Supporting information for the article

Formation of Formal Disilene Fluoride Adducts

Michaela Zirngast, Michaela Flock, Judith Baumgartner, Christoph Marschner*

Institut für Anorganische Chemie, Technische Universität Graz, Stremayrgasse 16,

A-8010 Graz, Austria

Tel: ++43-316-873-8209; Fax: ++43-316-873-8701

e-mail: christoph.marschner@tugraz.at

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Experimental details:

Synthesis of fluorosilanes

*Triisopropylsilylbis(trimethylsilyl)silane (**1a**):*

To a stirred solution of tris(trimethylsilyl)(tri-*iso*-propylsilyl)silane[1] (522 mg, 1.29 mmol) in THF (6 mL) KO^{t}Bu (159 mg, 1.42 mmol, 1.1 equiv) was added. After 16 h the mixture was added to ice cooled 0.5 M H_2SO_4/Et_2O. The aqueous phase was extracted twice with Et_2O and the combined organic layers were washed with brine and dried over Na_2SO_4. Removal of the solvent gave **1a** as the product (417 mg, 97 %) as a colorless oil. ^{29}Si NMR (C_6D_6, δ ppm): 14.5; -11.5; -125.7. ^{1}H NMR (C_6D_6, δ ppm): 2.55 (s, 1H); 1.42 (m, 3H); 1.14 (d, J = 7 Hz, 18H); 0.30 (s, 18H). ^{13}C NMR (C_6D_6, δ ppm): 20.2; 13.9; 2.7. MS (70 eV): *m/z* (%): 332 (7) [M^+], 289 (31) [M^+ - iPr], 160 (100) [M^+ - $HSi(SiMe_3)_2$ - Me], 115 (65) [$HSi(iPr)_2$]

*Chloro(triisopropylsilyl)bis(trimethylsilyl)silane (**1b**)*:

A solution of **1a** (1.57 g, 4.71 mmol) in CCl_4 (8 mL) was stirred for 5 days at r.t. (completeness of conversion was controlled by ^{29}Si-NMR). After the solvent was removed compound **1b** was obtained as a colorless crystalline solid (1.31g, 76%) which was used without further purification. ^{29}Si NMR (C_6D_6, δ ppm): 11.1 (*Si*^{i}Pr$_3$); -8.0 (*Si*-Cl); -10.6 (*Si*Me$_3$). ^{1}H NMR (C_6D_6, δ ppm): 1.37 (m, 3H); 1.18 (d, J = 7.2 Hz, 18H); 0.30 (s, 18H). ^{13}C NMR (C_6D_6, δ ppm): 20.3; 13.5; 0.5. Anal. calcd. for $C_{15}H_{39}ClSi_4$ (367.26): C 49.05, H 10.70. Found: C 48.64, H 10.66. GC/MS: 366 (2) M^+; 351 (5) M^+-Me; 281 (2); 258 (5); 239 (17); 216 (17); 194 (40); 174 (90); 157 (45); 129 (27); 115 (90); 87 (43); 73 (100) $SiMe_3$.

[1] Kayser, C.; Fischer, R.; Baumgartner, J.; Marschner, C.; *Organometallics* **2002**, *21*, 1023–1030.

Fluorobis(trimethylsilyl)(triisopropylsilyl)silane (**1**):

Compound **1b** (0.76g, 2.06 mmol) was dissolved in Et_2O (5 mL) and $[Ph_3SnF_2][NBu_4]$[2] (0.91g, 1.44 mmol, 0.7 equiv) was added. After stirring for 15 hours at r.t. the reaction was complete (controlled by ^{29}Si-NMR) and the precipitate was removed by filtration. The solvent was completely removed and the residue treated with pentane. Again precipitation occurred which was removed by centrifugation. The product was obtained as a colorless oil (0.67 g, 93%) after removal of the pentane. ^{29}Si-NMR (C_6D_6, δ ppm): 40.1 (d, J_{Si-F} = 324.0 Hz, *Si*-F); 6.4 (d, J_{Si-F} = 12.1 Hz, iPr_3Si-); -15.0 (d, J_{Si-F} = 17.7 Hz, Me_3Si-). ^{1}H NMR (C_6D_6, δ ppm): 1.14 (d, J_{H-H} = 6.7 Hz, 18H), 0.28 (s, 18 H). ^{13}C NMR (C_6D_6, δ ppm): 20.2; 17.2 (d, J_{C-F} = 1.9 Hz); 13.6; 0.7 (d, J_{C-F} = 1.5 Hz). ^{19}F NMR (C_6D_6, δ ppm): -250.5 (J_{Si-F} = 325.2 Hz). GC/MS: 350 (2) M^+; 335 M^+-Me; 258 (5); 223 (5); 216 (3); 193 (2); 174 (100); 159 (25); 129 (20); 115 (30); 87 (22); 73 (80) $SiMe_3$; 59 (55) $SiMe_2$.

*(tert-Butyldimethylsilyl)bis(trimethylsilyl)silane (**5a**)*:

Compound **5a** was obtained in an analogous way as described above for **1b** from the reaction of *tert*-butyldimethylsilyltris(trimethylsilyl)silane[1,3] (1.32 g, 3.64 mmol) and KO^tBu (449 mg, 4.00 mmol, 1.1 equiv) after hydrolysis as a colorless oil (994 mg, 94 %). ^{29}Si NMR (C_6D_6, δ ppm): 2.3; -11.2; -119.9. ^{1}H NMR (C_6D_6, δ ppm): 2.27 (s, 1H); 0.97 (s, 9H); 0.24 (s, 18H); 0.17 (s, 6H).

*Chloro(tert-butyldimethylsilyl)bis(trimethylsilyl)silane (**5b**):*

The preparation of **5b** was accomplished as described above for **1b** reacting **5a (**1.01 g, 3.47 mmol) in CCl_4 (8 mL) to give **5b** after 4 d as a colorless oil (0.82g, 73%). ^{29}Si-NMR (C_6D_6, δ

[2] a) Gingras, M., *Tetrahedron Lett.* **1991**, *32*, 7381–7384. b) Hummeltenberg, R.; Jurkschat, K.; Uhlig, F. *Phosphorus, Sulfur Silicon Relat. Elem.* **1997**, *123*, 255–261.

[3] Apeloig, Y.; Yuzefovich, M.; Bendikov, M.; Bravo-Zhivotovskii, D.; Klinkhammer, K.; *Organometallics* **1997**, *16*, 1265–1269.

ppm): 2.9; -11.2; -11.7. ^{1}H NMR (C_6D_6, δ ppm): 0.97 (s, 9H); 0.26 (s, 18H); 0.22 (s, 6H). ^{13}C NMR (C_6D_6, δ ppm): 27.8; 18.4, -0.4; -4.25. GC/MS: 324 (1) M^+; 309(1) M^+-Me; 267 (6); 216 (25); 194 (5); 174 (48); 158 (30); 143(17); 131 (30); 116 (46); 85 (4); 73 (100) $SiMe_3$; 59 (9) $SiMe_2$.

*Fluoro(tert-butyldimethylsilyl)bis(trimethylsilyl)silane (**5**):*

The preparation of **5** was carried out as described above for **1** using **5b** (300 mg, 0.92 mmol) and $[Ph_3SnF_2][NBu_4]$ (580 mg, 0.92 mmol) to give **5** as a colorless oil (150 mg, 51%). ^{29}Si-NMR (C_6D_6, δ ppm): 35.6 (d, J_{Si-F} = 327.7 Hz); -3.0 (d, J_{Si-F} =14.9 Hz); -15.5 (d, J_{Si-F} =17.5 Hz). ^{1}H NMR (C_6D_6, δ ppm): 1.01 (s, 9H); 0.23 (s, 18H); 0.15 (s, 6 H). ^{13}C NMR (C_6D_6, δ ppm): 27.6 (d, J_{C-F} = 0.7 Hz); 18.3, -0.4 (d, J_{C-F} =1.5 Hz); -4.2 (d, J_{C-F} = 2.0 Hz). ^{19}F NMR (C_6D_6, δ ppm): -252.6 (J_{Si-F} = 327.4 Hz). GC/MS: 308(1) M^+; 293(1); 251(1); 216(9); 201(2); 174(51); 159(22); 131(15); 116(25); 99(10); 73(100); 59(15).

*1,1-Bis(trimethylsilyl)-2,2-dimethyl-2-thexyldisilane (**7a**):*

The preparation of compound **7a** was accomplished in an analogous way as described above for **1a** from thexyldimethylsilyltris(trimethylsilyl)silane[1] (500 mg, 1.28 mmol) and KO^{t}Bu (158 mg, 1.41 mmol, 1.1 equiv). After hydrolysis **7a** was obtained as a colorless oil (400 mg, 98 %). ^{29}Si NMR (C_6D_6, δ ppm): 2.8; -11.4; -116.0. ^{1}H NMR (C_6D_6, δ ppm): 2.53 (s, 1H); 1.73, (hept, J = 7.0 Hz, 1H), 0.92 (s, 12H); 0.91 (d, J = 7.0 Hz, 6H), 0.27 (s, 18H); 0.25 (s, 6H). ^{13}C NMR (C_6D_6, δ ppm): 35.1; 31.5; 24.6; 21.5; 19.0; 2.5; 0.3.

*1-Chloro-1,1-bis(trimethylsilyl)-2,2-dimethyl-2-thexyldisilane (**7b**):*

The preparation of **7b** was carried out as described above for **1b** reacting **7a (**1.22 g, 3.83 mmol) in CCl_4 (10 mL) to give **7b** after 4 d as a colorless oil (1.04g, 77%).^{29}Si-NMR ($CDCl_3$,

δ ppm): 6.0; -10.0; -10.5. ^{1}H NMR ($CDCl_3$, δ ppm): 1.77 (hept, J = 6.8 Hz, 1H); 0.97 (s, 6H); 0.91 (d, J = 6.8 Hz, 6H); 0.30 (s, 6H); 0.29 (s, 18H). ^{13}C NMR ($CDCl_3$, δ ppm): 35.2; 25.4; 22.4; 19.1; 0.1; -2.1.

1-Fluoro-1,1-bis(trimethylsilyl)-2,2-dimethyl-2-thexyldisilane (**7**):

The preparation of **7** was carried out as described above for **1** using **7b** (1.04 g, 2.93 mmol) and $[Ph_3SnF_2][NBu_4]$ (1.29 g, 2.05 mmol, 0.7 equiv.) to give **7** as a colorless oil (700 mg, 71%). ^{29}Si-NMR (C_6D_6, δ ppm): 33.4 (d, J_{Si-F} =326.5 Hz); -1.7 (d, J_{Si-F} =14.3 Hz); -15.3 (d, J_{Si-F} =17.9 Hz). ^{1}H NMR (C_6D_6, δ ppm): 1.72 (hept, J = 6.9 Hz); 0.94 (s, 6H); 0.88 (d, J = 6.9 Hz); 0.25 (s, 18H); 0.21 (s, 6H). ^{13}C NMR (C_6D_6, δ ppm): 35.1; 25.6; 21.8; 18.7 (d, J_{C-F} = 0.6 Hz); -0.1 (d, J_{C-F} = 1.4 Hz); -2.3 (d, J_{C-F} = 1.8 Hz). ^{19}F NMR (C_6D_6, δ ppm): -249.1 (J_{Si-F} = 327.7 Hz).

*2,2-Bis(trimethylsilyl)-1,1,1,3,3,4,4,4-octamethyltetrasilane (**9a**)*

The preparation of **9a** was carried out in an analogous manner as for **1a** using 1,1,1-tris(trimethylsilyl)-2,2,3,3,3-pentamethyltrisilane[3] (500 mg, 1.32 mmol) and KO^{t}Bu (163 mg, 1.45 mmol, 1.1 equiv). After hydrolysis **9a** (385 mg, 95 %) was obtained as a colorless oil. ^{29}Si-NMR (C_6D_6, δ ppm): -11.2; -16.1; -41.7; -116.2. ^{1}H NMR (C_6D_6, δ ppm): 2.57 (s, 1H); 0.30 (s, 6H); 0.26 (s, 18H); 0.17 (s, 9H). ^{13}C NMR (C_6D_6, δ ppm): 2.2; -1.6; -2.6.

*2-Chloro-2-(trimethylsilyl)-1,1,1,3,3,4,4,4-octamethyltetrasilane (**9b**)*

The preparation of **9b** was carried out as described above for **1b** reacting **9a** (385 mg, 1.26 mmol) in CCl_4 (5 mL) to give **9b** after 18h as a colorless oil (264 mg, 62 %).^{29}Si-NMR (C_6D_6, δ ppm): -6.6; -10.8; - 14.8; -38.5. ^{1}H NMR (C_6D_6, δ ppm): 0.28 (s. 6H); 0.27 (s. 18H); 0.19 (s. 9H). ^{13}C NMR (C_6D_6, δ ppm): -0.2; -1.0; -4.4.

*2-Fluoro-2-(trimethylsilyl)-1,1,1,3,3,4,4,4-octamethyltetrasilane(**9**):*

The preparation of **9** was carried out as described above for **1** using **9b** (244 mg, 0.715 mmol) and $[Ph_3SnF_2][NBu_4]$ (316 mg, 0.500 mmol, 0.7 equiv.) to give **9** as a colorless oil (190 mg, 82 %). ^{29}Si-NMR (C_6D_6, δ ppm): 38.7 (d, J_{Si-F} = 329.4 Hz); -15.3 (d, J = 17.8 Hz); -15.3 (d, J = 1.8 Hz); -42.7 (d, J = 18.6 Hz). ^{1}H NMR (C_6D_6, δ ppm): 0.27 (s. 6H); 0.24 (s. 18H); 0.20 (s. 9H). ^{13}C NMR (C_6D_6, δ ppm): -0.4 (d, J = 1.4 Hz); -1.4; -4.9 (d, J = 2.8 Hz). ^{19}F NMR (C_6D_6, δ ppm): -250.2 (J_{Si-F} = 329.3 Hz, J = 17.8 Hz).

*Chloro(undecamethylcyclohexasilanyl)bis(trimethylsilyl)silane (**11b**)*

The preparation of **11b** was carried out as described above for **1a** reacting undecamethylcyclohexasilanylbis(trimethylsilyl)silane (120 mg, 0.258 mmol) in CCl_4 (3 mL) to give **11b** after 18h as a colorless oil (120 mg, 94 %).^{29}Si-NMR ($CDCl_3$, δ ppm): 1.1; -10.3; -36.3; -40.2; -42.7; -68.5. ^{1}H NMR ($CDCl_3$, δ ppm): 0.49 (s, 3H); 0.43 (s, 6H); 0.38 (s, 6H); 0.32 (s, 18H); 0.22 (s, 9H); 0.20 (s, 9H). ^{13}C NMR ($CDCl_3$, δ ppm): 0.0; -2.6; -4.1; -4.7; -5.1; -6.5; -6.7; -7.3.

*Fluoro(undecamethylcyclohexasilanyl)bis(trimethylsilyl)silane (**11**)*

The preparation of **11** was carried out as described above for **1** using **11b** (120 mg, 0.221 mmol) and $[Ph_3SnF_2][NBu_4]$ (97 mg, 0.154 mmol, 0.7 equiv.) to give **11** as a colorless oil (85 mg, 73 %). ^{29}Si-NMR (C_6D_6, δ ppm): 45.3 (d, J = 335.0 Hz); -15.0 (d, J = 18.2 Hz); -37.1 (d, J = 4.7 Hz); -40.3 (d, J = 1.1 Hz); -42.6; -72.1 (d, J = 15.0 Hz). ^{1}H NMR (C_6D_6, δ ppm): 0.46 (s, 3H); 0.39 (d, J = 1.2 Hz, 12H); 0.29 (s, 18H); 0.24 (d, J = 0.3 Hz, 6H); 0.22 (s, 12 H). ^{13}C NMR (C_6D_6, δ ppm): -0.1 (d, J = 1.3 Hz); -2.6; -4.3; -4.6; -6.8. ^{19}F NMR (C_6D_6, δ ppm): -241.5 (J_{Si-F} = 334.3 Hz, J = 18.3 Hz).

*Fluoromethylbis(trimethylsilyl)silane (**13**)*[4]*:*

The preparation of **13** was carried out as described above for **1** using chloromethylbis-(trimethylsilyl)silane (580 mg, 2.93 mmol) and $[Ph_3SnF_2][NBu_4]$ (1.13 g, 1.81 mmol, 0.7 equiv) to give **13** as a colorless oil (489 mg, 90%). ^{29}Si-NMR (C_6D_6, δ ppm): 36.2 (d, J_{Si-F} =324.3 Hz); -19.6 (d, J_{Si-F} = 20.8 Hz). ^{1}H NMR (C_6D_6, δ ppm): 0.44 (d, J_{H-F} = (9.8 Hz, 3H)); 0.12 (s, 18H). ^{13}C NMR (C_6D_6, δ ppm): -1.4 (d, J_{C-F} = 11.5 Hz); -2.3 (d, J_{C-F} = 1.4 Hz). ^{19}F NMR (C_6D_6, δ ppm): -209.7 (J_{Si-F} = 324.8 Hz; J_{F-H} = 9.8 Hz). GC/MS: 208(8) M^+; 193 (8); 175 (2); 145(2); 131(10); 116(65); 101(25); 73(100) $SiMe_3$.

*Chlorobis(trimethylsilyl)phenylsilane (**14b**)*[4]*:*

^{29}Si-NMR (C_6D_6, δ ppm): -2.5; -14.1. ^{1}H NMR (C_6D_6, δ ppm): 7.58 (m, 2H); 7.42 (m, 3H); 0.27 (s, 18H). ^{13}C NMR (C_6D_6, δ ppm): 135.5; 133.5; 129.2; 128.3; -1.7. GC/MS: 286(5) M+; 271(5); 251(1); 213(1); 193(8); 175(80); 163(100); 135(85); 105(25); 93 (5); 73(75); 45(39)

Fluorobis(trimethylsilyl)phenylsilane (**14**):

The preparation of **14** was carried out as described above for **1** using **14b** (440 mg, 1.54 mmol) and $[Ph_3SnF_2][NBu_4]$ (680 mg, 1.08 mmol, 0.7 equiv) to give **14** as a colorless oil (340 mg, 82%). ^{29}Si-NMR (C_6D_6, δ ppm): 26.9 (d, J_{Si-F} = 327.2 Hz); -18.5 (d, $^{2}J_{Si-F}$ =20.2 Hz). ^{1}H NMR (C_6D_6, δ ppm): 7.51 (m, 2H); 7.42 (m, 3H); 0.24 (s, 18H). ^{13}C NMR (C_6D_6, δ ppm): 132.5; 132.4; 129.1; 128.3; 1.7 (d, J_{C-F} = 1.4 Hz). ^{19}F NMR (C_6D_6, δ ppm): -216.9 (J_{Si-F} = 327.2 Hz).

[4] Schenzel, K.; Hassler, K.; in *Organosilicon Chemistry II: From Molecules to Materials*, Auner, N.; Weis, J., (eds).; Verlag Chemie, Weinheim, (1996), 95–100.

tert-Butylfluorobis(trimethylsilyl)silane (**15**):

To a cooled solution (-70°C) of difluorobis(trimethylsilyl)silane (450 mg, 2.09 mmol) in Et_2O (10 mL) ^{t}BuLi (1.40 mL, 1.5 molar in pentane, 2.09 mmol) was added slowly. The reaction mixture was stirred for 16 h at r.t. then the solvent was removed. The residue was suspended in pentane and the solid components removed by centrifugation. After the solvent was removed compound **15** was obtained as colorless oil (420 mg, 81%). ^{29}Si-NMR (C_6D_6, δ ppm): 39.0 (d, $J_{Si\text{-}F}$ = 333.1 Hz); -19.9 (d, $J_{Si\text{-}F}$ = 20.5 Hz). ^{1}H NMR (C_6D_6, δ ppm): 1.09 (d, J = 1.4 Hz, 9H); 0.19 (d, J = 0.3 Hz, 18H). ^{13}C NMR (C_6D_6, δ ppm): 27.4 (d, $J_{C\text{-}F}$ = 1.3 Hz); 22.8 (d, $J_{C\text{-}F}$ = 9.8 Hz); -0.5 (d, $J_{C\text{-}F}$ = 1.4 Hz). ^{19}F NMR (C_6D_6, δ ppm): -213.9 ($J_{Si\text{-}F}$ = 334.7 Hz).

Complete Reference 22:

Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

Minimum structures optimized at the mPW1PW91/6-31+G* level with Gaussian03

A, G = -2316.311356 hartree

Si	1.22455	0.90386	-0.55537
Si	1.73530	-0.99473	0.68604
Si	1.56931	3.02828	0.40811
Si	1.78698	1.10173	-2.83433
Si	3.06636	-2.18021	-0.84697
Si	3.39922	-0.09030	2.07465
H	0.95010	4.11028	-0.41491
H	0.95570	3.11526	1.76508
H	3.02115	3.32858	0.53387
H	3.22967	1.43976	-2.97565
H	1.53038	-0.16224	-3.58175
H	0.99878	2.17770	-3.50702
F	-0.51476	0.91135	-0.66883
Li	-1.82116	-0.19432	0.09099
O	-1.92704	-0.62780	2.01480
O	-3.40476	1.04295	-0.08496
O	-2.23179	-1.78775	-1.01547
C	-1.23616	-2.76564	-1.29280
C	-3.30758	-1.84221	-1.93159
C	-1.30562	0.29297	2.90115
C	-1.78137	-1.96897	2.46072
C	-4.53116	1.00234	0.77028
C	-3.40937	2.17514	-0.93882
H	-2.95435	-1.66659	-2.95552
H	-3.80297	-2.82022	-1.88552
H	-4.01474	-1.06085	-1.65270
H	-0.82476	-2.61973	-2.29807
H	-0.44000	-2.63787	-0.55706
H	-1.66343	-3.77286	-1.21430
H	-4.28978	2.15878	-1.59364
H	-3.41578	3.10013	-0.34939
H	-2.49999	2.13564	-1.53629
H	-5.45804	0.92502	0.18728
H	-4.42134	0.12749	1.41072
H	-4.57584	1.90415	1.39387
H	-0.23279	0.08550	2.97783
H	-1.45340	1.29287	2.49038
H	-1.77127	0.23389	3.89277
H	-0.72176	-2.24710	2.48702
H	-2.22859	-2.08417	3.45598
H	-2.31072	-2.60408	1.74934
H	3.94111	-1.14666	2.98396
H	4.59561	0.54406	1.43777
H	2.82037	0.95917	2.97347
H	3.75476	-3.31258	-0.15348
H	2.22913	-2.82077	-1.91321
H	4.14131	-1.44347	-1.58284

B, G = -2316.307266 hartree

Si	1.46013	1.07083	0.12162
Si	3.20628	-0.37699	0.48521
Si	0.95616	2.31805	2.05697
Si	1.82856	2.68187	-1.55819
Si	3.38037	-1.40570	-1.62472
Si	2.03081	-2.02694	1.66819
H	-0.41674	2.91550	1.98006
H	0.98484	1.50150	3.30374
H	1.90709	3.45051	2.23310
H	3.07637	3.45322	-1.31074
H	1.91524	2.07237	-2.91564
H	0.70173	3.66537	-1.60967
F	-0.13978	0.51595	-0.33857
Li	-1.79878	-0.25876	-0.17676
O	-2.26159	-1.21409	1.48100
O	-3.12386	1.21180	-0.30271
O	-2.01700	-1.50282	-1.68896
C	-0.85355	-2.19629	-2.12891
C	-2.98239	-1.36068	-2.71259
C	-1.89199	-0.67075	2.74118
C	-2.43694	-2.62177	1.53442
C	-4.33534	1.28136	0.42580
C	-2.79179	2.44396	-0.92553
H	-2.56890	-0.80413	-3.56296
H	-3.32314	-2.34414	-3.05906
H	-3.82563	-0.80968	-2.29488
H	-0.36360	-1.64920	-2.94124
H	-0.16930	-2.26463	-1.28437
H	-1.12082	-3.20313	-2.47053
H	-3.56731	2.72689	-1.64766
H	-2.68316	3.23599	-0.17588
H	-1.84118	2.30588	-1.43864
H	-5.17351	1.52043	-0.24074
H	-4.49685	0.30535	0.88374
H	-4.27150	2.04609	1.20972
H	-0.93969	-1.09193	3.07935
H	-1.78529	0.40717	2.61534
H	-2.67172	-0.87537	3.48507
H	-1.50649	-3.11387	1.83761
H	-3.23629	-2.87709	2.24100
H	-2.71428	-2.95061	0.53288
H	2.89790	-3.19633	2.00991
H	1.50708	-1.52739	2.98137
H	0.82527	-2.65537	1.01674
H	4.52814	-2.36427	-1.64921
H	2.21964	-2.21020	-2.13899
H	3.66600	-0.40605	-2.70001

C, G = -2316.312968 hartree

Si	-1.59785	-0.61485	-1.36286
Si	0.13043	0.86052	-0.79467
Si	-3.79691	0.18502	-1.07544
Si	-1.53294	-1.67778	-3.46351
Si	1.54620	0.86639	-2.66454
Si	-0.87901	2.96738	-0.97270
H	-4.80159	-0.90038	-1.27008
H	-4.01233	0.74112	0.29223
H	-4.09400	1.26393	-2.05800
H	-1.76758	-0.68005	-4.54391
H	-0.21144	-2.32240	-3.71035
H	-2.57550	-2.73814	-3.58391
F	-1.51814	-1.89804	-0.27440
Li	1.12062	-0.06774	1.48795
O	2.86221	0.78880	1.95777
O	-0.10702	0.21364	3.03655
O	1.51896	-2.01911	1.44526
C	1.96395	-2.55523	0.20717
C	0.73789	-2.94990	2.17656
C	3.21713	2.05435	1.42138
C	3.97352	0.08903	2.48341
C	0.14657	1.20524	4.01375
C	-1.49811	0.02152	2.81528
H	-0.15815	-3.22662	1.61032
H	1.32680	-3.84907	2.39741
H	0.45006	-2.46612	3.11036
H	1.11094	-2.85622	-0.40977
H	2.52064	-1.77290	-0.30904
H	2.61731	-3.41898	0.38343
H	-1.98587	-0.30558	3.74203
H	-1.96371	0.94887	2.46295
H	-1.60667	-0.74653	2.04998
H	-0.27819	0.90811	4.98084
H	1.22837	1.30375	4.10429
H	-0.28470	2.16783	3.71178
H	3.94455	1.93796	0.60959
H	2.30798	2.50376	1.02217
H	3.64174	2.69490	2.20457
H	4.73259	-0.07242	1.70761
H	4.42403	0.64706	3.31418
H	3.61151	-0.87532	2.83991
H	0.12329	4.03831	-0.67020
H	-1.48717	3.34448	-2.28482
H	-1.96201	3.13511	0.04710
H	2.58769	1.93074	-2.50537
H	2.31144	-0.41603	-2.78106
H	0.93367	1.09593	-4.00843

Dimer 1, G = -2888.522504 hartree

Si	-0.42457800	0.97724000	-0.52204400
Si	0.42457800	-0.97724000	0.52204400
Si	-0.08052800	0.46146500	-2.79534200
Si	0.08052800	-0.46146500	2.79534200
F	-0.51844900	2.84127700	-0.77128400
F	0.51844900	-2.84127700	0.77128400
Si	-2.74291300	0.62857800	-0.28369600
Si	2.74291300	-0.62857800	0.28369600
H	1.23893900	-0.19610400	-3.06271500
H	-1.23893900	0.19610400	3.06271500
H	-1.09344900	-0.44528800	-3.43231500
H	1.09344900	0.44528800	3.43231500
H	-0.08365700	1.68020800	-3.67336200
H	0.08365700	-1.68020800	3.67336200
H	-3.12067500	0.10447400	1.06786200
H	3.12067500	-0.10447400	-1.06786200
H	-3.54613200	1.88918000	-0.44072200
H	3.54613200	-1.88918000	0.44072200
H	-3.37115100	-0.32783400	-1.25439900
H	3.37115100	0.32783400	1.25439900
Li	0.13055900	4.26579400	0.06519100
Li	-0.13055900	-4.26579400	-0.06519100
O	-0.91112700	5.80205600	-0.66567000
O	0.91112700	-5.80205600	0.66567000
O	-0.19118800	4.33539000	2.02155500
O	0.19118800	-4.33539000	-2.02155500
O	2.07627700	4.54928600	-0.24593600
O	-2.07627700	-4.54928600	0.24593600
C	2.86258100	3.36974000	-0.36500500
C	-2.86258100	-3.36974000	0.36500500
C	2.64497100	5.65049600	-0.92090400
C	-2.64497100	-5.65049600	0.92090400
C	-1.44080900	3.78474800	2.41432000
C	1.44080900	-3.78474800	-2.41432000
C	0.84320500	4.01942700	2.93939100
C	-0.84320500	-4.01942700	-2.93939100
C	-1.66474500	5.59330900	-1.85005700
C	1.66474500	-5.59330900	1.85005700
C	-1.22490700	7.01614400	-0.01840200
C	1.22490700	-7.01614400	0.01840200
H	3.84294300	3.51828300	0.10367400
H	-3.84294300	-3.51828300	-0.10367400
H	2.32653700	2.56501000	0.13924700
H	-2.32653700	-2.56501000	-0.13924700
H	2.99388900	3.10019000	-1.41897000
H	-2.99388900	-3.10019000	1.41897000
H	3.63031400	5.89386500	-0.50270100
H	-3.63031400	-5.89386500	0.50270100
H	2.75313200	5.43798600	-1.99233400
H	-2.75313200	-5.43798600	1.99233400

H	1.97427800	6.50032800	-0.78834700
H	-1.97427800	-6.50032800	0.78834700
H	0.60754000	4.42593000	3.93120600
H	-0.60754000	-4.42593000	-3.93120600
H	0.98058900	2.93474500	3.01380400
H	-0.98058900	-2.93474500	-3.01380400
H	1.75747300	4.48118400	2.56528300
H	-1.75747300	-4.48118400	-2.56528300
H	-1.75578700	4.21069200	3.37540700
H	1.75578700	-4.21069200	-3.37540700
H	-2.16700600	4.04252900	1.64290400
H	2.16700600	-4.04252900	-1.64290400
H	-1.37650300	2.69471200	2.49601000
H	1.37650300	-2.69471200	-2.49601000
H	-0.99200800	7.87401400	-0.66319300
H	0.99200800	-7.87401400	0.66319300
H	-2.28897900	7.05099600	0.24927600
H	2.28897900	-7.05099600	-0.24927600
H	-0.62539600	7.06660700	0.89135100
H	0.62539600	-7.06660700	-0.89135100
H	-1.42919700	6.36565900	-2.59320600
H	1.42919700	-6.36565900	2.59320600
H	-1.39821700	4.60757100	-2.22888300
H	1.39821700	-4.60757100	2.22888300
H	-2.73874400	5.61713400	-1.62856500
H	2.73874400	-5.61713400	1.62856500

Dimer 2, G = -2888.522428 hartree

Si	-1.71413700	1.63797200	-0.04593900
Si	-0.39346500	-0.26314200	-0.06981100
Si	-1.85142300	3.02723200	1.85801700
Si	0.86198800	0.06219500	1.87397900
F	-3.37423300	1.07916700	-0.07724000
F	2.66608800	-0.75393100	0.19806100
Si	-1.79860500	3.08186200	-1.91065500
Si	1.05212700	0.29059500	-1.81428400
H	-2.35387500	2.29145600	3.05481300
H	-0.12950100	0.53317200	2.92365400
H	-0.52936700	3.62203300	2.20034800
H	1.92350900	1.11042800	1.95637600
H	-2.79848400	4.16544600	1.64281200
H	1.36938500	-1.19482600	2.50328700
H	-2.14251700	2.35961700	-3.16967900
H	0.22872600	0.83179600	-2.95997700
H	-2.84100100	4.14041500	-1.73575000
H	1.75510800	-0.86923900	-2.44172200
H	-0.49989700	3.78168900	-2.12119000
H	2.07628700	1.36178700	-1.60789800
Li	-3.86306100	-0.73372900	0.01925500
Li	4.30380700	-0.31450400	-0.01863800
O	-5.82898000	-0.43859200	-0.48698100

O	5.04024200	1.46043400	-0.68117800
O	-3.50344200	-2.15313200	-1.33691500
O	5.15485200	-1.73901300	-1.20062100
O	-3.96192200	-1.46686100	1.87950700
O	5.33208100	-0.40236000	1.72942300
C	-2.78647400	-1.77737000	2.61995700
C	4.70170900	-1.19004800	2.72435600
C	-5.06436100	-1.20175300	2.72387700
C	6.62277600	0.02282500	2.09192400
C	-3.07653900	-1.66445700	-2.60060200
C	4.26055100	-2.80325000	-1.48758700
C	-2.81022700	-3.33573700	-0.96892400
C	6.49936500	-2.06634700	-1.44844600
C	-6.43806300	0.83899200	-0.55841000
C	4.52131900	2.57839100	0.02027200
C	-6.67024900	-1.46700600	-0.96852300
C	5.19011800	1.72005400	-2.06362000
H	-2.94084100	-2.69505900	3.20169200
H	5.27746300	-2.10748700	2.90860600
H	-1.97614800	-1.91184200	1.90243500
H	3.70878200	-1.43389500	2.34729500
H	-2.52657900	-0.95217300	3.29188600
H	4.61226400	-0.62488700	3.66092500
H	-5.29706800	-2.08029300	3.33951800
H	7.29049800	-0.83550800	2.25267000
H	-4.85337500	-0.34858300	3.38060400
H	6.59397400	0.62390400	3.01123600
H	-5.91625600	-0.96747300	2.08541900
H	7.00662800	0.63490700	1.27427200
H	-2.98372900	-4.12047400	-1.71670000
H	6.65411600	-2.32283800	-2.50577600
H	-1.73715900	-3.13457800	-0.87188800
H	6.81995000	-2.91558900	-0.82889700
H	-3.21081800	-3.65814800	-0.00665600
H	7.10483500	-1.19298300	-1.19877400
H	-3.26989000	-2.41377900	-3.37890000
H	4.27674100	-3.03549100	-2.56040600
H	-3.65333900	-0.76301500	-2.81297500
H	3.27131700	-2.46265300	-1.18100800
H	-2.01021700	-1.41544400	-2.57323900
H	4.54155500	-3.69953700	-0.91817300
H	-7.58383000	-1.53694900	-0.36317900
H	5.91722400	2.52723100	-2.22540800
H	-6.94862600	-1.28231400	-2.01409900
H	4.22972000	1.99657700	-2.51372800
H	-6.11136300	-2.40007700	-0.90665500
H	5.55227400	0.80261800	-2.52858000
H	-7.34527500	0.86827600	0.05915100
H	5.21422500	3.42750700	-0.05008700
H	-5.71307300	1.56357300	-0.19211200
H	4.40573600	2.28113300	1.06273300

H	-6.70253000	1.08033900	-1.59563200
H	3.54253000	2.86524700	-0.37970000

$(H_3Si)_2FSiLi(OMe_2)_3$, G = -1444.256881 hartree

Si	-0.43265	-1.91008	0.50924
Si	1.20614	-3.52649	-0.08220
F	0.09635	-0.60940	-0.62484
Si	-2.13733	-2.83704	-0.86306
H	2.57018	-3.15556	0.42528
H	0.88462	-4.82936	0.58119
H	1.41184	-3.82952	-1.53623
H	-3.33236	-1.93204	-0.96118
H	-1.79836	-3.17004	-2.28535
H	-2.65345	-4.09825	-0.24368
Li	0.21979	1.08005	0.03137
O	0.09482	2.25120	-1.56556
O	-1.28475	1.68718	1.17561
O	1.94224	1.36375	0.98827
C	2.50951	0.28027	1.71532
C	2.90606	2.33182	0.62703
C	-2.56776	1.25711	0.74070
C	-1.14603	1.58014	2.58492
C	0.29013	1.69996	-2.85895
C	-0.39208	3.57760	-1.59941
H	2.95309	0.64409	2.65034
H	1.70467	-0.42472	1.93325
H	3.27633	-0.22343	1.11606
H	3.36845	2.76856	1.52125
H	3.68865	1.88659	-0.00035
H	2.39450	3.11358	0.06450
H	-1.89880	2.20132	3.08635
H	-1.25114	0.53528	2.89885
H	-0.14896	1.94161	2.83860
H	-3.34716	1.89277	1.17905
H	-2.59116	1.34807	-0.34591
H	-2.73556	0.21087	1.01933
H	0.32791	4.24362	-2.09225
H	-1.34814	3.62647	-2.13594
H	-0.54332	3.89661	-0.56760
H	1.05571	2.26558	-3.40437
H	0.60992	0.66749	-2.72436
H	-0.64762	1.71705	-3.42722

$(H_3Si)_2Si{=}Si(SiH_3)_2$, G = -1744.044943 hartree

Si	-0.00141	-0.00170	-1.08154
Si	0.00142	0.00166	1.08167
Si	1.99507	0.03050	-2.28615
Si	-1.99066	0.20270	-2.28120
Si	-1.99517	-0.03039	2.28609
Si	1.99075	-0.20278	2.28118

H	2.11733	1.29710	-3.05801
H	3.15382	-0.08868	-1.36482
H	2.02839	-1.09890	-3.25473
H	-2.12272	-0.91845	-3.25092
H	-3.15320	0.18188	-1.35716
H	-2.00597	1.47612	-3.05138
H	2.00647	-1.47652	3.05081
H	3.15321	-0.18124	1.35706
H	2.12258	0.91800	3.25137
H	-2.11587	-1.29547	3.06070
H	-2.03023	1.10108	3.25217
H	-3.15389	0.08521	1.36426

$FLi(OMe_2)_3$, G = -572.231507 hartree

F	-1.98316	-0.09389	-0.04482
Li	-0.29556	0.01553	0.00272
O	0.22324	1.99449	-0.02968
O	0.34545	-0.78428	1.74242
O	0.44335	-0.89439	-1.63639
C	-0.38862	2.55822	1.11912
H	-1.45477	2.30448	1.14608
H	0.10889	2.13038	1.99033
H	-0.25847	3.64860	1.12394
C	-0.34979	2.50406	-1.22272
H	-1.41070	2.23426	-1.28065
H	-0.23244	3.59500	-1.26689
H	0.18755	2.05001	-2.05641
C	1.71437	-1.12370	-2.19276
H	1.77863	-0.71444	-3.21044
H	2.44888	-0.62277	-1.55933
H	1.94042	-2.19830	-2.22942
C	-0.61221	-1.49703	-2.37276
H	-0.63478	-1.10116	-3.39689
H	-0.47521	-2.58587	-2.41075
H	-1.53134	-1.24156	-1.84017
C	1.60233	-1.12640	2.27286
H	1.80430	-2.19944	2.14928
H	2.35722	-0.55246	1.73195
H	1.65932	-0.87667	3.34119
C	-0.73580	-1.44476	2.38606
H	-0.60608	-2.53360	2.32685
H	-0.78871	-1.14493	3.44106
H	-1.63563	-1.14186	1.84584