Tuning Conductance in π–σ–π Single–Molecule Wires

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Supporting Information

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I. Comment on 10^{-3} G_0 Peak

The peak we observe at ~10^{-3} G_0 corresponds to molecular junctions where the first electrode binds to one thiomethyl group. The second electrode forms a weak contact with the π–system of the same thioanisole ring, the α–β σ–bond, or both; the thiomethyl group on the other end of the molecule may serve an auxillary role by directing the molecule's orientation towards forming this weak contact with the electrode, similar to what was previously described for the thioanisole-substituted silacyclobutane.[1] Furthermore, we see that when a conductance plateau is formed at 10^{-3} G_0, conductance typically jumps to the molecule–dependent, lower conductance value plateaus that comprise the major conductance peaks we observe. Once the weak contact is broken, conductance then occurs from one MeS–Au contact to the other MeS–Au contact at the other end of the junction.

II. General Synthesis and Characterization Information

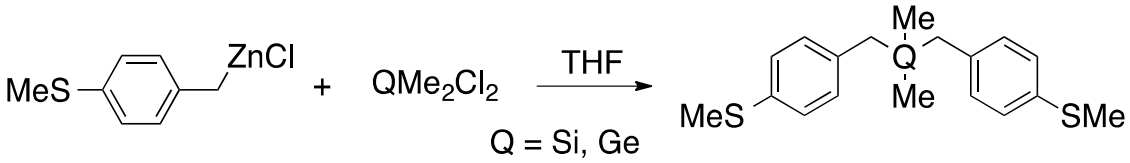
All reactions were performed in oven-dried or flame-dried round bottom flasks, unless otherwise noted. The flasks were fitted with rubber septa and reactions were conducted under a positive pressure of nitrogen or argon. Anhydrous and anaerobic solvents were obtained from a Schlenk manifold with purification 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. All chlorogermane precursors were purchased from Gelest. Zinc chloride was purchased from Acros as a THF solution. Lithium granules and lithium chloride were purchased from Strem. Trifluoromethanesulfonic acid was purchased from Alfa Aesar. Bis(chlorodimethylsilyl)methane,[2] bis(chlorodimethylgermyl)methane[3] (which was synthesized from bis(trimethylgermyl)methane[4]), 1,3-dichlorohexamethyltrigermane,[5] **CCC**[6] and **SiSiSi**[6] were synthesized from previously reported methods.

Instrumentation. ^{1}H and ^{13}C 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 7.16). 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 77.16; C_6D_6 δ 128.06).[7] 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 either a using a JEOL JMSHX110A/110A tandem mass spectrometer (FAB+) or a Waters XEVO G2XS QToF mass spectrometer equipped with a UPC2 SFC inlet, electrospray ionization (ESI) probe, atmospheric pressure chemical ionization (APCI) probe, and atmospheric solids analysis probe (ASAP).

III. Synthetic Procedures and Characterization of Compounds

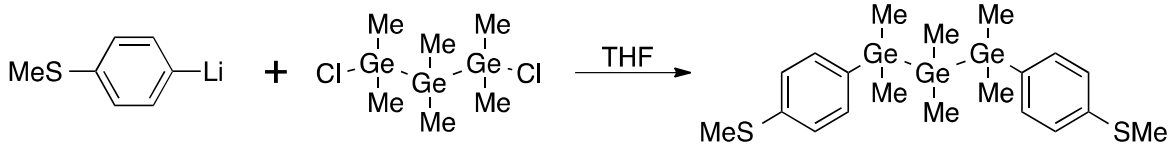
CGeC & CSiC



The preparation of the benzylic zinc chloride species was adapted from the procedure of Knochel *et al*.[8] A 25 mL Schlenk flask equipped with a stir bar was charged with lithium chloride (86 mg, 2.03 mmol, 2.1 equiv.) and magnesium turnings (99 mg, 4.06 mmol, 4.2 equiv.), then evacuated and backfilled with argon 3x. THF (2 mL) was added, followed by 0.7 M zinc chloride solution in THF (2.9 mL, 2.03 mmol, 2.1 equiv.). After stirring for 5 minutes, 4-(chloromethyl)thioanisole (351 mg, 2.03 mmol, 2.1 equiv.) was added and stirred for an hour, over which a white precipitate developed. Dichlorodimethylgermane (0.11 mL, 0.97 mmol, 1.0 equiv.) was then added to the reaction mixture and stirred overnight. The solution was then pipetted into water (10 mL), and the turnings were washed with ethyl ether (2x5 mL). The organic layer was separated from the aqueous layer, and the aqueous layer was extracted with ethyl ether. The organic layers were combined and washed with brine, dried over magnesium sulfate, then concentrated *in vacuo*. The crude material was purified using SiO_2 column chromatography with a gradient from 0-30% dichloromethane in hexanes. This yielded **CGeC** as a colorless oil (270 mg, 74% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.15 (d, J = 8.2 Hz, 4H), 6.90 (d, J = 8.3 Hz, 4H), 2.46 (s, 6H), 2.18 (s, 4H), 0.04 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.23, 133.22, 128.46, 127.69, 24.31, 16.82, -4.28. HRMS (TOF MS ASAP+) for [$C_{18}H_{24}GeS_2$+H]: calculated = 379.0611, found = 379.0610 [M+H].

CSiC was synthesized with the same general procedure described above, with the exception that dichlorodimethylsilane (0.11 mL, 0.90 mmol) was used instead of dichlorodimethylgermane. This process yielded a colorless oil (172 mg, 58% yield). ^{1}H NMR (400 MHz, C_6D_6) δ 7.14 (d, J = 8.3 Hz, 4H), 6.76 (d, J = 8.3 Hz, 4H), 2.06 (s, 6H), 1.88 (s, 4H), -0.14 (s, 6H). ^{13}C NMR (100 MHz, C_6D_6) δ 137.07, 134.30, 129.07, 127.87, 24.78, 16.26, -3.89. ^{29}Si NMR (99 MHz, C_6D_6) δ 1.85. HRMS (FAB+) for $C_{18}H_{24}S_2Si$: calculated = 332.11, found = 332.1088 $[M]^+$.

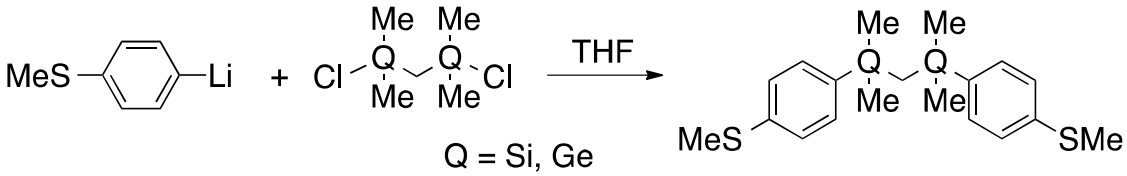
GeGeGe



A 10 mL round bottom flask equipped with a stir bar was charged with 4-bromothioanisole (26 mg, 0.13 mmol, 2.1 equiv.), which was evacuated and backfilled with argon 3x. THF (1.6 mL) was added to the flask, which was then cooled to -78˚C with an acetone/CO_2 bath. After 5 minutes, a 1.60 M *n*-butyllithium solution in hexanes (80 µL, 0.13 mmol, 2.1 equiv.) was added via syringe. The reaction was stirred for 1.5 hours over which a white precipitate developed. 1,3-

dichlorohexamethyltrigermane[5] (23 mg, 0.061 μmol, 1.00 equiv.) was added dropwise to the reaction mixture as a concentrated solution in THF. The reaction mixture was stirred at -78˚C for 20 minutes. The CO_2/acetone bath was removed and the reaction mixture was allowed to warm to room temperature, stirring for 2-3 hours. The reaction mixture was quenched with a saturated aqueous ammonium chloride solution, which was then extracted with ethyl ether 3x. The organic layer was washed with brine, dried with magnesium sulfate, concentrated *in vacuo*, then isolated with a 1000 μm preparatory TLC plate using 10% dichloromethane in hexanes as the eluent. Colorless semisolid (18 mg, 53% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 (d, J = 8.2 Hz, 4H), 7.17 (d, J = 8.2 Hz, 4H), 2.48 (s, 6H), 0.43 (s, 12H), 0.30 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.52, 138.34, 133.86, 126.20, 15.80, -2.69, -5.36. HRMS (TOF MS ASAP+) for [$C_{20}H_{32}Ge_3S_2$+H]: calculated = 554.9689, found = 554.9693 $[M+H]^+$.

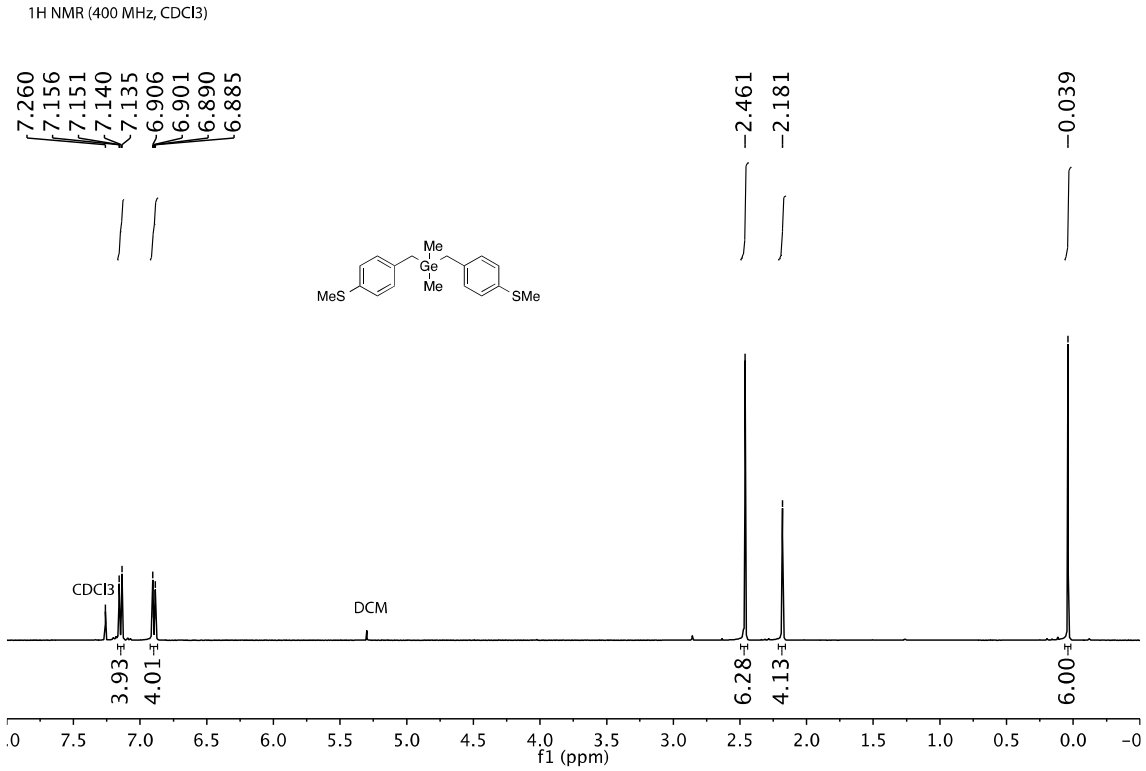
GeCGe & **SiCSi**

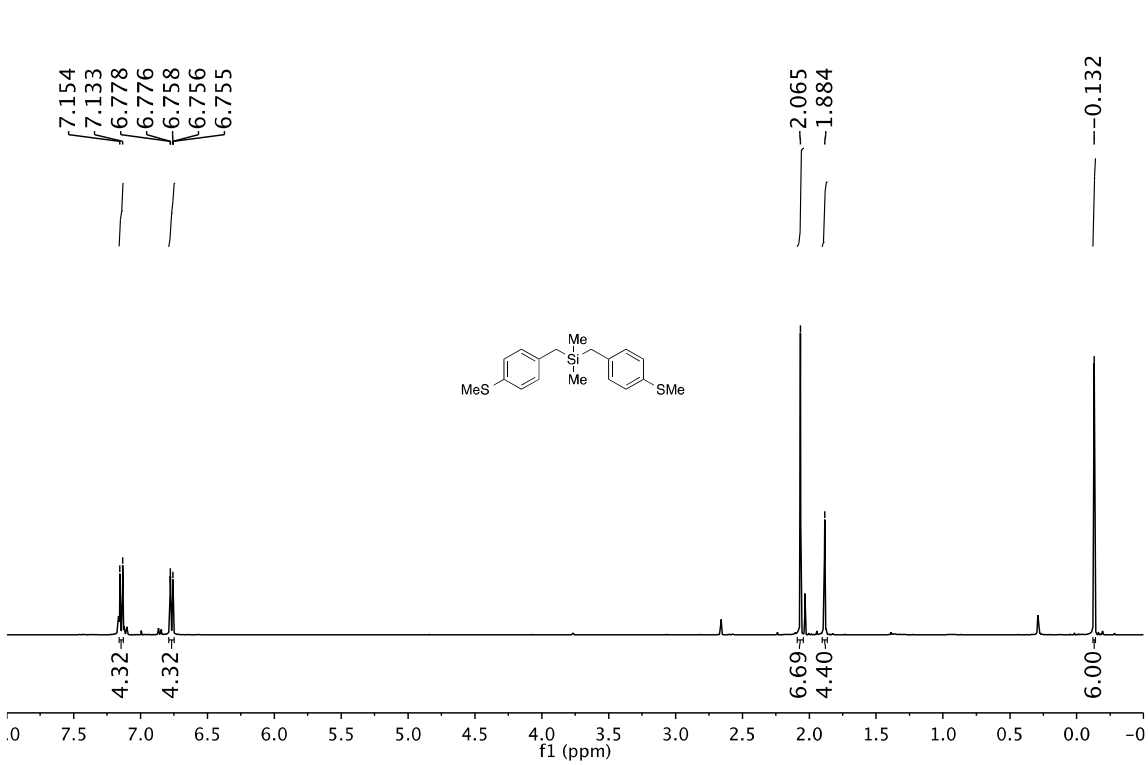


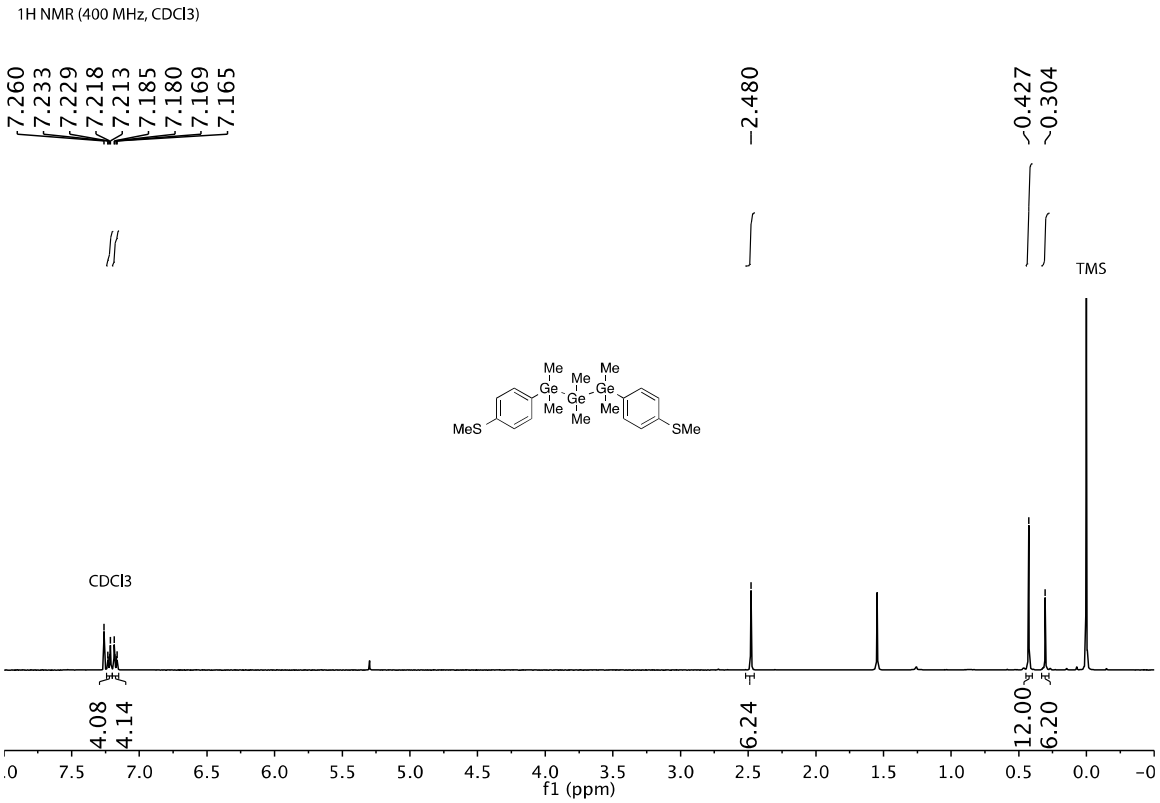
GeCGe was synthesized with the same general procedure described for **GeGeGe** with the following exceptions: bis(chlorodimethylgermyl)methane[3,4] (98 mg, 0.33 mmol) was used instead of 1,3-dichlorohexamethyltrigermane, and the crude material was isolated with a 2000 μm preparatory TLC plate using 2.5% ethyl acetate in hexanes as the eluent. Colorless oil (44 mg, 28% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.29 (m, 4H), 7.22 – 7.18 (m, 4H), 2.48 (s, 6H), 0.40 (s, 2H), 0.33 (s, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 139.58, 138.95, 133.73, 126.39, 15.23, 0.85, -0.77. HRMS (TOF MS ASAP+) for $C_{19}H_{28}Ge_2S_2$: calculated = 469.0134, found = 469.0145 $[M+H]^+$.

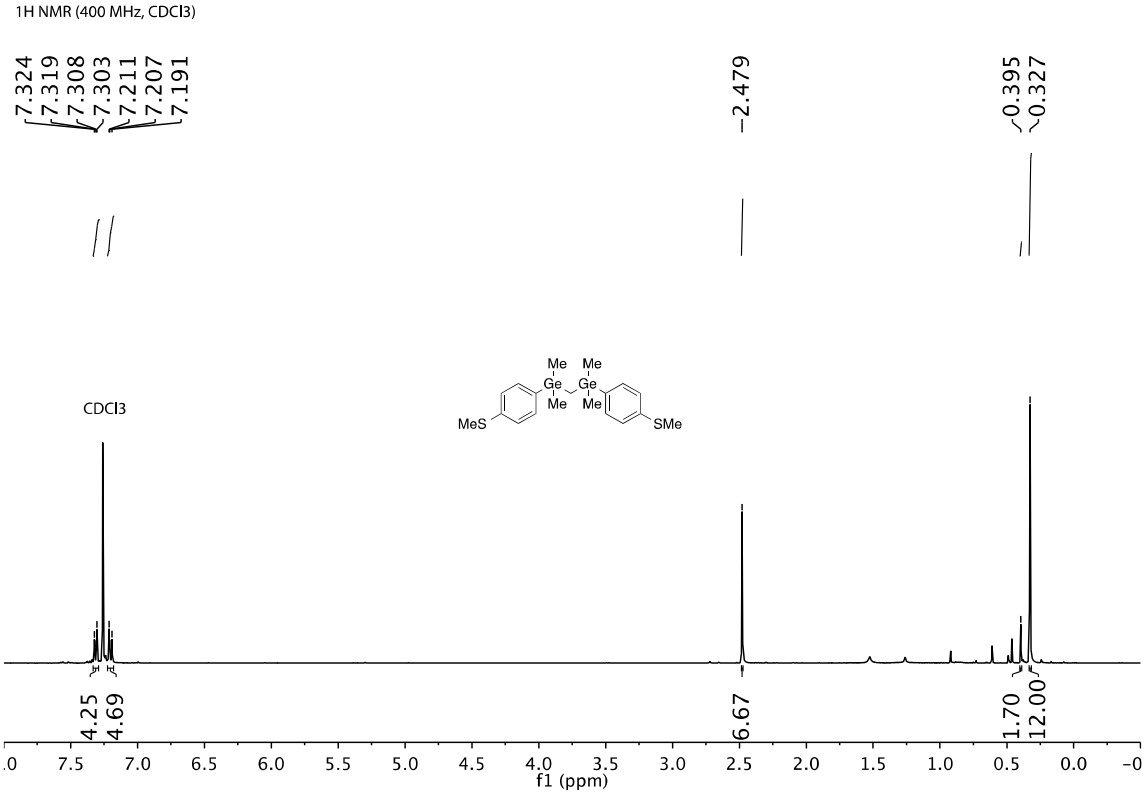
SiCSi was synthesized with the same general procedure described for **GeGeGe** with the following exceptions: Bis(chlorodimethylsilyl)methane[2] (100 mg, 0.50 mmol) was used instead of 1,3-dichlorohexamethyltrigermane, and the crude material was isolated using SiO_2 column chromatography with a gradient from 0-30% dichloromethane in hexanes. Colorless oil (175 mg, 93% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.32 (m, 4H), 7.22 – 7.17 (m, 4H), 2.48 (s, 6H), 0.22 (s, 3H), 0.21 (s, 12H).^{13}C NMR (126 MHz, C_6D_6) δ 140.19, 136.76, 134.13, 125.96, 15.06, 2.57, 0.06. ^{29}Si NMR (99 MHz, C_6D_6) δ -3.90. HRMS (FAB+) for $C_{19}H_{28}S_2Si_2$: calculated = 376.12, found = 376.1183 $[M]^+$.

^{1}H NMR Spectra:

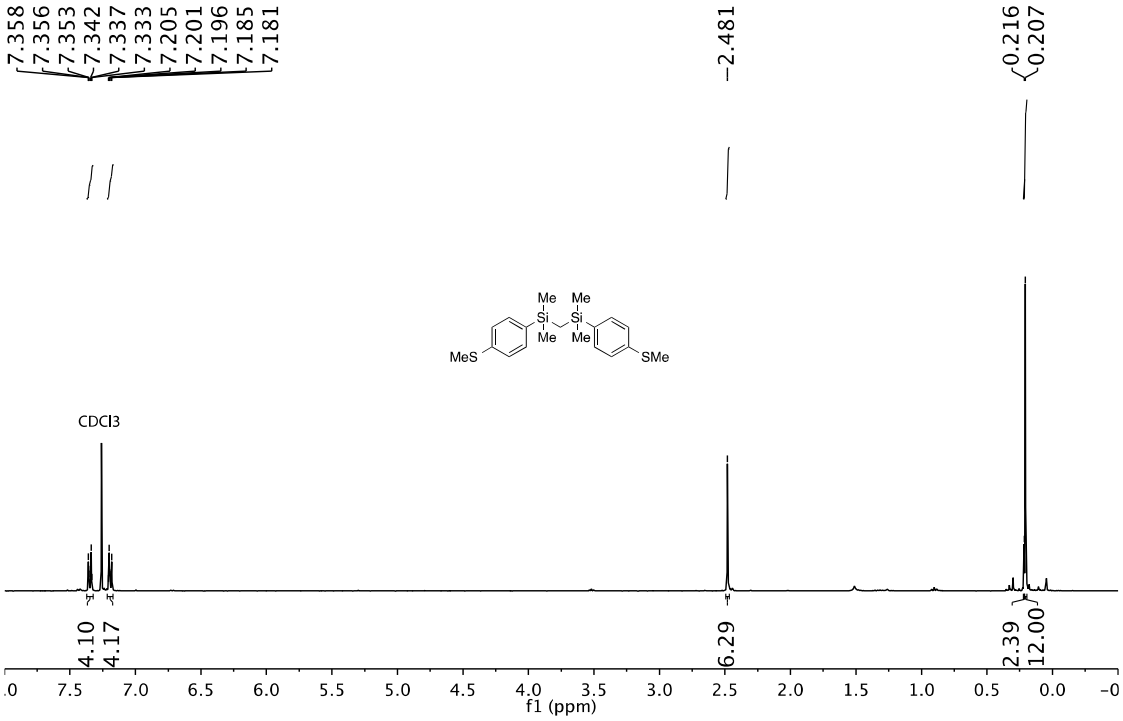




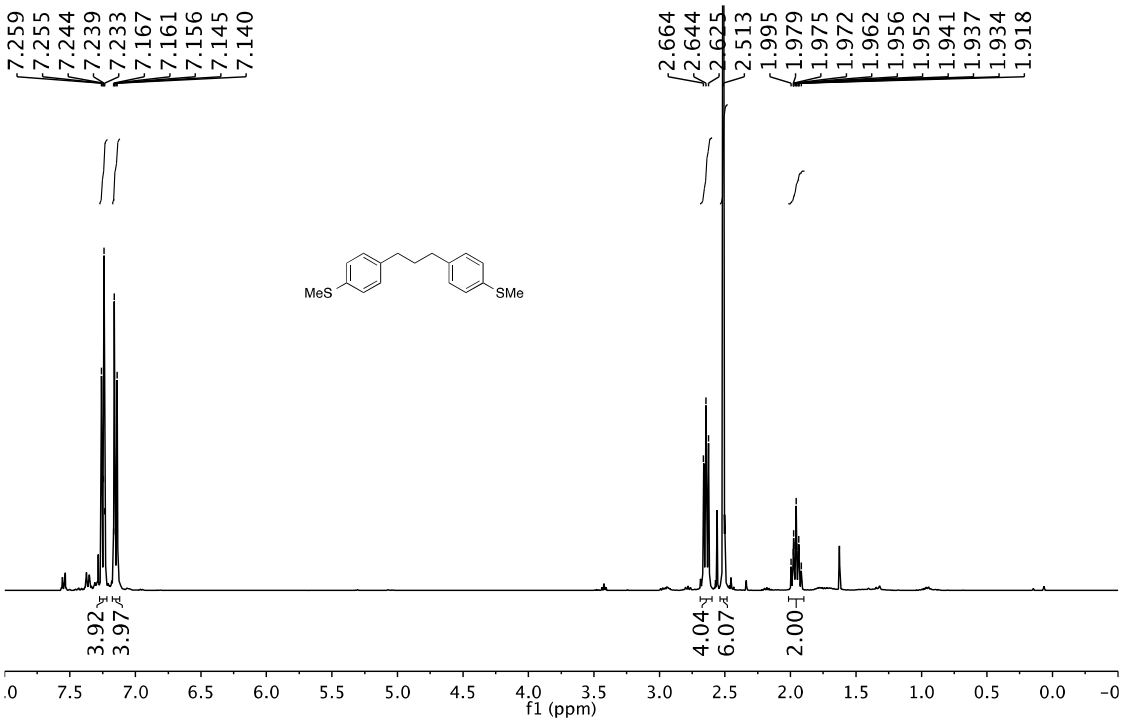

1H NMR (400 MHz, CDCl3)
7.260
7.233
7.229
7.218
7.213
7.185
7.180
7.169
7.165
2.480
0.427
0.304
TMS
Me
Ge
Me
Me
Ge
Me
Me
Ge
Me
Me
MeS
SMe
CDCl3
4.08
4.14
6.24
12.00
6.20
f1 (ppm)

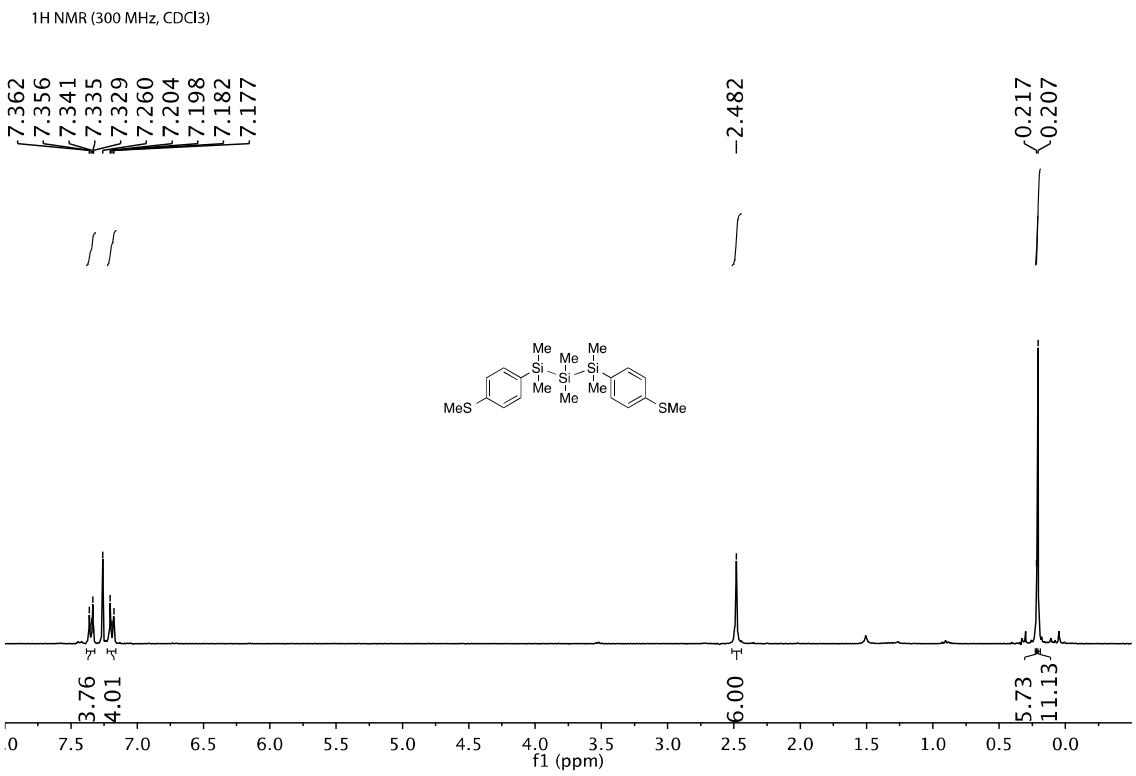

1H NMR (400 MHz, CDCl3)
7.324
7.319
7.308
7.303
7.211
7.207
7.191
2.479
0.395
0.327
Me
Ge
Me
Me
Ge
Me
Me
MeS
SMe
CDCl3
4.25
4.69
6.67
1.70
12.00
f1 (ppm)

1H NMR (400 MHz, CDCl3)



1H NMR (400 MHz, CDCl3)




1H NMR (300 MHz, CDCl3)
7.362
7.356
7.341
7.335
7.329
7.260
7.204
7.198
7.182
7.177
2.482
0.217
0.207
Me
Me
Si
Si
Me
Me
Me
Me
MeS
SMe
3.76
4.01
6.00
5.73
11.13
f1 (ppm)

IV. STM Break-Junction Experimental Details

We measured the conductance of single molecules bound to gold electrodes using a custom modified Scanning Tunneling Microscope (STM). We used a 0.25 mm diameter gold wire (99.998%, Alfa Aesar) as the tip and a gold-coated (99.999%, Alfa Aesar) mica surface as the substrate. A commercially available single-axis piezoelectric positioner (Nano-P15, Mad City Labs) was used to achieve sub-angstrom level control of the tip-substrate distance. The STM was controlled using a custom written software in Igor Pro (Wavemetrics, Inc.) and operated under ambient conditions at room temperature. The gold substrate was cleaned using UV/Ozone for 15 minutes prior to use. For each measurement, 1000 traces were first collected prior to adding molecular solutions to ensure that the gold was clean. Solutions of the target molecules at 0.1~12 mM concentration in 1,2,4-trichlorobenzene (Alfa Aesar, 99% purity) were added to the substrate for molecular conductance measurements. The applied bias was 700 mV (all molecules besides **CCC**) or 900 mV (**CCC**), and the substrate was displaced at a speed of 15-20 nm/s for all measurements. The current and voltage data were acquired at 40 kHz.

V. References

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(3) Barrau, J.; Hamida, N. B.; Satge, J. *J. Organomet. Chem.* **1985**, *282*, 315.
(4) Barton, T. J.; Hoekman, S. K. *J. Am. Chem. Soc.* **1980**, *102*, 1584.
(5) Su, T. A.; Li, H.; Zhang, V.; Neupane, M.; Batra, A.; Klausen, R. S.; Kumar, B.; Steigerwald, M. L.; Venkataraman, L.; Nuckolls, C. *J. Am. Chem. Soc.* **2015**, *137*, 12400.
(6) Klausen, R. S.; Widawsky, J. R.; Steigerwald, M. L.; Venkataraman, L.; Nuckolls, C. *J. Am. Chem. Soc.* **2012**, *134*, 4541.
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(8) Metzger, A.; Piller, F. M.; Knochel, P. *Chem. Commun.* **2008**, 5824.
(9) Klausen, R. S.; Widawsky, J. R.; Su, T. A.; Li, H.; Chen, Q.; Steigerwald, M. L.; Venkataraman, L.; Nuckolls, C. *Chem. Sci.* **2014**, *5*, 1561.

VI. Computational Chemistry

General Comments

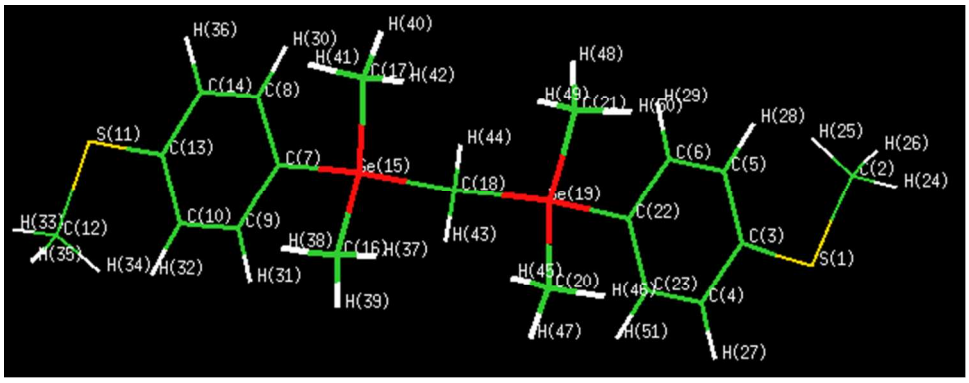
All quantum chemical calculations were performed using Jaguar, version 8.3, Schrodinger, LLC, New York, NY, 2014. Density functional theory methods with the B3LYP functional were used in each calculation. All geometries were optimized with the 6-31G** basis for light atoms and the LACVP** basis for heavy atoms. Single point energy calculations were then performed on the optimized geometries with the larger cc-PVTZ basis set to obtain more reliable energy values.

We constrain the dihedrals of the central σ–backbone to *anti* (ω=180˚) conformations and enforce coplanarity between the thioanisole π–orbitals and the σ–backbone to ensure that we are comparing consistent molecular geometries across the wires studied here. The resulting symmetry in molecular geometry enables us to use the HOMO/HOMO–1 splitting as a reasonable metric for evaluating the coupling between the S pπ orbitals, since the two S pπ orbitals interact similarly with the rest of the molecule (Ref. 9 gives further background and elaboration on orbital splitting). Furthermore, the energetic effects of imposing these constraints are negligible: without such constraints we find a <0.3 kcal/mol difference in total energy and ≤ 0.01 eV difference in HOMO & HOMO–1 energies.

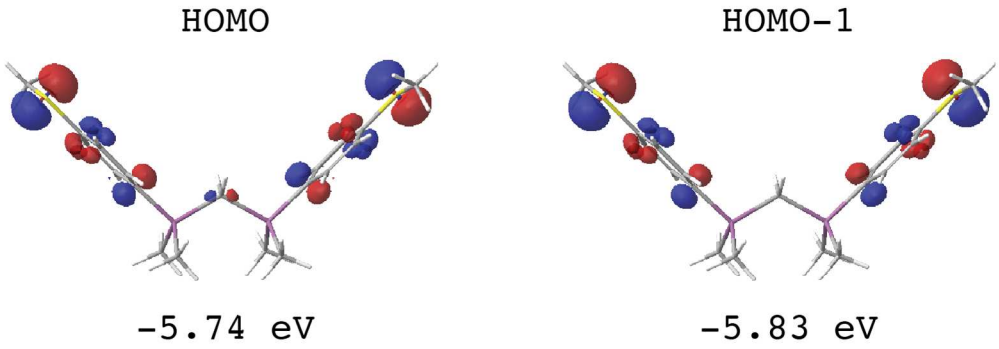
We give the calculation details below for the molecules discussed in this manuscript, ordered from least to most conductive.

Calculation Details

GeCGe



Final energy (B3LYP/cc-pVTZ): -5691.82326741602 hartrees



HOMO & HOMO–1 energies and surfaces (B3LYP/cc-pVTZ).

Optimized geometry:

Subjected to the constraints that ω(C(Ar)-α-β-α) = 180˚ and that the α-β σ-bond is orthogonal to the phenyl ring σ-plane. Optimized with LACVP** basis set.

atom	x	y	z
S1	-23.8566301465	2.0198923502	2.7365407475
C2	-24.9358225008	3.1894249517	-0.3154047389
C3	-21.4462504590	-0.1929618243	1.9315438744
C4	-20.1903913886	-1.3674492877	3.9525662808
C5	-20.7478114626	-0.8241549165	-0.5402708094
C6	-18.8285697053	-2.5877191460	-0.9625641271
C7	-5.5731065885	-3.3239488854	-0.2568326776
C8	-4.8344617791	-2.0597995865	-2.4754353991
C9	-4.3717963525	-2.5984849157	1.9909228487
C10	-2.5300900581	-0.7071222879	2.0504189860
S11	0.4913949329	2.9651541449	-0.3757758194
C12	1.5111629596	3.3777626162	2.8852376271
C13	-1.8289600917	0.5297318068	-0.1801324737
C14	-3.0056471963	-0.1711713924	-2.4525905000
Ge15	-8.2402773797	-5.9428447330	-0.3002812607
C16	-7.4915697787	-8.4394904181	2.3784206393
C17	-8.1732941475	-7.6432996687	-3.6280700696
C18	-11.5452590839	-4.2662816046	0.2902014616
Ge19	-14.7641297481	-6.1927099904	0.3993388145
C20	-14.7355060665	-8.7109268992	3.1613077167
C21	-15.4156581831	-7.9258836443	-2.8473032649
C22	-17.5456875514	-3.7764192396	1.0279070771
C23	-18.2849257347	-3.1202005043	3.4954169648
H24	-26.3941902919	4.5865542780	0.1101521358
H25	-23.4091184336	4.1118531856	-1.3555213364
H26	-25.7675438808	1.6834247239	-1.4572093890
H27	-20.7120257190	-0.9032116090	5.8848320306
H28	-21.6816196273	0.0367721807	-2.1487962384
H29	-18.3436565330	-3.0331578293	-2.9108131805
H30	-5.6956496585	-2.5527970072	-4.2763217195
H31	-4.8599107209	-3.5212608593	3.7628963594
H32	-1.6577792507	-0.2216214108	3.8405055216
H33	2.9246440860	4.8810000644	2.8386199733
H34	-0.0523454137	3.9677823556	4.0976008712
H35	2.3851745204	1.6627397818	3.6324844698

H36	-2.4818226734	0.7672949472	-4.2036390733
H37	-8.7926159801	-10.0429948447	2.2799526801
H38	-5.5666682916	-9.1657064987	2.1684966332
H39	-7.6591185661	-7.6098042732	4.2653575285
H40	-8.7444827660	-6.3650775794	-5.1502595811
H41	-6.2692835827	-8.3301697617	-4.0519299702
H42	-9.4564276350	-9.2640176106	-3.6552991333
H43	-11.3942265028	-3.2318436340	2.0818640288
H44	-11.7572032072	-2.8070842237	-1.1687294679
H45	-13.3742135065	-10.2179948222	2.7747510097
H46	-16.6025365807	-9.5755332932	3.3692021569
H47	-14.2243653853	-7.8524488871	4.9720527383
H48	-15.2936461262	-6.6219839564	-4.4479277489
H49	-14.0452590329	-9.4404896848	-3.1658487286
H50	-17.3057830403	-8.7651507006	-2.8497447910
H51	-17.3624578166	-3.9920521082	5.1131434702

angstroms

atom	x	y	z
S1	-12.6243850000	1.0688810000	1.4481150000
C2	-13.1954690000	1.6877710000	-0.1669050000
C3	-11.3488670000	-0.1021110000	1.0221290000
C4	-10.6842950000	-0.7236230000	2.0916080000
C5	-10.9792690000	-0.4361240000	-0.2858990000
C6	-9.9636500000	-1.3693620000	-0.5093670000
C7	-2.9491610000	-1.7589580000	-0.1359100000
C8	-2.5582870000	-1.0899990000	-1.3099440000
C9	-2.3134550000	-1.3750590000	1.0535510000
C10	-1.3388660000	-0.3741930000	1.0850350000
S11	0.2600350000	1.5690920000	-0.1988520000
C12	0.7996730000	1.7874350000	1.5268020000
C13	-0.9678440000	0.2803220000	-0.0953220000
C14	-1.5905200000	-0.0905800000	-1.2978550000
Ge15	-4.3605670000	-3.1448180000	-0.1589020000
C16	-3.9643680000	-4.4659860000	1.2586060000
C17	-4.3251210000	-4.0446600000	-1.9198920000
C18	-6.1094880000	-2.2576190000	0.1535680000
Ge19	-7.8128410000	-3.2770410000	0.2113210000
C20	-7.7976940000	-4.6096240000	1.6728920000
C21	-8.1576150000	-4.1941970000	-1.5067280000
C22	-9.2847780000	-1.9983950000	0.5439450000
C23	-9.6759660000	-1.6511390000	1.8496950000
H24	-13.9672040000	2.4271000000	0.0582900000
H25	-12.3875720000	2.1758990000	-0.7173110000
H26	-13.6355970000	0.8908300000	-0.7711220000
H27	-10.9603320000	-0.4779590000	3.1141190000
H28	-11.4734190000	0.0194590000	-1.1370940000
H29	-9.7070450000	-1.6050780000	-1.5403360000
H30	-3.0140080000	-1.3508820000	-2.2629320000
H31	-2.5717540000	-1.8633710000	1.9912390000
H32	-0.8772590000	-0.1172770000	2.0323080000
H33	1.5476550000	2.5829140000	1.5021330000
H34	-0.0277000000	2.0996600000	2.1683570000
H35	1.2621800000	0.8798840000	1.9222280000
H36	-1.3133240000	0.4060350000	-2.2244700000
H37	-4.6528520000	-5.3145240000	1.2064990000
H38	-2.9457540000	-4.8502830000	1.1475190000
H39	-4.0530310000	-4.0269350000	2.2571300000

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 H40          -4.6273810000     -3.3682540000     -2.7254000000
 H41          -3.3175620000     -4.4081360000     -2.1441890000
 H42          -5.0041260000     -4.9023070000     -1.9343010000
 H43          -6.0295650000     -1.7102180000      1.1016750000
 H44          -6.2216440000     -1.4854450000     -0.6184650000
 H45          -7.0773290000     -5.4071300000      1.4683350000
 H46          -8.7856840000     -5.0671540000      1.7829050000
 H47          -7.5272100000     -4.1553370000      2.6310970000
 H48          -8.0930490000     -3.5042030000     -2.3537420000
 H49          -7.4324310000     -4.9956920000     -1.6752950000
 H50          -9.1578260000     -4.6383180000     -1.5080200000
 H51          -9.1878170000     -2.1125030000      2.7057590000

 principal moments of inertia:
       amu*angstrom^2:     2351.10055     8018.52033     9521.72661
                g*cm^2: 3.90409382E-37 1.33150646E-36 1.58111970E-36

 rotational constants:
cm^(-1):      0.00717010      0.00210234      0.00177044
GHz:      0.21495423      0.06302647      0.05307640

 Molecular weight:     468.01 amu

 Stoichiometry: Ge2C19H28S2
 Molecular Point Group: C1
 Point Group used: C1


 bond lengths (angstroms):

S1      -C2      :   1.821387      S1      -C3      :   1.783152
C2      -H24     :   1.092197      C2      -H25     :   1.092663
C2      -H26     :   1.092660      C3      -C4      :   1.404179
C3      -C5      :   1.399680      C4      -C23     :   1.391235
C4      -H27     :   1.087233      C5      -C6      :   1.397266
C5      -H28     :   1.084561      C6      -C22     :   1.402147
C6      -H29     :   1.088258      C7      -C8      :   1.406643
C7      -C9      :   1.402255      C7      -Ge15    :   1.978182
C8      -C14     :   1.391243      C8      -H30     :   1.088084
C9      -C10     :   1.397336      C9      -H31     :   1.088313
C10     -C13     :   1.399746      C10     -H32     :   1.084626
S11     -C12     :   1.821199      S11     -C13     :   1.783069
C12     -H33     :   1.092187      C12     -H34     :   1.092531
C12     -H35     :   1.092668      C13     -C14     :   1.404058
C14     -H36     :   1.087235      Ge15    -C16     :   1.977824
Ge15    -C17     :   1.977892      Ge15    -C18     :   1.985821
C16     -H37     :   1.093957      C16     -H38     :   1.094349
C16     -H39     :   1.094384      C17     -H40     :   1.094408
C17     -H41     :   1.094349      C17     -H42     :   1.093990
C18     -Ge19    :   1.985943      C18     -H43     :   1.097699
C18     -H44     :   1.097664      Ge19    -C20     :   1.977927
Ge19    -C21     :   1.977811      Ge19    -C22     :   1.977921
C20     -H45     :   1.093977      C20     -H46     :   1.094331
C20     -H47     :   1.094393      C21     -H48     :   1.094392
C21     -H49     :   1.093938      C21     -H50     :   1.094380
C22     -C23     :   1.406626      C23     -H51     :   1.088114

 bond lengths (bohr):
```

S1	-C2	:	3.441923	S1	-C3	:	3.369670
C2	-H24	:	2.063954	C2	-H25	:	2.064835
C2	-H26	:	2.064828	C3	-C4	:	2.653514
C3	-C5	:	2.645012	C4	-C23	:	2.629053
C4	-H27	:	2.054573	C5	-C6	:	2.640451
C5	-H28	:	2.049524	C6	-C22	:	2.649674
C6	-H29	:	2.056509	C7	-C8	:	2.658170
C7	-C9	:	2.649877	C7	-Ge15	:	3.738222
C8	-C14	:	2.629068	C8	-H30	:	2.056182
C9	-C10	:	2.640582	C9	-H31	:	2.056614
C10	-C13	:	2.645137	C10	-H32	:	2.049646
S11	-C12	:	3.441567	S11	-C13	:	3.369511
C12	-H33	:	2.063934	C12	-H34	:	2.064584
C12	-H35	:	2.064843	C13	-C14	:	2.653285
C14	-H36	:	2.054576	Ge15	-C16	:	3.737546
Ge15	-C17	:	3.737675	Ge15	-C18	:	3.752657
C16	-H37	:	2.067279	C16	-H38	:	2.068019
C16	-H39	:	2.068087	C17	-H40	:	2.068132
C17	-H41	:	2.068019	C17	-H42	:	2.067341
C18	-Ge19	:	3.752888	C18	-H43	:	2.074350
C18	-H44	:	2.074285	Ge19	-C20	:	3.737741
Ge19	-C21	:	3.737521	Ge19	-C22	:	3.737730
C20	-H45	:	2.067316	C20	-H46	:	2.067986
C20	-H47	:	2.068102	C21	-H48	:	2.068101
C21	-H49	:	2.067244	C21	-H50	:	2.068078
C22	-C23	:	2.658139	C23	-H51	:	2.056237

bond angles:

C3	-S1	-C2	: 103.626684	H24	-C2	-S1	: 105.588887
H25	-C2	-S1	: 111.507425	H25	-C2	-H24	: 108.898961
H26	-C2	-S1	: 111.641131	H26	-C2	-H24	: 108.851438
H26	-C2	-H25	: 110.188129	C4	-C3	-S1	: 116.567957
C5	-C3	-S1	: 124.669980	C5	-C3	-C4	: 118.761802
C23	-C4	-C3	: 120.375857	H27	-C4	-C3	: 119.744193
H27	-C4	-C23	: 119.879948	C6	-C5	-C3	: 120.051562
H28	-C5	-C3	: 120.856192	H28	-C5	-C6	: 119.092121
C22	-C6	-C5	: 122.101027	H29	-C6	-C5	: 117.876684
H29	-C6	-C22	: 120.022038	C9	-C7	-C8	: 116.859598
Ge15	-C7	-C8	: 121.448572	Ge15	-C7	-C9	: 121.675826
C14	-C8	-C7	: 121.848557	H30	-C8	-C7	: 120.039674
H30	-C8	-C14	: 118.111619	C10	-C9	-C7	: 122.099969
H31	-C9	-C7	: 120.027421	H31	-C9	-C10	: 117.872244

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 C13     -C10     -C9      : 120.052628  H32     -C10     -C9      :
119.089452
 H32     -C10     -C13     : 120.857777  C13     -S11     -C12     :
103.632041
 H33     -C12     -S11     : 105.595545  H34     -C12     -S11     :
111.486353
 H34     -C12     -H33     : 108.890075  H35     -C12     -S11     :
111.638475
 H35     -C12     -H33     : 108.858560  H35     -C12     -H34     :
110.206680
 S11     -C13     -C10     : 124.712820  C14     -C13     -C10     :
118.761022
 C14     -C13     -S11     : 116.525817  C13     -C14     -C8      :
120.377891
 H36     -C14     -C8      : 119.872444  H36     -C14     -C13     :
119.749635
 C16     -Ge15    -C7      : 108.464670  C17     -Ge15    -C7      :
108.438539
 C17     -Ge15    -C16     : 109.305968  C18     -Ge15    -C7      :
108.273249
 C18     -Ge15    -C16     : 111.228369  C18     -Ge15    -C17     :
111.047067
 H37     -C16     -Ge15    : 110.972717  H38     -C16     -Ge15    :
110.382169
 H38     -C16     -H37     : 107.973553  H39     -C16     -Ge15    :
111.697457
 H39     -C16     -H37     : 107.677256  H39     -C16     -H38     :
107.993556
 H40     -C17     -Ge15    : 111.664602  H41     -C17     -Ge15    :
110.492779
 H41     -C17     -H40     : 107.981415  H42     -C17     -Ge15    :
110.932467
 H42     -C17     -H40     : 107.663075  H42     -C17     -H41     :
107.960477
 Ge19    -C18     -Ge15    : 122.047797  H43     -C18     -Ge15    :
107.132201
 H43     -C18     -Ge19    : 107.056436  H44     -C18     -Ge15    :
107.073827
 H44     -C18     -Ge19    : 107.092828  H44     -C18     -H43     :
105.314943
 C20     -Ge19    -C18     : 111.146728  C21     -Ge19    -C18     :
111.241036
 C21     -Ge19    -C20     : 109.317461  C22     -Ge19    -C18     :
108.140050
 C22     -Ge19    -C20     : 108.479760  C22     -Ge19    -C21     :
108.429204
 H45     -C20     -Ge19    : 110.978469  H46     -C20     -Ge19    :
110.429277
 H46     -C20     -H45     : 107.969188  H47     -C20     -Ge19    :
111.667014
 H47     -C20     -H45     : 107.672694  H47     -C20     -H46     :
107.979026
 H48     -C21     -Ge19    : 111.694356  H49     -C21     -Ge19    :
110.980477
 H49     -C21     -H48     : 107.671792  H50     -C21     -Ge19    :
110.397704
 H50     -C21     -H48     : 107.991076  H50     -C21     -H49     :
107.960164
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 Ge19     -C22      -C6       : 121.600519  C23      -C22      -C6       :
116.868229
 C23      -C22      -Ge19     : 121.510912  C22      -C23      -C4       :
121.840813
 H51      -C23      -C4       : 118.100687  H51      -C23      -C22      :
120.058427

torsional angles:

 S1       -C3       -C4       -C23      : 179.965582
 S1       -C3       -C4       -H27      :  -0.020546
 S1       -C3       -C5       -C6       :-179.988515
 S1       -C3       -C5       -H28      :  -0.118536
 C2       -S1       -C3       -C4       : 178.126780
 C2       -S1       -C3       -C5       :  -2.062126
 C3       -S1       -C2       -H24      :-178.842189
 C3       -S1       -C2       -H25      : -60.718401
 C3       -S1       -C2       -H26      :  63.020384
 C3       -C4       -C23      -C22      :   0.088801
 C3       -C4       -C23      -H51      :-179.813094
 C3       -C5       -C6       -C22      :  -0.009534
 C3       -C5       -C6       -H29      : 179.808079
 C4       -C3       -C5       -C6       :  -0.181252
 C4       -C3       -C5       -H28      : 179.688727
 C4       -C23      -C22      -C6       :  -0.271223
 C4       -C23      -C22      -Ge19     : 178.113132
 C5       -C3       -C4       -C23      :   0.142812
 C5       -C3       -C4       -H27      :-179.843316
 C5       -C6       -C22      -Ge19     :-178.150908
 C5       -C6       -C22      -C23      :   0.231894
 C6       -C22      -Ge19     -C18      :  89.999952
 C6       -C22      -Ge19     -C20      :-149.352347
 C6       -C22      -Ge19     -C21      : -30.731905
 C6       -C22      -C23      -H51      : 179.628790
 C7       -C8       -C14      -C13      :   0.106295
 C7       -C8       -C14      -H36      :-179.956196
 C7       -C9       -C10      -C13      :  -0.027446
 C7       -C9       -C10      -H32      :-179.891353
 C7       -Ge15     -C16      -H37      :-173.299945
 C7       -Ge15     -C16      -H38      : -53.632645
 C7       -Ge15     -C16      -H39      :  66.533353
 C7       -Ge15     -C17      -H40      : -67.023991
 C7       -Ge15     -C17      -H41      :  53.179753
 C7       -Ge15     -C17      -H42      : 172.876887
 C7       -Ge15     -C18      -Ge19     :-179.999966
 C7       -Ge15     -C18      -H43      : -56.282733
 C7       -Ge15     -C18      -H44      :  56.287094
 C8       -C7       -C9       -C10      :   0.171776
 C8       -C7       -C9       -H31      :-179.603488
 C8       -C7       -Ge15     -C16      : 149.185003
 C8       -C7       -Ge15     -C17      :  30.581521
 C8       -C7       -Ge15     -C18      : -89.999968
 C8       -C14      -C13      -C10      :   0.046220
 C8       -C14      -C13      -S11      : 179.843680
 C9       -C7       -C8       -C14      :  -0.210979
 C9       -C7       -C8       -H30      : 179.645638
 C9       -C7       -Ge15     -C16      : -32.316174
 C9       -C7       -Ge15     -C17      :-150.919655
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C9	-C7	-Ge15	-C18	: 88.498856
C9	-C10	-C13	-S11	:-179.864220
C9	-C10	-C13	-C14	: -0.084678
C10	-C9	-C7	-Ge15	:-178.392701
C10	-C13	-S11	-C12	: -1.348214
C10	-C13	-C14	-H36	:-179.891366
S11	-C13	-C10	-H32	: -0.002758
S11	-C13	-C14	-H36	: -0.093906
C12	-S11	-C13	-C14	: 178.867784
C13	-C10	-C9	-H31	: 179.752446
C13	-S11	-C12	-H33	:-179.326267
C13	-S11	-C12	-H34	: -61.220252
C13	-S11	-C12	-H35	: 62.525183
C13	-C14	-C8	-H30	:-179.752981
C14	-C8	-C7	-Ge15	: 178.356991
C14	-C13	-C10	-H32	: 179.776785
Ge15	-C7	-C8	-H30	: -1.786391
Ge15	-C7	-C9	-H31	: 1.832036
Ge15	-C18	-Ge19	-C20	: 61.029600
Ge15	-C18	-Ge19	-C21	: -61.035971
Ge15	-C18	-Ge19	-C22	: 179.999967
C16	-Ge15	-C17	-H40	: 174.906218
C16	-Ge15	-C17	-H41	: -64.890039
C16	-Ge15	-C17	-H42	: 54.807096
C16	-Ge15	-C18	-Ge19	: -60.916448
C16	-Ge15	-C18	-H43	: 62.800785
C16	-Ge15	-C18	-H44	: 175.370612
C17	-Ge15	-C16	-H37	: -55.246509
C17	-Ge15	-C16	-H38	: 64.420791
C17	-Ge15	-C16	-H39	:-175.413210
C17	-Ge15	-C18	-Ge19	: 61.055853
C17	-Ge15	-C18	-H43	:-175.226913
C17	-Ge15	-C18	-H44	: -62.657086
C18	-Ge15	-C16	-H37	: 67.731083
C18	-Ge15	-C16	-H38	:-172.601618
C18	-Ge15	-C16	-H39	: -52.435619
C18	-Ge15	-C17	-H40	: 51.820818
C18	-Ge15	-C17	-H41	: 172.024562
C18	-Ge15	-C17	-H42	: -68.278304
C18	-Ge19	-C20	-H45	: -68.074538
C18	-Ge19	-C20	-H46	: 172.229127
C18	-Ge19	-C20	-H47	: 52.069766
C18	-Ge19	-C21	-H48	: -52.211249
C18	-Ge19	-C21	-H49	: 67.951719
C18	-Ge19	-C21	-H50	:-172.382570
C18	-Ge19	-C22	-C23	: -88.307885
Ge19	-C22	-C6	-H29	: 2.035296
Ge19	-C22	-C23	-H51	: -1.986855
C20	-Ge19	-C18	-H43	: -62.722525
C20	-Ge19	-C18	-H44	:-175.266214
C20	-Ge19	-C21	-H48	:-175.331391
C20	-Ge19	-C21	-H49	: -55.168423
C20	-Ge19	-C21	-H50	: 64.497288
C20	-Ge19	-C22	-C23	: 32.339816
C21	-Ge19	-C18	-H43	: 175.211904
C21	-Ge19	-C18	-H44	: 62.668215
C21	-Ge19	-C20	-H45	: 55.101596
C21	-Ge19	-C20	-H46	: -64.594739

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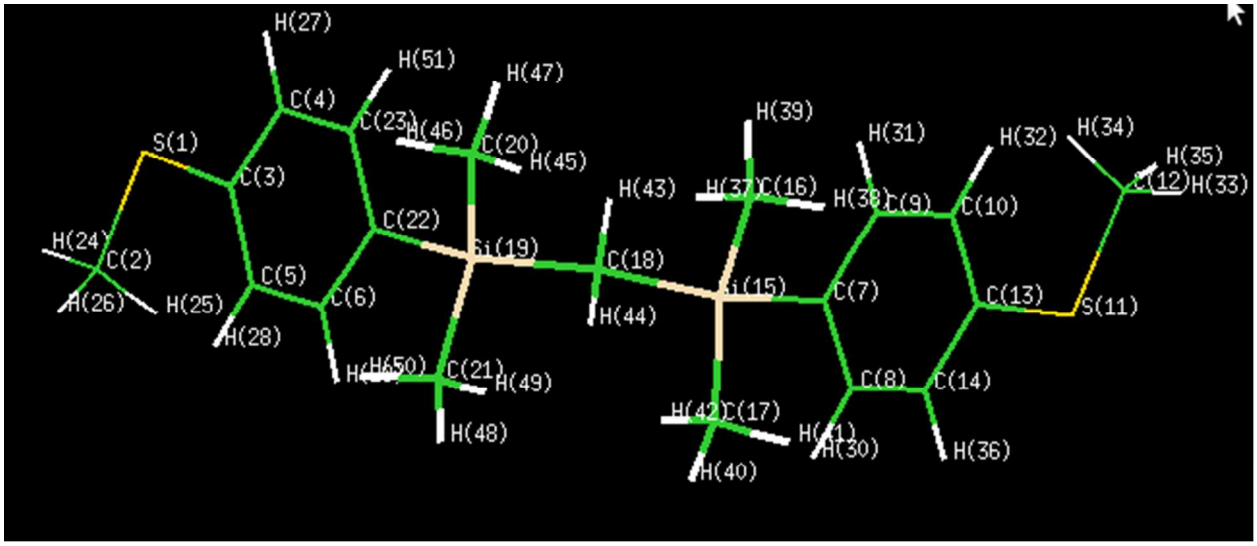
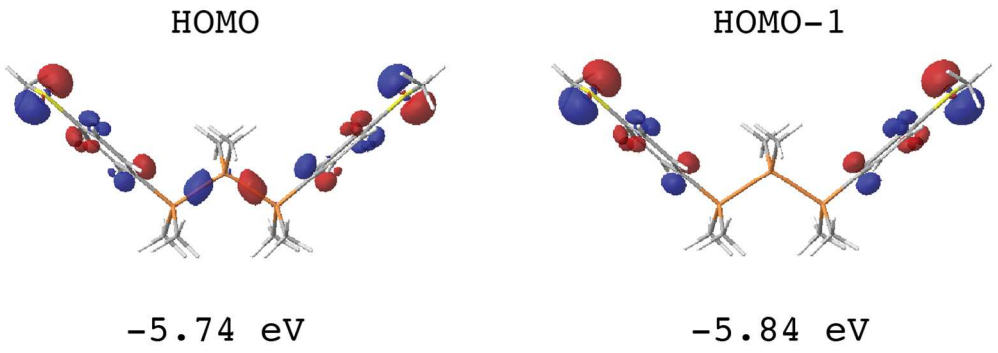
C21     -Ge19    -C20     -H47     : 175.245901
C21     -Ge19    -C22     -C23     : 150.960258
C22     -C6      -C5      -H28     :-179.881802
C22     -Ge19    -C18     -H43     :  56.247843
C22     -Ge19    -C18     -H44     : -56.295846
C22     -Ge19    -C20     -H45     : 173.158997
C22     -Ge19    -C20     -H46     :  53.462662
C22     -Ge19    -C20     -H47     : -66.696699
C22     -Ge19    -C21     -H48     :  66.579576
C22     -Ge19    -C21     -H49     :-173.257455
C22     -Ge19    -C21     -H50     : -53.591745
C22     -C23     -C4      -H27     :-179.925090
C23     -C22     -C6      -H29     :-179.581903
H27     -C4      -C23     -H51     :   0.173015
H28     -C5      -C6      -H29     :  -0.064188
H30     -C8      -C14     -H36     :   0.184528
H31     -C9      -C10     -H32     :  -0.111461

 nuclear repulsion energy.......    1810.510237682 hartrees
```

SiCSi



Final energy (B3LYP/cc-pVTZ): -2116.73442657136 hartrees



HOMO & HOMO–1 energies and surfaces (B3LYP/cc-pVTZ).

Optimized geometry:

Subjected to the constraints that ω(C(Ar)-α-β-α) = 180˚ and that the α-β σ-bond is orthogonal to the phenyl ring σ-plane. Optimized with 6-31G** basis set.

atom	x	y	z
S1	-23.4915596256	2.0985862152	2.7102338701
C2	-24.5854559389	3.2602367691	-0.3399088176
C3	-21.1202802613	-0.1553600539	1.8989215323
C4	-19.8825285467	-1.3530533541	3.9154067063
C5	-20.4364488479	-0.7971620686	-0.5725624494
C6	-18.5516927026	-2.5930236072	-0.9984519159
C7	-5.8508906597	-3.3674428219	-0.2255029082
C8	-5.1203225398	-2.0703574864	-2.4310476221
C9	-4.6518159697	-2.6401590459	2.0263476547
C10	-2.8351693334	-0.7287785493	2.1027587305
S11	0.1443089355	2.9994847994	-0.2918398541
C12	1.2602129993	3.3073854359	2.9498227969
C13	-2.1469272992	0.5335868481	-0.1156361210
C14	-3.3153733082	-0.1621101556	-2.3922269783
Si15	-8.3617187394	-5.9238529854	-0.2908156226
C16	-7.6029710235	-8.3198953208	2.2589389256
C17	-8.2485751671	-7.5411391847	-3.4825309223
C18	-11.5502933143	-4.3792702193	0.2719089127
Si19	-14.6557445062	-6.1729018811	0.3755150372
C20	-14.6723419708	-8.5945556747	3.0121591926
C21	-15.3148658608	-7.8255032822	-2.7309925116
C22	-17.2813904555	-3.8123674996	0.9856036680
C23	-18.0112499281	-3.1381963662	3.4542662887
H24	-26.0296999169	4.6700556063	0.0901134800
H25	-23.0606718335	4.1658407713	-1.3965076064
H26	-25.4369929870	1.7543026817	-1.4662460593
H27	-20.3923747655	-0.8817613277	5.8485360610
H28	-21.3564582324	0.0809445288	-2.1791320119
H29	-18.0805461852	-3.0451122367	-2.9475740228
H30	-5.9707200830	-2.5592504219	-4.2370985640
H31	-5.1254172414	-3.5832457659	3.7905184862
H32	-1.9695481565	-0.2483005642	3.8968930595
H33	2.6872340134	4.7973154327	2.9049777062
H34	-0.2591797175	3.8769129852	4.2255126532
H35	2.1365205775	1.5621137553	3.6187971835
H36	-2.7984935288	0.7922015375	-4.1361191588
H37	-8.8578776719	-9.9608673473	2.1441758580
H38	-5.6591269217	-9.0038457869	2.0619859996
H39	-7.7993022295	-7.5290449375	4.1617287273
H40	-8.8513146530	-6.2898097879	-5.0173211276
H41	-6.3272792775	-8.1801954273	-3.9127818767
H42	-9.4833902473	-9.2008459560	-3.5240878895
H43	-11.4025110622	-3.3382937964	2.0658297026
H44	-11.7626985308	-2.9014288005	-1.1753378402
H45	-13.3542050863	-10.1401513340	2.6189884442
H46	-16.5572114996	-9.4209725934	3.2343513006
H47	-14.1297978208	-7.7733884152	4.8331238530
H48	-15.1591354206	-6.5451968250	-4.3499435596
H49	-13.9870479094	-9.3801072659	-3.0484740595
H50	-17.2253373992	-8.6224990549	-2.7432360472

H51	-17.1044327217	-4.0272955005	5.0704148728

angstroms

atom	x	y	z
S1	-12.4311980000	1.1105240000	1.4341940000
C2	-13.0100630000	1.7252430000	-0.1798720000
C3	-11.1763710000	-0.0822130000	1.0048660000
C4	-10.5213810000	-0.7160050000	2.0719440000
C5	-10.8145030000	-0.4218400000	-0.3029870000
C6	-9.8171330000	-1.3721690000	-0.5283580000
C7	-3.0961580000	-1.7819740000	-0.1193310000
C8	-2.7095580000	-1.0955860000	-1.2864550000
C9	-2.4616350000	-1.3971120000	1.0722970000
C10	-1.5003070000	-0.3856530000	1.1127320000
S11	0.0763650000	1.5872590000	-0.1544350000
C12	0.6668760000	1.7501930000	1.5609790000
C13	-1.1361050000	0.2823620000	-0.0611920000
C14	-1.7544200000	-0.0857850000	-1.2659120000
Si15	-4.4248310000	-3.1347680000	-0.1538930000
C16	-4.0233190000	-4.4026990000	1.1953790000
C17	-4.3649580000	-3.9905990000	-1.8428760000
C18	-6.1121520000	-2.3174100000	0.1438880000
Si19	-7.7554860000	-3.2665590000	0.1987140000
C20	-7.7642690000	-4.5480430000	1.5939660000
C21	-8.1042780000	-4.1410780000	-1.4451790000
C22	-9.1449180000	-2.0174180000	0.5215590000
C23	-9.5311430000	-1.6606620000	1.8279190000
H24	-13.7743240000	2.4712870000	0.0476860000
H25	-12.2031820000	2.2044680000	-0.7390000000
H26	-13.4606770000	0.9283370000	-0.7759040000
H27	-10.7911800000	-0.4666080000	3.0949120000
H28	-11.3013510000	0.0428340000	-1.1531470000
H29	-9.5678130000	-1.6114040000	-1.5597890000
H30	-3.1595690000	-1.3542970000	-2.2421760000
H31	-2.7122540000	-1.8961720000	2.0058560000
H32	-1.0422400000	-0.1313950000	2.0621470000
H33	1.4220230000	2.5386300000	1.5372480000
H34	-0.1371520000	2.0515740000	2.2360450000
H35	1.1305980000	0.8266350000	1.9149850000
H36	-1.4808990000	0.4192150000	-2.1887400000
H37	-4.6873870000	-5.2710640000	1.1346490000
H38	-2.9946810000	-4.7646300000	1.0911560000
H39	-4.1272130000	-3.9841990000	2.2022920000
H40	-4.6839140000	-3.3284240000	-2.6550520000
H41	-3.3482520000	-4.3287730000	-2.0705550000
H42	-5.0183940000	-4.8688780000	-1.8648670000
H43	-6.0339490000	-1.7665490000	1.0931900000
H44	-6.2245520000	-1.5353700000	-0.6219620000
H45	-7.0667410000	-5.3659370000	1.3859090000
H46	-8.7616990000	-4.9853640000	1.7115450000
H47	-7.4771670000	-4.1135000000	2.5575790000
H48	-8.0218690000	-3.4635690000	-2.3018910000
H49	-7.4016270000	-4.9637390000	-1.6131830000
H50	-9.1152560000	-4.5628300000	-1.4516580000
H51	-9.0512760000	-2.1311530000	2.6831480000

principal moments of inertia:

amu*angstrom^2:	2038.83929	7283.56186	8503.94137

```
              g*cm^2: 3.38557186E-37 1.20946375E-36 1.41211251E-36

  rotational constants:
              cm^(-1):              0.00826825              0.00231448
0.00198233
                  GHz:              0.24787584              0.06938624
0.05942880

  Molecular weight:     376.12 amu

  Stoichiometry: Si2C19H28S2
  Molecular Point Group: C1
  Point Group used: C1


  bond lengths (angstroms):

 S1      -C2      :   1.821585      S1      -C3      :   1.783686
 C2      -H24     :   1.091998      C2      -H25     :   1.092400
 C2      -H26     :   1.092413      C3      -C4      :   1.403339
 C3      -C5      :   1.398848      C4      -C23     :   1.390143
 C4      -H27     :   1.086947      C5      -C6      :   1.395946
 C5      -H28     :   1.084304      C6      -C22     :   1.403761
 C6      -H29     :   1.087770      C7      -C8      :   1.408107
 C7      -C9      :   1.403822      C7      -Si15    :   1.896475
 C8      -C14     :   1.390111      C8      -H30     :   1.087586
 C9      -C10     :   1.396007      C9      -H31     :   1.087843
 C10     -C13     :   1.398923      C10     -H32     :   1.084371
 S11     -C12     :   1.821509      S11     -C13     :   1.783685
 C12     -H33     :   1.091990      C12     -H34     :   1.092248
 C12     -H35     :   1.092391      C13     -C14     :   1.403280
 C14     -H36     :   1.086945      Si15    -C16     :   1.894570
 Si15    -C17     :   1.894385      Si15    -C18     :   1.898368
 C16     -H37     :   1.094866      C16     -H38     :   1.095423
 C16     -H39     :   1.095358      C17     -H40     :   1.095371
 C17     -H41     :   1.095395      C17     -H42     :   1.094914
 C18     -Si19    :   1.898535      C18     -H43     :   1.100335
 C18     -H44     :   1.100339      Si19    -C20     :   1.894467
 Si19    -C21     :   1.894419      Si19    -C22     :   1.896076
 C20     -H45     :   1.094890      C20     -H46     :   1.095418
 C20     -H47     :   1.095356      C21     -H48     :   1.095338
 C21     -H49     :   1.094858      C21     -H50     :   1.095442
 C22     -C23     :   1.408198      C23     -H51     :   1.087681

  bond lengths (bohr):

 S1      -C2      :   3.442297      S1      -C3      :   3.370678
 C2      -H24     :   2.063577      C2      -H25     :   2.064337
 C2      -H26     :   2.064361      C3      -C4      :   2.651926
 C3      -C5      :   2.643439      C4      -C23     :   2.626989
 C4      -H27     :   2.054032      C5      -C6      :   2.637955
 C5      -H28     :   2.049037      C6      -C22     :   2.652724
 C6      -H29     :   2.055588      C7      -C8      :   2.660937
 C7      -C9      :   2.652839      C7      -Si15    :   3.583819
 C8      -C14     :   2.626929      C8      -H30     :   2.055240
 C9      -C10     :   2.638071      C9      -H31     :   2.055726
 C10     -C13     :   2.643581      C10     -H32     :   2.049165
 S11     -C12     :   3.442154      S11     -C13     :   3.370677
```

C12	-H33	:	2.063563	C12	-H34	:	2.064050
C12	-H35	:	2.064319	C13	-C14	:	2.651816
C14	-H36	:	2.054029	Si15	-C16	:	3.580219
Si15	-C17	:	3.579869	Si15	-C18	:	3.587395
C16	-H37	:	2.068997	C16	-H38	:	2.070050
C16	-H39	:	2.069927	C17	-H40	:	2.069952
C17	-H41	:	2.069997	C17	-H42	:	2.069087
C18	-Si19	:	3.587712	C18	-H43	:	2.079332
C18	-H44	:	2.079340	Si19	-C20	:	3.580024
Si19	-C21	:	3.579933	Si19	-C22	:	3.583064
C20	-H45	:	2.069042	C20	-H46	:	2.070040
C20	-H47	:	2.069923	C21	-H48	:	2.069889
C21	-H49	:	2.068983	C21	-H50	:	2.070085
C22	-C23	:	2.661108	C23	-H51	:	2.055420

bond angles:

C3	-S1	-C2	: 103.647197	H24	-C2	-S1	: 105.563855
H25	-C2	-S1	: 111.521117	H25	-C2	-H24	: 108.898895
H26	-C2	-S1	: 111.614452	H26	-C2	-H24	: 108.867862
H26	-C2	-H25	: 110.208630	C4	-C3	-S1	: 116.572540
C5	-C3	-S1	: 124.707080	C5	-C3	-C4	: 118.720043
C23	-C4	-C3	: 120.390703	H27	-C4	-C3	: 119.745626
H27	-C4	-C23	: 119.863657	C6	-C5	-C3	: 120.070099
H28	-C5	-C3	: 120.854526	H28	-C5	-C6	: 119.075218
C22	-C6	-C5	: 122.297304	H29	-C6	-C5	: 117.811848
H29	-C6	-C22	: 119.890422	C9	-C7	-C8	: 116.477103
Si15	-C7	-C8	: 121.665395	Si15	-C7	-C9	: 121.850058
C14	-C8	-C7	: 122.038592	H30	-C8	-C7	: 119.921206
H30	-C8	-C14	: 118.039695	C10	-C9	-C7	: 122.308507
H31	-C9	-C7	: 119.904442	H31	-C9	-C10	: 117.786578
C13	-C10	-C9	: 120.063261	H32	-C10	-C9	: 119.087181
H32	-C10	-C13	: 120.849246	C13	-S11	-C12	: 103.684600
H33	-C12	-S11	: 105.563421	H34	-C12	-S11	: 111.598051
H34	-C12	-H33	: 108.860157	H35	-C12	-S11	: 111.541992
H35	-C12	-H33	: 108.899758	H35	-C12	-H34	: 110.210966
S11	-C13	-C10	: 124.762781	C14	-C13	-C10	: 118.713740

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 C14      -C13      -S11      : 116.523345  C13      -C14      -C8       :
120.398365
 H36      -C14      -C8       : 119.858006  H36      -C14      -C13      :
119.743048
 C16      -Si15     -C7       : 108.416960  C17      -Si15     -C7       :
108.443169
 C17      -Si15     -C16      : 109.021008  C18      -Si15     -C7       :
108.223766
 C18      -Si15     -C16      : 111.395435  C18      -Si15     -C17      :
111.251339
 H37      -C16      -Si15     : 111.269229  H38      -C16      -Si15     :
110.632210
 H38      -C16      -H37      : 107.591125  H39      -C16      -Si15     :
112.264066
 H39      -C16      -H37      : 107.246708  H39      -C16      -H38      :
107.623695
 H40      -C17      -Si15     : 112.256799  H41      -C17      -Si15     :
110.739654
 H41      -C17      -H40      : 107.624876  H42      -C17      -Si15     :
111.188154
 H42      -C17      -H40      : 107.232150  H42      -C17      -H41      :
107.584111
 Si19     -C18      -Si15     : 123.961012  H43      -C18      -Si15     :
106.720928
 H43      -C18      -Si19     : 106.671738  H44      -C18      -Si15     :
106.715847
 H44      -C18      -Si19     : 106.678371  H44      -C18      -H43      :
104.591521
 C20      -Si19     -C18      : 111.312623  C21      -Si19     -C18      :
111.413326
 C21      -Si19     -C20      : 109.024704  C22      -Si19     -C18      :
108.050065
 C22      -Si19     -C20      : 108.471835  C22      -Si19     -C21      :
108.478995
 H45      -C20      -Si19     : 111.247594  H46      -C20      -Si19     :
110.690839
 H46      -C20      -H45      : 107.593246  H47      -C20      -Si19     :
112.230952
 H47      -C20      -H45      : 107.249712  H47      -C20      -H46      :
107.614667
 H48      -C21      -Si19     : 112.291710  H49      -C21      -Si19     :
111.214260
 H49      -C21      -H48      : 107.244994  H50      -C21      -Si19     :
110.657554
 H50      -C21      -H48      : 107.634895  H50      -C21      -H49      :
107.583400
 Si19     -C22      -C6       : 121.761467  C23      -C22      -C6       :
116.490770
 C23      -C22      -Si19     : 121.724929  C22      -C23      -C4       :
122.030499
 H51      -C23      -C4       : 118.046437  H51      -C23      -C22      :
119.922910

  torsional angles:

 S1       -C3       -C4       -C23      : 179.910301
 S1       -C3       -C4       -H27      :  -0.045212
 S1       -C3       -C5       -C6       :-179.935224
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S1      -C3     -C5     -H28    :  -0.080572
C2      -S1     -C3     -C4     : 178.857669
C2      -S1     -C3     -C5     :  -1.356731
C3      -S1     -C2     -H24    :-179.278558
C3      -S1     -C2     -H25    : -61.162554
C3      -S1     -C2     -H26    :  62.593408
C3      -C4     -C23    -C22    :   0.099422
C3      -C4     -C23    -H51    :-179.757549
C3      -C5     -C6     -C22    :  -0.011601
C3      -C5     -C6     -H29    : 179.750549
C4      -C3     -C5     -C6     :  -0.153876
C4      -C3     -C5     -H28    : 179.700776
C4      -C23    -C22    -C6     :  -0.255652
C4      -C23    -C22    -Si19   : 178.034913
C5      -C3     -C4     -C23    :   0.111279
C5      -C3     -C4     -H27    :-179.844234
C5      -C6     -C22    -Si19   :-178.077849
C5      -C6     -C22    -C23    :   0.212041
C6      -C22    -Si19   -C18    :  90.000001
C6      -C22    -Si19   -C20    :-149.209809
C6      -C22    -Si19   -C21    : -30.915477
C6      -C22    -C23    -H51    : 179.598699
C7      -C8     -C14    -C13    :   0.131846
C7      -C8     -C14    -H36    : 179.853791
C7      -C9     -C10    -C13    :  -0.122487
C7      -C9     -C10    -H32    :-179.920942
C7      -Si15   -C16    -H37    :-172.752579
C7      -Si15   -C16    -H38    : -53.207789
C7      -Si15   -C16    -H39    :  67.038665
C7      -Si15   -C17    -H40    : -67.673358
C7      -Si15   -C17    -H41    :  52.644307
C7      -Si15   -C17    -H42    : 172.198215
C7      -Si15   -C18    -Si19   :-179.999985
C7      -Si15   -C18    -H43    : -55.702126
C7      -Si15   -C18    -H44    :  55.697656
C8      -C7     -C9     -C10    :   0.233567
C8      -C7     -C9     -H31    :-179.510788
C8      -C7     -Si15   -C16    : 149.040536
C8      -C7     -Si15   -C17    :  30.801250
C8      -C7     -Si15   -C18    : -89.999964
C8      -C14    -C13    -C10    :  -0.008485
C8      -C14    -C13    -S11    : 179.864962
C9      -C7     -C8     -C14    :  -0.237925
C9      -C7     -C8     -H30    : 179.498032
C9      -C7     -Si15   -C16    : -31.987089
C9      -C7     -Si15   -C17    :-150.226376
C9      -C7     -Si15   -C18    :  88.972411
C9      -C10    -C13    -S11    :-179.858610
C9      -C10    -C13    -C14    :   0.003556
C10     -C9     -C7     -Si15   :-178.789309
C10     -C13    -S11    -C12    :   1.062329
C10     -C13    -C14    -H36    :-179.730750
S11     -C13    -C10    -H32    :  -0.063761
S11     -C13    -C14    -H36    :   0.142698
C12     -S11    -C13    -C14    :-178.802567
C13     -C10    -C9     -H31    : 179.627020
C13     -S11    -C12    -H33    : 179.445320
C13     -S11    -C12    -H34    : -62.444787
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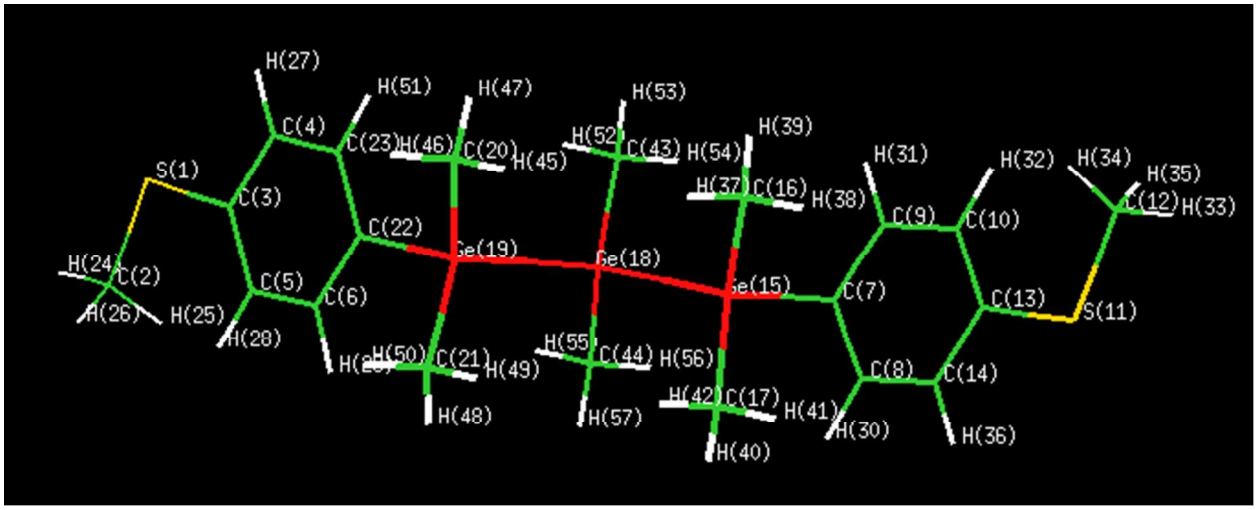
C13     -S11     -C12     -H35     :  61.317548
C13     -C14     -C8      -H30     :-179.608871
C14     -C8      -C7      -Si15    : 178.786898
C14     -C13     -C10     -H32     : 179.798405
Si15    -C7      -C8      -H30     :  -1.477145
Si15    -C7      -C9      -H31     :   1.466337
Si15    -C18     -Si19    -C20     :  60.997915
Si15    -C18     -Si19    -C21     : -60.929731
Si15    -C18     -Si19    -C22     :-179.999995
C16     -Si15    -C17     -H40     : 174.471545
C16     -Si15    -C17     -H41     : -65.210791
C16     -Si15    -C17     -H42     :  54.343118
C16     -Si15    -C18     -Si19    : -60.906877
C16     -Si15    -C18     -H43     :  63.390982
C16     -Si15    -C18     -H44     : 174.790764
C17     -Si15    -C16     -H37     : -54.880962
C17     -Si15    -C16     -H38     :  64.663828
C17     -Si15    -C16     -H39     :-175.089717
C17     -Si15    -C18     -Si19    :  60.960300
C17     -Si15    -C18     -H43     :-174.741842
C17     -Si15    -C18     -H44     : -63.342059
C18     -Si15    -C16     -H37     :  68.269548
C18     -Si15    -C16     -H38     :-172.185662
C18     -Si15    -C16     -H39     : -51.939208
C18     -Si15    -C17     -H40     :  51.235058
C18     -Si15    -C17     -H41     : 171.552722
C18     -Si15    -C17     -H42     : -68.893369
C18     -Si19    -C20     -H45     : -68.715540
C18     -Si19    -C20     -H46     : 171.712396
C18     -Si19    -C20     -H47     :  51.459142
C18     -Si19    -C21     -H48     : -51.568146
C18     -Si19    -C21     -H49     :  68.618947
C18     -Si19    -C21     -H50     :-171.865140
C18     -Si19    -C22     -C23     : -88.200545
Si19    -C22     -C6      -H29     :   2.164803
Si19    -C22     -C23     -H51     :  -2.110736
C20     -Si19    -C18     -H43     : -63.321565
C20     -Si19    -C18     -H44     :-174.683253
C20     -Si19    -C21     -H48     :-174.810713
C20     -Si19    -C21     -H49     : -54.623619
C20     -Si19    -C21     -H50     :  64.892294
C20     -Si19    -C22     -C23     :  32.589644
C21     -Si19    -C18     -H43     : 174.750788
C21     -Si19    -C18     -H44     :  63.389100
C21     -Si19    -C20     -H45     :  54.587054
C21     -Si19    -C20     -H46     : -64.985010
C21     -Si19    -C20     -H47     : 174.761736
C21     -Si19    -C22     -C23     : 150.883977
C22     -C6      -C5      -H28     :-179.868833
C22     -Si19    -C18     -H43     :  55.680525
C22     -Si19    -C18     -H44     : -55.681164
C22     -Si19    -C20     -H45     : 172.534725
C22     -Si19    -C20     -H46     :  52.962660
C22     -Si19    -C20     -H47     : -67.290594
C22     -Si19    -C21     -H48     :  67.246127
C22     -Si19    -C21     -H49     :-172.566779
C22     -Si19    -C21     -H50     : -53.050867
C22     -C23     -C4      -H27     :-179.945118
```

```
 C23      -C22      -C6       -H29      :-179.545307
 H27      -C4       -C23      -H51      :   0.197912
 H28      -C5       -C6       -H29      :  -0.106682
 H30      -C8       -C14      -H36      :   0.113074
 H31      -C9       -C10      -H32      :  -0.171435

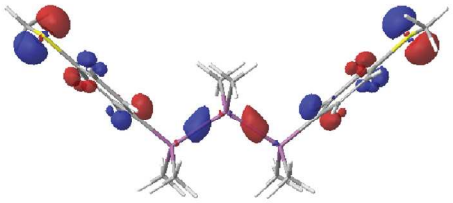
  nuclear repulsion energy.......    2316.783887988 hartrees
```

GeGeGe



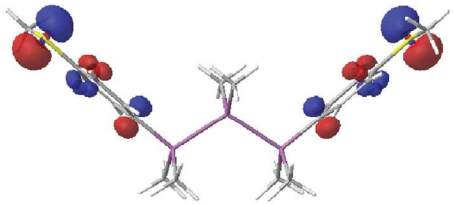
Final energy (B3LYP/cc-pVTZ): -7809.47806451385 hartrees

HOMO



-5.60 eV

HOMO−1



-5.81 eV

HOMO & HOMO–1 energies and surfaces (B3LYP/cc-pVTZ).

<u>Optimized geometry:</u>

Subjected to the constraints that ω(C(Ar)-α-β-α) = 180˚ and that the α-β σ-bond is orthogonal to the phenyl ring σ-plane. Optimized with LACVP** basis set.

atom	x	y	z
S1	-24.7959619806	2.0894796250	3.9681130577
C2	-26.3484683683	2.6459605051	0.9469039667
C3	-22.3016349895	-0.0388565486	3.1957158500
C4	-20.7015679746	-0.7692583726	5.1834563999
C5	-21.8481063886	-1.0136679907	0.7786295245
C6	-19.8354422409	-2.6745974148	0.3751503201
C7	-4.8085970977	-3.1081894050	-1.0061412116
C8	-4.3883560225	-2.2410847931	-3.4843280519
C9	-3.2448959724	-2.1199061054	0.8917145152
C10	-1.3478566073	-0.3594599240	0.3686515519

S11	1.3877071518	2.7074446343	-3.0390896796
C12	2.8789580672	3.5991761571	-0.0680339200
C13	-0.9619688634	0.4779495315	-2.1104121213
C14	-2.5094580282	-0.4875096560	-4.0380064681
Ge15	-7.5579747547	-5.5248486525	-0.2231861040
C16	-6.5406142392	-7.5707644211	2.7478148536
C17	-8.0059097662	-7.8158618995	-3.1566589904
Ge18	-11.5162045448	-3.0537728516	0.6561166901
Ge19	-15.3131140847	-5.7047411309	1.7087810691
C20	-14.7236990577	-7.7733298337	4.7781630584
C21	-16.1808271884	-7.9949191191	-1.1297859919
C22	-18.2170694491	-3.4264608585	2.3344939555
C23	-18.7064272572	-2.4256996972	4.7485567192
H24	-27.8760587171	3.9758250300	1.3447007647
H25	-25.0585224181	3.4990509081	-0.4213087704
H26	-27.1584654567	0.9097954148	0.1764966406
H27	-21.0247772824	-0.0343986847	7.0748265866
H28	-23.0451798587	-0.4996946101	-0.8038554785
H29	-19.5477427767	-3.3927462547	-1.5299147119
H30	-5.5447058946	-2.9446543959	-5.0316849359
H31	-3.4840143573	-2.7269125929	2.8415036954
H32	-0.1865915576	0.3387523052	1.9065465772
H33	4.3112306302	5.0000584795	-0.5642400956
H34	1.5228641437	4.4597990084	1.2293934560
H35	3.8051959890	1.9890557993	0.8336507903
H36	-2.2368045635	0.1412570278	-5.9749644079
H37	-7.9814151362	-8.9899374026	3.1795775889
H38	-4.7600557027	-8.5540512849	2.3702022204
H39	-6.2846848506	-6.4013924464	4.4331935543
H40	-8.5810271254	-6.7827202811	-4.8523933903
H41	-6.2394032332	-8.8073274980	-3.5762329922
H42	-9.4607551078	-9.2306658343	-2.7584370041
C43	-10.8323731314	-0.7036829863	3.5203235551
C44	-12.3336603822	-0.9437405652	-2.3573520827
H45	-13.1687643719	-9.1016353344	4.4701584870
H46	-16.4174379068	-8.8620048337	5.2526732884
H47	-14.2353673708	-6.6011081519	6.4093897673
H48	-16.4961960225	-6.9519868296	-2.8866775984
H49	-14.6493496730	-9.3432916216	-1.4661515730
H50	-17.8984616244	-9.0643075743	-0.6991249669
H51	-17.5133184326	-2.9453158001	6.3402616959
H52	-12.4893379101	0.4748806163	3.8960370135
H53	-10.3683206458	-1.7349254300	5.2507174219
H54	-9.2419210431	0.5366746606	3.0635729712
H55	-13.9948638166	0.2289875632	-1.9798074796
H56	-10.7482500832	0.3027284560	-2.8148358803
H57	-12.7341557090	-2.1123245242	-4.0151199950

angstroms

atom	x	y	z
S1	-13.1214580000	1.1057050000	2.0998350000
C2	-13.9430090000	1.4001820000	0.5010800000
C3	-11.8015170000	-0.0205620000	1.6911000000
C4	-10.9547980000	-0.4070740000	2.7429670000
C5	-11.5615200000	-0.5364100000	0.4120330000
C6	-10.4964640000	-1.4153360000	0.1985210000
C7	-2.5446000000	-1.6447830000	-0.5324270000
C8	-2.3222180000	-1.1859310000	-1.8438270000

C9	-1.7171250000	-1.1218060000	0.4718750000
C10	-0.7132550000	-0.1902180000	0.1950820000
S11	0.7343430000	1.4327180000	-1.6082170000
C12	1.5234790000	1.9046020000	-0.0360020000
C13	-0.5090520000	0.2529200000	-1.1167820000
C14	-1.3279480000	-0.2579790000	-2.1368210000
Ge15	-3.9995080000	-2.9236240000	-0.1181050000
C16	-3.4611440000	-4.0062760000	1.4540810000
C17	-4.2365450000	-4.1359760000	-1.6704320000
Ge18	-6.0941130000	-1.6159870000	0.3472020000
Ge19	-8.1033510000	-3.0188190000	0.9042480000
C20	-7.7914460000	-4.1134690000	2.5284950000
C21	-8.5625250000	-4.2307290000	-0.5978570000
C22	-9.6400580000	-1.8132050000	1.2353610000
C23	-9.8990150000	-1.2836250000	2.5128280000
H24	-14.7513750000	2.1039160000	0.7115850000
H25	-13.2603990000	1.8516180000	-0.2229470000
H26	-14.3716410000	0.4814430000	0.0933980000
H27	-11.1258330000	-0.0182030000	3.7438370000
H28	-12.1949840000	-0.2644270000	-0.4253820000
H29	-10.3442200000	-1.7953640000	-0.8095960000
H30	-2.9341320000	-1.5582440000	-2.6626530000
H31	-1.8436610000	-1.4430200000	1.5036590000
H32	-0.0987400000	0.1792600000	1.0089010000
H33	2.2814050000	2.6459170000	-0.2985830000
H34	0.8058650000	2.3600240000	0.6505670000
H35	2.0136230000	1.0525630000	0.4411490000
H36	-1.1836660000	0.0747500000	-3.1618150000
H37	-4.2235830000	-4.7572700000	1.6825600000
H38	-2.5189130000	-4.5266090000	1.2542570000
H39	-3.3257120000	-3.3874710000	2.3459450000
H40	-4.5408840000	-3.5892610000	-2.5677760000
H41	-3.3017500000	-4.6606370000	-1.8924610000
H42	-5.0064160000	-4.8846580000	-1.4597020000
C43	-5.7322450000	-0.3723730000	1.8628750000
C44	-6.5266920000	-0.4994060000	-1.2474570000
H45	-6.9686100000	-4.8163780000	2.3655060000
H46	-8.6877340000	-4.6895710000	2.7795950000
H47	-7.5330320000	-3.4931560000	3.3917030000
H48	-8.7294110000	-3.6788330000	-1.5275640000
H49	-7.7521020000	-4.9442570000	-0.7758540000
H50	-9.4714580000	-4.7966250000	-0.3699610000
H51	-9.2676490000	-1.5585940000	3.3551220000
H52	-6.6090730000	0.2512960000	2.0616940000
H53	-5.4866790000	-0.9180830000	2.7785600000
H54	-4.8906140000	0.2839960000	1.6211730000
H55	-7.4057630000	0.1211750000	-1.0476690000
H56	-5.6877290000	0.1601970000	-1.4895470000
H57	-6.7386250000	-1.1177940000	-2.1247100000

principal moments of inertia:

amu*angstrom^2:	2238.42561	10027.80138	11251.10485
g*cm^2:	3.71699271E-37	1.66515539E-36	1.86828968E-36

rotational constants:

cm^(-1):	0.00753102	0.00168109	0.00149831

GHz: 0.22577431 0.05039779 0.04491817

Molecular weight: 557.96 amu

Stoichiometry: Ge3C20H32S2
Molecular Point Group: C1
Point Group used: C1

bond lengths (angstroms):

S1	-C2	:	1.821450	S1	-C3	:	1.782635
C2	-H24	:	1.092250	C2	-H25	:	1.092687
C2	-H26	:	1.092708	C3	-C4	:	1.404546
C3	-C5	:	1.399896	C4	-C23	:	1.391396
C4	-H27	:	1.087297	C5	-C6	:	1.397298
C5	-H28	:	1.084673	C6	-C22	:	1.402415
C6	-H29	:	1.088071	C7	-C8	:	1.407043
C7	-C9	:	1.402442	C7	-Ge15	:	1.980872
C8	-C14	:	1.391227	C8	-H30	:	1.087902
C9	-C10	:	1.397221	C9	-H31	:	1.088011
C10	-C13	:	1.399663	C10	-H32	:	1.084640
S11	-C12	:	1.821337	S11	-C13	:	1.783105
C12	-H33	:	1.092222	C12	-H34	:	1.092591
C12	-H35	:	1.092650	C13	-C14	:	1.404311
C14	-H36	:	1.087262	Ge15	-C16	:	1.983366
Ge15	-C17	:	1.983861	Ge15	-Ge18	:	2.512727
C16	-H37	:	1.094307	C16	-H38	:	1.094749
C16	-H39	:	1.093930	C17	-H40	:	1.093959
C17	-H41	:	1.094718	C17	-H42	:	1.094364
Ge18	-Ge19	:	2.513021	Ge18	-C43	:	1.993687
Ge18	-C44	:	1.994195	Ge19	-C20	:	1.983361
Ge19	-C21	:	1.983907	Ge19	-C22	:	1.981063
C20	-H45	:	1.094397	C20	-H46	:	1.094658
C20	-H47	:	1.093935	C21	-H48	:	1.093981
C21	-H49	:	1.094345	C21	-H50	:	1.094684
C22	-C23	:	1.406924	C23	-H51	:	1.087975
C43	-H52	:	1.094221	C43	-H53	:	1.093883
C43	-H54	:	1.094341	C44	-H55	:	1.094441
C44	-H56	:	1.094323	C44	-H57	:	1.094026

bond lengths (bohr):

S1	-C2	:	3.442042	S1	-C3	:	3.368691
C2	-H24	:	2.064053	C2	-H25	:	2.064880
C2	-H26	:	2.064919	C3	-C4	:	2.654207
C3	-C5	:	2.645421	C4	-C23	:	2.629358
C4	-H27	:	2.054693	C5	-C6	:	2.640511
C5	-H28	:	2.049735	C6	-C22	:	2.650180
C6	-H29	:	2.056157	C7	-C8	:	2.658925
C7	-C9	:	2.650230	C7	-Ge15	:	3.743306
C8	-C14	:	2.629038	C8	-H30	:	2.055838
C9	-C10	:	2.640364	C9	-H31	:	2.056043
C10	-C13	:	2.644980	C10	-H32	:	2.049673
S11	-C12	:	3.441829	S11	-C13	:	3.369580
C12	-H33	:	2.064000	C12	-H34	:	2.064699
C12	-H35	:	2.064810	C13	-C14	:	2.653762

C14	-H36	:	2.054627	Ge15	-C16	:	3.748018
Ge15	-C17	:	3.748953	Ge15	-Ge18	:	4.748365
C16	-H37	:	2.067941	C16	-H38	:	2.068776
C16	-H39	:	2.067228	C17	-H40	:	2.067282
C17	-H41	:	2.068717	C17	-H42	:	2.068049
Ge18	-Ge19	:	4.748922	Ge18	-C43	:	3.767523
Ge18	-C44	:	3.768483	Ge19	-C20	:	3.748009
Ge19	-C21	:	3.749040	Ge19	-C22	:	3.743666
C20	-H45	:	2.068111	C20	-H46	:	2.068604
C20	-H47	:	2.067238	C21	-H48	:	2.067325
C21	-H49	:	2.068012	C21	-H50	:	2.068654
C22	-C23	:	2.658701	C23	-H51	:	2.055975
C43	-H52	:	2.067778	C43	-H53	:	2.067140
C43	-H54	:	2.068005	C44	-H55	:	2.068194
C44	-H56	:	2.067971	C44	-H57	:	2.067409

bond angles:

C3	-S1	-C2	: 103.583475	H24	-C2	-S1	: 105.593760
H25	-C2	-S1	: 111.507484	H25	-C2	-H24	: 108.896333
H26	-C2	-S1	: 111.621548	H26	-C2	-H24	: 108.863300
H26	-C2	-H25	: 110.194142	C4	-C3	-S1	: 116.648750
C5	-C3	-S1	: 124.697897	C5	-C3	-C4	: 118.653252
C23	-C4	-C3	: 120.459228	H27	-C4	-C3	: 119.743914
H27	-C4	-C23	: 119.796857	C6	-C5	-C3	: 120.137487
H28	-C5	-C3	: 120.856133	H28	-C5	-C6	: 119.006325
C22	-C6	-C5	: 122.069474	H29	-C6	-C5	: 117.899489
H29	-C6	-C22	: 120.030706	C9	-C7	-C8	: 116.908788
Ge15	-C7	-C8	: 121.437164	Ge15	-C7	-C9	: 121.622695
C14	-C8	-C7	: 121.786512	H30	-C8	-C7	: 120.066178
H30	-C8	-C14	: 118.147197	C10	-C9	-C7	: 122.051909
H31	-C9	-C7	: 120.025753	H31	-C9	-C10	: 117.921857
C13	-C10	-C9	: 120.105297	H32	-C10	-C9	: 119.048211
H32	-C10	-C13	: 120.846420	C13	-S11	-C12	: 103.629737
H33	-C12	-S11	: 105.603713	H34	-C12	-S11	: 111.460275
H34	-C12	-H33	: 108.900992	H35	-C12	-S11	: 111.671595
H35	-C12	-H33	: 108.842099	H35	-C12	-H34	: 110.197463
S11	-C13	-C10	: 124.717787	C14	-C13	-C10	: 118.720728

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 C14     -C13     -S11     : 116.561173  C13     -C14     -C8      :
120.426606
 H36     -C14     -C8      : 119.834574  H36     -C14     -C13     :
119.738812
 C16     -Ge15    -C7      : 108.592853  C17     -Ge15    -C7      :
108.579559
 C17     -Ge15    -C16     : 108.609029  Ge18    -Ge15    -C7      :
108.362109
 Ge18    -Ge15    -C16     : 111.318601  Ge18    -Ge15    -C17     :
111.304382
 H37     -C16     -Ge15    : 110.548284  H38     -C16     -Ge15    :
110.388517
 H38     -C16     -H37     : 108.155083  H39     -C16     -Ge15    :
111.782770
 H39     -C16     -H37     : 107.712497  H39     -C16     -H38     :
108.126819
 H40     -C17     -Ge15    : 111.695814  H41     -C17     -Ge15    :
110.460156
 H41     -C17     -H40     : 108.101985  H42     -C17     -Ge15    :
110.576337
 H42     -C17     -H40     : 107.706332  H42     -C17     -H41     :
108.173414
 Ge19    -Ge18    -Ge15    : 114.647338  C43     -Ge18    -Ge15    :
108.306079
 C43     -Ge18    -Ge19    : 108.954123  C44     -Ge18    -Ge15    :
108.912708
 C44     -Ge18    -Ge19    : 108.444091  C44     -Ge18    -C43     :
107.339532
 C20     -Ge19    -Ge18    : 111.339139  C21     -Ge19    -Ge18    :
110.991079
 C21     -Ge19    -C20     : 108.620722  C22     -Ge19    -Ge18    :
108.513292
 C22     -Ge19    -C20     : 108.722817  C22     -Ge19    -C21     :
108.588594
 H45     -C20     -Ge19    : 110.533726  H46     -C20     -Ge19    :
110.460153
 H46     -C20     -H45     : 108.164903  H47     -C20     -Ge19    :
111.740083
 H47     -C20     -H45     : 107.704841  H47     -C20     -H46     :
108.109814
 H48     -C21     -Ge19    : 111.751621  H49     -C21     -Ge19    :
110.490116
 H49     -C21     -H48     : 107.678412  H50     -C21     -Ge19    :
110.508060
 H50     -C21     -H48     : 108.122603  H50     -C21     -H49     :
108.161586
 Ge19    -C22     -C6      : 121.518555  C23     -C22     -C6      :
116.879094
 C23     -C22     -Ge19    : 121.574418  C22     -C23     -C4      :
121.801323
 H51     -C23     -C4      : 118.131978  H51     -C23     -C22     :
120.066528
 H52     -C43     -Ge18    : 110.378432  H53     -C43     -Ge18    :
111.466133
 H53     -C43     -H52     : 108.187738  H54     -C43     -Ge18    :
110.231485
 H54     -C43     -H52     : 108.333919  H54     -C43     -H53     :
108.146783
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 H55     -C44     -Ge18    : 110.227395  H56     -C44     -Ge18    :
110.370502
 H56     -C44     -H55     : 108.324066  H57     -C44     -Ge18    :
111.514701
 H57     -C44     -H55     : 108.136898  H57     -C44     -H56     :
108.169150

  torsional angles:

 S1      -C3      -C4      -C23     : 179.984065
 S1      -C3      -C4      -H27     :  -0.027239
 S1      -C3      -C5      -C6      :-179.993672
 S1      -C3      -C5      -H28     :  -0.079402
 C2      -S1      -C3      -C4      : 178.312423
 C2      -S1      -C3      -C5      :  -1.805089
 C3      -S1      -C2      -H24     :-179.041274
 C3      -S1      -C2      -H25     : -60.917698
 C3      -S1      -C2      -H26     :  62.814513
 C3      -C4      -C23     -C22     :  -0.076616
 C3      -C4      -C23     -H51     :-179.926148
 C3      -C5      -C6      -C22     :   0.116999
 C3      -C5      -C6      -H29     : 179.907361
 C4      -C3      -C5      -C6      :  -0.113359
 C4      -C3      -C5      -H28     : 179.800912
 C4      -C23     -C22     -C6      :   0.073691
 C4      -C23     -C22     -Ge19    : 178.178810
 C5      -C3      -C4      -C23     :   0.094162
 C5      -C3      -C4      -H27     :-179.917141
 C5      -C6      -C22     -Ge19    :-178.200221
 C5      -C6      -C22     -C23     :  -0.093968
 C6      -C22     -Ge19    -Ge18    :  90.000013
 C6      -C22     -Ge19    -C20     :-148.756356
 C6      -C22     -Ge19    -C21     : -30.742518
 C6      -C22     -C23     -H51     : 179.920368
 C7      -C8      -C14     -C13     :  -0.036987
 C7      -C8      -C14     -H36     : 179.995303
 C7      -C9      -C10     -C13     :   0.145598
 C7      -C9      -C10     -H32     :-179.757160
 C7      -Ge15    -C16     -H37     :-177.338281
 C7      -Ge15    -C16     -H38     : -57.713363
 C7      -Ge15    -C16     -H39     :  62.682021
 C7      -Ge15    -C17     -H40     : -62.427445
 C7      -Ge15    -C17     -H41     :  57.927402
 C7      -Ge15    -C17     -H42     : 177.639307
 C7      -Ge15    -Ge18    -Ge19    : 179.999966
 C7      -Ge15    -Ge18    -C43     : -58.114804
 C7      -Ge15    -Ge18    -C44     :  58.320530
 C8      -C7      -C9      -C10     :  -0.138205
 C8      -C7      -C9      -H31     :-179.880672
 C8      -C7      -Ge15    -C16     : 151.048378
 C8      -C7      -Ge15    -C17     :  33.126356
 C8      -C7      -Ge15    -Ge18    : -87.900120
 C8      -C14     -C13     -C10     :   0.038928
 C8      -C14     -C13     -S11     : 179.845487
 C9      -C7      -C8      -C14     :   0.083797
 C9      -C7      -C8      -H30     : 179.959179
 C9      -C7      -Ge15    -C16     : -31.051534
 C9      -C7      -Ge15    -C17     :-148.973555
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C9	-C7	-Ge15	-Ge18	: 89.999969
C9	-C10	-C13	-S11	:-179.880967
C9	-C10	-C13	-C14	: -0.091467
C10	-C9	-C7	-Ge15	:-178.129030
C10	-C13	-S11	-C12	: -2.531070
C10	-C13	-C14	-H36	:-179.993331
S11	-C13	-C10	-H32	: 0.020017
S11	-C13	-C14	-H36	: -0.186771
C12	-S11	-C13	-C14	: 177.675315
C13	-C10	-C9	-H31	: 179.893249
C13	-S11	-C12	-H33	:-178.884553
C13	-S11	-C12	-H34	: -60.774345
C13	-S11	-C12	-H35	: 62.964212
C13	-C14	-C8	-H30	:-179.914671
C14	-C8	-C7	-Ge15	: 178.078612
C14	-C13	-C10	-H32	: 179.809517
Ge15	-C7	-C8	-H30	: -2.046006
Ge15	-C7	-C9	-H31	: 2.128502
Ge15	-Ge18	-Ge19	-C20	: 60.380298
Ge15	-Ge18	-Ge19	-C21	: -60.755300
Ge15	-Ge18	-Ge19	-C22	: 179.999988
Ge15	-Ge18	-C43	-H52	: 177.149857
Ge15	-Ge18	-C43	-H53	: -62.594351
Ge15	-Ge18	-C43	-H54	: 57.511400
Ge15	-Ge18	-C44	-H55	:-176.912221
Ge15	-Ge18	-C44	-H56	: -57.293637
Ge15	-Ge18	-C44	-H57	: 62.965420
C16	-Ge15	-C17	-H40	: 179.660808
C16	-Ge15	-C17	-H41	: -59.984345
C16	-Ge15	-C17	-H42	: 59.727560
C16	-Ge15	-Ge18	-Ge19	: -60.649132
C16	-Ge15	-Ge18	-C43	: 61.236098
C16	-Ge15	-Ge18	-C44	: 177.671432
C17	-Ge15	-C16	-H37	: -59.434974
C17	-Ge15	-C16	-H38	: 60.189944
C17	-Ge15	-C16	-H39	:-179.414672
C17	-Ge15	-Ge18	-Ge19	: 60.673943
C17	-Ge15	-Ge18	-C43	:-177.440827
C17	-Ge15	-Ge18	-C44	: -61.005493
Ge18	-Ge15	-C16	-H37	: 63.448317
Ge18	-Ge15	-C16	-H38	:-176.926765
Ge18	-Ge15	-C16	-H39	: -56.531381
Ge18	-Ge15	-C17	-H40	: 56.768939
Ge18	-Ge15	-C17	-H41	: 177.123785
Ge18	-Ge15	-C17	-H42	: -63.164309
Ge18	-Ge19	-C20	-H45	: -62.464251
Ge18	-Ge19	-C20	-H46	: 177.861870
Ge18	-Ge19	-C20	-H47	: 57.467636
Ge18	-Ge19	-C21	-H48	: -56.328698
Ge18	-Ge19	-C21	-H49	: 63.547975
Ge18	-Ge19	-C21	-H50	:-176.779501
Ge18	-Ge19	-C22	-C23	: -88.017289
Ge19	-Ge18	-C43	-H52	: -57.535625
Ge19	-Ge18	-C43	-H53	: 62.720167
Ge19	-Ge18	-C43	-H54	:-177.174082
Ge19	-Ge18	-C44	-H55	: 57.709647
Ge19	-Ge18	-C44	-H56	: 177.328231
Ge19	-Ge18	-C44	-H57	: -62.412711

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Ge19    -C22     -C6      -H29     :   2.013779
Ge19    -C22     -C23     -H51     :  -1.974514
C20     -Ge19    -Ge18    -C43     : -61.151312
C20     -Ge19    -Ge18    -C44     :-177.684830
C20     -Ge19    -C21     -H48     :-179.050562
C20     -Ge19    -C21     -H49     : -59.173889
C20     -Ge19    -C21     -H50     :  60.498635
C20     -Ge19    -C22     -C23     :  33.226342
C21     -Ge19    -Ge18    -C43     : 177.713089
C21     -Ge19    -Ge18    -C44     :  61.179572
C21     -Ge19    -C20     -H45     :  60.047029
C21     -Ge19    -C20     -H46     : -59.626851
C21     -Ge19    -C20     -H47     : 179.978915
C21     -Ge19    -C22     -C23     : 151.240180
C22     -C6      -C5      -H28     :-179.798851
C22     -Ge19    -Ge18    -C43     :  58.468377
C22     -Ge19    -Ge18    -C44     : -58.065140
C22     -Ge19    -C20     -H45     : 178.040529
C22     -Ge19    -C20     -H46     :  58.366650
C22     -Ge19    -C20     -H47     : -62.027584
C22     -Ge19    -C21     -H48     :  62.870839
C22     -Ge19    -C21     -H49     :-177.252487
C22     -Ge19    -C21     -H50     : -57.579963
C22     -C23     -C4      -H27     : 179.934693
C23     -C22     -C6      -H29     :-179.879968
H27     -C4      -C23     -H51     :   0.085162
H28     -C5      -C6      -H29     :  -0.008489
H30     -C8      -C14     -H36     :   0.117619
H31     -C9      -C10     -H32     :  -0.009509
C43     -Ge18    -C44     -H55     : -59.860195
C43     -Ge18    -C44     -H56     :  59.758390
C43     -Ge18    -C44     -H57     :-179.982553
C44     -Ge18    -C43     -H52     :  59.701231
C44     -Ge18    -C43     -H53     : 179.957023
C44     -Ge18    -C43     -H54     : -59.937227

 nuclear repulsion energy.......    2019.475034921 hartrees
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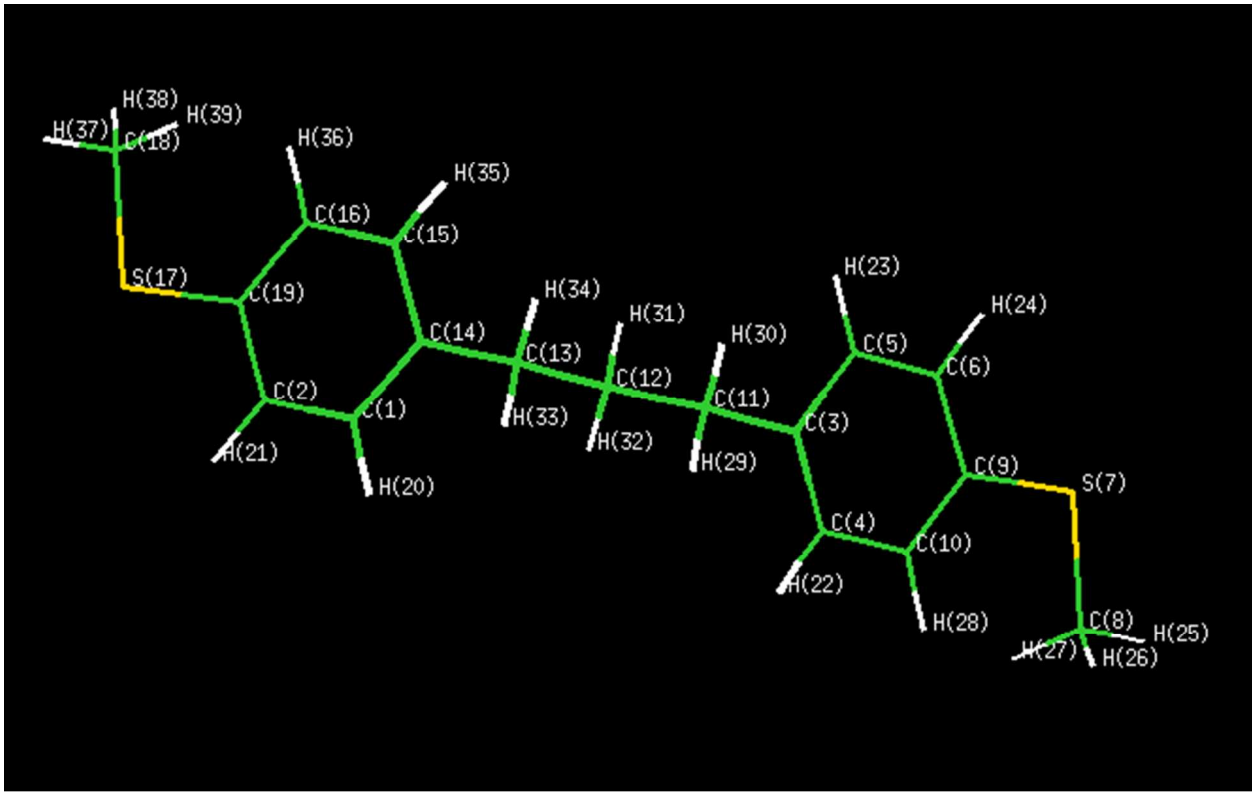
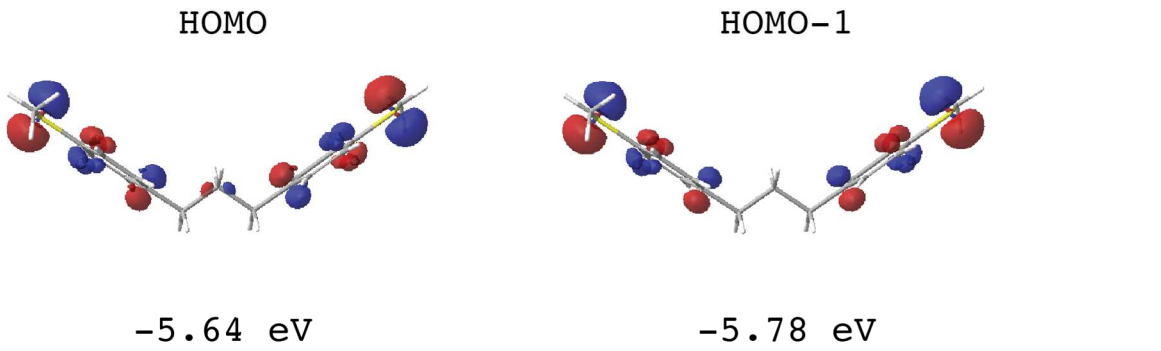
CCC



Final energy (B3LYP/cc-pVTZ): -1456.54711907804 hartrees



HOMO & HOMO–1 energies and surfaces (B3LYP/cc-pVTZ).

Optimized geometry:

Subjected to the constraints that ω(C(Ar)-α-β-α) = 180˚ and that the α-β σ-bond is orthogonal to the phenyl ring σ-plane. Optimized with 6-31G** basis set.

atom	x	y	z
C1	-6.9927179865	-4.1492111814	2.2924305417
C2	-4.8246843362	-2.6675978693	2.3488936686
C3	-17.7573595541	-4.8826838104	0.0587496955
C4	-18.8725209555	-4.1636770349	2.3426953669
C5	-18.9170013290	-4.0652941134	-2.1788825680
C6	-21.0930493079	-2.5944805860	-2.1389375372
S7	-24.9883398796	0.0013417055	-0.0114177252

C8	-25.9135951438	0.3924488730	3.2803661317
C9	-22.1937372969	-1.8842667062	0.1670347819
C10	-21.0565700347	-2.6852724777	2.4151361282
C11	-15.3586942788	-6.4377413284	-0.0056200455
C12	-12.9348748591	-4.8210976360	0.0332894154
C13	-10.5100179798	-6.4352355515	-0.0331571346
C14	-8.1128985005	-4.8770996697	0.0039967708
C15	-6.9695329367	-4.0521624065	-2.2293949473
C16	-4.7920695530	-2.5620963494	-2.2048870892
S17	-0.9098634449	0.0329662723	0.3942554512
C18	0.0591144126	0.5745409927	-2.8634320773
C19	-3.6930974353	-1.8536247971	0.0924378431
H20	-7.8268185316	-4.7665053380	4.0667000696
H21	-3.9932766508	-2.1465153389	4.1527733152
H22	-18.0303909641	-4.7756024795	4.1153359509
H23	-18.1078527277	-4.6023391603	-3.9903626931
H24	-21.9553426771	-2.0026939527	-3.9061602764
H25	-27.6501910917	1.5063536066	3.2392154556
H26	-26.3059948839	-1.4250254633	4.1776931336
H27	-24.4857596577	1.4247930270	4.3557412393
H28	-21.8545881492	-2.1808422140	4.2333663549
H29	-15.3275062389	-7.7348228844	1.6131117943
H30	-15.3484727502	-7.6271160542	-1.7049940579
H31	-12.9438397199	-3.5205314250	-1.5814210872
H32	-12.9267263601	-3.6284404559	1.7292486927
H33	-10.5200618741	-7.7325344261	1.5856087202
H34	-10.5397660484	-7.6245441369	-1.7324857936
H35	-7.7830581437	-4.5891866665	-4.0392366798
H36	-3.9701029393	-1.9754781171	-3.9874317279
H37	1.7919630336	1.6891014612	-2.7483080721
H38	0.4686520790	-1.1995924750	-3.8365654427
H39	-1.3570104406	1.6513541819	-3.9104197191

angstroms

atom	x	y	z
C1	-3.7003870000	-2.1956680000	1.2131020000
C2	-2.5531130000	-1.4116320000	1.2429810000
C3	-9.3967900000	-2.5838050000	0.0310890000
C4	-9.9869080000	-2.2033230000	1.2397010000
C5	-10.0104460000	-2.1512610000	-1.1530150000
C6	-11.1619610000	-1.3729400000	-1.1318770000
S7	-13.2232600000	0.0007100000	-0.0060420000
C8	-13.7128840000	0.2076750000	1.7358950000
C9	-11.7444200000	-0.9971110000	0.0883910000
C10	-11.1426570000	-1.4209850000	1.2780350000
C11	-8.1274710000	-3.4067060000	-0.0029740000
C12	-6.8448410000	-2.5512150000	0.0176160000
C13	-5.5616620000	-3.4053800000	-0.0175460000
C14	-4.2931610000	-2.5808500000	0.0021150000
C15	-3.6881180000	-2.1443120000	-1.1797450000
C16	-2.5358540000	-1.3558030000	-1.1667760000
S17	-0.4814790000	0.0174450000	0.2086310000
C18	0.0312820000	0.3040340000	-1.5152630000
C19	-1.9543030000	-0.9808960000	0.0489160000
H20	-4.1417740000	-2.5223260000	2.1520050000
H21	-2.1131510000	-1.1358870000	2.1975530000
H22	-9.5412720000	-2.5271400000	2.1777420000
H23	-9.5822630000	-2.4354530000	-2.1116090000

H24	-11.6182670000	-1.0597800000	-2.0670510000
H25	-14.6318510000	0.7971280000	1.7141190000
H26	-13.9205330000	-0.7540910000	2.2107400000
H27	-12.9573060000	0.7539680000	2.3049590000
H28	-11.5649500000	-1.1540520000	2.2402010000
H29	-8.1109670000	-4.0930920000	0.8536220000
H30	-8.1220620000	-4.0360960000	-0.9022440000
H31	-6.8495850000	-1.8629850000	-0.8368520000
H32	-6.8405290000	-1.9200880000	0.9150790000
H33	-5.5669770000	-4.0918810000	0.8390680000
H34	-5.5774040000	-4.0347350000	-0.9167920000
H35	-4.1186170000	-2.4284930000	-2.1374720000
H36	-2.1008880000	-1.0453780000	-2.1100580000
H37	0.9482660000	0.8938340000	-1.4543420000
H38	0.2480000000	-0.6347970000	-2.0302230000
H39	-0.7180990000	0.8738590000	-2.0693050000

principal moments of inertia:

amu*angstrom^2:	678.86523	6559.98917	6735.26816
g*cm^2:	1.12728209E-37	1.08931169E-36	1.11841745E-36

rotational constants:

cm^(-1):	0.02483207	0.00256976	0.00250289
GHz:	0.74444674	0.07703961	0.07503473

Molecular weight: 288.10 amu

Stoichiometry: C17H20S2
Molecular Point Group: C1
Point Group used: C1

bond lengths (angstroms):

C1	-C2	:	1.389907	C1	-C14	:	1.402225
C1	-H20	:	1.087689	C2	-C19	:	1.403531
C2	-H21	:	1.086651	C3	-C4	:	1.397766
C3	-C5	:	1.402059	C3	-C11	:	1.513108
C4	-C10	:	1.396165	C4	-H22	:	1.087828
C5	-C6	:	1.390042	C5	-H23	:	1.087662
C6	-C9	:	1.403410	C6	-H24	:	1.086662
S7	-C8	:	1.821239	S7	-C9	:	1.786486
C8	-H25	:	1.091984	C8	-H26	:	1.092515
C8	-H27	:	1.092322	C9	-C10	:	1.398943
C10	-H28	:	1.084135	C11	-C12	:	1.541891
C11	-H29	:	1.097795	C11	-H30	:	1.097655
C12	-C13	:	1.541876	C12	-H31	:	1.097178
C12	-H32	:	1.097169	C13	-C14	:	1.513054
C13	-H33	:	1.097770	C13	-H34	:	1.097715
C14	-C15	:	1.397654	C15	-C16	:	1.396290
C15	-H35	:	1.087809	C16	-C19	:	1.398808
C16	-H36	:	1.084131	S17	-C18	:	1.821227
S17	-C19	:	1.786450	C18	-H37	:	1.091987
C18	-H38	:	1.092499	C18	-H39	:	1.092353

bond lengths (bohr):

C1	-C2	:	2.626544	C1	-C14	:	2.649822
C1	-H20	:	2.055434	C2	-C19	:	2.652288
C2	-H21	:	2.053472	C3	-C4	:	2.641394
C3	-C5	:	2.649508	C3	-C11	:	2.859360
C4	-C10	:	2.638370	C4	-H22	:	2.055697
C5	-C6	:	2.626799	C5	-H23	:	2.055383
C6	-C9	:	2.652061	C6	-H24	:	2.053494
S7	-C8	:	3.441642	S7	-C9	:	3.375969
C8	-H25	:	2.063551	C8	-H26	:	2.064555
C8	-H27	:	2.064190	C9	-C10	:	2.643619
C10	-H28	:	2.048718	C11	-C12	:	2.913752
C11	-H29	:	2.074533	C11	-H30	:	2.074268
C12	-C13	:	2.913724	C12	-H31	:	2.073365
C12	-H32	:	2.073349	C13	-C14	:	2.859257
C13	-H33	:	2.074485	C13	-H34	:	2.074381
C14	-C15	:	2.641182	C15	-C16	:	2.638607
C15	-H35	:	2.055662	C16	-C19	:	2.643364
C16	-H36	:	2.048711	S17	-C18	:	3.441620
S17	-C19	:	3.375902	C18	-H37	:	2.063556
C18	-H38	:	2.064524	C18	-H39	:	2.064248

bond angles:

C14	-C1	-C2	: 121.497354	H20	-C1	-C2	: 119.065940
H20	-C1	-C14	: 119.435147	C19	-C2	-C1	: 120.463863
H21	-C2	-C1	: 119.750659	H21	-C2	-C19	: 119.784223
C5	-C3	-C4	: 117.483707	C11	-C3	-C4	: 121.444309
C11	-C3	-C5	: 121.059737	C10	-C4	-C3	: 121.719342
H22	-C4	-C3	: 119.448022	H22	-C4	-C10	: 118.831740
C6	-C5	-C3	: 121.498410	H23	-C5	-C3	: 119.433672
H23	-C5	-C6	: 119.066440	C9	-C6	-C5	: 120.463005
H24	-C6	-C5	: 119.744598	H24	-C6	-C9	: 119.790787
C9	-S7	-C8	: 103.618676	H25	-C8	-S7	: 105.575892
H26	-C8	-S7	: 111.516378	H26	-C8	-H25	: 108.899846
H27	-C8	-S7	: 111.663469	H27	-C8	-H25	: 108.816799
H27	-C8	-H26	: 110.200629	S7	-C9	-C6	: 116.562460
C10	-C9	-C6	: 118.668728	C10	-C9	-S7	: 124.768757
C9	-C10	-C4	: 120.166734	H28	-C10	-C4	: 118.998145
H28	-C10	-C9	: 120.834438	C12	-C11	-C3	: 113.314814
H29	-C11	-C3	: 109.577493	H29	-C11	-C12	: 108.903660

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 H30      -C11      -C3       : 109.537071  H30      -C11      -C12      :
108.964303
 H30      -C11      -H29      : 106.300674  C13      -C12      -C11      :
112.619935
 H31      -C12      -C11      : 109.513859  H31      -C12      -C13      :
109.471240
 H32      -C12      -C11      : 109.472222  H32      -C12      -C13      :
109.514712
 H32      -C12      -H31      : 106.034865  C14      -C13      -C12      :
113.298753
 H33      -C13      -C12      : 108.942002  H33      -C13      -C14      :
109.554631
 H34      -C13      -C12      : 108.926799  H34      -C13      -C14      :
109.578715
 H34      -C13      -H33      : 106.297812  C13      -C14      -C1       :
121.019263
 C15      -C14      -C1       : 117.482540  C15      -C14      -C13      :
121.476462
 C16      -C15      -C14      : 121.720086  H35      -C15      -C14      :
119.443804
 H35      -C15      -C16      : 118.835043  C19      -C16      -C15      :
120.166560
 H36      -C16      -C15      : 118.993461  H36      -C16      -C19      :
120.839441
 C19      -S17      -C18      : 103.617147  H37      -C18      -S17      :
105.581654
 H38      -C18      -S17      : 111.517921  H38      -C18      -H37      :
108.896740
 H39      -C18      -S17      : 111.655971  H39      -C18      -H37      :
108.821851
 H39      -C18      -H38      : 110.199349  C16      -C19      -C2       :
118.669477
 S17      -C19      -C2       : 116.563458  S17      -C19      -C16      :
124.766917

  torsional angles:

 C1       -C2       -C19      -C16      :   0.044944
 C1       -C2       -C19      -S17      :-179.822006
 C1       -C14      -C13      -C12      :  88.261266
 C1       -C14      -C13      -H33      : -33.610827
 C1       -C14      -C13      -H34      :-149.868671
 C1       -C14      -C15      -C16      :   0.088721
 C1       -C14      -C15      -H35      : 179.708387
 C2       -C1       -C14      -C13      :-178.447104
 C2       -C1       -C14      -C15      :  -0.118575
 C2       -C19      -C16      -C15      :  -0.074246
 C2       -C19      -C16      -H36      :-179.804699
 C2       -C19      -S17      -C18      : 177.427420
 C3       -C4       -C10      -C9       :   0.108563
 C3       -C4       -C10      -H28      : 179.810390
 C3       -C5       -C6       -C9       :   0.004613
 C3       -C5       -C6       -H24      :-179.532858
 C3       -C11      -C12      -C13      :-179.999976
 C3       -C11      -C12      -H31      : -57.941737
 C3       -C11      -C12      -H32      :  57.915918
 C4       -C3       -C5       -C6       :   0.022259
 C4       -C3       -C5       -H23      :-179.531331
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C4      -C3      -C11     -C12     : -88.694829
C4      -C3      -C11     -H29     :  33.155586
C4      -C3      -C11     -H30     : 149.406143
C4      -C10     -C9      -C6      :  -0.078082
C4      -C10     -C9      -S7      : 179.832508
C5      -C3      -C4      -C10     :  -0.078809
C5      -C3      -C4      -H22     : 179.572874
C5      -C3      -C11     -C12     :  89.999976
C5      -C3      -C11     -H29     :-148.149609
C5      -C3      -C11     -H30     : -31.899052
C5      -C6      -C9      -S7      :-179.894927
C5      -C6      -C9      -C10     :   0.022959
C6      -C5      -C3      -C11     :-178.722568
C6      -C9      -S7      -C8      : 177.336803
C6      -C9      -C10     -H28     :-179.774359
S7      -C9      -C6      -H24     :  -0.357670
S7      -C9      -C10     -H28     :   0.136231
C8      -S7      -C9      -C10     :  -2.575490
C9      -C6      -C5      -H23     : 179.559802
C9      -S7      -C8      -H25     :-178.733530
C9      -S7      -C8      -H26     : -60.611709
C9      -S7      -C8      -H27     :  63.166546
C9      -C10     -C4      -H22     :-179.545203
C10     -C4      -C3      -C11     : 178.660894
C10     -C9      -C6      -H24     : 179.560216
C11     -C3      -C4      -H22     :  -1.687423
C11     -C3      -C5      -H23     :   1.723842
C11     -C12     -C13     -C14     :-179.999996
C11     -C12     -C13     -H33     : -57.786128
C11     -C12     -C13     -H34     :  57.766285
C12     -C13     -C14     -C15     : -90.000026
C13     -C12     -C11     -H29     :  57.773785
C13     -C12     -C11     -H30     : -57.781564
C13     -C14     -C1      -H20     :   2.011578
C13     -C14     -C15     -C16     : 178.409135
C13     -C14     -C15     -H35     :  -1.971199
C14     -C1      -C2      -C19     :   0.053395
C14     -C1      -C2      -H21     :-179.538252
C14     -C13     -C12     -H31     :  57.917689
C14     -C13     -C12     -H32     : -57.939893
C14     -C15     -C16     -C19     :   0.006601
C14     -C15     -C16     -H36     : 179.742006
C15     -C14     -C1      -H20     :-179.659894
C15     -C14     -C13     -H33     : 148.127881
C15     -C14     -C13     -H34     :  31.870037
C15     -C16     -C19     -S17     : 179.780886
C16     -C19     -C2      -H21     : 179.636454
C16     -C19     -S17     -C18     :  -2.430472
S17     -C19     -C2      -H21     :  -0.230496
S17     -C19     -C16     -H36     :   0.050433
C19     -C2      -C1      -H20     : 179.596366
C19     -C16     -C15     -H35     :-179.615311
C19     -S17     -C18     -H37     :-178.625111
C19     -S17     -C18     -H38     : -60.502762
C19     -S17     -C18     -H39     :  63.269418
H20     -C1      -C2      -H21     :   0.004719
H22     -C4      -C10     -H28     :   0.156624
H23     -C5      -C6      -H24     :   0.022332
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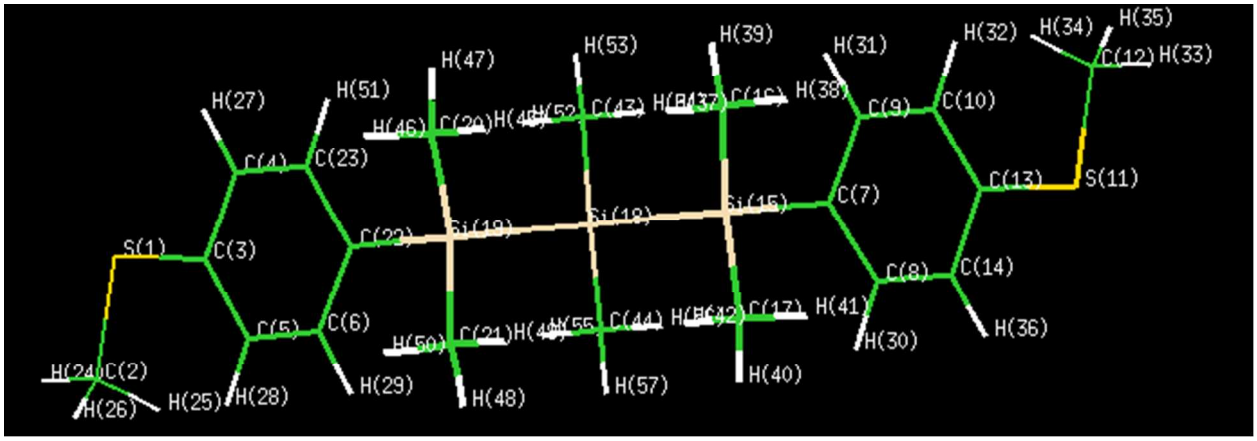
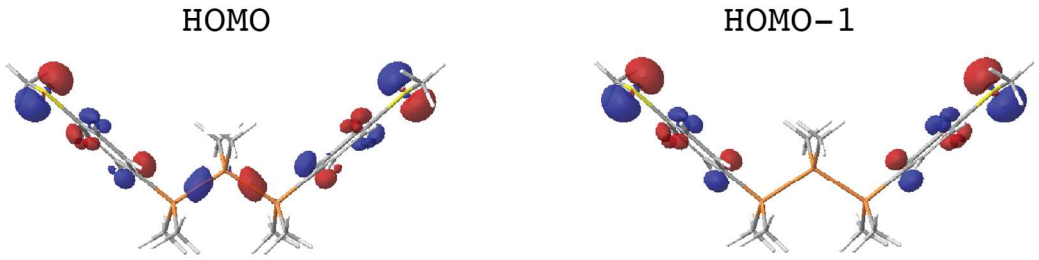
H29      -C11     -C12     -H31     : 179.832024
H29      -C11     -C12     -H32     : -64.310321
H30      -C11     -C12     -H31     :  64.276675
H30      -C11     -C12     -H32     :-179.865670
H31      -C12     -C13     -H33     :-179.868443
H31      -C12     -C13     -H34     : -64.316030
H32      -C12     -C13     -H33     :  64.273975
H32      -C12     -C13     -H34     : 179.826387
H35      -C15     -C16     -H36     :   0.120093

  nuclear repulsion energy.......    1443.139820844 hartrees
```

SiSiSi



Final energy (B3LYP/cc-pVTZ): -2446.80158907678 hartrees



HOMO & HOMO–1 energies and surfaces (B3LYP/cc-pVTZ).

<u>Optimized geometry:</u>

Subjected to the constraints that ω(C(Ar)-α-β-α) = 180˚ and that the α-β σ-bond is orthogonal to the phenyl ring σ-plane. Optimized with 6-31G** basis set.

atom	x	y	z
S1	-24.4602124503	2.9684838424	3.7379652026
C2	-26.0061577089	3.5174077077	0.7116614100
C3	-21.9791267701	0.8150521058	2.9847524946
C4	-20.4007594803	0.0764564293	4.9841923389
C5	-21.5183567387	-0.1689226183	0.5747715393
C6	-19.5190699622	-1.8461377022	0.1901007790

C7	-5.1659159620	-2.2920374786	-0.8976161299
C8	-4.6623738696	-1.4700651958	-3.3789247978
C9	-3.6707608725	-1.2377403763	1.0250913851
C10	-1.7788445549	0.5316120843	0.5280367225
S11	1.0322421088	3.5619901264	-2.8503835184
C12	2.4770567841	4.4635784607	0.1411814388
C13	-1.3182748345	1.3191932414	-1.9532341509
C14	-2.7869132871	0.2916886760	-3.9079026039
Si15	-7.8005135440	-4.6183508098	-0.1769728516
C16	-6.8508203415	-6.5934264152	2.6714453517
C17	-8.2099869596	-6.8091575496	-2.9963799794
Si18	-11.5466045689	-2.2844351104	0.6258243803
Si19	-15.1330383028	-4.8043754495	1.5813870721
C20	-14.5920701844	-6.7857514018	4.5311002648
C21	-15.9463707578	-7.0079359510	-1.1383048773
C22	-17.9135662053	-2.6124840068	2.1591878423
C23	-18.4190036930	-1.5965559037	4.5674151318
H24	-27.5282848594	4.8548764905	1.1023037049
H25	-24.7116650776	4.3592258943	-0.6584183765
H26	-26.8222850688	1.7814996201	-0.0513136232
H27	-20.7317998132	0.8178375621	6.8709591528
H28	-22.7008793176	0.3505234092	-1.0160320381
H29	-19.2278442691	-2.5725937781	-1.7101038774
H30	-5.7525360841	-2.2235197888	-4.9492059494
H31	-3.9656186192	-1.8045127048	2.9785126189
H32	-0.6789483611	1.2760016611	2.0884157092
H33	3.9228938012	5.8552937216	-0.3393267819
H34	1.1049738879	5.3368889332	1.4124814613
H35	3.3806255513	2.8533711754	1.0644543803
H36	-2.4535769370	0.8766552877	-5.8484642514
H37	-8.2776448241	-8.0390442241	3.0701057544
H38	-5.0508826636	-7.5586607253	2.3295126374
H39	-6.6395791963	-5.4509282356	4.3834805291
H40	-8.8312060773	-5.7981332858	-4.6914246293
H41	-6.4324217493	-7.7700228129	-3.4495098480
H42	-9.6287555398	-8.2617560068	-2.5942141347
C43	-10.9307787296	-0.0487549340	3.3956450945
C44	-12.3029069792	-0.2760115081	-2.2798544143
H45	-13.0735372930	-8.1589870310	4.2257772148
H46	-16.3029016064	-7.8373632034	5.0366964896
H47	-14.0560720458	-5.6313082634	6.1624025628
H48	-16.2138142476	-5.9908815710	-2.9201881118
H49	-14.4332349242	-8.3876136565	-1.4401621696
H50	-17.6876834621	-8.0558835736	-0.7405779992
H51	-17.2443518235	-2.1231469857	6.1690959727
H52	-12.5902247187	1.1300826789	3.7712867434
H53	-10.4842383360	-1.0813674291	5.1331575596
H54	-9.3377358268	1.2065825719	2.9811922505
H55	-13.9767337842	0.8948061072	-1.9437798511
H56	-10.7241409573	0.9834663878	-2.7333206542
H57	-12.6759502547	-1.4447523143	-3.9470123758

angstroms

atom	x	y	z
S1	-12.9437870000	1.5708540000	1.9780460000
C2	-13.7618660000	1.8613320000	0.3765950000
C3	-11.6308530000	0.4313070000	1.5794630000
C4	-10.7956170000	0.0404590000	2.6375210000

C5	-11.3870240000	-0.0893900000	0.3041560000
C6	-10.3290470000	-0.9769340000	0.1005970000
C7	-2.7336850000	-1.2128940000	-0.4749980000
C8	-2.4672220000	-0.7779250000	-1.7880500000
C9	-1.9424830000	-0.6549840000	0.5424550000
C10	-0.9413240000	0.2813170000	0.2794250000
S11	0.5462390000	1.8849240000	-1.5083580000
C12	1.3108020000	2.3620240000	0.0747100000
C13	-0.6976010000	0.6980870000	-1.0336070000
C14	-1.4747710000	0.1543550000	-2.0679730000
Si15	-4.1278540000	-2.4439260000	-0.0936500000
C16	-3.6252980000	-3.4890910000	1.4136680000
C17	-4.3445380000	-3.6032510000	-1.5856160000
Si18	-6.1102000000	-1.2088710000	0.3311720000
Si19	-8.0080590000	-2.5423660000	0.8368340000
C20	-7.7217910000	-3.5908650000	2.3977550000
C21	-8.4384560000	-3.7084400000	-0.6023650000
C22	-9.4794510000	-1.3824670000	1.1425930000
C23	-9.7469170000	-0.8448610000	2.4169720000
H24	-14.5673410000	2.5690900000	0.5833140000
H25	-13.0768500000	2.3068030000	-0.3484200000
H26	-14.1937420000	0.9427290000	-0.0271540000
H27	-10.9707960000	0.4327810000	3.6359550000
H28	-12.0127880000	0.1854890000	-0.5376610000
H29	-10.1749370000	-1.3613580000	-0.9049480000
H30	-3.0441110000	-1.1766360000	-2.6190070000
H31	-2.0985150000	-0.9549070000	1.5761610000
H32	-0.3592840000	0.6752310000	1.1051420000
H33	2.0759060000	3.0984880000	-0.1795640000
H34	0.5847270000	2.8241600000	0.7474530000
H35	1.7889500000	1.5099390000	0.5632850000
H36	-1.2983770000	0.4639060000	-3.0948740000
H37	-4.3803410000	-4.2540790000	1.6246300000
H38	-2.6728120000	-3.9998710000	1.2327250000
H39	-3.5135140000	-2.8845070000	2.3196380000
H40	-4.6732730000	-3.0682400000	-2.4825950000
H41	-3.4038910000	-4.1117190000	-1.8254020000
H42	-5.0953180000	-4.3719330000	-1.3727990000
C43	-5.7843190000	-0.0258000000	1.7968980000
C44	-6.5104180000	-0.1460590000	-1.2064470000
H45	-6.9182180000	-4.3175500000	2.2361850000
H46	-8.6271240000	-4.1473540000	2.6653050000
H47	-7.4381530000	-2.9799600000	3.2610030000
H48	-8.5799810000	-3.1702380000	-1.5452970000
H49	-7.6377390000	-4.4385340000	-0.7621010000
H50	-9.3599190000	-4.2629900000	-0.3918970000
H51	-9.1253180000	-1.1235210000	3.2645450000
H52	-6.6624600000	0.5980140000	1.9956790000
H53	-5.5480200000	-0.5722350000	2.7163500000
H54	-4.9413170000	0.6384960000	1.5775790000
H55	-7.3961690000	0.4735110000	-1.0286040000
H56	-5.6749710000	0.5204280000	-1.4464110000
H57	-6.7078240000	-0.7645300000	-2.0886690000

principal moments of inertia:

amu*angstrom^2:	1923.24269	8989.24686	9936.91500
g*cm^2:	3.19361922E-37	1.49269937E-36	1.65006335E-36

rotational constants:

cm^(-1):	0.00876521	0.00187531	0.00169647
GHz:	0.26277443	0.05622039	0.05085874

Molecular weight: 420.13 amu

Stoichiometry: Si3C20H32S2
Molecular Point Group: C1
Point Group used: C1

bond lengths (angstroms):

S1	-C2	:	1.821614	S1	-C3	:	1.783601
C2	-H24	:	1.091991	C2	-H25	:	1.092400
C2	-H26	:	1.092411	C3	-C4	:	1.403520
C3	-C5	:	1.398923	C4	-C23	:	1.390038
C4	-H27	:	1.086957	C5	-C6	:	1.395882
C5	-H28	:	1.084341	C6	-C22	:	1.404288
C6	-H29	:	1.087498	C7	-C8	:	1.408654
C7	-C9	:	1.404448	C7	-Si15	:	1.898571
C8	-C14	:	1.390130	C8	-H30	:	1.087318
C9	-C10	:	1.395766	C9	-H31	:	1.087588
C10	-C13	:	1.398982	C10	-H32	:	1.084319
S11	-C12	:	1.821616	S11	-C13	:	1.783566
C12	-H33	:	1.091979	C12	-H34	:	1.092400
C12	-H35	:	1.092419	C13	-C14	:	1.403407
C14	-H36	:	1.086951	Si15	-C16	:	1.901825
Si15	-C17	:	1.901828	Si15	-Si18	:	2.373927
C16	-H37	:	1.095355	C16	-H38	:	1.095840
C16	-H39	:	1.094897	C17	-H40	:	1.094931
C17	-H41	:	1.095835	C17	-H42	:	1.095369
Si18	-Si19	:	2.373978	Si18	-C43	:	1.911598
Si18	-C44	:	1.911548	Si19	-C20	:	1.902045
Si19	-C21	:	1.901648	Si19	-C22	:	1.898381
C20	-H45	:	1.095402	C20	-H46	:	1.095852
C20	-H47	:	1.094921	C21	-H48	:	1.094902
C21	-H49	:	1.095308	C21	-H50	:	1.095863
C22	-C23	:	1.408758	C23	-H51	:	1.087390
C43	-H52	:	1.095349	C43	-H53	:	1.095363
C43	-H54	:	1.095464	C44	-H55	:	1.095468
C44	-H56	:	1.095335	C44	-H57	:	1.095350

bond lengths (bohr):

S1	-C2	:	3.442351	S1	-C3	:	3.370517
C2	-H24	:	2.063564	C2	-H25	:	2.064337
C2	-H26	:	2.064357	C3	-C4	:	2.652268
C3	-C5	:	2.643582	C4	-C23	:	2.626791
C4	-H27	:	2.054050	C5	-C6	:	2.637834
C5	-H28	:	2.049107	C6	-C22	:	2.653721
C6	-H29	:	2.055074	C7	-C8	:	2.661970
C7	-C9	:	2.654022	C7	-Si15	:	3.587780
C8	-C14	:	2.626965	C8	-H30	:	2.054734
C9	-C10	:	2.637616	C9	-H31	:	2.055244
C10	-C13	:	2.643693	C10	-H32	:	2.049066

S11	-C12	:	3.442356	S11	-C13	:	3.370452
C12	-H33	:	2.063542	C12	-H34	:	2.064337
C12	-H35	:	2.064373	C13	-C14	:	2.652055
C14	-H36	:	2.054040	Si15	-C16	:	3.593929
Si15	-C17	:	3.593934	Si15	-Si18	:	4.486072
C16	-H37	:	2.069920	C16	-H38	:	2.070838
C16	-H39	:	2.069055	C17	-H40	:	2.069120
C17	-H41	:	2.070828	C17	-H42	:	2.069948
Si18	-Si19	:	4.486168	Si18	-C43	:	3.612397
Si18	-C44	:	3.612302	Si19	-C20	:	3.594343
Si19	-C21	:	3.593593	Si19	-C22	:	3.587419
C20	-H45	:	2.070010	C20	-H46	:	2.070860
C20	-H47	:	2.069101	C21	-H48	:	2.069066
C21	-H49	:	2.069833	C21	-H50	:	2.070882
C22	-C23	:	2.662167	C23	-H51	:	2.054869
C43	-H52	:	2.069910	C43	-H53	:	2.069936
C43	-H54	:	2.070128	C44	-H55	:	2.070134
C44	-H56	:	2.069884	C44	-H57	:	2.069911

bond angles:

C3	-S1	-C2	: 103.650841	H24	-C2	-S1	: 105.556599
H25	-C2	-S1	: 111.523712	H25	-C2	-H24	: 108.897654
H26	-C2	-S1	: 111.615773	H26	-C2	-H24	: 108.866695
H26	-C2	-H25	: 110.213677	C4	-C3	-S1	: 116.584428
C5	-C3	-S1	: 124.738691	C5	-C3	-C4	: 118.676779
C23	-C4	-C3	: 120.445621	H27	-C4	-C3	: 119.738596
H27	-C4	-C23	: 119.815779	C6	-C5	-C3	: 120.113278
H28	-C5	-C3	: 120.850337	H28	-C5	-C6	: 119.036287
C22	-C6	-C5	: 122.273212	H29	-C6	-C5	: 117.840201
H29	-C6	-C22	: 119.885929	C9	-C7	-C8	: 116.490924
Si15	-C7	-C8	: 121.759135	Si15	-C7	-C9	: 121.718422
C14	-C8	-C7	: 121.993905	H30	-C8	-C7	: 119.918640
H30	-C8	-C14	: 118.087083	C10	-C9	-C7	: 122.278874
H31	-C9	-C7	: 119.880259	H31	-C9	-C10	: 117.840244
C13	-C10	-C9	: 120.110799	H32	-C10	-C9	: 119.026424
H32	-C10	-C13	: 120.862684	C13	-S11	-C12	: 103.630855
H33	-C12	-S11	: 105.566441	H34	-C12	-S11	: 111.532184
H34	-C12	-H33	: 108.892051	H35	-C12	-S11	: 111.598008

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 H35     -C12     -H33     : 108.876044  H35     -C12     -H34     :
110.210253
 S11     -C13     -C10     : 124.719563  C14     -C13     -C10     :
118.676305
 C14     -C13     -S11     : 116.604050  C13     -C14     -C8      :
120.449055
 H36     -C14     -C8      : 119.807627  H36     -C14     -C13     :
119.743289
 C16     -Si15    -C7      : 108.752653  C17     -Si15    -C7      :
108.744346
 C17     -Si15    -C16     : 108.473339  Si18    -Si15    -C7      :
108.168191
 Si18    -Si15    -C16     : 111.391691  Si18    -Si15    -C17     :
111.246895
 H37     -C16     -Si15    : 110.750722  H38     -C16     -Si15    :
110.791498
 H38     -C16     -H37     : 107.783107  H39     -C16     -Si15    :
112.291970
 H39     -C16     -H37     : 107.256684  H39     -C16     -H38     :
107.774051
 H40     -C17     -Si15    : 112.272454  H41     -C17     -Si15    :
110.898097
 H41     -C17     -H40     : 107.769098  H42     -C17     -Si15    :
110.698779
 H42     -C17     -H40     : 107.233977  H42     -C17     -H41     :
107.772924
 Si19    -Si18    -Si15    : 114.422078  C43     -Si18    -Si15    :
108.471970
 C43     -Si18    -Si19    : 108.699495  C44     -Si18    -Si15    :
108.671816
 C44     -Si18    -Si19    : 108.437338  C44     -Si18    -C43     :
107.960219
 C20     -Si19    -Si18    : 111.353687  C21     -Si19    -Si18    :
111.356566
 C21     -Si19    -C20     : 108.489318  C22     -Si19    -Si18    :
108.103424
 C22     -Si19    -C20     : 108.740694  C22     -Si19    -C21     :
108.731239
 H45     -C20     -Si19    : 110.797091  H46     -C20     -Si19    :
110.851891
 H46     -C20     -H45     : 107.768969  H47     -C20     -Si19    :
112.236792
 H47     -C20     -H45     : 107.241043  H47     -C20     -H46     :
107.749440
 H48     -C21     -Si19    : 112.309594  H49     -C21     -Si19    :
110.710582
 H49     -C21     -H48     : 107.250505  H50     -C21     -Si19    :
110.809181
 H50     -C21     -H48     : 107.785668  H50     -C21     -H49     :
107.782361
 Si19    -C22     -C6      : 121.725903  C23     -C22     -C6      :
116.497679
 C23     -C22     -Si19    : 121.736992  C22     -C23     -C4      :
121.993292
 H51     -C23     -C4      : 118.087203  H51     -C23     -C22     :
119.919208
 H52     -C43     -Si18    : 110.790002  H53     -C43     -Si18    :
111.817496
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 H53      -C43      -H52      : 107.741495  H54      -C43      -Si18     :
110.669545
 H54      -C43      -H52      : 107.933715  H54      -C43      -H53      :
107.731506
 H55      -C44      -Si18     : 110.680546  H56      -C44      -Si18     :
110.783745
 H56      -C44      -H55      : 107.947172  H57      -C44      -Si18     :
111.818665
 H57      -C44      -H55      : 107.720802  H57      -C44      -H56      :
107.732700

  torsional angles:

 S1       -C3       -C4       -C23      : 179.998993
 S1       -C3       -C4       -H27      :   0.022903
 S1       -C3       -C5       -C6       : 179.983450
 S1       -C3       -C5       -H28      :  -0.131921
 C2       -S1       -C3       -C4       : 178.715038
 C2       -S1       -C3       -C5       :  -1.403276
 C3       -S1       -C2       -H24      :-179.278106
 C3       -S1       -C2       -H25      : -61.166545
 C3       -S1       -C2       -H26      :  62.598901
 C3       -C4       -C23      -C22      :  -0.055890
 C3       -C4       -C23      -H51      :-179.857389
 C3       -C5       -C6       -C22      :   0.113110
 C3       -C5       -C6       -H29      : 179.817652
 C4       -C3       -C5       -C6       :  -0.137148
 C4       -C3       -C5       -H28      : 179.747482
 C4       -C23      -C22      -C6       :   0.026590
 C4       -C23      -C22      -Si19     : 177.779758
 C5       -C3       -C4       -C23      :   0.109812
 C5       -C3       -C4       -H27      :-179.866278
 C5       -C6       -C22      -Si19     :-177.808681
 C5       -C6       -C22      -C23      :  -0.055244
 C6       -C22      -Si19     -Si18     :  90.000027
 C6       -C22      -Si19     -C20      :-148.972464
 C6       -C22      -Si19     -C21      : -31.025421
 C6       -C22      -C23      -H51      : 179.824539
 C7       -C8       -C14      -C13      :  -0.023826
 C7       -C8       -C14      -H36      : 179.914021
 C7       -C9       -C10      -C13      :   0.115043
 C7       -C9       -C10      -H32      :-179.774896
 C7       -Si15     -C16      -H37      :-176.460746
 C7       -Si15     -C16      -H38      : -56.908952
 C7       -Si15     -C16      -H39      :  63.659340
 C7       -Si15     -C17      -H40      : -64.105693
 C7       -Si15     -C17      -H41      :  56.517647
 C7       -Si15     -C17      -H42      : 176.092194
 C7       -Si15     -Si18     -Si19     :-179.999981
 C7       -Si15     -Si18     -C43      : -58.471380
 C7       -Si15     -Si18     -C44      :  58.661468
 C8       -C7       -C9       -C10      :  -0.036989
 C8       -C7       -C9       -H31      :-179.743749
 C8       -C7       -Si15     -C16      : 148.881080
 C8       -C7       -Si15     -C17      :  30.939027
 C8       -C7       -Si15     -Si18     : -90.000030
 C8       -C14      -C13      -C10      :   0.099573
 C8       -C14      -C13      -S11      : 179.999749
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C9	-C7	-C8	-C14	: -0.008623
C9	-C7	-C8	-H30	: 179.765277
C9	-C7	-Si15	-C16	: -33.232984
C9	-C7	-Si15	-C17	:-151.175037
C9	-C7	-Si15	-Si18	: 87.885905
C9	-C10	-C13	-S11	: 179.965103
C9	-C10	-C13	-C14	: -0.143486
C10	-C9	-C7	-Si15	:-178.028640
C10	-C13	-S11	-C12	: -0.734632
C10	-C13	-C14	-H36	:-179.838313
S11	-C13	-C10	-H32	: -0.147009
S11	-C13	-C14	-H36	: 0.061863
C12	-S11	-C13	-C14	: 179.371920
C13	-C10	-C9	-H31	: 179.827502
C13	-S11	-C12	-H33	:-179.537115
C13	-S11	-C12	-H34	: -61.421936
C13	-S11	-C12	-H35	: 62.332178
C13	-C14	-C8	-H30	:-179.801698
C14	-C8	-C7	-Si15	: 177.982144
C14	-C13	-C10	-H32	: 179.744402
Si15	-C7	-C8	-H30	: -2.243955
Si15	-C7	-C9	-H31	: 2.264600
Si15	-Si18	-Si19	-C20	: 60.610370
Si15	-Si18	-Si19	-C21	: -60.620244
Si15	-Si18	-Si19	-C22	:-179.999990
Si15	-Si18	-C43	-H52	: 177.342060
Si15	-Si18	-C43	-H53	: -62.453719
Si15	-Si18	-C43	-H54	: 57.655573
Si15	-Si18	-C44	-H55	:-177.416141
Si15	-Si18	-C44	-H56	: -57.709702
Si15	-Si18	-C44	-H57	: 62.479858
C16	-Si15	-C17	-H40	: 177.775560
C16	-Si15	-C17	-H41	: -61.601100
C16	-Si15	-C17	-H42	: 57.973447
C16	-Si15	-Si18	-Si19	: -60.531898
C16	-Si15	-Si18	-C43	: 60.996704
C16	-Si15	-Si18	-C44	: 178.129552
C17	-Si15	-C16	-H37	: -58.347276
C17	-Si15	-C16	-H38	: 61.204518
C17	-Si15	-C16	-H39	:-178.227189
C17	-Si15	-Si18	-Si19	: 60.628557
C17	-Si15	-Si18	-C43	:-177.842842
C17	-Si15	-Si18	-C44	: -60.709993
Si18	-Si15	-C16	-H37	: 64.418936
Si18	-Si15	-C16	-H38	:-176.029270
Si18	-Si15	-C16	-H39	: -55.460978
Si18	-Si15	-C17	-H40	: 54.921696
Si18	-Si15	-C17	-H41	: 175.545036
Si18	-Si15	-C17	-H42	: -64.880417
Si18	-Si19	-C20	-H45	: -64.522308
Si18	-Si19	-C20	-H46	: 175.873975
Si18	-Si19	-C20	-H47	: 55.332581
Si18	-Si19	-C21	-H48	: -54.979369
Si18	-Si19	-C21	-H49	: 64.876814
Si18	-Si19	-C21	-H50	:-175.586964
Si18	-Si19	-C22	-C23	: -87.635847
Si19	-Si18	-C43	-H52	: -57.679095
Si19	-Si18	-C43	-H53	: 62.525126

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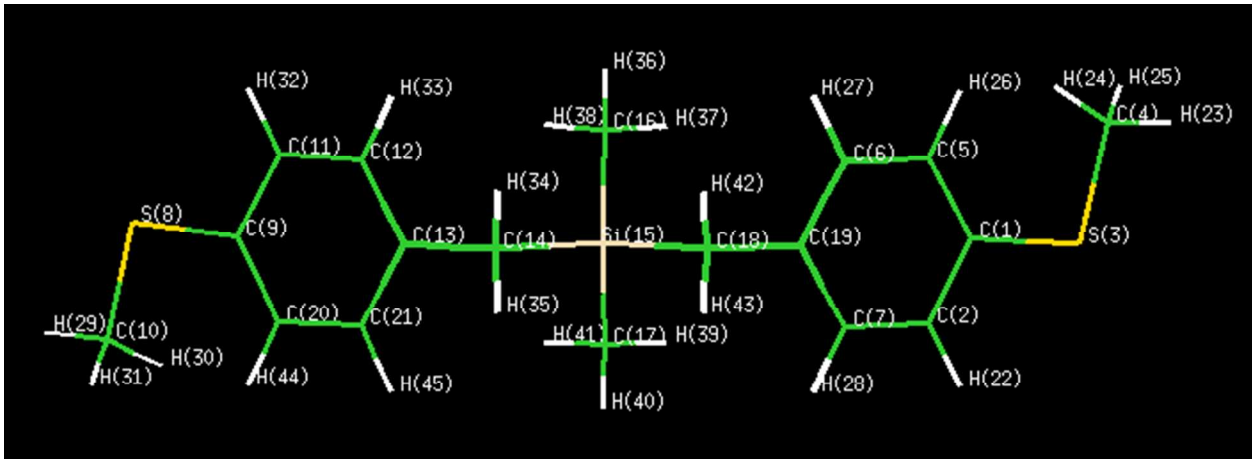
Si19    -Si18    -C43     -H54     :-177.365583
Si19    -Si18    -C44     -H55     :  57.645201
Si19    -Si18    -C44     -H56     : 177.351640
Si19    -Si18    -C44     -H57     : -62.458800
Si19    -C22     -C6      -H29     :   2.492649
Si19    -C22     -C23     -H51     :  -2.422293
C20     -Si19    -Si18    -C43     : -60.793216
C20     -Si19    -Si18    -C44     :-177.922158
C20     -Si19    -C21     -H48     :-177.867693
C20     -Si19    -C21     -H49     : -58.011510
C20     -Si19    -C21     -H50     :  61.524712
C20     -Si19    -C22     -C23     :  33.391662
C21     -Si19    -Si18    -C43     : 177.976170
C21     -Si19    -Si18    -C44     :  60.847229
C21     -Si19    -C20     -H45     :  58.367757
C21     -Si19    -C20     -H46     : -61.235960
C21     -Si19    -C20     -H47     : 178.222646
C21     -Si19    -C22     -C23     : 151.338705
C22     -C6      -C5      -H28     :-179.773605
C22     -Si19    -Si18    -C43     :  58.596424
C22     -Si19    -Si18    -C44     : -58.532517
C22     -Si19    -C20     -H45     : 176.467860
C22     -Si19    -C20     -H46     :  56.864142
C22     -Si19    -C20     -H47     : -63.677252
C22     -Si19    -C21     -H48     :  64.026199
C22     -Si19    -C21     -H49     :-176.117618
C22     -Si19    -C21     -H50     : -56.581397
C22     -C23     -C4      -H27     : 179.920182
C23     -C22     -C6      -H29     :-179.753914
H27     -C4      -C23     -H51     :   0.118683
H28     -C5      -C6      -H29     :  -0.069063
H30     -C8      -C14     -H36     :   0.136148
H31     -C9      -C10     -H32     :  -0.062437
C43     -Si18    -C44     -H55     : -59.956938
C43     -Si18    -C44     -H56     :  59.749501
C43     -Si18    -C44     -H57     : 179.939061
C44     -Si18    -C43     -H52     :  59.754000
C44     -Si18    -C43     -H53     : 179.958221
C44     -Si18    -C43     -H54     : -59.932487

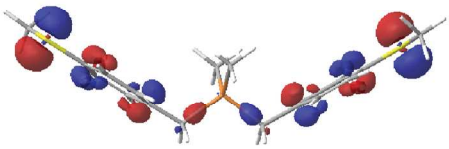
 nuclear repulsion energy.......    2833.798975932 hartrees
```

CSiC



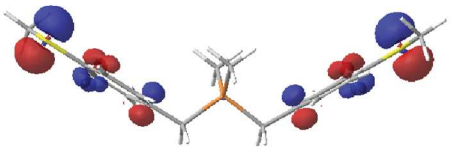
Final energy (B3LYP/cc-pVTZ): -1786.64296461976 hartrees

HOMO



−5.51 eV

HOMO−1



−5.68 eV

HOMO & HOMO–1 energies and surfaces (B3LYP/cc-pVTZ).

Optimized geometry:

Subjected to the constraints that ω(C(Ar)-α-β-α) = 180˚ and that the α-β σ-bond is orthogonal to the phenyl ring σ-plane. Optimized with 6-31G** basis set.

atom	x	y	z
C1	16.2666472107	2.1473505979	−2.5238974256
C2	14.3352941986	1.7745567663	−4.3010960290
S3	19.0788242463	3.6500419152	−3.6335918493
C4	20.9569380043	4.0518222558	−0.7773709669
C5	15.8788961968	1.3121464527	−0.0469748120
C6	13.6056766109	0.1559515382	0.6279352043
C7	12.0831923021	0.6160355989	−3.6047791951
S8	−4.9465093103	5.5350777400	5.7191956461
C9	−2.4906004512	3.6535662544	4.3675690352
C10	−6.6196425857	6.7644541884	2.9738015317
C11	−0.7074718872	2.6373433540	6.0451148211
C12	1.2614299830	1.1415438679	5.1586783109
C13	1.5517920712	0.6117043467	2.5746214542
C14	3.7257878075	−0.9708486864	1.6250926579
Si15	6.6804142882	0.9496176134	0.7820574877
C16	7.8821780585	2.6803554103	3.6667395353
C17	5.9142172719	3.2841077895	−1.8109982449
C18	9.1779368062	−1.4099057646	−0.3682849450
C19	11.6496513345	−0.2008155261	−1.1172174235

C20	-2.2497964306	3.1129723019	1.7920424021
C21	-0.2590946798	1.6138336696	0.9266253157
H22	14.6007005637	2.3934515209	-6.2411946936
H23	22.6584303997	5.0587647113	-1.3685509981
H24	19.9591985151	5.1899570578	0.6267862509
H25	21.5077345882	2.2370313306	0.0383689992
H26	17.3336432726	1.5395617638	1.3779769520
H27	13.3595681290	-0.4860148826	2.5645416551
H28	10.6242046809	0.3407743121	-5.0252164034
H29	-8.0700943140	8.0252152083	3.7255459225
H30	-5.3598358775	7.8474883560	1.7482007560
H31	-7.5387997037	5.2603417970	1.8989706652
H32	-0.8642397871	3.0213564896	8.0564013585
H33	2.6099933478	0.3707907219	6.5037872564
H34	4.2657109073	-2.3788949605	3.0484457136
H35	3.1594463365	-2.0335588495	-0.0631697649
H36	8.3502783374	1.3749930744	5.2052165962
H37	9.5903260693	3.7577525249	3.2176990340
H38	6.4621981639	4.0055560911	4.3792418734
H39	7.5925907579	4.3667961372	-2.3505774145
H40	5.2051391175	2.3370110707	-3.5110601176
H41	4.4650921313	4.6233831504	-1.1893331518
H42	9.4830330891	-2.7955002026	1.1442234995
H43	8.3761392394	-2.4577513420	-1.9679853530
H44	-3.6038721265	3.8378183311	0.4357009246
H45	-0.1233121886	1.2147499682	-1.0846952368

angstroms

atom	x	y	z
C1	8.6079390000	1.1363290000	-1.3355890000
C2	7.5859110000	0.9390550000	-2.2760420000
S3	10.0960790000	1.9315190000	-1.9228140000
C4	11.0899340000	2.1441320000	-0.4113670000
C5	8.4027500000	0.6943580000	-0.0248580000
C6	7.1998140000	0.0825260000	0.3322890000
C7	6.3941500000	0.3259920000	-1.9075670000
S8	-2.6175800000	2.9290370000	3.0264680000
C9	-1.3179690000	1.9333840000	2.3112180000
C10	-3.5029640000	3.5795950000	1.5736680000
C11	-0.3743780000	1.3956220000	3.1989370000
C12	0.6675200000	0.6040790000	2.7298550000
C13	0.8211730000	0.3237000000	1.3624310000
C14	1.9716020000	-0.5137510000	0.8599620000
Si15	3.5351230000	0.5025160000	0.4138470000
C16	4.1710690000	1.4183830000	1.9403550000
C17	3.1296690000	1.7378750000	-0.9583390000
C18	4.8567550000	-0.7460900000	-0.1948880000
C19	6.1647300000	-0.1062670000	-0.5912060000
C20	-1.1905410000	1.6473140000	0.9483080000
C21	-0.1371070000	0.8540040000	0.4903490000
H22	7.7263580000	1.2665600000	-3.3026980000
H23	11.9903250000	2.6769830000	-0.7242060000
H24	10.5619530000	2.7464070000	0.3316810000
H25	11.3814030000	1.1837860000	0.0203040000
H26	9.1725690000	0.8147010000	0.7291940000
H27	7.0695790000	-0.2571880000	1.3570970000
H28	5.6220870000	0.1803300000	-2.6592300000
H29	-4.2705100000	4.2467610000	1.9714740000

H30	-2.8363030000	4.1527120000	0.9251080000
H31	-3.9893610000	2.7836530000	1.0048920000
H32	-0.4573360000	1.5988330000	4.2632640000
H33	1.3811490000	0.1962140000	3.4416560000
H34	2.2573170000	-1.2588570000	1.6131680000
H35	1.6719070000	-1.0761130000	-0.0334280000
H36	4.4187770000	0.7276150000	2.7544820000
H37	5.0749820000	1.9885170000	1.7027330000
H38	3.4196480000	2.1196490000	2.3173950000
H39	4.0178260000	2.3108090000	-1.2438720000
H40	2.7544410000	1.2366930000	-1.8579730000
H41	2.3628250000	2.4465890000	-0.6293680000
H42	5.0182050000	-1.4793150000	0.6054970000
H43	4.4324620000	-1.3005860000	-1.0414130000
H44	-1.9070870000	2.0308860000	0.2305630000
H45	-0.0652540000	0.6428180000	-0.5739960000

principal moments of inertia:

amu*angstrom^2:	708.72888	7636.29332	7684.71983
g*cm^2:	1.17687185E-37	1.26803618E-36	1.27607759E-36

rotational constants:

cm^(-1):	0.02378572	0.00220757	0.00219366
GHz:	0.71307805	0.06618119	0.06576414

Molecular weight: 332.11 amu

Stoichiometry: SiC18H24S2
Molecular Point Group: C1
Point Group used: C1

bond lengths (angstroms):

C1	-C2	:	1.402822	C1	-S3	:	1.786539
C1	-C5	:	1.398376	C2	-C7	:	1.389933
C2	-H22	:	1.086742	S3	-C4	:	1.821380
C4	-H23	:	1.092018	C4	-H24	:	1.092529
C4	-H25	:	1.092501	C5	-C6	:	1.396047
C5	-H26	:	1.084296	C6	-C19	:	1.399959
C6	-H27	:	1.087473	C7	-C19	:	1.404382
C7	-H28	:	1.087334	S8	-C9	:	1.786588
S8	-C10	:	1.821471	C9	-C11	:	1.402711
C9	-C20	:	1.398427	C10	-H29	:	1.092011
C10	-H30	:	1.092488	C10	-H31	:	1.092525
C11	-C12	:	1.390011	C11	-H32	:	1.086724
C12	-C13	:	1.404304	C12	-H33	:	1.087327
C13	-C14	:	1.509068	C13	-C21	:	1.400018
C14	-Si15	:	1.917398	C14	-H34	:	1.097331
C14	-H35	:	1.097367	Si15	-C16	:	1.890361
Si15	-C17	:	1.890344	Si15	-C18	:	1.917364
C16	-H36	:	1.096049	C16	-H37	:	1.094795
C16	-H38	:	1.094791	C17	-H39	:	1.094808
C17	-H40	:	1.096048	C17	-H41	:	1.094782
C18	-C19	:	1.509053	C18	-H42	:	1.097407
C18	-H43	:	1.097313	C20	-C21	:	1.395991

C20	-H44	:	1.084308	C21	-H45	:	1.087471

bond lengths (bohr):

C1	-C2	:	2.650950	C1	-S3	:	3.376069
C1	-C5	:	2.642548	C2	-C7	:	2.626593
C2	-H22	:	2.053644	S3	-C4	:	3.441909
C4	-H23	:	2.063614	C4	-H24	:	2.064580
C4	-H25	:	2.064528	C5	-C6	:	2.638147
C5	-H26	:	2.049023	C6	-C19	:	2.645539
C6	-H27	:	2.055027	C7	-C19	:	2.653897
C7	-H28	:	2.054764	S8	-C9	:	3.376162
S8	-C10	:	3.442082	C9	-C11	:	2.650739
C9	-C20	:	2.642644	C10	-H29	:	2.063601
C10	-H30	:	2.064503	C10	-H31	:	2.064574
C11	-C12	:	2.626739	C11	-H32	:	2.053610
C12	-C13	:	2.653750	C12	-H33	:	2.054751
C13	-C14	:	2.851725	C13	-C21	:	2.645650
C14	-Si15	:	3.623357	C14	-H34	:	2.073655
C14	-H35	:	2.073723	Si15	-C16	:	3.572265
Si15	-C17	:	3.572232	Si15	-C18	:	3.623294
C16	-H36	:	2.071232	C16	-H37	:	2.068862
C16	-H38	:	2.068855	C17	-H39	:	2.068888
C17	-H40	:	2.071230	C17	-H41	:	2.068838
C18	-C19	:	2.851696	C18	-H42	:	2.073798
C18	-H43	:	2.073620	C20	-C21	:	2.638040
C20	-H44	:	2.049045	C21	-H45	:	2.055022

bond angles:

S3	-C1	-C2	:	116.685975	C5	-C1	-C2	:	118.491789
C5	-C1	-S3	:	124.819764	C7	-C2	-C1	:	120.595811
H22	-C2	-C1	:	119.788449	H22	-C2	-C7	:	119.615670
C4	-S3	-C1	:	103.515944	H23	-C4	-S3	:	105.612974
H24	-C4	-S3	:	111.409916	H24	-C4	-H23	:	108.923744
H25	-C4	-S3	:	111.768186	H25	-C4	-H23	:	108.792697
H25	-C4	-H24	:	110.168602	C6	-C5	-C1	:	120.314496
H26	-C5	-C1	:	120.836331	H26	-C5	-C6	:	118.848433
C19	-C6	-C5	:	121.832399	H27	-C6	-C5	:	118.762897
H27	-C6	-C19	:	119.404520	C19	-C7	-C2	:	121.622169
H28	-C7	-C2	:	118.988819	H28	-C7	-C19	:	119.388956
C10	-S8	-C9	:	103.492527	C11	-C9	-S8	:	116.719493
C20	-C9	-S8	:	124.782597	C20	-C9	-C11	:	118.493840
H29	-C10	-S8	:	105.623069	H30	-C10	-S8	:	111.361085

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 H30      -C10      -H29      : 108.945372  H31      -C10      -S8       :
111.804217
 H31      -C10      -H29      : 108.773471  H31      -C10      -H30      :
110.169648
 C12      -C11      -C9       : 120.595022  H32      -C11      -C9       :
119.786962
 H32      -C11      -C12      : 119.618016  C13      -C12      -C11      :
121.621972
 H33      -C12      -C11      : 118.988671  H33      -C12      -C13      :
119.389061
 C14      -C13      -C12      : 121.227215  C21      -C13      -C12      :
117.131194
 C21      -C13      -C14      : 121.641592  Si15     -C14      -C13      :
113.889915
 H34      -C14      -C13      : 110.289481  H34      -C14      -Si15     :
107.895341
 H35      -C14      -C13      : 110.320209  H35      -C14      -Si15     :
107.752091
 H35      -C14      -H34      : 106.376510  C16      -Si15     -C14      :
110.074110
 C17      -Si15     -C14      : 109.899190  C17      -Si15     -C16      :
109.981048
 C18      -Si15     -C14      : 106.905292  C18      -Si15     -C16      :
109.876459
 C18      -Si15     -C17      : 110.057133  H36      -C16      -Si15     :
111.746438
 H37      -C16      -Si15     : 110.781061  H37      -C16      -H36      :
107.627558
 H38      -C16      -Si15     : 110.949517  H38      -C16      -H36      :
107.638065
 H38      -C16      -H37      : 107.930537  H39      -C17      -Si15     :
110.935110
 H40      -C17      -Si15     : 111.741146  H40      -C17      -H39      :
107.634964
 H41      -C17      -Si15     : 110.803791  H41      -C17      -H39      :
107.928800
 H41      -C17      -H40      : 107.629217  C19      -C18      -Si15     :
113.873776
 H42      -C18      -Si15     : 107.755451  H42      -C18      -C19      :
110.323162
 H43      -C18      -Si15     : 107.906721  H43      -C18      -C19      :
110.291117
 H43      -C18      -H42      : 106.374343  C7       -C19      -C6       :
117.130785
 C18      -C19      -C6       : 121.653564  C18      -C19      -C7       :
121.215651
 C21      -C20      -C9       : 120.313659  H44      -C20      -C9       :
120.833521
 H44      -C20      -C21      : 118.852058  C20      -C21      -C13      :
121.831521
 H45      -C21      -C13      : 119.398171  H45      -C21      -C20      :
118.770065

  torsional angles:

 C1       -C2       -C7       -C19      :   0.485279
 C1       -C2       -C7       -H28      :-179.601535
 C1       -S3       -C4       -H23      :-177.129222
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C1      -S3      -C4      -H24     : -59.012802
C1      -S3      -C4      -H25     :  64.722056
C1      -C5      -C6      -C19     :  -0.223109
C1      -C5      -C6      -H27     : 179.619835
C2      -C1      -S3      -C4      : 174.915755
C2      -C1      -C5      -C6      :  -0.558178
C2      -C1      -C5      -H26     : 179.125084
C2      -C7      -C19     -C6      :  -1.228356
C2      -C7      -C19     -C18     : 178.771689
S3      -C1      -C2      -C7      : 179.885765
S3      -C1      -C2      -H22     :  -0.017155
S3      -C1      -C5      -C6      :-179.965905
S3      -C1      -C5      -H26     :  -0.282643
C4      -S3      -C1      -C5      :  -5.666843
C5      -C1      -C2      -C7      :   0.429958
C5      -C1      -C2      -H22     :-179.472961
C5      -C6      -C19     -C7      :   1.098772
C5      -C6      -C19     -C18     :-178.901272
C6      -C19     -C7      -H28     : 178.858798
C6      -C19     -C18     -Si15    :  90.000022
C6      -C19     -C18     -H42     : -31.302028
C6      -C19     -C18     -H43     :-148.525079
C7      -C19     -C6      -H27     :-178.743190
C7      -C19     -C18     -Si15    : -90.000025
C7      -C19     -C18     -H42     : 148.697925
C7      -C19     -C18     -H43     :  31.474875
S8      -C9      -C11     -C12     : 179.723966
S8      -C9      -C11     -H32     :  -0.278802
S8      -C9      -C20     -C21     :-179.843805
S8      -C9      -C20     -H44     :  -0.165121
C9      -S8      -C10     -H29     :-176.547339
C9      -S8      -C10     -H30     : -58.424760
C9      -S8      -C10     -H31     :  65.301809
C9      -C11     -C12     -C13     :   0.527003
C9      -C11     -C12     -H33     :-179.672256
C9      -C20     -C21     -C13     :  -0.156675
C9      -C20     -C21     -H45     : 179.662734
C10     -S8      -C9      -C11     : 173.976385
C10     -S8      -C9      -C20     :  -6.771021
C11     -C9      -C20     -C21     :  -0.603415
C11     -C9      -C20     -H44     : 179.075268
C11     -C12     -C13     -C14     : 178.749962
C11     -C12     -C13     -C21     :  -1.250054
C12     -C11     -C9      -C20     :   0.422431
C12     -C13     -C14     -Si15    : -90.000001
C12     -C13     -C14     -H34     :  31.470245
C12     -C13     -C14     -H35     : 148.693171
C12     -C13     -C21     -C20     :   1.066594
C12     -C13     -C21     -H45     :-178.751711
C13     -C12     -C11     -H32     :-179.470235
C13     -C14     -Si15    -C16     :  60.698996
C13     -C14     -Si15    -C17     : -60.579103
C13     -C14     -Si15    -C18     : 179.999994
C13     -C21     -C20     -H44     :-179.841672
C14     -C13     -C12     -H33     :  -1.050000
C14     -C13     -C21     -C20     :-178.933423
C14     -C13     -C21     -H45     :   1.248273
C14     -Si15    -C16     -H36     :  58.968018
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C14     -Si15    -C16     -H37     : 178.973968
C14     -Si15    -C16     -H38     : -61.166083
C14     -Si15    -C17     -H39     :-178.595756
C14     -Si15    -C17     -H40     : -58.479001
C14     -Si15    -C17     -H41     :  61.540965
C14     -Si15    -C18     -C19     :-179.999995
C14     -Si15    -C18     -H42     : -57.280315
C14     -Si15    -C18     -H43     :  57.210463
Si15    -C14     -C13     -C21     :  90.000016
C16     -Si15    -C14     -H34     : -62.090891
C16     -Si15    -C14     -H35     :-176.576829
C16     -Si15    -C17     -H39     :  60.070365
C16     -Si15    -C17     -H40     :-179.812880
C16     -Si15    -C17     -H41     : -59.792914
C16     -Si15    -C18     -C19     : -60.571313
C16     -Si15    -C18     -H42     :  62.148367
C16     -Si15    -C18     -H43     : 176.639145
C17     -Si15    -C14     -H34     : 176.631010
C17     -Si15    -C14     -H35     :  62.145072
C17     -Si15    -C16     -H36     :-179.802815
C17     -Si15    -C16     -H37     : -59.796865
C17     -Si15    -C16     -H38     :  60.063084
C17     -Si15    -C18     -C19     :  60.681129
C17     -Si15    -C18     -H42     :-176.599190
C17     -Si15    -C18     -H43     : -62.108412
C18     -Si15    -C14     -H34     :  57.210107
C18     -Si15    -C14     -H35     : -57.275831
C18     -Si15    -C16     -H36     : -58.504734
C18     -Si15    -C16     -H37     :  61.501215
C18     -Si15    -C16     -H38     :-178.638835
C18     -Si15    -C17     -H39     : -61.119516
C18     -Si15    -C17     -H40     :  58.997238
C18     -Si15    -C17     -H41     : 179.017205
C18     -C19     -C6      -H27     :   1.256765
C18     -C19     -C7      -H28     :  -1.141158
C19     -C6      -C5      -H26     :-179.912614
C19     -C7      -C2      -H22     :-179.611634
C20     -C9      -C11     -H32     :-179.580336
C21     -C13     -C12     -H33     : 178.949984
C21     -C13     -C14     -H34     :-148.529738
C21     -C13     -C14     -H35     : -31.306812
H22     -C2      -C7      -H28     :   0.301552
H26     -C5      -C6      -H27     :  -0.069670
H32     -C11     -C12     -H33     :   0.330506
H44     -C20     -C21     -H45     :  -0.022263

 nuclear repulsion energy.......    1882.293380580 hartrees
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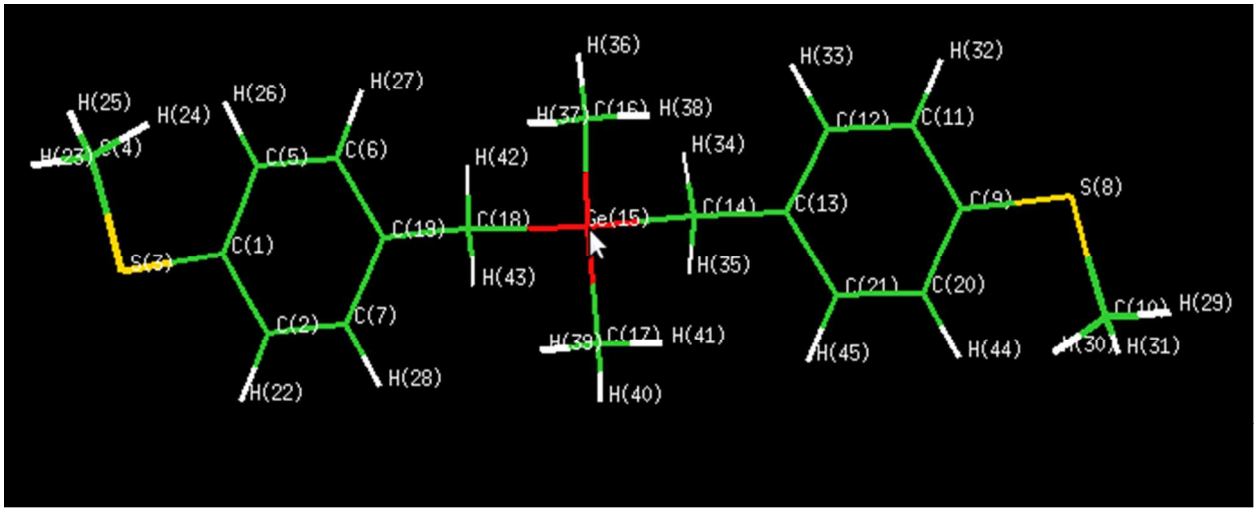
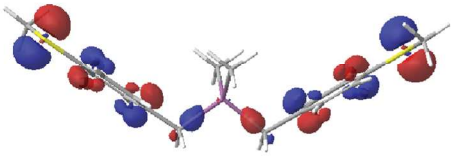
CGeC



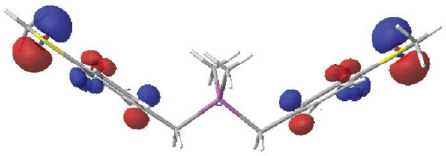
Final energy (B3LYP/cc-pVTZ): -3574.18874215465 hartrees

HOMO



-5.46 eV

HOMO-1



-5.68 eV

HOMO & HOMO–1 energies and surfaces (B3LYP/cc-pVTZ).

Optimized geometry:

Subjected to the constraints that ω(C(Ar)-α-β-α) = 180˚ and that the α-β σ-bond is orthogonal to the phenyl ring σ-plane. Optimized with LACVP** basis set.

atom	x	y	z
C1	16.3164263762	2.1176611107	-2.5556618320
C2	14.3936187057	1.7214157779	-4.3389812583
S3	19.1015066290	3.6796236880	-3.6482372268
C4	20.9655835013	4.0871431268	-0.7842722467
C5	15.9416313247	1.2574615581	-0.0840058852
C6	13.6906179105	0.0512663800	0.5798662409
C7	12.1634924344	0.5131740265	-3.6542427764
S8	-4.9540171922	5.5812116239	5.7384991984
C9	-2.5432085368	3.6387281249	4.3947300687
C10	-6.6294975075	6.7948806687	2.9882730543
C11	-0.7751694359	2.5979293362	6.0754165795
C12	1.1601104270	1.0550246470	5.1942278388
C13	1.4312010883	0.5006508115	2.6115467027
C14	3.5646149560	-1.1296518214	1.6680480224
Ge	6.6697637917	0.8577221217	0.7755719476
C16	7.9313695192	2.6627356040	3.7903521903
C17	5.8638711885	3.2978782237	-1.9325624368
C18	9.3002172043	-1.5917106459	-0.4361790253

C19	11.7433949784	-0.3309723027	-1.1717983831
C20	-2.3205969096	3.0758864267	1.8210969413
C21	-0.3645281695	1.5281591563	0.9604249571
H22	14.6489528305	2.3606477651	-6.2745445802
H23	22.6503612691	5.1309125650	-1.3606500531
H24	19.9434948910	5.1926404689	0.6291484085
H25	21.5473186813	2.2742513764	0.0152368617
H26	17.3905070214	1.5022642392	1.3448198174
H27	13.4533911414	-0.6074826985	2.5126951291
H28	10.7097280161	0.2226305245	-5.0780266897
H29	-8.0621423465	8.0811416530	3.7320654777
H30	-5.3653708853	7.8487809286	1.7409857817
H31	-7.5709061506	5.2869812662	1.9375002912
H32	-0.9191117646	2.9980240411	8.0852366895
H33	2.4977662927	0.2667990932	6.5412000543
H34	4.1058060620	-2.5289732299	3.0956113880
H35	2.9930559512	-2.1826506819	-0.0213331182
H36	8.3927159170	1.3445136818	5.3166972095
H37	9.6400523225	3.7315892667	3.3309370926
H38	6.5063667326	3.9836900701	4.4954562507
H39	7.5470143432	4.3727657820	-2.4658355904
H40	5.1558645087	2.3374287002	-3.6226654528
H41	4.4143851102	4.6286063534	-1.2991583650
H42	9.6114910019	-2.9691433568	1.0788843290
H43	8.4986142793	-2.6300509009	-2.0387499272
H44	-3.6633550358	3.8194690904	0.4628827451
H45	-0.2416147132	1.1134058459	-1.0492836590

angstroms

atom	x	y	z
C1	8.6342810000	1.1206180000	-1.3523980000
C2	7.6167750000	0.9109340000	-2.2960900000
S3	10.1080820000	1.9471730000	-1.9305640000
C4	11.0945090000	2.1628230000	-0.4150190000
C5	8.4359480000	0.6654200000	-0.0444540000
C6	7.2447630000	0.0271290000	0.3068520000
C7	6.4366430000	0.2715600000	-1.9337420000
S8	-2.6215530000	2.9534500000	3.0366830000
C9	-1.3458080000	1.9255320000	2.3255910000
C10	-3.5081790000	3.5956960000	1.5813260000
C11	-0.4102020000	1.3747650000	3.2149720000
C12	0.6139040000	0.5582950000	2.7486670000
C13	0.7573590000	0.2649330000	1.3819710000
C14	1.8863130000	-0.5977860000	0.8826930000
Ge	3.5294870000	0.4538870000	0.4104150000
C16	4.1971000000	1.4090590000	2.0057680000
C17	3.1030270000	1.7451620000	-1.0226680000
C18	4.9214630000	-0.8422970000	-0.2308160000
C19	6.2143370000	-0.1751430000	-0.6200890000
C20	-1.2280070000	1.6276890000	0.9636830000
C21	-0.1929000000	0.8086670000	0.5082350000
H22	7.7518920000	1.2492010000	-3.3203460000
H23	11.9860550000	2.7151620000	-0.7200250000
H24	10.5536430000	2.7478270000	0.3329310000
H25	11.4023500000	1.2034820000	0.0080630000
H26	9.2026600000	0.7949640000	0.7116480000
H27	7.1192280000	-0.3214660000	1.3296610000
H28	5.6673440000	0.1178110000	-2.6871760000

H29	-4.2663020000	4.2763560000	1.9749240000
H30	-2.8392320000	4.1533960000	0.9212900000
H31	-4.0063510000	2.7977500000	1.0252810000
H32	-0.4863730000	1.5864860000	4.2785230000
H33	1.3217610000	0.1411840000	3.4614540000
H34	2.1726990000	-1.3382750000	1.6381270000
H35	1.5838570000	-1.1550090000	-0.0112890000
H36	4.4412340000	0.7114860000	2.8134750000
H37	5.1012960000	1.9746720000	1.7626560000
H38	3.4430210000	2.1080780000	2.3788930000
H39	3.9937080000	2.3139680000	-1.3048640000
H40	2.7283660000	1.2369140000	-1.9170320000
H41	2.3359920000	2.4493530000	-0.6874850000
H42	5.0861820000	-1.5712030000	0.5709210000
H43	4.4972730000	-1.3917630000	-1.0788600000
H44	-1.9385640000	2.0211760000	0.2449470000
H45	-0.1278570000	0.5891890000	-0.5552570000

principal moments of inertia:

amu*angstrom^2:	764.38145	7717.42089	7806.73707
g*cm^2:	1.26928511E-37	1.28150773E-36	1.29633903E-36

rotational constants:

cm^(-1):		0.02205395	0.00218436
	0.00215937		
GHz:		0.66116074	0.06548548
	0.06473627		

Molecular weight: 378.05 amu

Stoichiometry: GeC18H24S2
Molecular Point Group: C1
Point Group used: C1

bond lengths (angstroms):

C1	-C2	:	1.403510	C1	-S3	:	1.785934
C1	-C5	:	1.399021	C2	-C7	:	1.390254
C2	-H22	:	1.087098	S3	-C4	:	1.821104
C4	-H23	:	1.092228	C4	-H24	:	1.092792
C4	-H25	:	1.092749	C5	-C6	:	1.396336
C5	-H26	:	1.084582	C6	-C19	:	1.400682
C6	-H27	:	1.087849	C7	-C19	:	1.405222
C7	-H28	:	1.087714	S8	-C9	:	1.785999
S8	-C10	:	1.821167	C9	-C11	:	1.403461
C9	-C20	:	1.399064	C10	-H29	:	1.092231
C10	-H30	:	1.092779	C10	-H31	:	1.092739
C11	-C12	:	1.390272	C11	-H32	:	1.087092
C12	-C13	:	1.405169	C12	-H33	:	1.087708
C13	-C14	:	1.506021	C13	-C21	:	1.400733
C14	-Ge	:	2.007258	C14	-H34	:	1.095911
C14	-H35	:	1.095984	Ge	-C16	:	1.975655
Ge	-C17	:	1.975598	Ge	-C18	:	2.007204
C16	-H36	:	1.094806	C16	-H37	:	1.093888
C16	-H38	:	1.093840	C17	-H39	:	1.093841
C17	-H40	:	1.094794	C17	-H41	:	1.093881
C18	-C19	:	1.506038	C18	-H42	:	1.096001

C18	-H43	:	1.095915	C20	-C21	:	1.396308
C20	-H44	:	1.084576	C21	-H45	:	1.087849

bond lengths (bohr):

C1	-C2	:	2.652250	C1	-S3	:	3.374925
C1	-C5	:	2.643766	C2	-C7	:	2.627200
C2	-H22	:	2.054317	S3	-C4	:	3.441388
C4	-H23	:	2.064011	C4	-H24	:	2.065078
C4	-H25	:	2.064996	C5	-C6	:	2.638692
C5	-H26	:	2.049564	C6	-C19	:	2.646906
C6	-H27	:	2.055737	C7	-C19	:	2.655484
C7	-H28	:	2.055482	S8	-C9	:	3.375049
S8	-C10	:	3.441507	C9	-C11	:	2.652156
C9	-C20	:	2.643848	C10	-H29	:	2.064017
C10	-H30	:	2.065054	C10	-H31	:	2.064978
C11	-C12	:	2.627234	C11	-H32	:	2.054306
C12	-C13	:	2.655384	C12	-H33	:	2.055470
C13	-C14	:	2.845968	C13	-C21	:	2.647002
C14	-Ge	:	3.793167	C14	-H34	:	2.070972
C14	-H35	:	2.071110	Ge	-C16	:	3.733446
Ge	-C17	:	3.733339	Ge	-C18	:	3.793066
C16	-H36	:	2.068883	C16	-H37	:	2.067150
C16	-H38	:	2.067057	C17	-H39	:	2.067059
C17	-H40	:	2.068861	C17	-H41	:	2.067135
C18	-C19	:	2.846000	C18	-H42	:	2.071142
C18	-H43	:	2.070978	C20	-C21	:	2.638640
C20	-H44	:	2.049551	C21	-H45	:	2.055738

bond angles:

S3	-C1	-C2	:	116.726973	C5	-C1	-C2	:	118.504100
C5	-C1	-S3	:	124.766425	C7	-C2	-C1	:	120.588169
H22	-C2	-C1	:	119.796163	H22	-C2	-C7	:	119.615564
C4	-S3	-C1	:	103.437617	H23	-C4	-S3	:	105.642141
H24	-C4	-S3	:	111.401426	H24	-C4	-H23	:	108.930190
H25	-C4	-S3	:	111.767608	H25	-C4	-H23	:	108.791669
H25	-C4	-H24	:	110.145713	C6	-C5	-C1	:	120.323538
H26	-C5	-C1	:	120.842066	H26	-C5	-C6	:	118.833329
C19	-C6	-C5	:	121.809112	H27	-C6	-C5	:	118.781682
H27	-C6	-C19	:	119.409180	C19	-C7	-C2	:	121.610104
H28	-C7	-C2	:	119.001878	H28	-C7	-C19	:	119.387716
C10	-S8	-C9	:	103.447237	C11	-C9	-S8	:	116.726937
C20	-C9	-S8	:	124.767235	C20	-C9	-C11	:	118.502703

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 H29      -C10      -S8       : 105.647239  H30      -C10      -S8       :
111.384822
 H30      -C10      -H29      : 108.936113  H31      -C10      -S8       :
111.781830
 H31      -C10      -H29      : 108.783815  H31      -C10      -H30      :
110.145146
 C12      -C11      -C9       : 120.596044  H32      -C11      -C9       :
119.791287
 H32      -C11      -C12      : 119.612620  C13      -C12      -C11      :
121.603105
 H33      -C12      -C11      : 118.998662  H33      -C12      -C13      :
119.397822
 C14      -C13      -C12      : 121.236362  C21      -C13      -C12      :
117.154543
 C21      -C13      -C14      : 121.609095  Ge       -C14      -C13      :
113.049387
 H34      -C14      -C13      : 110.758681  H34      -C14      -Ge       :
107.594508
 H35      -C14      -C13      : 110.780796  H35      -C14      -Ge       :
107.479978
 H35      -C14      -H34      : 106.909140  C16      -Ge       -C14      :
109.873224
 C17      -Ge       -C14      : 109.658601  C17      -Ge       -C16      :
110.041486
 C18      -Ge       -C14      : 107.729778  C18      -Ge       -C16      :
109.623313
 C18      -Ge       -C17      : 109.879479  H36      -C16      -Ge       :
111.287639
 H37      -C16      -Ge       : 110.477698  H37      -C16      -H36      :
108.004892
 H38      -C16      -Ge       : 110.576475  H38      -C16      -H36      :
108.013914
 H38      -C16      -H37      : 108.374060  H39      -C17      -Ge       :
110.564016
 H40      -C17      -Ge       : 111.286403  H40      -C17      -H39      :
108.017851
 H41      -C17      -Ge       : 110.478682  H41      -C17      -H39      :
108.376725
 H41      -C17      -H40      : 108.011591  C19      -C18      -Ge       :
113.069160
 H42      -C18      -Ge       : 107.457965  H42      -C18      -C19      :
110.773256
 H43      -C18      -Ge       : 107.611165  H43      -C18      -C19      :
110.754771
 H43      -C18      -H42      : 106.905089  C7       -C19      -C6       :
117.152934
 C18      -C19      -C6       : 121.631448  C18      -C19      -C7       :
121.215618
 C21      -C20      -C9       : 120.318604  H44      -C20      -C9       :
120.843144
 H44      -C20      -C21      : 118.837198  C20      -C21      -C13      :
121.812387
 H45      -C21      -C13      : 119.401434  H45      -C21      -C20      :
118.786151

  torsional angles:

 C1       -C2       -C7       -C19      :    0.524259
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C1      -C2      -C7      -H28     :-179.677015
C1      -S3      -C4      -H23     :-177.088530
C1      -S3      -C4      -H24     : -58.951545
C1      -S3      -C4      -H25     :  64.746713
C1      -C5      -C6      -C19     :  -0.261434
C1      -C5      -C6      -H27     : 179.679812
C2      -C1      -S3      -C4      : 175.022784
C2      -C1      -C5      -C6      :  -0.483643
C2      -C1      -C5      -H26     : 179.136230
C2      -C7      -C19     -C6      :  -1.229599
C2      -C7      -C19     -C18     : 178.770453
S3      -C1      -C2      -C7      : 179.806876
S3      -C1      -C2      -H22     :  -0.075824
S3      -C1      -C5      -C6      :-179.887930
S3      -C1      -C5      -H26     :  -0.268056
C4      -S3      -C1      -C5      :  -5.563340
C5      -C1      -C2      -C7      :   0.354782
C5      -C1      -C2      -H22     :-179.527918
C5      -C6      -C19     -C7      :   1.099564
C5      -C6      -C19     -C18     :-178.900489
C6      -C19     -C7      -H28     : 178.972434
C6      -C19     -C18     -Ge      :  90.000033
C6      -C19     -C18     -H42     : -30.684504
C6      -C19     -C18     -H43     :-149.131126
C7      -C19     -C6      -H27     :-178.841323
C7      -C19     -C18     -Ge      : -90.000022
C7      -C19     -C18     -H42     : 149.315441
C7      -C19     -C18     -H43     :  30.868820
S8      -C9      -C11     -C12     : 179.755450
S8      -C9      -C11     -H32     :  -0.164399
S8      -C9      -C20     -C21     :-179.846112
S8      -C9      -C20     -H44     :  -0.223890
C9      -S8      -C10     -H29     :-176.962659
C9      -S8      -C10     -H30     : -58.824312
C9      -S8      -C10     -H31     :  64.871382
C9      -C11     -C12     -C13     :   0.540474
C9      -C11     -C12     -H33     :-179.694045
C9      -C20     -C21     -C13     :  -0.246396
C9      -C20     -C21     -H45     : 179.692357
C10     -S8      -C9      -C11     : 174.569870
C10     -S8      -C9      -C20     :  -6.085042
C11     -C9      -C20     -C21     :  -0.511729
C11     -C9      -C20     -H44     : 179.110493
C11     -C12     -C13     -C14     : 178.741436
C11     -C12     -C13     -C21     :  -1.258561
C12     -C11     -C9      -C20     :   0.367643
C12     -C13     -C14     -Ge      : -90.000003
C12     -C13     -C14     -H34     :  30.836410
C12     -C13     -C14     -H35     : 149.295364
C12     -C13     -C21     -C20     :   1.113073
C12     -C13     -C21     -H45     :-178.825314
C13     -C12     -C11     -H32     :-179.539536
C13     -C14     -Ge      -C16     :  60.628250
C13     -C14     -Ge      -C17     : -60.441751
C13     -C14     -Ge      -C18     : 179.999981
C13     -C21     -C20     -H44     :-179.876130
C14     -C13     -C12     -H33     :  -1.023130
C14     -C13     -C21     -C20     :-178.886925
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C14     -C13     -C21     -H45     :   1.174689
C14     -Ge      -C16     -H36     :  59.230823
C14     -Ge      -C16     -H37     : 179.205351
C14     -Ge      -C16     -H38     : -60.820872
C14     -Ge      -C17     -H39     :-178.943205
C14     -Ge      -C17     -H40     : -58.895681
C14     -Ge      -C17     -H41     :  61.087118
C14     -Ge      -C18     -C19     : 179.999977
C14     -Ge      -C18     -H42     : -57.448711
C14     -Ge      -C18     -H43     :  57.363656
Ge      -C14     -C13     -C21     :  89.999994
C16     -Ge      -C14     -H34     : -61.988381
C16     -Ge      -C14     -H35     :-176.808123
C16     -Ge      -C17     -H39     :  60.088405
C16     -Ge      -C17     -H40     :-179.864070
C16     -Ge      -C17     -H41     : -59.881272
C16     -Ge      -C18     -C19     : -60.469399
C16     -Ge      -C18     -H42     :  62.081913
C16     -Ge      -C18     -H43     : 176.894280
C17     -Ge      -C14     -H34     : 176.941619
C17     -Ge      -C14     -H35     :  62.121876
C17     -Ge      -C16     -H36     :-179.929633
C17     -Ge      -C16     -H37     : -59.955105
C17     -Ge      -C16     -H38     :  60.018672
C17     -Ge      -C18     -C19     :  60.582091
C17     -Ge      -C18     -H42     :-176.866597
C17     -Ge      -C18     -H43     : -62.054229
C18     -Ge      -C14     -H34     :  57.383350
C18     -Ge      -C14     -H35     : -57.436392
C18     -Ge      -C16     -H36     : -58.976058
C18     -Ge      -C16     -H37     :  60.998470
C18     -Ge      -C16     -H38     :-179.027752
C18     -Ge      -C17     -H39     : -60.711341
C18     -Ge      -C17     -H40     :  59.336184
C18     -Ge      -C17     -H41     : 179.318982
C18     -C19     -C6      -H27     :   1.158625
C18     -C19     -C7      -H28     :  -1.027514
C19     -C6      -C5      -H26     :-179.888876
C19     -C7      -C2      -H22     :-179.592830
C20     -C9      -C11     -H32     :-179.552205
C21     -C13     -C12     -H33     : 178.976873
C21     -C13     -C14     -H34     :-149.163593
C21     -C13     -C14     -H35     : -30.704638
H22     -C2      -C7      -H28     :   0.205895
H26     -C5      -C6      -H27     :   0.052370
H32     -C11     -C12     -H33     :   0.225945
H44     -C20     -C21     -H45     :   0.062623

 nuclear repulsion energy.......    1643.375973249 hartrees
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