</sub>Cl and extracted with ether. The organic layer was dried over Na<sub>2</sub>SO<sub>4</sub>, filtrated and evaporated. The crude product was purified by FCC (hexane) and GPLC (CHCl<sub>3</sub>) to give the mixture of hydrosilane **6** (152 mg, 43%). **6:** white powder, mp. 167.5-170.8 °C; <sup>1</sup>H NMR (300 MHz, r.t., CDCl<sub>3</sub>) δ -0.19 (s, 9H), -0.16 (s, 9H),

0.04 (s, 18H), 0.06 (s, 18H), 1.32 (s, 1H), 2.30 (br s, 1H), 2.33 (br s, 1H), 3.76-3.79 (m, 2H), 5.58-5.60 (m, 1H), 6.14 (ddd,  $^3J = 14$  Hz,  $^4J = 2$  Hz, 1H), 6.29 (br s, 1H), 6.38 (br s, 1H), 6.94 (ddd,  $^3J = 14$  Hz,  $^3J = 4$  Hz,  $^3J = 4$  Hz, 1H), 7.11-7.19 (m, 2H), 7.26-7.32 (m, 1H), 7.44 (dd,  $^3J = 7.5$  Hz,  $^4J = 1.5$  Hz, 1H);  $^{13}\text{C}$  NMR (75 MHz, r.t.,  $\text{CDCl}_3$ )  $\delta$  0.52 (q), 0.72 (q), 0.76 (q), 0.98 (q), 1.27 (q), 28.17 (d), 28.48 (d), 30.53 (d), 36.08 (t), 121.93 (d), 123.72 (s), 124.95 (d), 125.56 (d), 126.91 (d), 128.99 (d), 129.17 (d), 131.33 (s), 136.09 (d), 144.25 (s), 144.97 (s), 146.07 (d), 152.69 (s), 152.87 (s);  $^{29}\text{Si}$  NMR (59 MHz, r.t.,  $\text{CDCl}_3$ )  $\delta$  -54.4, 1.8, 1.9; Anal. Calcd for  $\text{C}_{36}\text{H}_{68}\text{Si}_7$ : C, 61.99; H, 9.83. Found: C, 61.93; H, 10.06.

**Preparation of 1-Bromo-1,4-dihydro-1-[2,4,6-tris[bis(trimethylsilyl)methyl]phenyl]-1-silanaphthalene (7).** A solution of **6** (196 mg, 0.281 mmol) and NBS (55.9 mg, 0.300 mmol) in benzene (30 ml) was stirred under air. After 12 h, the solvent was evaporated. Separation of the mixture by GPC ( $\text{CHCl}_3$ ) afforded bromosilane **7** (193 mg, 0.249 mmol, 89%). **7**: white powder, mp. 207.5-210.4 °C;  $^1\text{H}$  NMR (300 MHz, r.t.,  $\text{CDCl}_3$ );  $\delta$  -0.17 (s, 9H), 0.14 (s, 9H), 0.03 (s, 9H), 0.04 (s, 18H), 0.06 (s, 9H), 1.30 (s, 1H), 2.50 (br s, 1H), 2.56 (br s, 1H), 3.49-3.64 (m, 2H), 6.26 (br s, 1H), 6.79 (br s, 1H), 6.49 (d,  $^3J = 14$  Hz, 1H), 6.94-7.01 (m, 1H), 7.14-7.17 (m, 1H), 7.28-7.39 (m, 2H), 8.01-8.04 (m, 1H);  $^{13}\text{C}$  NMR (75 MHz, r.t.,  $\text{CDCl}_3$ );  $\delta$  0.76 (q), 0.80 (q), 1.06 (q), 1.25 (q), 1.40 (q), 28.22 (d), 28.64 (d), 30.65 (d), 36.28 (t), 122.59 (d), 122.90 (s), 126.58 (d), 127.68 (d), 128.57 (d), 129.39 (d), 130.59 (d), 136.44 (s), 137.99 (d), 144.50 (s), 146.16 (s), 146.19 (d), 152.78 (s), 153.29 (s);  $^{29}\text{Si}$  NMR (59 MHz, r.t.,  $\text{CDCl}_3$ );  $\delta$  -23.4, -0.7, 2.6, 2.8; Anal. Calcd for  $\text{C}_{36}\text{H}_{67}\text{Si}_7\text{Br}$ : C, 55.69; H, 8.70. Found: C, 55.67; H, 8.74.

**Synthesis of 1-[2,4,6-Tris[bis(trimethylsilyl)methyl]phenyl]-1-silanaphthalene (4).** In a glovebox filled with argon, **7** (40.2 mg, 0.0519 mmol) was dissolved in THF (2 ml), to this solution was added lithium diisopropylamide (2.0 M solution in heptane/THF/ethylbenzene,

0.026 ml, 0.052 mmol, Aldrich chemicals co.) at -40 °C. After removal of solvents under reduced pressure, cold hexane was added to the residue and the resulting suspension was filtered through Celite®. Evaporation of the filtrate afforded **4** (34.8 mg, 97%). **4**: pale yellow crystals, mp. 127-132 °C (dec.); <sup>1</sup>H NMR (400 MHz, 10 °C, C<sub>6</sub>D<sub>6</sub>) δ 0.04 (s, 9H), 0.08 (s, 9H), 0.15 (s, 18H), 0.18 (s, 18H), 1.55 (s, 1H), 2.49 (br s, 1H), 2.57 (br s, 1H), 6.64 (br s, 1H), 6.77 (br s, 1H), 7.10 (d, <sup>3</sup>J = 11.6 Hz, 1H), 7.15 (ddd, <sup>3</sup>J = 7.8 Hz, <sup>3</sup>J = 6.9 Hz, <sup>4</sup>J = 1.0 Hz, 1H), 7.17 (d, <sup>3</sup>J = 9.2 Hz, 1H), 7.36 (ddd, <sup>3</sup>J = 8.2 Hz, <sup>3</sup>J = 6.9 Hz, <sup>4</sup>J = 1.5 Hz, 1H), 7.73 (dd, <sup>3</sup>J = 8.2 Hz, <sup>4</sup>J = 1.0 Hz, 1H), 8.07 (dd, <sup>3</sup>J = 11.6 Hz, <sup>3</sup>J = 9.2 Hz, 1H), 8.22 (dd, <sup>3</sup>J = 7.8 Hz, <sup>4</sup>J = 1.5 Hz, 1H); <sup>13</sup>C NMR (100 MHz, 10 °C, C<sub>6</sub>D<sub>6</sub>) δ 0.94 (q), 1.20 (q), 1.26 (q), 1.54 (q), 31.68 (d), 36.52 (d), 36.95 (d), 116.74 (d), 116.89 (d), 120.58 (d), 121.77 (d), 123.64 (s), 126.29 (d), 128.76 (d), 131.40 (d), 131.52 (s), 133.19 (d), 137.95 (d), 145.33 (s), 148.16 (s), 153.05 (s), 153.16 (s); <sup>29</sup>Si NMR (59 MHz, 10 °C, C<sub>6</sub>D<sub>6</sub>) δ 2.2, 2.5, 2.6, 3.3, 91.7. UV-vis (hexane) λ<sub>max</sub> 254 (4 × 10<sup>4</sup>), 354 (2 × 10<sup>4</sup>), 364 (2 × 10<sup>4</sup>), and 378 (1 × 10<sup>4</sup>) nm; High resolution FAB-MS *m/z* calcd for C<sub>36</sub>H<sub>66</sub>Si<sub>7</sub> ([M]<sup>+</sup>): 694.3549, found: 694.3556 ([M]<sup>+</sup>). Elemental analysis of **4** gave values [Anal. Found: C, 60.41; H, 9.31.] agreed with the calculated values for the corresponding hydrolyzed product [Calcd for C<sub>72</sub>H<sub>68</sub>OSi<sub>7</sub>: C, 60.60; H, 9.61] due to the high sensitivity of **4** to moisture.

**Dimerization of 4.** In a glovebox filled with argon, **7** (35.9 mg, 0.463 mmol) was dissolved in THF (2 ml), and lithium diisopropylamide (2.0 M solution in heptane/THF/ethylbenzene, 0.035 ml, 0.070 mmol, Aldrich chemicals co.) was added to the solution at -40 °C. After removal of the solvents under reduced pressure, cold hexane was added to the residue and the resulting suspension was filtered through Celite®. The residue was dissolved in C<sub>6</sub>D<sub>6</sub> (0.6 ml) and the solution was put into a 5 φ NMR tube. After heating at 100 °C for 12 h, the tube was opened. The solvent was evaporated and hexane was added to the residue. Filtration of the mixture through Celite® followed by separation with GPLC (CHCl<sub>3</sub>) and PTLC (hexane) afforded

**9** (15.9 mg, 49%). **9:** white powder, mp. 144.3–147.8 °C;  $^1\text{H}$  NMR (300 MHz, r.t.,  $\text{CDCl}_3$ )  $\delta$  –0.25 (s, 9H), –0.22 (s, 9H), –0.18 (s, 18H), 0.04 (s, 27H), 0.08 (s, 9H), 0.09 (s, 18H), 0.18 (s, 9H), 0.21 (s, 9H), 1.26 (d,  $^3J = 10$  Hz, 1H), 1.28 (s, 1H), 1.35 (s, 1H), 2.10–2.16 (m, 4H), 4.02 (d,  $^3J = 7$  Hz, 1H), 5.89 (d,  $^3J = 11$  Hz, 1H), 6.10 (d,  $^3J = 8$  Hz, 1H), 6.26–6.48 (m, 6H), 6.57–6.59 (m, 1H), 6.77–6.79 (m, 1H), 6.81–6.84 (m, 2H), 6.95–6.98 (m, 1H), 7.57–7.64 (m, 1H);  $^{13}\text{C}$  NMR (75 MHz, r.t.,  $\text{CDCl}_3$ )  $\delta$  0.81 (q), 0.91 (q), 0.98 (q), 0.99 (q), 1.14 (q), 1.27 (q), 1.37 (q), 1.49 (q), 1.69 (q), 1.75 (q), 2.06 (q), 2.12 (q), 15.36 (d), 27.11 (d), 27.21 (d), 28.48 (d  $\times 2$ ), 30.30 (d), 30.46 (d), 42.28 (d), 122.89 (d), 122.93 (d), 123.18 (d), 123.23 (s), 125.82 (d), 125.85 (d), 127.60 (d), 127.84 (d), 127.86 (d), 127.95 (d), 128.32 (s), 128.59 (d), 128.66 (d), 129.53 (d), 131.21 (d), 133.40 (d), 133.81 (d), 134.81 (s), 135.40 (s), 140.57 (s), 143.87 (s), 144.46 (s), 144.88 (s), 148.91 (d), 152.39 (s), 152.54 (s), 152.83 (s), 152.99 (s);  $^{29}\text{Si}$  NMR (59 MHz, r.t.,  $\text{CDCl}_3$ )  $\delta$  –33.2, –24.6, 1.67, 1.71, 1.9, 1.98, 2.04, 2.1, 2.2, 2.3, 2.7; Anal. Calcd for  $\text{C}_{72}\text{H}_{132}\text{Si}_{14}$ : C, 62.17; H, 9.56. Found: C, 61.85; H, 9.53.

**Spectroscopic Data and Elemental Analysis for the Dimer of 1.** White powder, mp. 152.1–154.4 °C (dec).  $^1\text{H}$  NMR (300 MHz, r.t.,  $\text{CDCl}_3$ )  $\delta$  0.02 (s, 18H), 0.03 (s, 18H), 0.037 (s, 9H), 0.043 (s, 18H), 0.07 (s, 27H), 0.10 (s, 9H), 0.14 (s, 9H), 1.25 (d,  $^3J = 1.8$  Hz, 1H), 1.29 (s, 1H), 1.34 (s, 1H), 2.04 (s, 1H), 2.13 (s, 1H), 2.33 (s, 1H), 2.55 (s, 1H), 4.14 (t,  $^3J = 7.2$  Hz, 1H), 5.54 (d,  $^3J = 13.8$  Hz, 1H), 5.69 (dd,  $^3J = 10.3$  Hz,  $^3J = 5.9$  Hz, 1H), 6.26–6.47 (m, 8H), 6.84 (dd,  $^3J = 12.2$  Hz,  $^3J = 7.7$  Hz, 1H), 7.47 (dd,  $^3J = 12.7$  Hz,  $^3J = 6.8$  Hz, 1H).  $^{13}\text{C}$  NMR (76 MHz, r.t.,  $\text{CDCl}_3$ )  $\delta$  0.77 (q), 0.79 (q), 0.90 (q), 1.00 (q), 1.08 (q), 1.10 (q), 1.24 (q), 1.38 (q), 1.55 (q), 1.66 (q), 1.79 (q), 2.12 (q), 14.36 (d), 27.06 (d), 27.45 (d), 29.10 (d), 29.17 (d), 30.36 (d), 30.55 (d), 39.88 (d), 122.42 (d), 122.50 (d), 122.82 (d), 124.05 (d), 127.37 (d), 127.93 (d), 128.22 (d), 129.01 (s), 129.35 (d), 130.26 (d), 135.50 (d), 140.75 (d), 144.07 (s), 144.99 (s), 148.01 (d), 150.68 (d), 151.97 (s), 153.10 (s), 153.24 (s), 153.58 (s).  $^{29}\text{Si}$  NMR (60 MHz, r.t.,  $\text{CDCl}_3$ )  $\delta$

-42.64, -24.12, 1.66, 1.72, 1.78, 1.84, 1.87, 1.95, 2.01, 2.08, 2.15, 2.23, 2.48. Anal. calcd for C<sub>64</sub>H<sub>128</sub>Si<sub>14</sub>H<sub>2</sub>O: C, 58.73; H, 10.01%. Found C, 58.88; H, 9.62%.

**X-ray Data Collection.** The intensity data of **9**·CHCl<sub>3</sub> were collected on a Rigaku/MSC Mercury CCD diffractometer with graphite monochromated MoK $\alpha$  radiation ( $\lambda = 0.71070 \text{ \AA}$ ). The structure was solved by direct method SHELX-97,<sup>1</sup> and refined by full-matrix least-square method. All hydrogen atoms were placed using AFIX instructions.

**Computational Methods.** The geometries of 1-silanaphthalenes **8a** and **8b** were optimized by using the Gaussian 98 program<sup>2</sup> at B3LYP/6-31G(d). GIAO-B3LYP calculations were carried out with 6-311G(3d) for Si and 6-311G(d) for C and H, and NICS calculations were carried out with 6-311G(d).

## References

- (1) Sheldrick, G. M. In; University of Göttingen: Göttingen, Germany, 1997.
- (2) Fisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Zakrzewski, V. G.; Jr., J. A. M.; Stratmann, R. E.; Burant, J. C.; Dapprich, S.; Millam, J. M.; Daniels, A. D.; Kudin, K. N.; Strain, M. C.; Farkas, O.; Tomasi, J.; Barone, V.; Cossi, M.; Cammi, R.; Mennucci, B.; Pomelli, C.; Adamo, C.; Clifford, S.; Ochterski, J.; Petersson, G. A.; Ayala, P. Y.; Cui, Q.; Morokuma, K.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Cioslowski, J.; Ortiz, J. V.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Gomperts, R.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Gonzalez, C.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Andres, J. L.; Head-Gordon, M.; Replogle, E. S.; Pople, J. A. In; Gaussian, Inc.: Pittsburgh, 1998.

## Crystallographic Data for 9·CHCl<sub>3</sub>

### Synthesis and Properties of the First 1-Silanaphthalene

Nobuhiro Takeda, Akihiro Shinohara, Norihiro Tokitoh\*

*Institute for Chemical Research, Kyoto University, Gokasho, Uji, Kyoto 611-0011, Japan*

Table 1. Crystal data and structure refinement for dimer 9·CHCl<sub>3</sub>.

Identification code	dimer	
Empirical formula	C <sub>73</sub> H <sub>133</sub> Cl <sub>3</sub> Si <sub>14</sub>	
Formula weight	1510.40	
Temperature	93(2) K	
Wavelength	0.71070 Å	
Crystal system	triclinic	
Space group	P-1(#2)	
Unit cell dimensions	a = 13.215(5) Å b = 18.439(7) Å c = 20.390(8) Å	α = 74.679(15)°. β = 79.450(18)°. γ = 78.132(17)°.
Volume	4645(3) Å <sup>3</sup>	
Z	2	
Density (calculated)	1.080 Mg/m <sup>3</sup>	
Absorption coefficient	0.314 mm <sup>-1</sup>	
F(000)	1636	
Crystal size	0.30 x 0.30 x 0.20 mm <sup>3</sup>	
Theta range for data collection	3.02 to 25.00°	
Index ranges	-12<=h<=15, -20<=k<=21, -24<=l<=24	
Reflections collected	30782	
Independent reflections	16026 [R(int) = 0.0804]	
Completeness to theta = 25.00°	97.9 %	
Max. and min. transmission	0.9398 and 0.9116	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	16026 / 61 / 921	
Goodness-of-fit on F <sup>2</sup>	1.164	
Final R indices [I>2sigma(I)]	R1 = 0.1006, wR2 = 0.2142	
R indices (all data)	R1 = 0.1328, wR2 = 0.2331	
Largest diff. peak and hole	0.797 and -0.563 e.Å <sup>-3</sup>	

Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for dimer 9-CHCl<sub>3</sub>. U(eq) is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	U(eq)
Si(1)	2707(1)	11142(1)	2924(1)	14(1)
C(1)	3759(4)	10331(3)	2701(3)	17(1)
C(2)	4736(4)	10258(3)	3009(3)	19(1)
C(3)	4824(4)	10493(3)	3564(3)	22(1)
C(4)	4213(5)	11058(3)	4566(3)	26(1)
C(5)	3507(5)	11542(3)	4917(3)	32(1)
C(6)	2634(5)	11966(3)	4637(3)	33(1)
C(7)	2447(4)	11895(3)	4008(3)	24(1)
C(8)	4036(4)	10978(3)	3934(2)	18(1)
C(9)	3128(4)	11389(3)	3658(2)	19(1)
Si(2)	3187(1)	9389(1)	3065(1)	15(1)
C(10)	1893(4)	9616(3)	2742(3)	20(1)
C(11)	1235(4)	10167(3)	2982(3)	22(1)
C(12)	1548(4)	10610(3)	3413(3)	18(1)
C(13)	1659(4)	10254(3)	4694(3)	25(1)
C(14)	2142(5)	9807(3)	5256(3)	27(1)
C(15)	2958(4)	9220(3)	5180(3)	24(1)
C(16)	3282(4)	9059(3)	4538(3)	19(1)
C(17)	1994(4)	10094(3)	4051(3)	18(1)
C(18)	2796(4)	9481(3)	3972(2)	14(1)
C(19)	2441(4)	12060(3)	2221(2)	16(1)
C(20)	3233(4)	12537(3)	1980(3)	18(1)
C(21)	2998(4)	13276(3)	1562(3)	22(1)
C(22)	2017(4)	13579(3)	1358(3)	21(1)
C(23)	1275(4)	13094(3)	1569(2)	20(1)
C(24)	1457(4)	12356(3)	1977(2)	19(1)
C(25)	4344(4)	12287(3)	2143(3)	21(1)
C(26)	1737(5)	14375(3)	922(3)	29(1)
C(27)	580(4)	11907(3)	2103(3)	19(1)
Si(3)	5291(1)	12081(1)	1368(1)	23(1)
Si(4)	4774(1)	12966(1)	2570(1)	24(1)
Si(5)	2376(2)	14491(1)	10(1)	40(1)
Si(6)	1618(2)	15148(1)	1389(1)	36(1)
Si(7)	487(1)	11607(1)	1300(1)	24(1)
Si(8)	-649(1)	12337(1)	2607(1)	24(1)

C(28)	4942(5)	11303(3)	1059(3)	29(1)
C(29)	5334(5)	12904(3)	602(3)	36(2)
C(30)	6627(4)	11762(3)	1618(3)	32(1)
C(31)	3646(5)	13476(3)	3060(3)	32(1)
C(32)	5467(5)	13714(3)	1943(3)	32(1)
C(33)	5697(5)	12401(3)	3186(3)	35(2)
C(34)	2585(6)	13563(4)	-234(3)	47(2)
C(35)	1512(7)	15195(5)	-568(4)	71(3)
C(36)	3666(6)	14835(5)	-126(5)	69(2)
C(37)	801(6)	14884(5)	2229(4)	59(2)
C(38)	983(8)	16075(4)	886(5)	83(3)
C(39)	2893(6)	15297(4)	1561(4)	56(2)
C(40)	1832(5)	11204(4)	969(3)	37(2)
C(41)	-349(5)	10852(4)	1509(3)	37(2)
C(42)	-46(6)	12395(4)	607(3)	45(2)
C(43)	-1365(5)	11551(3)	3128(3)	37(2)
C(44)	-1550(5)	13064(3)	2063(3)	36(2)
C(45)	-268(5)	12833(4)	3187(3)	38(2)
C(46)	3919(4)	8388(3)	3058(2)	15(1)
C(47)	4950(4)	8188(3)	2748(2)	15(1)
C(48)	5467(4)	7436(3)	2925(3)	17(1)
C(49)	5022(4)	6860(3)	3395(2)	15(1)
C(50)	3965(4)	7038(3)	3644(3)	19(1)
C(51)	3396(4)	7772(3)	3475(2)	16(1)
C(52)	5527(4)	8754(3)	2188(2)	17(1)
C(53)	5604(4)	6065(3)	3644(3)	21(1)
C(54)	2229(4)	7851(3)	3706(3)	20(1)
Si(9)	5265(1)	8730(1)	1308(1)	21(1)
Si(10)	6946(1)	8716(1)	2282(1)	21(1)
Si(11)	6088(1)	5526(1)	2940(1)	28(1)
Si(12)	6492(1)	6053(1)	4277(1)	24(1)
Si(13)	1637(1)	7428(1)	3128(1)	28(1)
Si(14)	1707(1)	7544(1)	4655(1)	22(1)
C(55)	3918(4)	9245(3)	1192(3)	29(1)
C(56)	6170(5)	9234(4)	592(3)	33(1)
C(57)	5381(6)	7732(3)	1218(3)	39(2)
C(58)	7074(4)	8579(3)	3202(3)	27(1)
C(59)	7376(5)	9649(3)	1826(3)	33(1)
C(60)	7882(4)	7956(3)	1931(3)	31(1)
C(61)	4964(5)	5632(3)	2466(4)	43(2)

C(62)	7212(6)	5860(4)	2320(3)	43(2)
C(63)	6488(6)	4494(3)	3349(3)	43(2)
C(64)	6717(5)	5076(3)	4850(3)	41(2)
C(65)	5801(5)	6715(4)	4819(3)	35(2)
C(66)	7775(5)	6327(4)	3864(3)	47(2)
C(67)	1825(5)	6358(3)	3331(3)	38(2)
C(68)	201(5)	7834(4)	3171(4)	46(2)
C(69)	2259(5)	7712(4)	2224(3)	39(2)
C(70)	963(5)	6723(3)	4890(3)	35(1)
C(71)	740(4)	8367(3)	4866(3)	30(1)
C(72)	2758(4)	7235(3)	5220(3)	25(1)
C(73)	1495(6)	8890(6)	632(4)	40(2)
Cl(1)	246(6)	8690(5)	968(5)	66(2)
Cl(2)	2266(6)	8136(3)	327(6)	80(2)
Cl(3)	1392(3)	9724(2)	-31(1)	75(1)
C(74)	1085(17)	8838(12)	358(12)	59(7)
Cl(4)	200(20)	8595(15)	1095(18)	70(6)
Cl(5)	2070(20)	8074(12)	280(20)	96(8)
Cl(6)	1581(12)	9627(8)	411(10)	105(4)
C(75)	9590(20)	5096(15)	5992(13)	138(16)
Cl(7)	8617(14)	5897(14)	5938(11)	82(6)
Cl(8)	10050(30)	4920(18)	5191(12)	98(9)
Cl(9)	10593(19)	5249(17)	6370(14)	112(9)

Table 3. Bond lengths [Å] and angles [°] for dimer 9-CHCl<sub>3</sub>.

Si(1)-C(9)	1.878(5)	C(26)-Si(6)	1.880(6)
Si(1)-C(1)	1.911(5)	C(27)-Si(7)	1.895(5)
Si(1)-C(19)	1.923(5)	C(27)-Si(8)	1.900(5)
Si(1)-C(12)	1.962(5)	Si(3)-C(30)	1.861(6)
C(1)-C(2)	1.504(7)	Si(3)-C(29)	1.870(6)
C(1)-Si(2)	1.946(5)	Si(3)-C(28)	1.877(6)
C(2)-C(3)	1.344(7)	Si(4)-C(31)	1.866(6)
C(3)-C(8)	1.464(7)	Si(4)-C(33)	1.871(6)
C(4)-C(5)	1.388(8)	Si(4)-C(32)	1.880(6)
C(4)-C(8)	1.401(7)	Si(5)-C(35)	1.858(7)
C(5)-C(6)	1.380(9)	Si(5)-C(34)	1.859(7)
C(6)-C(7)	1.393(8)	Si(5)-C(36)	1.887(8)
C(7)-C(9)	1.400(7)	Si(6)-C(37)	1.853(8)
C(8)-C(9)	1.406(7)	Si(6)-C(38)	1.865(7)
Si(2)-C(18)	1.868(5)	Si(6)-C(39)	1.870(7)
Si(2)-C(10)	1.873(5)	Si(7)-C(40)	1.857(6)
Si(2)-C(46)	1.903(5)	Si(7)-C(42)	1.860(6)
C(10)-C(11)	1.331(7)	Si(7)-C(41)	1.866(6)
C(11)-C(12)	1.504(7)	Si(8)-C(45)	1.864(6)
C(12)-C(17)	1.529(7)	Si(8)-C(44)	1.867(6)
C(13)-C(17)	1.392(7)	Si(8)-C(43)	1.872(6)
C(13)-C(14)	1.398(8)	C(46)-C(47)	1.412(7)
C(14)-C(15)	1.380(8)	C(46)-C(51)	1.444(6)
C(15)-C(16)	1.391(7)	C(47)-C(48)	1.398(7)
C(16)-C(18)	1.393(7)	C(47)-C(52)	1.535(7)
C(17)-C(18)	1.403(7)	C(48)-C(49)	1.381(7)
C(19)-C(24)	1.427(7)	C(49)-C(50)	1.398(7)
C(19)-C(20)	1.439(7)	C(49)-C(53)	1.511(7)
C(20)-C(21)	1.410(7)	C(50)-C(51)	1.396(7)
C(20)-C(25)	1.516(7)	C(51)-C(54)	1.517(7)
C(21)-C(22)	1.394(7)	C(52)-Si(9)	1.900(5)
C(22)-C(23)	1.396(7)	C(52)-Si(10)	1.906(5)
C(22)-C(26)	1.512(7)	C(53)-Si(12)	1.890(5)
C(23)-C(24)	1.393(7)	C(53)-Si(11)	1.902(5)
C(24)-C(27)	1.505(7)	C(54)-Si(14)	1.907(5)
C(25)-Si(3)	1.900(5)	C(54)-Si(13)	1.918(5)
C(25)-Si(4)	1.922(5)	Si(9)-C(55)	1.862(6)
C(26)-Si(5)	1.873(6)	Si(9)-C(57)	1.870(6)

Si(9)-C(56)	1.877(6)	C(6)-C(7)-C(9)	120.8(5)
Si(10)-C(58)	1.858(6)	C(4)-C(8)-C(9)	119.3(5)
Si(10)-C(60)	1.871(6)	C(4)-C(8)-C(3)	119.0(5)
Si(10)-C(59)	1.874(6)	C(9)-C(8)-C(3)	121.6(4)
Si(11)-C(62)	1.861(7)	C(7)-C(9)-C(8)	119.0(5)
Si(11)-C(61)	1.866(6)	C(7)-C(9)-Si(1)	119.5(4)
Si(11)-C(63)	1.871(6)	C(8)-C(9)-Si(1)	120.6(4)
Si(12)-C(65)	1.853(6)	C(18)-Si(2)-C(10)	101.7(2)
Si(12)-C(66)	1.856(7)	C(18)-Si(2)-C(46)	109.4(2)
Si(12)-C(64)	1.870(6)	C(10)-Si(2)-C(46)	114.5(2)
Si(13)-C(69)	1.861(6)	C(18)-Si(2)-C(1)	97.7(2)
Si(13)-C(67)	1.879(6)	C(10)-Si(2)-C(1)	103.7(2)
Si(13)-C(68)	1.887(7)	C(46)-Si(2)-C(1)	126.1(2)
Si(14)-C(71)	1.861(5)	C(11)-C(10)-Si(2)	113.3(4)
Si(14)-C(72)	1.869(6)	C(10)-C(11)-C(12)	122.6(5)
Si(14)-C(70)	1.883(6)	C(11)-C(12)-C(17)	112.5(4)
C(73)-Cl(2)	1.731(10)	C(11)-C(12)-Si(1)	111.5(3)
C(73)-Cl(1)	1.742(8)	C(17)-C(12)-Si(1)	102.8(3)
C(73)-Cl(3)	1.759(9)	C(17)-C(13)-C(14)	119.5(5)
C(74)-Cl(5)	1.726(14)	C(15)-C(14)-C(13)	120.9(5)
C(74)-Cl(4)	1.747(8)	C(14)-C(15)-C(16)	119.3(5)
C(74)-Cl(6)	1.750(13)	C(15)-C(16)-C(18)	121.0(5)
C(75)-Cl(8)	1.726(14)	C(13)-C(17)-C(18)	120.2(5)
C(75)-Cl(7)	1.740(11)	C(13)-C(17)-C(12)	120.9(5)
C(75)-Cl(9)	1.753(13)	C(18)-C(17)-C(12)	118.8(4)
		C(16)-C(18)-C(17)	119.0(5)
C(9)-Si(1)-C(1)	105.2(2)	C(16)-C(18)-Si(2)	126.7(4)
C(9)-Si(1)-C(19)	108.7(2)	C(17)-C(18)-Si(2)	114.0(4)
C(1)-Si(1)-C(19)	118.4(2)	C(24)-C(19)-C(20)	116.6(4)
C(9)-Si(1)-C(12)	100.1(2)	C(24)-C(19)-Si(1)	124.3(4)
C(1)-Si(1)-C(12)	102.6(2)	C(20)-C(19)-Si(1)	118.6(4)
C(19)-Si(1)-C(12)	119.5(2)	C(21)-C(20)-C(19)	120.1(5)
C(2)-C(1)-Si(1)	112.3(3)	C(21)-C(20)-C(25)	116.4(5)
C(2)-C(1)-Si(2)	108.8(3)	C(19)-C(20)-C(25)	123.5(4)
Si(1)-C(1)-Si(2)	107.4(2)	C(22)-C(21)-C(20)	123.0(5)
C(3)-C(2)-C(1)	127.4(5)	C(21)-C(22)-C(23)	115.9(5)
C(2)-C(3)-C(8)	127.7(5)	C(21)-C(22)-C(26)	124.2(5)
C(5)-C(4)-C(8)	120.7(5)	C(23)-C(22)-C(26)	119.9(5)
C(6)-C(5)-C(4)	120.2(5)	C(24)-C(23)-C(22)	124.0(5)
C(5)-C(6)-C(7)	119.9(5)	C(23)-C(24)-C(19)	120.2(5)

C(23)-C(24)-C(27)	115.6(4)	C(41)-Si(7)-C(27)	110.3(3)
C(19)-C(24)-C(27)	124.2(4)	C(45)-Si(8)-C(44)	106.4(3)
C(20)-C(25)-Si(3)	111.7(3)	C(45)-Si(8)-C(43)	109.7(3)
C(20)-C(25)-Si(4)	113.1(3)	C(44)-Si(8)-C(43)	109.0(3)
Si(3)-C(25)-Si(4)	113.2(3)	C(45)-Si(8)-C(27)	108.7(3)
C(22)-C(26)-Si(5)	113.1(4)	C(44)-Si(8)-C(27)	114.2(3)
C(22)-C(26)-Si(6)	113.7(4)	C(43)-Si(8)-C(27)	108.8(3)
Si(5)-C(26)-Si(6)	120.8(3)	C(47)-C(46)-C(51)	117.0(4)
C(24)-C(27)-Si(7)	110.4(3)	C(47)-C(46)-Si(2)	126.9(4)
C(24)-C(27)-Si(8)	113.0(4)	C(51)-C(46)-Si(2)	115.8(4)
Si(7)-C(27)-Si(8)	119.7(3)	C(48)-C(47)-C(46)	119.8(4)
C(30)-Si(3)-C(29)	108.3(3)	C(48)-C(47)-C(52)	117.3(4)
C(30)-Si(3)-C(28)	108.4(3)	C(46)-C(47)-C(52)	122.8(4)
C(29)-Si(3)-C(28)	105.2(3)	C(49)-C(48)-C(47)	123.4(5)
C(30)-Si(3)-C(25)	108.7(3)	C(48)-C(49)-C(50)	116.7(4)
C(29)-Si(3)-C(25)	114.9(3)	C(48)-C(49)-C(53)	124.0(5)
C(28)-Si(3)-C(25)	111.1(2)	C(50)-C(49)-C(53)	119.3(4)
C(31)-Si(4)-C(33)	107.9(3)	C(51)-C(50)-C(49)	122.5(5)
C(31)-Si(4)-C(32)	107.0(3)	C(50)-C(51)-C(46)	119.5(5)
C(33)-Si(4)-C(32)	107.2(3)	C(50)-C(51)-C(54)	116.0(4)
C(31)-Si(4)-C(25)	111.9(3)	C(46)-C(51)-C(54)	124.2(4)
C(33)-Si(4)-C(25)	109.1(3)	C(47)-C(52)-Si(9)	110.0(3)
C(32)-Si(4)-C(25)	113.5(2)	C(47)-C(52)-Si(10)	115.0(3)
C(35)-Si(5)-C(34)	108.1(4)	Si(9)-C(52)-Si(10)	116.2(3)
C(35)-Si(5)-C(26)	109.8(3)	C(49)-C(53)-Si(12)	110.9(3)
C(34)-Si(5)-C(26)	109.2(3)	C(49)-C(53)-Si(11)	113.6(4)
C(35)-Si(5)-C(36)	108.1(4)	Si(12)-C(53)-Si(11)	120.3(3)
C(34)-Si(5)-C(36)	109.5(4)	C(51)-C(54)-Si(14)	120.1(4)
C(26)-Si(5)-C(36)	112.0(4)	C(51)-C(54)-Si(13)	107.7(3)
C(37)-Si(6)-C(38)	109.2(5)	Si(14)-C(54)-Si(13)	113.3(3)
C(37)-Si(6)-C(39)	107.6(4)	C(55)-Si(9)-C(57)	109.3(3)
C(38)-Si(6)-C(39)	107.5(4)	C(55)-Si(9)-C(56)	106.7(3)
C(37)-Si(6)-C(26)	108.2(3)	C(57)-Si(9)-C(56)	108.2(3)
C(38)-Si(6)-C(26)	110.3(3)	C(55)-Si(9)-C(52)	108.1(2)
C(39)-Si(6)-C(26)	114.0(3)	C(57)-Si(9)-C(52)	111.9(2)
C(40)-Si(7)-C(42)	108.5(3)	C(56)-Si(9)-C(52)	112.4(2)
C(40)-Si(7)-C(41)	108.8(3)	C(58)-Si(10)-C(60)	109.0(3)
C(42)-Si(7)-C(41)	107.9(3)	C(58)-Si(10)-C(59)	106.3(3)
C(40)-Si(7)-C(27)	106.8(2)	C(60)-Si(10)-C(59)	107.1(3)
C(42)-Si(7)-C(27)	114.5(3)	C(58)-Si(10)-C(52)	109.8(2)

C(60)-Si(10)-C(52)	114.2(2)	C(67)-Si(13)-C(54)	115.5(3)
C(59)-Si(10)-C(52)	110.1(3)	C(68)-Si(13)-C(54)	108.1(3)
C(62)-Si(11)-C(61)	109.1(3)	C(71)-Si(14)-C(72)	112.4(3)
C(62)-Si(11)-C(63)	108.1(3)	C(71)-Si(14)-C(70)	105.1(3)
C(61)-Si(11)-C(63)	109.3(3)	C(72)-Si(14)-C(70)	104.6(3)
C(62)-Si(11)-C(53)	114.9(3)	C(71)-Si(14)-C(54)	106.2(2)
C(61)-Si(11)-C(53)	106.8(3)	C(72)-Si(14)-C(54)	113.1(2)
C(63)-Si(11)-C(53)	108.6(3)	C(70)-Si(14)-C(54)	115.3(3)
C(65)-Si(12)-C(66)	109.9(3)	Cl(2)-C(73)-Cl(1)	110.9(6)
C(65)-Si(12)-C(64)	107.7(3)	Cl(2)-C(73)-Cl(3)	110.5(5)
C(66)-Si(12)-C(64)	108.7(3)	Cl(1)-C(73)-Cl(3)	108.6(6)
C(65)-Si(12)-C(53)	107.6(2)	Cl(5)-C(74)-Cl(4)	110.5(9)
C(66)-Si(12)-C(53)	113.6(3)	Cl(5)-C(74)-Cl(6)	111.6(10)
C(64)-Si(12)-C(53)	109.2(3)	Cl(4)-C(74)-Cl(6)	108.0(9)
C(69)-Si(13)-C(67)	104.9(3)	Cl(8)-C(75)-Cl(7)	110.8(10)
C(69)-Si(13)-C(68)	108.4(3)	Cl(8)-C(75)-Cl(9)	111.1(10)
C(67)-Si(13)-C(68)	109.9(3)	Cl(7)-C(75)-Cl(9)	108.3(10)
C(69)-Si(13)-C(54)	109.8(3)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for dimer 9· $\text{CHCl}_3$ . The anisotropic displacement factor exponent takes the form:  $-2\pi^2[\ h^2\ a^{*2}\text{U}^{11} + \dots + 2\ h\ k\ a^{*}\ b^{*}\text{U}^{12}]$

	$\text{U}^{11}$	$\text{U}^{22}$	$\text{U}^{33}$	$\text{U}^{23}$	$\text{U}^{13}$	$\text{U}^{12}$
Si(1)	18(1)	12(1)	11(1)	1(1)	-6(1)	-2(1)
C(1)	12(3)	23(3)	16(3)	-5(2)	-3(2)	0(2)
C(2)	15(3)	18(3)	22(3)	-3(2)	-3(2)	-1(2)
C(3)	25(3)	18(3)	22(3)	2(2)	-13(2)	-4(2)
C(4)	38(3)	30(3)	15(3)	2(2)	-15(2)	-12(3)
C(5)	53(4)	34(3)	15(3)	-5(3)	-6(3)	-18(3)
C(6)	52(4)	28(3)	18(3)	-8(3)	0(3)	-8(3)
C(7)	35(3)	20(3)	15(3)	-2(2)	-4(2)	-5(2)
C(8)	24(3)	19(3)	14(2)	1(2)	-5(2)	-10(2)
C(9)	28(3)	12(2)	14(3)	5(2)	-6(2)	-8(2)
Si(2)	15(1)	14(1)	14(1)	-1(1)	-7(1)	-1(1)
C(10)	23(3)	20(3)	18(3)	-5(2)	-7(2)	0(2)
C(11)	22(3)	19(3)	26(3)	-2(2)	-8(2)	-3(2)
C(12)	18(3)	17(3)	17(3)	-2(2)	-4(2)	2(2)
C(13)	31(3)	20(3)	20(3)	-4(2)	5(2)	-2(2)
C(14)	37(3)	23(3)	18(3)	-1(2)	0(2)	-7(2)
C(15)	29(3)	24(3)	15(3)	2(2)	-8(2)	-5(2)
C(16)	18(3)	17(3)	23(3)	-1(2)	-5(2)	-5(2)
C(17)	18(3)	19(3)	18(3)	-4(2)	-1(2)	-7(2)
C(18)	19(3)	8(2)	14(2)	1(2)	-5(2)	-3(2)
C(19)	22(3)	14(2)	13(2)	-1(2)	-5(2)	-4(2)
C(20)	22(3)	16(3)	16(3)	-5(2)	-6(2)	-1(2)
C(21)	30(3)	17(3)	19(3)	-3(2)	-7(2)	-6(2)
C(22)	29(3)	19(3)	12(2)	-1(2)	-11(2)	5(2)
C(23)	24(3)	25(3)	12(2)	-4(2)	-11(2)	-1(2)
C(24)	21(3)	24(3)	10(2)	-3(2)	-7(2)	0(2)
C(25)	27(3)	20(3)	16(3)	2(2)	-6(2)	-9(2)
C(26)	33(3)	23(3)	29(3)	1(2)	-18(3)	5(2)
C(27)	18(3)	17(3)	18(3)	5(2)	-7(2)	0(2)
Si(3)	25(1)	22(1)	22(1)	0(1)	-4(1)	-6(1)
Si(4)	28(1)	20(1)	26(1)	-2(1)	-11(1)	-8(1)
Si(5)	50(1)	30(1)	25(1)	14(1)	-4(1)	0(1)
Si(6)	49(1)	18(1)	40(1)	-1(1)	-22(1)	1(1)
Si(7)	23(1)	28(1)	23(1)	-6(1)	-12(1)	-1(1)
Si(8)	21(1)	25(1)	21(1)	1(1)	-5(1)	1(1)
C(28)	34(3)	31(3)	21(3)	1(2)	-3(2)	-11(3)
C(29)	41(4)	34(3)	30(3)	-3(3)	3(3)	-10(3)
C(30)	22(3)	28(3)	45(4)	-7(3)	-4(3)	-5(2)
C(31)	41(4)	30(3)	28(3)	-9(3)	-11(3)	-9(3)
C(32)	38(4)	22(3)	39(4)	-3(3)	-12(3)	-9(3)
C(33)	41(4)	30(3)	38(4)	3(3)	-22(3)	-16(3)

C(34)	59(5)	51(4)	24(3)	-5(3)	-5(3)	3(3)
C(35)	89(7)	66(6)	34(4)	10(4)	-19(4)	21(5)
C(36)	49(5)	57(5)	78(6)	11(4)	8(4)	-11(4)
C(37)	74(6)	61(5)	52(5)	-31(4)	-11(4)	-4(4)
C(38)	132(9)	34(4)	94(7)	-20(5)	-75(7)	23(5)
C(39)	65(5)	42(4)	67(5)	-9(4)	-25(4)	-17(4)
C(40)	35(4)	50(4)	33(3)	-17(3)	-8(3)	-8(3)
C(41)	29(3)	46(4)	41(4)	-15(3)	-6(3)	-9(3)
C(42)	64(5)	45(4)	32(4)	-11(3)	-26(3)	-1(3)
C(43)	26(3)	36(3)	40(4)	-1(3)	-3(3)	4(3)
C(44)	27(3)	35(3)	38(4)	1(3)	-7(3)	2(3)
C(45)	37(4)	45(4)	31(3)	-13(3)	-4(3)	0(3)
C(46)	21(3)	13(2)	11(2)	-3(2)	-4(2)	-3(2)
C(47)	22(3)	15(2)	10(2)	-5(2)	-4(2)	-4(2)
C(48)	10(2)	24(3)	18(3)	-8(2)	-4(2)	2(2)
C(49)	20(3)	15(2)	10(2)	0(2)	-3(2)	-3(2)
C(50)	24(3)	13(2)	18(3)	2(2)	-4(2)	-5(2)
C(51)	21(3)	15(2)	11(2)	-1(2)	-3(2)	-6(2)
C(52)	16(3)	21(3)	14(2)	-4(2)	-1(2)	-4(2)
C(53)	20(3)	13(2)	29(3)	-3(2)	-11(2)	0(2)
C(54)	16(3)	16(3)	25(3)	-1(2)	-1(2)	-3(2)
Si(9)	27(1)	22(1)	12(1)	-2(1)	-4(1)	-1(1)
Si(10)	21(1)	23(1)	18(1)	-2(1)	-3(1)	-4(1)
Si(11)	40(1)	19(1)	27(1)	-8(1)	-14(1)	6(1)
Si(12)	26(1)	22(1)	22(1)	1(1)	-10(1)	0(1)
Si(13)	27(1)	29(1)	30(1)	-5(1)	-9(1)	-10(1)
Si(14)	20(1)	19(1)	24(1)	-2(1)	-1(1)	-5(1)
C(55)	34(3)	30(3)	21(3)	-1(2)	-15(2)	1(3)
C(56)	41(4)	43(4)	10(3)	2(3)	-1(2)	-7(3)
C(57)	67(5)	30(3)	22(3)	-11(3)	-15(3)	-1(3)
C(58)	24(3)	34(3)	25(3)	-6(3)	-5(2)	-7(2)
C(59)	26(3)	34(3)	33(3)	0(3)	4(3)	-8(3)
C(60)	20(3)	34(3)	31(3)	-3(3)	-3(2)	2(2)
C(61)	59(5)	25(3)	49(4)	-7(3)	-36(4)	10(3)
C(62)	64(5)	33(4)	26(3)	-11(3)	0(3)	4(3)
C(63)	61(5)	25(3)	45(4)	-13(3)	-17(3)	0(3)
C(64)	60(5)	27(3)	34(4)	9(3)	-28(3)	-5(3)
C(65)	35(4)	43(4)	32(3)	-14(3)	-16(3)	0(3)
C(66)	40(4)	68(5)	31(4)	-1(3)	-11(3)	-13(3)
C(67)	50(4)	34(3)	37(4)	-14(3)	-13(3)	-14(3)
C(68)	38(4)	47(4)	56(4)	1(3)	-22(3)	-20(3)
C(69)	51(4)	47(4)	27(3)	-14(3)	-8(3)	-15(3)
C(70)	34(4)	36(3)	31(3)	-5(3)	0(3)	-6(3)
C(71)	22(3)	27(3)	31(3)	0(3)	4(2)	0(2)
C(72)	31(3)	17(3)	26(3)	-3(2)	-6(2)	0(2)
C(73)	39(6)	72(7)	19(4)	-10(5)	-3(4)	-32(5)

Cl(1)	41(2)	92(4)	45(4)	14(3)	10(2)	-23(3)
Cl(2)	52(3)	142(4)	54(3)	-45(3)	-1(3)	-10(2)
Cl(3)	110(3)	108(3)	25(1)	5(2)	-12(2)	-82(2)
C(74)	54(10)	69(10)	48(11)	-2(9)	-5(8)	-16(7)
Cl(4)	31(8)	92(10)	45(10)	46(7)	2(5)	0(6)
Cl(5)	82(15)	141(10)	77(10)	-69(9)	-23(11)	23(10)
Cl(6)	88(9)	89(8)	135(12)	-5(9)	-9(9)	-44(7)
C(75)	136(18)	137(19)	141(19)	-33(11)	-18(10)	-25(9)
Cl(7)	70(13)	140(20)	49(12)	-21(12)	4(9)	-53(11)
Cl(8)	90(17)	67(18)	120(20)	0(20)	-19(19)	-19(14)
Cl(9)	117(19)	100(20)	100(20)	0(16)	-24(17)	12(16)

Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ )  
for dimer 9·CHCl<sub>3</sub>.

	x	y	z	U(eq)
H(1)	3933	10417	2190	20
H(2)	5362	10019	2787	23
H(3)	5475	10323	3736	26
H(4)	4822	10779	4757	31
H(5)	3625	11581	5351	39
H(6)	2161	12306	4872	39
H(7)	1850	12193	3814	28
H(8)	1723	9364	2437	24
H(9)	540	10286	2877	27
H(10)	936	10985	3552	21
H(11)	1108	10663	4749	30
H(12)	1904	9908	5697	32
H(13)	3295	8930	5563	28
H(14)	3843	8655	4485	23
H(15)	3533	13580	1413	26
H(16)	605	13278	1426	24
H(17)	4351	11789	2491	25
H(18)	992	14389	876	35
H(19)	830	11418	2427	23
H(20)	5349	11277	611	44
H(21)	4196	11411	1017	44
H(22)	5100	10814	1388	44
H(23)	5523	13333	727	54
H(24)	4647	13059	445	54
H(25)	5856	12753	233	54
H(26)	7092	11545	1260	48
H(27)	6602	11375	2053	48
H(28)	6889	12200	1674	48
H(29)	3362	13112	3460	47
H(30)	3104	13718	2764	47
H(31)	3880	13868	3213	47
H(32)	4999	14029	1616	48
H(33)	6090	13467	1693	48
H(34)	5672	14036	2191	48
H(35)	5962	12749	3378	52
H(36)	6282	12108	2945	52
H(37)	5332	12052	3558	52
H(38)	1913	13390	-173	71
H(39)	3051	13184	59	71
H(40)	2900	13625	-715	71

H(41)	1863	15271	-1042	106
H(42)	1356	15682	-430	106
H(43)	860	15005	-535	106
H(44)	4095	14514	221	103
H(45)	3542	15365	-86	103
H(46)	4029	14804	-585	103
H(47)	1159	14419	2510	89
H(48)	130	14792	2155	89
H(49)	681	15299	2464	89
H(50)	339	16005	753	124
H(51)	1459	16256	472	124
H(52)	816	16451	1167	124
H(53)	2771	15706	1805	84
H(54)	3344	15438	1125	84
H(55)	3233	14825	1844	84
H(56)	1810	10991	580	56
H(57)	2134	10801	1334	56
H(58)	2261	11608	818	56
H(59)	-312	10652	1104	56
H(60)	-1073	11070	1648	56
H(61)	-99	10438	1885	56
H(62)	356	12813	505	68
H(63)	-779	12581	758	68
H(64)	4	12208	193	68
H(65)	-888	11157	3401	55
H(66)	-1630	11327	2821	55
H(67)	-1950	11756	3434	55
H(68)	-2173	13248	2356	54
H(69)	-1757	12833	1737	54
H(70)	-1194	13493	1810	54
H(71)	156	13216	2916	57
H(72)	138	12460	3522	57
H(73)	-897	13084	3429	57
H(74)	6162	7316	2711	21
H(75)	3621	6643	3939	22
H(76)	5167	9268	2253	20
H(77)	5045	5786	3937	25
H(78)	1966	8412	3576	24
H(79)	3724	9168	777	43
H(80)	3893	9791	1147	43
H(81)	3430	9048	1592	43
H(82)	6000	9212	151	50
H(83)	6892	8985	638	50
H(84)	6090	9767	615	50
H(85)	4882	7468	1571	58
H(86)	6092	7461	1275	58

H(87)	5231	7742	762	58
H(88)	6783	8126	3472	41
H(89)	6693	9028	3364	41
H(90)	7813	8510	3253	41
H(91)	6919	10060	2010	50
H(92)	7337	9744	1334	50
H(93)	8097	9631	1893	50
H(94)	8599	8031	1920	46
H(95)	7758	7985	1465	46
H(96)	7781	7455	2225	46
H(97)	4651	6171	2341	65
H(98)	4441	5338	2759	65
H(99)	5210	5442	2049	65
H(100)	7446	5528	1999	64
H(101)	7785	5846	2570	64
H(102)	6997	6384	2064	64
H(103)	6692	4203	2993	64
H(104)	5902	4303	3671	64
H(105)	7081	4436	3596	64
H(106)	7022	5095	5247	61
H(107)	7197	4732	4596	61
H(108)	6051	4888	5007	61
H(109)	6244	6722	5153	52
H(110)	5149	6544	5063	52
H(111)	5643	7229	4529	52
H(112)	7668	6796	3503	70
H(113)	8199	5917	3663	70
H(114)	8136	6414	4209	70
H(115)	1650	6194	2952	56
H(116)	1369	6173	3753	56
H(117)	2555	6148	3394	56
H(118)	111	8381	2957	69
H(119)	-121	7754	3652	69
H(120)	-135	7577	2927	69
H(121)	3008	7508	2193	59
H(122)	2158	8269	2074	59
H(123)	1940	7507	1929	59
H(124)	636	6658	5369	52
H(125)	1443	6256	4833	52
H(126)	422	6829	4591	52
H(127)	361	8209	5327	45
H(128)	246	8541	4530	45
H(129)	1105	8784	4853	45
H(130)	3268	7584	5064	38
H(131)	3108	6717	5198	38
H(132)	2450	7241	5694	38

H(133)	1823	8980	1002	48
H(134)	708	8983	-53	71
H(135)	9291	4645	6293	166

Table 6. Torsion angles [°] for dimer 9·CHCl<sub>3</sub>.

C(9)-Si(1)-C(1)-C(2)	-15.7(4)
C(19)-Si(1)-C(1)-C(2)	106.0(4)
C(12)-Si(1)-C(1)-C(2)	-120.0(4)
C(9)-Si(1)-C(1)-Si(2)	103.9(3)
C(19)-Si(1)-C(1)-Si(2)	-134.5(2)
C(12)-Si(1)-C(1)-Si(2)	-0.4(3)
Si(1)-C(1)-C(2)-C(3)	23.8(7)
Si(2)-C(1)-C(2)-C(3)	-95.0(6)
C(1)-C(2)-C(3)-C(8)	-10.6(9)
C(8)-C(4)-C(5)-C(6)	-1.8(8)
C(4)-C(5)-C(6)-C(7)	1.6(9)
C(5)-C(6)-C(7)-C(9)	0.9(8)
C(5)-C(4)-C(8)-C(9)	-0.5(8)
C(5)-C(4)-C(8)-C(3)	177.0(5)
C(2)-C(3)-C(8)-C(4)	169.6(5)
C(2)-C(3)-C(8)-C(9)	-12.9(8)
C(6)-C(7)-C(9)-C(8)	-3.1(8)
C(6)-C(7)-C(9)-Si(1)	166.3(4)
C(4)-C(8)-C(9)-C(7)	2.9(7)
C(3)-C(8)-C(9)-C(7)	-174.5(5)
C(4)-C(8)-C(9)-Si(1)	-166.3(4)
C(3)-C(8)-C(9)-Si(1)	16.2(6)
C(1)-Si(1)-C(9)-C(7)	-171.1(4)
C(19)-Si(1)-C(9)-C(7)	61.1(4)
C(12)-Si(1)-C(9)-C(7)	-64.9(4)
C(1)-Si(1)-C(9)-C(8)	-1.9(5)
C(19)-Si(1)-C(9)-C(8)	-129.7(4)
C(12)-Si(1)-C(9)-C(8)	104.3(4)
C(2)-C(1)-Si(2)-C(18)	67.8(4)
Si(1)-C(1)-Si(2)-C(18)	-54.0(3)
C(2)-C(1)-Si(2)-C(10)	171.9(3)
Si(1)-C(1)-Si(2)-C(10)	50.2(3)
C(2)-C(1)-Si(2)-C(46)	-53.1(4)
Si(1)-C(1)-Si(2)-C(46)	-174.9(2)
C(18)-Si(2)-C(10)-C(11)	37.9(4)
C(46)-Si(2)-C(10)-C(11)	155.8(4)
C(1)-Si(2)-C(10)-C(11)	-63.2(4)
Si(2)-C(10)-C(11)-C(12)	5.7(7)
C(10)-C(11)-C(12)-C(17)	-55.4(7)
C(10)-C(11)-C(12)-Si(1)	59.4(6)
C(9)-Si(1)-C(12)-C(11)	-165.1(4)
C(1)-Si(1)-C(12)-C(11)	-56.8(4)
C(19)-Si(1)-C(12)-C(11)	76.6(4)
C(9)-Si(1)-C(12)-C(17)	-44.3(3)

C(1)-Si(1)-C(12)-C(17)	63.9(3)
C(19)-Si(1)-C(12)-C(17)	-162.7(3)
C(17)-C(13)-C(14)-C(15)	1.4(8)
C(13)-C(14)-C(15)-C(16)	-2.0(8)
C(14)-C(15)-C(16)-C(18)	0.1(8)
C(14)-C(13)-C(17)-C(18)	1.1(8)
C(14)-C(13)-C(17)-C(12)	-174.9(5)
C(11)-C(12)-C(17)-C(13)	-132.9(5)
Si(1)-C(12)-C(17)-C(13)	107.1(5)
C(11)-C(12)-C(17)-C(18)	51.1(6)
Si(1)-C(12)-C(17)-C(18)	-68.9(5)
C(15)-C(16)-C(18)-C(17)	2.2(7)
C(15)-C(16)-C(18)-Si(2)	175.4(4)
C(13)-C(17)-C(18)-C(16)	-2.8(7)
C(12)-C(17)-C(18)-C(16)	173.2(4)
C(13)-C(17)-C(18)-Si(2)	-176.8(4)
C(12)-C(17)-C(18)-Si(2)	-0.8(6)
C(10)-Si(2)-C(18)-C(16)	146.8(4)
C(46)-Si(2)-C(18)-C(16)	25.4(5)
C(1)-Si(2)-C(18)-C(16)	-107.4(4)
C(10)-Si(2)-C(18)-C(17)	-39.8(4)
C(46)-Si(2)-C(18)-C(17)	-161.2(3)
C(1)-Si(2)-C(18)-C(17)	66.0(4)
C(9)-Si(1)-C(19)-C(24)	-119.9(4)
C(1)-Si(1)-C(19)-C(24)	120.2(4)
C(12)-Si(1)-C(19)-C(24)	-6.1(5)
C(9)-Si(1)-C(19)-C(20)	51.9(4)
C(1)-Si(1)-C(19)-C(20)	-68.0(4)
C(12)-Si(1)-C(19)-C(20)	165.7(4)
C(24)-C(19)-C(20)-C(21)	4.1(7)
Si(1)-C(19)-C(20)-C(21)	-168.4(4)
C(24)-C(19)-C(20)-C(25)	-175.1(4)
Si(1)-C(19)-C(20)-C(25)	12.5(6)
C(19)-C(20)-C(21)-C(22)	-0.4(8)
C(25)-C(20)-C(21)-C(22)	178.8(5)
C(20)-C(21)-C(22)-C(23)	-2.7(7)
C(20)-C(21)-C(22)-C(26)	178.8(5)
C(21)-C(22)-C(23)-C(24)	2.0(8)
C(26)-C(22)-C(23)-C(24)	-179.3(5)
C(22)-C(23)-C(24)-C(19)	1.7(8)
C(22)-C(23)-C(24)-C(27)	-175.7(5)
C(20)-C(19)-C(24)-C(23)	-4.7(7)
Si(1)-C(19)-C(24)-C(23)	167.3(4)
C(20)-C(19)-C(24)-C(27)	172.5(5)
Si(1)-C(19)-C(24)-C(27)	-15.5(7)
C(21)-C(20)-C(25)-Si(3)	-72.6(5)

C(19)-C(20)-C(25)-Si(3)	106.6(5)
C(21)-C(20)-C(25)-Si(4)	56.5(5)
C(19)-C(20)-C(25)-Si(4)	-124.3(4)
C(21)-C(22)-C(26)-Si(5)	70.6(6)
C(23)-C(22)-C(26)-Si(5)	-107.9(5)
C(21)-C(22)-C(26)-Si(6)	-72.1(6)
C(23)-C(22)-C(26)-Si(6)	109.4(5)
C(23)-C(24)-C(27)-Si(7)	73.1(5)
C(19)-C(24)-C(27)-Si(7)	-104.3(5)
C(23)-C(24)-C(27)-Si(8)	-63.9(5)
C(19)-C(24)-C(27)-Si(8)	118.7(5)
C(20)-C(25)-Si(3)-C(30)	-179.0(4)
Si(4)-C(25)-Si(3)-C(30)	52.0(3)
C(20)-C(25)-Si(3)-C(29)	59.4(4)
Si(4)-C(25)-Si(3)-C(29)	-69.6(4)
C(20)-C(25)-Si(3)-C(28)	-59.8(4)
Si(4)-C(25)-Si(3)-C(28)	171.1(3)
C(20)-C(25)-Si(4)-C(31)	27.5(4)
Si(3)-C(25)-Si(4)-C(31)	155.8(3)
C(20)-C(25)-Si(4)-C(33)	146.8(4)
Si(3)-C(25)-Si(4)-C(33)	-84.9(3)
C(20)-C(25)-Si(4)-C(32)	-93.7(4)
Si(3)-C(25)-Si(4)-C(32)	34.6(4)
C(22)-C(26)-Si(5)-C(35)	148.0(5)
Si(6)-C(26)-Si(5)-C(35)	-72.3(5)
C(22)-C(26)-Si(5)-C(34)	29.7(5)
Si(6)-C(26)-Si(5)-C(34)	169.4(4)
C(22)-C(26)-Si(5)-C(36)	-91.8(5)
Si(6)-C(26)-Si(5)-C(36)	47.9(5)
C(22)-C(26)-Si(6)-C(37)	-47.7(5)
Si(5)-C(26)-Si(6)-C(37)	172.8(4)
C(22)-C(26)-Si(6)-C(38)	-167.0(5)
Si(5)-C(26)-Si(6)-C(38)	53.5(5)
C(22)-C(26)-Si(6)-C(39)	71.9(5)
Si(5)-C(26)-Si(6)-C(39)	-67.6(4)
C(24)-C(27)-Si(7)-C(40)	47.3(4)
Si(8)-C(27)-Si(7)-C(40)	-179.0(3)
C(24)-C(27)-Si(7)-C(42)	-72.8(4)
Si(8)-C(27)-Si(7)-C(42)	60.9(4)
C(24)-C(27)-Si(7)-C(41)	165.4(4)
Si(8)-C(27)-Si(7)-C(41)	-60.9(4)
C(24)-C(27)-Si(8)-C(45)	-30.3(4)
Si(7)-C(27)-Si(8)-C(45)	-162.9(3)
C(24)-C(27)-Si(8)-C(44)	88.3(4)
Si(7)-C(27)-Si(8)-C(44)	-44.3(4)
C(24)-C(27)-Si(8)-C(43)	-149.7(4)

Si(7)-C(27)-Si(8)-C(43)	77.7(4)
C(18)-Si(2)-C(46)-C(47)	-120.5(4)
C(10)-Si(2)-C(46)-C(47)	126.1(4)
C(1)-Si(2)-C(46)-C(47)	-4.8(5)
C(18)-Si(2)-C(46)-C(51)	52.6(4)
C(10)-Si(2)-C(46)-C(51)	-60.8(4)
C(1)-Si(2)-C(46)-C(51)	168.3(3)
C(51)-C(46)-C(47)-C(48)	-8.8(7)
Si(2)-C(46)-C(47)-C(48)	164.2(4)
C(51)-C(46)-C(47)-C(52)	168.1(4)
Si(2)-C(46)-C(47)-C(52)	-18.9(7)
C(46)-C(47)-C(48)-C(49)	0.4(7)
C(52)-C(47)-C(48)-C(49)	-176.7(4)
C(47)-C(48)-C(49)-C(50)	6.7(7)
C(47)-C(48)-C(49)-C(53)	-173.8(5)
C(48)-C(49)-C(50)-C(51)	-5.0(7)
C(53)-C(49)-C(50)-C(51)	175.4(5)
C(49)-C(50)-C(51)-C(46)	-3.4(7)
C(49)-C(50)-C(51)-C(54)	172.0(5)
C(47)-C(46)-C(51)-C(50)	10.3(7)
Si(2)-C(46)-C(51)-C(50)	-163.5(4)
C(47)-C(46)-C(51)-C(54)	-164.8(4)
Si(2)-C(46)-C(51)-C(54)	21.4(6)
C(48)-C(47)-C(52)-Si(9)	87.7(5)
C(46)-C(47)-C(52)-Si(9)	-89.3(5)
C(48)-C(47)-C(52)-Si(10)	-45.8(5)
C(46)-C(47)-C(52)-Si(10)	137.2(4)
C(48)-C(49)-C(53)-Si(12)	75.5(6)
C(50)-C(49)-C(53)-Si(12)	-105.0(5)
C(48)-C(49)-C(53)-Si(11)	-63.7(6)
C(50)-C(49)-C(53)-Si(11)	115.9(5)
C(50)-C(51)-C(54)-Si(14)	58.4(6)
C(46)-C(51)-C(54)-Si(14)	-126.4(4)
C(50)-C(51)-C(54)-Si(13)	-73.3(5)
C(46)-C(51)-C(54)-Si(13)	101.9(5)
C(47)-C(52)-Si(9)-C(55)	75.4(4)
Si(10)-C(52)-Si(9)-C(55)	-151.7(3)
C(47)-C(52)-Si(9)-C(57)	-45.0(4)
Si(10)-C(52)-Si(9)-C(57)	87.9(4)
C(47)-C(52)-Si(9)-C(56)	-167.0(4)
Si(10)-C(52)-Si(9)-C(56)	-34.1(4)
C(47)-C(52)-Si(10)-C(58)	-39.8(4)
Si(9)-C(52)-Si(10)-C(58)	-170.4(3)
C(47)-C(52)-Si(10)-C(60)	83.0(4)
Si(9)-C(52)-Si(10)-C(60)	-47.6(4)
C(47)-C(52)-Si(10)-C(59)	-156.4(4)

Si(9)-C(52)-Si(10)-C(59)	73.0(3)
C(49)-C(53)-Si(11)-C(62)	72.7(4)
Si(12)-C(53)-Si(11)-C(62)	-62.3(4)
C(49)-C(53)-Si(11)-C(61)	-48.4(4)
Si(12)-C(53)-Si(11)-C(61)	176.6(3)
C(49)-C(53)-Si(11)-C(63)	-166.2(4)
Si(12)-C(53)-Si(11)-C(63)	58.9(4)
C(49)-C(53)-Si(12)-C(65)	38.2(4)
Si(11)-C(53)-Si(12)-C(65)	174.3(3)
C(49)-C(53)-Si(12)-C(66)	-83.7(4)
Si(11)-C(53)-Si(12)-C(66)	52.3(4)
C(49)-C(53)-Si(12)-C(64)	154.8(4)
Si(11)-C(53)-Si(12)-C(64)	-69.2(4)
C(51)-C(54)-Si(13)-C(69)	-41.1(4)
Si(14)-C(54)-Si(13)-C(69)	-176.4(3)
C(51)-C(54)-Si(13)-C(67)	77.3(4)
Si(14)-C(54)-Si(13)-C(67)	-58.0(4)
C(51)-C(54)-Si(13)-C(68)	-159.2(4)
Si(14)-C(54)-Si(13)-C(68)	65.6(3)
C(51)-C(54)-Si(14)-C(71)	128.3(4)
Si(13)-C(54)-Si(14)-C(71)	-102.5(3)
C(51)-C(54)-Si(14)-C(72)	4.5(5)
Si(13)-C(54)-Si(14)-C(72)	133.8(3)
C(51)-C(54)-Si(14)-C(70)	-115.8(4)
Si(13)-C(54)-Si(14)-C(70)	13.5(4)

---

Symmetry transformations used to generate equivalent atoms: