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Electronic Supplementary Information

London dispersion-driven hetero-aryl-aryl interactions in 1,2-diaryldisilanes

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Experimental Section

All operations with air- and moisture-sensitive compounds were carried out under an anhydrous, inert atmosphere of nitrogen using the standard Schlenk techniques. Tetrahydrofuran was dried over potassium and diethyl ether over $LiAlH_4$; all were freshly distilled before being used for the reactions. NMR-spectra were recorded on a Bruker Avance III 500 instrument at ambient temperature; the chemical shifts (δ) were referenced to the residual proton or carbon peaks of the used solvents (^1H, ^{13}C). Elemental analyses were performed using a Euro EA Elemental Analyser. EI mass spectra were recorded using an AutospecX magnetic sector mass spectrometer with EBE geometry (Vacuum Generators, Manchester UK) equipped with a standard EI source. Samples were introduced by a push rod in aluminum crucibles. Ions were accelerated by 8 kV.

1-Chloro-1,1,2,2-tetramethyl-2-phenyldisilane (1). A solution of 1,2-dichloro-1,1,2,2-tetramethyldisilane (11 mL, 60 mmol, 1 eq.) in dry DE (200 mL) was cooled to 0 °C. Phenyllithium (1.9 M in dibutyl ether, 30 mL, 57 mmol, 0.9 eq.) in dry DE (120 mL) was added dropwise over a period of 1 h. The cloudy suspension was stirred for 4 h at 0 °C and for 14 h at room temperature. After removing the solvent under reduced pressure, the residue was suspended with dry *n*-pentane (100 mL) and filtered. The colorless solid was washed with dry *n*-pentane (50 mL) and the solvent of the filtrate removed in vacuo. Distillation of the remaining oil (0.29 mbar, 60 °C) yielded 1-chloro-1,1,2,2-tetramethyl-2-phenyldisilane (7.2 g, 32 mmol, 53%) as a colorless liquid. ^1H NMR (500 MHz, C_6D_6): δ [ppm] = 7.40 (m, 2H, Ar–**H**), 7.16 (m, 3H, Ar–**H**), 0.33 (s, 6H Si–(C**H**$_3$)$_2$, 0.30 (s, 6H Si–(C**H**$_3$)$_2$). $^{13}C\{^1H\}$ NMR (126 MHz, C_6D_6): δ [ppm] = 136.9 (Ar–**C**$_6$H$_5$), 134.2 (Ar–**C**$_6$H$_5$), 129.4 (Ar–**C**$_6$H$_5$), 128.4 (Ar–**C**$_6$H$_5$), 2.1 (Si–(**C**H$_3$)$_2$), −4.6 (Si–(**C**H$_3$)$_2$). $^{29}Si\{^1H\}$ NMR (99 MHz, C_6D_6): δ [ppm] = 21.9, −21.9. MS (EI, 70 eV): *m*/*z* [assignment] = 228.2 $[M]^+$, 212.9 $[M-CH_3]^+$, 135.0 $[M-C_2H_6ClSi]^+$. AT-IR: ν [cm^{-1}] = 3069, 3051, 3021, 2999, 2956, 2896, 2872, 1486, 1427, 1400, 1247, 1105, 998, 831, 814, 784, 767, 730, 696, 669, 644, 494, 464, 417.

1-Chloro-1,1,2,2-tetramethyl-2-(perfluorophenyl)disilane (2). A solution of 1,2-dichloro-1,1,2,2-tetramethyldisilane (11 mL, 60 mmol, 1 eq.) in dry DE (200 mL) was cooled to 0 °C. Freshly generated pentafluorophenylmagnesium bromide (7.0 mL, 56 mmol of bromopentafluorobenzene; 1.4 g, 57 mmol of Mg; 100 mL of dry THF) was added dropwise over a period of 1 h. The cloudy suspension was stirred for 4 h at 0 °C and for 13 h at room temperature. After removing the solvent under reduced pressure, the residue was suspended with dry *n*-pentane (100 mL) and filtered. The pale brown solid was washed with dry *n*-pentane (50 mL)

and the solvent of the filtrate removed in vacuo. Distillation of the remaining brown oil (0.21 mbar, 53 °C) yielded 1-chloro-1,1,2,2-tetramethyl-2-(perfluorophenyl)disilane (7.3 g, 23 mmol, 41%) as a colorless liquid. ^{1}H NMR (500 MHz, C_6D_6): δ [ppm] = 0.38 (s, 6H Si–(C**H**$_3$)$_2$), 0.37 (s, 6H Si–(C**H**$_3$)$_2$). ^{13}C{^{1}H} NMR (126 MHz, C_6D_6): δ [ppm] = 149.0 (Ar–**C**$_6$F$_5$), 142.2 (Ar–**C**$_6$F$_5$), 137.5 (Ar–**C**$_6$F$_5$), 108.8 (Ar–**C**$_6$F$_5$), 1.8 (Si–(**C**H$_3$)$_2$), −3.6 (Si–(**C**H$_3$)$_2$). ^{19}F{^{1}H} NMR (470 MHz, C_6D_6): δ [ppm] = −126.0 (m, 2F, *o*-**F**), −150.9 (m, *p*-**F**), −160.8 (m, 2F, *m*-**F**). ^{29}Si{^{1}H} NMR (99 MHz, C_6D_6): δ [ppm] = 21.1, −22.1. MS (EI, 70 eV): *m*/*z* [assignment] = 302.8 [M−CH$_3$]$^+$. AT-IR: $\tilde{\nu}$ [cm^{-1}] = 2963, 2903, 1640, 1515, 1456, 1405, 1373, 1284, 1252, 1079, 1014, 966, 848, 828, 781, 736, 699, 675, 657, 619, 507, 484, 421.

1,1,2,2-Tetramethyl-1-(perfluorophenyl)-2-phenyldisilane (3). To a solution of bromopentafluorobenzene (0.85 mL, 6.6 mmol, 1 eq.) in dry DE (100 mL) was added at −78 °C *n*-butyllithium (1.6 M in *n*-hexane, 4.3 mL, 6.6 mmol) and was stirred for 1 h. 1-Chloro-1,1,2,2-tetramethyl-2-phenyldisilane (1.5 g, 6.6 mmol, 1 eq.) was added dropwise via a syringe over a period of 5 min. After complete addition the solution was allowed to slowly warm to ambient temperature and was stirred for 12 h. The resulting colorless suspension was quenched with water (30 mL), the aqueous layer extracted with dichloromethane (3 × 30 mL) and the combined organic layers dried over $MgSO_4$. After removing the solvent under reduced pressure, the crude colorless oil was purified by column chromatography (*n*-pentane) to give 1,1,2,2-tetramethyl-1-(perfluorophenyl)-2-phenyldisilane (2.0 g, 5.7 mmol, 86%) as a colorless oil which slowly crystallized. ^{1}H NMR (500 MHz, C_6D_6): δ [ppm] = 7.33 (m, 2H, Ar–**H**), 7.14 (m, 3H, Ar–**H**), 0.33 (s, 6H Si–(C**H**$_3$)$_2$), 0.31 (s, 6H Si–(C**H**$_3$)$_2$). ^{13}C{^{1}H} NMR (126 MHz, C_6D_6): δ [ppm] = 149.0 (Ar–**C**$_6$F$_5$), 141.8 (Ar–**C**$_6$F$_5$), 137.5 (Ar–**C**$_6$H$_5$), 137.4 (Ar–**C**$_6$F$_5$), 134.0 (Ar–**C**$_6$H$_5$), 129.3 (Ar–**C**$_6$H$_5$), 110.4 (Ar–**C**$_6$H$_5$), −2.7 (C$_6$F$_5$Si–(**C**H$_3$)$_2$), −4.2 (C$_6$H$_5$Si–(**C**H$_3$)$_2$). ^{19}F{^{1}H} NMR (470 MHz, C_6D_6): δ [ppm] = −126.1 (m, 2F, *o*-**F**), −152.2 (m, *p*-**F**), −161.5 (m, 2F, *m*-**F**). ^{29}Si{^{1}H} NMR (99 MHz, C_6D_6): δ [ppm] = −20.1, −20.8. MS (EI, 70 eV): *m*/*z* [assignment] = 344.9 [M−CH$_3$]$^+$, 135 [M−C$_8$H$_6$F$_5$Si]$^+$. HRMS: calculated for $C_{16}H_{17}F_5Si_2^+$: 360.07835, measured: 360.07795. AT-IR: $\tilde{\nu}$ [cm^{-1}] = 3071, 3053, 2971, 2956, 2900, 1639, 1577, 1549, 1514, 1453, 1427, 1408, 1367, 1277, 1251, 1106, 1076, 1027, 997, 963, 845, 824, 806, 761, 731, 697, 671, 643, 616, 498, 472, 444.

1,1,2,2-Tetramethyl-1-(perchlorophenyl)-2-phenyldisilane (4). To a suspension of hexachlorobenzene (2.5 g, 8.7 mmol, 1 eq.) in dry DE (200 mL) was added at −20 °C *n*-butyllithium (1.6 M in *n*-hexane, 5.5 mL, 8.7 mmol) and stirred for 1 h. 1-Chloro-1,1,2,2-tetramethyl-2-phenyldisilane (2.0 g, 8.7 mmol, 1 eq.) was added dropwise via a syringe over a period of 5

min. After complete addition the solution was allowed to slowly warm to ambient temperature and was stirred for 12 h. The resulting yellow suspension was quenched with water (30 mL), the aqueous layer extracted with dichloromethane (3 × 30 mL) and the combined organic layers dried over $MgSO_4$. After removing the solvent under reduced pressure, the crude yellow oil was purified by column chromatography (*n*-pentane) and recrystallized from *n*-hexane to give 1,1,2,2-tetramethyl-1-(perchlorophenyl)-2-phenyldisilane (3.1 g, 6.9 mmol, 79%) as colorless crystals. ^{1}H NMR (500 MHz, C_6D_6): δ [ppm] = 7.36 (m, 2H, Ar–**H**), 7.18 (m, 3H, Ar–**H**), 0.52 (s, 6H, Si–(C**H**$_3$)$_2$),0.37 (s, 6H, Si–(C**H**$_3$)$_2$). ^{13}C{^{1}H} NMR (126 MHz, C_6D_6): δ [ppm] = 139.4 (Ar–**C**), 138.6 (Ar–**C**), 138.3 (Ar–**C**), 134.6 (Ar–**C**), 134.1 (Ar–**C**), 132.4 (Ar–**C**), 129.0 (Ar–**C**), 128.1 (Ar–**C**), 2.3 (Si–(**C**H$_3$)$_2$), −2.7 (Si–(**C**H$_3$)$_2$). ^{29}Si{^{1}H} NMR (99 MHz, C_6D_6): δ [ppm] = −9.1, −18.7. MS (EI, 70 eV): *m*/*z* [assignment] = 426.9 [M−CH$_3$]$^+$, 306.9 [M−C$_8$H$_{11}$Si]$^+$. AT-IR: *v* [cm^{-1}] = 3067, 3049, 2996, 2952, 2895, 1514, 1426, 1403, 1336, 1321, 1291, 1247, 1158, 1105, 1088, 1067, 998, 860, 833, 790, 762, 731, 696, 678, 646, 624, 584, 473, 440. Elemental analysis calculated (%) for $C_{16}H_{17}Cl_5Si_2$: C 43.41, H 3.87; found: C 43.52, H 3.80.

1,1,2,2-Tetramethyl-1-(perchlorophenyl)-2-(perfluorophenyl)disilane (5). To a suspension of hexachlorobenzene (0.92 g, 3.2 mmol, 1 eq.) in dry DE (200 mL) was added at −20 °C *n*-butyllithium (1.6 M in *n*-hexane, 2.0 mL, 3.2 mmol) and was stirred for 1 h. 1-Chloro-1,1,2,2-tetramethyl-2-(perfluorophenyl)disilane (1.0 g, 3.2 mmol, 1 eq.) was added dropwise via a syringe over a period of 5 min. After complete addition the solution was allowed to slowly warm to ambient temperature and stirred was for 12 h. The resulting yellow suspension was quenched with water (30 mL), the aqueous layer extracted with dichloromethane (3 × 30 mL) and the combined organic layers dried over $MgSO_4$. After removing the solvent under reduced pressure, the crude colorless oil was purified by column chromatography (*n*-pentane) and recrystallized from *n*-hexane to give 1,1,2,2-tetramethyl-1-(perchlorophenyl)-2-(perfluorophenyl)disilane (1.4 g, 2.6 mmol, 83%) as colorless crystals. ^{1}H NMR (500 MHz, C_6D_6): δ [ppm] = 0.47 (s, 6H Si–(C**H**$_3$)$_2$), 0.36 (s, 6H Si–(C**H**$_3$)$_2$). ^{13}C{^{1}H} NMR (126 MHz, C_6D_6): δ [ppm] = 148.9 (Ar–**C**$_6$F$_5$), 142.0 (Ar–**C**$_6$F$_5$), 138.2 (Ar–**C**$_6$Cl$_5$), 137.8 (Ar–**C**$_6$Cl$_5$), 137.4 (Ar–**C**$_6$F$_5$), 135.2 (Ar–**C**$_6$Cl$_5$), 132.6 (Ar–**C**$_6$Cl$_5$), 110.5 (Ar–**C**$_6$F$_5$), −1.5 (C$_6$F$_5$Si–(**C**H$_3$)$_2$), −1.7 (C$_6$Cl$_5$Si–(**C**H$_3$)$_2$). ^{19}F{^{1}H} NMR (470 MHz, C_6D_6): δ [ppm] = −126.2 (m, 2F, *o*-**F**), −151.3 (tt, $^{3}J_{F,F}$ = 21.1 Hz, $^{4}J_{F,F}$ = 3.7 Hz, *p*-**F**), −161.1 (m, 2F, *m*-**F**). ^{29}Si{^{1}H} NMR (99 MHz, C_6D_6): δ [ppm] = −8.5, −16.8. MS (EI, 70 eV): *m*/*z* [assignment] = 516.7 [M−CH$_3$]$^+$, 306.8 [M−C$_8$H$_6$F$_5$Si]$^+$. HRMS: calculated for $C_{16}H_{12}Cl_5F_5Si_2^+$: 529.88349, measured: 529.88354. AT-IR: *v* [cm^{-1}] = 1638, 1510, 1466, 1453, 1409, 1369, 1335, 1326, 1292, 1251, 1214, 1160, 1131, 1076, 1017, 964, 860, 830, 783, 739, 716, 696, 679, 663, 626, 585, 498, 443. Elemental analysis calculated (%) for $C_{16}H_{12}Cl_5F_5Si_2$: C 36.08, H 2.27, found: C 35.90, H 2.01.

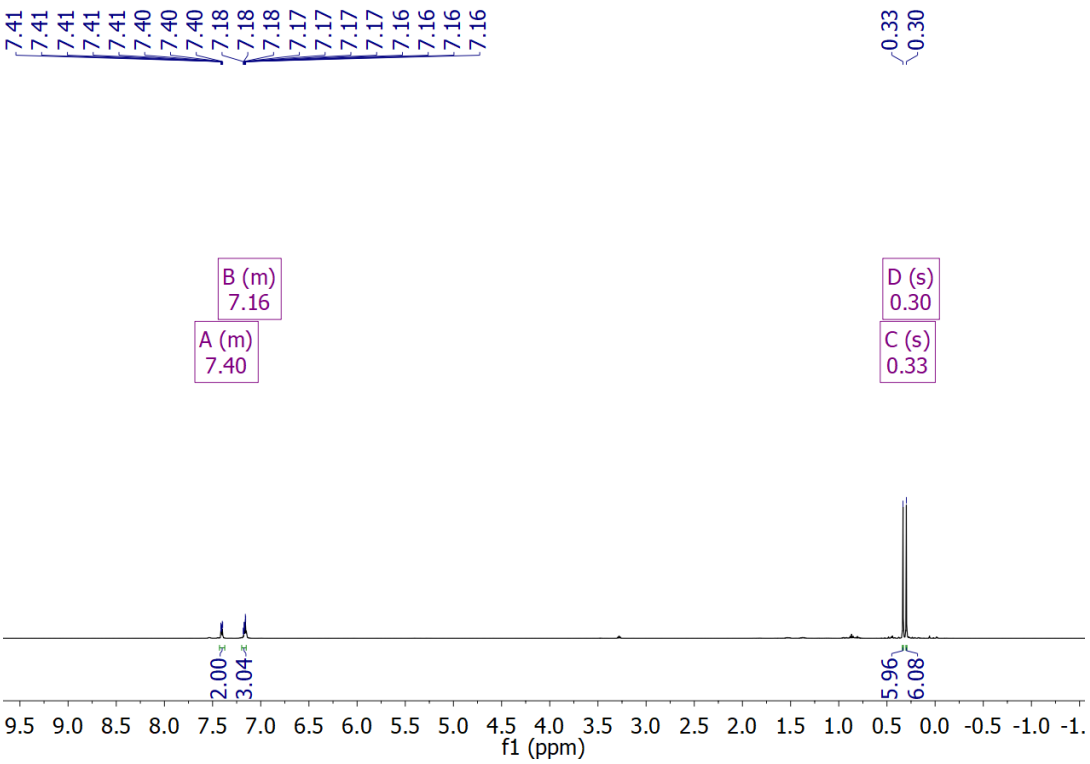

Figure S1: ^{1}H NMR spectrum of a solution of 1-chloro-1,1,2,2-tetramethyl-2-phenyldisilane (**1**) in C_6D_6 measured at 293 K, 500 MHz.

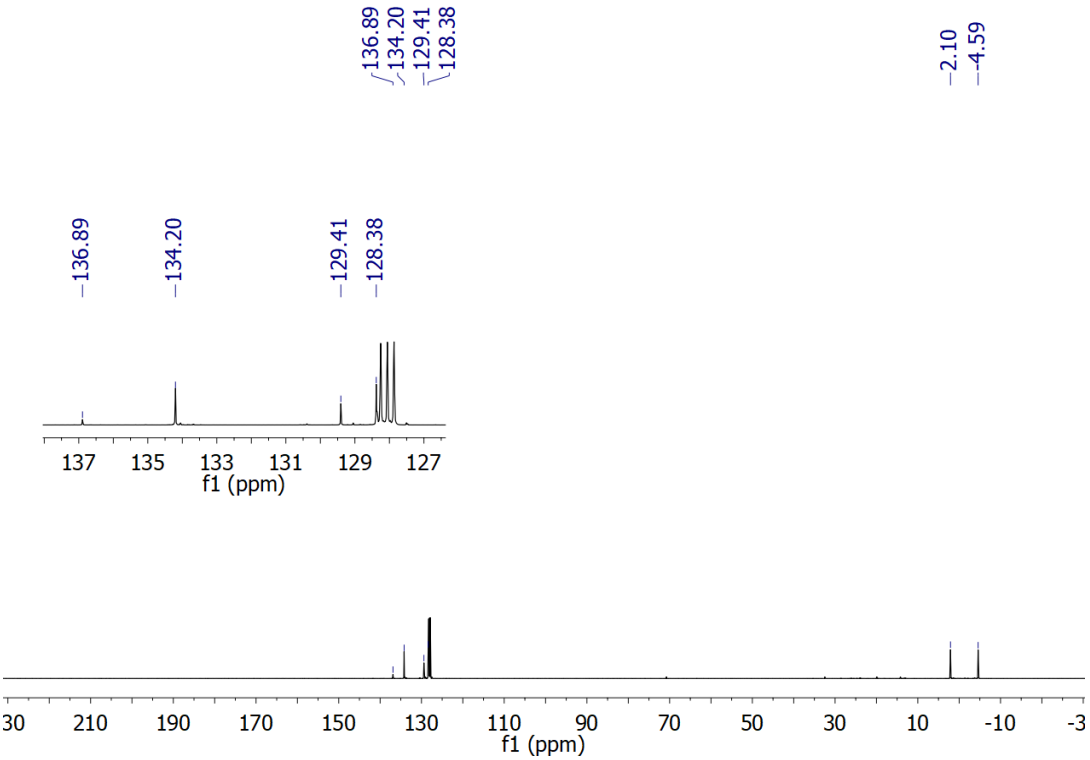

Figure S2: $^{13}C\{^{1}H\}$ NMR spectrum of a solution of 1-chloro-1,1,2,2-tetramethyl-2-phenyldisilane (**1**) in C_6D_6 measured at 293 K, 126 MHz.

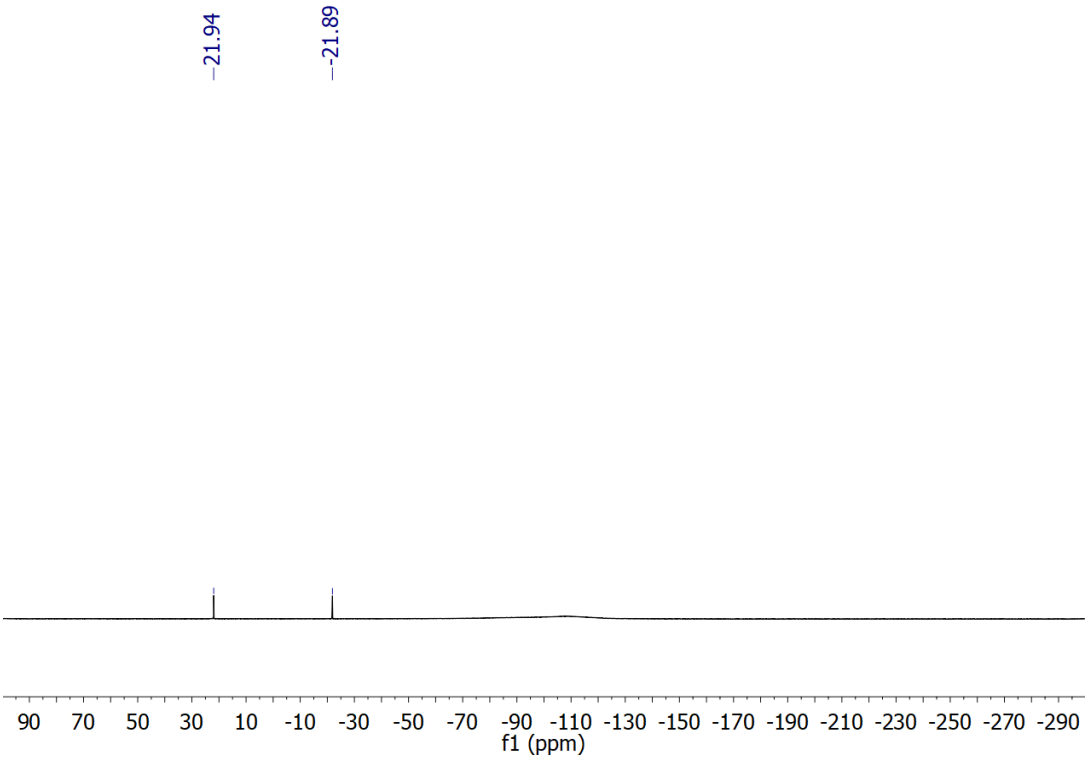

Figure S3: $^{29}Si\{^{1}H\}$ NMR spectrum of a solution of 1-chloro-1,1,2,2-tetramethyl-2-phenyldisilane (**1**) in C_6D_6 measured at 293 K, 99 MHz.

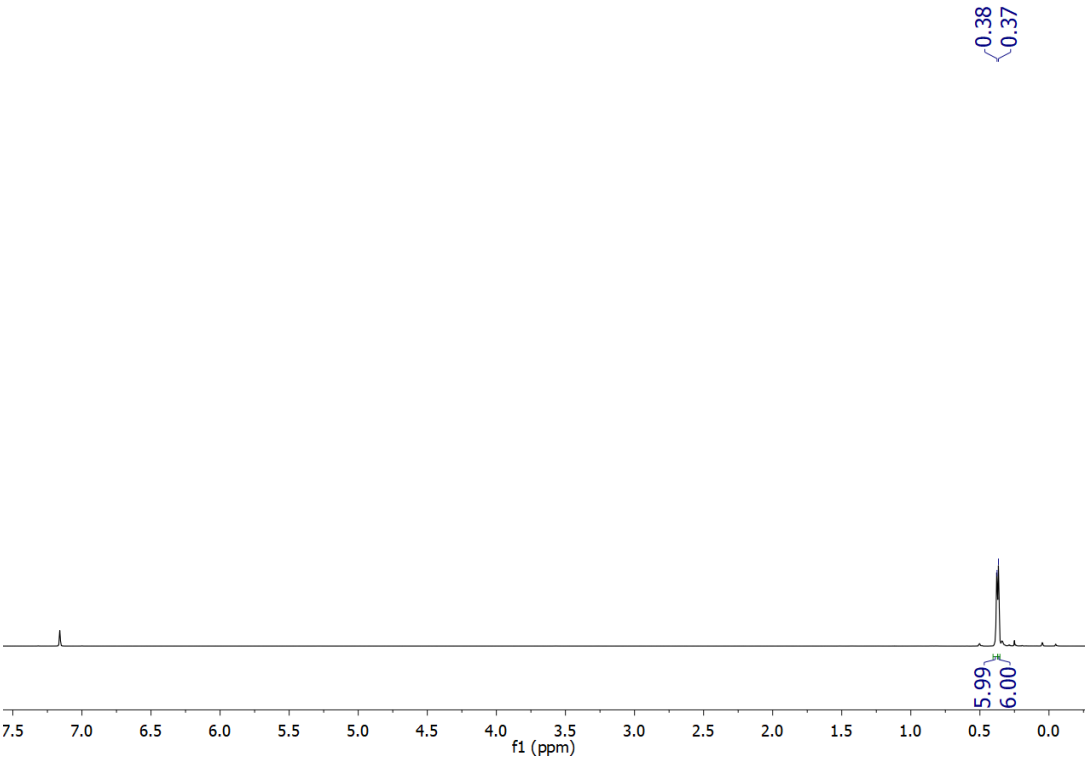

Figure S4: ^{1}H NMR spectrum of a solution of 1-chloro-1,1,2,2-tetramethyl-2-(perfluorophenyl)disilane (**2**) in C_6D_6 measured at 293 K, 500 MHz.

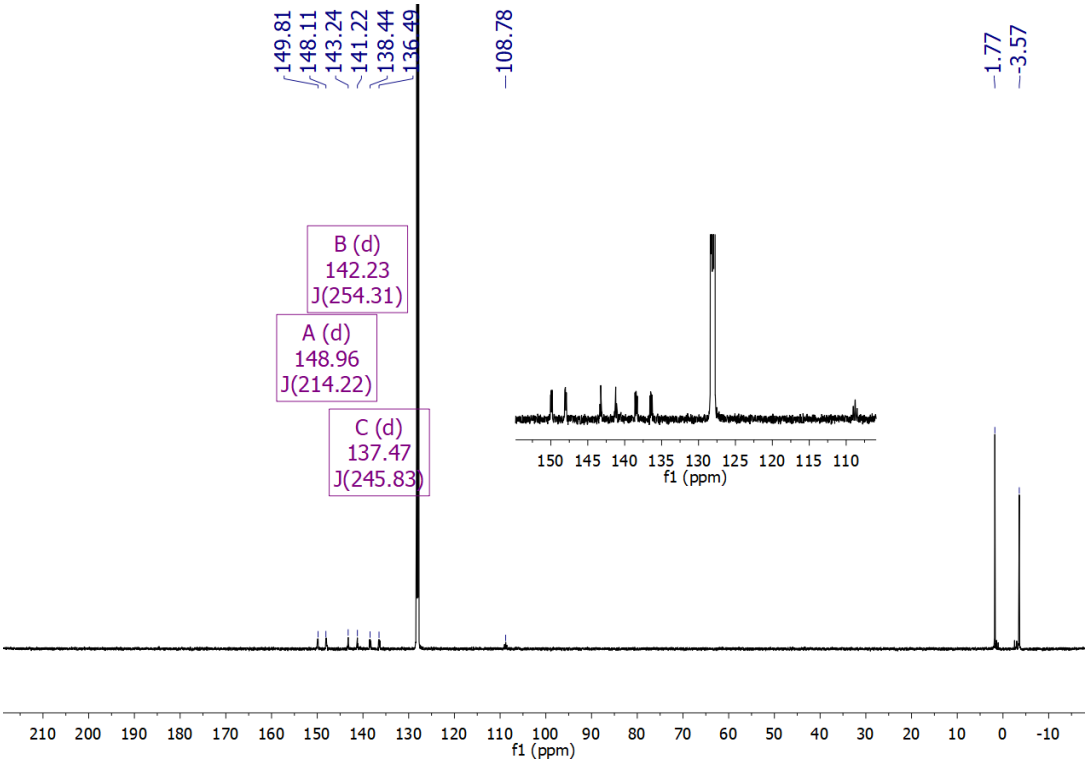

Figure S5: $^{13}C\{^{1}H\}$ NMR spectrum of a solution of 1-chloro-1,1,2,2-tetramethyl-2-(perfluorophenyl)disilane (**2**) in C_6D_6 measured at 293 K, 126 MHz.

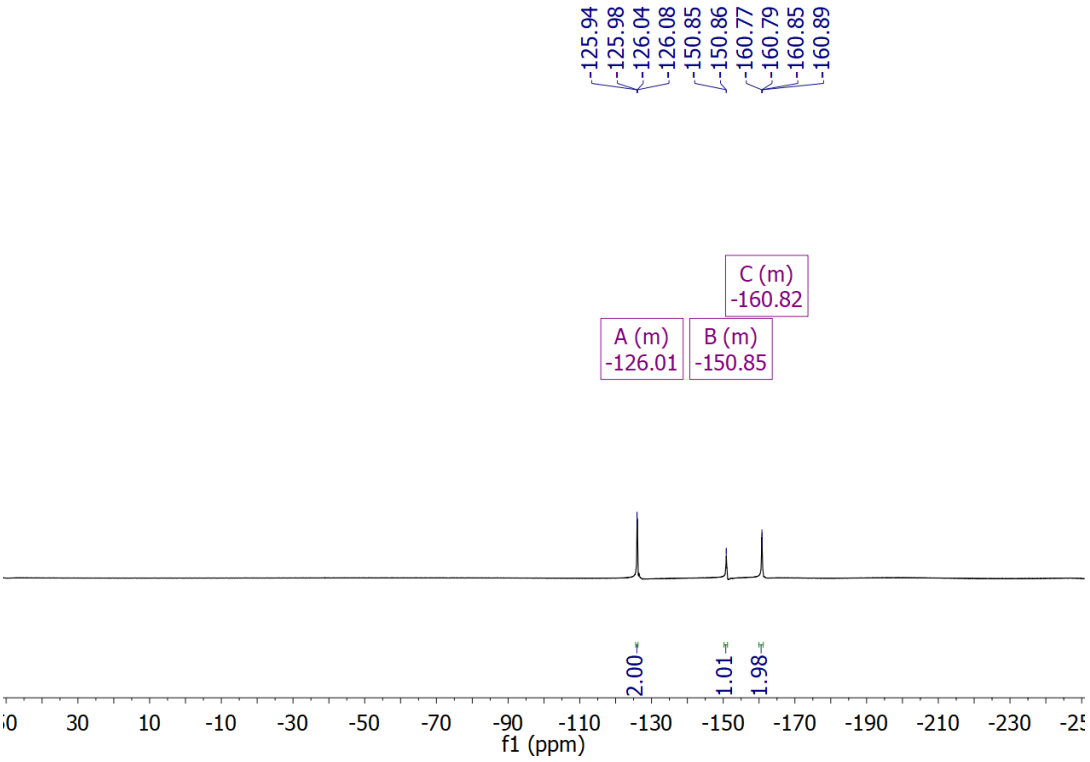

Figure S6: $^{19}F\{^{1}H\}$ NMR spectrum of a solution of 1-chloro-1,1,2,2-tetramethyl-2-(perfluorophenyl)disilane (**2**) in C_6D_6 measured at 293 K, 470 MHz.

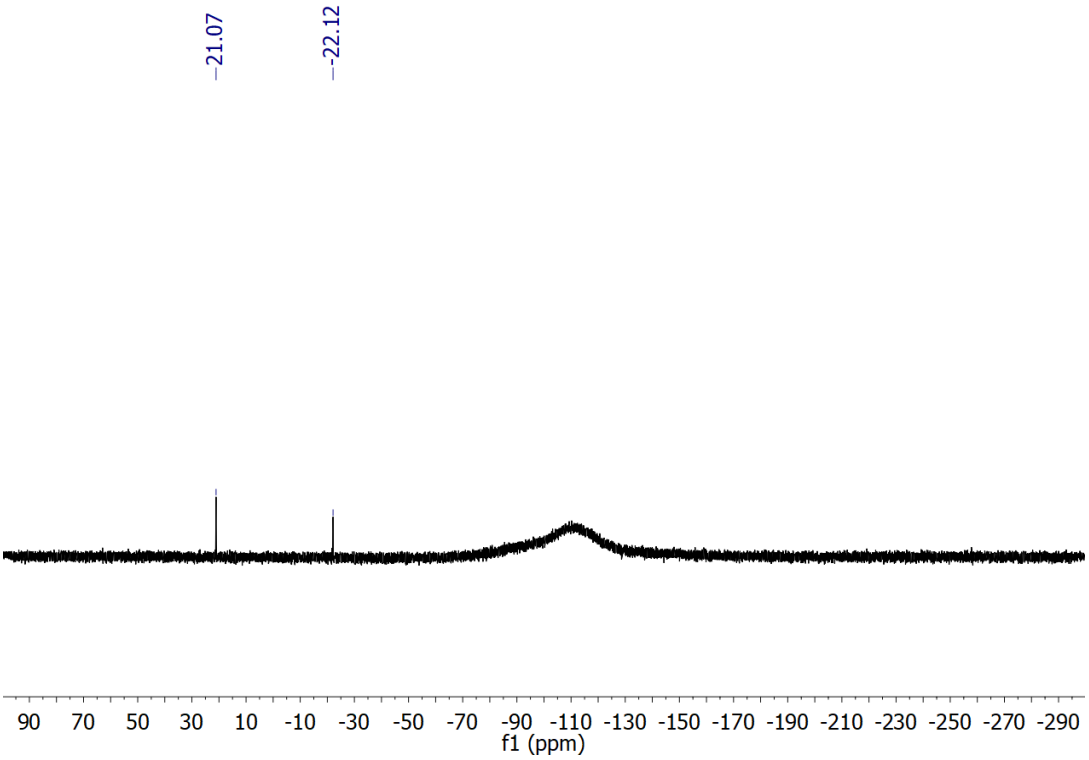

Figure S7: $^{29}Si\{^{1}H\}$ NMR spectrum of a solution of 1-chloro-1,1,2,2-tetramethyl-2-(perfluorophenyl)disilane (**2**) in C_6D_6 measured at 293 K, 99 MHz.

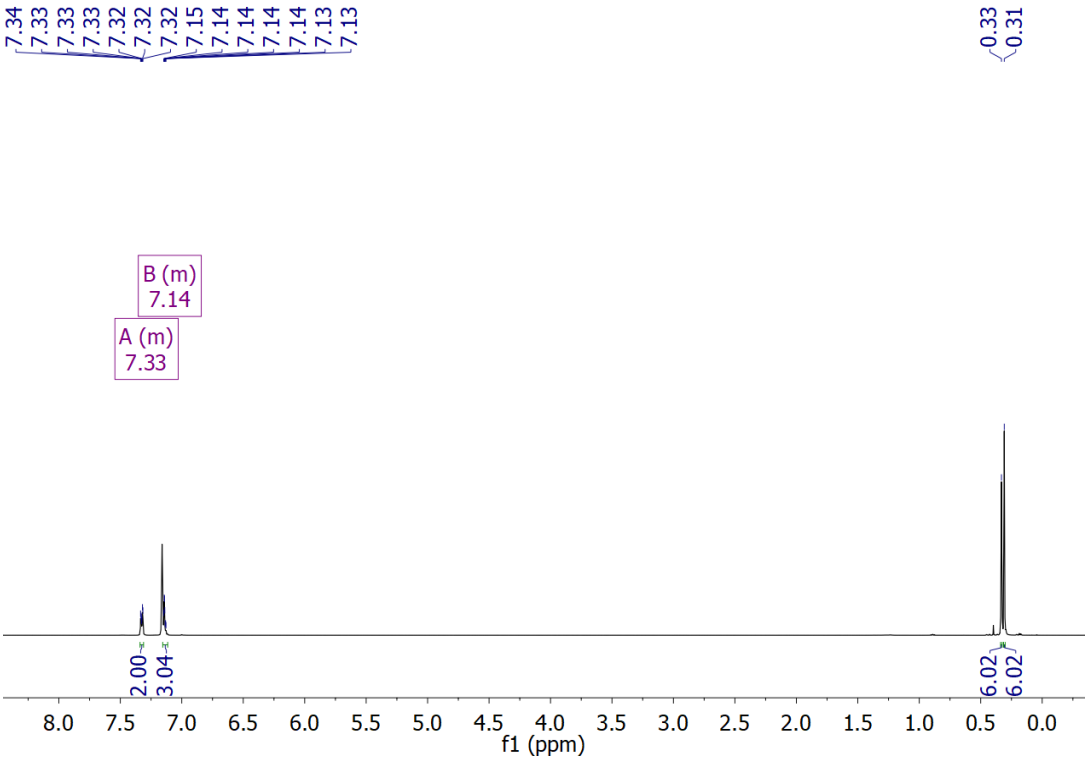

Figure S8: ^{1}H NMR spectrum of a solution of 1,1,2,2-tetramethyl-1-(perfluorophenyl)-2-phenyldisilane (**3**) in C_6D_6 measured at 293 K, 500 MHz.

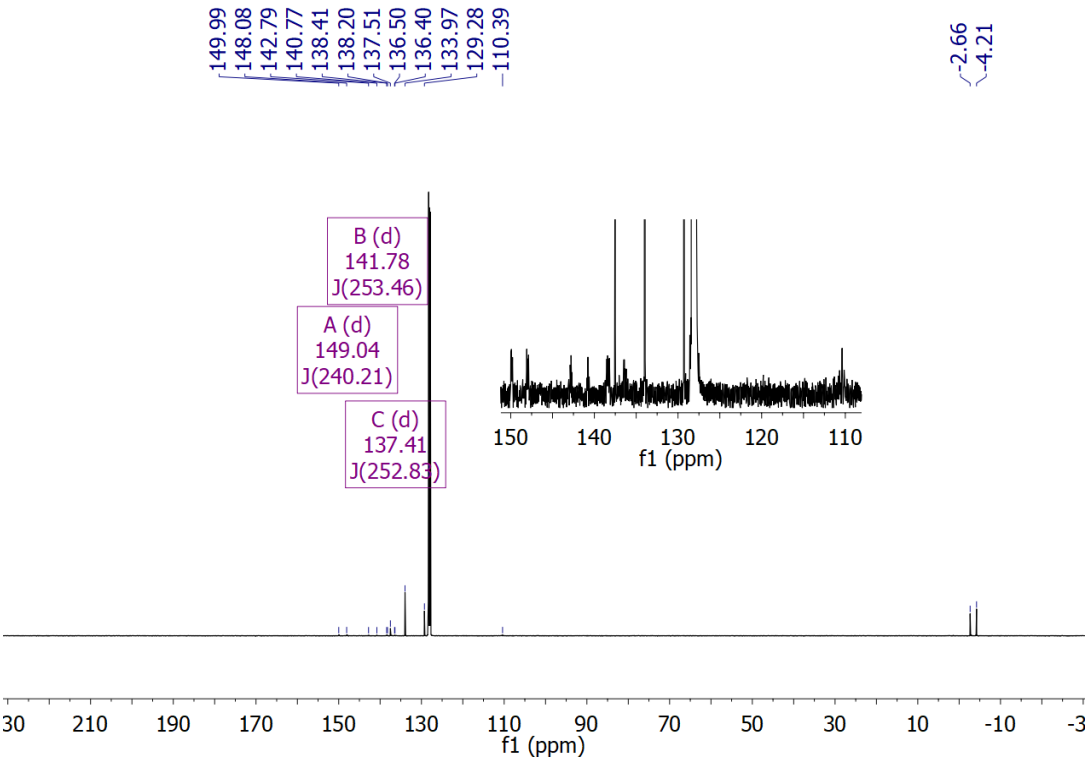

Figure S9: $^{13}C\{^{1}H\}$ NMR spectrum of a solution of 1,1,2,2-tetramethyl-1-(perfluorophenyl)-2-phenyldisilane (**3**) in C_6D_6 measured at 293 K, 126 MHz.

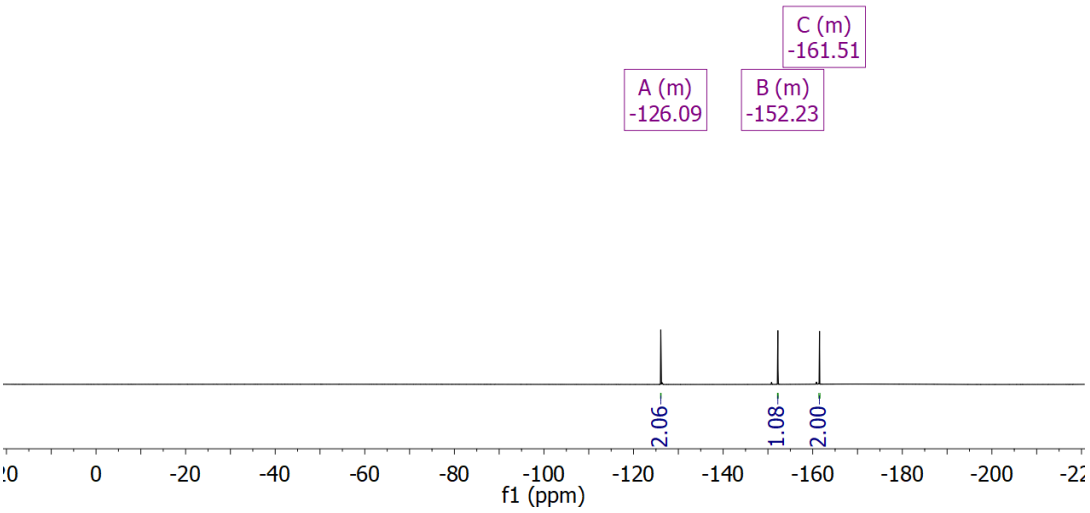

Figure S10: $^{19}F\{^{1}H\}$ NMR spectrum of a solution of 1,1,2,2-tetramethyl-1-(perfluorophenyl)-2-phenyldisilane (**3**) in C_6D_6 measured at 293 K, 470 MHz.

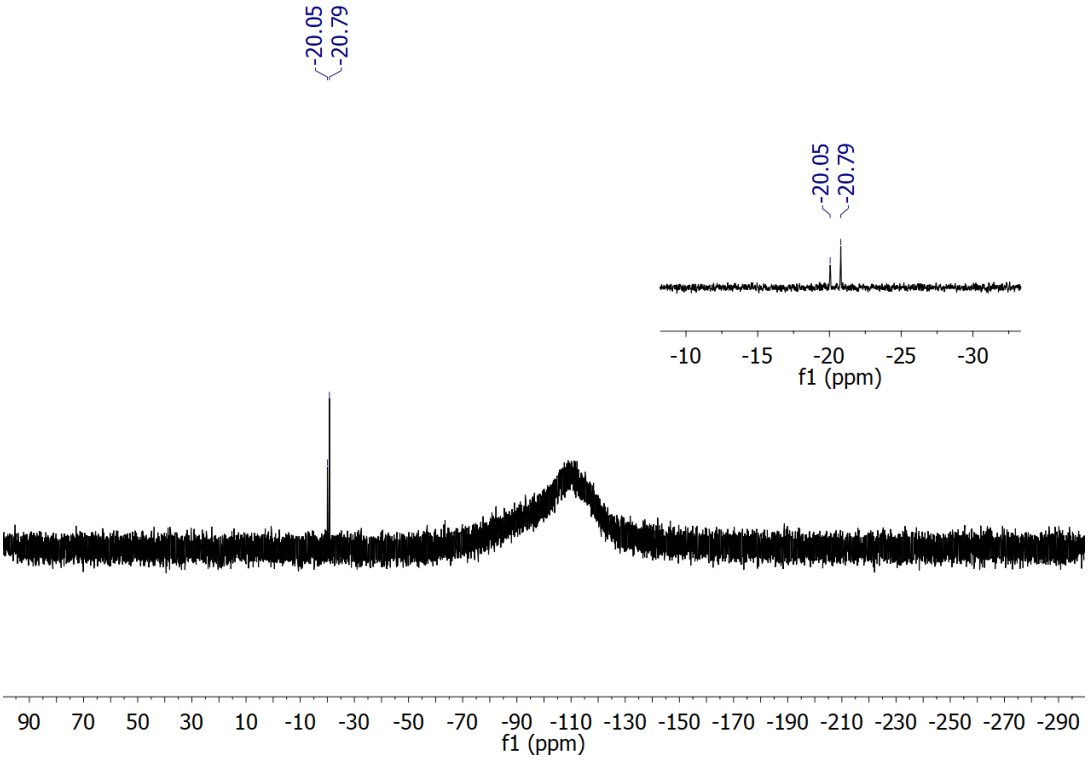

Figure S11: $^{29}Si\{^{1}H\}$ NMR spectrum of a solution of 1,1,2,2-tetramethyl-1-(perfluorophenyl)-2-phenyldisilane (**3**) in C_6D_6 measured at 293 K, 99 MHz.

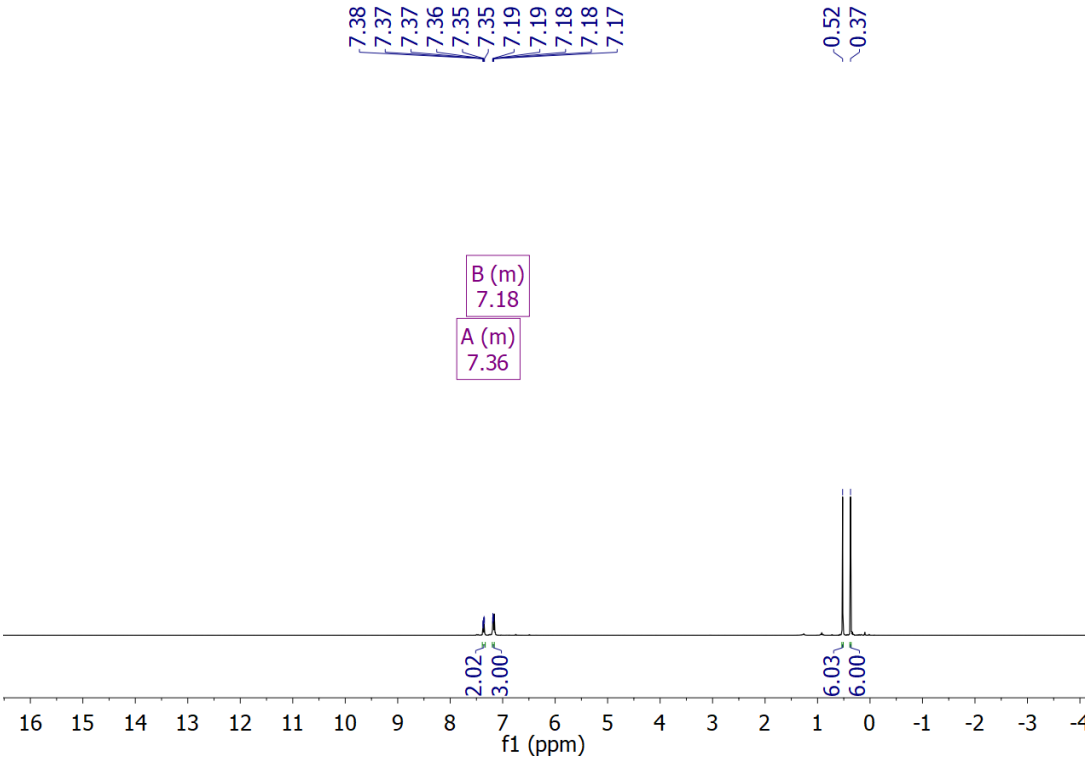

Figure S12: ^{1}H NMR spectrum of a solution of 1,1,2,2-tetramethyl-1-(perchlorophenyl)-2-phenyldisilane (**4**) in C_6D_6 measured at 293 K, 500 MHz.

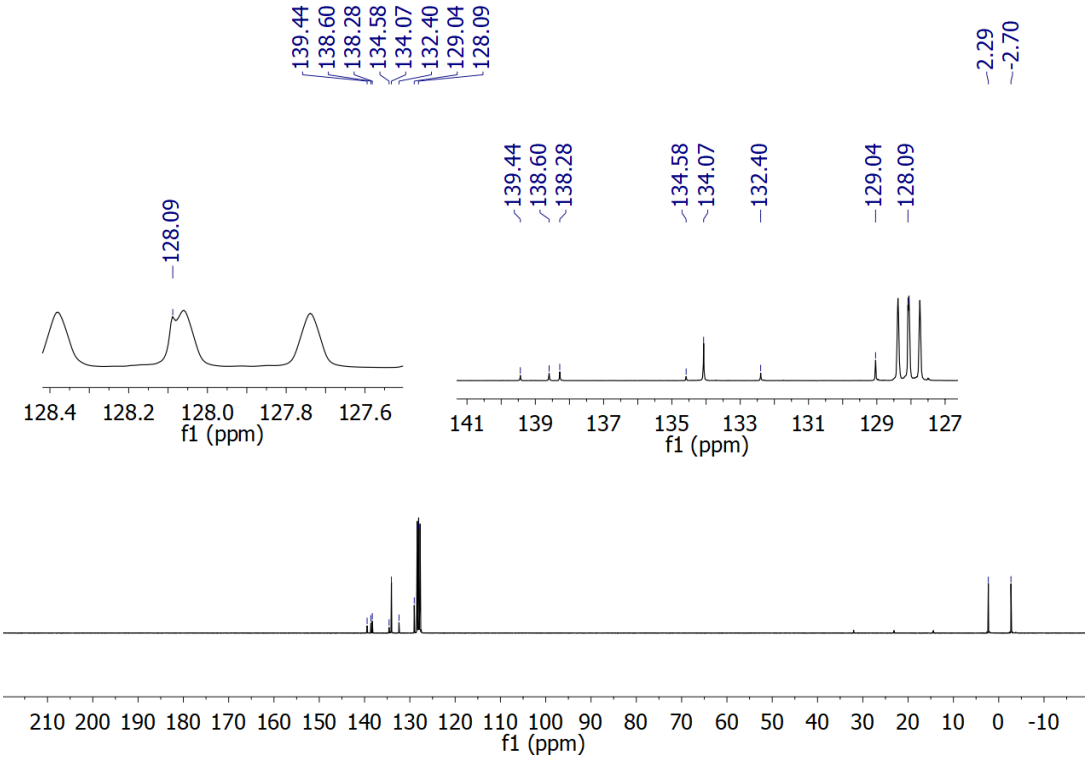

Figure S13: $^{13}C\{^{1}H\}$ NMR spectrum of a solution of 1,1,2,2-tetramethyl-1-(perchlorophenyl)-2-phenyldisilane (**4**) in C_6D_6 measured at 293 K, 126 MHz.

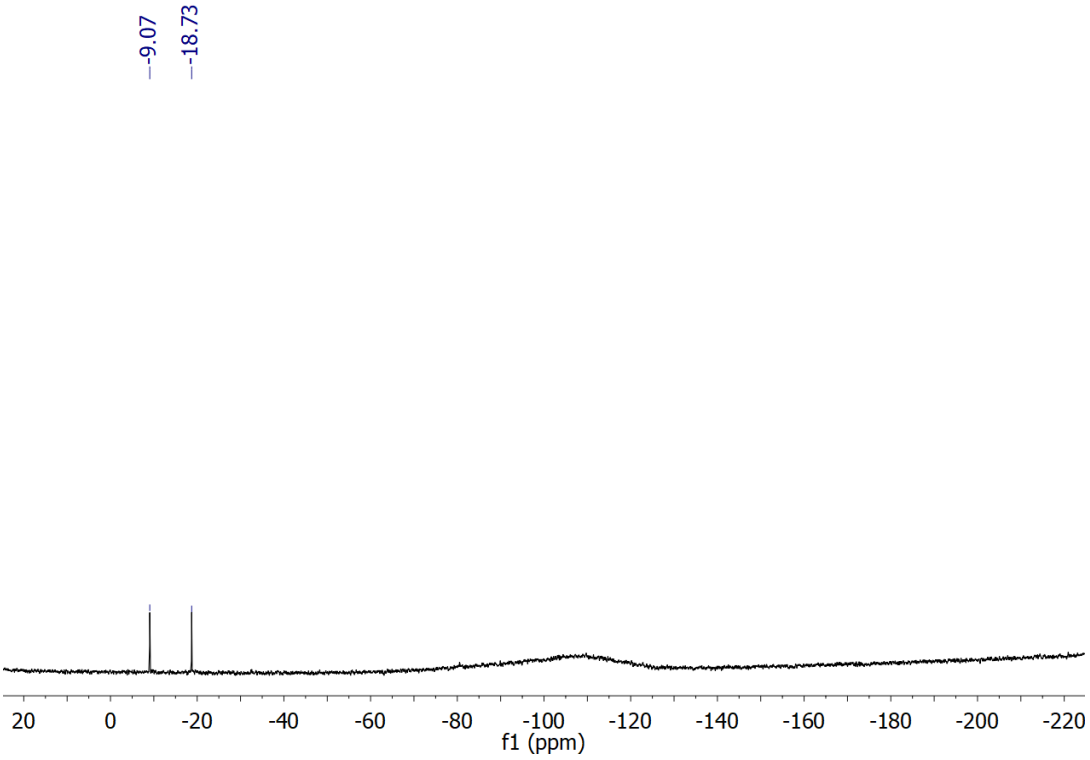

Figure S14: $^{29}Si\{^{1}H\}$ NMR spectrum of a solution of 1,1,2,2-tetramethyl-1-(perfluorophenyl)-2-phenyldisilane (**4**) in C_6D_6 measured at 293 K, 99 MHz.

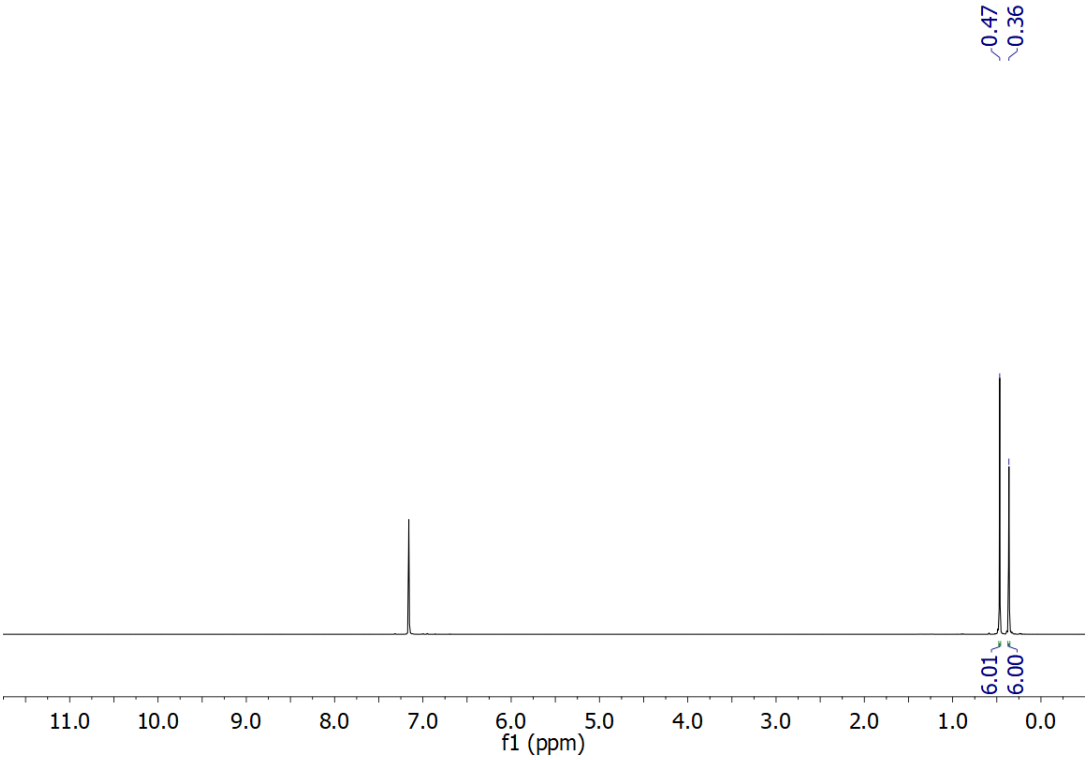

Figure S15: ^{1}H NMR spectrum of a solution of 1,1,2,2-tetramethyl-1-(perchlorophenyl)-2-(perfluorophenyl)disilane (**5**) in C_6D_6 measured at 293 K, 500 MHz.

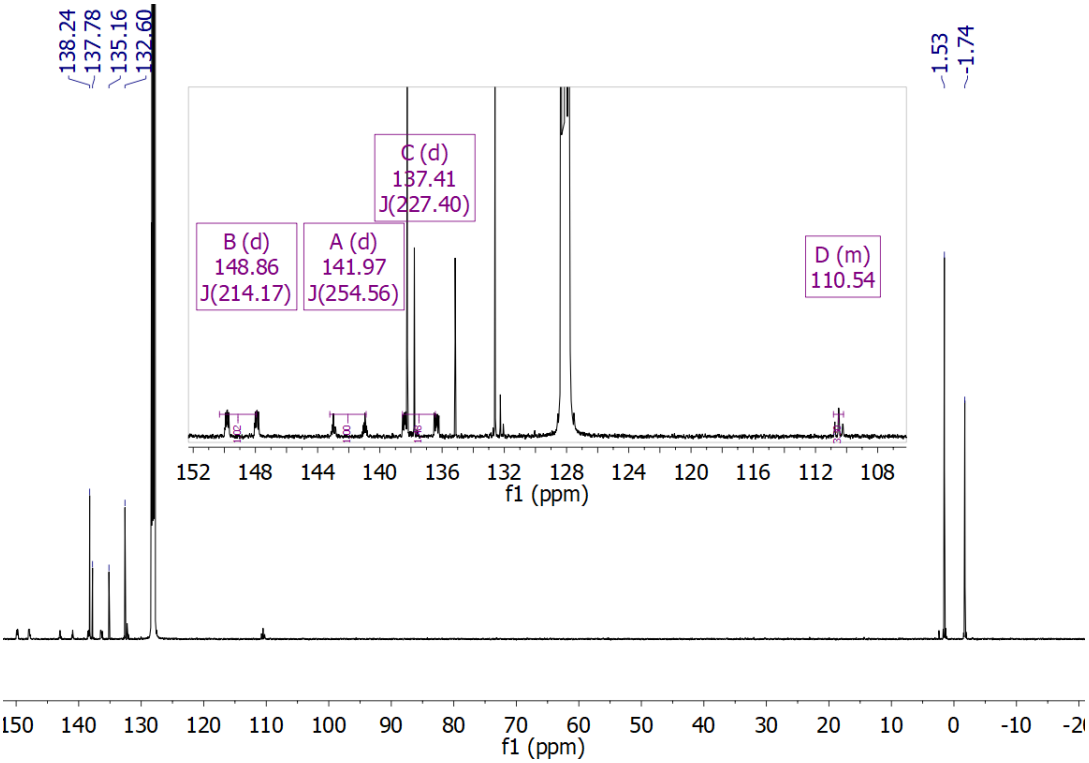

Figure S16: $^{13}C\{^{1}H\}$ NMR spectrum of a solution of 1,1,2,2-tetramethyl-1-(perchlorophenyl)-2-(perfluorophenyl)disilane (**5**) in C_6D_6 measured at 293 K, 126 MHz.

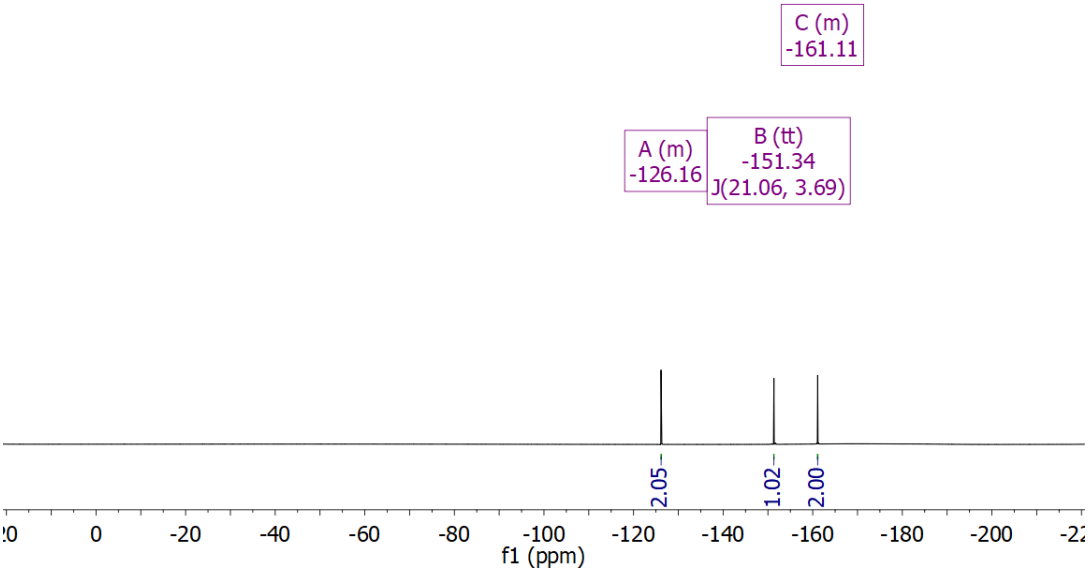

Figure S17: $^{19}F\{^{1}H\}$ NMR spectrum of a solution of 1,1,2,2-tetramethyl-1-(perchlorophenyl)-2-(perfluorophenyl)disilane (**5**) in C_6D_6 measured at 293 K, 470 MHz.

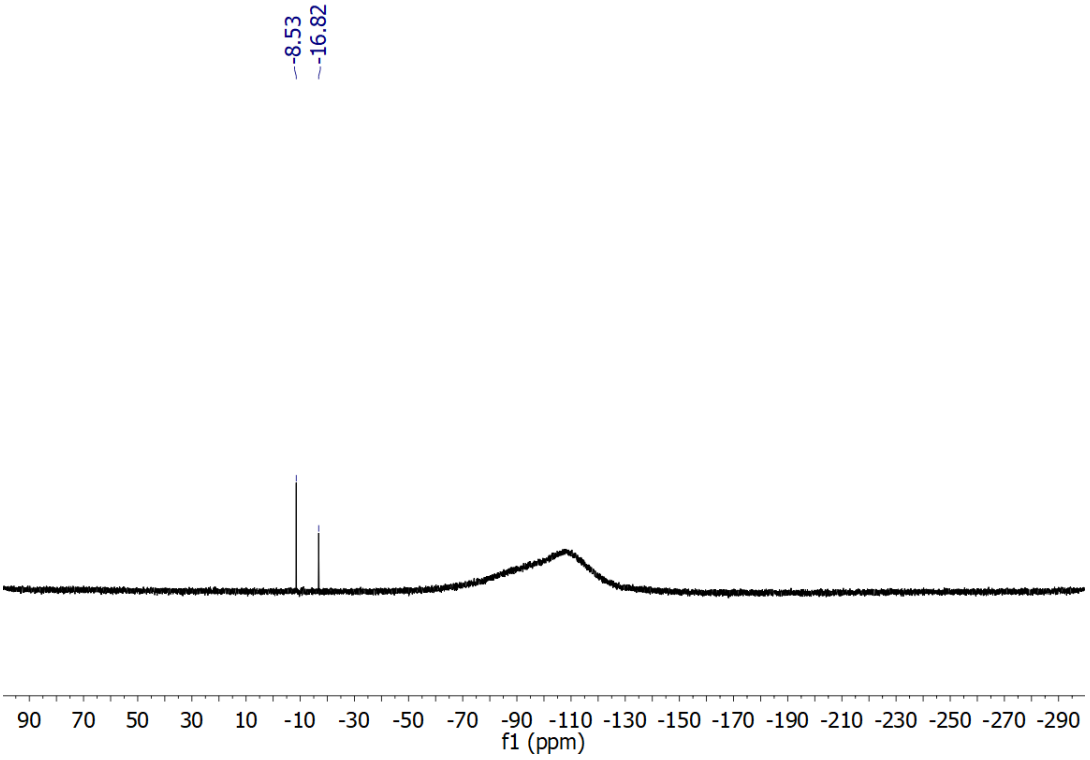

Figure S18: $^{29}Si\{^{1}H\}$ NMR spectrum of a solution of 1,1,2,2-tetramethyl-1-(perchlorophenyl)-2-(perfluorophenyl)disilane (**5**) in C_6D_6 measured at 293 K, 99 MHz.

Crystallographic Data

Suitable crystals were obtained by slow evaporation of a saturated *n*-hexane (**3**-**5**), methanol (**5**) or acetonitrile (**5**) solutions, respectively. Using Olex2,[1] the structures were solved with the ShelXS[2] or ShelXT[3] structure solution program using direct methods and refined with the ShelXL[4] refinement package using least squares minimization. CCDC 1971114-1971118 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge via http://www.ccdc.cam.ac.uk/conts/retrieving.html.

Several attempts have been made to crystallize compound **5** from benzene or toluene, all of them resulting in amorphous solids not suitable for X-ray diffraction. Attempts to co-crystallize **5** with naphthalene from *n*-hexane as the solvent led to the previously described structure of $\mathbf{5}_{Hex}$.

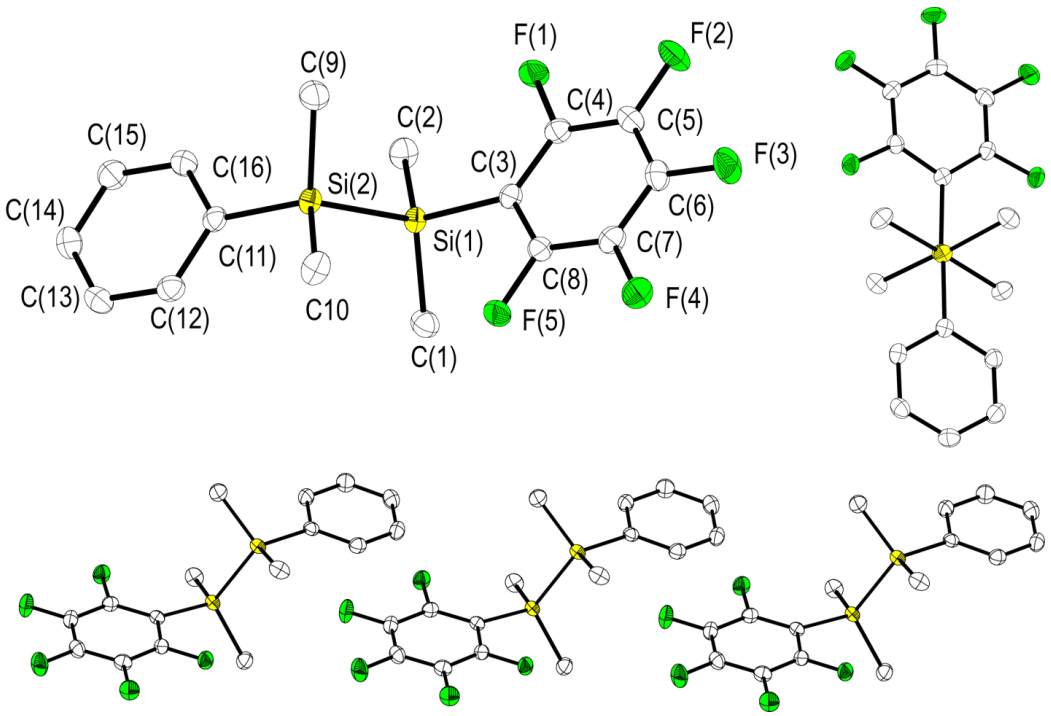

Figure S19: Molecular structure of 1,1,2,2-tetramethyl-1-(perfluorophenyl)-2-phenyldisilane (**3**) in the crystalline state (top left), view along the Si–Si- axis (top right) and the extended structure and packing by further π-stacking interactions (bottom). Hydrogen atoms are omitted for clarity. Displacement ellipsoids are drawn at 50% probability level.

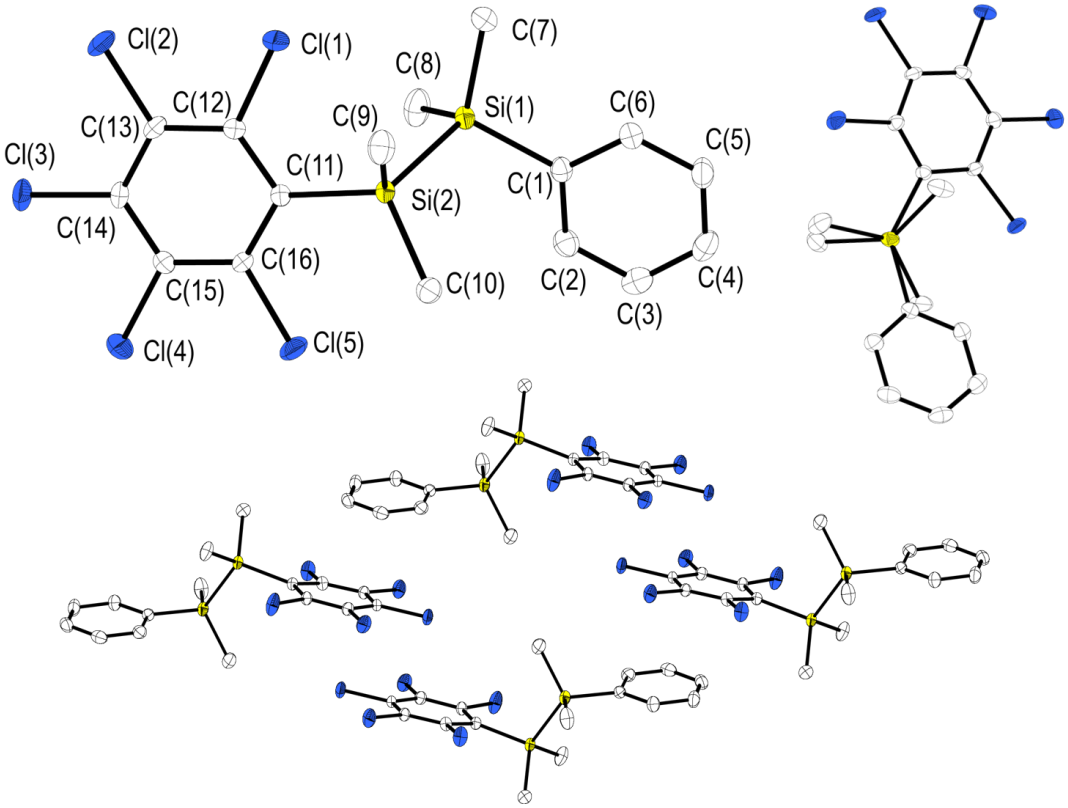

Figure S20: Molecular structure of 1,1,2,2-tetramethyl-1-(perchlorophenyl)-2-phenyldisilane (**4**) in the crystalline state (top left), view along the Si–Si- axis (top right) and the extended structure and packing by further π-stacking interactions (bottom). Hydrogen atoms were refined isotropically and are omitted for clarity in the figure. The C_6Cl_5 group is disordered in ratio 89:11. All 1-2 and 1-3 distances of disordered parts were restrained to be same, the U_{eq} values of neighboring atoms were constrained to be same pair wisely. Displacement ellipsoids are drawn at 50% probability level.

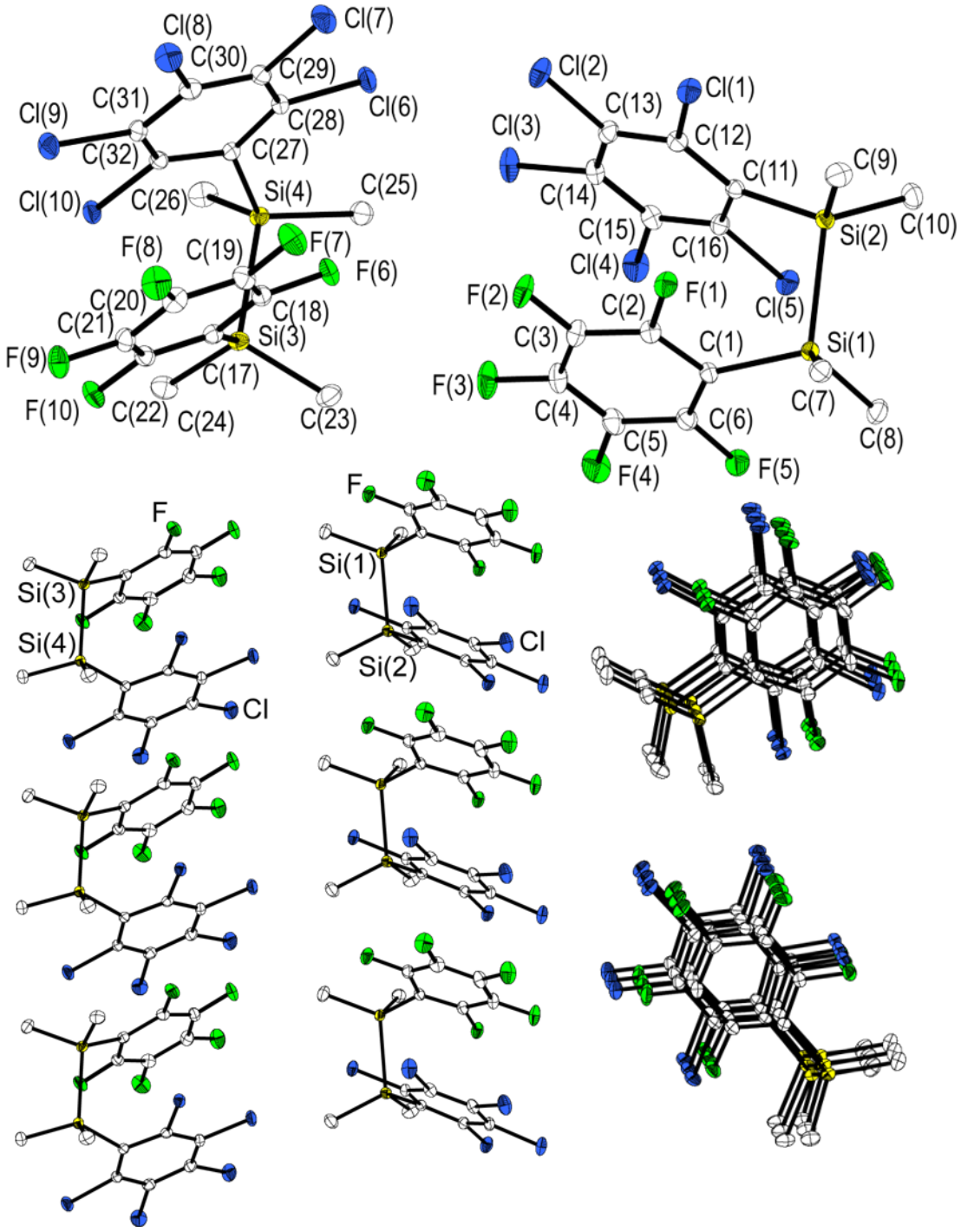

Figure S21: Molecular structure of 1,1,2,2-tetramethyl-1-(perchlorophenyl)-2-(perfluorophenyl)disilane (**5·*n*-hex**) (crystallized from n-hexane) in the crystalline state (top), extended structure and packing by further π-stacking interactions (bottom left) and the view along the Si–Si- axis (bottom right). Hydrogen atoms were taken into account using a riding model and are omitted for clarity in the figure. The hydrogen atoms of the methyl group C(10) are disordered, an idealized ratio 1:1 was applied. Displacement ellipsoids are drawn at 50% probability level.

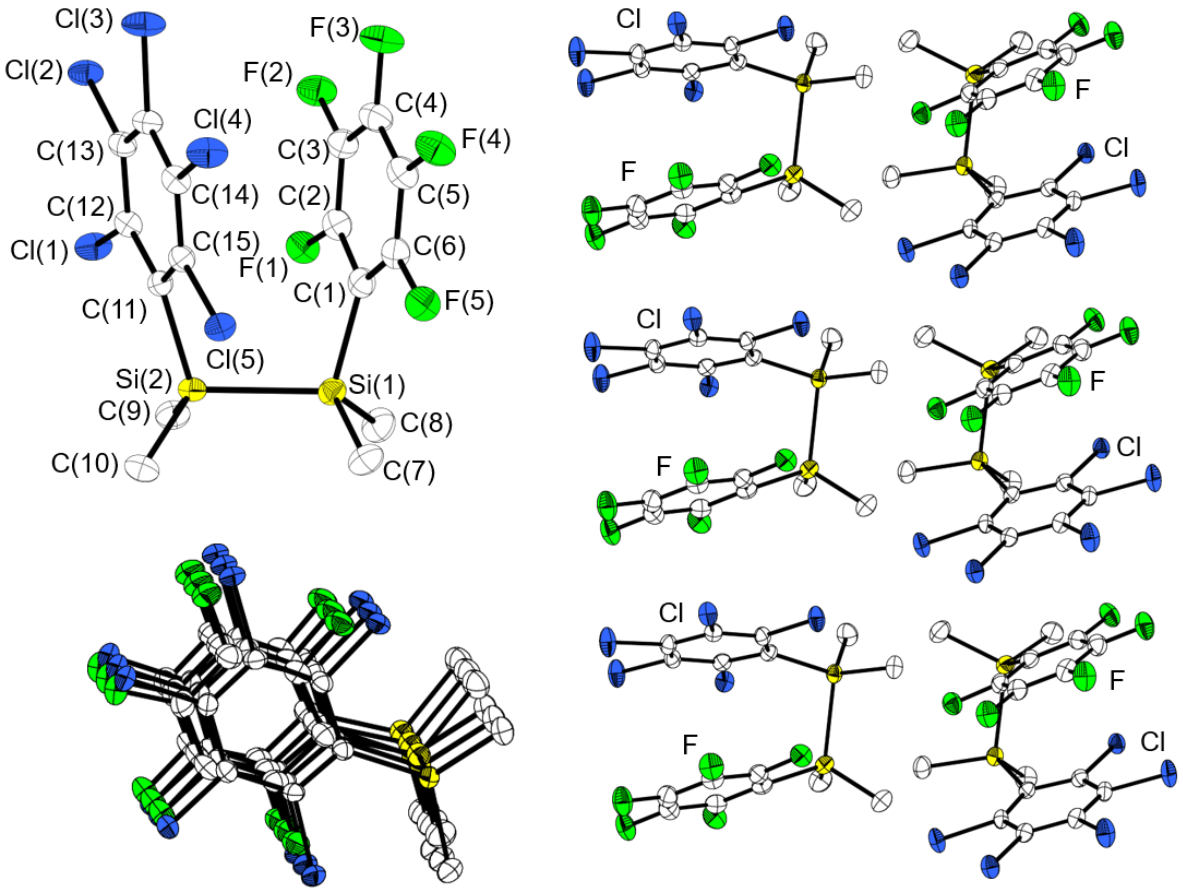

Figure S22 Molecular structure of 1,1,2,2-tetramethyl-1-(perchlorophenyl)-2-(perfluorophenyl)disilane (**5·ACN**) (crystallized from acetonitrile) in the crystalline state (top left), extended structure and packing by further π-stacking interactions (right) and the view along the Si–Si- axis (bottom left). Hydrogen atoms were refined isotropically and are omitted for clarity. Displacement ellipsoids are drawn at 50% probability level.

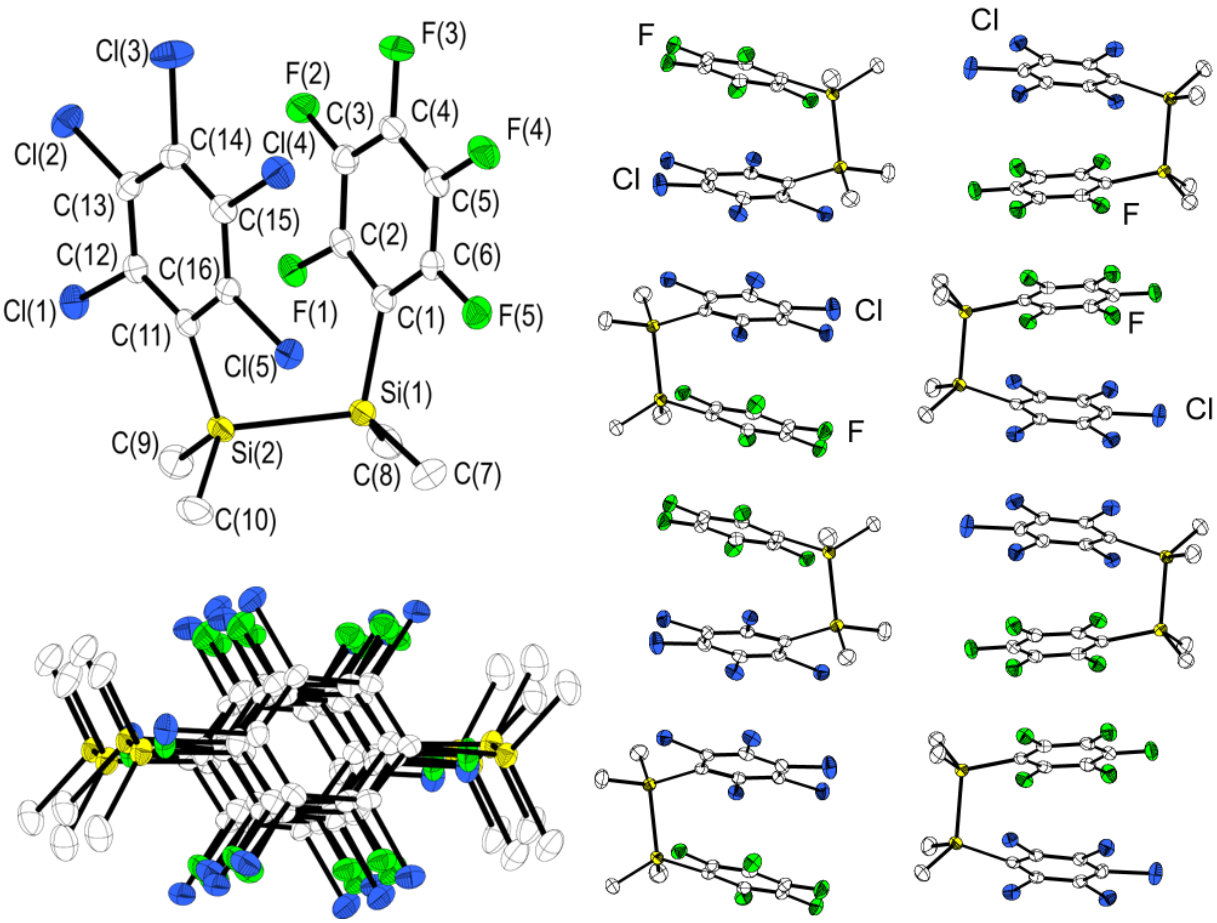

Figure S23 Molecular structure of 1,1,2,2-tetramethyl-1-(perchlorophenyl)-2-(perfluorophenyl)disilane (**5·MeOH**) (crystallized from methanol) in the crystalline state (top left), extended structure and packing by further π-stacking interactions (right) and the view along the Si–Si- axis (bottom left). Hydrogen atoms were refined isotropically and are omitted for clarity. Displacement ellipsoids are drawn at 50% probability level.

Table S1: Crystallographic data for **3**, **4** and **5**.

	3	**4**	**5 (*n*-hexane)**	**5 (MeOH)**	**5 (ACN)**
Empirical formula	$C_{16}H_{17}F_5Si_2$	$C_{16}H_{17}Cl_5Si_2$	$C_{16}H_{12}Cl_5F_5Si_2$	$C_{16}H_{12}Cl_5F_5Si_2$	$C_{16}H_{12}Cl_5F_5Si_2$
M [g mol^{-1}]	360.47	442.72	532.69	532.69	532.69
Diffraktometer	SuperNova	SuperNova	SuperNova	SuperNova	SuperNova
T [K]	100.0(1)	100.0(1)	100.0(1)	100.0(1)	100.0(1)
λ [Å]	1.54184	0.71073	0.71073	0.71073	1.54184
Crystal system	triclinic	triclinic	triclinic	monoclinic	monoclinic
Space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P2_1/n$	$P2_1/n$
a [Å]	7.7407(3)	9.0639(3)	7.4433(4)	7.4610(2)	7.5524(4)
b [Å]	9.4632(4)	9.3355(3)	15.7582(9)	19.0631(5)	14.9892(6)
c [Å]	13.1078(5)	13.4071(4)	18.0844(12)	14.6867(3)	18.8060(9)
α [°]	74.013(3)	94.436(2)	89.433(5)	90	90
β [°]	80.178(3)	104.175(3)	81.593(5)	91.567(2)	101.387(4)
γ [°]	67.671(4)	113.509(3)	80.330(5)	90	90
V [Å^3]	851.47(6)	988.89(5)	2068.3(2)	2088.10(9)	2087.02(17)
Z	2	2	4	4	4
μ [mm^{-1}]	2.321	0.850	0.862	0.854	7.873
ρ_{calcd} [Mg m^{-3}]	1.406	1.487	1.711	1.694	1.695
F(000)	372	452	1064	1064	1064
$2\Theta_{max}$ [°]	151.338	60.1	65.4	65.7	154.2
Index ranges	$-9 \le h \le 9$ $-11 \le k \le 11$ $-16 \le l \le 16$	$-12 \le h \le 12$ $-13 \le k \le 13$ $-18 \le l \le 18$	$-11 \le h \le 11$ $-23 \le k \le 23$ $-27 \le l \le 27$	$-11 \le h \le 11$ $-28 \le k \le 28$ $-21 \le l \le 22$	$-6 \le h \le 9$ $-18 \le k \le 18$ $-22 \le l \le 23$
Reflections collected/indep.	14007/3496	22666/5777	113759/16736	76664/7458	13183/4293
R_{int}	0.0194	0.0348	0.0344	0.0442	0.0371
data/restrains/parameters	3496/0/212	5777/21/307	16736/0/513	7458/0/301	4293/0/257
GoF on F^2	1.038	1.021	1.053	1.046	1.041
R_1/wR_2 [$I>2\sigma$(I)]	0.0265/0.0756	0.0323/0.0746	0.0293/0.0715	0.0395/0.0898	0.0375/0.1005
R_{ind} (all data)/wR_2	0.0279/0.0767	0.0428/0.0797	0.0358/0.0736	0.0606/0.1004	0.0423/0.1051
ρ_{fin} (max/min) [e Å^{-3}]	0.31/−0.21	0.40/−0.35	0.42/−0.33	0.74/−0.34	0.46/−0.47
CCDC number	1971114	1971115	1971116	1971117	1971118

Gas-Phase Electron Diffraction

Table S2. Experimental details of the gas-phase electron diffraction experiments for $C_6F_5Me_2SiSiMe_2C_6H_5$ (**3**), $C_6Cl_5Me_2SiSiMe_2C_6H_5$ (**4**) and $C_6Cl_5Me_2SiSiMe_2C_6F_5$ (**5**).

	$C_6F_5Me_2SiSiMe_2C_6H_5$ (**3**)		$C_6Cl_5Me_2SiSiMe_2C_6H_5$ (**6**)		$C_6Cl_5Me_2SiSiMe_2C_6F_5$ (**7**)	
detector distance	short	long	short	long	short	long
nozzle-to-plate distance. mm	250.0	500.0	250.0	500.0	250.0	500.0
accelerating voltage. kV	60	60	60	60	60	60
fast electron current. μA	1.5	1.51	1.55	1.6	1.55	1.55
electron wavelength.[a] Å	0.048738	0.048585	0.048784	0.048663	0.048784	0.048604
nozzle temperature. K	405	410	550	545	552	548
sample pressure.[b] mbar	6.3×10^{-6}	3.5×10^{-6}	3.1×10^{-7}	3.0×10^{-7}	2.9×10^{-7}	9.7×10^{-8}
residual gas pressure[c]. mbar	1.6×10^{-7}	2.3×10^{-7}	1.5×10^{-7}	2.5×10^{-7}	1.5×10^{-7}	5.7×10^{-7}
exposure time. s	10	10	10	10	10	10
used *s* range. $Å^{-1}$	5.0 – 30.0	3.0 – 15.9	8.0 – 29.0	3.0 – 14.0	6.8 – 30.2	2.6 – 16.4

[a] Determined from CCl_4 diffraction patterns measured in the same experiment. [b] During the measurement. [c] Between measurements.

Gas-phase electron diffraction experiment

Electron diffraction patterns were recorded on the heavily improved Balzers Eldigraph KD-G2 gas-phase electron diffractometer at Bielefeld University. Experimental details are listed in Table 5, instrumental details are reported elsewhere.[5] The electron diffraction patterns, three for each, long and short nozzle-to-plate distances were measured on Fuji BAS-IP MP 2025 imaging plates. which were scanned by using a calibrated Fuji BAS.1800II scanner. The intensity curves (Figure S24) were obtained by applying a method described earlier.[6] Sector function and electron wavelength were refined[7] using carbon tetrachloride diffraction patterns, recorded in the same experiment as the substance under investigation.

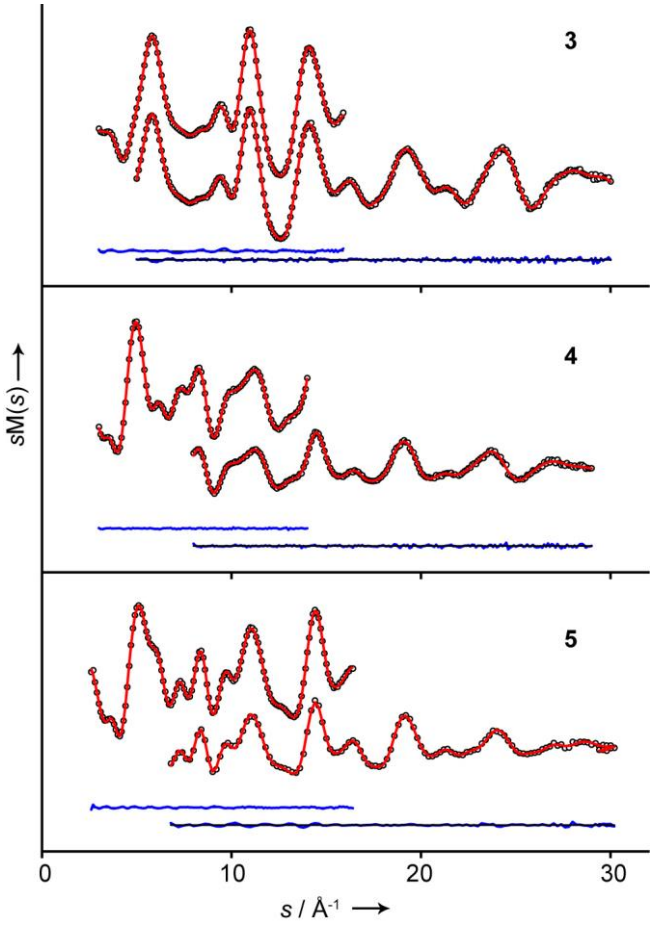

Figure S24. Experimental (dots) and model (solid line) molecular intensity curves of $C_6F_5Me_2SiSiMe_2C_6H_5$ (**3**), $C_6Cl_5Me_2SiSiMe_2C_6H_5$ (**4**) and $C_6Cl_5Me_2SiSiMe_2C_6F_5$ (**5**) for long (upper trace) and short (lower trace) nozzle-to-detector distance and the difference curves. respectively.

Gas-phase structure analysis

The structural analysis was performed using the UNEX program.[8] All refinements were performed using two averaged intensity curves simultaneously (Figure 11). one for the short and another for the long nozzle-to-plate distance. They were obtained by averaging independently measured intensity curves. For the definition of independent geometrical parameters and their groups in the least-squares refinement see the following Tables. The differences between values of parameters were kept fixed at the values taken from the dispersion corrected PBE0(D3)/TZVP calculations. Start values for amplitudes of vibrations and thermal corrections used in the gas-phase electron-diffraction refinements. were calculated using analytical quadratic force fields for all conformers employing the PBE0(D3)/TZVP approximation. The mean square amplitudes and vibrational corrections to the equilibrium structure were calculated using the VibModule program.[9]

Table S3. Z-Matrix used in the refinement of the gas-phase structure of the *syn*-conformer $C_6F_5Me_2SiSiMe_2C_6H_5$ (**3**). Distances *r* are given in Å, angles *a* and dihedrals *d* are given in deg. The numbers written in line with the parameter indicate the groups they were refined in.

1	Si						
2	Si	1	rsisi				
3	C	1	rsic1	2	asisic1		
4	C	2	rsic2	1	asisic2	3	dcsisic
5	C	1	rsic3	2	asisic3	3	acsic1 1
6	C	2	rsic4	1	asisic4	4	acsic2 1
7	C	1	rsic5	2	asisic5	3	acsic3 -1
8	C	2	rsic6	1	asisic6	4	acsic4 -1
9	C	3	rcc1	1	asicc1	2	dsisicc1
10	C	3	rcc2	1	asicc2	2	dsisicc3
11	C	9	rcc3	3	accc2	10	0
12	C	10	rcc4	3	accc3	9	0
13	C	11	rcc5	12	rcc6	9	180.00000000 4
14	C	4	rcc7	2	asicc3	1	dsisicc2
15	C	4	rcc8	2	asicc4	1	dsisicc4
16	C	14	rcc9	4	accc5	15	0
17	C	15	rcc10	4	accc6	14	0
18	C	16	rcc11	17	rcc12	14	180.00000000 4
19	F	9	rcl1	3	acccl1	10	180
20	F	10	rcl2	3	acccl2	9	180
21	F	11	rcl3	9	acccl3	3	180
22	F	12	rcl4	10	acccl4	3	180
23	F	13	rcl5	3	acccl10	2	dsicccl1
24	H	14	rcl6	4	acccl5	15	180
25	H	15	rcl7	4	acccl6	14	180
26	H	16	rcl8	14	acccl7	4	180
27	H	17	rcl9	15	acccl8	4	180
28	H	18	rcl10	4	acccl11	1	dsicccl2
29	H	5	rch1	1	asich1	3	dcsich1
30	H	5	rch2	1	asich2	3	dcsich2
31	H	5	rch3	1	asich3	3	dcsich3
32	H	6	rch4	2	asich4	4	dcsich4
33	H	6	rch5	2	asich5	4	dcsich5
34	H	6	rch6	2	asich6	4	dcsich6
35	H	7	rch7	1	asich7	3	dcsich7
36	H	7	rch8	1	asich8	3	dcsich8
37	H	7	rch9	1	asich9	3	dcsich9
38	H	8	rch10	2	asich10	4	dcsich10
39	H	8	rch11	2	asich11	4	dcsich11
40	H	8	rch12	2	asich12	4	dcsich12

Variables:

rsisi	2.37858683	3
rsic1	1.90890313	1
rsic2	1.88286213	1
rsic3	1.87921513	1
rsic4	1.88228513	1
rsic5	1.87737913	1
rsic6	1.87887013	1
rcc1	1.39769582	2
rcc2	1.39530582	2
rcc3	1.39163082	2
rcc4	1.39591382	2
rcc5	1.39584282	2
rcc6	1.39425982	2
rcc7	1.40849982	2
rcc8	1.40563482	2
rcc9	1.39655882	2
rcc10	1.39913482	2
rcc11	1.39945782	2
rcc12	1.39722782	2

rcl1	1.35025182	2
rcl2	1.34719282	2
rcl3	1.33691782	2
rcl4	1.33876982	2
rcl5	1.33445782	2
rcl6	1.09025673	4
rcl7	1.08838273	4
rcl8	1.08809673	4
rcl9	1.08785573	4
rcl10	1.08771873	4
rch1	1.09396173	4
rch2	1.09672473	4
rch3	1.09648273	4
rch4	1.09581773	4
rch5	1.09639573	4
rch6	1.09643073	4
rch7	1.09535173	4
rch8	1.09713773	4
rch9	1.09406373	4
rch10	1.09680173	4
rch11	1.09617773	4
rch12	1.09555473	4
asisic1	104.96315	5
asisic2	107.66615	5
asisic3	115.25115	5
acsic1	105.749365	6
asisic4	111.97615	5
acsic2	106.879365	6
asisic5	113.68715	5
acsic3	107.881365	6
asisic6	112.69015	5
acsic4	106.846365	6
asicc1	118.941437	7
asicc2	126.421437	7
accc2	124.461437	7
accc3	123.721437	7
asicc3	121.068437	7
asicc4	122.771437	7
accc5	122.311437	7
accc6	122.161437	7
acccl1	118.368604	8
acccl2	119.717604	8
acccl3	120.288604	8
acccl4	119.894604	8
acccl10	179.44	
acccl5	118.967604	8
acccl6	118.936604	8
acccl7	119.053604	8
acccl8	118.953604	8
acccl11	179.5	
asich1	111.647	
asich2	109.827	
asich3	110.554	
asich4	111.286	
asich5	111.022	
asich6	110.324	
asich7	111.47	
asich8	108.517	
asich9	112.339	
asich10	111.049	
asich11	110.491	
asich12	110.948	
dcsisic	9.3106755	10
dsisicc1	60.1791859	20
dsisicc3	-108.695314	20

dsisicc2	64.5471776	21
dsisicc4	-108.968422	21
dsicccl1	-34.81	
dsicccl2	-11.055	
dcsich1	58.8642	
dcsich2	178.9567	
dcsich3	-61.9632	
dcsich4	56.8906	
dcsich5	176.9477	
dcsich6	-63.0002	
dcsich7	61.016	
dcsich8	-179.8822	
dcsich9	-60.4897	
dcsich10	60.0179	
dcsich11	179.7991	
dcsich12	-60.7025	

Table S4. Cartesian coordinates for the refined structure of the *syn*−conformer $C_6F_5Me_2SiSiMe_2C_6H_5$ (**3**).

N	At	An	Mass	*X*	*Y*	*Z*
1	Si	14	27.9769265	1.60051546	1.69533559	0.32168878
2	Si	14	27.9769265	2.71783461	-0.3461935	-0.16966871
3	C	6	12.0000000	-0.25375894	1.24409481	0.36595315
4	C	6	12.0000000	1.40772852	-1.61891345	-0.62680735
5	C	6	12.0000000	1.98584257	2.43490671	2.00573363
6	C	6	12.0000000	3.86278638	-0.18282678	-1.65472563
7	C	6	12.0000000	1.84029974	3.02020799	-0.98665713
8	C	6	12.0000000	3.65331219	-1.03414489	1.30740866
9	C	6	12.0000000	-0.69742901	0.29694602	1.29310989
10	C	6	12.0000000	-1.21569427	1.59964163	-0.58016799
11	C	6	12.0000000	-1.97266875	-0.26013533	1.30087529
12	C	6	12.0000000	-2.50590245	1.06768559	-0.6111682
13	C	6	12.0000000	-2.90428023	0.12445782	0.33518108
14	C	6	12.0000000	0.61005203	-1.4601023	-1.77674777
15	C	6	12.0000000	1.072205	-2.69895597	0.20790299
16	C	6	12.0000000	-0.44991039	-2.31929503	-2.07447927
17	C	6	12.0000000	0.01188065	-3.56404703	-0.08348674
18	C	6	12.0000000	-0.76747851	-3.389003	-1.22987431
19	F	9	18.9984032	0.16055629	-0.1135148	2.25152688
20	F	9	18.9984032	-0.91432006	2.50487432	-1.53130198
21	F	9	18.9984032	-2.3089946	-1.16170714	2.22899299
22	F	9	18.9984032	-3.36862743	1.46420019	-1.55498302
23	F	9	18.9984032	-4.12986629	-0.40294228	0.3113987
24	H	1	1.00782503	0.82596455	-0.63819526	-2.45976339
25	H	1	1.00782503	1.65623416	-2.86808837	1.11061065
26	H	1	1.00782503	-1.03175425	-2.14738605	-2.97772868
27	H	1	1.00782503	-0.20202391	-4.3835588	0.5992104
28	H	1	1.00782503	-1.59840627	-4.05379814	-1.45512638
29	H	1	1.00782503	1.76816952	1.73147434	2.8147785
30	H	1	1.00782503	3.04788519	2.70308593	2.06005223
31	H	1	1.00782503	1.39758322	3.34553421	2.16999821
32	H	1	1.00782503	3.30666831	0.09505637	-2.55712805
33	H	1	1.00782503	4.62493787	0.58596956	-1.4810567
34	H	1	1.00782503	4.3719066	-1.13414394	-1.84953994
35	H	1	1.00782503	1.26868509	3.9243981	-0.75108901
36	H	1	1.00782503	2.90412445	3.28612384	-1.02239134
37	H	1	1.00782503	1.54247302	2.67965009	-1.98279718
38	H	1	1.00782503	4.12932252	-1.99113171	1.06131029
39	H	1	1.00782503	4.43839452	-0.33721121	1.62289999
40	H	1	1.00782503	2.9815294	-1.18940273	2.1587858

Table S5. Full listing of structural parameters of the *syn* conformer $C_6F_5Me_2SiSiMe_2C_6H_5$ (**3**). r_a, r_{h1} and r_e values are given in Å. Errors correspond to one time standard deviation. For atom numbering see Table S11.

No.	Type	i	j	k	l	r_a	r_{h1}	r_e	Error
1	stretch	1	2	0	0	2.37929	2.38116	2.37859	0.00297
2	stretch	1	3	0	0	1.90940	1.91150	1.90890	0.00053
3	stretch	1	5	0	0	1.87912	1.88116	1.87922	0.00053
4	stretch	1	7	0	0	1.87748	1.87951	1.87738	0.00053
5	stretch	2	4	0	0	1.88336	1.88535	1.88286	0.00053
6	stretch	2	6	0	0	1.88219	1.88424	1.88229	0.00053
7	stretch	2	8	0	0	1.87897	1.88100	1.87887	0.00053
8	stretch	3	9	0	0	1.39730	1.39878	1.39770	0.00019
9	stretch	3	10	0	0	1.39451	1.39598	1.39531	0.00019
10	stretch	4	14	0	0	1.40780	1.40930	1.40850	0.00019
11	stretch	4	15	0	0	1.40443	1.40592	1.40563	0.00019
12	stretch	5	29	0	0	1.09236	1.09766	1.09396	0.00135
13	stretch	5	30	0	0	1.09512	1.10045	1.09672	0.00135
14	stretch	5	31	0	0	1.09488	1.10021	1.09648	0.00135
15	stretch	6	32	0	0	1.09422	1.09953	1.09582	0.00135
16	stretch	6	33	0	0	1.09480	1.10012	1.09640	0.00135
17	stretch	6	34	0	0	1.09483	1.10016	1.09643	0.00135
18	stretch	7	35	0	0	1.09385	1.09915	1.09535	0.00135
19	stretch	7	36	0	0	1.09554	1.10086	1.09714	0.00135
20	stretch	7	37	0	0	1.09246	1.09774	1.09406	0.00135
21	stretch	8	38	0	0	1.09530	1.10062	1.09680	0.00135
22	stretch	8	39	0	0	1.09448	1.09980	1.09618	0.00135
23	stretch	8	40	0	0	1.09395	1.09927	1.09555	0.00135
24	stretch	9	11	0	0	1.39123	1.39267	1.39163	0.00019
25	stretch	9	19	0	0	1.34995	1.35140	1.35025	0.00019
26	stretch	10	12	0	0	1.39551	1.39697	1.39591	0.00019
27	stretch	10	20	0	0	1.34689	1.34832	1.34719	0.00019
28	stretch	11	13	0	0	1.39534	1.39678	1.39584	0.00019
29	stretch	11	21	0	0	1.33672	1.33810	1.33692	0.00019
30	stretch	12	13	0	0	1.39376	1.39519	1.39426	0.00019
31	stretch	12	22	0	0	1.33857	1.33995	1.33877	0.00019
32	stretch	13	23	0	0	1.33426	1.33563	1.33446	0.00019
33	stretch	14	16	0	0	1.39626	1.39772	1.39656	0.00019
34	stretch	14	24	0	0	1.08866	1.09390	1.09026	0.00135
35	stretch	15	17	0	0	1.39883	1.40030	1.39913	0.00019
36	stretch	15	25	0	0	1.08678	1.09199	1.08838	0.00135
37	stretch	16	18	0	0	1.39946	1.40092	1.39946	0.00019
38	stretch	16	26	0	0	1.08650	1.09169	1.08810	0.00135
39	stretch	17	18	0	0	1.39713	1.39858	1.39723	0.00019
40	stretch	17	27	0	0	1.08626	1.09146	1.08786	0.00135
41	stretch	18	28	0	0	1.08612	1.09130	1.08772	0.00135
42	bend	2	1	3	0	104.96315			0.19277
43	bend	2	1	5	0	115.25115			0.19277
44	bend	2	1	7	0	113.68715			0.19277

45	bend	1	2	4	0	107.66615			0.19277
46	bend	1	2	6	0	111.97615			0.19277
47	bend	1	2	8	0	112.69015			0.19277
48	bend	3	1	5	0	105.74936			0.66178
49	bend	3	1	7	0	107.88136			0.66178
50	bend	1	3	9	0	118.94144			0.06628
51	bend	1	3	10	0	126.42144			0.06628
52	bend	5	1	7	0	108.69928			1.10703
53	bend	1	5	29	0	111.64700			0.00000
54	bend	1	5	30	0	109.82700			0.00000
55	bend	1	5	31	0	110.55400			0.00000
56	bend	1	7	35	0	111.47000			0.00000
57	bend	1	7	36	0	108.51700			0.00000
58	bend	1	7	37	0	112.33900			0.00000
59	bend	4	2	6	0	106.87936			0.66178
60	bend	4	2	8	0	106.84636			0.66178
61	bend	2	4	14	0	121.06844			0.06628
62	bend	2	4	15	0	122.77144			0.06628
63	bend	6	2	8	0	110.43641			1.17209
64	bend	2	6	32	0	111.28600			0.00000
65	bend	2	6	33	0	111.02200			0.00000
66	bend	2	6	34	0	110.32400			0.00000
67	bend	2	8	38	0	111.04900			0.00000
68	bend	2	8	39	0	110.49100			0.00000
69	bend	2	8	40	0	110.94800			0.00000
70	bend	9	3	10	0	113.80569			0.13047
71	bend	3	9	11	0	124.46144			0.06628
72	bend	3	9	19	0	118.36860			0.38148
73	bend	3	10	12	0	123.72144			0.06628
74	bend	3	10	20	0	119.71760			0.38148
75	bend	14	4	15	0	115.86638			0.13181
76	bend	4	14	16	0	122.31144			0.06628
77	bend	4	14	24	0	118.96760			0.38148
78	bend	4	15	17	0	122.16144			0.06628
79	bend	4	15	25	0	118.93660			0.38148
80	bend	29	5	30	0	108.25763			0.00000
81	bend	29	5	31	0	108.45010			0.00000
82	bend	30	5	31	0	108.00087			0.00000
83	bend	32	6	33	0	107.78259			0.00000
84	bend	32	6	34	0	108.02030			0.00000
85	bend	33	6	34	0	108.28586			0.00000
86	bend	35	7	36	0	108.23655			0.00000
87	bend	35	7	37	0	108.10181			0.00000
88	bend	36	7	37	0	108.04386			0.00000
89	bend	38	8	39	0	107.96808			0.00000
90	bend	38	8	40	0	108.47200			0.00000
91	bend	39	8	40	0	107.79452			0.00000

92	bend	11	9	19	0	117.16996			0.39910
93	bend	9	11	13	0	119.83088			0.06584
94	bend	9	11	21	0	120.28860			0.38148
95	bend	12	10	20	0	116.56096			0.39910
96	bend	10	12	13	0	120.45232			0.06593
97	bend	10	12	22	0	119.89460			0.38148
98	bend	13	11	21	0	119.88051			0.39895
99	bend	11	13	12	0	117.72824			0.13387
100	bend	11	13	23	0	121.09134			0.06765
101	bend	13	12	22	0	119.65308			0.39898
102	bend	12	13	23	0	121.17722			0.06722
103	bend	16	14	24	0	118.72096			0.39910
104	bend	14	16	18	0	120.91887			0.06681
105	bend	14	16	26	0	119.05360			0.38148
106	bend	17	15	25	0	118.90196			0.39910
107	bend	15	17	18	0	121.07309			0.06705
108	bend	15	17	27	0	118.95360			0.38148
109	bend	18	16	26	0	120.02753			0.39930
110	bend	16	18	17	0	117.66879			0.13462
111	bend	16	18	28	0	121.03357			0.06681
112	bend	18	17	27	0	119.97330			0.39938
113	bend	17	18	28	0	121.29508			0.06881
114	torsion	4	2	1	3	9.31068			1.06511
115	torsion	6	2	1	3	126.51267			1.32200
116	torsion	8	2	1	3	-108.25902			1.31061
117	torsion	2	1	3	9	60.17919			1.00256
118	torsion	2	1	3	10	-108.69531			1.00256
119	torsion	4	2	1	5	125.20378			1.32495
120	torsion	6	2	1	5	-117.59422			1.88659
121	torsion	8	2	1	5	7.63409			1.06679
122	torsion	2	1	5	29	-56.57964			0.46538
123	torsion	2	1	5	30	63.51286			0.46538
124	torsion	2	1	5	31	-177.40704			0.46538
125	torsion	4	2	1	7	-108.35493			1.30417
126	torsion	6	2	1	7	8.84707			1.06446
127	torsion	8	2	1	7	134.07538			1.86418
128	torsion	2	1	7	35	176.97971			0.46359
129	torsion	2	1	7	36	-63.91849			0.46359
130	torsion	2	1	7	37	55.47401			0.46359
131	torsion	1	2	4	14	64.54718			1.06167
132	torsion	1	2	4	15	-108.96842			1.06167
133	torsion	1	2	6	32	-60.78261			0.44613
134	torsion	1	2	6	33	59.27449			0.44613
135	torsion	1	2	6	34	179.32659			0.44613
136	torsion	1	2	8	38	178.07036			0.45747
137	torsion	1	2	8	39	-62.14844			0.45747
138	torsion	1	2	8	40	57.34996			0.45747

139	torsion	9	3	1	5	-62.10741			1.11859
140	torsion	10	3	1	5	129.01809			1.11859
141	torsion	3	1	5	29	58.86420			0.00000
142	torsion	3	1	5	30	178.95670			0.00000
143	torsion	3	1	5	31	-61.96320			0.00000
144	torsion	9	3	1	7	-178.27524			1.02907
145	torsion	10	3	1	7	12.85026			1.02907
146	torsion	3	1	7	35	61.01600			0.00000
147	torsion	3	1	7	36	-179.88220			0.00000
148	torsion	3	1	7	37	-60.48970			0.00000
149	torsion	1	3	9	11	-170.22921			0.01833
150	torsion	1	3	9	19	9.77079			0.01833
151	torsion	1	3	10	12	169.36430			0.01769
152	torsion	1	3	10	20	-10.63570			0.01769
153	torsion	29	5	1	7	174.47500			0.69299
154	torsion	30	5	1	7	-65.43250			0.69299
155	torsion	31	5	1	7	53.64760			0.69299
156	torsion	5	1	7	35	-53.20775			0.68314
157	torsion	5	1	7	36	65.89405			0.68314
158	torsion	5	1	7	37	-174.71345			0.68314
159	torsion	14	4	2	6	-55.92122			1.09536
160	torsion	15	4	2	6	130.56318			1.09536
161	torsion	4	2	6	32	56.89060			0.00000
162	torsion	4	2	6	33	176.94770			0.00000
163	torsion	4	2	6	34	-63.00020			0.00000
164	torsion	14	4	2	8	-174.15874			1.18299
165	torsion	15	4	2	8	12.32566			1.18299
166	torsion	4	2	8	38	60.01790			0.00000
167	torsion	4	2	8	39	179.79910			0.00000
168	torsion	4	2	8	40	-60.70250			0.00000
169	torsion	2	4	14	16	-173.94226			0.01131
170	torsion	2	4	14	24	6.05774			0.01131
171	torsion	2	4	15	17	173.82861			0.01123
172	torsion	2	4	15	25	-6.17139			0.01123
173	torsion	32	6	2	8	172.75609			0.68121
174	torsion	33	6	2	8	-67.18681			0.68121
175	torsion	34	6	2	8	52.86529			0.68121
176	torsion	6	2	8	38	-55.86821			0.68137
177	torsion	6	2	8	39	63.91299			0.68137
178	torsion	6	2	8	40	-176.58861			0.68137
179	torsion	11	9	3	10	0.00000			0.00000
180	torsion	19	9	3	10	180.00000			0.00000
181	torsion	9	3	10	12	0.00000			0.00000
182	torsion	9	3	10	20	180.00000			0.00000
183	torsion	3	9	11	13	0.00000			0.00000
184	torsion	3	9	11	21	180.00000			0.00000
185	torsion	3	10	12	13	0.00000			0.00000

186	torsion	3	10	12	22	180.00000			0.00000
187	torsion	16	14	4	15	0.00000			0.00000
188	torsion	24	14	4	15	180.00000			0.00000
189	torsion	14	4	15	17	0.00000			0.00000
190	torsion	14	4	15	25	180.00000			0.00000
191	torsion	4	14	16	18	0.00000			0.00000
192	torsion	4	14	16	26	180.00000			0.00000
193	torsion	4	15	17	18	0.00000			0.00000
194	torsion	4	15	17	27	180.00000			0.00000
195	torsion	13	11	9	19	-180.00000			0.00000
196	torsion	21	11	9	19	0.00000			0.00000
197	torsion	9	11	13	12	0.00000			0.00000
198	torsion	9	11	13	23	179.35605			0.00171
199	torsion	13	12	10	20	-180.00000			0.00000
200	torsion	22	12	10	20	0.00000			0.00000
201	torsion	10	12	13	11	0.00000			0.00000
202	torsion	10	12	13	23	-179.35547			0.00182
203	torsion	12	13	11	21	-180.00000			0.00000
204	torsion	23	13	11	21	-0.64395			0.00171
205	torsion	11	13	12	22	-180.00000			0.00000
206	torsion	23	13	12	22	0.64453			0.00182
207	torsion	18	16	14	24	-180.00000			0.00000
208	torsion	26	16	14	24	0.00000			0.00000
209	torsion	14	16	18	17	0.00000			0.00000
210	torsion	14	16	18	28	179.42548			0.00177
211	torsion	18	17	15	25	-180.00000			0.00000
212	torsion	27	17	15	25	0.00000			0.00000
213	torsion	15	17	18	16	0.00000			0.00000
214	torsion	15	17	18	28	-179.42390			0.00168
215	torsion	17	18	16	26	-180.00000			0.00000
216	torsion	28	18	16	26	-0.57452			0.00177
217	torsion	16	18	17	27	-180.00000			0.00000
218	torsion	28	18	17	27	0.57610			0.00168
219	o.o.p	19	3	9	11	0.00000			0.00000
220	o.o.p	20	3	10	12	0.00000			0.00000
221	o.o.p	24	4	14	16	0.00000			0.00000
222	o.o.p	25	4	15	17	0.00000			0.00000
223	o.o.p	21	9	11	13	0.00000			0.00000
224	o.o.p	22	10	12	13	0.00000			0.00000
225	o.o.p	23	11	13	12	-0.55144			0.00146
226	o.o.p	26	14	16	18	0.00000			0.00000
227	o.o.p	27	15	17	18	0.00000			0.00000
228	o.o.p	28	16	18	17	-0.49228			0.00148

Table S6. Full listing of interatomic distances. refined vibrational amplitudes *l* and corrections of the *syn*-conformer $C_6F_5Me_2SiSiMe_2C_6H_5$ (**3**). All is given in Å. The numbers at the Gu column indicate the groups the amplitudes were refined in.

At1	At2	r_a	*l*	corr	*a*	Gr	Gu
C18	H28	1.086119	0.075053	0.0016	0	0	100
C17	H27	1.086256	0.075152	0.0016	0	0	100
C16	H26	1.086497	0.075152	0.0016	0	0	100
C15	H25	1.086783	0.075252	0.0016	0	0	100
C14	H24	1.088657	0.075552	0.0016	0	0	100
C5	H29	1.092362	0.076051	0.0016	0	0	100
C7	H37	1.092464	0.075951	0.0016	0	0	100
C7	H35	1.093852	0.07615	0.0015	0	0	100
C8	H40	1.093955	0.07625	0.0016	0	0	100
C6	H32	1.094218	0.07625	0.0016	0	0	100
C8	H39	1.094478	0.07635	0.0017	0	0	100
C6	H33	1.094796	0.07635	0.0016	0	0	100
C6	H34	1.094831	0.07635	0.0016	0	0	100
C5	H31	1.094883	0.07635	0.0016	0	0	100
C5	H30	1.095125	0.07635	0.0016	0	0	100
C8	H38	1.095302	0.07635	0.0015	0	0	100
C7	H36	1.095538	0.07635	0.0016	0	0	100
C13	F23	1.334258	0.042716	0.0002	0	0	100
C11	F21	1.336718	0.042916	0.0002	0	0	100
C12	F22	1.33857	0.043016	0.0002	0	0	100
C10	F20	1.346893	0.043914	0.0003	0	0	100
C9	F19	1.349952	0.044213	0.0003	0	0	100
C9	C11	1.391231	0.044712	0.0004	0	0	100
C12	C13	1.39376	0.044712	0.0005	0	0	100
C3	C10	1.394506	0.045311	0.0008	0	0	100
C11	C13	1.395343	0.044812	0.0005	0	0	100
C10	C12	1.395514	0.045012	0.0004	0	0	100
C14	C16	1.396259	0.045111	0.0003	0	0	100
C17	C18	1.397128	0.045111	0.0001	0	0	100
C3	C9	1.397296	0.045511	0.0004	0	0	100
C15	C17	1.398835	0.045311	0.0003	0	0	100
C16	C18	1.399458	0.045211	0.0000	0	0	100
C4	C15	1.404435	0.04571	0.0012	0	0	100
C4	C14	1.4078	0.04591	0.0007	0	0	100
H32	H33	1.75889	0.140325	0.0122	0	0	101
H39	H40	1.759036	0.139768	0.0118	0	0	101
H35	H37	1.760617	0.139768	0.0118	0	0	101
H36	H37	1.761713	0.139879	0.0115	0	0	101
H32	H34	1.761895	0.13999	0.0119	0	0	101
H38	H39	1.761899	0.13999	0.0119	0	0	101
H30	H31	1.762252	0.13999	0.0121	0	0	101
H29	H30	1.763394	0.139656	0.0118	0	0	101
H35	H36	1.764718	0.139768	0.0117	0	0	101
H33	H34	1.764944	0.139768	0.0123	0	0	101
H29	H31	1.765151	0.139545	0.012	0	0	101
H38	H40	1.767947	0.139656	0.011	0	0	101
Si1	C7	1.877479	0.061698	-0.0001	0	0	101
Si2	C8	1.87897	0.06181	-0.0001	0	0	101
Si1	C5	1.879115	0.061921	0.0001	0	0	101
Si2	C6	1.882185	0.062144	0.0001	0	0	101
Si2	C4	1.883362	0.061141	-0.0005	0	0	101
Si1	C3	1.909403	0.063257	-0.0005	0	0	101
C16	H24	2.13742	0.100244	0.0079	0	0	102
C14	H26	2.139847	0.100653	0.0073	0	0	102
C17	H25	2.140352	0.100346	0.0077	0	0	102
C15	H27	2.140978	0.100448	0.0072	0	0	102
C4	H25	2.147255	0.100142	0.007	0	0	102
C18	H27	2.149413	0.100448	0.008	0	0	102
C18	H26	2.152197	0.100244	0.008	0	0	102
C4	H24	2.1522	0.100346	0.0065	0	0	102

C16	H28	2.162816	0.100448	0.0077	0	0	102
C17	H28	2.163538	0.10004	0.0077	0	0	102
C12	F20	2.330115	0.062231	0.0034	0	0	102
C11	F19	2.336461	0.062435	0.0036	0	0	102
C9	C10	2.336526	0.057837	0.0033	0	0	102
C3	F19	2.357416	0.062027	0.0027	0	0	102
C13	F22	2.35839	0.063048	0.0045	0	0	102
C13	F21	2.360998	0.062844	0.0044	0	0	102
C9	F21	2.362978	0.062844	0.0036	0	0	102
C10	F22	2.36352	0.062844	0.0037	0	0	102
C3	F20	2.36861	0.06172	0.0032	0	0	102
C12	F23	2.373112	0.062742	0.0041	0	0	102
C11	F23	2.373495	0.063048	0.0041	0	0	102
Si1	Si2	2.379287	0.066829	-0.0007	0	0	102
C14	C15	2.382581	0.057837	0.0022	0	0	102
C11	C12	2.38417	0.057019	0.004	0	0	102
C16	C17	2.390554	0.057326	0.0025	0	0	102
H25	H40	2.400919	0.465148	-0.0191	0	0	102
C9	C13	2.407564	0.056917	0.0044	0	0	102
C10	C13	2.417549	0.056917	0.0043	0	0	102
C14	C18	2.429054	0.057122	0.0035	0	0	102
C15	C18	2.431508	0.057122	0.0032	0	0	102
H24	H26	2.43669	0.163599	0.0122	0	0	102
H25	H27	2.439796	0.163497	0.012	0	0	102
Si1	H36	2.44864	0.129571	0.0083	0	0	102
C4	C17	2.449722	0.057428	0.0053	0	0	102
C4	C16	2.452253	0.05753	0.0048	0	0	102
C3	C12	2.456408	0.05753	0.0049	0	0	102
C3	C11	2.463384	0.057428	0.0047	0	0	102
Si1	H30	2.467958	0.131615	0.0084	0	0	102
Si2	H39	2.475795	0.13141	0.0089	0	0	102
Si2	H34	2.477217	0.131819	0.0085	0	0	102
Si1	H31	2.477678	0.130695	0.0084	0	0	102
Si2	H40	2.481329	0.130389	0.0091	0	0	102
Si2	H38	2.481375	0.1309	0.0113	0	0	102
Si1	H35	2.484233	0.129162	0.0117	0	0	102
Si2	H33	2.486437	0.132024	0.0087	0	0	102
Si2	H32	2.486577	0.131002	0.0117	0	0	102
Si1	H29	2.488082	0.128856	0.0109	0	0	102
H26	H28	2.491159	0.164008	0.0136	0	0	102
H27	H28	2.492178	0.163905	0.0136	0	0	102
Si1	H37	2.498271	0.128447	0.0083	0	0	102
F20	H37	2.560542	0.495918	-0.0565	0	0	103
F19	H29	2.577707	0.391472	-0.0666	0	0	102
H24	H32	2.595635	0.666038	-0.007	0	0	103
H25	H38	2.598733	0.640572	0.0257	0	0	103
F20	F22	2.660631	0.139272	0.0053	0	0	103
F19	F21	2.67729	0.140322	0.0056	0	0	103
C9	C12	2.731549	0.083091	0.0054	0	0	103
F22	F23	2.73986	0.142947	0.0077	0	0	103
F20	H35	2.742325	0.540942	-0.024	0	0	103
F21	F23	2.743184	0.143341	0.0079	0	0	103
C8	H25	2.743929	0.3871	-0.0254	0	0	103
C10	C11	2.746082	0.082959	0.0053	0	0	103
C14	C17	2.761739	0.083484	0.0044	0	0	103
C15	C16	2.765621	0.083878	0.0039	0	0	103
Si1	C9	2.850318	0.103699	0.0097	0	0	103
C4	C18	2.861324	0.084141	0.0072	0	0	103
Si2	C14	2.862208	0.113675	0.0129	0	0	103
C3	C13	2.870464	0.084403	0.007	0	0	103
F19	H40	2.8804	1.166419	0.1402	0	0	103
Si2	C15	2.893285	0.111444	0.0026	0	0	103
C7	F20	2.911244	0.25426	-0.0564	0	0	103
Si1	C10	2.956038	0.101336	0.0026	0	0	103
Si2	H24	2.96509	0.22	0.0197	0	0	103

H31	H35	2.992679	0.514821	-0.012	0	0	103
Si1	F19	2.998094	0.169463	0.0135	0	0	103
C3	C5	3.013785	0.154499	0.0066	0	0	103
C4	C8	3.014293	0.146885	0.0066	0	0	103
C4	C6	3.01528	0.160012	0.009	0	0	103
Si2	H25	3.019138	0.2179	0.0018	0	0	103
C5	C7	3.045567	0.156205	0.007	0	0	103
H34	H38	3.052264	0.532279	-0.0082	0	0	103
C3	C7	3.054617	0.134678	0.0063	0	0	103
C6	C8	3.081252	0.159224	0.0079	0	0	103
C15	H40	3.117929	0.436837	0.0014	0	0	104
C5	F19	3.131686	0.356778	0.0126	0	0	103
C6	H24	3.131845	0.425624	0.0427	0	0	104
H30	H36	3.157791	0.518759	-0.0174	0	0	103
C4	H32	3.184453	0.328142	0.0202	0	0	104
C7	H31	3.192008	0.363341	0.0121	0	0	103
C5	H35	3.195594	0.331837	0.0189	0	0	103
C14	H32	3.198245	0.46853	0.011	0	0	104
C3	H29	3.199662	0.311209	0.0132	0	0	104
C4	H38	3.206884	0.292559	0.0173	0	0	104
C3	H31	3.207824	0.328257	0.0167	0	0	104
C4	H40	3.211235	0.303086	0.0169	0	0	104
C8	H34	3.223744	0.365573	0.0155	0	0	103
C4	H34	3.225604	0.309836	0.0173	0	0	104
Si1	F20	3.228068	0.140044	-0.0011	0	0	104
C15	H38	3.233267	0.435235	0.0187	0	0	104
C6	H38	3.254614	0.344701	0.0192	0	0	103
C9	H29	3.257036	0.365785	-0.024	0	0	104
H33	H39	3.261103	0.539236	-0.0174	0	0	103
C5	H36	3.26239	0.336169	0.0144	0	0	103
C3	H35	3.263665	0.262697	0.015	0	0	104
C8	C15	3.266303	0.233521	-0.004	0	0	104
C3	H37	3.272928	0.266587	0.014	0	0	104
C7	H30	3.279708	0.368854	0.0129	0	0	103
H32	H37	3.293267	0.724019	-0.1117	0	0	104
C10	H37	3.293788	0.342559	-0.0164	0	0	104
H24	H37	3.312978	0.941636	0.1147	0	0	104
C6	H39	3.318264	0.308349	0.0131	0	0	104
H33	H36	3.331464	0.649763	-0.0969	0	0	104
H29	H40	3.336084	0.704454	-0.1059	0	0	104
C8	H33	3.35304	0.325168	0.0151	0	0	104
C14	H25	3.366926	0.108008	0.0115	0	0	104
C15	H24	3.368313	0.108122	0.0116	0	0	104
C16	H27	3.374123	0.108237	0.0128	0	0	104
C17	H26	3.374243	0.108008	0.0129	0	0	104
F19	H25	3.377729	0.526767	-0.0421	0	0	104
C18	H24	3.395311	0.108466	0.0133	0	0	104
C18	H25	3.396341	0.108466	0.013	0	0	104
Si2	C3	3.405964	0.128374	0.0067	0	0	104
C10	H35	3.407336	0.359835	-0.0006	0	0	104
C7	C10	3.407857	0.163499	-0.0134	0	0	104
C14	H28	3.408294	0.108122	0.0134	0	0	104
C4	H27	3.411431	0.10858	0.0146	0	0	104
C15	H28	3.412209	0.108008	0.0132	0	0	104
C4	H26	3.414776	0.108923	0.0141	0	0	104
H30	H39	3.44445	0.718298	-0.0728	0	0	104
Si1	C4	3.444789	0.135696	0.0079	0	0	104
C6	C14	3.466056	0.283406	0.0306	0	0	104
C15	F19	3.470158	0.380773	-0.0508	0	0	104
H31	H36	3.471517	0.487866	0.059	0	0	104
C4	C9	3.474108	0.247594	-0.0407	0	0	104
C4	F19	3.475336	0.346563	0.0041	0	0	104
H32	H36	3.477658	0.894497	0.0861	0	0	104
Si2	F19	3.478506	0.43226	0.0508	0	0	104
H30	H35	3.480463	0.486722	0.0635	0	0	104

C5	C9	3.492591	0.204231	0.0115	0	0	104
C3	C4	3.495654	0.181806	-0.0398	0	0	104
H34	H39	3.502736	0.499994	0.0606	0	0	104
H24	H34	3.510885	0.635805	0.1212	0	0	104
C3	H24	3.531993	0.491413	0.0308	0	0	104
Si1	C6	3.534721	0.162927	0.0081	0	0	104
H29	H39	3.545918	0.804567	0.036	0	0	104
Si1	C8	3.54817	0.160296	0.0065	0	0	104
C10	H24	3.560991	0.602968	0.004	0	0	104
Si2	C7	3.565241	0.165101	0.0083	0	0	104
F19	H31	3.567694	0.581801	0.1068	0	0	104
C10	F19	3.576236	0.070823	0.0081	0	0	104
C9	F20	3.583158	0.070937	0.0084	0	0	104
C3	C14	3.589586	0.294161	-0.0329	0	0	104
H33	H38	3.589963	0.489925	0.0639	0	0	104
Si2	C5	3.597227	0.162469	0.0087	0	0	104
C8	F19	3.598098	0.848731	0.1353	0	0	104
C12	F21	3.606103	0.071166	0.0099	0	0	104
C11	F22	3.606346	0.071395	0.01	0	0	104
C13	F20	3.611185	0.071624	0.0096	0	0	104
C13	F19	3.612863	0.071738	0.0096	0	0	104
C9	F23	3.628025	0.071166	0.01	0	0	104
C10	F23	3.636692	0.071166	0.0099	0	0	104
H33	H37	3.648698	0.877221	0.1112	0	0	104
C3	F22	3.656076	0.071624	0.0101	0	0	104
C7	H32	3.65928	0.608574	-0.0298	0	0	104
C3	F21	3.662292	0.071853	0.0096	0	0	104
Si1	H24	3.667381	0.408347	0.045	0	0	104
Si1	H33	3.680574	0.333177	0.011	0	0	104
Si1	H40	3.681338	0.322651	0.007	0	0	104
C6	H36	3.681907	0.537408	-0.0278	0	0	104
Si1	H32	3.691772	0.361208	0.0176	0	0	104
C14	H34	3.703452	0.492557	0.0732	0	0	104
Si2	H37	3.70825	0.320477	0.0099	0	0	104
Si1	H39	3.710113	0.334893	0.0152	0	0	104
C9	C15	3.715819	0.341415	-0.071	0	0	104
C8	H29	3.716973	0.544501	-0.0462	0	0	104
Si2	H36	3.717415	0.316701	0.0183	0	0	104
C6	H37	3.720659	0.566698	-0.0213	0	0	104
C7	H33	3.740009	0.578597	-0.0085	0	0	104
C9	H31	3.740465	0.469674	0.0611	0	0	104
F20	H24	3.74393	0.610633	-0.0332	0	0	104
Si2	H29	3.74629	0.339012	0.0121	0	0	104
Si2	C9	3.751593	0.246679	0.019	0	0	104
C5	H39	3.75565	0.543472	-0.0346	0	0	104
C9	C14	3.770441	0.387717	0.0006	0	0	105
H25	H39	3.771413	0.362353	0.0244	0	0	104
C5	H40	3.775307	0.592213	-0.0136	0	0	104
Si2	H30	3.776125	0.356746	0.0158	0	0	104
H30	H40	3.780906	0.875733	0.1134	0	0	104
C10	C14	3.827715	0.37654	-0.0691	0	0	104
C14	H27	3.838231	0.10858	0.0155	0	0	104
C17	H24	3.840868	0.108809	0.0153	0	0	104
C15	H26	3.842247	0.108923	0.0151	0	0	104
C16	H25	3.842896	0.108923	0.0148	0	0	104
C8	H30	3.85574	0.604226	0.0043	0	0	104
C6	C7	3.874583	0.33844	-0.028	0	0	104
Si1	C14	3.89339	0.258235	0.0234	0	0	104
C4	H28	3.937713	0.108923	0.0185	0	0	104
C3	H30	3.938715	0.141863	0.0487	0	0	105
C5	C8	3.939032	0.342101	-0.0272	0	0	104
F20	H36	3.942331	0.234491	-0.0117	0	0	105
C4	H39	3.945086	0.137427	0.041	0	0	105
C4	H33	3.945904	0.141863	0.0468	0	0	105
C7	H24	3.959502	0.719381	0.1127	0	0	105

C7	H29	3.966192	0.150799	0.0484	0	0	104
C3	H36	3.974992	0.133856	0.0337	0	0	105
F19	H30	3.975739	0.325496	0.0624	0	0	105
C9	H25	3.975778	0.48543	-0.0273	0	0	105
C5	H37	3.984254	0.147595	0.0363	0	0	104
C9	H40	3.989402	0.779329	0.0718	0	0	105
C8	H32	3.990327	0.153659	0.0507	0	0	104
C6	H40	3.999571	0.150456	0.0418	0	0	104
H24	H33	4.01988	0.424725	0.0897	0	0	105
C9	F22	4.063465	0.071094	0.012	0	0	105
C12	F19	4.075195	0.071094	0.0114	0	0	105
C10	F21	4.076399	0.070878	0.0116	0	0	105
C9	H24	4.083735	0.529039	0.0731	0	0	105
C11	F20	4.085546	0.070986	0.0116	0	0	105
F19	H39	4.115363	0.932446	0.2142	0	0	105
C12	H24	4.137566	0.710291	0.0372	0	0	105
C11	C15	4.138181	0.416933	-0.0868	0	0	105
H29	H35	4.1486	0.279723	0.0673	0	0	105
C14	H37	4.15026	0.780086	0.0982	0	0	105
C10	H31	4.152315	0.373433	0.0239	0	0	105
H31	H37	4.162637	0.288921	0.0457	0	0	105
C6	C15	4.164562	0.164263	0.0292	0	0	105
C4	C11	4.166611	0.322791	-0.0448	0	0	105
C15	H34	4.167727	0.338156	0.0239	0	0	105
C5	C10	4.169432	0.185147	0.0299	0	0	105
Si2	C16	4.171193	0.087434	0.0188	0	0	105
Si1	C11	4.17281	0.086243	0.0165	0	0	105
H34	H40	4.18698	0.292708	0.056	0	0	105
H32	H38	4.187399	0.291734	0.0696	0	0	105
Si2	C17	4.193658	0.08646	0.0116	0	0	105
C4	C10	4.193744	0.273771	-0.0412	0	0	105
C11	C14	4.194105	0.621526	-0.001	0	0	106
C3	C15	4.195629	0.306884	-0.0326	0	0	105
C3	F23	4.198378	0.072068	0.0135	0	0	105
C17	F21	4.212367	0.677533	-0.1497	0	0	106
C17	F19	4.213801	0.514288	-0.0448	0	0	106
C14	F19	4.221205	0.506458	0.0499	0	0	106
H29	H36	4.230957	0.282212	0.0622	0	0	105
C11	C17	4.232808	0.463355	-0.1376	0	0	105
Si1	C12	4.245762	0.084187	0.0118	0	0	105
C12	C14	4.246212	0.476557	-0.068	0	0	105
C9	C17	4.246977	0.368022	-0.087	0	0	105
H24	H25	4.269611	0.138725	0.021	0	0	105
H30	H37	4.269899	0.296063	0.0442	0	0	105
H26	H27	4.275334	0.139699	0.0239	0	0	105
C11	C16	4.277674	0.691071	-0.0407	0	0	106
H24	H28	4.283544	0.14024	0.0238	0	0	105
H25	H28	4.287038	0.140024	0.0236	0	0	105
H32	H39	4.289245	0.291193	0.0628	0	0	105
C9	C16	4.298809	0.503538	-0.0272	0	0	106
C15	H39	4.304711	0.22973	0.044	0	0	105
C14	F20	4.307396	0.456631	-0.0524	0	0	104
C15	F21	4.318128	0.604007	-0.0896	0	0	106
H33	H40	4.319491	0.300932	0.051	0	0	105
C8	C14	4.322722	0.112214	0.031	0	0	105
C13	C16	4.32288	0.706599	-0.1036	0	0	106
F21	H27	4.331012	0.872631	-0.1506	0	0	106
C7	C9	4.335438	0.112538	0.0296	0	0	105
C11	C18	4.337232	0.569234	-0.1364	0	0	106
H25	H34	4.342878	0.426348	0.0325	0	0	105
C10	C16	4.360203	0.384795	-0.0967	0	0	105
C12	C16	4.361145	0.482617	-0.1374	0	0	105
C3	C16	4.369217	0.306884	-0.0458	0	0	105
C12	H26	4.372232	0.643958	-0.1166	0	0	105
Si2	C10	4.381656	0.233517	0.026	0	0	105

C3	H40	4.400156	0.500255	0.0274	0	0	105
C6	H25	4.402962	0.263708	0.0385	0	0	105
F20	H31	4.407835	0.573216	0.0364	0	0	106
C17	H40	4.408642	0.553573	0.0056	0	0	106
Si1	C15	4.409699	0.207114	0.0177	0	0	105
F19	H38	4.418874	0.974427	0.1301	0	0	106
C13	C14	4.430535	0.661872	-0.0349	0	0	106
C14	H33	4.435578	0.336842	0.0803	0	0	106
H30	H33	4.441569	0.68497	-0.0247	0	0	105
C10	H36	4.448155	0.20691	0.0254	0	0	106
C9	H30	4.451599	0.210577	0.0656	0	0	105
C4	H37	4.454781	0.539644	0.0546	0	0	105
C13	H26	4.462142	0.962615	-0.0301	0	0	106
C15	H32	4.462185	0.403467	0.0594	0	0	106
C16	H32	4.465039	0.588877	0.0265	0	0	106
C10	H29	4.465079	0.418067	0.0567	0	0	106
Si1	H34	4.465124	0.159502	0.0516	0	0	105
C8	C9	4.47313	0.70275	0.0767	0	0	106
C18	F21	4.483977	0.888252	-0.0907	0	0	107
Si1	H38	4.485619	0.157229	0.0456	0	0	105
F21	H25	4.486522	0.839584	-0.0272	0	0	106
H24	H36	4.487048	0.825967	0.1804	0	0	105
C11	H25	4.495069	0.591584	-0.0222	0	0	105
Si2	H35	4.505991	0.15777	0.0411	0	0	105
Si2	H31	4.511837	0.159285	0.0539	0	0	105
C14	H38	4.512724	0.333922	0.0394	0	0	106
C11	H29	4.512954	0.458679	-0.0127	0	0	106
C5	F20	4.530645	0.327817	0.0439	0	0	106
C17	H38	4.530994	0.531011	0.0229	0	0	106
C9	C18	4.542478	0.446867	-0.0752	0	0	106
C10	H26	4.54383	0.487919	-0.0916	0	0	105
C14	H40	4.563783	0.347991	0.039	0	0	106
C9	H35	4.565546	0.304326	0.0391	0	0	106
C12	H37	4.575975	0.422446	-0.0077	0	0	106
C13	C18	4.576469	0.613828	-0.1765	0	0	106
C3	C8	4.577432	0.377189	0.0423	0	0	106
C9	H37	4.591123	0.320783	0.0377	0	0	106
C3	H25	4.596749	0.41293	-0.0019	0	0	105
Si1	H25	4.603951	0.374933	0.0275	0	0	106
C11	H24	4.617044	0.90965	0.0859	0	0	107
C4	C7	4.617221	0.430542	0.0559	0	0	106
C7	C14	4.620548	0.707793	0.0923	0	0	106
C8	C17	4.637444	0.287736	0.0096	0	0	106
F19	H27	4.644817	0.705533	-0.0519	0	0	107
C13	H24	4.650843	1.031058	0.0723	0	0	107
C11	H27	4.652141	0.766986	-0.1101	0	0	106
H32	H35	4.677731	0.724118	0.0211	0	0	106
F22	H26	4.678665	0.750978	-0.1478	0	0	105
C8	H24	4.67886	0.216598	0.0479	0	0	106
H34	H36	4.684768	0.645548	0.0457	0	0	106
F19	H24	4.69129	0.675484	0.0956	0	0	107
C3	H32	4.692172	0.604803	0.0556	0	0	106
F20	F23	4.694599	0.102858	0.0161	0	0	106
H36	H39	4.698819	0.834408	0.0425	0	0	106
F19	F23	4.701383	0.10299	0.0162	0	0	106
H34	H37	4.705229	0.6847	0.0454	0	0	106
F21	F22	4.70927	0.102725	0.0169	0	0	106
F19	F20	4.710723	0.098212	0.0138	0	0	106
C5	H33	4.725047	0.489975	0.0227	0	0	105
C12	H35	4.72531	0.43678	0.0105	0	0	106
Si2	C18	4.727592	0.102858	0.019	0	0	106
H29	H38	4.727906	0.662934	0.0163	0	0	106
C4	F21	4.733723	0.568797	-0.0243	0	0	107
C11	H26	4.743262	1.020435	0.0268	0	0	107
C3	C6	4.747024	0.342416	0.0556	0	0	106

C6	H30	4.74741	0.615155	0.0267	0	0	106
Si1	C13	4.752751	0.105777	0.0181	0	0	106
H33	H35	4.754122	0.675542	0.0357	0	0	106
F22	H24	4.76452	0.951201	0.0139	0	0	106
H31	H40	4.76541	0.695716	0.0382	0	0	106
C7	F19	4.766416	0.17811	0.0427	0	0	106
Si2	F20	4.766961	0.448857	0.0471	0	0	106
H24	H35	4.769019	0.889221	0.1231	0	0	106
H31	H39	4.772226	0.658289	0.0349	0	0	106
C7	C12	4.776315	0.200805	0.0031	0	0	106
H27	H40	4.776384	0.623384	-0.0046	0	0	106
C4	H29	4.784989	0.511634	0.0316	0	0	106
C6	C16	4.787253	0.339497	0.0439	0	0	106
C4	C12	4.794659	0.415014	-0.0476	0	0	106
C4	C13	4.799746	0.432798	-0.0502	0	0	106
C16	F21	4.810572	0.980823	0.0181	0	0	108
C5	C11	4.816543	0.251769	0.0239	0	0	106
H32	H40	4.820709	0.213678	0.0778	0	0	106
H29	H37	4.823981	0.207042	0.0716	0	0	106
F21	H28	4.824084	1.043535	-0.0868	0	0	108
C4	C5	4.825154	0.273004	0.0429	0	0	106
C9	H27	4.827925	0.687473	-0.0704	0	0	107
C5	C6	4.831001	0.36113	0.0449	0	0	106
C4	F20	4.832062	0.363586	-0.0138	0	0	105
F20	H32	4.837323	1.220223	0.1302	0	0	106
F23	H26	4.838426	1.355218	0.0051	0	0	107
C13	C17	4.83883	0.674348	-0.1182	0	0	106
C11	H28	4.838887	0.772459	-0.1349	0	0	107
C3	H26	4.849226	0.569859	-0.0235	0	0	107
C16	F19	4.855326	0.640148	0.0388	0	0	108
H30	H38	4.859421	0.718411	0.0602	0	0	106
C18	F19	4.872415	0.632574	-0.0031	0	0	108
C3	C17	4.874402	0.448725	-0.038	0	0	106
C16	F23	4.876615	1.000554	-0.0905	0	0	107
H25	H29	4.881893	1.031665	0.0245	0	0	107
H26	H32	4.883771	0.761684	0.018	0	0	107
Si2	C11	4.889073	0.323836	0.0273	0	0	106
C16	H34	4.893222	0.696579	0.0772	0	0	107
C7	H34	4.893674	0.422181	0.0472	0	0	106
C8	H36	4.905377	0.550122	0.0599	0	0	106
C6	H35	4.911076	0.411431	0.0301	0	0	106
H25	H32	4.913345	0.473947	0.0823	0	0	107
H24	H27	4.915668	0.157405	0.0282	0	0	106
C9	H26	4.9176	0.734822	0.0146	0	0	108
H25	H26	4.917826	0.157538	0.0278	0	0	106
C13	H28	4.918117	0.837109	-0.1886	0	0	107
C7	H39	4.926187	0.596574	0.057	0	0	106
C16	F20	4.933315	0.505882	-0.0565	0	0	105
C14	F21	4.935364	0.805259	0.0301	0	0	108
C7	C8	4.941953	0.325561	0.0568	0	0	106
F20	H26	4.943343	0.725843	-0.07	0	0	106
C18	F23	4.943407	0.880816	-0.1897	0	0	107
C11	H31	4.946969	0.591	0.0645	0	0	106
C16	F22	4.947223	0.721463	-0.1406	0	0	106
C13	C15	4.948155	0.568172	-0.0696	0	0	106
H27	H38	4.948189	0.702194	0.0215	0	0	107
C12	C18	4.955187	0.626967	-0.1316	0	0	106
H24	H38	4.955337	0.402771	0.0587	0	0	107
C10	C15	4.958998	0.468765	-0.0261	0	0	106
C8	H31	4.959296	0.414881	0.0421	0	0	106
C5	H38	4.96872	0.41873	0.0389	0	0	106
C3	C18	4.975885	0.47167	-0.0488	0	0	107
Si2	H26	4.987956	0.194101	0.0309	0	0	107
F23	H28	5.003967	1.053215	-0.223	0	0	107
C11	H40	5.009984	1.256877	0.1031	0	0	107

C14	F22	5.013934	0.676737	-0.0712	0	0	106
C3	H39	5.016298	0.496636	0.0922	0	0	106
Si2	H27	5.021234	0.192584	0.0203	0	0	107
C9	H39	5.039125	0.93211	0.1462	0	0	107
C4	H36	5.04495	0.605371	0.0985	0	0	107
C15	H33	5.059062	0.262241	0.0659	0	0	107
C10	H32	5.059936	1.118775	0.0999	0	0	107
C10	H30	5.064028	0.267705	0.0708	0	0	107
H24	H40	5.065928	0.380159	0.0606	0	0	107
F21	H29	5.068878	0.57168	-0.0353	0	0	107
F20	H29	5.073893	0.508245	0.0916	0	0	107
Si1	C16	5.076106	0.380918	0.0291	0	0	107
F19	H35	5.096413	0.348745	0.0561	0	0	107
F22	H37	5.104027	0.537079	-0.0267	0	0	107
C10	C18	5.123602	0.55145	-0.0729	0	0	106
C8	H27	5.146742	0.420375	0.0092	0	0	107
C15	H29	5.161977	0.846518	0.0254	0	0	107
F21	H40	5.162662	1.495899	0.1284	0	0	107
C9	H36	5.164169	0.208974	0.0577	0	0	107
C3	H33	5.165971	0.500657	0.092	0	0	107
C14	H36	5.173868	0.924522	0.1514	0	0	107
C14	H39	5.174431	0.210188	0.0672	0	0	107
H25	H33	5.176073	0.441318	0.0642	0	0	107
Si1	F21	5.180203	0.154188	0.0241	0	0	107
H29	H33	5.197248	0.715756	0.0874	0	0	106
C5	H32	5.199804	0.597631	0.0954	0	0	107
F19	H37	5.200567	0.360734	0.0569	0	0	107
H30	H32	5.204856	0.756103	0.1043	0	0	106
C6	H29	5.212189	0.554835	0.082	0	0	107
C17	H34	5.255539	0.531083	0.0391	0	0	108
C9	H38	5.25604	0.813131	0.0906	0	0	107
C16	H37	5.257442	1.238514	0.1247	0	0	107
C12	H31	5.271064	0.577436	0.0356	0	0	108
C4	H30	5.271269	0.461958	0.0756	0	0	107
F20	H30	5.280079	0.403993	0.0712	0	0	108
C7	H40	5.284957	0.505665	0.0925	0	0	107
C9	H28	5.288022	0.612276	-0.0637	0	0	108
C6	F19	5.29189	0.519116	0.0905	0	0	108
Si1	F22	5.299638	0.147663	0.0171	0	0	107
C8	H37	5.300773	0.488516	0.0912	0	0	107
C12	C15	5.303003	0.6251	-0.0436	0	0	107
F22	H35	5.310596	0.575921	0.0001	0	0	108
C14	F23	5.313281	0.875999	-0.027	0	0	108
C6	C17	5.317323	0.248576	0.0428	0	0	108
C5	H25	5.327002	0.766935	0.0611	0	0	108
C13	H27	5.33632	1.016337	-0.0738	0	0	107
C5	C12	5.336643	0.26433	0.0386	0	0	108
C6	F20	5.340674	1.084022	0.142	0	0	107
C17	F23	5.353088	0.903731	-0.1279	0	0	107
F21	H26	5.35935	1.281536	0.0916	0	0	110
H36	H40	5.364868	0.76138	0.1266	0	0	107
C12	C17	5.367872	0.776253	-0.0697	0	0	107
C10	C17	5.368089	0.662129	-0.0373	0	0	107
C6	H26	5.381096	0.49594	0.0564	0	0	108
C6	C9	5.382891	0.301139	0.0683	0	0	108
H24	H39	5.384205	0.336282	0.0755	0	0	108
C6	C10	5.385527	0.781023	0.1029	0	0	108
Si2	C12	5.395878	0.365894	0.0338	0	0	107
F19	H36	5.396135	0.284325	0.0631	0	0	108
C12	H28	5.400989	0.859266	-0.1317	0	0	107
H37	H39	5.402372	0.77875	0.1193	0	0	108
F19	F22	5.405496	0.103308	0.0198	0	0	108
F20	F21	5.414237	0.103005	0.0198	0	0	108
C14	H35	5.414344	0.807986	0.1064	0	0	108
H26	H37	5.423389	1.401629	0.1369	0	0	108

C3	H38	5.423959	0.442468	0.068	0	0	108
C8	C16	5.433994	0.191317	0.0364	0	0	108
C17	H32	5.444114	0.539263	0.0662	0	0	108
C5	H24	5.456659	0.495789	0.0868	0	0	108
C5	C15	5.461848	0.563197	0.0539	0	0	108
C12	H29	5.463537	0.518056	0.0542	0	0	108
C4	H35	5.470048	0.475188	0.0764	0	0	108
C7	F22	5.470793	0.28387	-0.0048	0	0	108
C18	H32	5.471985	0.621364	0.0506	0	0	108
C9	H32	5.478187	0.379494	0.0804	0	0	109
Si1	C17	5.483496	0.340372	0.0255	0	0	108
C18	H40	5.487272	0.585615	0.0242	0	0	108
C7	C11	5.489094	0.173897	0.0365	0	0	108
C13	H29	5.504153	0.527599	0.0242	0	0	108
H26	H34	5.509599	0.818892	0.1028	0	0	108
C16	H38	5.516198	0.443832	0.0435	0	0	108
C13	H25	5.516829	0.832101	-0.0073	0	0	107
C16	H40	5.526247	0.488821	0.039	0	0	108
H31	H33	5.533009	0.727234	0.0671	0	0	107
C5	C14	5.536987	0.306592	0.064	0	0	108
C18	H38	5.549305	0.534416	0.0348	0	0	108
C10	H25	5.560706	0.63375	0.0131	0	0	107
F21	H24	5.563692	0.9841	0.1008	0	0	110
C3	H34	5.566525	0.405962	0.0869	0	0	108
H30	H34	5.567803	0.743153	0.068	0	0	108
C5	F21	5.578245	0.366123	0.0281	0	0	108
C8	C11	5.581478	0.895389	0.0975	0	0	108
C8	C18	5.587151	0.182285	0.0277	0	0	109
C18	H34	5.587784	0.41449	0.0586	0	0	109
Si2	F21	5.589579	0.340176	0.0396	0	0	109
C11	H37	5.59817	0.286756	0.0393	0	0	109
C6	C18	5.600057	0.209561	0.0479	0	0	109
C13	H37	5.608012	0.316811	0.0201	0	0	109
F23	H24	5.609764	0.765473	0.0731	0	0	109
C4	H31	5.614867	0.250526	0.0832	0	0	109
C5	C13	5.625085	0.178065	0.0355	0	0	109
C13	H31	5.628525	0.424062	0.0502	0	0	109
C18	F22	5.631109	0.895688	-0.1152	0	0	107
C11	H35	5.632105	0.263598	0.0448	0	0	109
Si2	C13	5.632624	0.350521	0.0317	0	0	108
F19	H32	5.64079	0.325045	0.1094	0	0	109
C14	H29	5.648174	0.348307	0.0623	0	0	109
F20	H33	5.648931	0.838551	0.2135	0	0	109
C3	H27	5.649823	0.648933	-0.0171	0	0	108
F19	H26	5.663644	0.781676	0.0725	0	0	110
Si1	H26	5.664921	0.335338	0.0431	0	0	109
C6	H31	5.669044	0.435803	0.089	0	0	108
C10	H40	5.671519	0.657416	0.0641	0	0	108
C17	H39	5.671743	0.233852	0.0657	0	0	109
F19	H28	5.680102	0.765572	0.0084	0	0	110
F23	H27	5.681251	1.182743	-0.0816	0	0	108
C5	H34	5.685444	0.430199	0.0847	0	0	108
C7	C13	5.687463	0.140393	0.026	0	0	109
H29	H32	5.689161	0.582283	0.1334	0	0	108
H25	H30	5.709319	0.609229	0.111	0	0	109
H36	H38	5.713111	0.619395	0.0914	0	0	108
C13	H35	5.715349	0.304254	0.0321	0	0	109
H37	H40	5.719792	0.337088	0.1277	0	0	109
H35	H39	5.741676	0.461836	0.0759	0	0	109
C15	H37	5.742939	0.497346	0.0837	0	0	109
F19	H33	5.746372	0.443206	0.1147	0	0	109
F21	H31	5.750474	0.53193	0.0854	0	0	109
C15	F23	5.755273	0.747546	-0.0681	0	0	108
H24	H29	5.760258	0.370539	0.0984	0	0	109
C16	H33	5.774452	0.269567	0.1032	0	0	109

C8	C10	5.776975	0.235395	0.0717	0	0	109
C4	F23	5.787731	0.404403	-0.0411	0	0	109
C7	H38	5.788397	0.244762	0.0893	0	0	109
Si1	C18	5.790185	0.243733	0.0292	0	0	109
C11	H30	5.79283	0.209252	0.0862	0	0	109
C8	H35	5.794107	0.254849	0.0805	0	0	109
C4	F22	5.794867	0.581374	-0.0346	0	0	108
C10	H28	5.796233	0.748455	-0.0627	0	0	108
C3	H28	5.797157	0.386082	-0.0359	0	0	109
C7	C16	5.799098	0.613037	0.1118	0	0	109
Si2	H28	5.80001	0.109618	0.0334	0	0	109
C12	H36	5.815152	0.170036	0.0465	0	0	109
C7	C15	5.817658	0.299622	0.0752	0	0	109
C15	F20	5.827621	0.588796	0.0077	0	0	108
C10	H33	5.836508	0.591113	0.1595	0	0	109
F19	H34	5.85993	0.678451	0.1063	0	0	110
C9	H33	5.90462	0.261024	0.1043	0	0	109
C8	F21	5.912559	0.774942	0.1219	0	0	109
F22	H28	5.912857	1.072921	-0.117	0	0	108
H31	H32	5.92195	0.454528	0.1242	0	0	109
C18	F20	5.924507	0.778599	-0.0211	0	0	108
H34	H35	5.927348	0.342029	0.108	0	0	109
H24	H30	5.939691	0.384023	0.1043	0	0	109
C15	H30	5.941033	0.719193	0.1018	0	0	110
H29	H34	5.955837	0.423033	0.1061	0	0	109
C12	H25	5.97339	0.740275	0.0081	0	0	108
H31	H38	5.984351	0.338529	0.1125	0	0	109
H24	H31	6.023155	0.643667	0.1113	0	0	110
H35	H40	6.025782	0.589719	0.1022	0	0	110
H37	H38	6.036903	0.5588	0.1092	0	0	110
C9	H34	6.044913	0.415316	0.0888	0	0	110
C14	H30	6.068806	0.429004	0.0953	0	0	110
C12	H27	6.068807	0.970825	-0.0282	0	0	108
H27	H34	6.073458	0.615324	0.0483	0	0	110
Si1	F23	6.074871	0.136882	0.0276	0	0	110
C12	H32	6.082047	1.315515	0.1243	0	0	110
C7	H26	6.109256	1.139501	0.1291	0	0	110
H27	H39	6.170042	0.486011	0.0713	0	0	110
C7	H25	6.171955	0.432708	0.0814	0	0	110
C14	H31	6.174465	0.441082	0.0938	0	0	110
C10	H27	6.188402	0.546031	-0.0064	0	0	109
H25	H31	6.18859	0.896818	0.12	0	0	110
C13	H40	6.205859	1.172836	0.0945	0	0	110
C6	H27	6.206507	0.317405	0.0584	0	0	110
C10	H34	6.210714	0.856075	0.138	0	0	110
C11	H38	6.234386	1.011798	0.1129	0	0	110
F20	H34	6.239168	1.185558	0.1864	0	0	110
C11	H39	6.242208	1.056084	0.1774	0	0	110
C10	H39	6.244143	0.487944	0.1256	0	0	110
C17	H29	6.256353	0.94835	0.0307	0	0	110
C15	H31	6.259597	0.683765	0.1037	0	0	110
H25	H37	6.259814	0.656389	0.0931	0	0	110
C15	H36	6.264229	0.530135	0.1147	0	0	110
C17	H33	6.270314	0.266517	0.0902	0	0	110
C17	F22	6.284295	0.611184	-0.0492	0	0	109
C12	H30	6.285189	0.279078	0.0909	0	0	110
F22	H31	6.293356	0.672331	0.0416	0	0	110
C17	F20	6.3023	0.494979	0.0053	0	0	109
Si1	H27	6.307284	0.457185	0.0393	0	0	110
H26	H33	6.335383	0.564275	0.1229	0	0	110
C8	F20	6.342672	0.382464	0.0952	0	0	110
F23	H25	6.344225	0.98249	-0.0043	0	0	110
C16	H39	6.358545	0.224969	0.0831	0	0	110
C15	F22	6.363341	0.47954	-0.0261	0	0	109
C11	H36	6.389737	0.226741	0.0722	0	0	110

C8	H26	6.38975	0.229156	0.0563	0	0	110
H27	H32	6.415858	0.586821	0.0904	0	0	110
C18	H37	6.41602	1.204238	0.1209	0	0	110
F20	H40	6.425758	0.535289	0.089	0	0	110
C16	H36	6.441831	1.042396	0.1746	0	0	110
C11	H32	6.443716	0.793915	0.1047	0	0	110
Si2	F22	6.449157	0.508234	0.0502	0	0	110
C5	F22	6.449478	0.334153	0.0537	0	0	110
C6	C11	6.451119	0.452676	0.0906	0	0	110
C6	C12	6.451359	0.905031	0.1223	0	0	110
F21	H38	6.453207	1.319219	0.1425	0	0	110
H28	H32	6.454617	0.705344	0.0636	0	0	110
C12	H40	6.461906	0.902615	0.0863	0	0	110
H28	H40	6.465203	0.669916	0.0341	0	0	110
F20	H25	6.475641	0.660737	0.0402	0	0	110
C16	H35	6.479438	1.003908	0.1303	0	0	110
H26	H38	6.492329	0.477476	0.0632	0	0	110
F22	H36	6.510361	0.336407	0.0433	0	0	110
F21	H30	6.512072	0.432708	0.0956	0	0	110
H25	H36	6.520537	0.502437	0.1113	0	0	110
H26	H40	6.529072	0.522406	0.0594	0	0	110
H28	H38	6.540206	0.6084	0.0472	0	0	110
C10	H38	6.549397	0.431258	0.0957	0	0	110
H31	H34	6.569679	0.460406	0.1438	0	0	110
H28	H34	6.583171	0.701157	0.0745	0	0	110
C5	C17	6.587678	0.63014	0.0643	0	0	110
C18	H39	6.592094	0.289223	0.0827	0	0	110
C17	H37	6.594571	0.974921	0.1087	0	0	110
C18	H33	6.598754	0.313862	0.1051	0	0	110
C15	H35	6.599304	0.491003	0.096	0	0	110
F20	H28	6.602492	0.960588	-0.0078	0	0	110
F21	H39	6.611144	1.341281	0.2134	0	0	110
C13	H30	6.615137	0.278595	0.097	0	0	110
C8	H28	6.615312	0.32755	0.0428	0	0	110
C6	H28	6.631331	0.372319	0.0656	0	0	110
C8	C13	6.634355	0.757198	0.0954	0	0	110
C5	C16	6.648965	0.382625	0.0729	0	0	110
C7	F21	6.658092	0.195822	0.0535	0	0	110
C16	H29	6.661682	0.637547	0.0639	0	0	110
F22	H29	6.668591	0.583761	0.0807	0	0	110
C13	H36	6.682952	0.24365	0.0681	0	0	110
H35	H38	6.69077	0.378599	0.1255	0	0	110
F20	H39	6.69193	0.544629	0.1402	0	0	110
C8	C12	6.693977	0.510167	0.0909	0	0	110
H26	H35	6.710847	1.224529	0.1533	0	0	110
F23	H29	6.722978	0.587465	0.0305	0	0	110
C13	H32	6.733438	1.11454	0.118	0	0	110
F22	H32	6.738956	1.592177	0.1486	0	0	110
H27	H29	6.764084	1.117761	0.0318	0	0	110
Si1	H28	6.770289	0.454126	0.0446	0	0	110
H26	H36	6.787884	1.238378	0.2005	0	0	110
C7	C17	6.79604	0.622088	0.0968	0	0	110
C7	C18	6.814702	0.829987	0.109	0	0	110
F21	H37	6.821008	0.462661	0.0586	0	0	110
Si2	F23	6.821113	0.442209	0.0437	0	0	110
F23	H37	6.825161	0.528364	0.0262	0	0	110
F21	H35	6.832489	0.410162	0.0631	0	0	110
F23	H31	6.8721	0.709853	0.0603	0	0	110
C5	F23	6.904094	0.302267	0.0476	0	0	110
H25	H35	6.948551	0.488266	0.1051	0	0	110
C6	C13	6.950365	0.700996	0.1099	0	0	110
C18	H29	6.954273	0.808247	0.0463	0	0	110
F23	H35	6.959137	0.501632	0.0408	0	0	110
C7	F23	6.96667	0.238013	0.0366	0	0	110
F22	H27	6.994794	1.163496	-0.0045	0	0	110

C12	H33	7.012836	0.949155	0.187	0	0	110
C11	H34	7.029212	0.565886	0.1082	0	0	110
C11	H33	7.070055	0.458152	0.1399	0	0	110
F20	H38	7.113491	0.479086	0.1235	0	0	110
F22	H25	7.124859	0.826122	0.0252	0	0	110
H27	H33	7.128383	0.340594	0.1051	0	0	110
C5	C18	7.138474	0.496156	0.0704	0	0	110
C17	H30	7.166123	0.707277	0.1201	0	0	110
C12	H34	7.170065	0.972022	0.157	0	0	110
F20	H27	7.210779	0.87701	0.0347	0	0	110
C16	H31	7.212776	0.540442	0.1029	0	0	110
C5	H27	7.220008	0.802128	0.0777	0	0	110
C6	F21	7.25107	0.622478	0.1064	0	0	111
C6	F22	7.262077	1.16575	0.1552	0	0	110
C13	H38	7.268888	0.83353	0.1118	0	0	110
C16	H30	7.269316	0.438344	0.1167	0	0	110
C12	H39	7.269566	0.575226	0.1593	0	0	110
H26	H39	7.270066	0.269416	0.1032	0	0	110
F23	H40	7.282205	1.279282	0.1072	0	0	110
C17	H31	7.285494	0.763962	0.1132	0	0	110
C13	H39	7.294518	0.822418	0.1745	0	0	110
H28	H37	7.311283	1.298606	0.1374	0	0	110
C5	H26	7.31743	0.599662	0.0946	0	0	111
C17	H36	7.349262	0.640768	0.1455	0	0	110
F21	H32	7.35789	0.914636	0.1269	0	0	111
F22	H30	7.362763	0.425417	0.1055	0	0	111
C12	H38	7.384916	0.590202	0.1104	0	0	110
H26	H29	7.419541	0.817317	0.093	0	0	111
C18	H36	7.453892	0.865254	0.1672	0	0	110
C18	H35	7.478844	1.106246	0.1278	0	0	111
F21	H36	7.49564	0.320426	0.0893	0	0	111
C17	H35	7.506371	0.835287	0.1161	0	0	111
C13	H34	7.565748	0.990755	0.1349	0	0	111
C13	H33	7.58822	0.864564	0.1707	0	0	111
H27	H37	7.591836	1.191652	0.1282	0	0	111
H28	H39	7.625433	0.418552	0.1031	0	0	111
H28	H33	7.634311	0.45005	0.1283	0	0	111
F21	H34	7.709292	0.840941	0.1182	0	0	111
F22	H40	7.711669	1.059201	0.1087	0	0	111
C7	H27	7.72751	0.766437	0.1148	0	0	111
C18	H31	7.739706	0.820952	0.1089	0	0	111
C7	H28	7.75105	1.145012	0.1284	0	0	111
C8	F23	7.760096	1.055769	0.1119	0	0	111
C18	H30	7.780625	0.678204	0.1247	0	0	111
H26	H31	7.791106	0.823778	0.1192	0	0	111
H27	H30	7.792292	1.096554	0.1397	0	0	111
F22	H33	7.809105	1.543777	0.2329	0	0	111
F23	H32	7.850744	1.544787	0.1354	0	0	111
C8	F22	7.869499	0.59199	0.1144	0	0	111
H28	H29	7.879177	1.101602	0.0603	0	0	111
F21	H33	7.899246	0.645697	0.1567	0	0	111
F23	H30	7.89927	0.377363	0.1148	0	0	111
H27	H31	7.91347	1.201142	0.1342	0	0	111
H26	H30	7.958581	0.637015	0.1377	0	0	111
F22	H34	7.969414	1.58961	0.2009	0	0	111
F23	H36	7.970795	0.330319	0.0831	0	0	111
C5	H28	8.092534	0.717172	0.0884	0	0	111
C6	F23	8.104669	1.000649	0.1292	0	0	111
H27	H36	8.269387	0.754525	0.1628	0	0	111
F23	H38	8.316168	1.193065	0.1277	0	0	111
H28	H35	8.358209	1.245965	0.1487	0	0	111
H27	H35	8.409098	0.857093	0.1354	0	0	111
H28	H36	8.429846	1.168433	0.1919	0	0	111
F22	H39	8.433774	0.656802	0.1856	0	0	111
F23	H39	8.467901	1.119571	0.2004	0	0	111

F22	H38	8.52536	0.745641	0.1351	0	0	111
H28	H31	8.641217	0.947547	0.1262	0	0	111
F23	H34	8.648325	1.155309	0.1542	0	0	111
H28	H30	8.773283	0.735949	0.1486	0	0	111
F23	H33	8.792464	0.950778	0.1985	0	0	111

Table S7. Z-Matrix used in the refinement of the gas-phase structure of the *syn*-conformer $C_6Cl_5Me_2SiSiMe_2C_6H_5$ (**4**). Distances *r* are given in Å, angles *a* and dihedrals *d* are given in deg. The numbers written in line with the parameter indicate the groups they were refined in.

1	Si							
2	Si	1	rsisi					
3	C	1	rsic1	2	asisic1			
4	C	2	rsic2	1	asisic2	3	dcsisic	
5	C	1	rsic3	2	asisic3	3	acsic1	1
6	C	2	rsic4	1	asisic4	4	acsic2	1
7	C	1	rsic5	2	asisic5	3	acsic3	-1
8	C	2	rsic6	1	asisic6	4	acsic4	-1
9	C	3	rcc1	1	asicc1	2	dsisicc1	
10	C	3	rcc2	1	asicc2	2	dsisicc3	
11	C	9	rcc3	3	accc2	10	0	
12	C	10	rcc4	3	accc3	9	0	
13	C	11	rcc5	12	rcc6	9	180	4
14	C	4	rcc7	2	asicc3	1	dsisicc2	
15	C	4	rcc8	2	asicc4	1	dsisicc4	
16	C	14	rcc9	4	accc5	15	0	
17	C	15	rcc10	4	accc6	14	0	
18	C	16	rcc11	17	rcc12	14	180	4
19	Cl	9	rcl1	3	acccl1	10	180	
20	Cl	10	rcl2	3	acccl2	9	180	
21	Cl	11	rcl3	9	acccl3	3	180	
22	Cl	12	rcl4	10	acccl4	3	180	
23	Cl	13	rcl5	3	acccl5	1	dsicccl	
24	H	14	rcha1	4	acch1	15	180	
25	H	15	rcha2	4	acch2	14	180	
26	H	16	rcha3	14	acch3	4	180	
27	H	17	rcha4	15	acch4	4	180	
28	H	18	rcha5	4	acch5	2	dsicch	
29	H	5	rch1	1	asich1	3	dcsich1	
30	H	5	rch2	1	asich2	3	dcsich2	
31	H	5	rch3	1	asich3	3	dcsich3	
32	H	6	rch4	2	asich4	4	dcsich4	
33	H	6	rch5	2	asich5	4	dcsich5	
34	H	6	rch6	2	asich6	4	dcsich6	
35	H	7	rch7	1	asich7	3	dcsich7	
36	H	7	rch8	1	asich8	3	dcsich8	
37	H	7	rch9	1	asich9	3	dcsich9	
38	H	8	rch10	2	asich10	4	dcsich10	
39	H	8	rch11	2	asich11	4	dcsich11	
40	H	8	rch12	2	asich12	4	dcsich12	

Variables:

rsisi	2.375364	3
rsic1	1.938329	1
rsic2	1.888643	1
rsic3	1.895282	1
rsic4	1.890117	1
rsic5	1.888438	1
rsic6	1.885520	1
rcc1	1.406132	2
rcc2	1.403860	2
rcc3	1.400227	2
rcc4	1.405218	2
rcc5	1.401723	2
rcc6	1.401054	2
rcc7	1.407394	2
rcc8	1.404192	2
rcc9	1.395238	2
rcc10	1.397725	2
rcc11	1.397975	2
rcc12	1.395980	2

rcl1	1.735163	5
rcl2	1.733569	5
rcl3	1.718651	5
rcl4	1.721140	5
rcl5	1.717358	5
rcha1	1.080912	4
rcha2	1.079108	4
rcha3	1.078823	4
rcha4	1.078514	4
rcha5	1.078350	4
rch1	1.083538	4
rch2	1.087063	4
rch3	1.086282	4
rch4	1.086321	4
rch5	1.086933	4
rch6	1.087285	4
rch7	1.085302	4
rch8	1.089633	4
rch9	1.082839	4
rch10	1.087645	4
rch11	1.087021	4
rch12	1.085294	4
asisic1	102.071519	6
asisic2	106.752519	6
asisic3	117.466519	6
acsic1	110.508298	7
asisic4	108.519519	6
acsic2	108.688298	7
asisic5	107.708519	6
acsic3	115.454298	7
asisic6	113.831519	6
acsic4	110.589298	7
asicc1	118.026131	8
asicc2	127.414131	8
accc2	124.515131	8
accc3	123.635131	8
asicc3	120.767131	8
asicc4	123.362131	8
accc5	122.430131	8
accc6	122.263131	8
acccl1	119.833678	9
acccl2	121.191678	9
acccl3	121.798678	9
acccl4	121.599678	9
acccl5	179.120000	
acch1	119.977000	
acch2	119.867000	
acch3	119.971000	
acch4	119.888000	
acch5	178.160000	
asich1	112.746000	
asich2	108.553000	
asich3	110.972000	
asich4	111.464000	
asich5	111.268000	
asich6	109.970000	
asich7	112.377000	
asich8	105.734000	
asich9	113.821000	
asich10	110.451000	
asich11	110.271000	
asich12	111.796000	
dcsisic	9.808445	20
dsisicc1	63.779206	21
dsisicc3	-104.067094	21

dsisicc2	62.824467	22
dsisicc4	-111.345533	22
dsicccl	-24.150000	
dsicch	-14.940000	
dcsich1	95.836300	
dcsich2	-143.815300	
dcsich3	-25.253500	
dcsich4	55.600900	
dcsich5	175.979300	
dcsich6	-64.031800	
dcsich7	175.326000	
dcsich8	-67.083600	
dcsich9	51.178200	
dcsich10	-179.793200	
dcsich11	-60.645200	
dcsich12	59.410800	

Table S8. Cartesian coordinates for the refined structure of the *syn*−conformer $C_6Cl_5Me_2SiSiMe_2C_6H_5$ (**4**).

N	At	An	Mass	*X*	*Y*	*Z*
1	Si	14	27.976927	-2.20892096	1.11305562	-0.99125648
2	Si	14	27.976927	-3.03723535	-0.38028927	0.65985469
3	C	6	12.000000	-0.29793618	0.80281691	-0.89634613
4	C	6	12.000000	-1.53797135	-1.03252197	1.60524979
5	C	6	12.000000	-2.83118882	0.88540175	-2.76693941
6	C	6	12.000000	-4.13059769	0.59315617	1.85547361
7	C	6	12.000000	-2.77262483	2.85421542	-0.52564062
8	C	6	12.000000	-4.05018768	-1.80701305	-0.04269215
9	C	6	12.000000	0.18188465	-0.47406187	-1.23775595
10	C	6	12.000000	0.67148329	1.62667062	-0.30278502
11	C	6	12.000000	1.49366227	-0.91295935	-1.02039666
12	C	6	12.000000	1.99706781	1.22388386	-0.06778062
13	C	6	12.000000	2.43222577	-0.05919699	-0.42456389
14	C	6	12.000000	-0.71720725	-0.15990407	2.34392637
15	C	6	12.000000	-1.09727827	-2.36368001	1.53065773
16	C	6	12.000000	0.45864591	-0.5838821	2.96384731
17	C	6	12.000000	0.07940799	-2.7958264	2.14895784
18	C	6	12.000000	0.87984269	-1.9140898	2.87738486
19	Cl	17	34.968853	-0.88171624	-1.62527588	-1.98223522
20	Cl	17	34.968853	0.29251689	3.2430801	0.19607933
21	Cl	17	34.968853	2.00597095	-2.49175429	-1.4661622
22	Cl	17	34.968853	3.14365214	2.27820812	0.66438532
23	Cl	17	34.968853	4.04057843	-0.57996541	-0.12237224
24	H	1	1.007825	-0.99020231	0.88090027	2.44673965
25	H	1	1.007825	-1.67486587	-3.09097347	0.98119377
26	H	1	1.007825	1.05814728	0.11929755	3.52061957
27	H	1	1.007825	0.38195647	-3.82777237	2.06683484
28	H	1	1.007825	1.80554217	-2.23683077	3.32655883
29	H	1	1.007825	-3.22861562	-0.10628155	-2.94768943
30	H	1	1.007825	-3.61691321	1.61295463	-2.95404829
31	H	1	1.007825	-2.03386246	1.06004409	-3.48372327
32	H	1	1.007825	-3.5742597	1.386342	2.34683639
33	H	1	1.007825	-4.97199455	1.04790915	1.33906853
34	H	1	1.007825	-4.51987929	-0.06863088	2.62533477
35	H	1	1.007825	-3.83832078	2.99683045	-0.67340163
36	H	1	1.007825	-2.56345848	2.95778116	0.53870117
37	H	1	1.007825	-2.24102435	3.64017402	-1.04737819
38	H	1	1.007825	-4.91086997	-1.42883796	-0.58966659
39	H	1	1.007825	-3.44773355	-2.39297687	-0.73211936
40	H	1	1.007825	-4.4055419	-2.47176836	0.73813217

Table S9. Full listing of structural parameters of the *syn* conformer $C_6Cl_5Me_2SiSiMe_2C_6H_5$ (**4**). r_a, r_{h1} and r_e values are given in Å. Errors correspond to one time standard deviation. For atom numbering see Table S8.

No.	Type	i	j	k	l	r_a	r_{h1}	r_e	Error
1	stretch	1	2	0	0	2.37646	2.37951	2.37536	0.00336
2	stretch	1	3	0	0	1.93863	1.94094	1.93833	0.00065
3	stretch	1	5	0	0	1.89558	1.89772	1.89528	0.00065
4	stretch	1	7	0	0	1.88864	1.89073	1.88844	0.00065
5	stretch	2	4	0	0	1.88954	1.89156	1.88864	0.00065
6	stretch	2	6	0	0	1.89032	1.89240	1.89012	0.00065
7	stretch	2	8	0	0	1.88582	1.88788	1.88552	0.00065
8	stretch	3	9	0	0	1.40563	1.40799	1.40613	0.00034
9	stretch	3	10	0	0	1.40276	1.40510	1.40386	0.00034
10	stretch	4	14	0	0	1.40679	1.40910	1.40739	0.00034
11	stretch	4	15	0	0	1.40309	1.40539	1.40419	0.00034
12	stretch	5	29	0	0	1.08174	1.09069	1.08354	0.00164
13	stretch	5	30	0	0	1.08486	1.09408	1.08706	0.00164
14	stretch	5	31	0	0	1.08348	1.09333	1.08628	0.00164
15	stretch	6	32	0	0	1.08492	1.09299	1.08632	0.00164
16	stretch	6	33	0	0	1.08543	1.09349	1.08693	0.00164
17	stretch	6	34	0	0	1.08578	1.09384	1.08728	0.00164
18	stretch	7	35	0	0	1.08400	1.09201	1.08530	0.00164
19	stretch	7	36	0	0	1.08823	1.09634	1.08963	0.00164
20	stretch	7	37	0	0	1.08144	1.08940	1.08284	0.00164
21	stretch	8	38	0	0	1.08634	1.09440	1.08764	0.00164
22	stretch	8	39	0	0	1.08552	1.09358	1.08702	0.00164
23	stretch	8	40	0	0	1.08379	1.09183	1.08529	0.00164
24	stretch	9	11	0	0	1.39983	1.40213	1.40023	0.00034
25	stretch	9	19	0	0	1.73506	1.73689	1.73516	0.00045
26	stretch	10	12	0	0	1.40472	1.40705	1.40522	0.00034
27	stretch	10	20	0	0	1.73347	1.73528	1.73357	0.00045
28	stretch	11	13	0	0	1.40132	1.40361	1.40172	0.00034
29	stretch	11	21	0	0	1.71885	1.72058	1.71865	0.00045
30	stretch	12	13	0	0	1.40055	1.40284	1.40105	0.00034
31	stretch	12	22	0	0	1.72134	1.72308	1.72114	0.00045
32	stretch	13	23	0	0	1.71756	1.71928	1.71736	0.00045
33	stretch	14	16	0	0	1.39504	1.39729	1.39524	0.00034
34	stretch	14	24	0	0	1.07951	1.08745	1.08091	0.00164
35	stretch	15	17	0	0	1.39753	1.39978	1.39773	0.00034
36	stretch	15	25	0	0	1.07771	1.08559	1.07911	0.00164
37	stretch	16	18	0	0	1.39798	1.40022	1.39798	0.00034
38	stretch	16	26	0	0	1.07742	1.08529	1.07882	0.00164
39	stretch	17	18	0	0	1.39598	1.39822	1.39598	0.00034
40	stretch	17	27	0	0	1.07711	1.08498	1.07851	0.00164
41	stretch	18	28	0	0	1.07695	1.08482	1.07835	0.00164
42	bend	2	1	3	0	102.07152			0.20638
43	bend	2	1	5	0	117.46652			0.20638
44	bend	2	1	7	0	107.70852			0.20638
45	bend	1	2	4	0	106.75252			0.20638
46	bend	1	2	6	0	108.51952			0.20638
47	bend	1	2	8	0	113.83152			0.20638
48	bend	3	1	5	0	110.50830			0.43152
49	bend	3	1	7	0	115.45430			0.43152
50	bend	1	3	9	0	118.02613			0.05656
51	bend	1	3	10	0	127.41413			0.05656
52	bend	5	1	7	0	104.10768			1.10697
53	bend	1	5	29	0	112.74600			0.00000
54	bend	1	5	30	0	108.55300			0.00000
55	bend	1	5	31	0	110.97200			0.00000
56	bend	1	7	35	0	112.37700			0.00000
57	bend	1	7	36	0	105.73400			0.00000
58	bend	1	7	37	0	113.82100			0.00000
59	bend	4	2	6	0	108.68830			0.43152
60	bend	4	2	8	0	110.58930			0.43152
61	bend	2	4	14	0	120.76713			0.05656

62	bend	2	4	15	0	123.36213			0.05656
63	bend	6	2	8	0	108.33843			1.14403
64	bend	2	6	32	0	111.46400			0.00000
65	bend	2	6	33	0	111.26800			0.00000
66	bend	2	6	34	0	109.97000			0.00000
67	bend	2	8	38	0	110.45100			0.00000
68	bend	2	8	39	0	110.27100			0.00000
69	bend	2	8	40	0	111.79600			0.00000
70	bend	9	3	10	0	113.57361			0.11100
71	bend	3	9	11	0	124.51513			0.05656
72	bend	3	9	19	0	119.83368			0.12464
73	bend	3	10	12	0	123.63513			0.05656
74	bend	3	10	20	0	121.19168			0.12464
75	bend	14	4	15	0	115.63460			0.11261
76	bend	4	14	16	0	122.43013			0.05656
77	bend	4	14	24	0	119.97700			0.00000
78	bend	4	15	17	0	122.26313			0.05656
79	bend	4	15	25	0	119.86700			0.00000
80	bend	29	5	30	0	108.58565			0.00000
81	bend	29	5	31	0	107.83570			0.00000
82	bend	30	5	31	0	108.02019			0.00000
83	bend	32	6	33	0	107.80956			0.00000
84	bend	32	6	34	0	107.90917			0.00000
85	bend	33	6	34	0	108.29446			0.00000
86	bend	35	7	36	0	107.99839			0.00000
87	bend	35	7	37	0	108.72861			0.00000
88	bend	36	7	37	0	107.90340			0.00000
89	bend	38	8	39	0	107.88136			0.00000
90	bend	38	8	40	0	108.40210			0.00000
91	bend	39	8	40	0	107.91447			0.00000
92	bend	11	9	19	0	115.65119			0.11805
93	bend	9	11	13	0	120.15574			0.05547
94	bend	9	11	21	0	121.79868			0.12464
95	bend	12	10	20	0	115.17319			0.11805
96	bend	10	12	13	0	120.85753			0.05547
97	bend	10	12	22	0	121.59968			0.12464
98	bend	13	11	21	0	118.04558			0.11792
99	bend	11	13	12	0	117.26285			0.11306
100	bend	11	13	23	0	121.14321			0.05593
101	bend	13	12	22	0	117.54279			0.11792
102	bend	12	13	23	0	121.58574			0.05712
103	bend	16	14	24	0	117.59287			0.05656
104	bend	14	16	18	0	121.03627			0.05729
105	bend	14	16	26	0	119.97100			0.00000
106	bend	17	15	25	0	117.86987			0.05656
107	bend	15	17	18	0	121.21493			0.05751
108	bend	15	17	27	0	119.88800			0.00000
109	bend	18	16	26	0	118.99273			0.05729
110	bend	16	18	17	0	117.42093			0.11532
111	bend	16	18	28	0	121.17549			0.05654
112	bend	18	17	27	0	118.89707			0.05751
113	bend	17	18	28	0	121.36769			0.05870
114	torsion	4	2	1	3	9.80845			0.52550
115	torsion	6	2	1	3	126.79155			0.76001
116	torsion	8	2	1	3	-112.49790			0.89262
117	torsion	2	1	3	9	63.77921			0.51007
118	torsion	2	1	3	10	-104.06709			0.51007
119	torsion	4	2	1	5	130.80252			0.80743
120	torsion	6	2	1	5	-112.21438			1.32138
121	torsion	8	2	1	5	8.49618			0.52745
122	torsion	2	1	5	29	-20.65680			0.59024
123	torsion	2	1	5	30	99.69160			0.59024
124	torsion	2	1	5	31	-141.74660			0.59024
125	torsion	4	2	1	7	-112.17392			0.81289
126	torsion	6	2	1	7	4.80918			0.52297

127	torsion	8	2	1	7	125.51974			1.39852
128	torsion	2	1	7	35	-71.40026			0.50715
129	torsion	2	1	7	36	46.19014			0.50715
130	torsion	2	1	7	37	164.45194			0.50715
131	torsion	1	2	4	14	62.82447			0.52965
132	torsion	1	2	4	15	-111.34553			0.52965
133	torsion	1	2	6	32	-60.13383			0.47050
134	torsion	1	2	6	33	60.24457			0.47050
135	torsion	1	2	6	34	-179.76653			0.47050
136	torsion	1	2	8	38	-59.62506			0.57698
137	torsion	1	2	8	39	59.52294			0.57698
138	torsion	1	2	8	40	179.57894			0.57698
139	torsion	9	3	1	5	-61.92287			0.81910
140	torsion	10	3	1	5	130.23083			0.81910
141	torsion	3	1	5	29	95.83630			0.00000
142	torsion	3	1	5	30	-143.81530			0.00000
143	torsion	3	1	5	31	-25.25350			0.00000
144	torsion	9	3	1	7	-179.71484			0.55778
145	torsion	10	3	1	7	12.43886			0.55778
146	torsion	3	1	7	35	175.32600			0.00000
147	torsion	3	1	7	36	-67.08360			0.00000
148	torsion	3	1	7	37	51.17820			0.00000
149	torsion	1	3	9	11	-169.48773			0.01702
150	torsion	1	3	9	19	10.51227			0.01702
151	torsion	1	3	10	12	168.30114			0.01626
152	torsion	1	3	10	20	-11.69886			0.01626
153	torsion	29	5	1	7	-139.61182			0.38931
154	torsion	30	5	1	7	-19.26342			0.38931
155	torsion	31	5	1	7	99.29838			0.38931
156	torsion	5	1	7	35	54.01360			0.41518
157	torsion	5	1	7	36	171.60400			0.41518
158	torsion	5	1	7	37	-70.13420			0.41518
159	torsion	14	4	2	6	-54.04678			0.70963
160	torsion	15	4	2	6	131.78322			0.70963
161	torsion	4	2	6	32	55.60090			0.00000
162	torsion	4	2	6	33	175.97930			0.00000
163	torsion	4	2	6	34	-64.03180			0.00000
164	torsion	14	4	2	8	-172.85460			0.73909
165	torsion	15	4	2	8	12.97540			0.73909
166	torsion	4	2	8	38	-179.79320			0.00000
167	torsion	4	2	8	39	-60.64520			0.00000
168	torsion	4	2	8	40	59.41080			0.00000
169	torsion	2	4	14	16	-174.60044			0.00863
170	torsion	2	4	14	24	5.39956			0.00863
171	torsion	2	4	15	17	174.44453			0.00853
172	torsion	2	4	15	25	-5.55547			0.00853
173	torsion	32	6	2	8	175.81422			0.39589
174	torsion	33	6	2	8	-63.80738			0.39589
175	torsion	34	6	2	8	56.18152			0.39589
176	torsion	6	2	8	38	61.18688			0.40189
177	torsion	6	2	8	39	-179.66512			0.40189
178	torsion	6	2	8	40	-59.60912			0.40189
179	torsion	11	9	3	10	0.00000			0.00000
180	torsion	19	9	3	10	180.00000			0.00000
181	torsion	9	3	10	12	0.00000			0.00000
182	torsion	9	3	10	20	180.00000			0.00000
183	torsion	3	9	11	13	0.00000			0.00000
184	torsion	3	9	11	21	180.00000			0.00000
185	torsion	3	10	12	13	0.00000			0.00000
186	torsion	3	10	12	22	180.00000			0.00000
187	torsion	16	14	4	15	0.00000			0.00000
188	torsion	24	14	4	15	180.00000			0.00000
189	torsion	14	4	15	17	0.00000			0.00000
190	torsion	14	4	15	25	180.00000			0.00000
191	torsion	4	14	16	18	0.00000			0.00000

192	torsion	4	14	16	26	-180.00000			0.00000
193	torsion	4	15	17	18	0.00000			0.00000
194	torsion	4	15	17	27	180.00000			0.00000
195	torsion	13	11	9	19	-180.00000			0.00000
196	torsion	21	11	9	19	0.00000			0.00000
197	torsion	9	11	13	12	0.00000			0.00000
198	torsion	9	11	13	23	178.97443			0.00054
199	torsion	13	12	10	20	-180.00000			0.00000
200	torsion	22	12	10	20	0.00000			0.00000
201	torsion	10	12	13	11	0.00000			0.00000
202	torsion	10	12	13	23	-178.96959			0.00057
203	torsion	12	13	11	21	-180.00000			0.00000
204	torsion	23	13	11	21	-1.02557			0.00054
205	torsion	11	13	12	22	180.00000			0.00000
206	torsion	23	13	12	22	1.03041			0.00057
207	torsion	18	16	14	24	-180.00000			0.00000
208	torsion	26	16	14	24	0.00000			0.00000
209	torsion	14	16	18	17	0.00000			0.00000
210	torsion	14	16	18	28	177.84983			0.00126
211	torsion	18	17	15	25	-180.00000			0.00000
212	torsion	27	17	15	25	0.00000			0.00000
213	torsion	15	17	18	16	0.00000			0.00000
214	torsion	15	17	18	28	-177.84544			0.00132
215	torsion	17	18	16	26	-180.00000			0.00000
216	torsion	28	18	16	26	-2.15017			0.00126
217	torsion	16	18	17	27	-180.00000			0.00000
218	torsion	28	18	17	27	2.15456			0.00132
219	o.o.p	19	3	9	11	0.00000			0.00000
220	o.o.p	20	3	10	12	0.00000			0.00000
221	o.o.p	24	4	14	16	0.00000			0.00000
222	o.o.p	25	4	15	17	0.00000			0.00000
223	o.o.p	21	9	11	13	0.00000			0.00000
224	o.o.p	22	10	12	13	0.00000			0.00000
225	o.o.p	23	11	13	12	-0.87775			0.00005
226	o.o.p	26	14	16	18	0.00000			0.00000
227	o.o.p	27	15	17	18	0.00000			0.00000
228	o.o.p	28	16	18	17	-1.83954			0.00002

Table S10. Full listing of interatomic distances. refined vibrational amplitudes *l* and corrections of the *syn*-conformer $C_6Cl_5Me_2SiSiMe_2C_6H_5$ (**4**). All is given in Å. The numbers at the Gu column indicate the groups the amplitudes were refined in.

At1	At2	r_a	*l*	corr	*a*	Gr	Gu
C18	H28	1.07695	0.092073	0.0014	0.0000	0	100
C17	H27	1.077114	0.092073	0.0014	0.0000	0	100
C16	H26	1.077423	0.092073	0.0014	0.0000	0	100
C15	H25	1.077708	0.092195	0.0014	0.0000	0	100
C14	H24	1.079512	0.092562	0.0014	0.0000	0	100
C7	H37	1.081439	0.092807	0.0014	0.0000	0	100
C5	H29	1.081738	0.098431	0.0018	0.0000	0	100
C5	H31	1.083482	0.103322	0.0028	0.0000	0	100
C8	H40	1.083794	0.093296	0.0015	0.0000	0	100
C7	H35	1.084002	0.093173	0.0013	0.0000	0	100
C5	H30	1.084863	0.100021	0.0022	0.0000	0	100
C6	H32	1.084921	0.093540	0.0014	0.0000	0	100
C6	H33	1.085433	0.093540	0.0015	0.0000	0	100
C8	H39	1.085521	0.093540	0.0015	0.0000	0	100
C6	H34	1.085785	0.093540	0.0015	0.0000	0	100
C8	H38	1.086345	0.093540	0.0013	0.0000	0	100
C7	H36	1.088233	0.093907	0.0014	0.0000	0	100
C14	C16	1.395038	0.056002	0.0002	0.0000	0	100
C17	C18	1.39598	0.055880	0.0000	0.0000	0	100
C15	C17	1.397525	0.056124	0.0002	0.0000	0	100
C16	C18	1.397975	0.056002	0.0000	0.0000	0	100
C9	C11	1.399827	0.056736	0.0004	0.0000	0	100
C12	C13	1.400554	0.056613	0.0005	0.0000	0	100
C11	C13	1.401323	0.056613	0.0004	0.0000	0	100
C3	C10	1.40276	0.057347	0.0011	0.0000	0	100
C4	C15	1.403092	0.056736	0.0011	0.0000	0	100
C10	C12	1.404718	0.057225	0.0005	0.0000	0	100
C3	C9	1.405632	0.057591	0.0005	0.0000	0	100
C4	C14	1.406794	0.056980	0.0006	0.0000	0	100
C13	Cl23	1.717558	0.054360	-0.0002	0.0000	0	101
C11	Cl21	1.718851	0.054468	-0.0002	0.0000	0	101
C12	Cl22	1.72134	0.054683	-0.0002	0.0000	0	101
C10	Cl20	1.733469	0.055978	0.0001	0.0000	0	101
H29	H31	1.734791	0.144636	0.0188	0.0000	0	101
C9	Cl19	1.735063	0.056301	0.0001	0.0000	0	101
H30	H31	1.741298	0.145606	0.0172	0.0000	0	101
H29	H30	1.741352	0.140537	0.0212	0.0000	0	101
H32	H33	1.743774	0.136546	0.0123	0.0000	0	101
H39	H40	1.744286	0.136223	0.0122	0.0000	0	101
H36	H37	1.744994	0.136115	0.0115	0.0000	0	101
H32	H34	1.745171	0.136331	0.0123	0.0000	0	101
H38	H39	1.745617	0.136439	0.0124	0.0000	0	101
H35	H36	1.747943	0.136223	0.0116	0.0000	0	101
H38	H40	1.750016	0.136007	0.0124	0.0000	0	101
H33	H34	1.750057	0.136223	0.0122	0.0000	0	101
H35	H37	1.750431	0.135684	0.0117	0.0000	0	101
Si2	C8	1.88582	0.062341	-0.0003	0.0000	0	101
Si1	C7	1.888638	0.062880	-0.0002	0.0000	0	101
Si2	C4	1.889543	0.061802	-0.0009	0.0000	0	101
Si2	C6	1.890317	0.062773	-0.0002	0.0000	0	101
Si1	C5	1.895582	0.063635	-0.0003	0.0000	0	101
Si1	C3	1.938629	0.066979	-0.0003	0.0000	0	101
C16	H24	2.115882	0.120199	0.0083	0.0000	0	102
C17	H25	2.120071	0.120320	0.0079	0.0000	0	102
C18	H27	2.128669	0.120442	0.0084	0.0000	0	102
C18	H26	2.131842	0.120442	0.0083	0.0000	0	102
C14	H26	2.140926	0.120684	0.0072	0.0000	0	102
C15	H27	2.14183	0.120684	0.0074	0.0000	0	102
C4	H25	2.148321	0.119956	0.0070	0.0000	0	102
C4	H24	2.154566	0.120320	0.0063	0.0000	0	102

C16	H28	2.154952	0.120442	0.0079	0.0000	0	102
C17	H28	2.155244	0.120199	0.0078	0.0000	0	102
C9	C10	2.347048	0.071634	0.0039	0.0000	0	102
Si1	Si2	2.376464	0.085110	-0.0011	0.0000	0	102
C14	C15	2.376998	0.070905	0.0026	0.0000	0	102
C16	C17	2.384585	0.070298	0.0030	0.0000	0	102
C11	C12	2.388214	0.070905	0.0049	0.0000	0	102
Si1	H36	2.413001	0.160022	0.0097	0.0000	0	102
H24	H26	2.422152	0.197417	0.0128	0.0000	0	102
C9	C13	2.423362	0.071148	0.0051	0.0000	0	102
H25	H27	2.427174	0.197417	0.0125	0.0000	0	102
C14	C18	2.427825	0.070177	0.0037	0.0000	0	102
C15	C18	2.430794	0.070055	0.0033	0.0000	0	102
C10	C13	2.435336	0.071148	0.0054	0.0000	0	102
C4	C17	2.448227	0.070541	0.0055	0.0000	0	102
H32	H36	2.450195	0.901976	0.1499	0.0000	0	102
C4	C16	2.451428	0.070541	0.0049	0.0000	0	102
H27	H28	2.46463	0.198024	0.0142	0.0000	0	102
H26	H28	2.465535	0.198146	0.0139	0.0000	0	102
Si1	H30	2.467558	0.171071	-0.0008	0.0000	0	102
C3	C12	2.469258	0.071269	0.0068	0.0000	0	102
Si2	H38	2.471203	0.161965	0.0130	0.0000	0	102
Si2	H34	2.472628	0.161722	0.0090	0.0000	0	102
Si2	H39	2.473633	0.160993	0.0077	0.0000	0	102
C3	C11	2.477368	0.071027	0.0064	0.0000	0	102
Si2	H32	2.488957	0.161115	0.0121	0.0000	0	102
Si2	H33	2.489875	0.161236	0.0090	0.0000	0	102
Si2	H40	2.492135	0.160751	0.0084	0.0000	0	102
Si1	H35	2.498793	0.157351	0.0121	0.0000	0	102
Si1	H31	2.502769	0.178598	-0.0036	0.0000	0	102
Si1	H29	2.512352	0.151281	0.0084	0.0000	0	103
H25	H39	2.518662	0.339439	0.0437	0.0000	0	103
Si1	H37	2.520145	0.141618	0.0078	0.0000	0	103
C12	Cl20	2.652511	0.073641	0.0031	0.0000	0	103
H24	H32	2.65502	0.500827	-0.0201	0.0000	0	103
C11	Cl19	2.656278	0.073863	0.0036	0.0000	0	103
C13	Cl22	2.671358	0.073530	0.0036	0.0000	0	103
C13	Cl21	2.67659	0.073530	0.0037	0.0000	0	103
C11	Cl23	2.71745	0.073530	0.0036	0.0000	0	103
C3	Cl19	2.720858	0.076529	0.0023	0.0000	0	103
C12	Cl23	2.722714	0.073419	0.0036	0.0000	0	103
C9	Cl21	2.726268	0.073530	0.0033	0.0000	0	103
C10	Cl22	2.730011	0.073641	0.0034	0.0000	0	103
C3	Cl20	2.734649	0.076973	0.0034	0.0000	0	103
C9	C12	2.740735	0.073752	0.0064	0.0000	0	103
C14	C17	2.755761	0.073975	0.0048	0.0000	0	103
C10	C11	2.757075	0.073752	0.0071	0.0000	0	103
C15	C16	2.760128	0.073863	0.0044	0.0000	0	103
H30	H35	2.762542	0.535926	-0.0857	0.0000	0	103
H25	H40	2.823731	0.525597	-0.0132	0.0000	0	103
Cl19	H39	2.854074	0.646360	0.1017	0.0000	0	104
Si2	C14	2.860673	0.100632	0.0146	0.0000	0	103
C4	C18	2.862969	0.074308	0.0078	0.0000	0	103
Si1	C9	2.871518	0.090302	0.0087	0.0000	0	103
C3	C13	2.892026	0.073863	0.0096	0.0000	0	103
Si2	C15	2.906246	0.097744	0.0016	0.0000	0	103
C8	H25	2.911541	0.325612	-0.0238	0.0000	0	104
Cl20	H37	2.933235	0.343675	-0.0832	0.0000	0	104
Cl20	H36	2.937668	0.225450	-0.0471	0.0000	0	104
H33	H35	2.965176	0.553698	0.0570	0.0000	0	103
Si2	H24	2.973647	0.199512	0.0220	0.0000	0	104
C5	C7	2.977302	0.143700	0.0065	0.0000	0	104
H34	H40	2.987124	0.327349	0.0706	0.0000	0	104
C7	H30	2.991046	0.354444	-0.1361	0.0000	0	104
Cl19	H31	2.999747	1.108261	0.2855	0.0000	0	104

Si1	C10	3.003048	0.091361	0.0027	0.0000	0	104
Cl20	Cl22	3.048788	0.126447	-0.0026	0.0000	0	104
Si2	H25	3.051257	0.194996	-0.0005	0.0000	0	104
C6	C8	3.051396	0.149953	0.0097	0.0000	0	104
H33	H38	3.05345	0.557430	0.0863	0.0000	0	104
Cl19	Cl21	3.057434	0.127141	0.0013	0.0000	0	104
C4	C6	3.061167	0.143005	0.0092	0.0000	0	104
Cl19	H29	3.081497	0.600737	-0.1239	0.0000	0	104
H24	H36	3.084824	0.778017	0.1446	0.0000	0	104
C6	H36	3.086602	0.583021	0.0409	0.0000	0	104
Cl22	Cl23	3.095496	0.127026	0.0017	0.0000	0	104
C4	C8	3.095805	0.135247	0.0069	0.0000	0	104
Cl21	Cl23	3.096241	0.127720	0.0022	0.0000	0	104
C5	H35	3.121923	0.287631	0.0174	0.0000	0	104
C3	C5	3.142928	0.144510	0.0072	0.0000	0	104
C6	H24	3.1749	0.370887	0.0336	0.0000	0	104
H30	H37	3.193526	0.343212	-0.0890	0.0000	0	104
Si1	Cl19	3.194408	0.153311	0.0059	0.0000	0	104
H33	H36	3.201557	0.681214	-0.0252	0.0000	0	104
C15	H39	3.202069	0.243977	0.0607	0.0000	0	104
C8	H34	3.203743	0.326885	0.0151	0.0000	0	104
C6	H40	3.219606	0.162227	0.0542	0.0000	0	104
C4	H32	3.228464	0.332443	0.0192	0.0000	0	104
C3	C7	3.229298	0.123320	0.0064	0.0000	0	104
C3	H31	3.23116	0.437468	-0.1048	0.0000	0	104
C14	H32	3.241636	0.439321	0.0070	0.0000	0	104
C6	H38	3.243614	0.343560	0.0238	0.0000	0	104
C7	Cl20	3.246183	0.199976	-0.0733	0.0000	0	104
C4	H39	3.259889	0.155974	0.0509	0.0000	0	104
C5	Cl19	3.267296	0.288210	0.0068	0.0000	0	104
C5	H37	3.267699	0.155395	0.0329	0.0000	0	104
C10	H24	3.273269	0.512387	0.0248	0.0000	0	104
C4	H34	3.275269	0.329201	0.0204	0.0000	0	104
C8	H33	3.282164	0.344718	0.0208	0.0000	0	104
H29	H39	3.28481	0.887674	-0.0933	0.0000	0	104
H29	H38	3.298844	0.697425	-0.1146	0.0000	0	104
C7	H32	3.305813	0.567041	0.0181	0.0000	0	104
C4	H40	3.310495	0.321675	0.0131	0.0000	0	104
Si2	H36	3.345001	0.357455	0.0287	0.0000	0	104
C3	C4	3.345378	0.190365	-0.0041	0.0000	0	104
C16	H27	3.352602	0.110930	0.0139	0.0000	0	104
C17	H26	3.353296	0.110930	0.0138	0.0000	0	104
Si2	C3	3.357303	0.145437	0.0080	0.0000	0	104
C14	H25	3.359049	0.110699	0.0122	0.0000	0	104
C15	H24	3.360925	0.110930	0.0122	0.0000	0	104
C3	H24	3.363401	0.476491	0.0515	0.0000	0	104
C4	C9	3.375942	0.227650	-0.0066	0.0000	0	104
C18	H24	3.376253	0.111278	0.0141	0.0000	0	104
C18	H25	3.378616	0.111162	0.0136	0.0000	0	104
H32	H35	3.378664	0.570862	0.0543	0.0000	0	104
C7	H33	3.390815	0.551872	0.0117	0.0000	0	104
C8	C15	3.394899	0.229156	-0.0030	0.0000	0	104
C14	H28	3.397951	0.110930	0.0143	0.0000	0	104
C3	C14	3.398769	0.289021	0.0074	0.0000	0	104
C15	H28	3.401904	0.110814	0.0139	0.0000	0	104
Cl19	H25	3.402592	0.554642	-0.0027	0.0000	0	105
C15	H40	3.404585	0.456690	-0.0010	0.0000	0	104
C4	H27	3.407069	0.111509	0.0153	0.0000	0	104
C3	H36	3.407123	0.151458	0.0332	0.0000	0	104
C4	H26	3.411162	0.111625	0.0145	0.0000	0	104
C7	H31	3.423065	0.583600	0.1146	0.0000	0	104
Si1	C4	3.425761	0.144858	0.0087	0.0000	0	104
C3	H37	3.428537	0.264357	0.0137	0.0000	0	104
H31	H37	3.436882	0.534156	0.1178	0.0000	0	104
Si2	C7	3.44546	0.174154	0.0096	0.0000	0	104

C6	H35	3.449283	0.331170	0.0519	0.0000	0	104
Si1	C6	3.46596	0.164080	0.0078	0.0000	0	104
Cl20	H24	3.470014	0.637328	0.0358	0.0000	0	104
C9	H31	3.489988	0.900762	0.0182	0.0000	0	105
C10	C14	3.490653	0.336728	-0.0085	0.0000	0	104
C6	C14	3.501836	0.285954	0.0276	0.0000	0	105
Si1	Cl20	3.502917	0.169076	-0.0095	0.0000	0	105
H34	H38	3.53033	0.567127	-0.0176	0.0000	0	105
H33	H40	3.544962	0.388090	0.0703	0.0000	0	105
C6	C7	3.552934	0.357277	0.0004	0.0000	0	105
H24	H34	3.554325	0.664349	0.1052	0.0000	0	105
C10	H36	3.571189	0.197498	0.0267	0.0000	0	105
Si1	C8	3.573961	0.204006	0.0061	0.0000	0	105
C9	C15	3.597722	0.368168	-0.0101	0.0000	0	105
Si1	H24	3.601595	0.491023	0.0534	0.0000	0	105
Si1	H32	3.602063	0.402700	0.0148	0.0000	0	105
Si1	H33	3.60324	0.408013	0.0119	0.0000	0	105
C15	Cl19	3.604426	0.415583	-0.0083	0.0000	0	105
Si2	Cl19	3.609899	0.340010	0.0201	0.0000	0	105
C10	H37	3.622792	0.371090	-0.0046	0.0000	0	105
C5	C9	3.625936	0.245844	0.0162	0.0000	0	105
C3	H29	3.645082	0.474421	0.0459	0.0000	0	105
C8	H29	3.646236	0.770868	-0.1812	0.0000	0	105
Si2	C5	3.649772	0.199491	0.0091	0.0000	0	105
C7	C10	3.668215	0.180099	-0.0051	0.0000	0	105
Si1	H38	3.672857	0.207592	0.0585	0.0000	0	105
Si2	H35	3.677697	0.199225	0.0404	0.0000	0	105
C4	Cl19	3.679172	0.362589	0.0157	0.0000	0	105
C9	C14	3.683845	0.424615	0.0223	0.0000	0	105
C8	Cl19	3.700118	0.502578	0.0193	0.0000	0	105
H29	H35	3.700909	0.421560	0.1944	0.0000	0	105
C7	H29	3.703215	0.408145	0.1489	0.0000	0	105
C5	H38	3.715438	0.429795	0.0821	0.0000	0	105
Si1	H39	3.719275	0.427669	0.0082	0.0000	0	105
Si2	C9	3.723574	0.229640	0.0144	0.0000	0	105
H31	H35	3.723915	0.961725	0.1368	0.0000	0	105
Si2	H29	3.728193	0.505102	-0.1052	0.0000	0	105
C14	H34	3.745763	0.542689	0.0684	0.0000	0	105
C14	H27	3.822436	0.128965	0.0166	0.0000	0	105
C17	H24	3.824411	0.129098	0.0163	0.0000	0	105
C16	H25	3.827054	0.128965	0.0159	0.0000	0	105
C15	H26	3.827204	0.128832	0.0161	0.0000	0	105
H30	H38	3.831827	0.993070	0.2323	0.0000	0	105
Si1	C14	3.83689	0.315705	0.0321	0.0000	0	105
C9	H29	3.841538	0.624238	-0.0087	0.0000	0	105
C3	H30	3.857941	0.374941	0.1303	0.0000	0	105
C9	H25	3.875316	0.552384	0.0259	0.0000	0	105
C12	C16	3.880393	0.519446	-0.0300	0.0000	0	105
C12	H24	3.882524	0.685599	0.0372	0.0000	0	105
C12	H26	3.887281	0.678958	-0.0171	0.0000	0	105
C5	H36	3.893815	0.346917	0.0169	0.0000	0	105
C7	H24	3.898339	0.759047	0.0899	0.0000	0	105
C12	C14	3.898977	0.464327	-0.0133	0.0000	0	105
C5	H39	3.903778	0.677763	0.0037	0.0000	0	105
C11	C15	3.919672	0.486507	-0.0049	0.0000	0	105
C14	H36	3.922941	0.709639	0.1252	0.0000	0	105
H25	H38	3.927177	0.667238	0.0354	0.0000	0	106
C4	H28	3.929015	0.124040	0.0197	0.0000	0	106
C4	C10	3.941672	0.344261	0.0072	0.0000	0	105
C10	C16	3.948329	0.482257	0.0017	0.0000	0	105
C11	Cl22	3.956135	0.087707	0.0118	0.0000	0	106
C12	Cl21	3.958378	0.087580	0.0117	0.0000	0	106
C8	H32	3.963999	0.176562	0.0527	0.0000	0	106
C10	Cl19	3.965045	0.089747	0.0109	0.0000	0	106
C13	Cl20	3.970239	0.088345	0.0133	0.0000	0	106

C13	Cl19	3.970807	0.088090	0.0118	0.0000	0	106
C9	Cl20	3.972233	0.090639	0.0134	0.0000	0	106
C4	H33	3.974474	0.171718	0.0494	0.0000	0	106
C11	C17	3.976232	0.505209	-0.0278	0.0000	0	106
C13	C16	3.982616	0.574166	-0.0264	0.0000	0	105
C6	H39	3.995454	0.379258	0.0144	0.0000	0	106
C9	Cl23	4.006261	0.087835	0.0118	0.0000	0	106
C4	C11	4.01107	0.361410	0.0013	0.0000	0	106
C5	C8	4.015025	0.394555	0.0045	0.0000	0	106
C10	Cl23	4.019651	0.087707	0.0118	0.0000	0	106
C9	H24	4.024477	0.575834	0.0725	0.0000	0	106
C4	H38	4.024558	0.367784	0.0191	0.0000	0	106
C3	Cl22	4.043546	0.088217	0.0132	0.0000	0	106
C3	Cl21	4.048704	0.087962	0.0117	0.0000	0	106
H24	H33	4.050263	0.458551	0.0861	0.0000	0	106
C3	C15	4.053806	0.356566	0.0151	0.0000	0	106
C9	H39	4.054369	0.517320	0.0823	0.0000	0	106
H34	H36	4.068128	0.657422	0.0961	0.0000	0	106
Si2	H30	4.069054	0.631416	0.0986	0.0000	0	106
C11	C14	4.072071	0.504572	0.0235	0.0000	0	106
H30	H36	4.077039	0.584885	-0.1889	0.0000	0	106
C14	Cl20	4.103366	0.610127	0.0455	0.0000	0	106
C11	C18	4.11204	0.474231	-0.0412	0.0000	0	106
C10	H26	4.116866	0.579021	0.0111	0.0000	0	106
C9	C17	4.120223	0.407941	-0.0128	0.0000	0	106
C11	C16	4.124119	0.556457	0.0055	0.0000	0	106
C13	C18	4.13329	0.550338	-0.0402	0.0000	0	106
Cl21	H27	4.1383	0.782609	-0.0268	0.0000	0	106
Cl19	H30	4.148377	0.371354	0.2004	0.0000	0	106
H34	H39	4.149717	0.604900	0.0722	0.0000	0	106
C17	Cl21	4.1522	0.598143	-0.0445	0.0000	0	106
H29	H37	4.152474	0.409216	0.1629	0.0000	0	106
C3	H35	4.155958	0.283774	0.0151	0.0000	0	106
Cl22	H26	4.157065	0.827738	-0.0136	0.0000	0	106
C3	C16	4.157704	0.378238	0.0132	0.0000	0	106
C13	H26	4.159538	0.762085	0.0219	0.0000	0	106
Si2	C16	4.17128	0.108869	0.0205	0.0000	0	106
H32	H40	4.174421	0.208815	0.0875	0.0000	0	106
C4	H36	4.176081	0.480350	0.0797	0.0000	0	106
C13	C14	4.189074	0.516810	0.0054	0.0000	0	106
Cl19	H38	4.195042	0.545876	0.0725	0.0000	0	106
C9	C16	4.19874	0.443891	0.0134	0.0000	0	106
Si2	C17	4.203339	0.105682	0.0116	0.0000	0	106
Si1	C11	4.203347	0.107722	0.0174	0.0000	0	106
H32	H38	4.209317	0.372119	0.0726	0.0000	0	106
C6	C15	4.22336	0.194792	0.0251	0.0000	0	106
H26	H27	4.234692	0.166363	0.0256	0.0000	0	106
C15	H34	4.243474	0.413805	0.0203	0.0000	0	106
H24	H28	4.253679	0.167128	0.0254	0.0000	0	106
H25	H28	4.258136	0.166873	0.0248	0.0000	0	106
H24	H25	4.266633	0.164961	0.0220	0.0000	0	106
H31	H36	4.288137	0.700893	0.1909	0.0000	0	106
C11	H25	4.290506	0.644419	0.0442	0.0000	0	106
Si1	C12	4.293002	0.106702	0.0146	0.0000	0	106
Cl20	H35	4.294029	0.413805	-0.0655	0.0000	0	106
Si2	C10	4.303808	0.267711	0.0216	0.0000	0	106
H33	H39	4.318182	0.557222	-0.0225	0.0000	0	106
C5	C10	4.324391	0.197086	0.0219	0.0000	0	106
C15	Cl21	4.327657	0.548171	-0.0117	0.0000	0	106
C10	H31	4.331363	0.453197	-0.1173	0.0000	0	106
C8	H30	4.348495	0.906521	0.1637	0.0000	0	106
Si2	H31	4.349562	0.391496	0.1505	0.0000	0	106
H32	H37	4.359553	0.670170	-0.0726	0.0000	0	106
H33	H37	4.370433	0.839976	0.0875	0.0000	0	106
C11	H27	4.380966	0.690312	0.0080	0.0000	0	106

C8	C14	4.388981	0.141250	0.0289	0.0000	0	106
C17	Cl19	4.39358	0.576068	0.0065	0.0000	0	107
Si1	H34	4.398589	0.190330	0.0530	0.0000	0	106
H31	H39	4.407031	0.795230	0.2291	0.0000	0	106
C13	H28	4.414736	0.671318	-0.0323	0.0000	0	106
Si1	C15	4.415508	0.239793	0.0211	0.0000	0	106
C13	C17	4.422696	0.640340	0.0099	0.0000	0	106
Cl21	H25	4.423725	0.857616	0.0369	0.0000	0	107
C9	C18	4.424838	0.468903	-0.0095	0.0000	0	107
H34	H35	4.430274	0.394300	0.1242	0.0000	0	106
Si2	H37	4.433801	0.330815	0.0061	0.0000	0	106
H35	H38	4.434549	0.311565	0.1200	0.0000	0	106
C15	H38	4.437019	0.629429	0.0254	0.0000	0	107
C3	H39	4.437033	0.402842	0.0531	0.0000	0	106
H30	H39	4.439302	1.163141	0.1447	0.0000	0	106
C12	C18	4.440342	0.607959	0.0059	0.0000	0	106
H25	H34	4.445011	0.551156	0.0195	0.0000	0	107
C9	Cl22	4.453143	0.106133	0.0151	0.0000	0	107
C14	H33	4.454411	0.346260	0.0812	0.0000	0	107
C9	H30	4.460977	0.451509	0.2008	0.0000	0	107
Cl23	H28	4.462521	0.896960	-0.0313	0.0000	0	106
C12	Cl19	4.464783	0.106575	0.0152	0.0000	0	107
H31	H38	4.465482	0.732254	0.3144	0.0000	0	106
C10	Cl21	4.467526	0.105986	0.0153	0.0000	0	107
C11	Cl20	4.47501	0.107607	0.0189	0.0000	0	107
C7	C9	4.482768	0.158463	0.0243	0.0000	0	107
C6	H25	4.483669	0.332698	0.0294	0.0000	0	107
C17	H39	4.490348	0.328866	0.0817	0.0000	0	107
H29	H36	4.493105	0.808529	0.1958	0.0000	0	107
C13	H24	4.498514	0.819585	0.0667	0.0000	0	107
C3	H25	4.499716	0.545407	0.0371	0.0000	0	107
C4	C12	4.506985	0.392516	0.0082	0.0000	0	106
C16	H32	4.510053	0.604665	0.0206	0.0000	0	107
C15	H32	4.51584	0.449298	0.0519	0.0000	0	107
C14	Cl19	4.520164	0.527276	0.0504	0.0000	0	107
C18	Cl21	4.537586	0.781554	-0.0134	0.0000	0	107
Si1	H40	4.539385	0.472883	0.0067	0.0000	0	107
H24	H37	4.543909	1.024776	0.0807	0.0000	0	107
Cl20	H26	4.546365	0.825953	0.0793	0.0000	0	106
C11	H24	4.548037	0.765486	0.0789	0.0000	0	107
C16	Cl22	4.551744	0.695922	-0.0033	0.0000	0	106
H30	H33	4.554921	1.127666	-0.0177	0.0000	0	107
C4	C13	4.557286	0.476420	0.0067	0.0000	0	107
C4	C7	4.560281	0.391072	0.0410	0.0000	0	107
C7	C14	4.566459	0.649034	0.0751	0.0000	0	107
C7	H34	4.569858	0.428661	0.0696	0.0000	0	107
C8	C9	4.573247	0.396526	0.0219	0.0000	0	107
C11	H28	4.58377	0.682349	-0.0290	0.0000	0	107
C18	Cl23	4.588567	0.863660	-0.0313	0.0000	0	107
C3	Cl23	4.600956	0.106281	0.0179	0.0000	0	107
Cl19	H40	4.604778	0.688392	-0.0733	0.0000	0	107
C14	H39	4.607619	0.213593	0.0726	0.0000	0	107
C14	H40	4.608231	0.386944	0.0315	0.0000	0	107
C11	H26	4.623785	0.850983	0.0534	0.0000	0	107
C13	C15	4.626304	0.639158	0.0203	0.0000	0	107
H24	H35	4.627351	0.816342	0.0975	0.0000	0	107
C5	H33	4.629439	0.562949	0.0040	0.0000	0	107
C6	H37	4.630472	0.572677	-0.0173	0.0000	0	107
C3	H32	4.63113	0.540837	0.0157	0.0000	0	107
C3	C8	4.632559	0.249708	0.0171	0.0000	0	107
C3	H26	4.636833	0.578132	0.0339	0.0000	0	107
Si1	H25	4.646859	0.411119	0.0275	0.0000	0	107
C16	Cl20	4.651963	0.831083	0.0739	0.0000	0	107
C9	H36	4.68428	0.218163	0.0560	0.0000	0	107
C8	H31	4.688951	0.809561	0.2229	0.0000	0	107

C3	C6	4.691198	0.322969	0.0317	0.0000	0	107
Cl22	H24	4.695798	0.840074	0.0178	0.0000	0	107
C10	C15	4.698729	0.534499	0.0355	0.0000	0	107
C9	H27	4.702707	0.637684	0.0098	0.0000	0	107
C7	H38	4.706761	0.353483	0.0808	0.0000	0	107
C3	C17	4.707423	0.487476	0.0219	0.0000	0	107
Cl23	H26	4.711654	1.125602	0.0481	0.0000	0	107
C17	H40	4.715972	0.615720	-0.0032	0.0000	0	107
C10	H35	4.725099	0.390187	0.0028	0.0000	0	107
C8	H24	4.728733	0.248824	0.0447	0.0000	0	107
C10	C18	4.734609	0.631493	0.0292	0.0000	0	107
Si2	C18	4.735264	0.120432	0.0201	0.0000	0	107
C16	Cl23	4.736508	0.855552	-0.0084	0.0000	0	107
C11	H31	4.747002	1.043644	-0.0137	0.0000	0	107
C9	H37	4.747659	0.352009	0.0308	0.0000	0	107
H29	H33	4.749767	0.905965	0.0197	0.0000	0	107
Cl20	H32	4.752457	1.085508	0.0460	0.0000	0	107
H29	H40	4.754371	1.083739	-0.2194	0.0000	0	107
Cl19	H27	4.769017	0.698563	0.0104	0.0000	0	107
C8	C17	4.769661	0.307934	0.0089	0.0000	0	107
C3	C18	4.779852	0.468018	0.0170	0.0000	0	107
C5	C6	4.780465	0.335204	0.0300	0.0000	0	107
C8	H35	4.7934	0.336384	0.0563	0.0000	0	107
Si1	C13	4.798728	0.129571	0.0216	0.0000	0	107
Cl21	H28	4.803379	0.942522	0.0003	0.0000	0	107
C4	Cl20	4.811755	0.605402	0.0480	0.0000	0	107
H32	H39	4.812795	0.423354	0.0636	0.0000	0	107
C6	C16	4.825003	0.332993	0.0407	0.0000	0	107
C7	C8	4.827207	0.316336	0.0300	0.0000	0	107
C9	H26	4.829033	0.669671	0.0456	0.0000	0	107
C12	H28	4.829065	0.843170	0.0222	0.0000	0	107
Si2	C11	4.835889	0.336678	0.0258	0.0000	0	107
C12	H36	4.860266	0.247202	0.0563	0.0000	0	107
H27	H39	4.865735	0.431609	0.0900	0.0000	0	107
C14	Cl22	4.866035	0.672620	-0.0007	0.0000	0	107
C5	Cl20	4.883434	0.355252	0.0253	0.0000	0	107
H24	H27	4.889122	0.177626	0.0301	0.0000	0	107
H25	H26	4.892177	0.177478	0.0296	0.0000	0	107
C4	Cl21	4.895162	0.539953	0.0163	0.0000	0	107
C6	H30	4.895214	0.918937	0.0480	0.0000	0	107
Si2	Cl20	4.898587	0.531109	0.0442	0.0000	0	107
Cl20	H31	4.901578	0.804697	-0.0314	0.0000	0	107
C13	H27	4.906132	0.950188	0.0550	0.0000	0	107
C10	H30	4.918998	0.524623	0.1228	0.0000	0	107
C4	C5	4.919801	0.246465	0.0266	0.0000	0	107
C10	H29	4.922698	0.525949	0.0982	0.0000	0	107
H26	H32	4.932422	0.670556	0.0115	0.0000	0	107
C12	C17	4.933379	0.754873	0.0415	0.0000	0	107
C6	H29	4.941418	0.694436	-0.0045	0.0000	0	107
C16	H34	4.944451	0.654636	0.0721	0.0000	0	107
C12	H37	4.962491	0.513121	0.0134	0.0000	0	108
C12	C15	4.96486	0.621174	0.0352	0.0000	0	107
C5	C11	4.970185	0.299384	0.0287	0.0000	0	107
H25	H32	4.981136	0.452688	0.0705	0.0000	0	107
Si2	H26	4.98703	0.195315	0.0335	0.0000	0	107
C10	H32	4.990748	0.772120	0.0197	0.0000	0	107
C8	H36	4.998302	0.497352	0.0268	0.0000	0	107
Cl19	H24	5.00934	0.664030	0.0807	0.0000	0	108
H36	H38	5.015967	0.580195	0.0856	0.0000	0	107
Si1	C16	5.020833	0.386797	0.0426	0.0000	0	107
C16	Cl21	5.020889	0.907196	0.0446	0.0000	0	108
H24	H40	5.027459	0.399464	0.0543	0.0000	0	108
Si2	H27	5.034655	0.204963	0.0206	0.0000	0	108
C7	C12	5.044782	0.236191	0.0166	0.0000	0	108
C10	C17	5.045876	0.644465	0.0453	0.0000	0	107

C7	Cl19	5.052231	0.223985	0.0235	0.0000	0	108
C17	Cl23	5.053516	0.930435	0.0219	0.0000	0	107
C4	H29	5.060135	0.546886	-0.1159	0.0000	0	108
C11	H39	5.060428	0.678614	0.1059	0.0000	0	108
C3	H38	5.069165	0.355396	0.0644	0.0000	0	108
C5	H40	5.084022	0.848386	0.0184	0.0000	0	108
C15	H33	5.099947	0.273443	0.0662	0.0000	0	108
C16	H36	5.102555	0.871213	0.1470	0.0000	0	108
C4	H35	5.106295	0.395026	0.0628	0.0000	0	108
H24	H39	5.108141	0.352702	0.0748	0.0000	0	108
C3	H33	5.125204	0.518828	0.0617	0.0000	0	108
C5	H32	5.126405	0.563213	0.0653	0.0000	0	108
C18	Cl19	5.145304	0.662762	0.0318	0.0000	0	108
C9	H28	5.148549	0.625669	0.0067	0.0000	0	108
C9	H38	5.153255	0.538326	0.0686	0.0000	0	108
H27	H40	5.162978	0.747886	-0.0128	0.0000	0	108
C11	H29	5.170426	0.798294	-0.0066	0.0000	0	108
C16	Cl19	5.177726	0.646276	0.0515	0.0000	0	108
C14	Cl21	5.186335	0.750898	0.0453	0.0000	0	108
C18	Cl22	5.203638	0.953136	0.0497	0.0000	0	107
C13	H25	5.232306	0.838875	0.0626	0.0000	0	108
C14	H38	5.236452	0.439886	0.0364	0.0000	0	108
H25	H33	5.243223	0.432119	0.0605	0.0000	0	108
C14	H37	5.246148	0.932242	0.0702	0.0000	0	108
H30	H32	5.247898	0.998344	0.0580	0.0000	0	108
Cl20	H30	5.256461	0.663396	0.0222	0.0000	0	108
C14	H35	5.27795	0.669578	0.0896	0.0000	0	108
Cl23	H27	5.282801	1.265287	0.0769	0.0000	0	108
C7	H39	5.292372	0.596185	0.0021	0.0000	0	108
C8	H27	5.299046	0.423242	0.0092	0.0000	0	108
Si2	C12	5.303676	0.379174	0.0299	0.0000	0	108
C9	H35	5.309027	0.359993	0.0321	0.0000	0	108
C6	C10	5.312879	0.591588	0.0524	0.0000	0	108
H26	H36	5.313243	1.027986	0.1699	0.0000	0	108
Cl21	Cl22	5.325896	0.141715	0.0207	0.0000	0	108
C6	Cl20	5.331007	0.944448	0.0856	0.0000	0	108
C17	H34	5.332138	0.590319	0.0361	0.0000	0	108
Cl22	H28	5.333655	1.220744	0.0759	0.0000	0	108
Cl20	Cl23	5.342606	0.143617	0.0207	0.0000	0	108
Cl19	Cl23	5.344769	0.143141	0.0200	0.0000	0	108
H30	H40	5.351192	1.222805	0.2111	0.0000	0	108
C14	Cl23	5.356663	0.805269	0.0188	0.0000	0	108
C10	H25	5.36431	0.657848	0.0588	0.0000	0	108
Cl21	H39	5.373169	0.877870	0.1306	0.0000	0	108
C6	C17	5.37323	0.269163	0.0393	0.0000	0	108
C6	C9	5.374266	0.313072	0.0391	0.0000	0	108
C10	H28	5.374281	0.798770	0.0465	0.0000	0	108
H25	H29	5.375576	0.943021	-0.2027	0.0000	0	108
H35	H39	5.37716	0.635021	0.0271	0.0000	0	108
C4	H37	5.38523	0.634229	0.0337	0.0000	0	108
C4	H31	5.385907	0.740911	0.1388	0.0000	0	108
C12	H31	5.4019	0.651983	-0.1157	0.0000	0	108
H24	H38	5.415693	0.435923	0.0548	0.0000	0	108
C6	H26	5.417248	0.455104	0.0527	0.0000	0	108
C9	H40	5.41774	0.622340	-0.0382	0.0000	0	108
Cl19	Cl20	5.437706	0.147421	0.0235	0.0000	0	108
Cl19	H36	5.447942	0.327180	0.0464	0.0000	0	108
H29	H32	5.449951	0.742972	0.0618	0.0000	0	108
H31	H33	5.450308	0.677821	0.1970	0.0000	0	108
C5	H24	5.451768	0.562420	0.0774	0.0000	0	108
C6	Cl19	5.454879	0.394550	0.0410	0.0000	0	108
Si1	C17	5.476911	0.351750	0.0346	0.0000	0	108
C9	H32	5.480745	0.523425	0.0346	0.0000	0	108
Cl19	H37	5.482347	0.341288	0.0355	0.0000	0	108
C3	H34	5.495048	0.394550	0.0715	0.0000	0	108

C3	H27	5.496209	0.654519	0.0432	0.0000	0	108
C17	H32	5.498185	0.558933	0.0587	0.0000	0	108
C5	C12	5.507249	0.261713	0.0346	0.0000	0	108
C15	H36	5.515474	0.500757	0.0927	0.0000	0	108
C3	H40	5.521632	0.486649	-0.0201	0.0000	0	108
C8	C16	5.52222	0.204012	0.0334	0.0000	0	108
C18	H32	5.524264	0.623291	0.0447	0.0000	0	108
C4	H30	5.53177	0.542923	0.1346	0.0000	0	108
Si1	Cl21	5.542262	0.172150	0.0242	0.0000	0	108
C5	H25	5.54834	0.684003	0.0371	0.0000	0	108
Si2	C13	5.553065	0.390270	0.0321	0.0000	0	108
H26	H34	5.557842	0.804318	0.0947	0.0000	0	108
C18	H39	5.560696	0.287075	0.0949	0.0000	0	108
C6	H31	5.562811	0.393916	0.1923	0.0000	0	108
C5	C14	5.574024	0.344300	0.0547	0.0000	0	108
C3	H28	5.578219	0.608549	0.0340	0.0000	0	108
C16	H39	5.583169	0.233021	0.0907	0.0000	0	108
Si1	H26	5.599073	0.539435	0.0594	0.0000	0	108
H35	H40	5.603944	0.606488	0.0723	0.0000	0	108
H36	H39	5.606137	0.757080	-0.0359	0.0000	0	108
Cl19	H35	5.608082	0.360786	0.0327	0.0000	0	108
C13	H31	5.609548	0.890076	-0.0817	0.0000	0	108
C15	H29	5.610524	0.746459	-0.1613	0.0000	0	108
Cl21	H26	5.613736	1.112001	0.0945	0.0000	0	108
C5	C15	5.62471	0.474126	0.0350	0.0000	0	108
Cl20	H29	5.625408	0.497111	0.1625	0.0000	0	108
C12	H27	5.638327	0.982650	0.0787	0.0000	0	108
C16	H40	5.644487	0.496001	0.0281	0.0000	0	108
H34	H37	5.64467	0.650239	0.0507	0.0000	0	108
C6	C18	5.649582	0.310536	0.0456	0.0000	0	108
C7	H40	5.651436	0.550373	0.0608	0.0000	0	108
C15	Cl23	5.65184	0.844582	0.0325	0.0000	0	108
H36	H40	5.65239	0.717768	0.0846	0.0000	0	108
C5	H34	5.655486	0.402793	0.0750	0.0000	0	108
C18	H34	5.655639	0.658006	0.0563	0.0000	0	108
C8	C11	5.661657	0.531034	0.0383	0.0000	0	108
H37	H38	5.666487	0.539277	0.0809	0.0000	0	108
C7	C11	5.676132	0.189270	0.0368	0.0000	0	108
Cl20	H33	5.68504	1.128645	0.1322	0.0000	0	108
Cl21	H31	5.691392	1.410806	0.0537	0.0000	0	108
Cl22	H36	5.692102	0.338276	0.0567	0.0000	0	108
C12	H25	5.694969	0.761994	0.0671	0.0000	0	108
Si1	Cl22	5.700554	0.169772	0.0221	0.0000	0	108
C10	H39	5.702168	0.463347	0.0693	0.0000	0	108
C8	C18	5.705426	0.274552	0.0255	0.0000	0	108
C18	H40	5.71681	0.598404	0.0123	0.0000	0	108
H29	H34	5.721885	0.828254	-0.0011	0.0000	0	108
C11	H36	5.743907	0.245702	0.0762	0.0000	0	108
C18	Cl20	5.747853	0.917658	0.0943	0.0000	0	108
H31	H40	5.755949	1.314269	0.2376	0.0000	0	108
Si1	C18	5.760225	0.382503	0.0424	0.0000	0	108
Cl23	H24	5.765857	0.985345	0.0688	0.0000	0	108
C7	C16	5.771903	0.768335	0.0965	0.0000	0	108
C8	H37	5.776933	0.481259	0.0501	0.0000	0	108
H30	H34	5.781929	1.072213	0.1149	0.0000	0	108
C4	Cl22	5.782359	0.643898	0.0283	0.0000	0	108
C11	H30	5.782637	0.567651	0.2371	0.0000	0	108
C7	C15	5.793639	0.374577	0.0597	0.0000	0	108
C16	H33	5.794687	0.385990	0.1040	0.0000	0	108
Si2	H28	5.796257	0.173894	0.0356	0.0000	0	108
C5	C13	5.800224	0.292465	0.0378	0.0000	0	108
C8	C10	5.807572	0.305622	0.0364	0.0000	0	108
C10	H33	5.808086	0.747569	0.0978	0.0000	0	108
Cl22	H37	5.811441	0.571773	0.0006	0.0000	0	108
C17	H38	5.828595	0.719670	0.0256	0.0000	0	108

Si2	Cl21	5.830788	0.476979	0.0354	0.0000	0	108
C4	Cl23	5.835048	0.665615	0.0224	0.0000	0	108
C13	H36	5.835172	0.265517	0.0798	0.0000	0	108
H31	H32	5.84543	0.619328	0.1940	0.0000	0	108
C11	H37	5.848742	0.454311	0.0402	0.0000	0	108
C15	Cl20	5.854108	0.706196	0.0745	0.0000	0	108
Cl19	H33	5.854745	0.496001	0.0535	0.0000	0	108
Cl19	H32	5.86409	0.480152	0.0571	0.0000	0	109
H25	H31	5.867789	1.359288	0.2392	0.0000	0	108
C10	H27	5.88138	0.816365	0.0726	0.0000	0	108
Cl21	H24	5.883122	0.902184	0.0887	0.0000	0	109
H24	H29	5.88995	0.580967	0.0333	0.0000	0	108
C14	H29	5.89178	0.496636	-0.0342	0.0000	0	108
C9	H33	5.892273	0.405805	0.0675	0.0000	0	108
H24	H31	5.90246	0.670688	0.1218	0.0000	0	108
C7	C13	5.929323	0.236485	0.0363	0.0000	0	109
H24	H30	5.934126	0.698428	0.1160	0.0000	0	108
Cl19	H28	5.934826	0.801812	0.0467	0.0000	0	109
C13	H37	5.957205	0.547624	0.0355	0.0000	0	109
C15	H31	5.959241	1.123255	0.1843	0.0000	0	108
C14	H31	5.988016	0.655512	0.1098	0.0000	0	109
Cl21	H29	6.007327	0.926234	-0.0671	0.0000	0	109
C5	Cl21	6.008436	0.426876	0.0327	0.0000	0	109
Cl19	H26	6.012693	0.777595	0.0773	0.0000	0	109
Cl19	H34	6.014538	0.517228	0.0591	0.0000	0	109
C12	H29	6.024581	0.692087	0.0886	0.0000	0	109
C9	H34	6.031724	0.432554	0.0670	0.0000	0	109
C17	Cl22	6.034795	1.000721	0.0758	0.0000	0	108
C12	H32	6.043245	0.948780	0.0310	0.0000	0	109
H25	H36	6.044468	0.529253	0.0852	0.0000	0	109
C7	Cl22	6.048101	0.312140	0.0141	0.0000	0	109
C7	H26	6.091697	0.982850	0.1153	0.0000	0	109
C10	H34	6.096926	0.694091	0.0997	0.0000	0	109
C12	H35	6.107074	0.463117	0.0217	0.0000	0	109
H37	H39	6.115418	0.739016	0.0453	0.0000	0	109
C12	H30	6.147853	0.653340	0.1766	0.0000	0	109
C14	H30	6.155731	0.536100	0.1387	0.0000	0	109
C13	H29	6.155763	0.790789	0.0421	0.0000	0	109
H27	H34	6.159204	0.668371	0.0433	0.0000	0	109
C7	H25	6.168342	0.408505	0.0623	0.0000	0	109
Cl19	Cl22	6.171934	0.131937	0.0285	0.0000	0	109
Cl20	H34	6.178158	1.069862	0.1486	0.0000	0	109
Cl20	Cl21	6.179067	0.134108	0.0328	0.0000	0	109
C8	Cl21	6.209569	0.776426	0.0492	0.0000	0	109
C13	H39	6.224244	0.611922	0.1094	0.0000	0	109
H25	H30	6.237288	0.882978	0.1958	0.0000	0	109
C17	Cl20	6.256197	0.877634	0.0942	0.0000	0	109
Cl23	H25	6.263405	1.032118	0.0761	0.0000	0	109
C18	H36	6.263977	0.762565	0.1439	0.0000	0	109
C6	H27	6.266493	0.337025	0.0543	0.0000	0	109
C15	Cl22	6.287092	0.843230	0.0598	0.0000	0	109
C10	H38	6.29253	0.445080	0.0778	0.0000	0	109
C17	H33	6.307376	0.288759	0.0916	0.0000	0	109
Si1	H27	6.312803	0.464954	0.0493	0.0000	0	109
C15	H30	6.319505	0.660355	0.1824	0.0000	0	109
C16	H37	6.322543	1.106103	0.0978	0.0000	0	109
C15	H35	6.328717	0.420195	0.0827	0.0000	0	109
H26	H33	6.356613	0.457298	0.1229	0.0000	0	110
C11	H38	6.360597	0.615909	0.0791	0.0000	0	110
H27	H38	6.364315	0.731790	0.0252	0.0000	0	110
C11	H40	6.370133	0.662742	-0.0201	0.0000	0	110
Cl20	H28	6.375182	1.082387	0.1147	0.0000	0	109
C6	C12	6.387994	0.677724	0.0653	0.0000	0	109
C17	H36	6.409921	0.502999	0.1232	0.0000	0	110
H31	H34	6.433296	0.394618	0.2581	0.0000	0	110

C6	C11	6.438644	0.379337	0.0553	0.0000	0	110
C16	H38	6.454583	0.469466	0.0395	0.0000	0	110
C11	H32	6.458128	0.576292	0.0464	0.0000	0	110
C8	H26	6.466529	0.205727	0.0529	0.0000	0	110
H27	H32	6.46941	0.513470	0.0817	0.0000	0	110
C12	H39	6.475404	0.432254	0.0949	0.0000	0	110
Si1	Cl23	6.497804	0.141349	0.0350	0.0000	0	110
H28	H32	6.501388	0.592422	0.0583	0.0000	0	110
H28	H39	6.523843	0.292461	0.1165	0.0000	0	110
H26	H37	6.529974	1.086083	0.1144	0.0000	0	110
C13	H30	6.53927	0.550823	0.2273	0.0000	0	110
C16	H35	6.557357	0.695002	0.1146	0.0000	0	110
C15	H37	6.572701	0.538089	0.0606	0.0000	0	110
H26	H39	6.577126	0.245769	0.1087	0.0000	0	110
C11	H35	6.577344	0.346511	0.0436	0.0000	0	110
H25	H35	6.581901	0.395184	0.0874	0.0000	0	110
Cl20	H25	6.590565	0.630483	0.0883	0.0000	0	110
C10	H40	6.600036	0.432820	0.0073	0.0000	0	110
C8	Cl20	6.604398	0.427443	0.0604	0.0000	0	110
H26	H40	6.608207	0.438480	0.0482	0.0000	0	110
C18	H33	6.629554	0.274916	0.1072	0.0000	0	110
H37	H40	6.641753	0.494086	0.0835	0.0000	0	110
H28	H34	6.650874	0.633595	0.0725	0.0000	0	110
C6	H28	6.674644	0.315949	0.0641	0.0000	0	110
C8	C13	6.676858	0.429283	0.0479	0.0000	0	110
Si2	Cl22	6.681973	0.448809	0.0464	0.0000	0	110
C5	C16	6.701422	0.353444	0.0679	0.0000	0	110
H28	H40	6.711257	0.570349	0.0217	0.0000	0	110
C8	C12	6.716638	0.337738	0.0477	0.0000	0	110
Si1	H28	6.720243	0.405937	0.0607	0.0000	0	110
C13	H32	6.727823	0.723725	0.0433	0.0000	0	110
C8	H28	6.728403	0.280576	0.0411	0.0000	0	110
Cl22	H27	6.730065	1.038259	0.1166	0.0000	0	110
C18	H38	6.733503	0.572613	0.0332	0.0000	0	110
C5	C17	6.744353	0.462250	0.0519	0.0000	0	110
Cl20	H39	6.757103	0.524789	0.0705	0.0000	0	110
C17	H29	6.777134	0.696700	-0.1324	0.0000	0	110
C7	C17	6.787593	0.433245	0.0834	0.0000	0	110
Cl21	H40	6.799883	0.844134	-0.0200	0.0000	0	110
C7	C18	6.806866	0.581244	0.0966	0.0000	0	110
Cl21	H30	6.845937	0.536816	0.2730	0.0000	0	110
Cl22	H31	6.849275	0.574311	-0.1041	0.0000	0	110
C6	C13	6.912065	0.498613	0.0661	0.0000	0	110
H26	H35	6.924828	0.866631	0.1353	0.0000	0	110
Cl20	H38	6.931906	0.519554	0.1051	0.0000	0	110
C13	H35	6.938341	0.374526	0.0417	0.0000	0	110
Cl22	H32	6.945579	0.995812	0.0370	0.0000	0	110
Cl21	H38	6.96221	0.827296	0.0905	0.0000	0	110
C17	H31	6.97948	1.071368	0.1662	0.0000	0	110
C5	Cl22	6.979711	0.241071	0.0497	0.0000	0	111
H25	H37	6.984842	0.475975	0.0681	0.0000	0	110
C12	H33	6.993823	0.664016	0.1180	0.0000	0	110
C11	H34	7.001362	0.506678	0.0815	0.0000	0	110
C16	H31	7.002168	0.686371	0.1032	0.0000	0	110
C16	H29	7.009871	0.508093	-0.0263	0.0000	0	110
C12	H34	7.058765	0.680853	0.1102	0.0000	0	110
C11	H33	7.061291	0.366402	0.0953	0.0000	0	111
Si2	Cl23	7.075907	0.399397	0.0478	0.0000	0	111
Cl22	H35	7.129711	0.400037	0.0155	0.0000	0	111
Cl22	H25	7.13136	0.748203	0.0899	0.0000	0	110
H28	H36	7.168368	0.621029	0.1695	0.0000	0	111
H27	H33	7.171323	0.275856	0.1065	0.0000	0	111
C7	Cl21	7.180101	0.164977	0.0517	0.0000	0	111
Cl20	H27	7.195889	0.719631	0.1188	0.0000	0	111
Cl23	H31	7.205023	0.781402	-0.0715	0.0000	0	111

C5	C18	7.247634	0.359240	0.0645	0.0000	0	111
Cl21	H36	7.295951	0.227770	0.0930	0.0000	0	111
C12	H38	7.333847	0.436869	0.0843	0.0000	0	111
C16	H30	7.334538	0.391212	0.1793	0.0000	0	111
C5	H26	7.340349	0.420883	0.0925	0.0000	0	111
C13	H40	7.34333	0.558107	0.0002	0.0000	0	111
H26	H38	7.352826	0.421138	0.0580	0.0000	0	111
H27	H29	7.358364	0.749813	-0.1451	0.0000	0	111
Cl20	H40	7.369189	0.426893	0.0487	0.0000	0	111
C18	H37	7.385075	0.759405	0.0978	0.0000	0	111
C13	H38	7.387561	0.533425	0.0840	0.0000	0	111
C5	H27	7.411177	0.545830	0.0657	0.0000	0	111
H27	H36	7.413336	0.435462	0.1401	0.0000	0	111
Cl21	H37	7.414703	0.373947	0.0561	0.0000	0	111
Cl23	H36	7.415635	0.249128	0.1054	0.0000	0	111
C12	H40	7.424748	0.456691	0.0117	0.0000	0	111
C18	H29	7.426949	0.553887	-0.0731	0.0000	0	111
C17	H35	7.435566	0.424591	0.1056	0.0000	0	111
C5	Cl23	7.453378	0.260893	0.0541	0.0000	0	111
C17	H37	7.465762	0.604403	0.0856	0.0000	0	111
C6	Cl22	7.47387	0.694181	0.0874	0.0000	0	111
C17	H30	7.476306	0.469864	0.2140	0.0000	0	111
C18	H31	7.478555	0.816059	0.1240	0.0000	0	111
C13	H34	7.491189	0.570896	0.1005	0.0000	0	111
Cl22	H30	7.531809	0.648508	0.1650	0.0000	0	112
C6	Cl21	7.560678	0.467292	0.0687	0.0000	0	112
C18	H35	7.562853	0.550946	0.1174	0.0000	0	111
Cl22	H29	7.57296	0.603504	0.1302	0.0000	0	112
Cl23	H37	7.574093	0.553250	0.0498	0.0000	0	112
C13	H33	7.57526	0.481758	0.1162	0.0000	0	111
H27	H31	7.584064	1.144862	0.1964	0.0000	0	111
C7	Cl23	7.585516	0.244222	0.0549	0.0000	0	112
Cl23	H39	7.591353	0.526263	0.1374	0.0000	0	111
H26	H31	7.612036	0.747367	0.1020	0.0000	0	112
H28	H33	7.657993	0.333030	0.1314	0.0000	0	112
Cl21	H32	7.721248	0.611005	0.0709	0.0000	0	112
C7	H27	7.72889	0.460842	0.1019	0.0000	0	112
H26	H29	7.733434	0.585653	0.0297	0.0000	0	112
C7	H28	7.737068	0.683312	0.1190	0.0000	0	112
H28	H38	7.77134	0.648358	0.0453	0.0000	0	112
Cl23	H29	7.77242	0.751868	0.0409	0.0000	0	112
H26	H30	7.933163	0.564501	0.1914	0.0000	0	112
C18	H30	7.952754	0.468042	0.2122	0.0000	0	112
Cl21	H34	7.989165	0.641908	0.0854	0.0000	0	112
Cl21	H35	7.997598	0.373084	0.0590	0.0000	0	112
Cl22	H39	8.082571	0.478243	0.1160	0.0000	0	112
Cl22	H33	8.086752	0.914332	0.1493	0.0000	0	112
Cl22	H34	8.107824	0.964137	0.1434	0.0000	0	112
C8	Cl23	8.116772	0.570351	0.0669	0.0000	0	112
H27	H30	8.166977	0.675211	0.2474	0.0000	0	112
Cl23	H32	8.181825	0.880729	0.0613	0.0000	0	112
C5	H28	8.183119	0.504946	0.0860	0.0000	0	112
Cl23	H30	8.191766	0.629157	0.2619	0.0000	0	112
Cl21	H33	8.203272	0.460091	0.1088	0.0000	0	112
C8	Cl22	8.231831	0.427239	0.0712	0.0000	0	112
H28	H37	8.250602	0.965337	0.1187	0.0000	0	112
H27	H35	8.353282	0.531048	0.1258	0.0000	0	112
H28	H31	8.356613	1.042444	0.1281	0.0000	0	112
H28	H29	8.369749	0.721565	-0.0482	0.0000	0	112
H27	H37	8.399597	0.688712	0.1062	0.0000	0	112
C6	Cl23	8.401293	0.645658	0.0873	0.0000	0	112
H28	H35	8.533335	0.737766	0.1410	0.0000	0	112
Cl23	H35	8.611403	0.418088	0.0589	0.0000	0	112
Cl23	H40	8.681265	0.767169	0.0168	0.0000	0	112
Cl22	H38	8.849996	0.603654	0.1049	0.0000	0	112

Cl22	H40	8.877232	0.551450	0.0423	0.0000	0	112
Cl23	H34	8.884554	0.834075	0.1206	0.0000	0	112
H28	H30	8.900725	0.525347	0.2464	0.0000	0	112
Cl23	H38	8.905242	0.780220	0.0985	0.0000	0	112
Cl23	H33	9.128679	0.637707	0.1456	0.0000	0	112

Table S11. Z-Matrix used in the refinement of the gas-phase structure of the *syn*-conformer $C_6Cl_5Me_2SiSiMe_2C_6F_5$ (**5**). Distances *r* are given in Å, angles *a* and dihedrals *d* are given in deg. The numbers written in line with the parameter indicate the groups they were refined in.

1	Si							
2	Si	1	rsisi					
3	C	1	rsic1	2	asisic1			
4	C	2	rsic2	1	asisic2	3	dcsisic	
5	C	1	rsic3	2	asisic3	3	acsic1	1
6	C	2	rsic4	1	asisic4	4	acsic2	1
7	C	1	rsic5	2	asisic5	3	acsic3	-1
8	C	2	rsic6	1	asisic6	4	acsic4	-1
9	C	3	rcc1	1	asicc1	2	dsisicc1	
10	C	3	rcc2	1	asicc2	2	dsisicc3	
11	C	9	rcc3	3	accc2	10	0	
12	C	10	rcc4	3	accc3	9	0	
13	C	11	rcc5	12	rcc6	9	180	4
14	C	4	rcc7	2	asicc3	1	dsisicc2	
15	C	4	rcc8	2	asicc4	1	dsisicc4	
16	C	14	rcc9	4	accc5	15	0	
17	C	15	rcc10	4	accc6	14	0	
18	C	16	rcc11	17	rcc12	14	180	4
19	Cl	9	rcl1	3	acccl1	10	180	
20	Cl	10	rcl2	3	acccl2	9	180	
21	Cl	11	rcl3	9	acccl3	3	180	
22	Cl	12	rcl4	10	acccl4	3	180	
23	Cl	13	rcl5	3	acccl5	1	dsicccl	
24	F	14	rf1	4	accf1	15	180	
25	F	15	rf2	4	accf2	14	180	
26	F	16	rf3	14	accf3	4	180	
27	F	17	rf4	15	accf4	4	180	
28	F	18	rf5	4	accf5	2	dsiccf	
29	H	5	rch1	1	asich1	3	dcsich1	
30	H	5	rch2	1	asich2	3	dcsich2	
31	H	5	rch3	1	asich3	3	dcsich3	
32	H	6	rch4	2	asich4	4	dcsich4	
33	H	6	rch5	2	asich5	4	dcsich5	
34	H	6	rch6	2	asich6	4	dcsich6	
35	H	7	rch7	1	asich7	3	dcsich7	
36	H	7	rch8	1	asich8	3	dcsich8	
37	H	7	rch9	1	asich9	3	dcsich9	
38	H	8	rch10	2	asich10	4	dcsich10	
39	H	8	rch11	2	asich11	4	dcsich11	
40	H	8	rch12	2	asich12	4	dcsich12	

Variables:

rsisi	2.39254462	3
rsic1	1.91065594	2
rsic2	1.88956694	2
rsic3	1.85869894	2
rsic4	1.85419094	2
rsic5	1.85965094	2
rsic6	1.86012894	2
rcc1	1.40472562	3
rcc2	1.40576762	3
rcc3	1.40559562	3
rcc4	1.40031262	3
rcc5	1.40200362	3
rcc6	1.40189962	3
rcc7	1.39452462	3
rcc8	1.39586462	3
rcc9	1.39467262	3
rcc10	1.39079262	3
rcc11	1.39351062	3
rcc12	1.39459662	3

rcl1	1.71882668	4
rcl2	1.72454168	4
rcl3	1.70735168	4
rcl4	1.70856968	4
rcl5	1.70496568	4
rf1	1.34215162	3
rf2	1.34845162	3
rf3	1.33430762	3
rf4	1.33486962	3
rf5	1.33067462	3
rch1	1.09047774	10
rch2	1.09656974	10
rch3	1.09164774	10
rch4	1.09010274	10
rch5	1.09497374	10
rch6	1.09340574	10
rch7	1.09472074	10
rch8	1.09482074	10
rch9	1.08920274	10
rch10	1.09444074	10
rch11	1.09440374	10
rch12	1.09158874	10
asisic1	105.76858736	6
asisic2	106.90858736	6
asisic3	107.05958736	6
acsic1	119.86609488	7
asisic4	116.34958736	6
acsic2	116.14009488	7
asisic5	117.49358736	6
acsic3	114.82209488	7
asisic6	111.40758736	6
acsic4	111.43909488	7
asicc1	125.71431275	8
asicc2	117.63731275	8
accc2	122.37631275	8
accc3	123.28231275	8
asicc3	125.29031275	8
asicc4	118.38331275	8
accc5	122.60231275	8
accc6	123.38431275	8
acccl1	119.90922598	9
acccl2	118.76722598	9
acccl3	120.36822598	9
acccl4	120.56722598	9
acccl5	177.09722598	9
accf1	120.10522598	9
accf2	118.93722598	9
accf3	120.31822598	9
accf4	120.68022598	9
accf5	179.00222598	9
asich1	113.02500000	
asich2	106.22400000	
asich3	112.45000000	
asich4	112.71800000	
asich5	108.48700000	
asich6	110.71500000	
asich7	109.40200000	
asich8	108.74100000	
asich9	113.80300000	
asich10	109.92500000	
asich11	110.21500000	
asich12	112.01100000	
dcsisic	9.85967593	20
dsisicc1	116.93447386	21
dsisicc3	-52.71082614	21

dsisicc2	116.92291914	22
dsisicc4	-55.45408086	22
dsicccl	41.00000000	
dsiccf	20.30000000	
dcsich1	54.65760000	
dcsich2	172.92180000	
dcsich3	-69.08060000	
dcsich4	59.79410000	
dcsich5	179.87160000	
dcsich6	-61.67880000	
dcsich7	59.99600000	
dcsich8	177.31900000	
dcsich9	-61.51200000	
dcsich10	62.02370000	
dcsich11	-179.17010000	
dcsich12	-58.57400000	

Table S12. Cartesian coordinates for the refined structure of the *syn*−conformer $C_6Cl_5Me_2SiSiMe_2C_6F_5$ (**5**).

N	At	An	Mass	*X*	*Y*	*Z*
1	Si	14	27.97692653	0.512391090783	2.748556954851	-0.656921045490
2	Si	14	27.97692653	2.374178662160	1.867306532899	0.560212682553
3	C	6	12.00000000	-0.782519791836	1.344761075277	-0.713215377302
4	C	6	12.00000000	2.062584046613	0.016249354366	0.776913707733
5	C	6	12.00000000	0.075951083762	4.379774261160	0.119874915945
6	C	6	12.00000000	4.057979580775	2.346212888905	-0.050923314515
7	C	6	12.00000000	0.862103053573	3.554265710534	-2.296078316472
8	C	6	12.00000000	2.577140639582	2.719299387746	2.201247197945
9	C	6	12.00000000	-2.063519030783	1.387273681522	-0.138334774415
10	C	6	12.00000000	-0.362799426887	0.088988852325	-1.185500834122
11	C	6	12.00000000	-2.881532962333	0.248661752938	-0.037760708129
12	C	6	12.00000000	-1.150367732208	-1.065849103553	-1.102068791261
13	C	6	12.00000000	-2.423935854189	-0.985036748192	-0.521710144912
14	C	6	12.00000000	2.858566429609	-1.001557532278	0.252337578725
15	C	6	12.00000000	0.869650288744	-0.390024700871	1.377154068451
16	C	6	12.00000000	2.497017433817	-2.347018389288	0.316595922552
17	C	6	12.00000000	0.470254472405	-1.719451787702	1.463239644386
18	C	6	12.00000000	1.296193371380	-2.706197222675	0.925598382844
19	Cl	17	34.96885271	-2.679861904184	2.870857667131	0.472783199886
20	Cl	17	34.96885271	1.198311132797	-0.047538495622	-1.905457855306
21	Cl	17	34.96885271	-4.430912754289	0.358832411750	0.670994854797
22	Cl	17	34.96885271	-0.570499614450	-2.558017990332	-1.699057345019
23	Cl	17	34.96885271	-3.383564618281	-2.380295807263	-0.323536570119
24	F	9	18.99840320	4.024009448556	-0.705271625552	-0.343756552735
25	F	9	18.99840320	0.053300739997	0.544666789987	1.904645314010
26	F	9	18.99840320	3.293801038407	-3.284028408061	-0.200632216985
27	F	9	18.99840320	-0.683089852519	-2.047526378618	2.049789595141
28	F	9	18.99840320	0.921789455062	-3.982057488718	0.977533386679
29	H	1	1.00782503	-0.290730480788	4.280887464202	1.142082196324
30	H	1	1.00782503	1.003566132315	4.963927288801	0.147456570188
31	H	1	1.00782503	-0.657633528264	4.937293265001	-0.465548825128
32	H	1	1.00782503	4.288938106899	1.918829235465	-1.026794897645
33	H	1	1.00782503	4.100466873966	3.437335840097	-0.132243776705
34	H	1	1.00782503	4.830407903692	2.028086317895	0.654545376522
35	H	1	1.00782503	-0.060752751323	3.991308189875	-2.690723124103
36	H	1	1.00782503	1.576214851306	4.369698367166	-2.141979755304
37	H	1	1.00782503	1.268463520076	2.873356755817	-3.042802339459
38	H	1	1.00782503	3.447985251631	2.314719443608	2.726361713860
39	H	1	1.00782503	2.741677874884	3.791074211434	2.053106175194
40	H	1	1.00782503	1.700359235788	2.592832922221	2.839076776566

Table S13. Full listing of structural parameters of the *syn* conformer $C_6Cl_5Me_2SiSiMe_2C_6F_5$ (**5**). r_a, r_{h1} and r_e values are given in Å. Errors correspond to one time standard deviation. For atom numbering see Table S11.

No.	Type	i	j	k	l	r_a	r_{h1}	r_e	Error
1	stretch	1	2	0	0	2.39404	2.39689	2.39254	0.00025
2	stretch	1	3	0	0	1.91126	1.91423	1.91066	0.00107
3	stretch	1	5	0	0	1.85880	1.86151	1.85870	0.00107
4	stretch	1	7	0	0	1.85975	1.86247	1.85965	0.00107
5	stretch	2	4	0	0	1.89067	1.89348	1.88957	0.00107
6	stretch	2	6	0	0	1.85429	1.85696	1.85419	0.00107
7	stretch	2	8	0	0	1.86043	1.86314	1.86013	0.00107
8	stretch	3	9	0	0	1.40433	1.40646	1.40473	0.00025
9	stretch	3	10	0	0	1.40487	1.40701	1.40577	0.00025
10	stretch	4	14	0	0	1.39432	1.39638	1.39452	0.00025
11	stretch	4	15	0	0	1.39516	1.39724	1.39586	0.00025
12	stretch	5	29	0	0	1.08908	1.09624	1.09048	0.00271
13	stretch	5	30	0	0	1.09527	1.10257	1.09657	0.00271
14	stretch	5	31	0	0	1.09015	1.09735	1.09165	0.00271
15	stretch	6	32	0	0	1.08870	1.09587	1.09010	0.00271
16	stretch	6	33	0	0	1.09357	1.10084	1.09497	0.00271
17	stretch	6	34	0	0	1.09191	1.09915	1.09341	0.00271
18	stretch	7	35	0	0	1.09322	1.10065	1.09472	0.00271
19	stretch	7	36	0	0	1.09332	1.10073	1.09482	0.00271
20	stretch	7	37	0	0	1.08770	1.09501	1.08920	0.00271
21	stretch	8	38	0	0	1.09304	1.10031	1.09444	0.00271
22	stretch	8	39	0	0	1.09290	1.10018	1.09440	0.00271
23	stretch	8	40	0	0	1.09019	1.09741	1.09159	0.00271
24	stretch	9	11	0	0	1.40530	1.40742	1.40560	0.00025
25	stretch	9	19	0	0	1.71863	1.72095	1.71883	0.00077
26	stretch	10	12	0	0	1.39991	1.40201	1.40031	0.00025
27	stretch	10	20	0	0	1.72444	1.72680	1.72454	0.00077
28	stretch	11	13	0	0	1.40150	1.40359	1.40200	0.00025
29	stretch	11	21	0	0	1.70755	1.70978	1.70735	0.00077
30	stretch	12	13	0	0	1.40140	1.40348	1.40190	0.00025
31	stretch	12	22	0	0	1.70877	1.71101	1.70857	0.00077
32	stretch	13	23	0	0	1.70527	1.70748	1.70497	0.00077
33	stretch	14	16	0	0	1.39437	1.39640	1.39467	0.00025
34	stretch	14	24	0	0	1.34195	1.34395	1.34215	0.00025
35	stretch	15	17	0	0	1.39049	1.39251	1.39079	0.00025
36	stretch	15	25	0	0	1.34825	1.35029	1.34845	0.00025
37	stretch	16	18	0	0	1.39301	1.39502	1.39351	0.00025
38	stretch	16	26	0	0	1.33431	1.33624	1.33431	0.00025
39	stretch	17	18	0	0	1.39410	1.39611	1.39460	0.00025
40	stretch	17	27	0	0	1.33477	1.33671	1.33487	0.00025
41	stretch	18	28	0	0	1.33067	1.33259	1.33067	0.00025
42	bend	2	1	3	0	105.76859			0.25034
43	bend	2	1	5	0	107.05959			0.25034
44	bend	2	1	7	0	117.49359			0.25034
45	bend	1	2	4	0	106.90859			0.25034
46	bend	1	2	6	0	116.34959			0.25034
47	bend	1	2	8	0	111.40759			0.25034
48	bend	3	1	5	0	119.86609			0.37356
49	bend	3	1	7	0	114.82209			0.37356
50	bend	1	3	9	0	125.71431			0.08614
51	bend	1	3	10	0	117.63731			0.08614
52	bend	5	1	7	0	91.85076			0.53150
53	bend	1	5	29	0	113.02500			0.00000
54	bend	1	5	30	0	106.22400			0.00000
55	bend	1	5	31	0	112.45000			0.00000
56	bend	1	7	35	0	109.40200			0.00000
57	bend	1	7	36	0	108.74100			0.00000
58	bend	1	7	37	0	113.80300			0.00000
59	bend	4	2	6	0	116.14009			0.37356
60	bend	4	2	8	0	111.43909			0.37356
61	bend	2	4	14	0	125.29031			0.08614

62	bend	2	4	15	0	118.38331			0.08614
63	bend	6	2	8	0	94.20869			0.53695
64	bend	2	6	32	0	112.71800			0.00000
65	bend	2	6	33	0	108.48700			0.00000
66	bend	2	6	34	0	110.71500			0.00000
67	bend	2	8	38	0	109.92500			0.00000
68	bend	2	8	39	0	110.21500			0.00000
69	bend	2	8	40	0	112.01100			0.00000
70	bend	9	3	10	0	115.89984			0.16978
71	bend	3	9	11	0	122.37631			0.08614
72	bend	3	9	19	0	119.90923			0.16006
73	bend	3	10	12	0	123.28231			0.08614
74	bend	3	10	20	0	118.76723			0.16006
75	bend	14	4	15	0	115.92138			0.17092
76	bend	4	14	16	0	122.60231			0.08614
77	bend	4	14	24	0	120.10523			0.16006
78	bend	4	15	17	0	123.38431			0.08614
79	bend	4	15	25	0	118.93723			0.16006
80	bend	29	5	30	0	108.00969			0.00000
81	bend	29	5	31	0	108.84744			0.00000
82	bend	30	5	31	0	108.05237			0.00000
83	bend	32	6	33	0	108.41961			0.00000
84	bend	32	6	34	0	108.29142			0.00000
85	bend	33	6	34	0	108.08532			0.00000
86	bend	35	7	36	0	107.65319			0.00000
87	bend	35	7	37	0	108.47781			0.00000
88	bend	36	7	37	0	108.58806			0.00000
89	bend	38	8	39	0	107.89918			0.00000
90	bend	38	8	40	0	108.41727			0.00000
91	bend	39	8	40	0	108.25898			0.00000
92	bend	11	9	19	0	117.71446			0.16541
93	bend	9	11	13	0	119.87872			0.08563
94	bend	9	11	21	0	120.36823			0.16006
95	bend	12	10	20	0	117.95046			0.16541
96	bend	10	12	13	0	119.21341			0.08580
97	bend	10	12	22	0	120.56723			0.16006
98	bend	13	11	21	0	119.75306			0.16525
99	bend	11	13	12	0	119.34941			0.17393
100	bend	11	13	23	0	119.75441			0.09123
101	bend	13	12	22	0	120.21936			0.16530
102	bend	12	13	23	0	120.81479			0.09547
103	bend	16	14	24	0	117.29246			0.16541
104	bend	14	16	18	0	119.48410			0.08842
105	bend	14	16	26	0	120.31823			0.16006
106	bend	17	15	25	0	117.67846			0.16541
107	bend	15	17	18	0	118.84179			0.08840
108	bend	15	17	27	0	120.68023			0.16006
109	bend	18	16	26	0	120.19768			0.16616
110	bend	16	18	17	0	119.76611			0.17817
111	bend	16	18	28	0	120.44087			0.10013
112	bend	18	17	27	0	120.47798			0.16615
113	bend	17	18	28	0	119.78330			0.08706
114	torsion	4	2	1	3	9.85968			0.50381
115	torsion	6	2	1	3	141.49828			0.62349
116	torsion	8	2	1	3	-112.11300			0.56878
117	torsion	2	1	3	9	116.93447			0.73162
118	torsion	2	1	3	10	-52.71083			0.73162
119	torsion	4	2	1	5	138.75625			0.58891
120	torsion	6	2	1	5	-89.60515			0.81156
121	torsion	8	2	1	5	16.78357			0.50356
122	torsion	2	1	5	29	-65.60801			0.37962
123	torsion	2	1	5	30	52.65619			0.37962
124	torsion	2	1	5	31	170.65379			0.37962
125	torsion	4	2	1	7	-119.83626			0.57300
126	torsion	6	2	1	7	11.80235			0.50626

127	torsion	8	2	1	7	118.19106			0.75933
128	torsion	2	1	7	35	-174.67661			0.38731
129	torsion	2	1	7	36	-57.35361			0.38731
130	torsion	2	1	7	37	63.81539			0.38731
131	torsion	1	2	4	14	116.92292			1.14594
132	torsion	1	2	4	15	-55.45408			1.14594
133	torsion	1	2	6	32	-67.40778			0.40151
134	torsion	1	2	6	33	52.66972			0.40151
135	torsion	1	2	6	34	171.11932			0.40151
136	torsion	1	2	8	38	-178.66382			0.32655
137	torsion	1	2	8	39	-59.85762			0.32655
138	torsion	1	2	8	40	60.73848			0.32655
139	torsion	9	3	1	5	-3.97455			0.85328
140	torsion	10	3	1	5	-173.61985			0.85328
141	torsion	3	1	5	29	54.65760			0.00000
142	torsion	3	1	5	30	172.92180			0.00000
143	torsion	3	1	5	31	-69.08060			0.00000
144	torsion	9	3	1	7	-111.83124			0.77919
145	torsion	10	3	1	7	78.52346			0.77919
146	torsion	3	1	7	35	59.99600			0.00000
147	torsion	3	1	7	36	177.31900			0.00000
148	torsion	3	1	7	37	-61.51200			0.00000
149	torsion	1	3	9	11	-169.80420			0.02294
150	torsion	1	3	9	19	10.19580			0.02294
151	torsion	1	3	10	12	170.66342			0.02374
152	torsion	1	3	10	20	-9.33658			0.02374
153	torsion	29	5	1	7	174.84978			0.59511
154	torsion	30	5	1	7	-66.88602			0.59511
155	torsion	31	5	1	7	51.11158			0.59511
156	torsion	5	1	7	35	-64.32957			0.55791
157	torsion	5	1	7	36	52.99343			0.55791
158	torsion	5	1	7	37	174.16243			0.55791
159	torsion	14	4	2	6	-14.83163			1.02741
160	torsion	15	4	2	6	172.79137			1.02741
161	torsion	4	2	6	32	59.79410			0.00000
162	torsion	4	2	6	33	179.87160			0.00000
163	torsion	4	2	6	34	-61.67880			0.00000
164	torsion	14	4	2	8	-121.12421			1.31775
165	torsion	15	4	2	8	66.49879			1.31775
166	torsion	4	2	8	38	62.02370			0.00000
167	torsion	4	2	8	39	-179.17010			0.00000
168	torsion	4	2	8	40	-58.57400			0.00000
169	torsion	2	4	14	16	-172.54414			0.01696
170	torsion	2	4	14	24	7.45586			0.01696
171	torsion	2	4	15	17	173.08545			0.01747
172	torsion	2	4	15	25	-6.91455			0.01747
173	torsion	32	6	2	8	176.17722			0.57240
174	torsion	33	6	2	8	-63.74528			0.57240
175	torsion	34	6	2	8	54.70432			0.57240
176	torsion	6	2	8	38	-58.20777			0.54144
177	torsion	6	2	8	39	60.59843			0.54144
178	torsion	6	2	8	40	-178.80547			0.54144
179	torsion	11	9	3	10	0.00000			0.00000
180	torsion	19	9	3	10	180.00000			0.00000
181	torsion	9	3	10	12	0.00000			0.00000
182	torsion	9	3	10	20	180.00000			0.00000
183	torsion	3	9	11	13	0.00000			0.00000
184	torsion	3	9	11	21	180.00000			0.00000
185	torsion	3	10	12	13	0.00000			0.00000
186	torsion	3	10	12	22	180.00000			0.00000
187	torsion	16	14	4	15	0.00000			0.00000
188	torsion	24	14	4	15	-180.00000			0.00000
189	torsion	14	4	15	17	0.00000			0.00000
190	torsion	14	4	15	25	180.00000			0.00000
191	torsion	4	14	16	18	0.00000			0.00000

192	torsion	4	14	16	26	-180.00000			0.00000
193	torsion	4	15	17	18	0.00000			0.00000
194	torsion	4	15	17	27	180.00000			0.00000
195	torsion	13	11	9	19	-180.00000			0.00000
196	torsion	21	11	9	19	0.00000			0.00000
197	torsion	9	11	13	12	0.00000			0.00000
198	torsion	9	11	13	23	176.74675			0.17893
199	torsion	13	12	10	20	-180.00000			0.00000
200	torsion	22	12	10	20	0.00000			0.00000
201	torsion	10	12	13	11	0.00000			0.00000
202	torsion	10	12	13	23	-176.71136			0.18333
203	torsion	12	13	11	21	-180.00000			0.00000
204	torsion	23	13	11	21	-3.25325			0.17893
205	torsion	11	13	12	22	-180.00000			0.00000
206	torsion	23	13	12	22	3.28864			0.18333
207	torsion	18	16	14	24	180.00000			0.00000
208	torsion	26	16	14	24	0.00000			0.00000
209	torsion	14	16	18	17	0.00000			0.00000
210	torsion	14	16	18	28	178.86337			0.18282
211	torsion	18	17	15	25	-180.00000			0.00000
212	torsion	27	17	15	25	0.00000			0.00000
213	torsion	15	17	18	16	0.00000			0.00000
214	torsion	15	17	18	28	-178.87091			0.18091
215	torsion	17	18	16	26	-180.00000			0.00000
216	torsion	28	18	16	26	-1.13663			0.18282
217	torsion	16	18	17	27	-180.00000			0.00000
218	torsion	28	18	17	27	1.12909			0.18091
219	o.o.p	19	3	9	11	0.00000			0.00000
220	o.o.p	20	3	10	12	0.00000			0.00000
221	o.o.p	24	4	14	16	0.00000			0.00000
222	o.o.p	25	4	15	17	0.00000			0.00000
223	o.o.p	21	9	11	13	0.00000			0.00000
224	o.o.p	22	10	12	13	0.00000			0.00000
225	o.o.p	23	11	13	12	-2.82397			0.15589
226	o.o.p	26	14	16	18	0.00000			0.00000
227	o.o.p	27	15	17	18	0.00000			0.00000
228	o.o.p	28	16	18	17	-0.97993			0.15714

Table S14. Full listing of interatomic distances. refined vibrational amplitudes *l* and corrections of the *syn*-conformer $C_6Cl_5Me_2SiSiMe_2C_6F_5$ (**5**). All is given in Å. The numbers at the Gu column indicate the groups the amplitudes were refined in.

At1	At2	r_a	*l*	corr	*a*	Gr	Gu
C7	H37	1.087703	0.089163	0.001500	0.000000	0	100
C6	H32	1.088703	0.088348	0.001400	0.000000	0	100
C5	H29	1.089078	0.088348	0.001400	0.000000	0	100
C5	H31	1.090148	0.088581	0.001500	0.000000	0	100
C8	H40	1.090189	0.088698	0.001400	0.000000	0	100
C6	H34	1.091906	0.088930	0.001500	0.000000	0	100
C8	H39	1.092904	0.089163	0.001500	0.000000	0	100
C8	H38	1.093041	0.089163	0.001400	0.000000	0	100
C7	H35	1.093221	0.090095	0.001500	0.000000	0	100
C7	H36	1.093321	0.089978	0.001500	0.000000	0	100
C6	H33	1.093574	0.089163	0.001400	0.000000	0	100
C5	H30	1.095270	0.089396	0.001300	0.000000	0	100
C18	F28	1.330675	0.050518	0.000000	0.000000	0	100
C16	F26	1.334308	0.050751	0.000000	0.000000	0	100
C17	F27	1.334770	0.050867	0.000100	0.000000	0	100
C14	F24	1.341952	0.051799	0.000200	0.000000	0	100
C15	F25	1.348252	0.052381	0.000200	0.000000	0	100
C15	C17	1.390493	0.052963	0.000300	0.000000	0	100
C16	C18	1.393011	0.052963	0.000500	0.000000	0	100
C17	C18	1.394097	0.052963	0.000500	0.000000	0	100
C4	C14	1.394325	0.053545	0.000200	0.000000	0	100
C14	C16	1.394373	0.053195	0.000300	0.000000	0	100
C4	C15	1.395165	0.053777	0.000700	0.000000	0	100
C10	C12	1.399913	0.054127	0.000400	0.000000	0	100
C12	C13	1.401400	0.054010	0.000500	0.000000	0	100
C11	C13	1.401504	0.054010	0.000500	0.000000	0	100
C3	C9	1.404326	0.054709	0.000400	0.000000	0	100
C3	C10	1.404868	0.054825	0.000900	0.000000	0	100
C9	C11	1.405296	0.054592	0.000300	0.000000	0	100
C13	Cl23	1.705266	0.061445	-0.000300	0.000000	0	101
C11	Cl21	1.707552	0.061690	-0.000200	0.000000	0	101
C12	Cl22	1.708770	0.061812	-0.000200	0.000000	0	101
C9	Cl19	1.718627	0.063159	0.000200	0.000000	0	101
C10	Cl20	1.724442	0.063771	0.000100	0.000000	0	101
H35	H36	1.752873	0.156306	0.014600	0.000000	0	101
H38	H39	1.757480	0.154837	0.012200	0.000000	0	101
H29	H30	1.757771	0.154592	0.011700	0.000000	0	101
H32	H34	1.758055	0.154347	0.011700	0.000000	0	101
H35	H37	1.758771	0.155571	0.013400	0.000000	0	101
H39	H40	1.759205	0.154592	0.012200	0.000000	0	101
H30	H31	1.759395	0.154470	0.011500	0.000000	0	101
H33	H34	1.759594	0.154592	0.011800	0.000000	0	101
H36	H37	1.759980	0.155449	0.013500	0.000000	0	101
H32	H33	1.760657	0.154347	0.011800	0.000000	0	101
H38	H40	1.760903	0.154470	0.012300	0.000000	0	101
H29	H31	1.763414	0.153858	0.011400	0.000000	0	101
Si2	C6	1.854291	0.070380	-0.000100	0.000000	0	101
Si1	C5	1.858799	0.070992	-0.000100	0.000000	0	101
Si1	C7	1.859751	0.071115	-0.000100	0.000000	0	101
Si2	C8	1.860429	0.070992	-0.000300	0.000000	0	101
Si2	C4	1.890667	0.072951	-0.001100	0.000000	0	101
Si1	C3	1.911256	0.075399	-0.000600	0.000000	0	101
C16	F24	2.333028	0.075339	0.004300	0.000000	0	102
C17	F25	2.340325	0.075694	0.003800	0.000000	0	102
C17	F28	2.353291	0.076404	0.004500	0.000000	0	102
C18	F26	2.359893	0.076404	0.005000	0.000000	0	102
C16	F28	2.360243	0.076286	0.004400	0.000000	0	102
C4	F25	2.360642	0.074866	0.003300	0.000000	0	102
C14	C15	2.361969	0.069189	0.003400	0.000000	0	102
C14	F26	2.363537	0.076286	0.003800	0.000000	0	102

C18	F27	2.364645	0.076522	0.005000	0.000000	0	102
C15	F27	2.364703	0.076286	0.004000	0.000000	0	102
C4	F24	2.369131	0.074748	0.002300	0.000000	0	102
C9	C10	2.378731	0.069662	0.003400	0.000000	0	102
C15	C18	2.393519	0.068125	0.004500	0.000000	0	102
Si1	Si2	2.394045	0.082554	-0.001500	0.000000	0	102
Si1	H30	2.396818	0.155764	0.010700	0.000000	0	102
C14	C18	2.403737	0.068125	0.004600	0.000000	0	102
C16	C17	2.407321	0.068361	0.004400	0.000000	0	102
C10	C13	2.411712	0.069308	0.005400	0.000000	0	102
C11	C12	2.415253	0.069189	0.005000	0.000000	0	102
Si2	H33	2.423942	0.155410	0.010100	0.000000	0	102
C9	C13	2.424966	0.069426	0.005000	0.000000	0	102
Si1	H36	2.434580	0.161796	0.007800	0.000000	0	102
Si1	H35	2.441182	0.163807	0.010200	0.000000	0	102
C4	C16	2.441561	0.068834	0.005000	0.000000	0	102
Si2	H38	2.446748	0.156829	0.012000	0.000000	0	102
C4	C17	2.448209	0.068716	0.005200	0.000000	0	102
Si2	H39	2.454255	0.157539	0.008400	0.000000	0	102
Si2	H34	2.454593	0.154700	0.008700	0.000000	0	102
C3	C11	2.456123	0.069308	0.006300	0.000000	0	102
C3	C12	2.463024	0.069189	0.006300	0.000000	0	102
Si2	H32	2.476079	0.151743	0.011400	0.000000	0	102
Si2	H40	2.476482	0.153281	0.008200	0.000000	0	102
Si1	H31	2.481806	0.151743	0.007400	0.000000	0	102
Si1	H29	2.484087	0.150915	0.011800	0.000000	0	102
H31	H35	2.488793	0.502522	0.001700	0.000000	0	104
H30	H36	2.495630	0.443481	-0.062000	0.000000	0	104
Si1	H37	2.500723	0.152453	0.005200	0.000000	0	102
H34	H38	2.525925	0.393485	-0.018800	0.000000	0	104
H33	H39	2.617836	0.414647	-0.020300	0.000000	0	105
C5	C7	2.664291	0.118369	0.007100	0.000000	0	104
C11	Cl19	2.675037	0.069216	0.004000	0.000000	0	103
F24	F26	2.677066	0.119403	0.006900	0.000000	0	103
C12	Cl20	2.679936	0.069425	0.003100	0.000000	0	103
C11	Cl23	2.688076	0.069112	0.003600	0.000000	0	103
C13	Cl21	2.689887	0.069112	0.003900	0.000000	0	103
F25	F27	2.692367	0.120240	0.006300	0.000000	0	103
C3	Cl20	2.695420	0.072039	0.003400	0.000000	0	103
C13	Cl22	2.697245	0.069216	0.003800	0.000000	0	103
C10	Cl22	2.700753	0.069112	0.003600	0.000000	0	103
C12	Cl23	2.701944	0.069112	0.003800	0.000000	0	103
C9	Cl21	2.702043	0.069216	0.003000	0.000000	0	103
F24	H32	2.703751	0.478529	0.020700	0.000000	0	102
C3	Cl19	2.706807	0.072248	0.001600	0.000000	0	103
C6	C8	2.713093	0.117036	0.008000	0.000000	0	104
C5	H36	2.721500	0.348442	-0.007300	0.000000	0	104
F27	F28	2.723924	0.123167	0.008800	0.000000	0	103
F26	F28	2.730134	0.122749	0.008800	0.000000	0	103
C7	H31	2.742645	0.227787	0.009300	0.000000	0	104
C15	C16	2.751641	0.069112	0.005700	0.000000	0	103
C10	C11	2.766012	0.069321	0.006500	0.000000	0	103
C14	C17	2.766508	0.069112	0.005800	0.000000	0	103
C9	C12	2.782844	0.069425	0.006500	0.000000	0	103
H31	H36	2.785529	0.533304	0.064500	0.000000	0	105
C5	H35	2.799908	0.388438	0.040700	0.000000	0	104
C7	H30	2.801839	0.264442	0.022700	0.000000	0	105
C8	H34	2.806291	0.262546	0.012800	0.000000	0	104
C4	Cl20	2.812392	0.221026	0.006500	0.000000	0	104
C6	H38	2.822959	0.272926	0.020700	0.000000	0	104
C4	C18	2.824768	0.064089	0.007400	0.000000	0	104
Si2	C15	2.830915	0.079802	0.002200	0.000000	0	104
H30	H39	2.841893	0.512426	-0.008500	0.000000	0	104
F25	H40	2.846235	0.404609	-0.056800	0.000000	0	102
Si1	C10	2.846726	0.075421	0.002600	0.000000	0	104

C3	C13	2.847175	0.063422	0.009200	0.000000	0	104
C3	F25	2.852157	0.242072	0.010000	0.000000	0	104
C6	H39	2.857696	0.287148	0.014100	0.000000	0	105
C8	H33	2.858421	0.282426	0.019300	0.000000	0	105
C14	Cl20	2.871506	0.268831	0.013400	0.000000	0	104
C10	C15	2.880576	0.196457	0.003100	0.000000	0	104
Cl19	H29	2.883386	0.356709	-0.029600	0.000000	0	102
Si2	C14	2.915714	0.077326	0.010000	0.000000	0	104
Si1	C9	2.951480	0.074850	0.007800	0.000000	0	104
F24	H34	2.987124	0.495206	0.032500	0.000000	0	102
Si2	F25	2.990943	0.129987	-0.000400	0.000000	0	104
H34	H39	3.002924	0.650376	0.067400	0.000000	0	106
C9	F25	3.046976	0.275878	0.013200	0.000000	0	104
H30	H35	3.055199	0.773508	0.128200	0.000000	0	106
H33	H38	3.058286	0.654202	0.081400	0.000000	0	106
C6	F24	3.063091	0.209740	0.002600	0.000000	0	103
Cl19	Cl21	3.068307	0.103990	0.000200	0.000000	0	104
Cl20	Cl22	3.076954	0.104371	0.001000	0.000000	0	104
Cl19	H31	3.078342	0.346656	-0.038600	0.000000	0	102
C4	C8	3.089782	0.117227	0.008600	0.000000	0	104
Cl21	Cl23	3.094388	0.104561	0.002200	0.000000	0	104
C12	C17	3.098136	0.299876	0.005800	0.000000	0	104
H29	H39	3.112364	0.555946	0.091600	0.000000	0	104
C4	C10	3.116213	0.173602	0.004500	0.000000	0	104
Cl22	Cl23	3.133996	0.104942	0.002400	0.000000	0	104
C10	F25	3.134156	0.256927	0.017000	0.000000	0	104
Si1	Cl20	3.141770	0.120084	-0.003700	0.000000	0	104
H29	H40	3.149380	0.472811	-0.035900	0.000000	0	104
C3	C7	3.168414	0.121036	0.008400	0.000000	0	104
C3	C15	3.172533	0.187315	0.006900	0.000000	0	104
C4	C6	3.173265	0.105418	0.004100	0.000000	0	104
Si2	F24	3.174946	0.123131	0.012100	0.000000	0	104
C5	Cl19	3.197826	0.166558	-0.036200	0.000000	0	103
C18	Cl22	3.205577	0.635215	0.018600	0.000000	0	106
C12	C15	3.257502	0.274489	0.011100	0.000000	0	105
C3	C5	3.260156	0.101895	0.002100	0.000000	0	104
C13	F27	3.261579	0.450817	0.020500	0.000000	0	105
Cl20	F24	3.277559	0.339695	0.017300	0.000000	0	105
C4	H38	3.297024	0.276640	0.020000	0.000000	0	104
C15	Cl20	3.299354	0.264843	0.017400	0.000000	0	105
C10	C17	3.302248	0.275393	0.011400	0.000000	0	105
C4	H40	3.303516	0.266641	0.016500	0.000000	0	104
C12	F27	3.305804	0.411633	0.028300	0.000000	0	105
C5	H39	3.317453	0.460864	0.027700	0.000000	0	105
Cl20	H37	3.318599	0.385289	-0.183300	0.000000	0	103
Si2	Cl20	3.333090	0.212297	0.002900	0.000000	0	105
Cl22	F28	3.338294	0.786544	0.040900	0.000000	0	106
C8	F25	3.338363	0.213027	0.006300	0.000000	0	104
H33	H36	3.366199	1.006737	-0.007600	0.000000	0	106
C3	H35	3.381871	0.337300	-0.000200	0.000000	0	104
Si1	Cl19	3.387461	0.123078	0.001000	0.000000	0	105
Si2	H30	3.391652	0.272278	0.019800	0.000000	0	105
Si1	F25	3.397408	0.263437	0.012800	0.000000	0	105
C8	H30	3.399881	0.593273	0.025400	0.000000	0	106
C17	Cl22	3.402945	0.595399	0.030200	0.000000	0	106
C4	H34	3.413632	0.247500	0.010300	0.000000	0	104
C16	Cl20	3.417243	0.508540	0.034100	0.000000	0	106
C8	H29	3.418239	0.366923	0.014700	0.000000	0	105
Si2	C5	3.424701	0.139254	0.008700	0.000000	0	105
C4	H32	3.429152	0.241405	0.010300	0.000000	0	104
Si2	C3	3.434051	0.117451	0.009700	0.000000	0	105
C15	H40	3.435440	0.316445	-0.011300	0.000000	0	104
Si1	C4	3.443685	0.118557	0.009500	0.000000	0	105
C3	H37	3.445485	0.340824	0.014300	0.000000	0	104
C3	C4	3.461936	0.234504	0.013700	0.000000	0	106

C14	H32	3.477496	0.325873	0.016900	0.000000	0	104
H30	H33	3.489031	0.434583	-0.025000	0.000000	0	107
C3	H29	3.496123	0.217598	0.011700	0.000000	0	104
C11	F25	3.501128	0.499897	0.030700	0.000000	0	106
Si1	C8	3.519770	0.198797	0.006300	0.000000	0	106
H30	H40	3.545797	0.917611	0.108300	0.000000	0	106
C6	C14	3.556751	0.145795	0.012300	0.000000	0	104
Cl23	F27	3.557337	0.845064	0.053200	0.000000	0	106
C12	C18	3.574509	0.479635	0.001500	0.000000	0	106
C13	C17	3.579589	0.507549	0.005900	0.000000	0	106
C12	F25	3.586130	0.463198	0.030900	0.000000	0	106
C14	F25	3.595826	0.091818	0.008400	0.000000	0	106
C3	H31	3.597324	0.207976	0.005900	0.000000	0	105
C15	F24	3.598862	0.091818	0.008200	0.000000	0	106
C18	F24	3.602401	0.093093	0.010900	0.000000	0	106
C15	F28	3.603670	0.092385	0.010900	0.000000	0	106
C18	F25	3.605144	0.093235	0.010300	0.000000	0	106
C5	H37	3.609228	0.168958	0.091300	0.000000	0	107
C14	H34	3.611124	0.336253	0.026000	0.000000	0	104
Si1	C6	3.613035	0.211691	0.006400	0.000000	0	106
C14	F28	3.616826	0.092526	0.010900	0.000000	0	106
C9	H29	3.618816	0.269593	0.008200	0.000000	0	104
C17	F26	3.620537	0.092810	0.011100	0.000000	0	106
C5	H40	3.620946	0.653210	0.015800	0.000000	0	106
Si2	H29	3.622909	0.358345	0.019300	0.000000	0	106
C16	F27	3.623008	0.092668	0.011100	0.000000	0	106
C8	C15	3.628978	0.165222	0.012800	0.000000	0	104
Si2	C7	3.637528	0.219484	0.008100	0.000000	0	106
C7	Cl20	3.642691	0.185887	-0.004200	0.000000	0	104
C4	F26	3.644888	0.092951	0.010700	0.000000	0	106
C5	C8	3.645113	0.350126	0.008000	0.000000	0	106
Si1	H39	3.648312	0.441519	0.012400	0.000000	0	106
C4	F27	3.651974	0.093235	0.011100	0.000000	0	106
C7	H29	3.664972	0.137886	0.033400	0.000000	0	107
C16	Cl22	3.669753	0.452996	0.006800	0.000000	0	107
Si1	H33	3.679669	0.429333	0.011400	0.000000	0	106
C10	C14	3.682607	0.327030	0.009800	0.000000	0	106
C5	C9	3.684391	0.136441	0.003300	0.000000	0	105
H32	H36	3.685107	1.043436	0.137100	0.000000	0	106
C6	H40	3.689320	0.141025	0.048500	0.000000	0	107
Si1	H40	3.689508	0.426925	0.006100	0.000000	0	106
Si2	C10	3.691783	0.226427	0.009700	0.000000	0	106
C8	H32	3.693289	0.141025	0.047200	0.000000	0	107
H30	H37	3.701003	0.347645	0.122400	0.000000	0	107
H31	H37	3.703154	0.288850	0.119400	0.000000	0	107
Cl22	F27	3.728620	0.523717	0.056500	0.000000	0	107
C9	C15	3.735230	0.359478	0.014300	0.000000	0	106
Si1	C15	3.744499	0.262984	0.012600	0.000000	0	106
C13	F25	3.749573	0.532912	0.040400	0.000000	0	106
H29	H36	3.760882	0.399198	0.017800	0.000000	0	108
Si2	H36	3.763062	0.401524	0.005300	0.000000	0	107
C10	H37	3.779844	0.369012	-0.056500	0.000000	0	104
C6	H36	3.781117	0.622895	0.043300	0.000000	0	107
C11	F27	3.786891	0.466910	0.016200	0.000000	0	107
H32	H37	3.787320	1.046553	-0.032500	0.000000	0	106
H34	H40	3.796339	0.288013	0.062200	0.000000	0	107
C17	Cl20	3.797498	0.343775	0.033100	0.000000	0	107
H29	H35	3.799803	0.389179	0.050800	0.000000	0	107
H32	H38	3.802638	0.295546	0.063900	0.000000	0	107
F25	H29	3.803934	0.497536	0.024800	0.000000	0	105
C9	H31	3.826361	0.250376	0.005900	0.000000	0	105
C13	C15	3.827243	0.338858	0.020800	0.000000	0	107
C7	C10	3.828220	0.158946	0.011300	0.000000	0	105
Cl19	F25	3.828639	0.581229	0.035500	0.000000	0	106
Cl20	H32	3.834945	0.360392	-0.067900	0.000000	0	105

F25	H38	3.841434	0.418666	0.074200	0.000000	0	105
C18	Cl20	3.843462	0.392003	0.041500	0.000000	0	107
H33	H40	3.847634	0.324210	0.064200	0.000000	0	108
C4	C12	3.858954	0.285607	0.017200	0.000000	0	107
C10	C18	3.859031	0.318980	0.016800	0.000000	0	107
H32	H39	3.863185	0.329717	0.059200	0.000000	0	108
C10	F27	3.864294	0.365012	0.026000	0.000000	0	107
Si1	H32	3.868971	0.419273	0.015300	0.000000	0	106
C7	H33	3.878218	0.511477	0.018300	0.000000	0	107
Si2	H37	3.901728	0.419204	-0.000900	0.000000	0	107
C15	H38	3.918485	0.546514	0.054400	0.000000	0	106
C3	C17	3.942693	0.292198	0.019100	0.000000	0	107
C9	Cl20	3.967855	0.073756	0.009700	0.000000	0	107
C7	H32	3.970915	0.506769	0.032700	0.000000	0	107
C10	Cl19	3.971945	0.074488	0.010200	0.000000	0	107
C13	Cl19	3.977293	0.072082	0.013000	0.000000	0	107
C13	Cl20	3.977777	0.072186	0.011500	0.000000	0	107
C12	Cl21	3.980023	0.071873	0.011900	0.000000	0	107
C10	Cl23	3.983469	0.071977	0.012200	0.000000	0	107
H33	H37	3.984559	0.867387	0.115400	0.000000	0	107
C9	Cl23	3.984823	0.072082	0.011600	0.000000	0	107
C11	Cl22	3.985578	0.071873	0.011700	0.000000	0	107
C4	H39	3.992170	0.190579	0.050000	0.000000	0	106
C3	H36	3.999417	0.223735	0.093900	0.000000	0	106
Cl20	F25	4.002168	0.285921	0.020100	0.000000	0	107
C15	Cl22	4.003854	0.369092	0.025700	0.000000	0	107
C6	H30	4.009058	0.355728	0.018500	0.000000	0	108
C3	Cl21	4.012781	0.072186	0.012000	0.000000	0	107
C3	Cl22	4.018845	0.072186	0.012100	0.000000	0	107
C10	C16	4.030659	0.296592	0.015200	0.000000	0	107
C11	C15	4.040414	0.317202	0.019300	0.000000	0	107
C4	H33	4.042128	0.137573	0.042400	0.000000	0	107
C6	C7	4.074144	0.320654	0.014100	0.000000	0	107
C15	F26	4.078698	0.072291	0.012900	0.000000	0	107
F24	H33	4.092608	0.321504	0.056100	0.000000	0	106
C16	F25	4.093344	0.072291	0.012200	0.000000	0	107
C14	F27	4.093893	0.072291	0.013200	0.000000	0	107
C3	H30	4.098748	0.137573	0.027900	0.000000	0	107
C17	F24	4.101154	0.072291	0.012600	0.000000	0	107
C6	H37	4.107193	0.677297	0.017200	0.000000	0	107
C12	C16	4.109939	0.403885	0.008000	0.000000	0	108
C10	H35	4.118350	0.711730	0.075100	0.000000	0	106
C12	F28	4.120877	0.505003	0.017100	0.000000	0	108
C5	H33	4.136772	0.385138	0.004300	0.000000	0	108
C4	F28	4.148006	0.073442	0.014700	0.000000	0	107
Si2	C17	4.148354	0.087461	0.011600	0.000000	0	107
C11	C17	4.152048	0.431655	0.014600	0.000000	0	108
Cl20	H35	4.153309	0.825369	0.149500	0.000000	0	106
F25	H39	4.156750	0.419698	0.060900	0.000000	0	106
C6	Cl20	4.162879	0.292826	0.002100	0.000000	0	107
C14	H38	4.163023	0.336137	0.016200	0.000000	0	107
Cl20	F26	4.170330	0.494458	0.045400	0.000000	0	108
Si1	C12	4.172408	0.087147	0.012400	0.000000	0	107
Cl22	F26	4.185453	0.630844	0.022300	0.000000	0	108
C8	C14	4.186077	0.159961	0.023700	0.000000	0	107
C5	F25	4.193926	0.422029	0.036200	0.000000	0	107
C9	H35	4.195439	0.379659	-0.035300	0.000000	0	107
Si2	C16	4.205947	0.084845	0.017200	0.000000	0	107
C7	C9	4.209136	0.174398	0.023000	0.000000	0	107
C12	C14	4.215633	0.375296	0.016400	0.000000	0	108
C14	Cl22	4.227045	0.469969	0.014300	0.000000	0	108
Si1	C11	4.243264	0.088298	0.017200	0.000000	0	107
Cl19	H30	4.258049	0.257600	-0.009000	0.000000	0	106
C17	Cl23	4.266177	0.586085	0.032800	0.000000	0	108
C9	F27	4.275054	0.488834	0.025100	0.000000	0	108

C9	C17	4.294035	0.401425	0.023000	0.000000	0	108
Cl20	H36	4.314177	0.387609	0.125500	0.000000	0	107
Cl19	H35	4.322202	0.500902	-0.065100	0.000000	0	108
H31	H39	4.328136	0.564525	0.055100	0.000000	0	108
C13	C18	4.335505	0.475476	0.011500	0.000000	0	108
F24	H38	4.336756	0.351621	0.008100	0.000000	0	107
H30	H38	4.347482	0.511096	0.084700	0.000000	0	108
C3	F27	4.351065	0.405877	0.025200	0.000000	0	108
Si2	H31	4.401562	0.170248	0.033400	0.000000	0	108
C3	C14	4.412206	0.260703	0.025700	0.000000	0	108
C4	C9	4.415810	0.272186	0.027400	0.000000	0	108
C4	Cl22	4.416488	0.402831	0.020900	0.000000	0	108
C6	C15	4.423649	0.113615	0.013900	0.000000	0	107
H29	H38	4.435613	0.463290	0.075900	0.000000	0	108
Si1	H38	4.445781	0.173880	0.054500	0.000000	0	108
C5	C6	4.451894	0.225787	0.022600	0.000000	0	108
C10	Cl21	4.465137	0.084011	0.014700	0.000000	0	108
C8	F24	4.477048	0.228599	0.028300	0.000000	0	108
Si2	H35	4.479342	0.204930	0.104200	0.000000	0	108
C11	Cl20	4.482294	0.084480	0.014500	0.000000	0	108
C9	Cl22	4.483209	0.084011	0.014600	0.000000	0	108
C12	Cl19	4.490957	0.084948	0.016500	0.000000	0	108
C5	C10	4.493267	0.127715	0.013100	0.000000	0	108
Si1	C14	4.493743	0.180676	0.022300	0.000000	0	108
Si2	C9	4.495916	0.191925	0.022000	0.000000	0	108
C10	F24	4.509902	0.359361	0.027000	0.000000	0	108
C3	H40	4.518417	0.351393	-0.008300	0.000000	0	108
Si1	H34	4.522433	0.178098	0.047500	0.000000	0	108
C7	Cl19	4.523834	0.285543	0.023600	0.000000	0	108
H36	H39	4.524550	0.668108	-0.132300	0.000000	0	110
C14	H40	4.533669	0.361001	0.043700	0.000000	0	108
C3	Cl23	4.542471	0.084597	0.017500	0.000000	0	108
C14	H33	4.561764	0.175967	0.063600	0.000000	0	107
H30	H32	4.562092	0.592073	0.068800	0.000000	0	109
C15	H39	4.564457	0.232465	0.066200	0.000000	0	108
H29	H37	4.572666	0.205282	0.109800	0.000000	0	108
C9	H37	4.595012	0.491294	0.068300	0.000000	0	108
H29	H33	4.605427	0.564315	0.044100	0.000000	0	109
Cl21	F25	4.610425	0.507815	0.044100	0.000000	0	108
Cl21	F27	4.619583	0.687788	0.042800	0.000000	0	108
H32	H40	4.621362	0.186886	0.079700	0.000000	0	108
C3	C8	4.635487	0.198838	0.019700	0.000000	0	108
H31	H40	4.641382	0.561010	0.046600	0.000000	0	108
C5	H38	4.661510	0.316476	0.074400	0.000000	0	108
C10	H36	4.670538	0.265859	0.125200	0.000000	0	108
C15	H34	4.677191	0.290933	0.019300	0.000000	0	108
F24	F28	4.683398	0.096900	0.018400	0.000000	0	108
F25	F28	4.683900	0.096782	0.017700	0.000000	0	108
C9	H30	4.686290	0.177278	0.034000	0.000000	0	108
C17	H40	4.694317	0.384052	-0.003700	0.000000	0	107
Si2	C18	4.694513	0.097603	0.018500	0.000000	0	108
C8	H31	4.695296	0.315656	0.047600	0.000000	0	108
F26	F27	4.714814	0.096782	0.019000	0.000000	0	108
C13	F28	4.716271	0.737015	0.019100	0.000000	0	109
F24	F25	4.717793	0.091861	0.013400	0.000000	0	108
Si1	C13	4.731644	0.103696	0.020200	0.000000	0	108
Cl23	F28	4.731858	0.984587	0.042500	0.000000	0	109
C4	C13	4.744404	0.482541	0.032400	0.000000	0	109
C7	H39	4.747468	0.558463	-0.003600	0.000000	0	109
Cl22	F25	4.753887	0.547210	0.042200	0.000000	0	109
C10	F28	4.754135	0.571217	0.031500	0.000000	0	109
C15	H32	4.757771	0.281677	0.017300	0.000000	0	108
H33	H35	4.760142	0.779327	0.156000	0.000000	0	109
Cl20	F27	4.770535	0.543609	0.044400	0.000000	0	109
C10	H29	4.773295	0.278748	0.022000	0.000000	0	108

F25	H30	4.776002	0.576477	0.073800	0.000000	0	108
C15	H29	4.791527	0.498910	0.027100	0.000000	0	108
H30	H34	4.792047	0.447883	0.057800	0.000000	0	110
C6	F25	4.794102	0.164272	0.012900	0.000000	0	108
C16	H32	4.799101	0.423218	0.018900	0.000000	0	108
H34	H36	4.804295	0.920218	0.083800	0.000000	0	109
C8	H36	4.804719	0.514782	-0.051900	0.000000	0	110
Cl20	H33	4.806309	0.512150	0.063100	0.000000	0	108
C3	C18	4.809314	0.460484	0.029800	0.000000	0	109
C4	C5	4.810093	0.242425	0.029200	0.000000	0	108
C4	C7	4.817461	0.180442	0.020100	0.000000	0	108
C18	Cl23	4.821953	0.826141	0.032600	0.000000	0	109
Cl20	F28	4.829044	0.651790	0.056500	0.000000	0	109
Cl20	H34	4.851684	0.405643	0.052800	0.000000	0	108
Si2	C12	4.855498	0.324545	0.021900	0.000000	0	109
C4	H29	4.857024	0.382326	0.027500	0.000000	0	108
C15	Cl19	4.860208	0.566715	0.043900	0.000000	0	109
C6	H29	4.861484	0.412320	0.045400	0.000000	0	109
C7	C8	4.862926	0.323944	0.022200	0.000000	0	109
C4	H37	4.879492	0.376467	-0.043800	0.000000	0	108
C10	H31	4.892627	0.237972	0.017700	0.000000	0	108
Si1	F24	4.907430	0.299337	0.028000	0.000000	0	109
C11	H29	4.915402	0.384904	0.020500	0.000000	0	108
Si1	C17	4.921401	0.342700	0.024300	0.000000	0	109
H32	H35	4.928515	0.831693	0.168900	0.000000	0	109
C6	C16	4.934746	0.187941	0.024900	0.000000	0	108
C16	H34	4.936756	0.437044	0.033200	0.000000	0	108
C8	C17	4.943715	0.229302	0.024800	0.000000	0	108
C15	Cl23	4.951633	0.657642	0.042700	0.000000	0	109
C5	H32	4.959622	0.388165	0.052400	0.000000	0	110
C9	H40	4.960245	0.449933	-0.012000	0.000000	0	108
C5	C15	4.960668	0.363813	0.035500	0.000000	0	108
C3	C6	4.968081	0.230167	0.019100	0.000000	0	109
Cl23	F25	4.972715	0.695903	0.060400	0.000000	0	109
H31	H33	4.976648	0.464009	0.023400	0.000000	0	110
C4	C11	4.981674	0.439928	0.034500	0.000000	0	109
F25	H31	4.985968	0.485670	0.055700	0.000000	0	108
C5	Cl20	4.987275	0.202709	0.009000	0.000000	0	109
Cl19	H40	4.997779	0.597216	-0.011500	0.000000	0	108
C9	H36	5.003603	0.324095	0.110800	0.000000	0	109
C6	H35	5.008683	0.520202	0.152600	0.000000	0	109
C3	C16	5.012515	0.419372	0.031800	0.000000	0	109
C12	F26	5.023323	0.544263	0.024800	0.000000	0	110
C10	H32	5.025916	0.370257	-0.024700	0.000000	0	108
C10	F26	5.041586	0.444859	0.029700	0.000000	0	110
C4	H30	5.043950	0.472338	0.054800	0.000000	0	109
C14	H39	5.051708	0.260326	0.069400	0.000000	0	109
C12	H37	5.058135	0.502308	-0.044700	0.000000	0	108
C3	H39	5.059901	0.439478	0.044700	0.000000	0	109
C5	C11	5.062975	0.182785	0.020100	0.000000	0	108
C6	C10	5.073920	0.320944	0.017800	0.000000	0	109
F24	H40	5.074501	0.446230	0.064300	0.000000	0	109
Cl22	F24	5.099451	0.625776	0.036600	0.000000	0	110
C7	H34	5.099815	0.477439	0.075400	0.000000	0	109
C17	H38	5.111073	0.507815	0.059700	0.000000	0	108
C3	H32	5.116370	0.409319	-0.002900	0.000000	0	109
C8	Cl20	5.124693	0.316292	0.015500	0.000000	0	109
Si2	Cl19	5.125154	0.344500	0.028300	0.000000	0	109
Cl19	H36	5.127441	0.538957	0.087700	0.000000	0	109
F25	H34	5.134971	0.339699	0.021000	0.000000	0	109
H34	H37	5.137606	0.995540	0.065500	0.000000	0	109
C13	C16	5.145515	0.530530	0.028800	0.000000	0	110
C7	C12	5.154515	0.208563	0.024400	0.000000	0	108
Cl19	H37	5.163246	0.655841	0.123400	0.000000	0	109
C10	H40	5.163937	0.414571	0.005500	0.000000	0	109

Si2	F27	5.168516	0.160847	0.017200	0.000000	0	109
C11	C18	5.176081	0.535821	0.030900	0.000000	0	110
C8	C10	5.177116	0.260926	0.022100	0.000000	0	109
C15	H33	5.180571	0.214863	0.050600	0.000000	0	109
C11	H31	5.185818	0.302299	0.021100	0.000000	0	108
F24	H39	5.188084	0.383062	0.066100	0.000000	0	109
C10	H30	5.194537	0.222065	0.040800	0.000000	0	109
C3	F24	5.202298	0.327691	0.036200	0.000000	0	110
C7	F25	5.203980	0.392364	0.026500	0.000000	0	109
C12	F24	5.204564	0.500419	0.037500	0.000000	0	110
C4	H36	5.210235	0.500546	0.053700	0.000000	0	109
C7	H40	5.245404	0.438938	0.045800	0.000000	0	110
Si2	F26	5.261801	0.128128	0.026000	0.000000	0	110
C5	H34	5.271051	0.280194	0.060100	0.000000	0	110
C3	H33	5.296752	0.374055	0.047400	0.000000	0	110
F27	H40	5.298453	0.454620	-0.022400	0.000000	0	108
H36	H40	5.299351	0.600075	-0.009400	0.000000	0	110
C16	H38	5.303208	0.562514	0.030000	0.000000	0	109
C13	C14	5.303937	0.473836	0.035000	0.000000	0	110
F25	H32	5.308356	0.327095	0.022900	0.000000	0	109
H37	H39	5.308986	0.703636	0.074400	0.000000	0	110
C8	C9	5.330540	0.384562	0.034500	0.000000	0	109
Cl19	Cl23	5.336405	0.113514	0.021200	0.000000	0	110
F24	H37	5.338003	0.793281	-0.076400	0.000000	0	109
F25	H33	5.339700	0.246682	0.035800	0.000000	0	110
C8	H37	5.341572	0.552704	0.065500	0.000000	0	110
C12	H35	5.341647	0.815938	0.070000	0.000000	0	109
F26	H32	5.342510	0.608127	0.018700	0.000000	0	109
C17	Cl21	5.342626	0.619099	0.039600	0.000000	0	110
C6	H31	5.351738	0.275029	0.044800	0.000000	0	110
Cl20	Cl23	5.359388	0.113388	0.020000	0.000000	0	110
C15	Cl21	5.360276	0.505585	0.039300	0.000000	0	110
C7	C15	5.363316	0.229800	0.026500	0.000000	0	110
C9	C18	5.365193	0.475600	0.036300	0.000000	0	110
Cl21	Cl22	5.367260	0.112506	0.020500	0.000000	0	110
C8	C16	5.372699	0.259276	0.033400	0.000000	0	109
Cl19	Cl20	5.387232	0.118805	0.017700	0.000000	0	110
Cl20	H30	5.392049	0.247438	0.027100	0.000000	0	110
H35	H39	5.393504	0.621618	0.119900	0.000000	0	110
C14	H37	5.395590	0.609028	-0.066300	0.000000	0	109
C11	H35	5.398689	0.631984	-0.013300	0.000000	0	109
F25	F26	5.418548	0.090962	0.021300	0.000000	0	110
C15	H30	5.424688	0.502057	0.070300	0.000000	0	110
F24	F27	5.426723	0.090836	0.021900	0.000000	0	110
Cl20	H40	5.429010	0.323030	0.023900	0.000000	0	110
C7	C11	5.446642	0.222241	0.034400	0.000000	0	110
C9	C14	5.447677	0.354779	0.037400	0.000000	0	110
Cl19	F27	5.471858	0.708297	0.065700	0.000000	0	110
C3	H38	5.471931	0.285360	0.066000	0.000000	0	110
Cl20	H29	5.474992	0.268100	0.024100	0.000000	0	110
C8	Cl19	5.494240	0.473080	0.041700	0.000000	0	110
Cl20	H31	5.494773	0.260163	0.015800	0.000000	0	110
Si1	Cl22	5.498091	0.134554	0.017200	0.000000	0	110
C4	Cl19	5.498652	0.381110	0.045000	0.000000	0	110
Si2	C11	5.499435	0.265076	0.032300	0.000000	0	110
H29	H32	5.517270	0.397866	0.073500	0.000000	0	110
C15	H37	5.521505	0.341172	-0.012900	0.000000	0	110
Si1	C16	5.522701	0.245422	0.031700	0.000000	0	110
H29	H34	5.548147	0.399378	0.067800	0.000000	0	110
C7	C14	5.554501	0.292289	0.034400	0.000000	0	110
F26	H34	5.558128	0.628983	0.037500	0.000000	0	109
C16	H40	5.560644	0.440198	0.042900	0.000000	0	110
F25	H37	5.572687	0.363472	0.028800	0.000000	0	110
C8	H35	5.574267	0.380480	0.127300	0.000000	0	110
C4	H35	5.581013	0.315849	0.105300	0.000000	0	110

H36	H38	5.596298	0.641360	0.009700	0.000000	0	111
C17	Cl19	5.596360	0.587350	0.058300	0.000000	0	110
C6	C17	5.603650	0.147908	0.026100	0.000000	0	110
Si1	F27	5.605212	0.361582	0.030200	0.000000	0	110
C7	F24	5.613487	0.405425	0.039200	0.000000	0	110
C10	H33	5.614162	0.433772	0.064000	0.000000	0	110
Si1	Cl21	5.622629	0.135058	0.026300	0.000000	0	110
C18	H40	5.625504	0.559213	0.022900	0.000000	0	109
Cl20	H38	5.627649	0.341550	0.037600	0.000000	0	110
Cl19	H39	5.646353	0.644170	0.075300	0.000000	0	110
C6	F26	5.652537	0.250588	0.031300	0.000000	0	110
Si2	C13	5.652600	0.298085	0.033200	0.000000	0	110
C8	C18	5.684752	0.238745	0.034000	0.000000	0	110
C5	C12	5.687877	0.160255	0.026300	0.000000	0	110
F25	H35	5.690412	0.415252	0.055000	0.000000	0	110
C11	H37	5.699789	0.576011	0.057100	0.000000	0	110
Cl20	H39	5.700607	0.341550	0.025400	0.000000	0	110
Si1	C18	5.701003	0.282840	0.032500	0.000000	0	110
C18	H38	5.703744	0.530026	0.048000	0.000000	0	110
H31	H38	5.705285	0.369645	0.119000	0.000000	0	110
Cl21	H29	5.706073	0.465269	0.016300	0.000000	0	110
C4	H31	5.706269	0.263438	0.052200	0.000000	0	110
C7	H38	5.709039	0.335359	0.074400	0.000000	0	111
C9	H39	5.731736	0.467537	0.070900	0.000000	0	110
C11	F28	5.739747	0.640264	0.039100	0.000000	0	110
F25	H36	5.740408	0.395472	0.032400	0.000000	0	110
C8	F27	5.747781	0.295187	0.029300	0.000000	0	110
Si2	Cl22	5.750219	0.349235	0.025500	0.000000	0	110
H31	H32	5.756615	0.479962	0.065300	0.000000	0	111
C3	H34	5.758444	0.249832	0.059000	0.000000	0	110
C10	H39	5.769410	0.305392	0.047100	0.000000	0	110
C17	H34	5.774942	0.361078	0.031000	0.000000	0	110
C10	H34	5.781728	0.359818	0.059100	0.000000	0	110
C15	H31	5.782945	0.405929	0.057300	0.000000	0	110
C3	F28	5.802299	0.462245	0.040500	0.000000	0	110
C6	C18	5.808997	0.178271	0.031200	0.000000	0	110
C17	H32	5.809141	0.352385	0.023500	0.000000	0	110
H37	H40	5.810382	0.538971	0.094000	0.000000	0	110
F24	H36	5.811742	0.667982	0.102700	0.000000	0	110
C18	H32	5.821290	0.416764	0.023300	0.000000	0	110
C12	H29	5.830478	0.361330	0.031500	0.000000	0	110
C11	C14	5.840532	0.472042	0.041300	0.000000	0	111
C10	H38	5.841841	0.315471	0.055500	0.000000	0	110
C7	C13	5.842169	0.225138	0.035900	0.000000	0	110
H35	H40	5.848384	0.609682	0.121200	0.000000	0	111
C16	Cl23	5.869714	0.754967	0.045700	0.000000	0	111
C9	C16	5.870686	0.470404	0.041200	0.000000	0	111
C18	H34	5.878185	0.427725	0.036000	0.000000	0	110
C13	H29	5.887697	0.416512	0.032500	0.000000	0	110
C13	H35	5.889779	0.624516	0.030800	0.000000	0	110
C13	H37	5.895468	0.575507	0.010200	0.000000	0	110
C11	H40	5.897091	0.533932	-0.000900	0.000000	0	110
C17	H39	5.902524	0.268352	0.086900	0.000000	0	110
C15	H36	5.904018	0.344700	0.057400	0.000000	0	110
C5	C13	5.922041	0.192886	0.031300	0.000000	0	110
C14	H36	5.925834	0.519947	0.093100	0.000000	0	110
C16	H33	5.935941	0.224256	0.083300	0.000000	0	110
C11	C16	5.941236	0.558613	0.041400	0.000000	0	111
F27	H38	5.970885	0.604610	0.075000	0.000000	0	110
C15	H35	5.972866	0.344700	0.077700	0.000000	0	110
Cl22	H37	5.987290	0.542625	-0.097700	0.000000	0	110
C4	Cl23	6.002729	0.568991	0.048300	0.000000	0	111
Si2	F28	6.012611	0.120025	0.028800	0.000000	0	111
C5	C14	6.016739	0.261351	0.042900	0.000000	0	111
H34	H35	6.017977	0.488155	0.224500	0.000000	0	111

Cl21	H31	6.019334	0.370023	0.021500	0.000000	0	110
C12	H36	6.019447	0.298463	0.149900	0.000000	0	110
C17	H29	6.021523	0.600075	0.035400	0.000000	0	110
C12	H31	6.026569	0.273265	0.030300	0.000000	0	110
C5	Cl21	6.041043	0.243532	0.023900	0.000000	0	110
C11	H30	6.055449	0.225264	0.057000	0.000000	0	110
C12	H40	6.071179	0.426465	0.015300	0.000000	0	110
H37	H38	6.096086	0.679730	0.096300	0.000000	0	111
C13	F26	6.127278	0.679320	0.043700	0.000000	0	111
C3	F26	6.144889	0.442548	0.044200	0.000000	0	111
C13	H31	6.146970	0.303124	0.033400	0.000000	0	110
C6	C9	6.163169	0.223254	0.033600	0.000000	0	111
C14	H29	6.171612	0.436404	0.042400	0.000000	0	111
Cl20	Cl21	6.177544	0.106780	0.026600	0.000000	0	111
C14	H30	6.180723	0.390797	0.067400	0.000000	0	111
Cl19	Cl22	6.186827	0.107599	0.029200	0.000000	0	111
C9	H38	6.191492	0.455247	0.088900	0.000000	0	111
C9	F28	6.198753	0.608726	0.045200	0.000000	0	111
C5	C17	6.210248	0.476685	0.047600	0.000000	0	111
H31	H34	6.217632	0.356708	0.094000	0.000000	0	112
C8	C12	6.218283	0.330307	0.037400	0.000000	0	111
C12	H32	6.218738	0.464387	-0.013900	0.000000	0	110
C7	Cl22	6.278951	0.269864	0.027300	0.000000	0	110
C6	C12	6.283083	0.367038	0.031500	0.000000	0	111
C11	H36	6.285422	0.286202	0.139700	0.000000	0	111
F26	H38	6.289876	0.528163	0.029700	0.000000	0	111
C16	H39	6.294291	0.242644	0.089400	0.000000	0	111
C8	C11	6.347931	0.415102	0.048500	0.000000	0	111
C14	H35	6.349133	0.518741	0.140300	0.000000	0	111
C14	Cl23	6.369069	0.725872	0.049400	0.000000	0	112
F27	H29	6.372109	0.751963	0.033100	0.000000	0	111
F24	H30	6.377974	0.422437	0.064400	0.000000	0	112
C16	H37	6.386287	0.566123	-0.058000	0.000000	0	111
C9	F24	6.392215	0.442096	0.048200	0.000000	0	112
C13	H40	6.397984	0.558067	0.013400	0.000000	0	111
C13	F24	6.405365	0.627728	0.051100	0.000000	0	112
C5	F24	6.406441	0.278073	0.048000	0.000000	0	112
Si1	Cl23	6.415799	0.151717	0.033600	0.000000	0	112
C9	H32	6.420774	0.367994	0.015500	0.000000	0	111
C17	H33	6.432711	0.197583	0.072400	0.000000	0	111
C9	H33	6.437061	0.418085	0.058900	0.000000	0	112
Cl19	H38	6.442641	0.598758	0.110100	0.000000	0	111
C18	Cl21	6.445990	0.811560	0.054700	0.000000	0	112
C7	C17	6.446006	0.323070	0.042300	0.000000	0	111
C4	Cl21	6.452090	0.542941	0.051300	0.000000	0	112
C8	F26	6.460680	0.260395	0.044900	0.000000	0	111
C12	H30	6.463622	0.223391	0.060100	0.000000	0	111
H35	H38	6.471158	0.450650	0.197200	0.000000	0	112
F24	H35	6.479772	0.633987	0.172400	0.000000	0	111
C17	H37	6.489875	0.442002	-0.006400	0.000000	0	111
Cl22	H35	6.535562	0.856422	0.108000	0.000000	0	111
C7	C16	6.609240	0.405180	0.048400	0.000000	0	112
Si1	F26	6.614868	0.338850	0.043700	0.000000	0	112
Cl21	H35	6.632400	0.635532	-0.029800	0.000000	0	112
C18	H39	6.654243	0.280774	0.096700	0.000000	0	112
Cl22	H32	6.664303	0.630846	-0.022900	0.000000	0	111
F27	H39	6.671922	0.377552	0.097000	0.000000	0	111
F26	H33	6.673543	0.307230	0.096400	0.000000	0	111
Cl23	F26	6.677866	0.969141	0.061500	0.000000	0	113
C5	F27	6.701185	0.645436	0.052400	0.000000	0	112
C14	Cl19	6.705037	0.483664	0.056500	0.000000	0	112
F24	H29	6.705777	0.432492	0.053400	0.000000	0	112
C13	H36	6.720875	0.306736	0.156600	0.000000	0	112
C6	Cl19	6.737798	0.301484	0.040700	0.000000	0	112
C8	C13	6.742485	0.449899	0.050700	0.000000	0	112

F26	H40	6.744114	0.538139	0.061500	0.000000	0	112
C17	H30	6.747415	0.619925	0.085100	0.000000	0	112
C18	H33	6.748540	0.239056	0.087100	0.000000	0	112
C6	F27	6.760840	0.182031	0.035900	0.000000	0	112
Cl19	H33	6.782899	0.457762	0.047900	0.000000	0	113
C18	Cl19	6.798926	0.691299	0.065300	0.000000	0	113
C12	H38	6.803807	0.522832	0.068600	0.000000	0	112
C7	Cl21	6.809967	0.307486	0.047900	0.000000	0	112
C13	H30	6.828341	0.274622	0.069900	0.000000	0	112
Cl21	F28	6.832357	0.968089	0.066100	0.000000	0	113
F28	H40	6.849350	0.589461	0.028200	0.000000	0	112
Cl21	H40	6.871924	0.780346	0.004400	0.000000	0	112
C14	H31	6.873146	0.309680	0.065800	0.000000	0	113
C11	H39	6.875431	0.560048	0.091700	0.000000	0	112
C18	H37	6.875826	0.572504	-0.028900	0.000000	0	112
C12	H34	6.890109	0.552695	0.068900	0.000000	0	112
Si1	F28	6.893815	0.394084	0.044500	0.000000	0	113
C9	H34	6.899097	0.332358	0.069800	0.000000	0	113
C12	H33	6.902120	0.535888	0.082900	0.000000	0	112
C12	H39	6.905426	0.401143	0.072600	0.000000	0	113
C6	Cl22	6.908048	0.545942	0.033900	0.000000	0	112
C11	F24	6.923332	0.546071	0.054500	0.000000	0	113
Si2	Cl21	6.923857	0.393333	0.047300	0.000000	0	113
F28	H38	6.949187	0.677100	0.057200	0.000000	0	112
C17	H31	6.950924	0.576706	0.070800	0.000000	0	112
F27	H34	6.955755	0.414334	0.041100	0.000000	0	112
C8	F28	6.964410	0.310938	0.046000	0.000000	0	112
C17	H35	6.995377	0.549394	0.086300	0.000000	0	112
C7	C18	7.002450	0.398877	0.051700	0.000000	0	112
F27	H32	7.031496	0.407130	0.033800	0.000000	0	112
F28	H32	7.052266	0.525233	0.031200	0.000000	0	112
C9	F26	7.054352	0.578210	0.053800	0.000000	0	113
C11	F26	7.061361	0.699860	0.054900	0.000000	0	113
C17	H36	7.068897	0.431630	0.093400	0.000000	0	113
Cl21	H30	7.077947	0.335849	0.064500	0.000000	0	112
C16	H36	7.091771	0.598936	0.119800	0.000000	0	113
C6	F28	7.093356	0.227351	0.043900	0.000000	0	112
C5	C16	7.097723	0.353985	0.054200	0.000000	0	113
Cl22	H36	7.099311	0.482764	0.166900	0.000000	0	112
C11	H38	7.109645	0.620112	0.099500	0.000000	0	113
C18	H29	7.124101	0.658859	0.044200	0.000000	0	113
F28	H34	7.129990	0.536638	0.046600	0.000000	0	112
F26	H37	7.142163	0.738778	-0.064500	0.000000	0	112
Cl19	H32	7.153111	0.420066	0.038500	0.000000	0	113
Cl21	H37	7.157949	0.730197	0.094500	0.000000	0	113
Si2	Cl23	7.159951	0.454608	0.049400	0.000000	0	113
C5	Cl22	7.163945	0.205903	0.037400	0.000000	0	113
C5	C18	7.179873	0.457913	0.055400	0.000000	0	113
C16	H29	7.188948	0.555232	0.048600	0.000000	0	113
Cl22	H40	7.193180	0.553580	0.037500	0.000000	0	113
C7	F27	7.202926	0.452506	0.053400	0.000000	0	113
C6	C11	7.204502	0.310131	0.045100	0.000000	0	113
C8	Cl22	7.232356	0.449953	0.045700	0.000000	0	113
C6	C13	7.258319	0.387025	0.044700	0.000000	0	113
F24	H31	7.261582	0.309080	0.071300	0.000000	0	113
C16	Cl19	7.287018	0.590225	0.064900	0.000000	0	113
F27	H37	7.315421	0.551177	0.030200	0.000000	0	113
C13	H32	7.324154	0.528950	0.007300	0.000000	0	113
C16	H35	7.324498	0.677482	0.142800	0.000000	0	113
F26	H39	7.343488	0.315237	0.102400	0.000000	0	113
F27	H31	7.346167	0.732750	0.077800	0.000000	0	113
F27	H30	7.364561	0.724941	0.093600	0.000000	0	113
Cl22	H29	7.367569	0.440942	0.043300	0.000000	0	113
C14	Cl21	7.368042	0.617228	0.059100	0.000000	0	114
C16	H30	7.378942	0.459549	0.084900	0.000000	0	114

C16	Cl21	7.384435	0.745380	0.061600	0.000000	0	114
C13	H38	7.386822	0.630775	0.091000	0.000000	0	113
Cl22	H34	7.394430	0.730197	0.071600	0.000000	0	113
C13	H39	7.398027	0.490503	0.093600	0.000000	0	113
C11	H32	7.409947	0.450704	0.018600	0.000000	0	113
Cl23	H29	7.443094	0.561690	0.045900	0.000000	0	113
Cl19	H34	7.480993	0.364821	0.078600	0.000000	0	114
C8	Cl21	7.484275	0.601489	0.067300	0.000000	0	113
C7	F26	7.491425	0.510928	0.062800	0.000000	0	113
C7	Cl23	7.506712	0.293911	0.052100	0.000000	0	113
Cl23	H37	7.513032	0.718332	0.012700	0.000000	0	113
F27	H33	7.517955	0.239966	0.079900	0.000000	0	114
Cl23	H35	7.522444	0.800634	0.043400	0.000000	0	113
Cl23	F24	7.529821	0.776406	0.064800	0.000000	0	114
Cl22	H31	7.553533	0.322746	0.043100	0.000000	0	113
C5	Cl23	7.557600	0.269581	0.049200	0.000000	0	113
Cl19	F24	7.577715	0.447408	0.064100	0.000000	0	114
C11	H33	7.595655	0.430621	0.080600	0.000000	0	114
C18	H36	7.597502	0.504664	0.119800	0.000000	0	114
Cl21	H36	7.600181	0.395847	0.151300	0.000000	0	114
C18	H35	7.614072	0.653903	0.117400	0.000000	0	113
C18	H30	7.623347	0.543334	0.091700	0.000000	0	114
F27	H35	7.629821	0.638961	0.072600	0.000000	0	114
Cl22	H38	7.647277	0.626821	0.064800	0.000000	0	114
Cl22	H33	7.664468	0.653950	0.095500	0.000000	0	114
Cl19	F28	7.682564	0.787947	0.075600	0.000000	0	114
Cl23	H40	7.749042	0.740259	0.034300	0.000000	0	113
Cl23	H31	7.759220	0.380718	0.050900	0.000000	0	113
C13	H33	7.800371	0.486378	0.091200	0.000000	0	114
Cl22	H30	7.832604	0.278937	0.071000	0.000000	0	114
C13	H34	7.864295	0.543934	0.078500	0.000000	0	114
C11	H34	7.866089	0.440963	0.078700	0.000000	0	114
F27	H36	7.886805	0.470190	0.104200	0.000000	0	114
C16	H31	7.899314	0.398695	0.077200	0.000000	0	114
C18	H31	7.932372	0.516355	0.078600	0.000000	0	114
F26	H36	7.934947	0.704911	0.145800	0.000000	0	114
F28	H39	7.940659	0.306965	0.114800	0.000000	0	114
Cl21	H39	7.954223	0.699215	0.116500	0.000000	0	114
F28	H37	7.967772	0.652601	-0.012900	0.000000	0	114
Cl22	H39	8.002667	0.443661	0.081900	0.000000	0	114
F28	H33	8.042476	0.255854	0.105100	0.000000	0	114
C7	F28	8.148328	0.479333	0.068500	0.000000	0	114
C8	Cl23	8.167777	0.582305	0.073000	0.000000	0	114
F26	H35	8.218124	0.817775	0.171400	0.000000	0	114
Cl21	H38	8.247690	0.789446	0.126500	0.000000	0	114
C5	F26	8.249922	0.229674	0.068200	0.000000	0	115
F28	H29	8.300656	0.708058	0.052400	0.000000	0	114
C5	F28	8.380051	0.339544	0.068100	0.000000	0	115
Cl23	H36	8.387981	0.222048	0.183400	0.000000	0	115
F26	H29	8.414990	0.359411	0.063200	0.000000	0	115
F26	H30	8.468895	0.293288	0.098200	0.000000	0	115
Cl23	H30	8.474251	0.218637	0.093500	0.000000	0	115
Cl21	F26	8.508750	0.554669	0.076200	0.000000	0	115
Cl21	F24	8.509227	0.407573	0.072600	0.000000	0	115
Cl19	F26	8.525532	0.410282	0.078000	0.000000	0	115
C6	Cl21	8.684365	0.234992	0.063900	0.000000	0	115
F28	H35	8.704338	0.509717	0.127200	0.000000	0	115
Cl23	H38	8.721417	0.536307	0.111200	0.000000	0	115
C6	Cl23	8.757008	0.325597	0.062900	0.000000	0	115
F28	H36	8.792021	0.360013	0.147300	0.000000	0	115
Cl23	H32	8.801544	0.411587	0.021400	0.000000	0	115
F28	H30	8.876985	0.570742	0.107800	0.000000	0	116
Cl23	H39	8.890935	0.382087	0.123100	0.000000	0	115
Cl21	H32	8.977228	0.458244	0.042300	0.000000	0	116
Cl21	H33	9.008418	0.436794	0.096900	0.000000	0	116

F26	H31	9.033767	0.405744	0.091700	0.000000	0	116
F28	H31	9.080243	0.593542	0.092100	0.000000	0	116
Cl23	H34	9.279257	0.683541	0.094100	0.000000	0	116
Cl21	H34	9.314665	0.497693	0.095900	0.000000	0	116
Cl23	H33	9.365048	0.536393	0.116100	0.000000	0	116

SAPT Calculations

For the energy decomposition analysis. the optimized geometries of the different conformers were used in the PSI4[10] program. The different contributions in kJ mol^{-1} of the aryl interactions are given in Table S22.

The SAPT calculation was performed using the density-fitted self-consistent field method at the Hartree-Fock level of theory with the jun-cc-pvdz basis set. The separation for the F-SAPT calculation, based on the SAPT0 approximation, was set at the bond of the ipso carbon atom of the aryl group and the respective silicon atom in order to determine only the energetic contributions occurring between the aryl moieties.

	3	**4**	**5**
total SAPT	–9.71469	–19.52462	–17.14793
electrostatics	–10.60639	–16.15416	–13.39899
exchange	34.87594	51.18166	51.63418
induction	–4.20696	–5.679	–5.62762
Induction from heavy to light	–1.5598	–1.85052	–1.95755
Induction from light to heavy	–2.64717	–3.82848	–3.67007
dispersion	–29.77718	–48.87312	–49.75549

References

[1] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, *J. Appl. Crystallogr.* **2009**, *42*, 339.

[2] G. M. Sheldrick, *Acta Crystallogr., Sect. A: Found. Crystallogr.* **2008**, *64*, 112.

[3] G. M. Sheldrick, *Acta Crystallogr., Sect. A: Found. Crystallogr.* **2015**, *71*, 3.

[4] G. M. Sheldrick, *Acta Crystallogr., Sect. C: Cryst. Struct. Chem.* **2009**, *42*, 339.

[5] a) C. G. Reuter, Yu. V. Vishnevskiy, S. Blomeyer, N. W. Mitzel, *Z. Naturforsch.* **2016**, *71b*, 1; b) R. J. F. Berger, M. Hoffmann, S. A. Hayes, N. W. Mitzel, *Z. Naturforsch.* **2009**, *64b*, 1259.

[6] Yu. V. Vishnevskiy, *J. Mol. Struct.* **2007**, *833*, 30.

[7] Yu. V. Vishnevskiy, *J. Mol. Struct.* **2007**, *871*, 24.

[8] Yu. V. Vishnevskiy, "UNEX, v. 1.6.0", http://unexprog.org, **2013**.

[9] a) V. A. Sipachev, *J. Mol. Struct. THEOCHEM* **1985**, *121*, 143; b) V. A. Sipachev, *J. Mol, Struct,* **2001**, *567-568*, 67; c) V. A. Sipachev, *J. Mol. Struct.* **2004**, *693*, 235. d) Yu. V. Vishnevskiy, Yu. A. Zhabanov, *J. Phys.: Conf. Ser.* **2015**, *633*, 012076.