Silicon Ring Strain Creates High-Conductance Pathways in Single-Molecule Circuits

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Supporting Information

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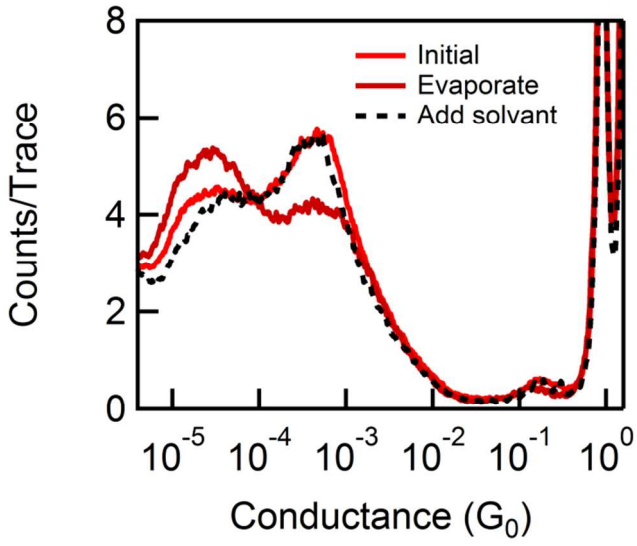
I. Table of Conductances

Molecule	High *G* state (G_0) *(S-to-silane conductance)*	Low *G* state (G_0) *(S-to-S conductance)*
1	4.2×10^{-4}	4.0×10^{-5}
2	———	6.4×10^{-5}
3	———	———
4	———	5.1×10^{-5}
5	———	1.7×10^{-4}
6	———	———
7	2.5×10^{-4}	———
8	———	7.6×10^{-5}
9	3.1×10^{-4}	1.8×10^{-5}
10	———	2.6×10^{-5}
11	2.7×10^{-4}	1.4×10^{-5}
12	———	1.7×10^{-5}
13	———	1.2×10^{-4}
19	———	———

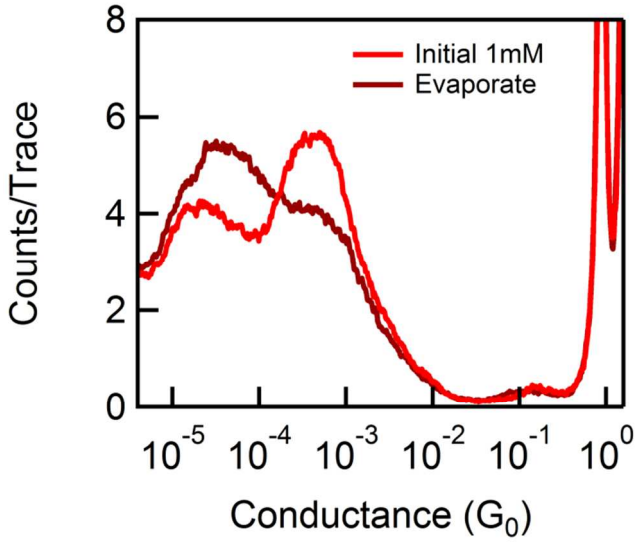
II. Additional Figures

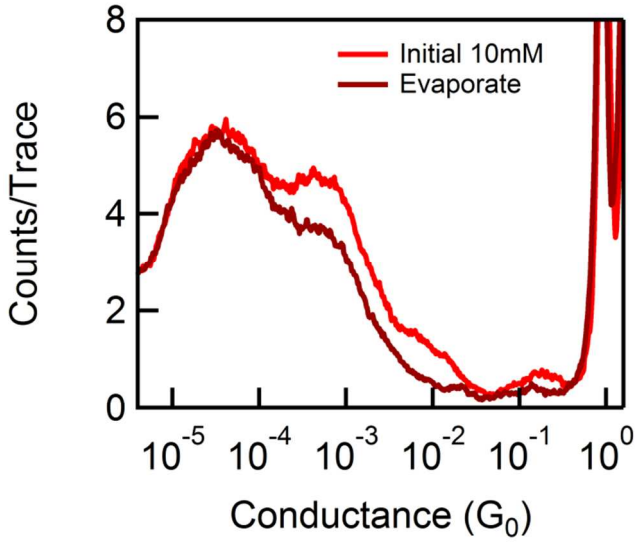
Figure S1



2 drops of fresh solvent were added after the end of 20,000 traces ("Evaporate"). The 5000 traces immediately after solvent re-addition are plotted above.

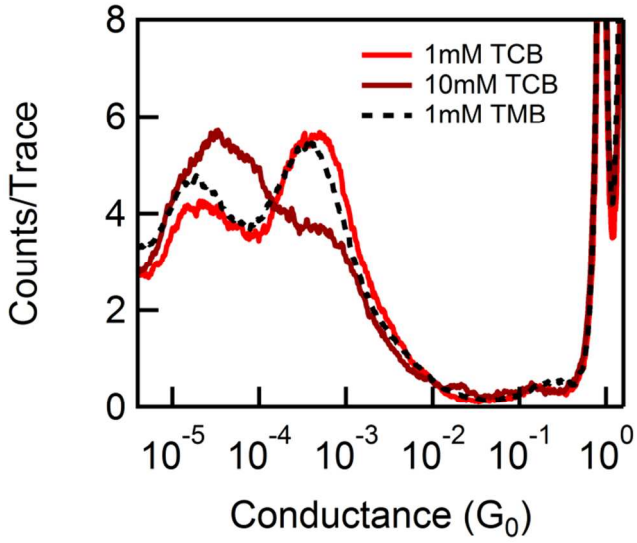
Figure S2





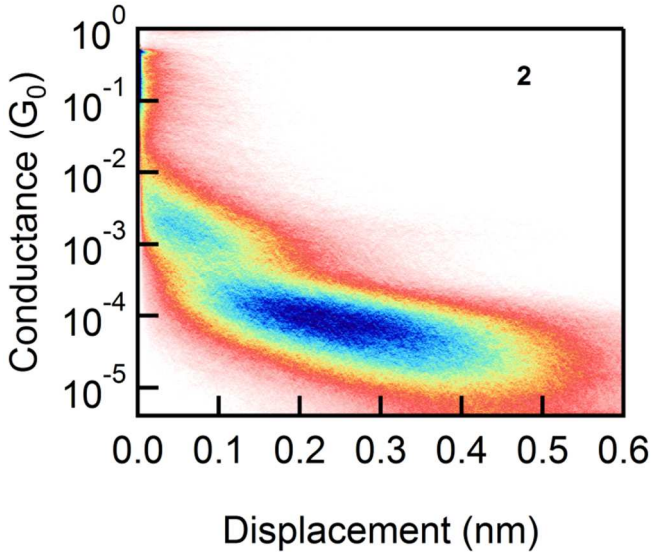
"Evaporate" describes the last 5000 traces, where most the solvent has evaporated. Here, we demonstrate that at 10 mM, the measurement nears the upper limit of the shifting peak distribution towards the low *G* state.

Figure S3



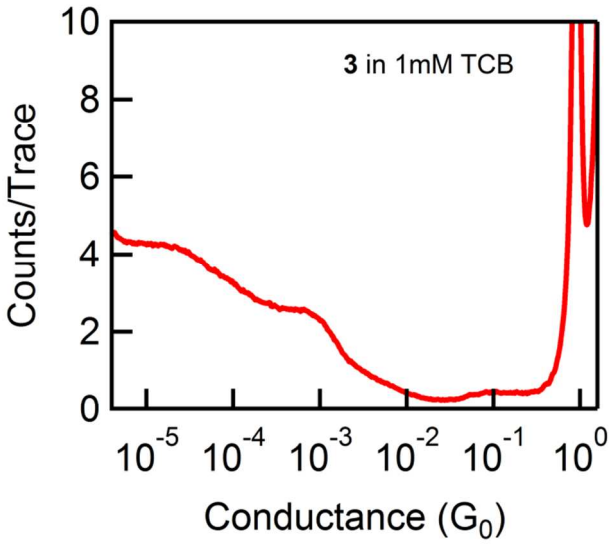
1D histogram of **1** in 1,2,4-trimethoxybenzene at 1 and 10 mM compared with TCB.

Figure S4



2D histogram showing the conductance profile of **2**, which is very similar in appearance to the low *G* state in **1**.

Figure S5



No conductive junction is observed for **3** in 1 mM TCB.

Figure S6

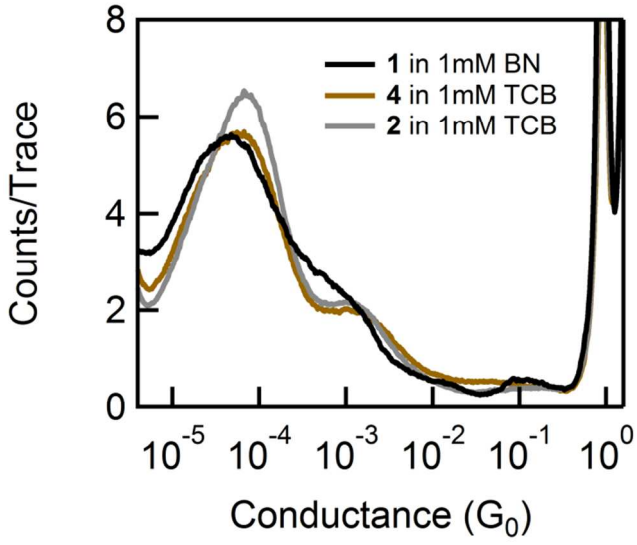


Figure S7

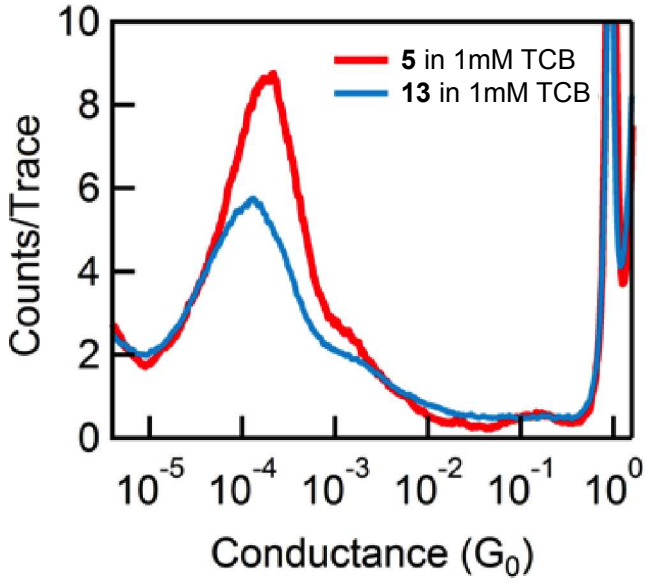


Figure S8

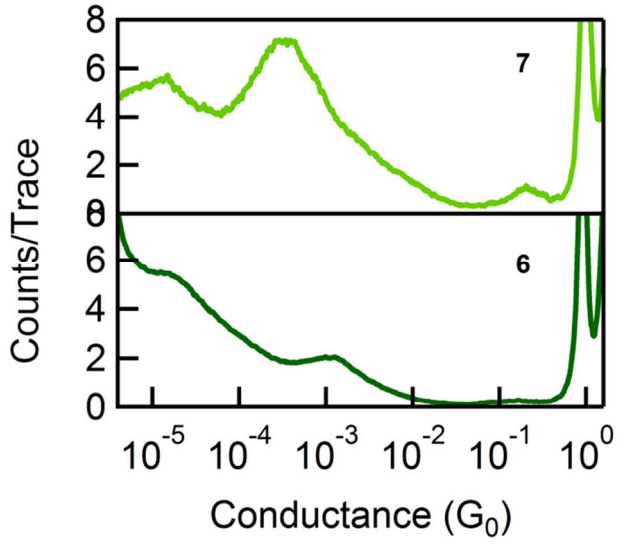


Figure S9

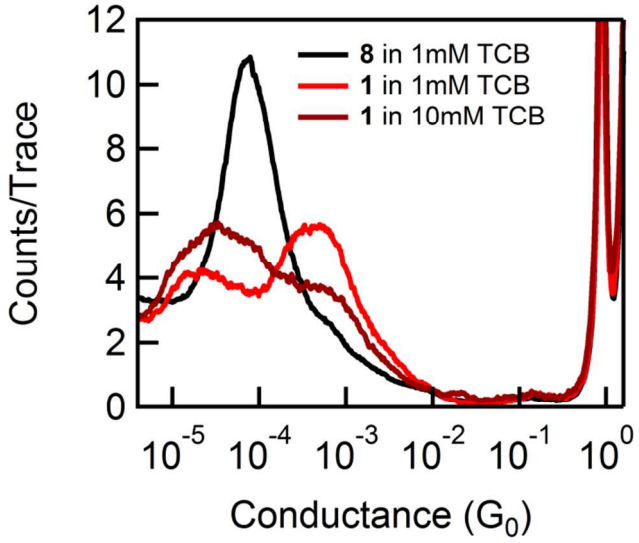
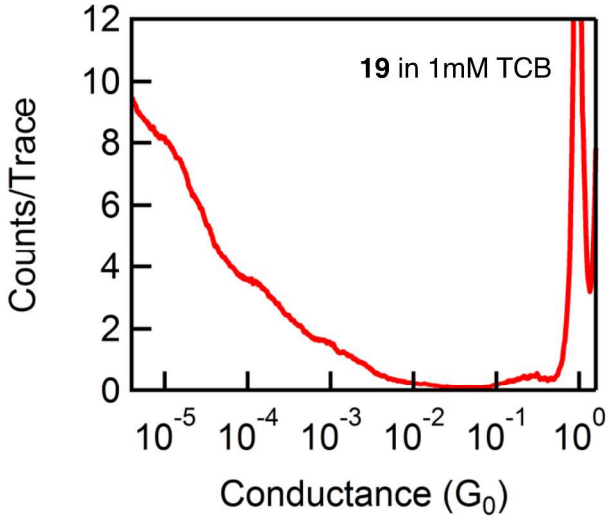
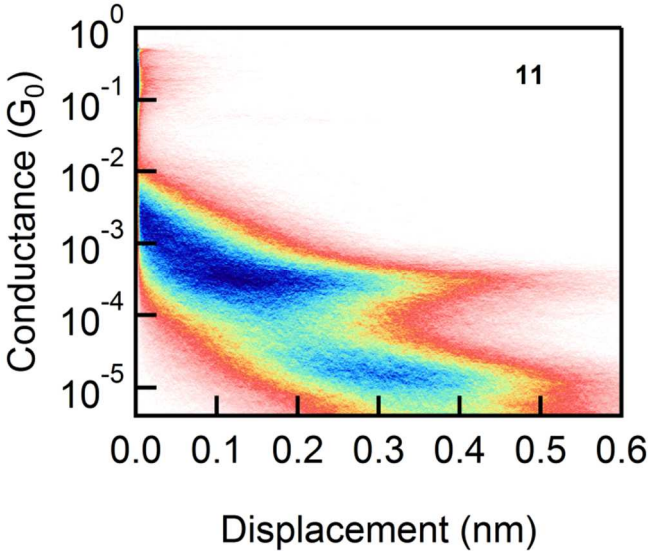


Figure S10



Oligosilanes of n ≥ 2 with *meta*-thioanisole linkers do not conduct. Here, we show that bis(3-thioanisole)tetramethyldisilane **19** does not yield conductive junctions.

Figure S11



III. General Information

All reactions were performed in oven-dried or flame-dried round bottom flasks, unless otherwise noted. The flasks were fitted with rubber septa and reactions were conducted under a positive pressure of nitrogen, unless otherwise noted. Anhydrous and anaerobic solvents were obtained from a Schlenk manifold with purification columns packed with activated alumina and supported copper catalyst (Glass Contour, Irvine, CA). Automated flash chromatography was performed using a Teledyne Isco Combiflash R_f200 and Redisep R_f Gold Silica columns.

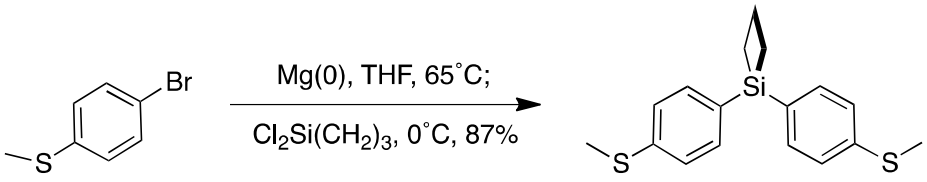
Materials. Commercial reagents were used without further purification. All reagents were purchased from Sigma-Aldrich, with the following exceptions. 1,1-dichlorosilacyclobutane and 1,1-dichlorosilacyclopentane were purchased from Gelest. 1-bromo-4-chlorobutane was purchased from Alfa Aesar. 3,5-dimethylthioanisole was purchased from Oakwood. 3-Bromothioanisole was purchased from America TCI Fine Chemicals. All magnesium turnings were pre-treated by washing with 1 M HCl (2x), distilled water (2x), ethanol (2x), and ethyl ether (2x) to remove the MgO layer, then heated (110˚C) under vacuum overnight to dry the turnings.

Instrumentation. ^{1}H, ^{13}C, and ^{29}Si NMR spectra were recorded on a Bruker DRX300 (300 MHz), Bruker DRX400 (400 MHz) or a Bruker DMX500 (500 MHz) spectrometer. Chemical shifts for protons are reported in parts per million downfield from tetramethylsilane and are referenced to residual protium in the NMR solvent ($CHCl_3$: δ 7.26; C_6H_6 δ 7.15). Chemical shifts for carbon are reported in parts per million downfield from tetramethylsilane and are referenced to the carbon resonances of the solvent ($CDCl_3$ δ 77.0; C_6D_6 δ 128.5). Chemical shifts for silicon are reported in parts per

million downfield from tetramethylsilane and referenced to the silicon resonance of tetramethylsilane (TMS δ 0.0). Data are represented as follows: chemical shift, multiplicity (s = singlet, d = doublet, dd= doublet of doublets, t = triplet, m = multiplet), coupling constants in Hertz, and integration. The mass spectroscopic data were obtained at the Columbia University mass spectrometry facility using a JEOL JMSHX110A/110A tandem mass spectrometer.

II. Synthetic Procedures and Characterization of Organic Compounds

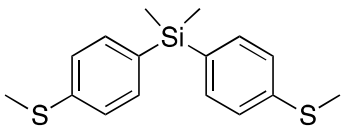
*1,1-bis(4-(methylthio)phenyl)silacyclobutane (**1**)*



The synthesis of **1** was adapted from Denmark et al.[1] Magnesium turnings (0.614 g, 25.29 mmol, 3.00 equiv.) were flame-dried with a 100 mL Schlenk flask equipped with a stir bar and rubber septum, cooling under vacuum. A fleck of iodine was added to the flask under a positive N_2 pressure, and 5 mL THF was added to the flask through the septum. After stirring at room temperature for an hour, the color changed from a translucent orange-yellow to a white precipitate denoting the formation of MgI_2. An oven-dried reflux condenser with a rubber septum was equipped under positive N_2 flow. 4-bromothioanisole (3.60 g, 17.70 mmol, 2.10 equiv.) was dissolved in 10 mL THF and added in two portions via syringe. A significant exotherm was observed after addition of the first portion. After the exotherm subsided, the second portion was added, followed by an additional 25 mL of THF. The reaction was heated to reflux with an oil bath and stirred at reflux overnight. The solution turned to a gray-black color over this period. 1,1-dichlorosilacyclobutane (1.00 mL, 8.43 mmol, 1.00 equiv.) was added by syringe into a second flame-dried 100 mL Schlenk flask equipped with a stir bar, followed by 3 mL THF. This second Schlenk flask was cooled to 0˚C with an ice bath. The aryl Grignard was added to the dichlorosilane slowly via cannula under vacuum. The reaction mixture was stirred to room temperature overnight.

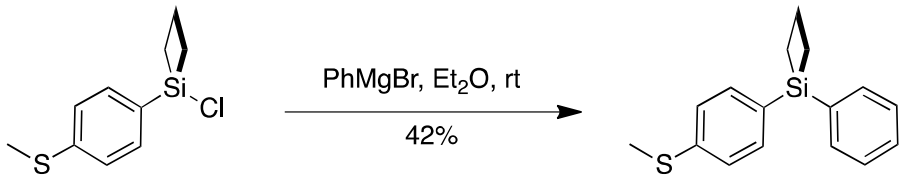
The reaction mixture was quenched with 1 mL of a saturated NH_4Cl solution, followed by 3 mL of distilled water. Over 5 minutes of stirring, the reaction mixture turned from gray-black to colorless. The organic and aqueous layers were separated with a separatory funnel, and the aqueous layer was extracted with diethyl ether (3 x 40 mL). The organic layers were combined, washed with brine (15 mL), dried over $MgSO_4$, filtered, then concentrated under vacuum to yield a white paste. Purification by column chromatography on silica gel (gradient of 100% hexanes to 30% dichloromethane/hexanes) yielded a clear oil (2.332 g, 87% yield) that solidified upon standing over the weekend. Alternatively, this material can be recrystallized from hot *n*-hexane or ethanol to yield white crystals. We note that synthesis of this molecule in particular from the 4-(methylthio)phenyl lithiate was unsuccessful, leading to substantial ring-opening of the silacycle. Single crystals suitable for x-ray diffraction were grown from methanol vapor diffusion into a concentrated solution of **1** in 1,2,4-trichlorobenzene (5 mg in 0.2 mL solvent). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55 – 7.49 (m, 4H), 7.32 – 7.26 (m, 4H), 2.50 (s, 6H), 2.30 - 2.20 (m, 2H), 1.48 (t, J = 8.3 Hz, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.96, 135.00, 132.26, 125.73, 18.38, 15.35, 14.14. ^{29}Si NMR (99 MHz, $CDCl_3$) δ 6.51. HRMS (FAB+) predicted for $C_{17}H_{20}S_2Si$ 316.08, observed 316.0786.

*bis(4-(methylthio)phenyl)dimethylsilane (**2**)*



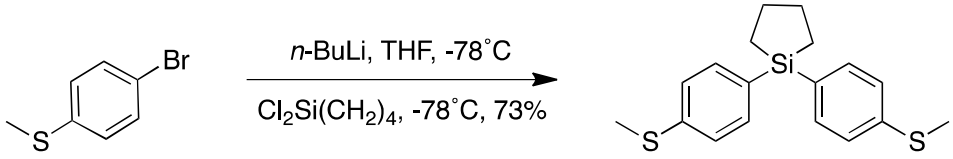
For synthesis and characterization of this molecule, refer to Nuckolls et al.[2]

*1-(4-(methylthio)phenyl)-1-phenylsilacyclobutane (**3**)*



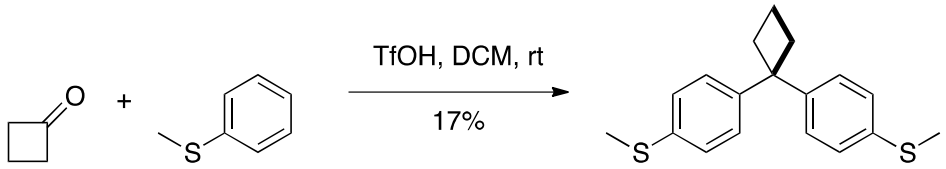
Chlorosilacyclobutane **14** (0.061 g, 0.266 mmol, 1.2 equiv.) was added to a flame-dried 10 mL round-bottom flask equipped with a stir bar, followed by 3 mL diethyl ether. Phenylmagnesium bromide (3.0 M in Et_2O, 0.075 mL, 0.222 mmol, 1.00 equiv.) was added via microsyringe to the reaction mixture, and the reaction stirred over night. The lightly cloudy solution was quenched with 1 mL distilled water. The organic and aqueous layers were separated with a separatory funnel, and the aqueous layer was extracted with diethyl ether (3 x 5 mL). The organic layers were combined, washed with brine (2 mL), dried over $MgSO_4$, filtered, then concentrated under vacuum to yield a cloudy white oil. Purification by preparative thin layer chromatography (100% hexanes) yielded the title compound as a clear, colorless oil (25 mg, 42% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66 - 7.60 (m, 2H), 7.56-7.51 (m, 2H), 7.47 - 7.38 (m, 3H), 7.33 - 7.27 (m, 2H), 2.50 (s, 3H), 2.31 - 2.22 (m, 2H), 1.54 - 1.41 (m, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.88, 136.44, 135.01, 134.61, 132.27, 129.84, 128.12, 125.65, 18.42, 15.32, 14.06. ^{29}Si NMR (99 MHz, $CDCl_3$) δ 6.60. HRMS (FAB+) predicted for $C_{16}H_{18}SSi$ 270.09, observed 270.0884.

*1,1-bis(4-(methylthio)phenyl)silacyclopentane (**4**)*



4-bromothioanisole (0.960 g, 4.726 mmol, 2.10 equiv.) was added to a flame-dried 25 mL round bottom flask with a stir bar and dissolved in 10 mL THF. The reaction mixture was cooled to -78˚C and stirred at that temperature for 5 minutes. A 1.39 M solution of *n*-butyllithium in hexanes (3.40 mL, 4.726 mmol, 2.10 equiv.) was added slowly to the reaction mixture at -78˚C, and was stirred at this temperature for 70 minutes to yield a cloudy white solution. 1,1-dichlorosilacyclopentane (0.295 mL, 2.250 mmol, 1.00 equiv.) was added neat to the reaction mixture, and stirred at -78˚C for 15 minutes. The reaction mixture was warmed to room temperature after removing the dry ice-acetone bath and was stirred at rt for 2 hours. The mixture was quenched with 2 mL of a saturated NH_4Cl solution, followed by 2 mL of distilled water. The organic and aqueous layers were separated with a separatory funnel, and the aqueous layer was extracted with diethyl ether (3 x 20 mL). The organic layers were combined, washed with brine (5 mL), dried over $MgSO_4$, filtered, then concentrated under vacuum to yield a yellow oil. Purification by column chromatography on silica gel (gradient of 100% hexanes to 25% dichloromethane/hexanes) yielded a slight yellow oil (541 mg, 73% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46 - 7.40 (m, 4H), 7.25 - 7.21 (m, 4H), 2.48 (s, 6H), 1.83 - 1.75 (m, 4H), 1.16 - 1.01 (m, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.32, 135.26, 132.84, 125.77, 27.83, 15.43, 12.34. ^{29}Si NMR (99 MHz, $CDCl_3$) δ 8.97. HRMS (FAB+) predicted for $C_{18}H_{22}S_2Si$ 330.09, observed 330.0926.

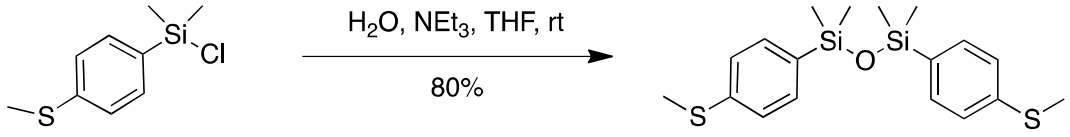
*1,1-bis(4-(methylthio)phenyl)cyclobutane (**5**)*



Cyclobutanone (0.079 g, 0.084 mL, 1.13 mmol, 1.00 equiv.) and thioanisole (0.148 g, 0.140 mL, 1.19 mmol, 1.05 equiv.) were added under nitrogen to a flame-dried 10 mL round bottom flask equipped with a stir bar. 3 mL of dichloromethane was added to the mixture, followed by a dropwise addition of triflic acid (0.100 mL, 1.13 mmol, 1.00 equiv.) to the solution. After stirring at room temperature for 30 minutes, a light purple color was observed. After stirring for 1.5 hours, this color deepened significantly. From 1.5 to 3 hours, no significant difference in color. The reaction mixture was stirred overnight, then poured slowly into a saturated $NaHCO_3$ solution (15 mL). After stirring for 10 minutes, the reaction mixture was extracted with DCM (3x15 mL) and the organic layers were combined. The organic layers were then washed with brine (10 mL), dried over $MgSO_4$, filtered, then concentrated to yield a white paste. Purification by column chromatography on silica gel (gradient of 100% hexanes to 30% dichloromethane/ hexanes) yielded a white solid (58 mg, 17%) of substantial purity. Recrystallization from hot ethyl acetate yielded analytically pure white crystals (20 mg). Single crystals suitable for x-ray diffraction were grown from methanol vapor diffusion into a concentrated solution of toluene (5 mg in 0.2 mL solvent). We note that attempts to synthesize the cyclobutane from ring-closing ((4-bromobutane-1,1-diyl)bis(4,1-phenylene))bis(methylsulfane) with NaH or KH and 18-crown-6 were unsuccessful. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.24 - 7.16 (m, 8H), 2.69 (t, J = 7.6 Hz, 4H), 2.45 (s, 6H), 1.96 (p, J = 7.6 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 146.88, 135.27, 127.05, 126.82,

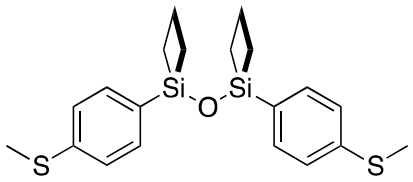
50.61, 35.06, 16.74, 16.29. HRMS (FAB+) predicted for $C_{18}H_{20}S_2$ 300.10, observed 301.1084.

*1,1'-oxybis(1-(4-(methylthio)phenyl))dimethylsilane (**6**)*



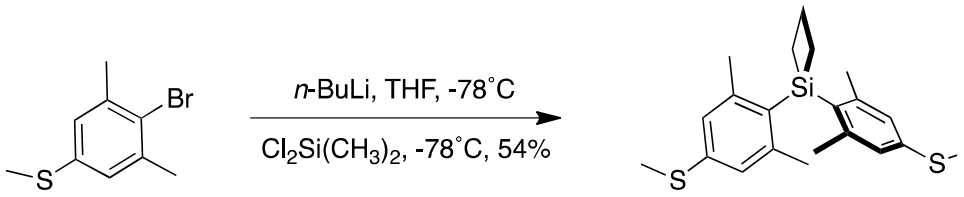
Chlorosilane **15** (0.650 g, 3.05 mmol, 2.00 equiv.) was added to a flame-dried 10 mL round bottom flask with a stir bar, followed by 2 mL THF. Distilled water (0.0275 mL, 1.52 mmol, 1.00 equiv.) was added to the reaction mixture by microsyringe at room temperature, with no perceptible color change. Triethylamine (0.1 mL, 0.717 mmol, 0.47 equiv.) was added and immediately yielded a cloudy precipitate denoting triethylamine hydrochloride salt formation. The reaction mixture was stirred for 30 minutes, then 1 mL distilled water was added. The organic and aqueous layers were separated, and the aqueous layer was extracted with ethyl acetate (3x10 mL), dried over $MgSO_4$, filtered, then reduced to a slight yellow oil. Purification by column chromatography on silica gel (gradient of 100% hexanes to 30% dichloromethane/hexanes) yielded a clear oil (440 mg, 80% yield). ^{1}H, ^{13}C, ^{29}Si NMR and HRMS data matches previously reported.[2]

1,1'-oxybis(1-(4-(methylthio)phenyl))silacyclobutane (7)



Disiloxane **7** (8.0 mg) was isolated from the reaction mixture of **9**, likely forming upon quenching with water. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 - 7.53 (m, 4H), 7.29 - 7.25 (m, 4H), 2.50 (s, 6H), 2.17 - 2.01 (m, 2H), 1.84 - 1.67 (m, 2H), 1.60 - 1.37 (m, 8H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.27, 133.69, 133.01, 125.66, 20.11, 15.32, 14.00. ^{29}Si NMR (99 MHz, $CDCl_3$) δ -21.92. HRMS (FAB+) predicted for $C_{20}H_{26}OS_2Si_2$ 402.72, observed 402.0964.

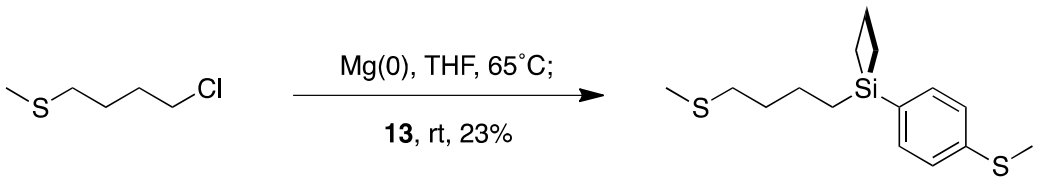
*1,1-bis(2,6-dimethyl-4-(methylthio)phenyl)silacyclobutane (**8**)*



4-bromo-3,5-dimethylthioanisole **16** (0.8306 g, 3.591 mmol, 2.05 equiv.) was added to a 50 mL flame-dried round bottom flask with a stir bar and dissolved in 14 mL THF. The reaction mixture was cooled to -78˚C with a dry ice-acetone bath and stirred for 5 minutes. A 1.53 M solution of *n*-butyllithium in hexanes (2.35 mL, 3.595 mmol, 2.05 equiv.) was added slowly to the reaction mixture and stirred for 3 hours at room temperature to yield a cloudy white solution. 1,1-dichlorosilacyclobutane (0.208 mL, 1.752 mmol, 1.00 equiv.) was added to the reaction mixture at -78˚C, and stirred at this

temperature for an hour. The dry ice-acetone bath was removed, and the reaction mixture stirred at room temperature for 5 hours to yield a yellow clear solution. The mixture was quenched with 1 mL of a saturated NH_4Cl solution, followed by 2 mL of distilled water. The organic and aqueous layers were separated with a separatory funnel, and the aqueous layer was extracted with diethyl ether (3 x 20 mL). The organic layers were combined, washed with brine (5 mL), dried over $MgSO_4$, filtered, then concentrated under vacuum to yield a whitish solid. Purification by column chromatography on silica gel (gradient of 100% hexanes to 15% dichloromethane/hexanes) yielded a white solid (350 mg, 54% yield) with an unidentified impurity. The white solid was recrystallized with boiling ethyl acetate and cooled to -30˚C to yield pure white crystals. ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.83 (s, 4H), 2.45 (s, 3H), 2.44 (s, 6H), 2.24 - 2.16 (m, 2H), 1.62 (t, J = 7.8 Hz, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 144.57, 139.75, 132.16, 125.36, 23.43, 21.91, 20.21, 15.06. ^{29}Si NMR (99 MHz, $CDCl_3$) δ 0.28. HRMS (FAB+) predicted for $C_{21}H_{28}S_2Si$ 372.14, observed 372.1392.

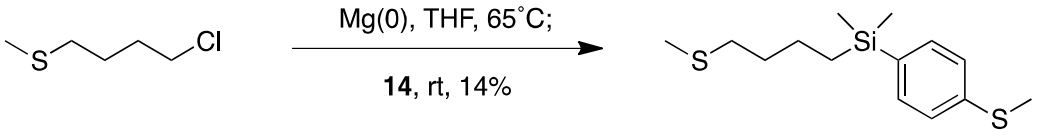
*1-(4-(methylthio)butyl)-1-(4-(methylthio)phenyl)silacyclobutane (**9**)*



Magnesium turnings (0.110 g, 4.5 mmol, 4.71 equiv.) were added to an oven-dried 25 mL Schlenk flask. 3 mL THF was added to the flask, followed by 2 drops of ethylene dibromide to initiate the Grignard reaction. The reaction mixture was stirred at room temperature for 20 minutes, then at 35˚C for 40 minutes. Over the course of this period, the evolution of ethylene was observed and the reaction mixture turned to a gray color. An oven-dried reflux condenser with a rubber septum was equipped under positive

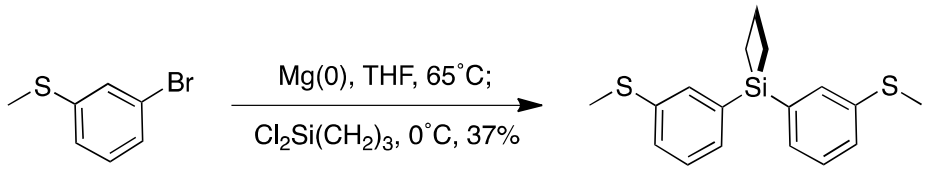
N_2 flow. Chloro-4-(methylthio)butane **17** (0.133 g, 0.960 mmol) was added with 2 mL THF, and the reaction mixture was brought to reflux and then stirred for 4 hours. After quenching an aliquot with water, there was no evidence of the chloro compound by NMR, though strong peaks corresponding to the cyclized thioether were observed. In a separate, flame-dried 25 mL round bottom flask equipped with a stir bar, chlorosilacyclobutane **14** (0.241 g, 1.06 mmol, 1.10 equiv.) was added with 4 mL THF. The Grignard was added to **14** by syringe at room temperature, and the reaction mixture was allowed to stir overnight. The light-yellow reaction mixture was quenched with 1 mL of a saturated NH_4Cl solution, followed by 2 mL of distilled water. The organic and aqueous layers were separated with a separatory funnel, and the aqueous layer was extracted with diethyl ether (3 x 15 mL). The organic layers were combined, washed with brine (5 mL), dried over $MgSO_4$, filtered, then concentrated under vacuum to yield a white, cloudy oil. Purification by column chromatography on silica gel (gradient of 100% hexanes to 30% dichloromethane/hexanes) yielded a clear oil (65.7 mg, 23% yield). Chromatography additionally furnished bis(silacyclobutyl)disiloxane **7** (8.0 mg) as a clear oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53 - 7.49 (m, 2H), 7.29 - 7.26 (m, 2H), 2.50 (s, 3H), 2.50 (t, 2H, obscured by overlapping singlet), 2.26 - 2.11 (m, 2H), 2.09 (s, 3H), 1.74 - 1.62 (m, 2H), 1.62 - 1.51 (m, 2H), 1.31 - 1.16 (m, 4H), 1.07 - 0.90 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.39, 134.15, 133.79, 125.77, 34.00, 32.75, 23.08, 18.57, 15.70, 15.42, 14.96, 13.08. ^{29}Si NMR (99 MHz, $CDCl_3$) δ 13.82. HRMS (FAB+) predicted for $C_{15}H_{24}S_2Si$ 296.11, observed 295.1020 (65.8%), 297.1166 (42.9%).

(4-(methylthio)butyl)(4-(methylthio)phenyl)dimethylsilane (***10***)



10 was prepared with the same procedure described for **9**, with the following modification: Chlorodimethylsilane **15** (0.320 g, 1.480 mmol) was used instead of chlorosilacyclobutane **14**. Purification by column chromatography on silica gel (gradient of 100% hexanes to 30% dichloromethane/hexanes) yielded a clear oil (61.1 mg, 14% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 - 7.38 (m, 2H), 7.26 - 7.21 (m, 2H), 2.48 (s, 3H), 2.47 (t, 2H, J = 7.6 Hz, partially obscured by overlapping singlet), 2.07 (s, 3H), 1.61 (p, J = 7.4 Hz, 2H), 1.49 - 1.33 (m, 2H), 0.80 - 0.67 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 139.60, 135.49, 134.11, 125.77, 34.00, 33.06, 23.29, 15.71, 15.58, 15.53, -2.89. ^{29}Si NMR (99 MHz, $CDCl_3$) δ -3.09. HRMS (FAB+) predicted for $C_{14}H_{24}S_2Si$ 284.11, observed 284.1097.

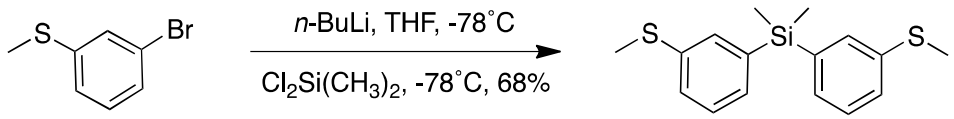
1,1-bis(3-(methylthio)phenyl)silacyclobutane ***(11)***



Magnesium turnings (0.160 g, 6.58 mmol, 4.39 equiv.) were flame-dried with a 25 mL Schlenk flask equipped with a stir bar and rubber septum, cooling under vacuum. A fleck of iodine was added to the flask under a positive N_2 pressure, and 3 mL THF was added to the flask through the septum. After stirring at room temperature for an hour, the color changed from a translucent orange-yellow to a white precipitate denoting the formation of MgI_2. An oven-dried reflux condenser with a rubber septum was equipped

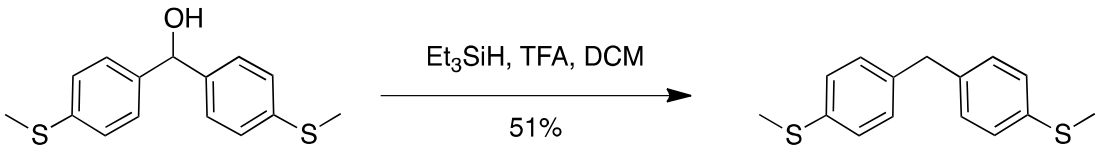
under positive N_2 flow. 3-bromothioanisole (0.405 mL, 2.00 equiv.) was dissolved in 6 mL THF and added in two portions via syringe. A significant exotherm was observed after addition of the first portion. After the exotherm subsided, the second portion was added. The reaction was heated to reflux with an oil bath and stirred at reflux overnight. The solution turned to a gray color over this period. 1,1-dichlorosilacyclobutane (0.178 mL, 1.50 mmol, 1.00 equiv.) was added by syringe into a second flame-dried 50 mL Schlenk flask equipped with a stir bar, followed by 8 mL THF. This second Schlenk flask was cooled to 0˚C with an ice bath. The aryl Grignard was added to the dichlorosilane slowly via syringe. The yellow reaction mixture was stirred to room temperature overnight. The mixture was quenched with 1 mL of a saturated NH_4Cl solution, followed by 3 mL of distilled water. The organic and aqueous layers were separated with a separatory funnel, and the aqueous layer was extracted with diethyl ether (3 x 20 mL). The organic layers were combined, washed with brine (5 mL), dried over $MgSO_4$, filtered, then concentrated under vacuum to yield a yellow oil. Purification by column chromatography on silica gel (gradient of 100% hexanes to 30% dichloromethane/hexanes) yielded a clear oil (173.5 mg, 37% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52 - 7.49 (m, 2H), 7.39 - 7.34 (m, 2H), 7.34 - 7.30 (m, 4H), 2.48 (s, 6H), 2.32 - 2.22 (m, 2H), 1.50 (t, J = 8.0 Hz, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 138.44, 137.09, 132.68, 131.25, 128.65, 128.12, 18.49, 16.06, 14.00. ^{29}Si NMR (99 MHz, $CDCl_3$) δ 7.14. HRMS (FAB+) predicted for $C_{17}H_{20}S_2Si$ 316.08, observed 316.0774.

1,1-bis(3-(methylthio)phenyl)dimethylsilane ***(12)***



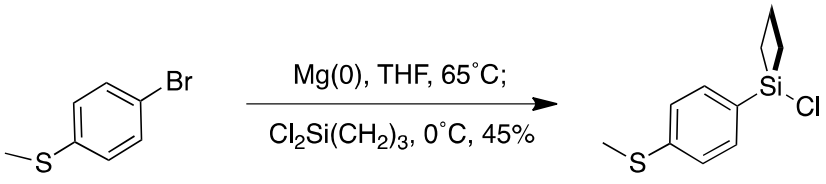
3-bromothioanisole (0.455 mL, 3.38 mmol, 2.05 equiv.) was added to a flame-dried 50 mL Schlenk flask equipped with a stir bar and dissolved in 17 mL THF. The flask was cooled to -78˚C with a dry ice/acetone bath and stirred at that temperature for 5 minutes. A 1.50 M solution of *n*-BuLi in hexanes was added (2.25 mL, 3.38 mmol, 2.05 equiv.), and the reaction mixture was stirred for 1 hour at -78˚C. Dichlorodimethylsilane (0.200 mL, 1.65 mmol, 1.00 equiv.) was added to the reaction mixture at -78˚C, and stirred at -78˚ for 20 minutes. The dry ice/acetone bath was removed, and the reaction mixture was allowed to stir at room temperature for 3 hours. The yellow reaction mixture was quenched with 2 mL of a saturated NH_4Cl solution, followed by 2 mL of distilled water. The organic and aqueous layers were separated with a separatory funnel, and the aqueous layer was extracted with diethyl ether (3 x 20 mL). The organic layers were combined, washed with brine (5 mL), dried over $MgSO_4$, filtered, then concentrated under vacuum to yield a yellow oil. Purification by column chromatography on silica gel (gradient of 100% hexanes to 30% dichloromethane/hexanes) yielded a clear oil (343 mg, 68% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42 - 7.38 (m, 1H), 7.29 - 7.26 (m, 3H), 2.46 (s, 3H), 0.54 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 138.88, 138.10, 132.57, 131.07, 128.51, 127.60, 16.11, -2.33. ^{29}Si NMR (99 MHz, $CDCl_3$) δ -7.21. HRMS (FAB+) predicted for $C_{16}H_{20}S_2Si$ 304.08, observed 304.0768.

*bis(4-(methylthio)phenyl)methane (**13**)*



18 (392 mg, 1.42 mmol, 1.00 equiv.) was added to a 20 mL scintillation vial equipped with a stir bar. 1 mL dichloromethane was added to the flask, giving a heterogeneous mixture. Trifluoroacetic acid (0.45 mL, 6.04 mmol, 4.25 equiv.) was added to the flask to give a navy-blue heterogeneous solution. Triethylsilane (0.60 mL, 3.69 mmol, 2.60 equiv.) was added to the reaction, giving an exotherm. The reaction was stirred for 1 hour at room temperature, then poured into a concentrated $NaHCO_3$ solution (10 mL) and extracted with ethyl acetate (3x15 mL). The organic layer was washed with brine (7 mL), dried with $MgSO_4$, filtered, and reduced to give a white solid (189 mg, 51% yield). This solid was found to be pure by NMR without any further purification. ^{1}H NMR (400 MHz, C_6D_6) δ 7.10 (d, J = 8.3 Hz, 4H), 6.89 (d, J = 8.4 Hz, 4H), 3.62 (s, 2H), 2.01 (s, 6H). ^{13}C NMR (101 MHz, C_6D_6) δ 138.33, 136.72, 129.75, 127.46, 41.04, 15.80. HRMS (FAB+) predicted for $C_{15}H_{16}S_2$ 260.07, observed 260.0695.

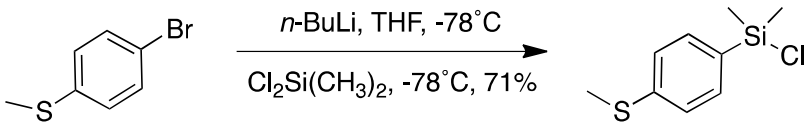
*1-chloro-1-(4-(methylthio)phenyl)silacyclobutane (**14**)*



The synthesis of **14** was adapted from Denmark et al.[1] Magnesium turnings (0.410 g, 16.87 mmol, 1.20 equiv.) were flame-dried with a 100 mL Schlenk flask equipped with

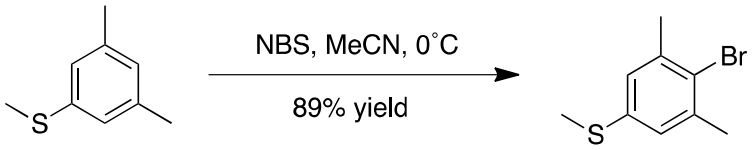
a stir bar and rubber septum, cooling under vacuum. The magnesium was activated, as described for **1.** An oven-dried reflux condenser with a rubber septum was equipped under positive N_2 flow. 4-bromothioanisole (2.86 g, 14.05 mmol, 1.00 equiv.) was dissolved in 8 mL THF and added in two portions via syringe. A significant exotherm was observed after addition of the first portion. After the exotherm subsided, the second portion was added, followed by an additional 25 mL of THF. The reaction was heated to reflux with an oil bath and stirred at reflux overnight. The solution turned to a gray color over this period. 1,1-dichlorosilacyclobutane (8.00 mL, 67.48 mmol, 4.80 equiv.) was added by syringe into a second flame-dried 200 mL Schlenk flask equipped with a stir bar, followed by 40 mL THF. This second Schlenk flask was cooled to 0˚C with an ice bath. The aryl Grignard was added to the dichlorosilane slowly via cannula under vacuum. The reaction mixture was stirred to room temperature overnight. Solvent and the excess 1,1-dichlorosilacyclobutane were removed *in vacuo* to yield a yellow solid. The solids were washed with hot hexanes (3x15 mL) and the slurry was transferred to a Schlenk filter and the solids were filtered over Celite. The filtrate was reduced *in vacuo*, and the residue was subjected to short-path distillation under vacuum (0.05 torr, 130˚ C) to yield 1.445 g (45% yield) of a clear oil. This material was stored in a dry box for further use. We note that the starting dichlorosilane and bis-adduct are easily separable by distillation, and would suggest an equimolar reaction for a more economical synthesis. The product hydrolyzes readily; therefore, only ^{1}H NMR is provided. ^{1}H NMR (500 MHz, C_6D_6) δ 7.47 - 7.38 (m, 2H), 7.09 - 7.03 (m, 2H), 2.17 - 2.02 (m, 1H), 1.92 (s, 3H), 1.87 - 1.74 (m, 1H), 1.60 - 1.41 (m, 4H).

chloro(4-(methylthio)phenyl)dimethylsilane (***15***)



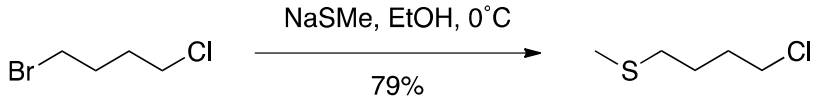
4-bromothioanisole (3.114 g, 15.33 mmol, 1.00 equiv.) was added to a flame-dried 100 mL Schlenk flask equipped with a stir bar, and was dissolved in 38 mL THF. The flask was cooled to -78˚C with a dry ice/acetone bath and stirred at that temperature for 10 minutes. A 1.61 M solution of *n*-BuLi in hexanes was added (10.0 mL, 16.1 mmol, 1.05 equiv.), and the reaction mixture was stirred for 2.5 hours at -78˚C. Dichlorodimethylsilane (12.63 mL, 91.98 mmol, 6.00 equiv.) was added to a separate oven-dried 250 mL Schlenk flask with a stir bar along with 30 mL THF. This flask was also cooled to -78˚C. The aryl lithiate was added slowly by vacuum cannula into the chlorosilane-containing flask at -78˚C. The reaction mixture was warmed slowly from -78˚ C to room temperature overnight. The reaction mixture exhibited a deep yellow color after stirring overnight. Solvent and the excess dichlorosilane were removed under moisture-free *in vacuo* conditions to yield a blue-black oily solid. The lithate salts were washed with hot hexanes (3x15 mL) and the slurry was transferred to a Schlenk filter and the solids were filtered over Celite. The filtrate was reduced *in vacuo*, and the residue was subjected to short-path distillation under vacuum (0.05 torr, 120˚ C) to yield 2.3503 g (71% yield) of **15** as a clear oil. This material was stored in a dry box. The product hydrolyzes readily; therefore, only ^{1}H NMR is provided. ^{1}H NMR (500 MHz, C_6D_6) δ 7.50 - 7.39 (m, 2H), 7.19 ?-7.14 (m, 2H), 2.04 (s, 3H), 0.53 (s, 6H).

*4-bromo-3,5-dimethylthioanisole (**16**)*



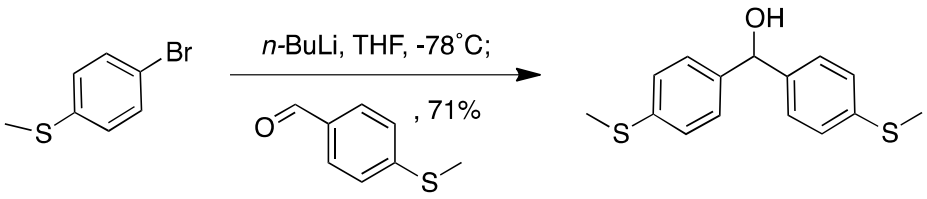
The synthesis of **16** was adapted from Siegel *et al.*[4] 3,5-dimethylthioanisole (0.510 g, 3.35 mmol, 1.00 equiv.) was added to a 25 mL flame-dried round bottom flask, dissolved in 3.3 mL non-anhydrous acetonitrile, and cooled to 0˚C with an ice-water bath. N-bromosuccinimide (0.600 g, 3.37 mmol, 1.01 equiv.) was dissolved in 3.4 mL acetonitrile, and heated (~40˚C) to homogeneity. The solution of N-bromosuccinimide was added slowly to the 0˚C solution of the thioanisole, giving an immediate yellow color. The reaction mixture was stirred at 0˚C for 5 minutes, then the ice bath was removed, and the reaction was stirred at room temperature for 18 hours. The reaction mixture was quenched with 5 mL water, then extracted with hexanes (3 x 15 mL), washed with brine (5 mL), dried with $MgSO_4$, and concentrated to give a yellow oil. Purification by column chromatography on silica gel (gradient of 100% hexanes to 10% dichloromethane/hexanes) yielded a slight yellow oil (680 mg, 89% yield).^{1}H NMR (500 MHz, $CDCl_3$) δ 6.97 (s, 2H), 2.46 (s, 3H), 2.39 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 138.76, 136.77, 126.36, 124.24, 23.95, 16.09. HRMS (FAB+) predicted for $C_9H_{11}BrS$ 231.97 (100%), 229.98 (98.2%). Observed 231.9742 (100%), 229.9765 (97.7990%).

*1-chloro-4-(methylthio)butane (**17**)*



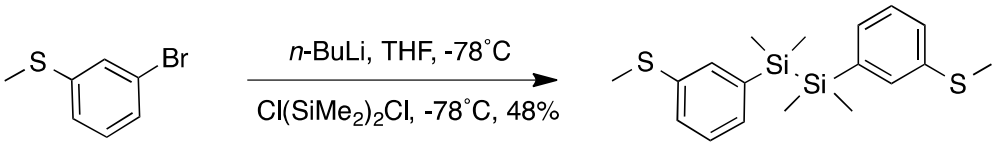
This procedure was adapted from Serif et al.[5] Sodium thiomethoxide has an unpleasant odor; for this reason, a quantity of the sodium thiomethoxide (1.5916 g, 22.7 mmol, 1.08 equiv.) was added in a fume hood to a tared 200 mL, 24/40 round bottom flask with a stir bar capped by a rubber septum, then weighed on a scale outside the fume hood. 40 mL of absolute ethanol was added (non-anhydrous) to dissolve the NaSMe. The flask was cooled to 0˚C with an ice-water bath, and 1-bromo-4-chlorobutane (3.605 g, 21.0 mmol, 1.00 equiv.) was added quickly via syringe. After stirring for 15 minutes at 0˚C, a cloudy precipitate was observed due to the insoluble NaBr. The reaction mixture was warmed to room temperature and stirred under ambient conditions overnight. The reaction mixture was concentrated, dissolved in hexanes, and filtered over a neutral alumina plug. The filtrate was reduced to yield a clear, colorless oil (2.27 g, 79% yield) with a strong garlic odor that required no further purification based on NMR. We note that silica chromatography results in significant decomposition of the material. **17** was stored at -30˚C to prevent cyclization of the material (the cyclized product is a crystalline solid). ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.57 (t, J = 6.5 Hz, 2H), 2.53 (t, J = 7.2 Hz, 2H), 2.10 (s, 3H), 1.95 - 1.84 (m, 2H), 1.81 - 1.71 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 44.74, 33.55, 31.55, 26.32, 15.58. HRMS (FAB+) could not be obtained.

*bis(4-(methylthio)phenyl)methanol (**18**)*



4-bromothioanisole (0.404 g, 2.00 mmol, 1.00 equiv.) was added to an oven-dried 25 mL round-bottom flask equipped with a stir bar. 8 mL THF was added to the flask, which was then cooled to -78˚C and stirred for 5 minutes. A 1.50 M solution of *n*-butyllithium in hexanes (1.50 mL, 2.20 mmol, 1.10 equiv.) was added to the flask slowly, and the reaction was stirred at -78˚C for 90 minutes. 4-(methylthio)benzaldehyde (0.330 mL, 2.50 mmol, 1.25 equiv.) was added neat to the flask. The reaction was stirred at -78˚C for 15 minutes, then warmed to room temperature and stirred for an hour. The reaction mixture was quenched with water. The aqueous and organic layers were separated with a separatory funnel, and the aqueous layer was extracted with ethyl acetate (3 x 10 mL), washed with brine, dried with Na_2SO_4, filtered, then concentrated. Purification by column chromatography on silica gel (gradient of 100% hexanes to 10% ethyl acetate/hexanes) yielded a yellow solid (392 mg, 71%). ^{1}H NMR (400 MHz, C_6D_6) δ 7.14 (d, J = 8.3 Hz, 4H), 7.09 (d, J = 8.3 Hz, 4H), 5.40 (s, 1H), 1.98 (s, 6H). ^{13}C NMR (101 MHz, C_6D_6) δ 141.59, 138.23, 127.49, 126.93, 75.45, 15.51. HRMS (FAB+) predicted for $C_{15}H_{16}OS_2$ 276.06, observed 276.0650.

*1,1,2,2-tetramethyl-1,2-bis(3-(methylthio)phenyl)disilane (**19**)*



3-bromothioanisole (0.200 g, 1.00 mmol, 2.10 equiv.) was added to an oven-dried 25 mL Schlenk flask equipped with a stir bar and dissolved in 2 mL THF. The flask was cooled to -78˚C with a dry ice/acetone bath and stirred at that temperature for 5 minutes. A 1.23 M solution of *n*-BuLi in hexanes was added (0.820 mL, 1.00 mmol, 2.10 equiv.), and the reaction mixture was stirred for 1 hour at -78˚C. tetramethyldichlorodisilane (0.089 mL, 0.475 mmol, 1.00 equiv.) was added to the reaction mixture at -78˚C, and stirred at -78˚ for 20 minutes. The dry ice/acetone bath was removed, and the reaction mixture was allowed to stir at room temperature for 3 hours. The yellow reaction mixture was quenched with 2 mL of a saturated NH_4Cl solution, followed by 2 mL of distilled water. The organic and aqueous layers were separated with a separatory funnel, and the aqueous layer was extracted with diethyl ether (3 x 20 mL). The organic layers were combined, washed with brine (5 mL), dried over $MgSO_4$, filtered, then concentrated under vacuum to yield a yellow oil. Purification by column chromatography on silica gel (gradient of 100% hexanes to 30% dichloromethane/hexanes) yielded a white solid (83 mg, 48% yield). ^{1}H NMR 400 MHz, C_6D_6) δ 7.44 (dd, J = 1.4, 0.6 Hz, 2H), 7.15 - 7.10 (m, 4H), 7.06 (dd, J = 7.1, 0.5 Hz, 2H), 2.03 (s, 6H), 0.26 (s, 12H). ^{13}C NMR (76 MHz, C_6D_6) δ 139.90, 138.91, 132.38, 130.75, 128.64, 127.31, 15.50, -3.90. .88, 138.10, 132.57, 131.07, 128.51, 127.60, 16.11, -2.33. ^{29}Si NMR (59 MHz, C_6D_6) δ -20.99.

HRMS (FAB+) predicted for $C_{18}H_{26}S_2Si_2$ 362.10, observed 347.0784 (100%); 361.0922 (15%).

V. STM Break-Junction Experiments:

i. General Details

We measure the conductance of single molecules attached to gold electrodes using a home-built modified Scanning Tunneling Microscope (STM). A hand-cut 0.25 mm diameter gold wire (99.998%, Alfa Aesar) is used as the STM tip and a gold-coated (99.999%, Alfa Aesar) mounted mica surface is used as the substrate. A commercially available single-axis piezoelectric positioner (Nano-P15, Mad City Labs) is used to achieve sub-angstrom level control of the tip-substrate distance. The STM is controlled using a custom written program in IgorPro (Wavemetrics, Inc.) and operates in ambient conditions at room temperature. The break junction technique is carried out in 1 mM solutions of the molecules in 1,2,4-trichlorobenzene (Sigma-Aldrich or Alfa Aesar, 99% purity) unless otherwise specified, which is introduced after collection of at least a thousand clean gold breaks to ensure the cleanliness of the system. The substrate is UV/Ozone cleaned for 15 minutes immediately before use.

Measurement of conductance is achieved by repeatedly moving the tip in and out of contact with the substrate, requiring that a gold metal contact with a conductance of at least 5 G_0 is formed before pulling out. The tip is withdrawn from the substrate at a speed of about 16 nm/s for about 4 nm and the measured current is recorded as a function of tip/substrate displacement while holding the applied voltage at 225 mV. The data is collected at a 40 kHz acquisition rate and plotted as conductance traces. Directly after the gold point contact breaks, a target molecule in the vicinity can bridge the gap so that its conductance (G=I/V) can be measured. Tens of thousands of conductance vs.

displacement traces were collected for each molecule studied and conductance histograms were constructed without any sort of data selection. The measurements were repeated on multiple days with multiple tip/substrate pairs to ensure reproducibility.

ii. Elongation and Compression Experiments

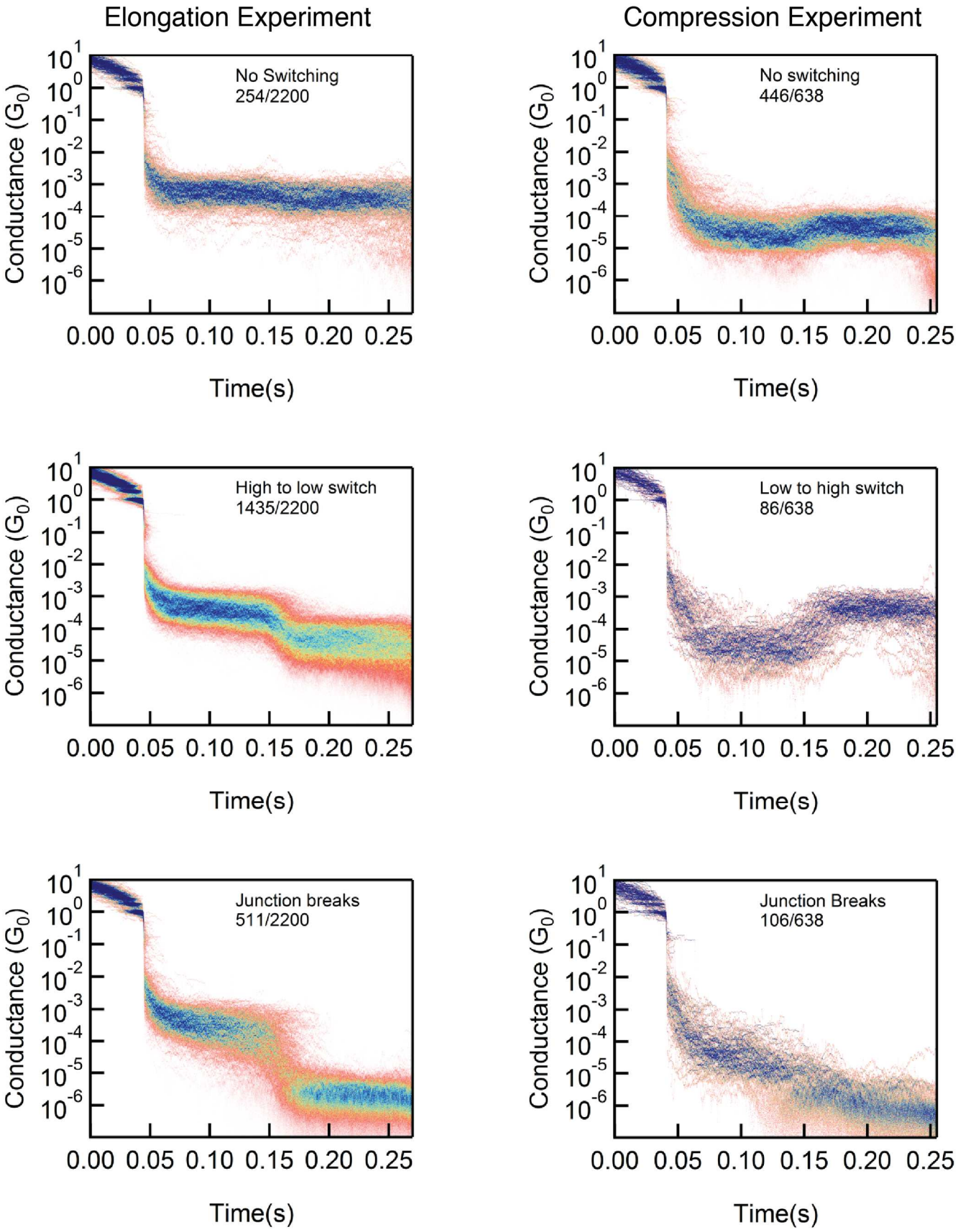
Here, we describe our modified STM-BJ studies regarding the junction elongation and compression experiments, as detailed in Figure 1b of the main text. We begin both experiments by reaching a gold-gold contact of $5G_0$ to ensure a new Au point contact configuration each time. We then pull out the gold tip (20nm/s) to the desired tip-substrate displacement and hold the tip for 70 ms. In the elongation experiment, we pull the tip for another 0.2nm. In the compression experiment, we push back for another 0.2nm. We hold for another 70ms, then pull until junction breaks. The push/pull 0.2 nm distance was chosen based on the difference in extension displacement between the high and low *G* molecular plateaus, as seen in Figure 1a from the main text. The high *G* state was defined by a range between $\log(G/G_0) = -2.9$ to -3.7; the low *G* state was defined by a range between $\log(G/G_0) = -3.7$ to -5.2. Traces starting in the high *G* state during the first hold period were selected for the elongation experiment; traces starting in the low *G* state during the first hold period were selected for the compression experiment. We used the same range to determine whether we were observing the high or low *G* state in the second hold period.

We used an algorithm to select traces based on this criteria from a set of 20,000 traces for both the elongation and compression experiments. We started our measurement at 1 mM, and every 5000 traces, we added solvent to the experimental setup to maintain a

dilute concentration. On the next page, 2-dimensional histograms can be found for the selected traces from the elongation and compression experiments.

Elongation: Among 2200 traces selected with the criteria stipulated above, 254 traces (12%) show no switching after pulling the gold tip by 0.2 nm, 1435 traces (65%) switch from high to low *G* state, and the remaining 511 traces (23%) result in a junction break.

Compression: 638 traces demonstrated a molecule bridging the gap in the low *G* conformer during the first hold. 446 of these traces (70%) resulted in no switching after pushing the tip from 0.6 to 0.4 nm, 86 traces (13%) showed switching from low to high *G* state, while the remaining 106 traces (17%) resulted in a junction break.


Elongation Experiment
Compression Experiment
No Switching
254/2200
No switching
446/638
High to low switch
1435/2200
Low to high switch
86/638
Junction breaks
511/2200
Junction Breaks
106/638
Conductance (G0)
Time(s)
0.00 0.05 0.10 0.15 0.20 0.25

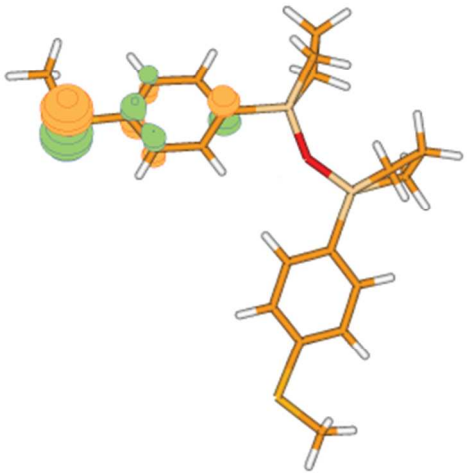
VI. Computational Chemistry

i. General Methods

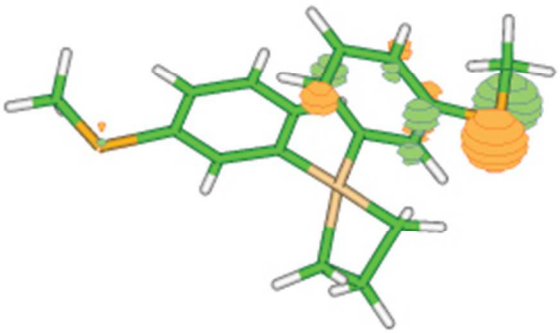
All DFT calculations were done using Jaguar (version 7.8, Schrodinger, LLC, New York, NY, 2010). We optimized the geometries of each of the subject molecules and calculated frontier orbital energies using the B3LYP functional and the 6-31G** basis set. All orbital surfaces shown are plotted at a 0.075 isovalue. The DFT geometry optimizations of **4**, **7**, and **11** are alluded to in the main text. These and the HOMO images (for **7** and **11**) are given here.

ii. HOMO Images

7:

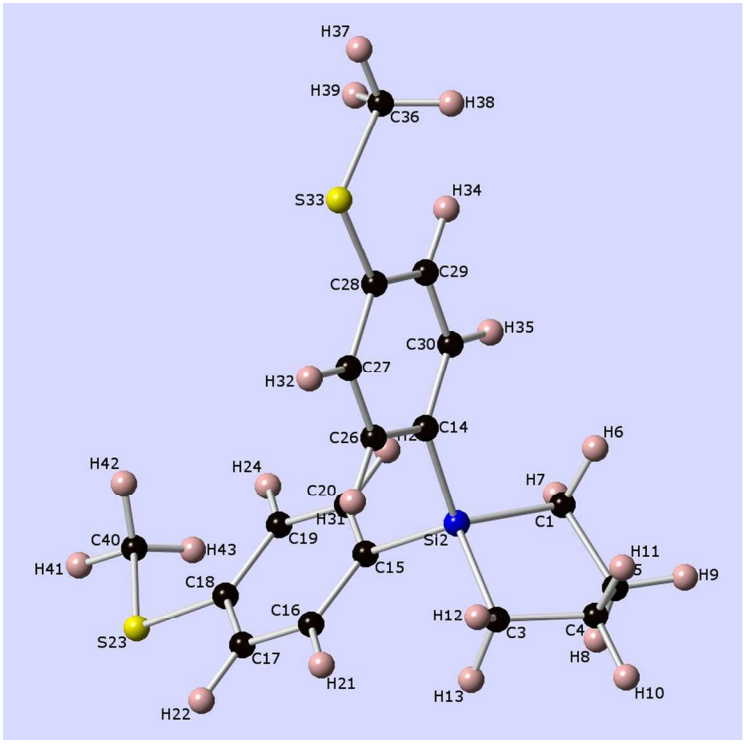


11:



Geometry Optimization for **4**:

B3LYP - 6-31G**
Final total energy = -1785.10060 hartree



final geometry:

	angstroms		
atom	x	y	z
C1	0.3811464333	0.0292910861	0.1042254102
Si2	0.1775236297	0.0175993588	2.0032798343
C3	2.0446158647	0.0701698708	2.3965528890
C4	2.6812918464	0.4475967198	1.0334839643
C5	1.8938071368	-0.2530590692	-0.0926205784
H6	0.1339627961	1.0217928105	-0.2929671956
H7	-0.2435127795	-0.6944055982	-0.4286278841
H8	2.0737058563	-1.3349262385	-0.0326735526
H9	2.2435418712	0.0675099085	-1.0814482500
H10	3.7463211792	0.1886060043	0.9947682412
H11	2.6182193746	1.5347772268	0.8900211548
H12	2.3282269937	0.7697790044	3.1890075151
H13	2.3931180568	-0.9232994869	2.7057609212
C14	-0.7449323040	1.5469875565	2.6262347859
C15	-0.6538650358	-1.5555366459	2.6477151474
C16	-0.1290984417	-2.2948213396	3.7242772603
C17	-0.7616910047	-3.4332919088	4.2120776880
C18	-1.9577357411	-3.8852210923	3.6337639992
C19	-2.4979422833	-3.1677456482	2.5597804793

C20	-1.8513875360	-2.0265193704	2.0850033849
H21	0.7971857117	-1.9795741788	4.1986462270
H22	-0.3265722638	-3.9773152633	5.0463330180
S23	-2.6786516216	-5.3570000883	4.3354582296
H24	-3.4188342230	-3.4871595459	2.0849548627
H25	-2.3038352130	-1.4956072463	1.2498225566
C26	-0.5360890893	2.0495529166	3.9257211093
C27	-1.2267529360	3.1554054680	4.4062446418
C28	-2.1683307351	3.8125697753	3.5976645962
C29	-2.3927159901	3.3327475755	2.3028933167
C30	-1.6879585647	2.2215882062	1.8355412009
H31	0.1841355230	1.5685735697	4.5839887296
H32	-1.0375242600	3.5147681499	5.4143659294
S33	-2.9921897938	5.2205906059	4.3165770289
H34	-3.1088267022	3.8154853165	1.6473109357
H35	-1.8865033789	1.8824981018	0.8212547918
C36	-4.1497768854	5.7513948990	3.0141603057
H37	-4.6867912374	6.6063421106	3.4301578988
H38	-3.6223347344	6.0703468622	2.1122552320
H39	-4.8686841335	4.9650463212	2.7730520945
C40	-4.2075390948	-5.5868921544	3.3720878806
H41	-4.6866126686	-6.4745073922	3.7903794225
H42	-4.8822023260	-4.7349540784	3.4830324366
H43	-3.9947471287	-5.7651339873	2.3155413950

principal moments of inertia:

amu*angstrom^2: 1743.22262 4311.65847 5422.37590

g*cm^2: 2.89468891E-37 7.15967644E-37 9.00406589E-37

rotational constants:

cm^(-1): 0.00967038 0.00390978 0.00310890

GHz: 0.28991077 0.11721221 0.09320250

Z-matrix: (angstroms and degrees)

C1
Si2 C1 sic2
C3 Si2 csi3 C1 csic3
C4 C3 cc4 Si2 ccsi4 C1 dih4
C5 C4 cc5 C3 ccc5 Si2 dih5
H6 C1 hc6 C5 hcc6 C4 dih6
H7 C1 hc7 C5 hcc7 C4 dih7
H8 C5 hc8 C1 hcc8 Si2 dih8
H9 C5 hc9 C1 hcc9 Si2 dih9
H10 C4 hc10 C5 hcc10 C1 dih10
H11 C4 hc11 C5 hcc11 C1 dih11
H12 C3 hc12 Si2 hcsi12 C1 dih12

H13 C3 hc13 Si2 hcsi13 C1 dih13
C14 Si2 csi14 C1 csic14 C5 dih14
C15 Si2 csi15 C1 csic15 C5 dih15
C16 C15 cc16 Si2 ccsi16 C1 dih16
C17 C16 cc17 C15 ccc17 Si2 dih17
C18 C17 cc18 C16 ccc18 C15 dih18
C19 C18 cc19 C17 ccc19 C16 dih19
C20 C19 cc20 C18 ccc20 C17 dih20
H21 C16 hc21 C15 hcc21 C17 dih21
H22 C17 hc22 C16 hcc22 C18 dih22
S23 C18 sc23 C17 scc23 C19 dih23
H24 C19 hc24 C18 hcc24 C17 dih24
H25 C20 hc25 C19 hcc25 C18 dih25
C26 C14 cc26 Si2 ccsi26 C1 dih26
C27 C26 cc27 C14 ccc27 Si2 dih27
C28 C27 cc28 C26 ccc28 C14 dih28
C29 C28 cc29 C27 ccc29 C26 dih29
C30 C29 cc30 C28 ccc30 C27 dih30
H31 C26 hc31 C14 hcc31 C27 dih31
H32 C27 hc32 C26 hcc32 C28 dih32
S33 C28 sc33 C27 scc33 C29 dih33
H34 C29 hc34 C28 hcc34 C27 dih34
H35 C30 hc35 C29 hcc35 C28 dih35
C36 S33 cs36 C28 csc36 C27 dih36
H37 C36 hc37 S33 hcs37 C28 dih37
H38 C36 hc38 S33 hcs38 H37 dih38
H39 C36 hc39 S33 hcs39 H37 dih39
C40 S23 cs40 C18 csc40 C17 dih40
H41 C40 hc41 S23 hcs41 C18 dih41
H42 C40 hc42 S23 hcs42 H41 dih42
H43 C40 hc43 S23 hcs43 H41 dih43

Z-variables: (angstroms and degrees)
sic2 = 1.9099755622
csi3 = 1.908785155
csic3 = 95.7624913347
cc4 = 1.5510526185
ccsi4 = 103.1295325372
dih4 = 13.5833798341
cc5 = 1.5424532874
ccc5 = 108.7530096299
dih5 = -37.1158422655
hc6 = 1.0972335164
hcc6 = 109.7772394562
dih6 = 80.9105127684
hc7 = 1.0944718618

hcc7 = 111.9866617119
dih7 = -160.3185674895
hc8 = 1.09835958
hcc8 = 109.3934700181
dih8 = 82.5612234479
hc9 = 1.0967492959
hcc9 = 111.8476286976
dih9 = -159.6296866716
hc10 = 1.0967509187
hcc10 = 111.2682175478
dih10 = 174.0509125498
hc11 = 1.098417575
hcc11 = 108.9613841969
dih11 = -68.757204306
hc12 = 1.0944736392
hcsi12 = 114.850595851
dih12 = 135.7030724867
hc13 = 1.0972897292
hcsi13 = 110.1078599204
dih13 = -103.4519029985
csi14 = 1.8915670965
csic14 = 111.9928325944
dih14 = 129.877922694
csi15 = 1.8924219601
csic15 = 112.9864026951
dih15 = -104.9287103682
cc16 = 1.4074472706
ccsi16 = 122.2299391889
dih16 = 131.4720329764
cc17 = 1.3907687964
ccc17 = 121.915683703
dih17 = 178.5244266099
cc18 = 1.4032853313
ccc18 = 120.4482401665
dih18 = 0.1376571508
cc19 = 1.4000124007
ccc19 = 118.6836193336
dih19 = -0.0130237148
cc20 = 1.3949350335
ccc20 = 120.1006093963
dih20 = -0.1100292531
hc21 = 1.087386326
hcc21 = 119.9349087607
dih21 = 179.9777464687
hc22 = 1.0868632318
hcc22 = 119.7929308315

dih22 = 179.9510824643
sc23 = 1.7827585122
scc23 = 116.6363973356
dih23 = 179.8276377174
hc24 = 1.0842170304
hcc24 = 120.8446749652
dih24 = 179.8277016208
hc25 = 1.0881652448
hcc25 = 117.8830648309
dih25 = -179.8965599713
cc26 = 1.4088478037
ccsi26 = 121.32537084
dih26 = -152.7904779318
cc27 = 1.3895428312
ccc27 = 121.9502381595
dih27 = -178.6511951473
cc28 = 1.4043629761
ccc28 = 120.4344951358
dih28 = 0.0722796888
cc29 = 1.3989320042
ccc29 = 118.6810265576
dih29 = -0.1097094125
cc30 = 1.3963438591
ccc30 = 120.116605167
dih30 = -0.0029201783
hc31 = 1.0878331142
hcc31 = 119.9052727892
dih31 = -179.978183917
hc32 = 1.0868567336
hcc32 = 119.8257004154
dih32 = -179.9962639481
sc33 = 1.7827230558
scc33 = 116.5673689805
dih33 = -179.7988301892
hc34 = 1.0842686645
hcc34 = 120.8532140826
dih34 = -179.7630300847
hc35 = 1.0877403467
hcc35 = 117.907104824
dih35 = -179.6550982586
cs36 = 1.8215516444
csc36 = 103.621173785
dih36 = -178.115690588
hc37 = 1.0919583996
hcs37 = 105.5626500244
dih37 = 179.016536926

hc38 = 1.0924094193
hcs38 = 111.6270486001
dih38 = 118.1333754438
hc39 = 1.0923849535
hcs39 = 111.4859728653
dih39 = -118.1067509176
cs40 = 1.821655757
csc40 = 103.616648196
dih40 = 178.3297346489
hc41 = 1.0919432739
hcs41 = 105.5585895523
dih41 = -178.9688149483
hc42 = 1.0923724893
hcs42 = 111.4826436164
dih42 = 118.1061707948
hc43 = 1.092401505
hcs43 = 111.6286984415
dih43 = -118.1280563107

bond lengths (angstroms):

C1	-Si2	:	1.909976	C1	-C5	:	1.551326
C1	-H6	:	1.097234	C1	-H7	:	1.094472
Si2	-C3	:	1.908785	Si2	-C14	:	1.891567
Si2	-C15	:	1.892422	C3	-C4	:	1.551053
C3	-H12	:	1.094474	C3	-H13	:	1.097290
C4	-C5	:	1.542453	C4	-H10	:	1.096751
C4	-H11	:	1.098418	C5	-H8	:	1.098360
C5	-H9	:	1.096749	C14	-C26	:	1.408848
C14	-C30	:	1.403418	C15	-C16	:	1.407447
C15	-C20	:	1.404468	C16	-C17	:	1.390769
C16	-H21	:	1.087386	C17	-C18	:	1.403285
C17	-H22	:	1.086863	C18	-C19	:	1.400012
C18	-S23	:	1.782759	C19	-C20	:	1.394935
C19	-H24	:	1.084217	C20	-H25	:	1.088165
S23	-C40	:	1.821656	C26	-C27	:	1.389543
C26	-H31	:	1.087833	C27	-C28	:	1.404363
C27	-H32	:	1.086857	C28	-C29	:	1.398932
C28	-S33	:	1.782723	C29	-C30	:	1.396344
C29	-H34	:	1.084269	C30	-H35	:	1.087740
S33	-C36	:	1.821552	C36	-H37	:	1.091958
C36	-H38	:	1.092409	C36	-H39	:	1.092385
C40	-H41	:	1.091943	C40	-H42	:	1.092372
C40	-H43	:	1.092402				

bond angles:

C5 -C1 -Si2 : 103.238334 H6 -C1 -Si2 : 109.964924
H6 -C1 -C5 : 109.777239 H7 -C1 -Si2 : 114.782868
H7 -C1 -C5 : 111.986662 H7 -C1 -H6 : 107.055521
C3 -Si2 -C1 : 95.762491 C14 -Si2 -C1 : 111.992833
C14 -Si2 -C3 : 112.761382 C15 -Si2 -C1 : 112.986403
C15 -Si2 -C3 : 112.486291 C15 -Si2 -C14 : 110.225887
C4 -C3 -Si2 : 103.129533 H12 -C3 -Si2 : 114.850596
H12 -C3 -C4 : 111.986300 H13 -C3 -Si2 : 110.107860
H13 -C3 -C4 : 109.729690 H13 -C3 -H12 : 107.002127
C5 -C4 -C3 : 108.753010 H10 -C4 -C3 : 111.849346
H10 -C4 -C5 : 111.268218 H11 -C4 -C3 : 109.393583
H11 -C4 -C5 : 108.961384 H11 -C4 -H10 : 106.551537
C4 -C5 -C1 : 108.814291 H8 -C5 -C1 : 109.393470
H8 -C5 -C4 : 108.902565 H9 -C5 -C1 : 111.847629
H9 -C5 -C4 : 111.263564 H9 -C5 -H8 : 106.551671
C26 -C14 -Si2 : 121.325371 C30 -C14 -Si2 : 122.058689
C30 -C14 -C26 : 116.603213 C16 -C15 -Si2 : 122.229939
C20 -C15 -Si2 : 121.125920 C20 -C15 -C16 : 116.630213
C17 -C16 -C15 : 121.915684 H21 -C16 -C15 : 119.934909
H21 -C16 -C17 : 118.149404 C18 -C17 -C16 : 120.448240
H22 -C17 -C16 : 119.792931 H22 -C17 -C18 : 119.758811
C19 -C18 -C17 : 118.683619 S23 -C18 -C17 : 116.636397
S23 -C18 -C19 : 124.679736 C20 -C19 -C18 : 120.100609
H24 -C19 -C18 : 120.844675 H24 -C19 -C20 : 119.054687
C19 -C20 -C15 : 122.221404 H25 -C20 -C15 : 119.895530
H25 -C20 -C19 : 117.883065 C40 -S23 -C18 : 103.616648
C27 -C26 -C14 : 121.950238 H31 -C26 -C14 : 119.905273
H31 -C26 -C27 : 118.144486 C28 -C27 -C26 : 120.434495
H32 -C27 -C26 : 119.825700 H32 -C27 -C28 : 119.739804
C29 -C28 -C27 : 118.681027 S33 -C28 -C27 : 116.567369
S33 -C28 -C29 : 124.751267 C30 -C29 -C28 : 120.116605
H34 -C29 -C28 : 120.853214 H34 -C29 -C30 : 119.029754
C29 -C30 -C14 : 122.214112 H35 -C30 -C14 : 119.878524
H35 -C30 -C29 : 117.907105 C36 -S33 -C28 : 103.621174
H37 -C36 -S33 : 105.562650 H38 -C36 -S33 : 111.627049
H38 -C36 -H37 : 108.867373 H39 -C36 -S33 : 111.485973
H39 -C36 -H37 : 108.907217 H39 -C36 -H38 : 110.224427
H41 -C40 -S23 : 105.558590 H42 -C40 -S23 : 111.482644
H42 -C40 -H41 : 108.910215 H43 -C40 -S23 : 111.628698
H43 -C40 -H41 : 108.864236 H43 -C40 -H42 : 110.229903

torsional angles:

C1 -Si2 -C3 -C4 : 13.583380
C1 -Si2 -C3 -H12 : 135.703072
C1 -Si2 -C3 -H13 :-103.451903
C1 -Si2 -C14 -C26 :-152.790478
C1 -Si2 -C14 -C30 : 28.551611
C1 -Si2 -C15 -C16 : 131.472033
C1 -Si2 -C15 -C20 : -49.931562
C1 -C5 -C4 -C3 : 50.415203
C1 -C5 -C4 -H10 : 174.050913
C1 -C5 -C4 -H11 : -68.757204
Si2 -C1 -C5 -C4 : -36.305333
Si2 -C1 -C5 -H8 : 82.561223
Si2 -C1 -C5 -H9 :-159.629687
Si2 -C3 -C4 -C5 : -37.115842
Si2 -C3 -C4 -H10 :-160.404159
Si2 -C3 -C4 -H11 : 81.785798
Si2 -C14 -C26 -C27 :-178.651195
Si2 -C14 -C26 -H31 : 1.370621
Si2 -C14 -C30 -C29 : 178.525200
Si2 -C14 -C30 -H35 : -1.663961
Si2 -C15 -C16 -C17 : 178.524427
Si2 -C15 -C16 -H21 : -1.497827
Si2 -C15 -C20 -C19 :-178.666654
Si2 -C15 -C20 -H25 : 1.345470
C3 -Si2 -C1 -C5 : 12.482132
C3 -Si2 -C1 -H6 :-104.601438
C3 -Si2 -C1 -H7 : 134.639289
C3 -Si2 -C14 -C26 : -46.118902
C3 -Si2 -C14 -C30 : 135.223187
C3 -Si2 -C15 -C16 : 24.396764
C3 -Si2 -C15 -C20 :-157.006831
C3 -C4 -C5 -H8 : -68.758602
C3 -C4 -C5 -H9 : 174.088163
C4 -C3 -Si2 -C14 :-103.193719
C4 -C3 -Si2 -C15 : 131.394911
C4 -C5 -C1 -H6 : 80.910513
C4 -C5 -C1 -H7 :-160.318567
C5 -C1 -Si2 -C14 : 129.877923
C5 -C1 -Si2 -C15 :-104.928710
C5 -C4 -C3 -H12 :-161.140822
C5 -C4 -C3 -H13 : 80.186442
H6 -C1 -Si2 -C14 : 12.794353
H6 -C1 -Si2 -C15 : 137.987720
H6 -C1 -C5 -H8 :-160.222931
H6 -C1 -C5 -H9 : -42.413841
H7 -C1 -Si2 -C14 :-107.964920

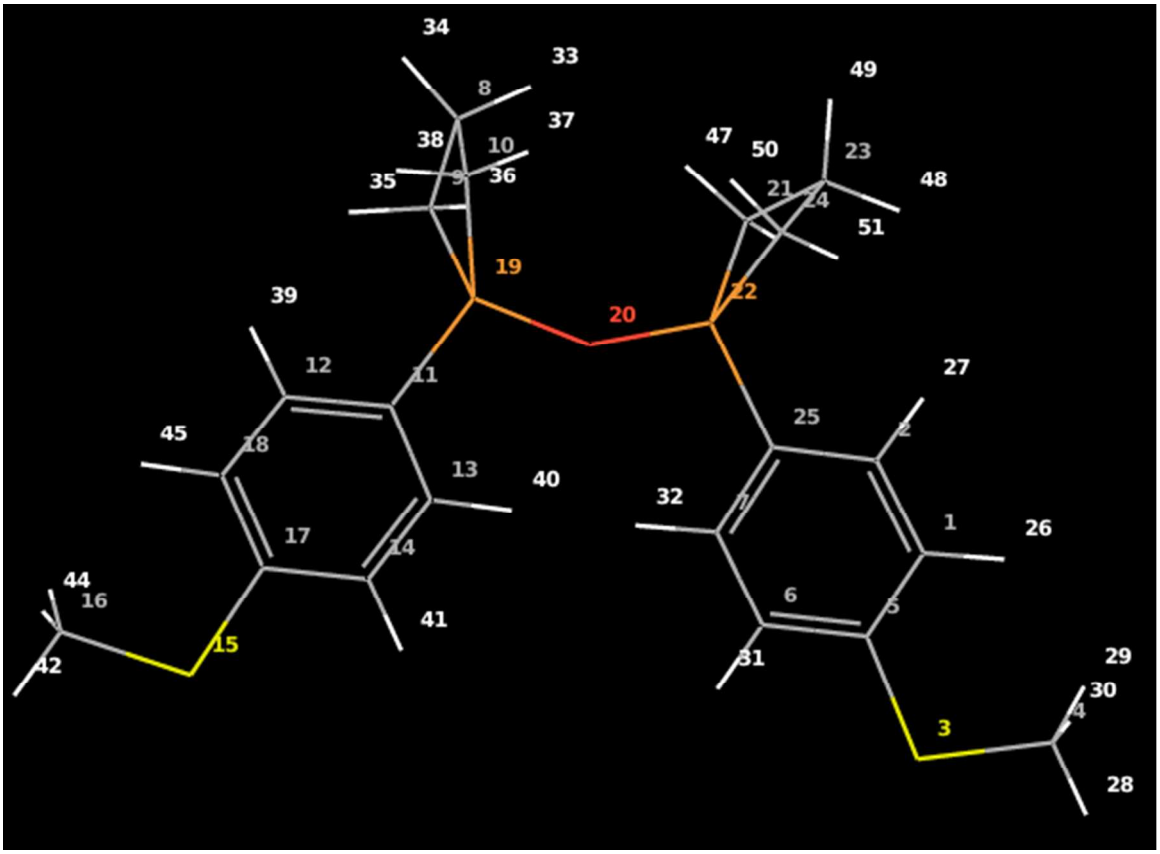
H7 -C1 -Si2 -C15 : 17.228447
H7 -C1 -C5 -H8 : -41.452011
H7 -C1 -C5 -H9 : 76.357078
H8 -C5 -C4 -H10 : 54.877107
H8 -C5 -C4 -H11 : 172.068990
H9 -C5 -C4 -H10 : -62.276128
H9 -C5 -C4 -H11 : 54.915756
H10 -C4 -C3 -H12 : 75.570861
H10 -C4 -C3 -H13 : -43.101875
H11 -C4 -C3 -H12 : -42.239182
H11 -C4 -C3 -H13 :-160.911918
H12 -C3 -Si2 -C14 : 18.925973
H12 -C3 -Si2 -C15 :-106.485396
H13 -C3 -Si2 -C14 : 139.770998
H13 -C3 -Si2 -C15 : 14.359628
C14 -Si2 -C15 -C16 :-102.384151
C14 -Si2 -C15 -C20 : 76.212255
C14 -C26 -C27 -C28 : 0.072280
C14 -C26 -C27 -H32 :-179.923984
C14 -C30 -C29 -C28 : 0.159299
C14 -C30 -C29 -H34 : 179.923767
C15 -Si2 -C14 -C26 : 80.508229
C15 -Si2 -C14 -C30 : -98.149683
C15 -C16 -C17 -C18 : 0.137657
C15 -C16 -C17 -H22 :-179.911260
C15 -C20 -C19 -C18 : 0.115331
C15 -C20 -C19 -H24 :-179.823510
C16 -C15 -C20 -C19 : 0.005138
C16 -C15 -C20 -H25 :-179.982738
C16 -C17 -C18 -C19 : -0.013024
C16 -C17 -C18 -S23 : 179.814614
C17 -C16 -C15 -C20 : -0.131475
C17 -C18 -C19 -C20 : -0.110029
C17 -C18 -C19 -H24 : 179.827702
C17 -C18 -S23 -C40 : 178.329735
C18 -C17 -C16 -H21 :-179.840471
C18 -C19 -C20 -H25 :-179.896560
C18 -S23 -C40 -H41 :-178.968815
C18 -S23 -C40 -H42 : -60.862644
C18 -S23 -C40 -H43 : 62.903129
C19 -C18 -C17 -H22 :-179.964123
C19 -C18 -S23 -C40 : -1.854143
C20 -C15 -C16 -H21 : 179.846272
C20 -C19 -C18 -S23 :-179.922676
H21 -C16 -C17 -H22 : 0.110611
H22 -C17 -C18 -S23 : -0.136485

S23 -C18 -C19 -H24 : 0.015055
H24 -C19 -C20 -H25 : 0.164598
C26 -C14 -C30 -C29 : -0.192612
C26 -C14 -C30 -H35 : 179.618227
C26 -C27 -C28 -C29 : -0.109709
C26 -C27 -C28 -S33 :-179.908540
C27 -C26 -C14 -C30 : 0.076711
C27 -C28 -C29 -C30 : -0.002920
C27 -C28 -C29 -H34 :-179.763030
C27 -C28 -S33 -C36 :-178.115691
C28 -C27 -C26 -H31 :-179.949167
C28 -C29 -C30 -H35 :-179.655098
C28 -S33 -C36 -H37 : 179.016537
C28 -S33 -C36 -H38 : -62.850088
C28 -S33 -C36 -H39 : 60.909786
C29 -C28 -C27 -H32 : 179.886558
C29 -C28 -S33 -C36 : 2.099110
C30 -C14 -C26 -H31 :-179.901473
C30 -C29 -C28 -S33 : 179.778092
H31 -C26 -C27 -H32 : 0.054569
H32 -C27 -C28 -S33 : 0.087728
S33 -C28 -C29 -H34 : 0.017982
H34 -C29 -C30 -H35 : 0.109370

Geometry Optimization for **7**:

Final total energy: -2228.50715178186 hartrees

B3LYP - 6-31G**



final geometry:

angstroms

atom	x	y	z
C1	-15.7005770090	-2.8607428850	-0.4228521780
C2	-14.8863323332	-1.7285640505	-0.4542748031
S3	-16.1508352000	-5.5715247913	0.2254522865
C4	-17.7834928504	-5.1193664274	-0.4448636612
C5	-15.2183741011	-4.0555405640	0.1238510744
C6	-13.9090862095	-4.0888691519	0.6295897735
C7	-13.1103744586	-2.9519190247	0.5928312628
C8	-8.9175959367	2.0349075281	0.8560320984
C9	-8.9529024005	0.8228445420	1.8509656854

C10	-8.7967705818	1.2985941039	-0.5230807101
C11	-8.3583831934	-1.8749240536	0.1262694777
C12	-6.9992450756	-1.9347574480	0.4722605044
C13	-8.9331307438	-3.0370225555	-0.4210307561
C14	-8.1883898242	-4.1946305071	-0.6137067881
S15	-5.9746476557	-5.7702773283	-0.5542650551
C16	-4.2791191002	-5.4359138201	0.0225176815
C17	-6.8294476912	-4.2338045477	-0.2631438734
C18	-6.2391562173	-3.0885278318	0.2843323758
Si19	-9.3394853242	-0.2954922261	0.3632876339
O20	-10.9397420961	-0.7015209522	0.1703475057
C21	-13.0916893530	1.2207792542	1.1925417798
Si22	-12.5148358804	-0.1921733405	0.0569256136
C23	-13.7604762825	1.8606182563	-0.0735062594
C24	-12.9951501069	1.1222886826	-1.2271768789
C25	-13.5779379210	-1.7389075174	0.0533894804
H26	-16.7034373970	-2.8003985022	-0.8303250064
H27	-15.2933170415	-0.8203975727	-0.8938189825
H28	-18.3906529815	-6.0240613382	-0.3720985839
H29	-18.2534891574	-4.3292251712	0.1451284459
H30	-17.7199732443	-4.8207772679	-1.4935581591
H31	-13.5187271562	-5.0100953676	1.0541103577
H32	-12.1000091826	-3.0093880060	0.9886697185
H33	-9.8588817887	2.5926168779	0.9059581339
H34	-8.1106032874	2.7495392508	1.0524670660
H35	-7.9657109183	0.6222660044	2.2835019575
H36	-9.6641586073	0.9109875041	2.6764450539
H37	-9.3909614671	1.7197765979	-1.3384098839
H38	-7.7563411488	1.2436636672	-0.8639343363
H39	-6.5072070042	-1.0652034117	0.9041003303
H40	-9.9834610972	-3.0358533666	-0.6987861576
H41	-8.6609649289	-5.0766903896	-1.0377967516
H42	-3.7265361838	-6.3635417828	-0.1405171968
H43	-3.8080981353	-4.6378042280	-0.5558434288
H44	-4.2574102945	-5.1942400761	1.0876466136
H45	-5.1933299747	-3.0837892766	0.5698574210
H46	-13.7583321929	1.0309003243	2.0372565397
H47	-12.2559081538	1.8329061973	1.5507052644
H48	-14.8266817825	1.6111712262	-0.1037184469
H49	-13.6846971305	2.9526466023	-0.1152542759
H50	-12.1292927779	1.7044267236	-1.5621166418
H51	-13.5888241855	0.8670483819	-2.1089099630

bond lengths (angstroms):

C1 -C2 : 1.394923 C1 -C5 : 1.399623
C1 -H26 : 1.084161 C2 -C25 : 1.403469
C2 -H27 : 1.087935 S3 -C4 : 1.821906
S3 -C5 : 1.782699 C4 -H28 : 1.091976
C4 -H29 : 1.092387 C4 -H30 : 1.092223
C5 -C6 : 1.403965 C6 -C7 : 1.389945
C6 -H31 : 1.086856 C7 -C25 : 1.407484
C7 -H32 : 1.086659 C8 -C9 : 1.568514
C8 -C10 : 1.568027 C8 -H33 : 1.095240
C8 -H34 : 1.095683 C9 -Si19 : 1.900871
C9 -H35 : 1.096297 C9 -H36 : 1.093193
C10 -Si19 : 1.902971 C10 -H37 : 1.093261
C10 -H38 : 1.096217 C11 -C12 : 1.403761
C11 -C13 : 1.407247 C11 -Si19 : 1.874392
C12 -C18 : 1.394359 C12 -H39 : 1.088444
C13 -C14 : 1.389899 C13 -H40 : 1.086436
C14 -C17 : 1.403977 C14 -H41 : 1.086834
S15 -C16 : 1.821893 S15 -C17 : 1.782185
C16 -H42 : 1.091981 C16 -H43 : 1.092402
C16 -H44 : 1.092418 C17 -C18 : 1.399940
C18 -H45 : 1.084112 Si19 -O20 : 1.662199
O20 -Si22 : 1.659283 C21 -Si22 : 1.902319
C21 -C23 : 1.568294 C21 -H46 : 1.092708
C21 -H47 : 1.096134 Si22 -C24 : 1.899324
Si22 -C25 : 1.876855 C23 -C24 : 1.569016
C23 -H48 : 1.095414 C23 -H49 : 1.095450
C24 -H50 : 1.095800 C24 -H51 : 1.093183

bond angles:

C5 -C1 -C2 : 120.036903 H26 -C1 -C2 : 119.098008
H26 -C1 -C5 : 120.864458 C25 -C2 -C1 : 122.008648
H27 -C2 -C1 : 117.921786 H27 -C2 -C25 : 120.068897
C5 -S3 -C4 : 103.692574 H28 -C4 -S3 : 105.553175
H29 -C4 -S3 : 111.491032 H29 -C4 -H28 : 108.907849
H30 -C4 -S3 : 111.653257 H30 -C4 -H28 : 108.832833
H30 -C4 -H29 : 110.233881 S3 -C5 -C1 : 124.610432
C6 -C5 -C1 : 118.833139 C6 -C5 -S3 : 116.555937
C7 -C6 -C5 : 120.460238 H31 -C6 -C5 : 119.720232
H31 -C6 -C7 : 119.819453 C25 -C7 -C6 : 121.614705
H32 -C7 -C6 : 118.776694 H32 -C7 -C25 : 119.608196
C10 -C8 -C9 : 101.347737 H33 -C8 -C9 : 110.195899
H33 -C8 -C10 : 110.208184 H34 -C8 -C9 : 114.007863
H34 -C8 -C10 : 114.029035 H34 -C8 -H33 : 107.019470
Si19 -C9 -C8 : 87.866490 H35 -C9 -C8 : 111.800589
H35 -C9 -Si19 : 112.598562 H36 -C9 -C8 : 115.551170

H36 -C9 -Si19 : 120.403647 H36 -C9 -H35 : 107.619889
Si19 -C10 -C8 : 87.806097 H37 -C10 -C8 : 115.666986
H37 -C10 -Si19 : 121.003191 H38 -C10 -C8 : 111.724216
H38 -C10 -Si19 : 111.933630 H38 -C10 -H37 : 107.653472
C13 -C11 -C12 : 117.135470 Si19 -C11 -C12 : 120.766122
Si19 -C11 -C13 : 122.089795 C18 -C12 -C11 : 121.994542
H39 -C12 -C11 : 120.094173 H39 -C12 -C18 : 117.911059
C14 -C13 -C11 : 121.523934 H40 -C13 -C11 : 119.563445
H40 -C13 -C14 : 118.912425 C17 -C14 -C13 : 120.481574
H41 -C14 -C13 : 119.805311 H41 -C14 -C17 : 119.713082
C17 -S15 -C16 : 103.676064 H42 -C16 -S15 : 105.531568
H43 -C16 -S15 : 111.576585 H43 -C16 -H42 : 108.868654
H44 -C16 -S15 : 111.578203 H44 -C16 -H42 : 108.871556
H44 -C16 -H43 : 110.243846 S15 -C17 -C14 : 116.584586
C18 -C17 -C14 : 118.878278 C18 -C17 -S15 : 124.537083
C17 -C18 -C12 : 119.986056 H45 -C18 -C12 : 119.127349
H45 -C18 -C17 : 120.886348 C10 -Si19 -C9 : 79.263138
C11 -Si19 -C9 : 119.226416 C11 -Si19 -C10 : 119.847097
O20 -Si19 -C9 : 115.489703 O20 -Si19 -C10 : 115.158403
O20 -Si19 -C11 : 106.463725 Si22 -O20 -Si19 : 147.869363
C23 -C21 -Si22 : 87.158619 H46 -C21 -Si22 : 121.158934
H46 -C21 -C23 : 115.772131 H47 -C21 -Si22 : 112.248873
H47 -C21 -C23 : 111.167619 H47 -C21 -H46 : 108.036477
C21 -Si22 -O20 : 118.362397 C24 -Si22 -O20 : 119.914920
C24 -Si22 -C21 : 79.215100 C25 -Si22 -O20 : 106.549339
C25 -Si22 -C21 : 116.197871 C25 -Si22 -C24 : 115.202848
C24 -C23 -C21 : 101.162068 H48 -C23 -C21 : 110.147058
H48 -C23 -C24 : 110.324183 H49 -C23 -C21 : 114.077721
H49 -C23 -C24 : 114.037491 H49 -C23 -H48 : 107.054955
C23 -C24 -Si22 : 87.243264 H50 -C24 -Si22 : 111.992596
H50 -C24 -C23 : 111.111114 H51 -C24 -Si22 : 121.403394
H51 -C24 -C23 : 115.978554 H51 -C24 -H50 : 107.855218
C7 -C25 -C2 : 117.044440 Si22 -C25 -C2 : 121.511110
Si22 -C25 -C7 : 121.423123

torsional angles:

C1 -C2 -C25 -C7 : 0.446979
C1 -C2 -C25 -Si22 :-177.895796
C1 -C5 -S3 -C4 : -2.692937
C1 -C5 -C6 -C7 : 0.321387
C1 -C5 -C6 -H31 :-179.779872
C2 -C1 -C5 -S3 :-179.968906
C2 -C1 -C5 -C6 : -0.233607
C2 -C25 -C7 -C6 : -0.356678
C2 -C25 -C7 -H32 : 179.408869

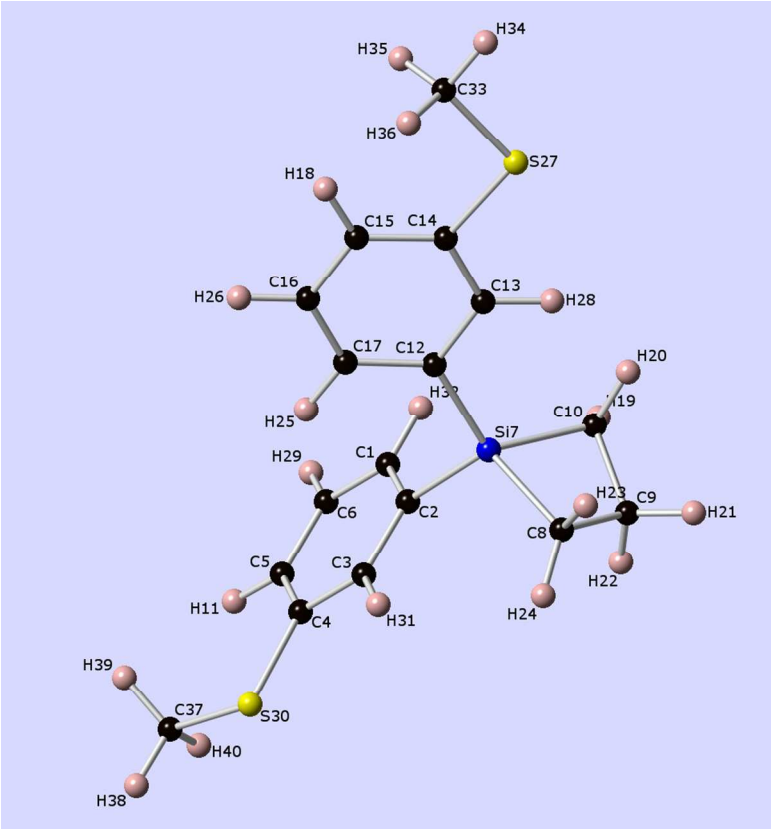
C2 -C25 -Si22 -O20 :-159.024567
C2 -C25 -Si22 -C21 : 66.667451
C2 -C25 -Si22 -C24 : -23.393756
S3 -C5 -C1 -H26 : -0.260568
S3 -C5 -C6 -C7 :-179.922166
S3 -C5 -C6 -H31 : -0.023424
C4 -S3 -C5 -C6 : 177.566298
C5 -C1 -C2 -C25 : -0.158051
C5 -C1 -C2 -H27 : 179.544461
C5 -S3 -C4 -H28 :-178.544338
C5 -S3 -C4 -H29 : -60.439809
C5 -S3 -C4 -H30 : 63.355518
C5 -C6 -C7 -C25 : -0.020798
C5 -C6 -C7 -H32 :-179.788238
C6 -C5 -C1 -H26 : 179.474731
C6 -C7 -C25 -Si22 : 177.987654
C7 -C25 -C2 -H27 :-179.249289
C7 -C25 -Si22 -O20 : 22.705144
C7 -C25 -Si22 -C21 :-111.602837
C7 -C25 -Si22 -C24 : 158.335956
C8 -C9 -Si19 -C10 : 13.135377
C8 -C9 -Si19 -C11 : 131.453010
C8 -C9 -Si19 -O20 : -99.754132
C8 -C10 -Si19 -C9 : -13.140063
C8 -C10 -Si19 -C11 :-130.795893
C8 -C10 -Si19 -O20 : 100.117470
C9 -C8 -C10 -Si19 : 16.026157
C9 -C8 -C10 -H37 : 139.632541
C9 -C8 -C10 -H38 : -96.749337
C9 -Si19 -C10 -H37 :-132.000735
C9 -Si19 -C10 -H38 : 99.434659
C9 -Si19 -C11 -C12 : -34.969517
C9 -Si19 -C11 -C13 : 146.128923
C9 -Si19 -O20 -Si22 : 51.557094
C10 -C8 -C9 -Si19 : -16.043687
C10 -C8 -C9 -H35 : 97.488083
C10 -C8 -C9 -H36 :-138.967835
C10 -Si19 -C9 -H35 : -99.634819
C10 -Si19 -C9 -H36 : 131.727776
C10 -Si19 -C11 -C12 : 59.326582
C10 -Si19 -C11 -C13 :-119.574977
C10 -Si19 -O20 -Si22 : -38.208131
C11 -C12 -C18 -C17 : -0.067673
C11 -C12 -C18 -H45 :-179.888763
C11 -C13 -C14 -C17 : 0.007207
C11 -C13 -C14 -H41 : 179.941688

C11 -Si19 -C9 -H35 : 18.682813
C11 -Si19 -C9 -H36 :-109.954592
C11 -Si19 -C10 -H37 : 110.343435
C11 -Si19 -C10 -H38 : -18.221171
C11 -Si19 -O20 -Si22 :-173.618850
C12 -C11 -C13 -C14 : -0.106825
C12 -C11 -C13 -H40 : 179.730407
C12 -C11 -Si19 -O20 :-167.778020
C12 -C18 -C17 -C14 : -0.036830
C12 -C18 -C17 -S15 :-179.950234
C13 -C11 -C12 -C18 : 0.137418
C13 -C11 -C12 -H39 :-179.686254
C13 -C11 -Si19 -O20 : 13.320420
C13 -C14 -C17 -S15 : 179.986632
C13 -C14 -C17 -C18 : 0.066400
C14 -C13 -C11 -Si19 : 178.832593
C14 -C17 -S15 -C16 :-179.711863
C14 -C17 -C18 -H45 : 179.781059
S15 -C17 -C14 -H41 : 0.052092
S15 -C17 -C18 -H45 : -0.132345
C16 -S15 -C17 -C18 : 0.203345
C17 -C14 -C13 -H40 :-179.831057
C17 -S15 -C16 -H42 : 179.862055
C17 -S15 -C16 -H43 : -62.048200
C17 -S15 -C16 -H44 : 61.767986
C17 -C18 -C12 -H39 : 179.759685
C18 -C12 -C11 -Si19 :-178.816870
C18 -C17 -C14 -H41 :-179.868141
Si19 -C9 -C8 -H33 : 100.650095
Si19 -C9 -C8 -H34 :-139.002422
Si19 -C10 -C8 -H33 :-100.658633
Si19 -C10 -C8 -H34 : 138.970336
Si19 -C11 -C12 -H39 : 1.359459
Si19 -C11 -C13 -H40 : -1.330175
Si19 -O20 -Si22 -C21 : -39.509530
Si19 -O20 -Si22 -C24 : 54.233355
Si19 -O20 -Si22 -C25 :-172.650324
O20 -Si19 -C9 -H35 : 147.475672
O20 -Si19 -C9 -H36 : 18.838267
O20 -Si19 -C10 -H37 : -18.743202
O20 -Si19 -C10 -H38 :-147.307808
O20 -Si22 -C21 -C23 : 133.841960
O20 -Si22 -C21 -H46 :-107.556941
O20 -Si22 -C21 -H47 : 22.106543
O20 -Si22 -C24 -C23 :-132.168659
O20 -Si22 -C24 -H50 : -20.487151

O20 -Si22 -C24 -H51 : 108.857601
C21 -Si22 -C24 -C23 : -15.532623
C21 -Si22 -C24 -H50 : 96.148886
C21 -Si22 -C24 -H51 :-134.506363
C21 -C23 -C24 -Si22 : 18.979921
C21 -C23 -C24 -H50 : -93.558543
C21 -C23 -C24 -H51 : 142.817168
Si22 -C21 -C23 -C24 : -18.950315
Si22 -C21 -C23 -H48 : 97.760940
Si22 -C21 -C23 -H49 :-141.833460
Si22 -C24 -C23 -H48 : -97.601205
Si22 -C24 -C23 -H49 : 141.890832
Si22 -C25 -C2 -H27 : 2.407936
Si22 -C25 -C7 -H32 : -2.246799
C23 -C21 -Si22 -C24 : 15.541098
C23 -C21 -Si22 -C25 : -97.375200
C23 -C24 -Si22 -C25 : 98.486711
C24 -Si22 -C21 -H46 : 134.142198
C24 -Si22 -C21 -H47 : -96.194318
C24 -C23 -C21 -H46 :-142.407214
C24 -C23 -C21 -H47 : 93.836708
C25 -C2 -C1 -H26 :-179.871532
C25 -C7 -C6 -H31 :-179.919440
C25 -Si22 -C21 -H46 : 21.225900
C25 -Si22 -C21 -H47 : 150.889384
C25 -Si22 -C24 -H50 :-149.831781
C25 -Si22 -C24 -H51 : -20.487029
H26 -C1 -C2 -H27 : -0.169020
H31 -C6 -C7 -H32 : 0.313121
H33 -C8 -C9 -H35 :-145.818134
H33 -C8 -C9 -H36 : -22.274053
H33 -C8 -C10 -H37 : 22.947751
H33 -C8 -C10 -H38 : 146.565873
H34 -C8 -C9 -H35 : -25.470651
H34 -C8 -C9 -H36 : 98.073430
H34 -C8 -C10 -H37 : -97.423280
H34 -C8 -C10 -H38 : 26.194842
H39 -C12 -C18 -H45 : -0.061405
H40 -C13 -C14 -H41 : 0.103423
H46 -C21 -C23 -H48 : -25.695960
H46 -C21 -C23 -H49 : 94.709640
H47 -C21 -C23 -H48 :-149.452037
H47 -C21 -C23 -H49 : -29.046437
H48 -C23 -C24 -H50 : 149.860331
H48 -C23 -C24 -H51 : 26.236042
H49 -C23 -C24 -H50 : 29.352368

H49 -C23 -C24 -H51 : -94.271921

Geometry Optimization for **11**:
B3LYP, 6-31G**
Final total energy = -1745.75838 hartree



final geometry:

	angstroms		
atom	x	y	z
C1	-0.2016047877	-0.0712794308	0.1037129240
C2	0.1517650841	-0.0366552570	1.4662511883
C3	1.5065393352	0.0987745679	1.7964103009
C4	2.5000631545	0.1891580663	0.8074622521
C5	2.1258744774	0.1503007735	-0.5398916867
C6	0.7775901487	0.0216339333	-0.8809697623
Si7	-1.1609341528	-0.2294400929	2.8117517341
C8	-0.9123657716	0.9400948044	4.2970623105
C9	-1.9176008314	1.9177907381	3.5985222496
C10	-2.6491807696	0.9431184215	2.6130695616

H11	2.8677637214	0.2206504913	-1.3270623860
C12	-1.4766860155	-2.0689548085	3.1176736383
C13	-2.6384723638	-2.4856613581	3.7831635262
C14	-2.8884627435	-3.8403334515	4.0495771762
C15	-1.9534450293	-4.7981663309	3.6417623036
C16	-0.7942229238	-4.3960367169	2.9767787481
C17	-0.5531264126	-3.0507183210	2.7116803801
H18	-2.1164170890	-5.8527010053	3.8333898635
H19	-2.9094374644	1.3621255014	1.6378057918
H20	-3.5641779743	0.5372344837	3.0593446515
H21	-2.5856871068	2.4461616835	4.2882215263
H22	-1.3679024461	2.6771092611	3.0327650013
H23	-1.3357787698	0.5214197345	5.2169050406
H24	0.0681733800	1.3591552841	4.5364950715
H25	0.3519225652	-2.7621625387	2.1858539972
H26	-0.0760620129	-5.1485784317	2.6619201574
S27	-4.4123127998	-4.2170205529	4.9034852168
H28	-3.3739788545	-1.7499865921	4.1021437566
H29	0.4971459184	-0.0047083594	-1.9306562630
S30	4.1820503839	0.3528948018	1.3858105625
H31	1.8057233625	0.1335040721	2.8419435304
H32	-1.2439954642	-0.1714426639	-0.1875210476
C33	-4.4065946996	-6.0356442083	5.0099944829
H34	-5.3392168118	-6.3024333402	5.5114177217
H35	-4.3944570907	-6.4954267974	4.0190434125
H36	-3.5681359699	-6.4024576797	5.6066300314
C37	5.1665467568	0.3331945910	-0.1466601228
H38	6.2083967510	0.3990354416	0.1736885655
H39	5.0252389597	-0.5976277604	-0.7008879790
H40	4.9391507824	1.1905572964	-0.7843922673

Z-matrix: (angstroms and degrees)

C1
C2 C1 cc2
C3 C2 cc3 C1 ccc3
C4 C3 cc4 C2 ccc4 C1 dih4
C5 C4 cc5 C3 ccc5 C2 dih5
C6 C5 cc6 C4 ccc6 C3 dih6
Si7 C2 sic7 C3 sicc7 C4 dih7
C8 Si7 csi8 C2 csic8 C3 dih8
C9 C8 cc9 Si7 ccsi9 C2 dih9
C10 C9 cc10 C8 ccc10 Si7 dih10
H11 C5 hc11 C4 hcc11 C3 dih11
C12 Si7 csi12 C10 csic12 C9 dih12
C13 C12 cc13 Si7 ccsi13 C10 dih13

C14 C13 cc14 C12 ccc14 Si7 dih14
C15 C14 cc15 C13 ccc15 C12 dih15
C16 C15 cc16 C14 ccc16 C13 dih16
C17 C16 cc17 C15 ccc17 C14 dih17
H18 C15 hc18 C16 hcc18 C17 dih18
H19 C10 hc19 Si7 hcsi19 C12 dih19
H20 C10 hc20 Si7 hcsi20 C12 dih20
H21 C9 hc21 C10 hcc21 Si7 dih21
H22 C9 hc22 C10 hcc22 Si7 dih22
H23 C8 hc23 Si7 hcsi23 C12 dih23
H24 C8 hc24 Si7 hcsi24 C12 dih24
H25 C17 hc25 C12 hcc25 C13 dih25
H26 C16 hc26 C17 hcc26 C12 dih26
S27 C14 sc27 C13 scc27 C12 dih27
H28 C13 hc28 C12 hcc28 C17 dih28
H29 C6 hc29 C5 hcc29 C4 dih29
S30 C4 sc30 C3 scc30 C2 dih30
H31 C3 hc31 C2 hcc31 Si7 dih31
H32 C1 hc32 C2 hcc32 Si7 dih32
C33 S27 cs33 C14 csc33 C13 dih33
H34 C33 hc34 S27 hcs34 C14 dih34
H35 C33 hc35 S27 hcs35 H34 dih35
H36 C33 hc36 S27 hcs36 H34 dih36
C37 S30 cs37 C4 csc37 C3 dih37
H38 C37 hc38 S30 hcs38 C4 dih38
H39 C37 hc39 S30 hcs39 H38 dih39
H40 C37 hc40 S30 hcs40 H38 dih40

Z-variables: (angstroms and degrees)
cc2 = 1.4080410582
cc3 = 1.4009852064
ccc3 = 118.2364308418
cc4 = 1.4047337824
ccc4 = 121.6178016134
dih4 = -0.4579848873
cc5 = 1.3988887345
ccc5 = 119.1502123183
dih5 = 0.3577217893
cc6 = 1.396696116
ccc6 = 119.7346770452
dih6 = -0.0609668002
sic7 = 1.8896340911
sicc7 = 120.919361547
dih7 = 177.4086818223
csi8 = 1.9067631275
csic8 = 113.6734358553

dih8 = 42.9338021105
cc9 = 1.5666349546
ccsi9 = 87.2375427076
dih9 = 95.2647153888
cc10 = 1.5672626873
ccc10 = 101.0560136063
dih10 = 19.7126603611
hc11 = 1.083967916
hcc11 = 120.9682287206
dih11 = 179.8162135163
csi12 = 1.8913227751
csic12 = 119.0181024319
dih12 = 133.7575455196
cc13 = 1.4022370193
ccsi13 = 120.2728028385
dih13 = -29.1787723905
cc14 = 1.4030708833
ccc14 = 121.6452119952
dih14 = -178.673656575
cc15 = 1.3992908637
ccc15 = 119.1110978882
dih15 = 0.0747110624
cc16 = 1.3956028251
ccc16 = 119.7794688109
dih16 = -0.1688591615
cc17 = 1.3922234945
ccc17 = 120.8641550289
dih17 = -0.0124170243
hc18 = 1.0841237907
hcc18 = 119.2987370628
dih18 = 179.8854266543
hc19 = 1.092904342
hcsi19 = 121.0022772238
dih19 = -107.6782728724
hc20 = 1.0959576231
hcsi20 = 112.4453981022
dih20 = 21.7551844059
hc21 = 1.0959928009
hcc21 = 114.2646603935
dih21 = -142.9521778494
hc22 = 1.0949037392
hcc22 = 109.9218803267
dih22 = 96.401410483
hc23 = 1.095754548
hcsi23 = 111.6652255957
dih23 = -21.2986124517

hc24 = 1.0928846053
hcsi24 = 121.5209218467
dih24 = 108.0497574184
hc25 = 1.0857584799
hcc25 = 120.0795738593
dih25 = 179.4233521555
hc26 = 1.086834881
hcc26 = 119.9665610002
dih26 = -179.8976494288
sc27 = 1.7869446293
scc27 = 116.5004215017
dih27 = -179.923586755
hc28 = 1.0880880234
hcc28 = 119.8847407633
dih28 = -179.5379158855
hc29 = 1.0868231837
hcc29 = 119.1559350819
dih29 = 179.8268927468
sc30 = 1.786162794
scc30 = 116.3569326247
dih30 = -179.7995874869
hc31 = 1.0880519081
hcc31 = 119.6988226355
dih31 = -2.4563717814
hc32 = 1.0869352427
hcc32 = 120.1475301067
dih32 = 2.3746466526
cs33 = 1.8217488632
csc33 = 103.632857954
dih33 = 178.0637971713
hc34 = 1.0919641522
hcs34 = 105.5493014718
dih34 = -178.8841797357
hc35 = 1.0924886153
hcs35 = 111.5393027982
dih35 = 118.0648049007
hc36 = 1.0924921703
hcs36 = 111.6860615903
dih36 = -118.1053103649
cs37 = 1.8215618595
csc37 = 103.6239721889
dih37 = 176.5625251362
hc38 = 1.0919751417
hcs38 = 105.5571483843
dih38 = -178.197881337
hc39 = 1.0925047643

hcs39 = 111.4751558273
dih39 = 118.0663409008
hc40 = 1.0924660296
hcs40 = 111.7232764097
dih40 = -118.1192491791

bond lengths (angstroms):

C1	-C2	: 1.408041	C1	-C6	: 1.391781
C1	-H32	: 1.086935	C2	-C3	: 1.400985
C2	-Si7	: 1.889634	C3	-C4	: 1.404734
C3	-H31	: 1.088052	C4	-C5	: 1.398889
C4	-S30	: 1.786163	C5	-C6	: 1.396696
C5	-H11	: 1.083968	C6	-H29	: 1.086823
Si7	-C8	: 1.906763	Si7	-C10	: 1.905058
Si7	-C12	: 1.891323	C8	-C9	: 1.566635
C8	-H23	: 1.095755	C8	-H24	: 1.092885
C9	-C10	: 1.567263	C9	-H21	: 1.095993
C9	-H22	: 1.094904	C10	-H19	: 1.092904
C10	-H20	: 1.095958	C12	-C13	: 1.402237
C12	-C17	: 1.407712	C13	-C14	: 1.403071
C13	-H28	: 1.088088	C14	-C15	: 1.399291
C14	-S27	: 1.786945	C15	-C16	: 1.395603
C15	-H18	: 1.084124	C16	-C17	: 1.392223
C16	-H26	: 1.086835	C17	-H25	: 1.085758
S27	-C33	: 1.821749	S30	-C37	: 1.821562
C33	-H34	: 1.091964	C33	-H35	: 1.092489
C33	-H36	: 1.092492	C37	-H38	: 1.091975
C37	-H39	: 1.092505	C37	-H40	: 1.092466

bond angles:

C6	-C1	-C2	: 120.425963	H32	-C1	-C2	: 120.147530
H32	-C1	-C6	: 119.426503	C3	-C2	-C1	: 118.236431
Si7	-C2	-C1	: 120.809256	Si7	-C2	-C3	: 120.919362
C4	-C3	-C2	: 121.617802	H31	-C3	-C2	: 119.698823
H31	-C3	-C4	: 118.683242	C5	-C4	-C3	: 119.150212
S30	-C4	-C3	: 116.356933	S30	-C4	-C5	: 124.492650
C6	-C5	-C4	: 119.734677	H11	-C5	-C4	: 120.968229
H11	-C5	-C6	: 119.296982	C5	-C6	-C1	: 120.833512
H29	-C6	-C1	: 120.010534	H29	-C6	-C5	: 119.155935
C8	-Si7	-C2	: 113.673436	C10	-Si7	-C2	: 113.931125
C10	-Si7	-C8	: 78.787826	C12	-Si7	-C2	: 109.291640
C12	-Si7	-C8	: 119.493506	C12	-Si7	-C10	: 119.018102

C9 -C8 -Si7 : 87.237543 H23 -C8 -Si7 : 111.665226
H23 -C8 -C9 : 111.396040 H24 -C8 -Si7 : 121.520922
H24 -C8 -C9 : 115.726818 H24 -C8 -H23 : 108.016329
C10 -C9 -C8 : 101.056014 H21 -C9 -C8 : 114.292994
H21 -C9 -C10 : 114.264660 H22 -C9 -C8 : 109.940953
H22 -C9 -C10 : 109.921880 H22 -C9 -H21 : 107.269730
C9 -C10 -Si7 : 87.279714 H19 -C10 -Si7 : 121.002277
H19 -C10 -C9 : 115.710373 H20 -C10 -Si7 : 112.445398
H20 -C10 -C9 : 111.345645 H20 -C10 -H19 : 107.851014
C13 -C12 -Si7 : 120.272803 C17 -C12 -Si7 : 121.475542
C17 -C12 -C13 : 118.241723 C14 -C13 -C12 : 121.645212
H28 -C13 -C12 : 119.884741 H28 -C13 -C14 : 118.469532
C15 -C14 -C13 : 119.111098 S27 -C14 -C13 : 116.500422
S27 -C14 -C15 : 124.388481 C16 -C15 -C14 : 119.779469
H18 -C15 -C14 : 120.921714 H18 -C15 -C16 : 119.298737
C17 -C16 -C15 : 120.864155 H26 -C16 -C15 : 119.169017
H26 -C16 -C17 : 119.966561 C16 -C17 -C12 : 120.357281
H25 -C17 -C12 : 120.079574 H25 -C17 -C16 : 119.562849
C33 -S27 -C14 : 103.632858 C37 -S30 -C4 : 103.623972
H34 -C33 -S27 : 105.549301 H35 -C33 -S27 : 111.539303
H35 -C33 -H34 : 108.855368 H36 -C33 -S27 : 111.686062
H36 -C33 -H34 : 108.824636 H36 -C33 -H35 : 110.214309
H38 -C37 -S30 : 105.557148 H39 -C37 -S30 : 111.475156
H39 -C37 -H38 : 108.880925 H40 -C37 -S30 : 111.723276
H40 -C37 -H38 : 108.815940 H40 -C37 -H39 : 110.217844

torsional angles:

C1 -C2 -C3 -C4 : -0.457985
C1 -C2 -C3 -H31 : 179.676962
C1 -C2 -Si7 -C8 :-139.254515
C1 -C2 -Si7 -C10 : -51.415786
C1 -C2 -Si7 -C12 : 84.442679
C1 -C6 -C5 -C4 : -0.122482
C1 -C6 -C5 -H11 : 179.998276
C2 -C1 -C6 -C5 : 0.016595
C2 -C1 -C6 -H29 :-179.932349
C2 -C3 -C4 -C5 : 0.357722
C2 -C3 -C4 -S30 :-179.799587
C2 -Si7 -C8 -C9 : 95.264715
C2 -Si7 -C8 -H23 :-152.783144
C2 -Si7 -C8 -H24 : -23.434774
C2 -Si7 -C10 -C9 : -94.979457
C2 -Si7 -C10 -H19 : 23.584725
C2 -Si7 -C10 -H20 : 153.018182
C2 -Si7 -C12 -C13 :-162.464387

C2 -Si7 -C12 -C17 : 18.702324
C3 -C2 -C1 -C6 : 0.268069
C3 -C2 -C1 -H32 :-179.756237
C3 -C2 -Si7 -C8 : 42.933802
C3 -C2 -Si7 -C10 : 130.772531
C3 -C2 -Si7 -C12 : -93.369005
C3 -C4 -C5 -C6 : -0.060967
C3 -C4 -C5 -H11 : 179.816214
C3 -C4 -S30 -C37 : 176.562525
C4 -C3 -C2 -Si7 : 177.408682
C4 -C5 -C6 -H29 : 179.826893
C4 -S30 -C37 -H38 :-178.197881
C4 -S30 -C37 -H39 : -60.131540
C4 -S30 -C37 -H40 : 63.682869
C5 -C4 -C3 -H31 :-179.775895
C5 -C4 -S30 -C37 : -3.604164
C5 -C6 -C1 -H32 :-179.959274
C6 -C1 -C2 -Si7 :-177.601048
C6 -C5 -C4 -S30 :-179.889945
Si7 -C2 -C1 -H32 : 2.374647
Si7 -C2 -C3 -H31 : -2.456372
Si7 -C8 -C9 -C10 : 19.712660
Si7 -C8 -C9 -H21 : 142.915005
Si7 -C8 -C9 -H22 : -96.404960
Si7 -C10 -C9 -C8 : -19.730312
Si7 -C10 -C9 -H21 :-142.952178
Si7 -C10 -C9 -H22 : 96.401410
Si7 -C12 -C13 -C14 :-178.673657
Si7 -C12 -C13 -H28 : 1.591580
Si7 -C12 -C17 -C16 : 178.478236
Si7 -C12 -C17 -H25 : -1.720412
C8 -Si7 -C10 -C9 : 16.112381
C8 -Si7 -C10 -H19 : 134.676563
C8 -Si7 -C10 -H20 : -95.889980
C8 -Si7 -C12 -C13 : 64.163641
C8 -Si7 -C12 -C17 :-114.669649
C8 -C9 -C10 -H19 :-143.058620
C8 -C9 -C10 -H20 : 93.337289
C9 -C8 -Si7 -C10 : -16.119597
C9 -C8 -Si7 -C12 :-133.250753
C9 -C10 -Si7 -C12 : 133.757546
C10 -Si7 -C8 -H23 : 95.832544
C10 -Si7 -C8 -H24 :-134.819086
C10 -Si7 -C12 -C13 : -29.178772
C10 -Si7 -C12 -C17 : 151.987938
C10 -C9 -C8 -H23 : -92.501244

C10 -C9 -C8 -H24 : 143.613817
H11 -C5 -C4 -S30 : -0.012764
H11 -C5 -C6 -H29 : -0.052350
C12 -Si7 -C8 -H23 : -21.298612
C12 -Si7 -C8 -H24 : 108.049757
C12 -Si7 -C10 -H19 :-107.678273
C12 -Si7 -C10 -H20 : 21.755184
C12 -C13 -C14 -C15 : 0.074711
C12 -C13 -C14 -S27 :-179.923587
C12 -C17 -C16 -C15 : 0.291900
C12 -C17 -C16 -H26 :-179.897649
C13 -C12 -C17 -C16 : -0.378001
C13 -C12 -C17 -H25 : 179.423352
C13 -C14 -C15 -C16 : -0.168859
C13 -C14 -C15 -H18 : 179.934989
C13 -C14 -S27 -C33 : 178.063797
C14 -C13 -C12 -C17 : 0.196847
C14 -C15 -C16 -C17 : -0.012417
C14 -C15 -C16 -H26 :-179.824359
C14 -S27 -C33 -H34 :-178.884180
C14 -S27 -C33 -H35 : -60.819375
C14 -S27 -C33 -H36 : 63.010510
C15 -C14 -C13 -H28 : 179.813107
C15 -C14 -S27 -C33 : -1.934401
C15 -C16 -C17 -H25 :-179.510477
C16 -C15 -C14 -S27 : 179.829295
C17 -C12 -C13 -H28 :-179.537916
C17 -C16 -C15 -H18 : 179.885427
H18 -C15 -C14 -S27 : -0.066857
H18 -C15 -C16 -H26 : 0.073485
H19 -C10 -C9 -H21 : 93.719514
H19 -C10 -C9 -H22 : -26.926897
H20 -C10 -C9 -H21 : -29.884577
H20 -C10 -C9 -H22 :-150.530989
H21 -C9 -C8 -H23 : 30.701100
H21 -C9 -C8 -H24 : -93.183839
H22 -C9 -C8 -H23 : 151.381135
H22 -C9 -C8 -H24 : 27.496197
H25 -C17 -C16 -H26 : 0.299974
S27 -C14 -C13 -H28 : -0.185191
H29 -C6 -C1 -H32 : 0.091782
S30 -C4 -C3 -H31 : 0.066796

VII. References

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