Single-Molecule Conductance in Atomically Precise Germanium Wires

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I. Supplemental Figures from Main Text

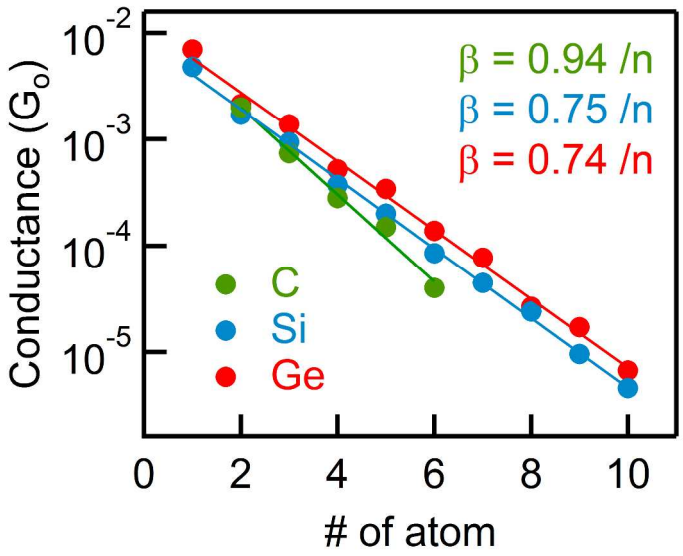


Figure S1. Conductance peak positions for measurements with **C4-C8**; **Si1-Si10**; **Ge1-10** plotted against the number (*n*) of atoms in the backbone chain between the distal methylene units. Based on how we defined the nomenclature of **C4-C8**, n=2 for **C4** and n=6 for **C8**. $\beta_C = 0.94 \pm 0.05\ n^{-1}$, $\beta_{Si} = 0.75 \pm 0.01\ n^{-1}$, $\beta_{Ge} = 0.74 \pm 0.02\ n^{-1}$.

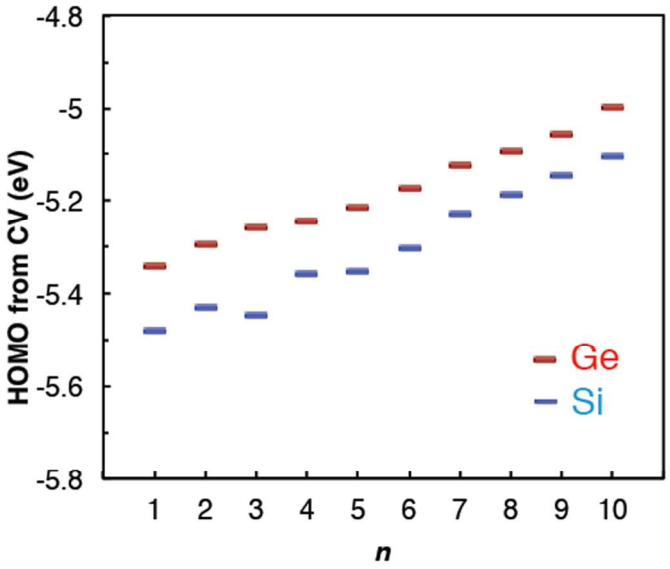


Figure S2. Cyclic voltammetry-derived HOMO levels (eV) for **Si***n*, **Ge***n* series plotted against *n*. The HOMO energies are determined from the onset of the first oxidation by CV vs. Fc^+/Fc and the equation $E_{HOMO} = -(4.80\ V + E_{onset}^{ox})$.[1] Numerical values are given in Table ST1.

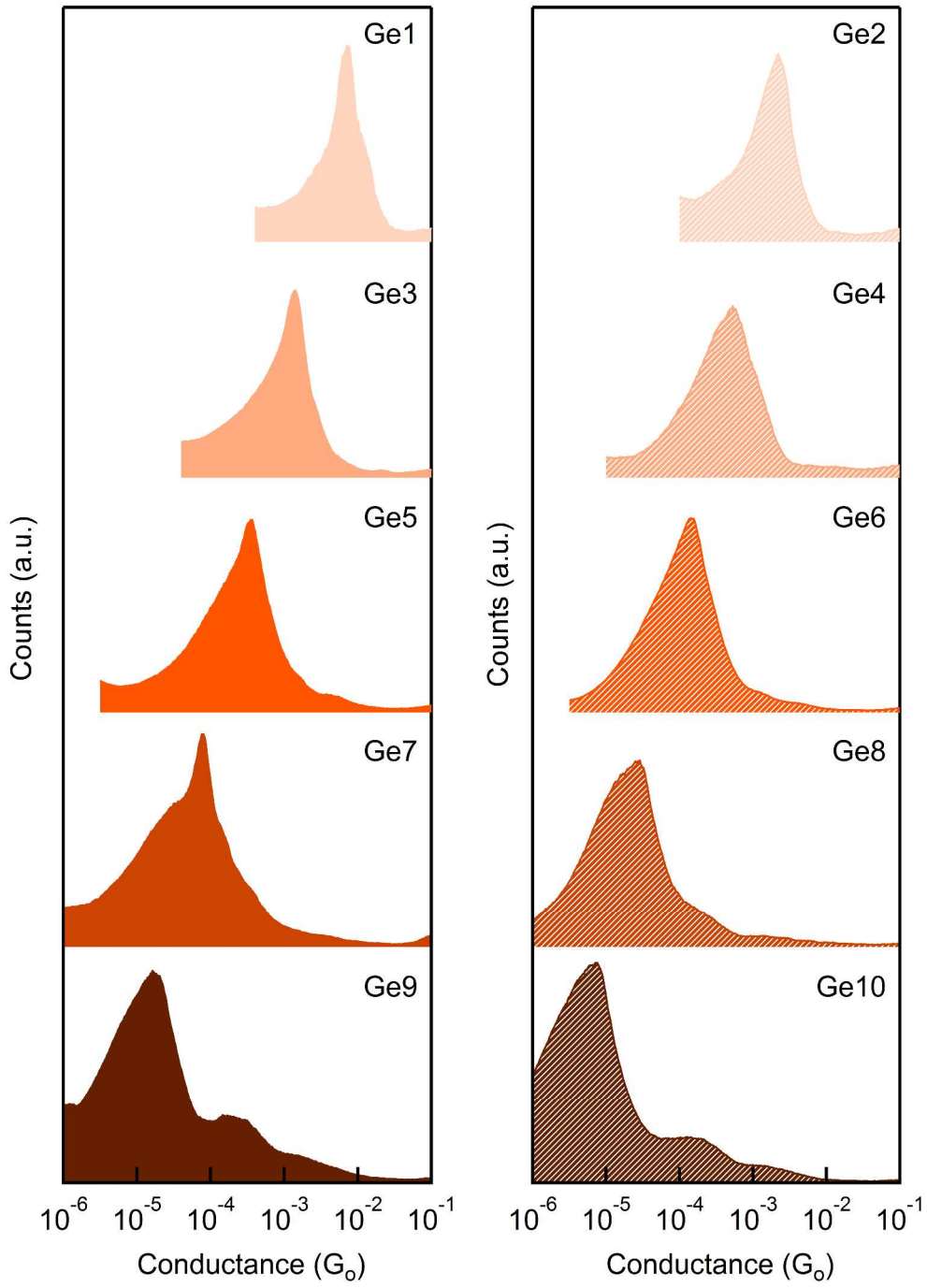
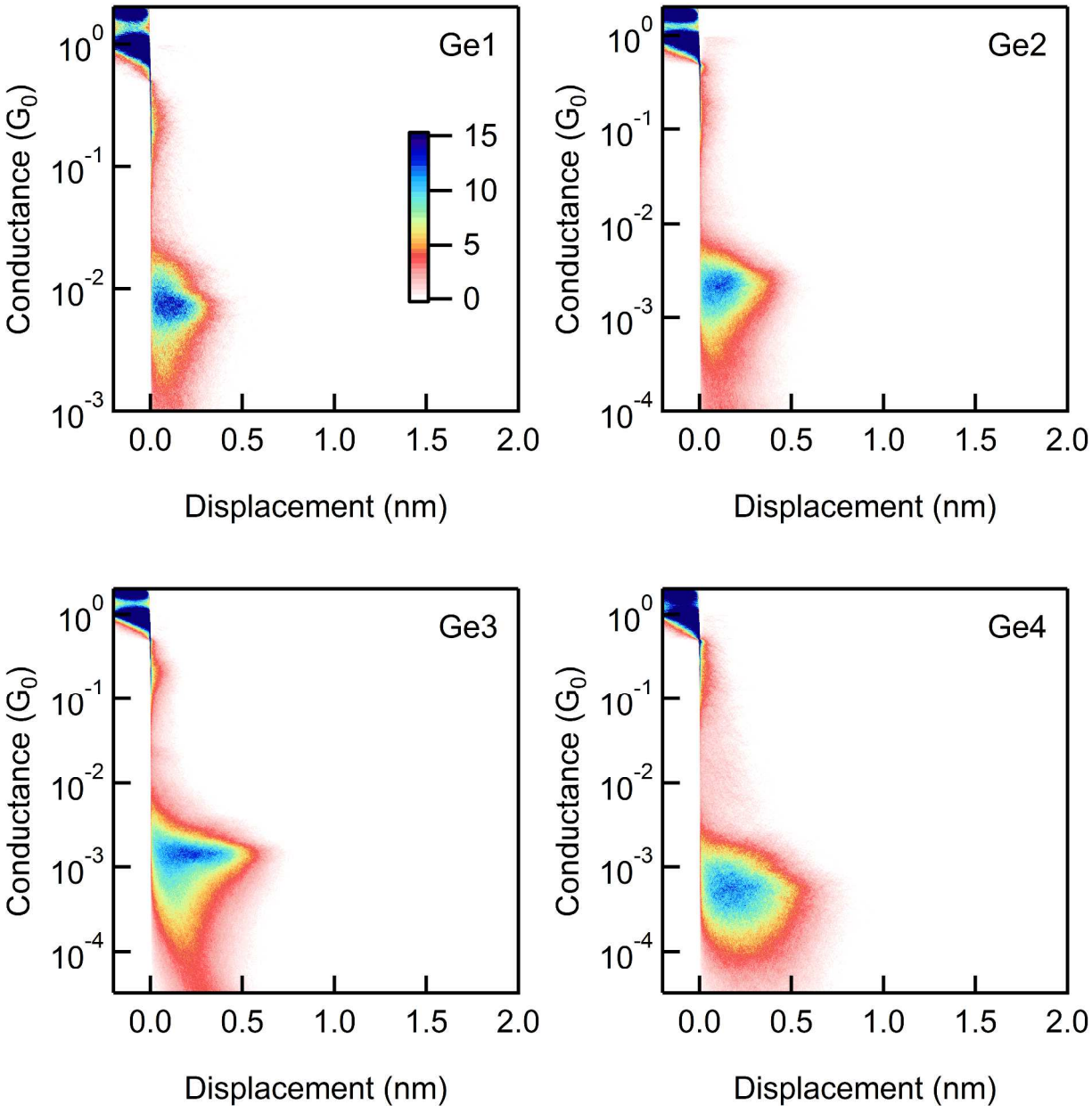
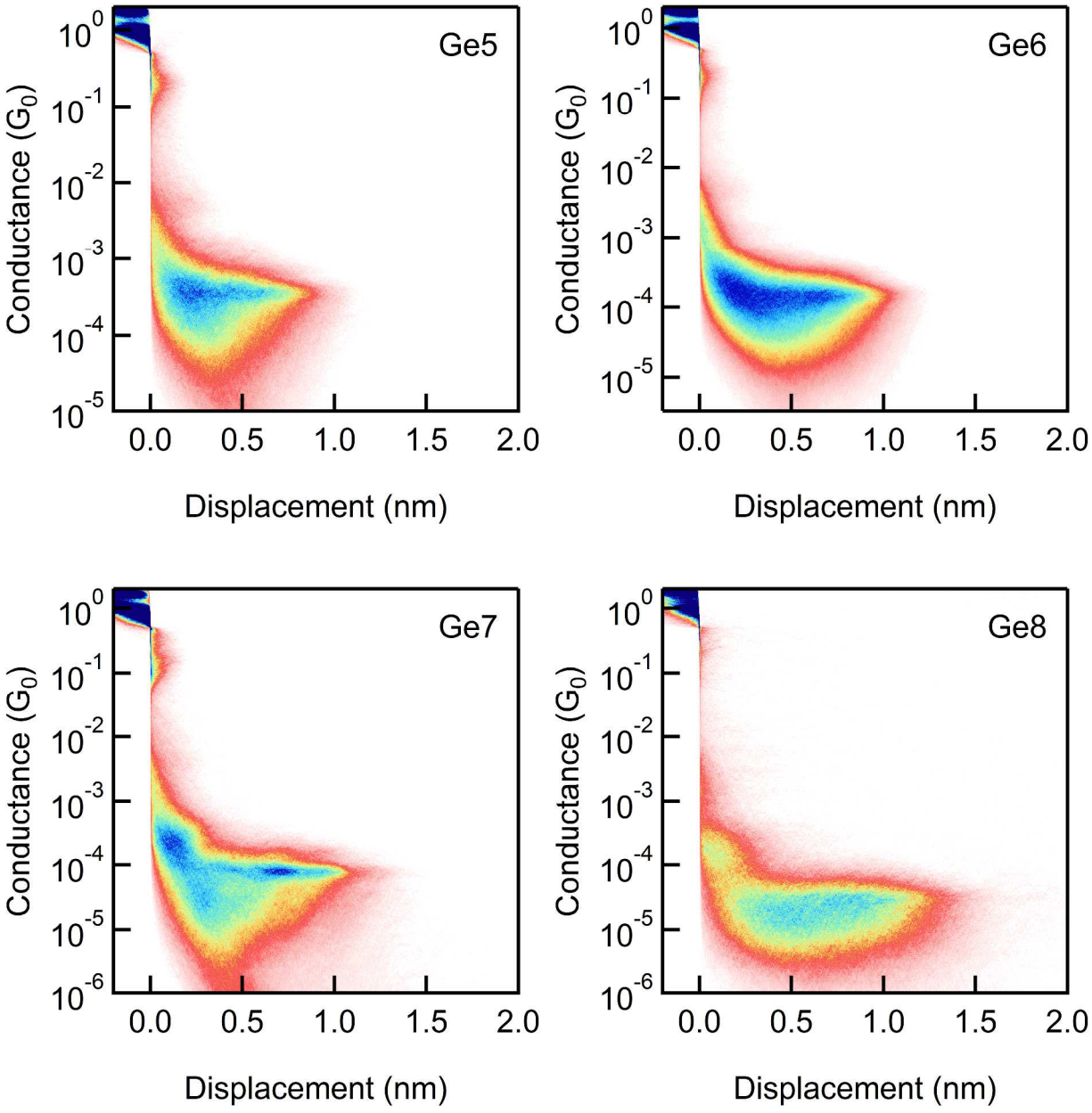


Figure S3. Log-binned 1D histograms of **Ge1-10** shown as comparison between odd (left) and even (right) series.


Ge1
Ge2
Ge3
Ge4
Conductance (G0)
Displacement (nm)
15
10
5
0


Ge5
Ge6
Ge7
Ge8
Conductance (G0)
Displacement (nm)
10^0
10^-1
10^-2
10^-3
10^-4
10^-5
10^-6
0.0
0.5
1.0
1.5
2.0

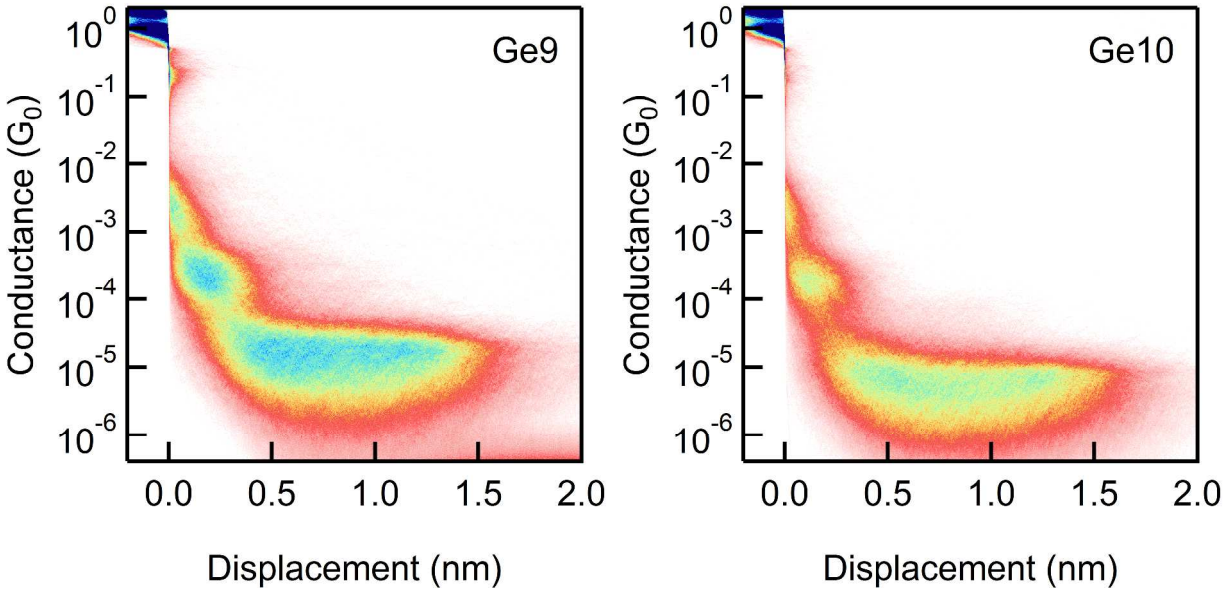
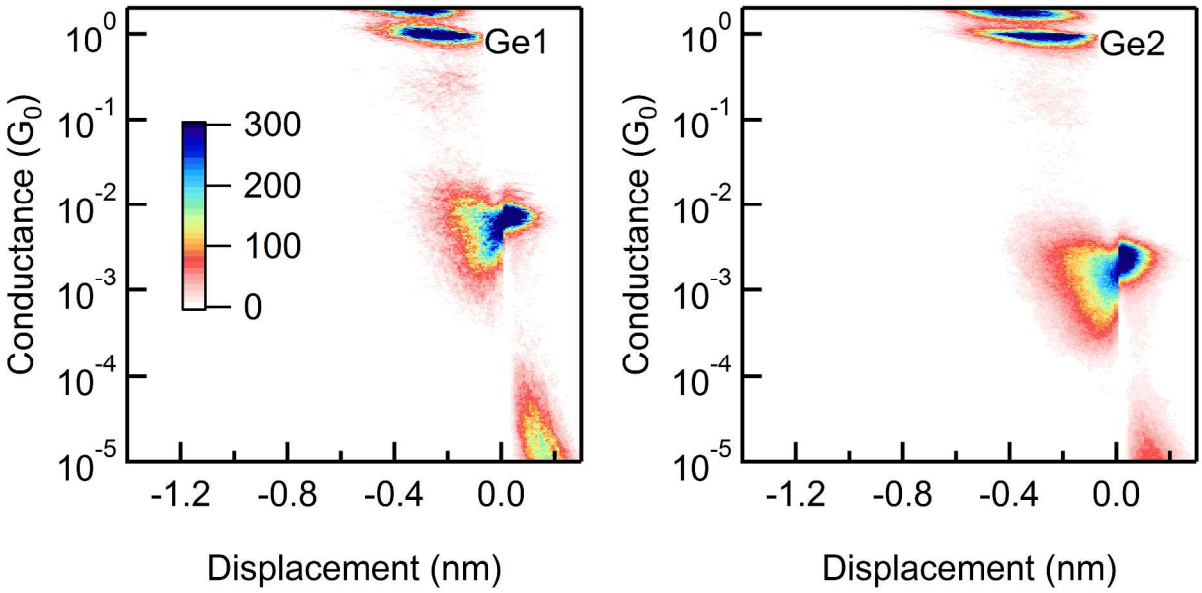
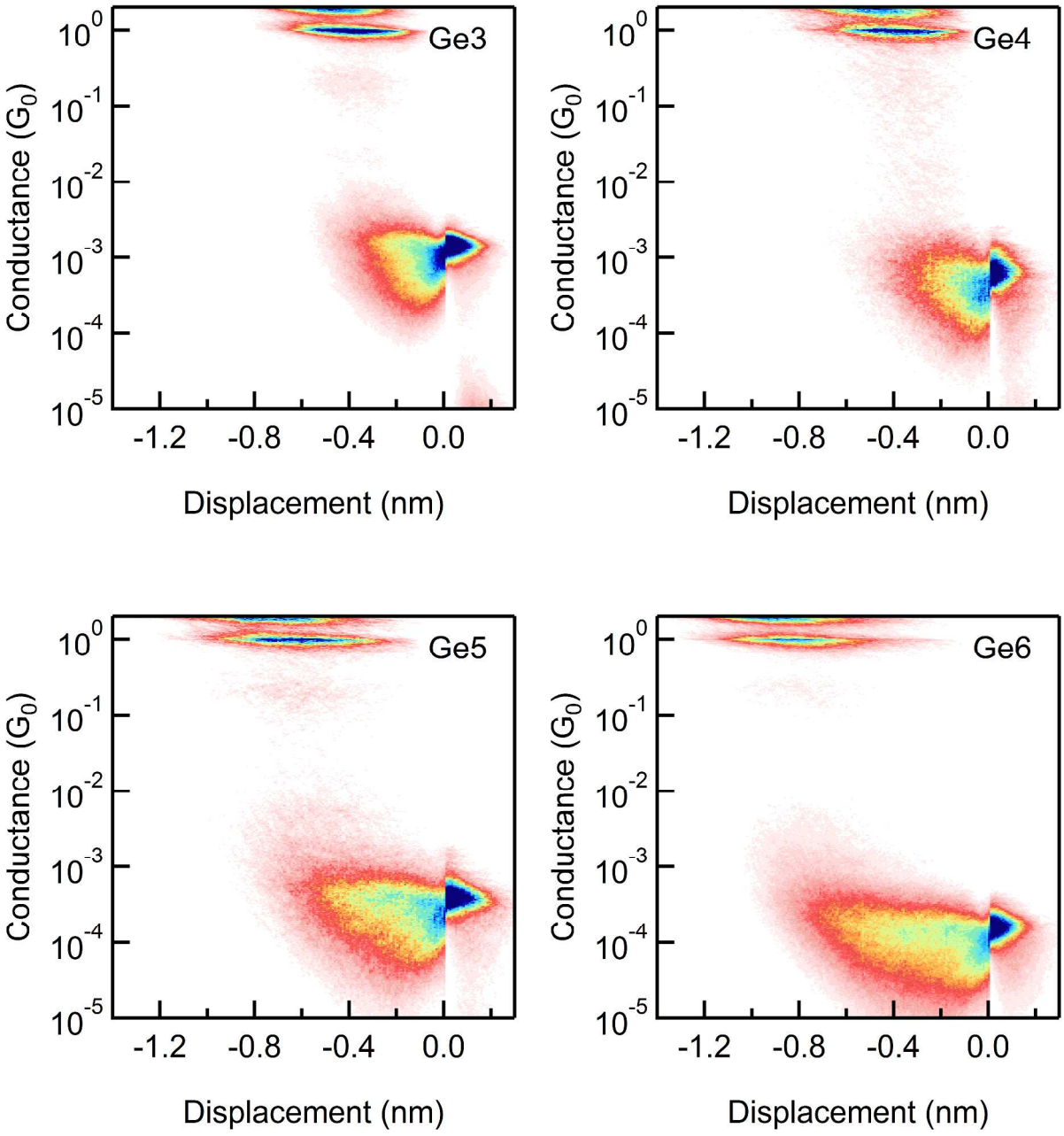


Figure S4. 2D histograms of conductance measurements for **Ge1-Ge10**. Histograms are created by aligning all traces to the displacement point where conductance crosses $0.5G_0$. The color bar indicates the number of counts per 1000 traces.




Ge3
Ge4
Ge5
Ge6
Conductance (G0)
Displacement (nm)
10^0
10^-1
10^-2
10^-3
10^-4
10^-5
-1.2
-0.8
-0.4
0.0

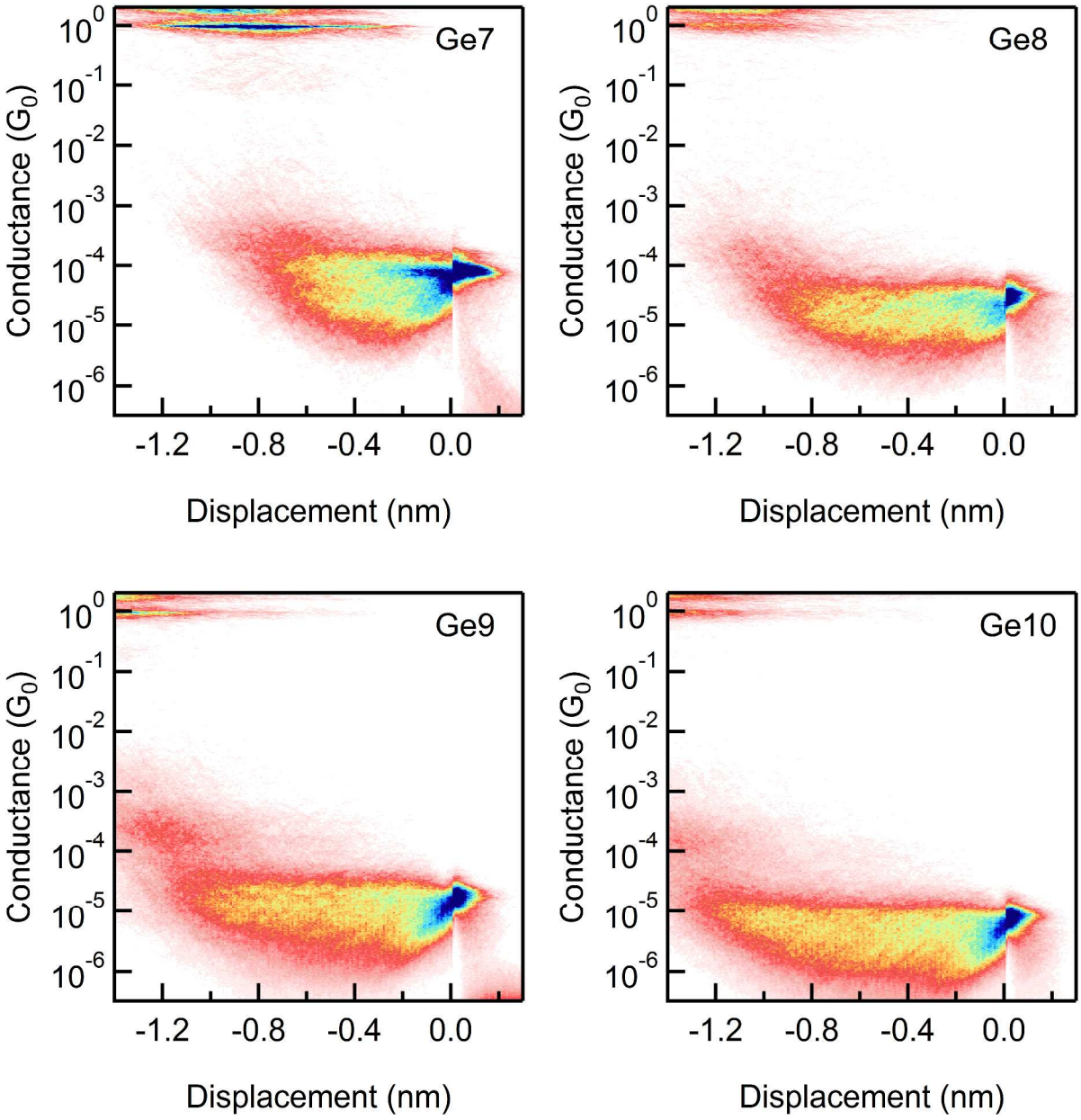


Figure S5. 2D histograms with displacement aligned to the switching event for **Ge1-10**. Histograms are made from the traces showing a low to high G switching event during the molecular junction elongation. The color bar indicates the number of counts per 1000 traces. The method for 2D histogram switching analysis is detailed in a previous publication.[2] The consistent factor of 1.6 switching ratio (see Figure S7) and ~2 Å high G displacement length indicate that the source of switching comes from a structural feature common to all germanes studied here. These results evidence that it is the terminal dihedral angles that account for switching, and not rotations to the internal Ge-Ge-Ge-Ge angles.

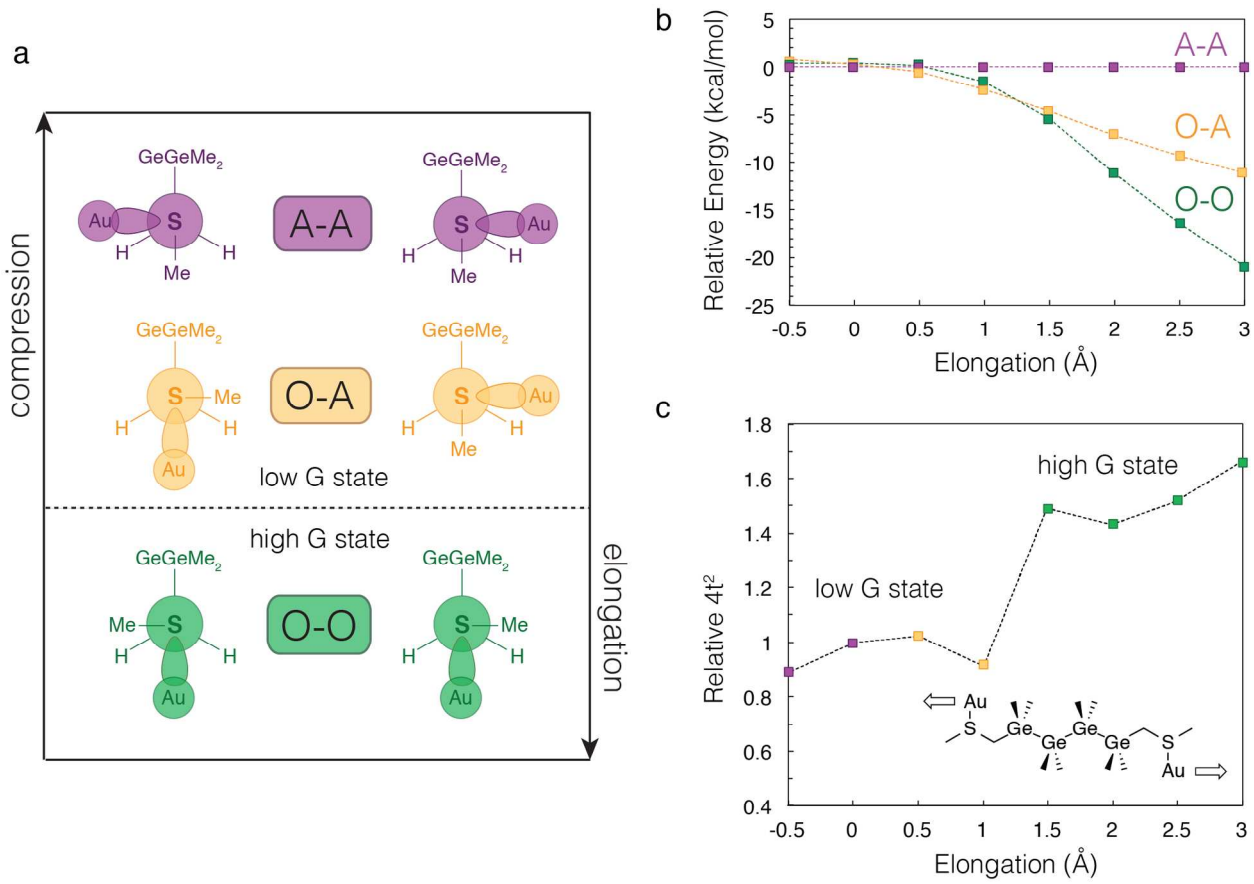


Figure S6. (a) Newman projections for the A-A (purple), O-A (yellow), and O-O (green) dihedral configurations from the perspective of the sulfur-methylene σ-bond in the Au-**Ge4**-Au system. (b) The relative energies of the A-A, O-A, and O-O conformers in the [Au-**Ge4**-Au]$^{2+}$ model system (B3LYP/LACVP**) are obtained by subtracting the total energy of the A-A conformer at each particular Au-Au distance. (c) Tunnel coupling squared as a function of Au-Au distance plotted relative to $4t^2$ at the elongation = 0 point for the Au-**Ge4**-Au model system (B3LYP/LACVP**). Tunnel coupling calculations were performed on the lowest energy geometries optimized without Me-S-CH_2-$GeMe_2$- dihedral constraint.

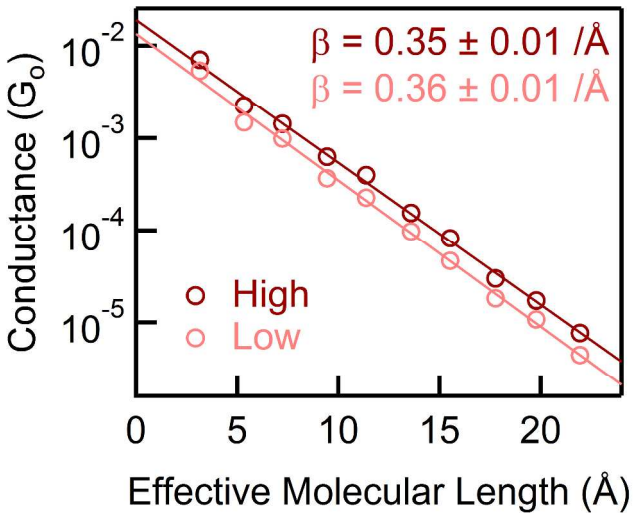


Figure S7. Conductance peak positions plotted from the low G (pre-switching) and high G (post switching) regions in Figure S5 against the DFT-optimized effective molecular lengths of **Ge1-Ge10**. Fitting a line through each set of peak values demonstrates that the low G and high G states decay with nearly the same β value, and are offset in conductance by a factor of 1.6.

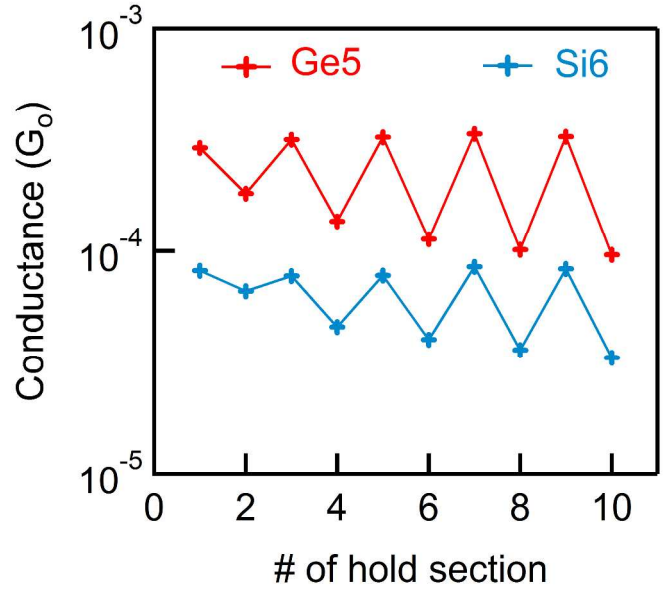


Figure S8. A comparison of junction training in **Ge5** vs. **Si6**. The conductance peak positions of **Si6** were determined with the same method described for **Ge5**. For **Ge5**, the switching factors upon compression from cycles 1-5 are 1.6, 2.3, 2.9, 3.3, and 3.4 respectively. For **Si6**, the switching factors upon compression from cycles 1-5 are 1.2, 1.7, 1.9, 2.4, and 2.5 respectively.

II. General Synthesis and Characterization Information

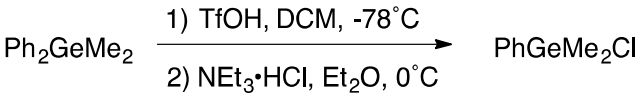
All reactions were performed in oven-dried or flame-dried round bottom flasks, unless otherwise noted. The flasks were fitted with rubber septa and reactions were conducted under a positive pressure of nitrogen or argon. Anhydrous and anaerobic solvents were obtained from a Schlenk manifold with purification 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. Trifluoromethanesulfonic acid and Lithium metal were purchased from Alfa Aesar. Anhydrous magnesium bromide was purchased from Strem and stored in a glovebox. Chlorodimethylphenylgermane, diphenyldimethylgermane, and hexamethyldigermane were purchased from Gelest. Chlorodimethylphenylgermane was either purchased from Gelest or synthesized as below. The triethylamine hydrochloride was recrystallized from ethanol, collected, dried under high vacuum overnight, and stored in a desiccator. 1,2-dichlorotetramethyldigermane was synthesized from a known procedure.[3]

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).[4] Data are represented as follows: chemical shift, multiplicity (s = singlet, d = doublet, dd= doublet of doublets, t = triplet, m = multiplet), coupling constants in Hertz, and integration. The mass spectroscopic data were obtained at the Columbia University mass spectrometry facility using a 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). We note that permethylgermanes commonly lose methyl groups upon ionization in the absence of phenyl rings, and report our masses for the α,ω-bis(methylthiomethyl) permethyloligogermanes as $[M\text{-}Me]^+$.[5] Absorption spectra were obtained on Shimadzu UV 1800 UV-Vis spectrophotometer. Cyclic voltammograms (CVs) were recorded on a CH166 electrochemical workstation with a standard three-electrode electrochemical cell.

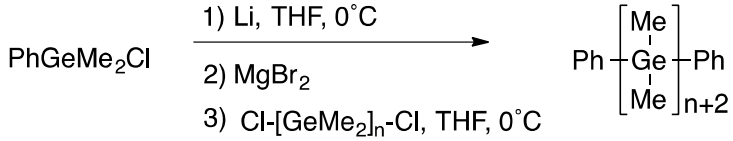
III. Synthetic Procedures and Characterization of Compounds

Chlorodimethylphenylgermane



Chlorodimethylphenylgermane was either purchased from Gelest or synthesized from diphenyldimethylgermane. A 250 mL oven-dried flask equipped with a stir bar was charged with diphenyldimethylgermane (9.88 g, 38.45 mmol, 1.00 equiv.). 125 mL dichloromethane was added to this flask, which was subsequently cooled to -78˚C with a CO_2-acetone bath. Trifluoromethanesulfonic acid (3.4 mL, 38.45 mmol, 1.00 equiv.) was added quickly via syringe and the reaction was warmed to room temperature. The solvent was stripped off *in vacuo* and was replaced with 100 mL diethyl ether and cooled to 0˚C with an ice-water bath. Triethylamine hydrochloride (5.29 g, 38.45 mmol, 1.00 equiv.) was added under a heavy flow of nitrogen. The reaction mixture was stirred at 0˚C for 30 minutes, then room temperature for an hour. Over this period, a biphasic mixture formed due to the formation of the NEt_3•TfOH ionic liquid. The reaction flask was then cooled to -78˚C to solidify the NEt_3•TfOH. The ether solution was then cannulated into a Schlenk flask. The ether was removed under vacuum and the remaining crude liquid was distilled (50-80˚C, 0.05 torr) to yield a colorless oil (7.23 g, 87% yield). This material was stored in a glovebox. The structure was confirmed by checking the ^{1}H NMR against the material purchased from Gelest. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.74 - 7.53 (m, 2H), 7.49 - 7.36 (m, 3H), 0.94 (s, 6H).

α,ω-diphenylpermethyloligogermanes **2** (n=3-11)



Our previous strategy for attenuating the reactivity of the phenyldimethylsilyl nucleophile employed isopropylmagnesium chloride to generate the phenyldimethylsilylmagnesium species with isopropyl lithium as a byproduct.[2] For the oligogermane system, we found that the presence of the isopropyl anion caused significant base-initiated disproportionation sideproducts to form. We find that magnesium bromide both attenuates the nucleophilicity of the phenyldimethylgermyl anion and effectively eliminates such disproportionation processes.

A representative procedure is given here for the *n*=3 oligomer, 1,3-diphenylhexamethyltrigermane. Lithium granules (0.59 g, 85.05 mmol, 8.10 equiv.) were added to a 2-neck 50 mL round bottom flask equipped with a stir bar. This flask was evacuated and cycled with argon 3x. 25 mL THF was added to this flask, which was subsequently cooled to 0˚C. Chlorodimethylphenylgermane (4.52 g, 21.00 mmol, 2.00 equiv.) was slowly added by syringe with 3 mL THF. After 15 minutes we observed green wisps coming off the lithium granules, indicative of germyl lithium generation. This reaction mixture was allowed to warm to room temperature overnight and turned a dark green color. Under positive argon pressure, a coarse Schlenk filter stick capped with a 100 mL Schlenk flask was fitted onto the 2-neck round

bottom flask. This apparatus was inverted and the mixture was vacuum filtered. The 2-neck round-bottom was rinsed 2x5 mL THF to wash the residual germyl lithium off the remaining granules. The Schlenk flask was then capped with a septum. Magnesium bromide (3.87 g, 21.00 mmol, 2.00 equiv.) was weighed out in the glovebox and added directly as a solid to the Schlenk flask under a strong flow of argon. The color of the reaction mixture transitioned from dark green to an orange-brown color and was stirred for 30 minutes.

Dichlorodimethylgermane (1.82 g, 10.50 mmol, 1.00 equiv.) was added to a separate 100 mL Schlenk flask with 10 mL THF and cooled to 0˚C. The phenyldimethylgermylmagnesium bromide solution was cannulated into the dichlorodimethylgermane solution and stirred for 1-2 hours. The reaction was quenched with a NH_4Cl (aq) solution (5 mL) and water (5 mL). The organic and aqueous layers were separated, and the aqueous layer was extracted with diethyl ether 3x30 mL. The organic layers were combined, washed with brine, dried with $MgSO_4$, filtered, and concentrated. The crude brown oil was purified by running a SiO_2 gel plug eluted with hexanes to yield 1,3-diphenylhexamethyltrigermane as a colorless oil (4.20 g, 87% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.39 - 7.32 (m, 4H), 7.32 - 7.27 (m, 6H), 0.44 (s, 12H), 0.32 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.39, 133.50, 128.05, 128.00, -2.77, -5.38. HRMS (TOF MS ASAP+) for $C_{18}H_{28}Ge_3$: calculated = 461.9858, found = 461.9849 (M+).

n=4: 1,4-diphenyloctamethyltetragermane was synthesized with the same general procedure with the following exceptions: 1,2-dichlorotetramethyldigermane was used instead of dichlorodimethylgermane. Colorless oil (6.05 g, 85% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.43 - 7.34 (m, 4H), 7.34 - 7.27 (m, 6H), 0.48 (s, 6H), 0.27 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.44, 133.34, 127.91, 127.85, -2.71, -4.58. HRMS (TOF MS ASAP+) for $C_{20}H_{34}Ge_4$: calculated = 565.9544, found = 565.9556 (M+).

n=5: 1,5-diphenyldecamethylpentagermane was synthesized with the same general procedure with the following exceptions: 1,3-dichlorohexamethyltrigermane was used instead of dichlorodimethylgermane. Colorless oil (2.99 g, 87% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42 - 7.37 (m, 4H), 7.33 - 7.27 (m, 6H), 0.50 (s, 12H), 0.30 (s, 12H), 0.23 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.65, 133.50, 128.06, 127.99, -2.48, -3.40, -4.20. HRMS (TOF MS ASAP+) for $C_{22}H_{40}Ge_5$: calculated = 667.9241, found = 667.9257 (M+).

n=6: 1,6-diphenyldodecamethylhexagermane was synthesized with the same general procedure with the following exceptions: 1,4-dichlorooctamethyltetragermane was used instead of dichlorodimethylgermane. White semisolid (3.71 g, 79%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.43 - 7.37 (m, 4H), 7.36 - 7.27 (m, 6H), 0.51 (s, 12H), 0.33 (s, 12H), 0.27 (s, 12H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.69, 133.52, 128.06, 127.99, -2.45, -3.18, -4.13. HRMS (TOF MS ASAP+) for $C_{24}H_{46}Ge_6$: calculated = 769.8937, found = 769.8947 (M+).

n=7: 1,7-diphenyltetradecamethylheptagermane was synthesized with the same general procedure with the following exceptions: 1,5-dichlorodecamethylpentagermane was used instead of dichlorodimethylgermane, and the product was isolated using automated silica gel column chromatography with hexanes. White semisolid (0.98 g, 78% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.43 - 7.38 (m, 4H), 7.35 - 7.28 (m, 6H), 0.51 (s, 12H), 0.34 (s, 12H), 0.30 (s, 6H), 0.29 (s, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.69, 133.50, 128.05, 127.98, -2.46, -2.98, -3.13, -4.11. HRMS (TOF MS ASAP+) for $C_{26}H_{52}Ge_7$: calculated = 873.8624, found = 873.8641 (M+).

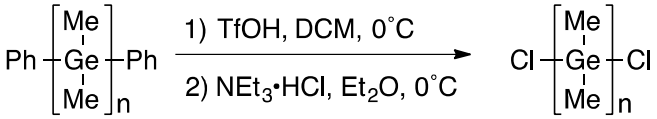
n=8: 1,8-diphenylhexadecamethyloctagermane was synthesized with the same general procedure with the following exceptions: 1,6-dichlorododecamethylhexagermane was used instead of dichlorodimethylgermane. White semisolid (2.36 g, 64% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.45 - 7.39 (m, 4H), 7.35 - 7.28 (m, 6H), 0.52 (s, 12H), 0.34 (s, 12H), 0.33 (s, 12H), 0.30 (s, 12H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.71, 133.52, 128.07, 128.00, -2.45, -2.91, -3.09, -4.10. HRMS (TOF MS ASAP+) for $C_{28}H_{58}Ge_8$: calculated = 975.8321, found = 975.8333 (M+).

n=9: 1,9-diphenyloctadecamethylnonagermane was synthesized with the same general procedure with the following exceptions: 1,7-dichlorotetradecamethylheptagermane was used instead of dichlorodimethylgermane. White semisolid (0.40 g, 64% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.47 - 7.37 (m, 4H), 7.35 - 7.27 (m, 6H), 0.52 (s, 12H), 0.35 (s, 6H), 0.35 (s, 12H), 0.34 (s, 12H), 0.31 (s, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.71, 133.52, 128.06, 127.99, -2.45, -2.85, -2.87, -3.08, -4.09. HRMS (TOF MS ASAP+) for $C_{30}H_{64}Ge_9$: calculated = 1077.8019, found = 1077.8031 (M+).

n=10: 1,10-diphenylicosamethyldecagermane was synthesized with the same general procedure with the following exceptions: 1,8-dichlorohexadecamethyloctagermane was used instead of dichlorodimethylgermane. White semisolid (0.76 g, 64%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52 - 7.48 (m, 4H), 7.42 - 7.34 (m, 6H), 0.61 (s, 12H), 0.46 (s, 12H), 0.44 (s, 12 H) 0.44 (s, 12H), 0.40 (s, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.68, 133.52, 128.08, 128.01, -2.41, -2.77, -2.83, -3.04, -4.05. HRMS (TOF MS ASAP+) for $C_{32}H_{70}Ge_{10}$: calculated = 1181.7705, found = 1181.7717 (M+).

n=11: 1,11-diphenyldocosamethylundecagermane was synthesized with the same general procedure with the following exceptions: 1,9-dichlorooctadecamethylnonagermane was used instead of dichlorodimethylgermane. White semisolid (0.14 g, 62% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45 - 7.39 (m, 4H), 7.35 - 7.27 (m, 6H), 0.52 (s, 12H), 0.36 (s, 6H), 0.36 (s, 12H) 0.35 (s, 12H), 0.35 (s, 12H), 0.31 (s, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.72, 133.53, 128.07, 128.00, -2.45, -2.78, -2.81, -2.87, -3.08, -4.09. HRMS (TOF MS ASAP+) for $C_{34}H_{76}Ge_{11}$: calculated = 1283.7402, found = 1283.7406 (M+).

α,ω-dichloropermethyloligogermanes **3** (n=3-10)



A representative procedure is given here for the *n*=3 oligomer, 1,3-dichlorohexamethyltrigermane. A 250 mL Schlenk flask equipped with a stir bar was charged with 1,3-diphenylhexamethyltrigermane (4.16 g, 9.00 mmol, 1.00 equiv.) and dissolved in dichloromethane (90 mL). The flask was cooled to 0˚C and trifluoromethanesulfonic acid [TfOH] (1.60 mL, 18.00 mmol, 2.00 equiv.) was added to the reaction flask via syringe. We would like to emphasize that these reactions require near-exact stoichiometric quantities of TfOH; in our hands, using an excess of TfOH resulted in significant disproportionation.

This reaction mixture was stirred at 0˚C for 30 minutes then room temperature for an hour. The dichloromethane was removed *in vacuo*. The silyl triflate was reconstituted in diethyl ether (90 mL) and cooled to 0˚C. Triethylamine hydrochloride (2.48 g, 18.00 mmol, 2.00 equiv.) was added under a heavy flow of nitrogen. The reaction mixture was stirred at 0˚C for 30 minutes, then room temperature for an hour. Over this period, a biphasic mixture formed due to the formation of the NEt_3•TfOH ionic liquid. The reaction flask was then cooled to -78˚C to solidify the NEt_3•TfOH salt. The ether solution was then cannulated into a separate Schlenk flask and concentrated *in vacuo*. There was occasionally 1,2-dichlorotetramethyldigermane in the residue from incomplete cleavage of the $PhGeMe_2$-$GeMe_2Ph$ dimer generated *in situ* during the first lithiation step from the preceding reaction.[6] This material is easily removed by sublimation (60˚C, 0.05 torr). The residue was then distilled (85-100˚C, 0.05 torr) to yield a colorless oil (2.94 g, 86% yield) that was stored in a glovebox. ^{1}H NMR (300 MHz, C_6D_6) δ 0.66 (s, 12H), 0.43 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 6.06, -5.25. We did not obtain mass spectrometry samples due to the moisture-sensitivity of these compounds.

n=4: 1,4-dichlorooctamethyltetragermane was synthesized with the same general procedure with the following exceptions: 1,4-diphenyloctamethyltetragermane was used instead of 1,3-diphenylhexamethyltrigermane and the material was distilled at 120-140˚C, 0.05 torr. Colorless oil (3.31 g, 65% yield). ^{1}H NMR (300 MHz, C_6D_6) δ 0.66 (s, 12H), 0.45 (s, 12H). ^{13}C NMR (101 MHz, C_6D_6) δ 5.75, -4.45.

n=5: 1,5-dichlorodecamethylpentagermane was synthesized with the same general procedure with the following exceptions: 1,5-diphenyldecamethylpentagermane was used instead of 1,3-diphenylhexamethyltrigermane and the material was carried forward to the next reaction without distillation. Colorless oil (1.94 g, 74%). ^{1}H NMR (300 MHz, C_6D_6) δ 0.67 (s, 12H), 0.49 (s, 6H), 0.45 (s, 12H). ^{13}C NMR (101 MHz, C_6D_6) δ 5.85, 1.43, -4.23.

n=6: 1,6-dichlorododecamethylhexagermane was synthesized with the same general procedure with the following exceptions: 1,6-diphenyldodecamethylhexagermane was used instead of 1,3-diphenylhexamethyltrigermane and the material was carried forward to the next reaction without distillation. Colorless oil (2.84 g, 91% yield). ^{1}H NMR (300 MHz, C_6D_6) δ 0.69 (s, 12H), 0.48 (s, 12H), 0.47 (s, 12H). ^{13}C NMR (101 MHz, C_6D_6) δ 5.90, -3.00, -4.16.

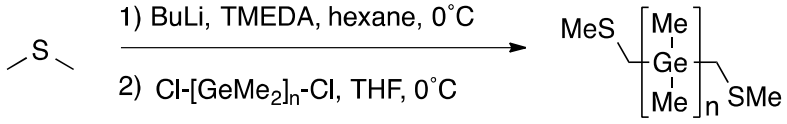
n=7: 1,7-dichlorotetradecamethylheptagermane was synthesized with the same general procedure with the following exceptions: 1,7-diphenyltetradecamethylheptagermane was used instead of 1,3-diphenylhexamethyltrigermane and the material was carried forward to the next reaction without distillation. Colorless oil (0.60 g, 92% yield). ^{1}H NMR (500 MHz, C_6D_6) δ 0.70 (s, 12H), 0.49 (s, 12H), 0.48 (s, 12H), 0.47 (s, 6H). ^{13}C NMR (126 MHz, C_6D_6) δ 5.95, -2.78, -2.93, -4.10.

n=8: 1,8-dichlorohexadecamethyloctagermane was synthesized with the same general procedure with the following exceptions: 1,8-diphenylhexadecamethyloctagermane was used instead of 1,3-diphenylhexamethyltrigermane and the material was carried forward to the next reaction without distillation. White semisolid (1.62 g, 83% yield) ^{1}H NMR (300 MHz, C_6D_6) δ 0.71 (s, 12H), 0.51 (s, 12H), 0.50 (s, 12H), 0.48 (s, 12H). ^{13}C NMR (101 MHz, C_6D_6) δ 5.94, -2.74, -2.91, -4.10.

n=9: 1,9-dichlorooctadecamethylnonagermane was synthesized with the same general procedure with the following exceptions: 1,9-diphenyloctadecamethylnonagermane was used instead of 1,3-diphenylhexamethyltrigermane and the material was carried forward to the next reaction without distillation. White semisolid (0.34 g, 94% yield). ^{1}H NMR (300 MHz, C_6D_6) δ 0.72 (s, 12H), 0.53 (s, 12H), 0.52 (s, 12H), 0.52 (s, 6H) 0.29 (s, 12H). ^{13}C NMR (101 MHz, C_6D_6) δ 5.97, 1.43, -2.63, -2.86, -4.07.

n=10: 1,10-dichloroicosamethyldecagermane was synthesized with the same general procedure with the following exceptions: 1,10-diphenylicosamethyldecagermane was used instead of 1,3-diphenylhexamethyltrigermane and the material was carried forward to the next reaction without distillation. White semisolid (0.26 g, 81% yield). ^{1}H NMR (300 MHz, C_6D_6) δ 0.69 (s, 12H), 0.50 (s, 12H), 0.49 (s, 12H), 0.49 (s, 12H), 0.26 (s, 12H). ^{13}C NMR (101 MHz, C_6D_6) δ 5.97, 1.43, -2.66, -2.86, -4.07.

α,ω-bis(methylthiomethyl)permethyloligogermanes **Ge1-Ge10** (n=1-10)



A representative procedure is given here for the *n*=1 oligomer, bis(methylthiomethyl)dimethylgermane. This procedure was adapted from the literature.[7] A 10 mL Schlenk flask equipped with a stir bar was charged with a solution of 1.61 M *n*-butyllithium in *n*-hexane (1.37 mL, 2.20 mmol, 2.20 equiv.) and was cooled to 0˚C with an ice-water bath. Tetramethylethylenediamine (TMEDA) (0.33 mL, 2.20 mmol, 2.20 equiv.) was added dropwise, followed by 1 mL hexanes, and was stirred for 20 minutes. Dimethylsulfide (0.17 mL, 2.20 mmol, 2.20 equiv.) was added via syringe, and this mixture was stirred slowly for 4 hours to generate methylthiomethyl lithium. This light cloudy solution was then cannulated into a 25 mL Schlenk flask charged with dichlorodimethylgermane (0.17 g, 1.00 mmol, 1.00 equiv.) and 4 mL THF at 0˚C. The reaction was stirred for 3 hours or let stir overnight. The reaction mixture was quenched with methanol, then concentrated *in vacuo*. This material was then separated using automated silica gel column chromatography with a gradient from 100% hexanes to 70%/30% hexanes/dichloromethane to yield a colorless oil (90 mg, 40% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.16 (s, 6H), 2.02 (s, 4H), 0.33 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 20.53, 19.72, -3.42. HRMS (TOF MS ASAP+) for $C_5H_{13}Ge_1S_2$: calculated = 210.9669, found = 210.9655 ([M-Me]+).

n=2: 1,2-bis(methylthiomethyl)tetramethyldigermane was synthesized with the same general procedure with the following exceptions: 1,2-dichlorotetramethyldigermane was used instead of dichlorodimethylgermane. Colorless oil (79 mg, 63% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.16 (s, 6H), 2.09 (s, 4H), 0.37 (s, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 20.86, 20.43, -3.29. HRMS (TOF MS ASAP+) for $C_7H_{19}Ge_2S_2$: calculated =312.9364, found = 312.9347 ([M-Me]+).

n=3: 1,3-bis(methylthiomethyl)hexamethyltrigermane was synthesized with the same general procedure with the following exceptions: 1,3-dichlorohexamethyltrigermane was used instead of dichlorodimethylgermane. Colorless oil (66 mg, 84% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.16 (s, 6H), 2.07 (s, 4H), 0.39 (s, 6H), 0.36 (s, 12H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 20.93, 20.88, -2.70, -5.14. HRMS (TOF MS ASAP+) for $C_9H_{25}Ge_3S_2$: calculated =414.9060, found = 414.9057 ([M-Me]+).

n=4: 1,4-bis(methylthiomethyl)octamethyltetragermane was synthesized with the same general procedure with the following exceptions: 1,4-dichlorooctamethyltetragermane was used instead of dichlorodimethylgermane. Colorless oil (60 mg, 70% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.15 (s, 6H), 2.06 (s, 4H), 0.40 (s, 12H), 0.35 (s, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 21.00, 20.89, -2.57, -4.23. HRMS (TOF MS ASAP+) for $C_{11}H_{31}Ge_4S_2$: calculated =518.8745, found = 518.8740 ([M-Me]+).

n=5: 1,5-bis(methylthiomethyl)decamethylpentagermane was synthesized with the same general procedure with the following exceptions: 1,5-dichlorodecamethylpentagermane was used instead of dichlorodimethylgermane. Colorless oil (76 mg, 68% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.15 (s, 6H), 2.06 (s, 4H), 0.41 (s, 6H), 0.40 (s, 12H), 0.35 (s, 12H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 21.05, 20.89, -2.54, -3.19, -4.04. HRMS (TOF MS ASAP+) for $C_{13}H_{37}Ge_5S_2$: calculated = 620.8442, found = 620.8459 ([M-Me]+).

n=6: 1,6-bis(methylthiomethyl)dodecamethylhexagermane was synthesized with the same general procedure with the following exceptions: 1,6-dichlorododecamethylhexagermane was used instead of dichlorodimethylgermane. Colorless oil (119 mg, 55% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.15 (s, 6H), 2.06 (s, 4H), 0.40 (s, 12H), 0.40 (s, 12H), 0.35 (s, 12H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 21.05, 20.91, -2.53, -3.00, -4.00. HRMS (TOF MS ASAP+) for $C_{15}H_{43}Ge_6S_2$: calculated = 722.8139, found = 722.8148 ([M-Me]+).

n=7: 1,7-bis(methylthiomethyl)tetradecamethylheptagermane was synthesized with the same general procedure with the following exceptions: 1,7-dichlorotetradecamethylheptagermane was used instead of dichlorodimethylgermane. Colorless oil (76 mg, 56% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.18 (s, 6H), 2.08 (s, 4H), 0.43 (s, 12H), 0.42 (s, 6H), 0.42 (s, 12H), 0.37 (s, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 21.04, 20.90, -2.53, -2.84, -2.99, -4.00. HRMS (TOF MS ASAP+) for $C_{17}H_{49}Ge_7S_2$: calculated = 826.7825, found = 826.7803 ([M-Me]+).

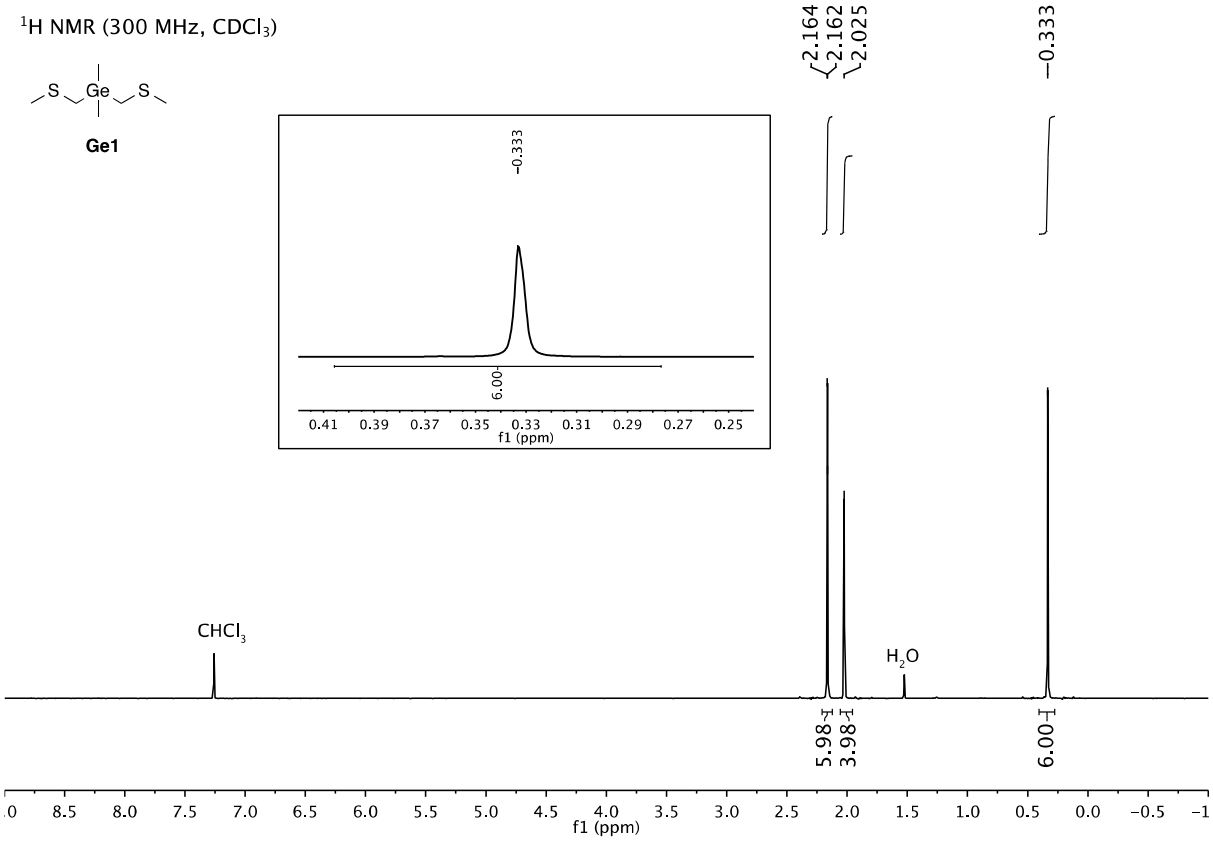
n=8: 1,8-bis(methylthiomethyl)hexadecamethyloctagermane was synthesized with the same general procedure with the following exceptions: 1,8-dichlorohexadecamethyloctagermane was used instead of dichlorodimethylgermane. White semisolid (130 mg, 48% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.15 (s, 6H), 2.06 (s, 4H), 0.40 (s, 12H), 0.40 (s, 12H), 0.39 (s, 12H), 0.35 (s, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 21.02, 20.91, -2.54, -2.82, -2.99, -4.01. HRMS (TOF MS ASAP+) for $C_{19}H_{55}Ge_8S_2$: calculated = 928.7522, found = 928.7549 ([M-Me]+).

n=9: 1,9-bis(methylthiomethyl)octadecamethylnonagermane was synthesized with the same general procedure with the following exceptions: 1,9-dichlorooctadecamethylnonagermane was used instead of dichlorodimethylgermane. White semisolid (89 mg, 53% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.15 (s, 6H), 2.06 (s, 4H), 0.42 (s, 12H), 0.42 (s, 6H), 0.42 (s, 12H), 0.42 (s,

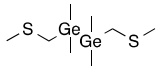
12H), 0.35 (s, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 21.02, 20.92, -2.52, -2.54, -2.79, -2.98, -4.00. HRMS (TOF MS ASAP+) for $C_{21}H_{61}Ge_9S_2$: calculated = 1030.7219, found = 1030.7234 ([M-Me]+).

n=10: 1,10-bis(methylthiomethyl)icosamethyldecagermane was synthesized with the same general procedure with the following exceptions: 1,10-dichloroicosamethyldecagermane was used instead of dichlorodimethylgermane. White semisolid (87 mg, 47% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.18 (s, 6H), 2.08 (s, 4H), 0.43 (s, 12H), 0.43 (s, 12H), 0.43 (s, 12H), 0.42 (s, 12H), 0.38 (s, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 21.04, 20.91, -2.52, -2.76, -2.79, -2.97, -3.99. HRMS (TOF MS ASAP+) for $C_{23}H_{67}Ge_{10}S_2$: calculated = 1134.6906, found = 1134.6929 ([M-Me]+).

^{1}H NMR Spectra for Ge1-Ge10

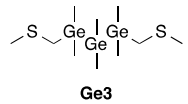


^{1}H NMR (300 MHz, $CDCl_3$)



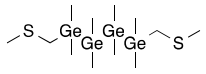
Ge2

^{1}H NMR (300 MHz, $CDCl_3$)



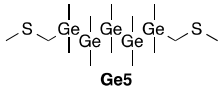
Ge3

^{1}H NMR (300 MHz, $CDCl_3$)

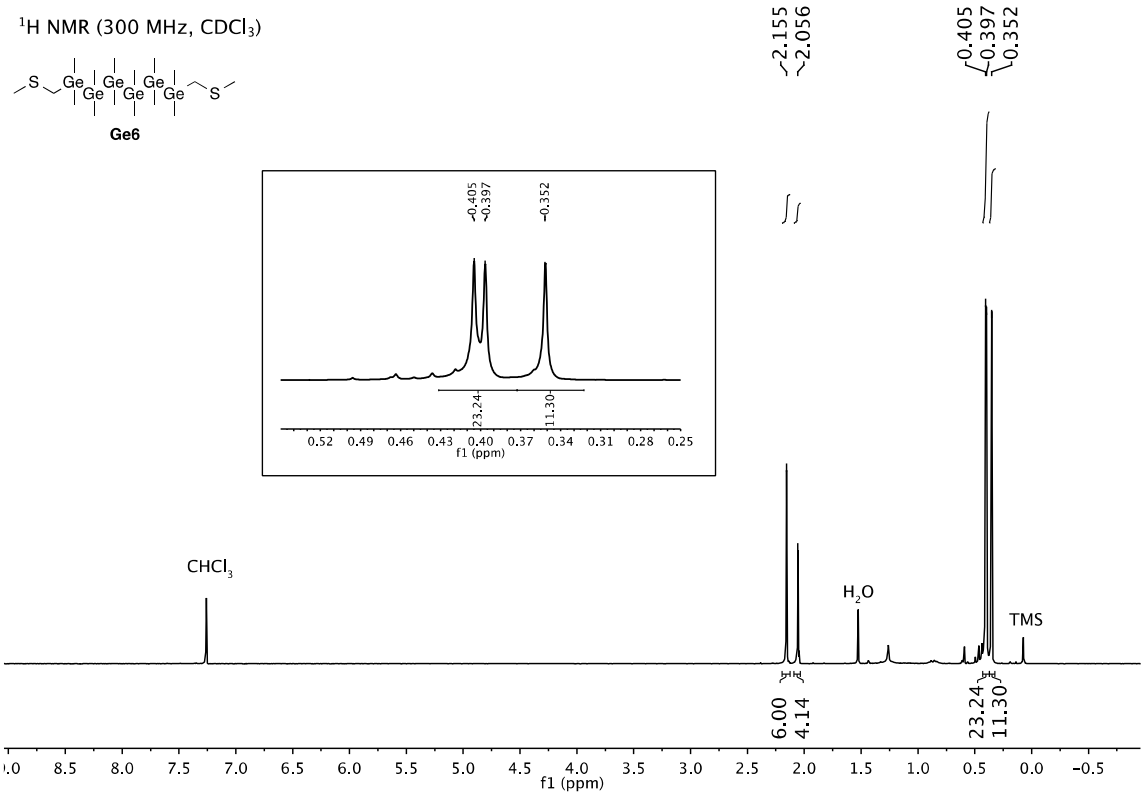


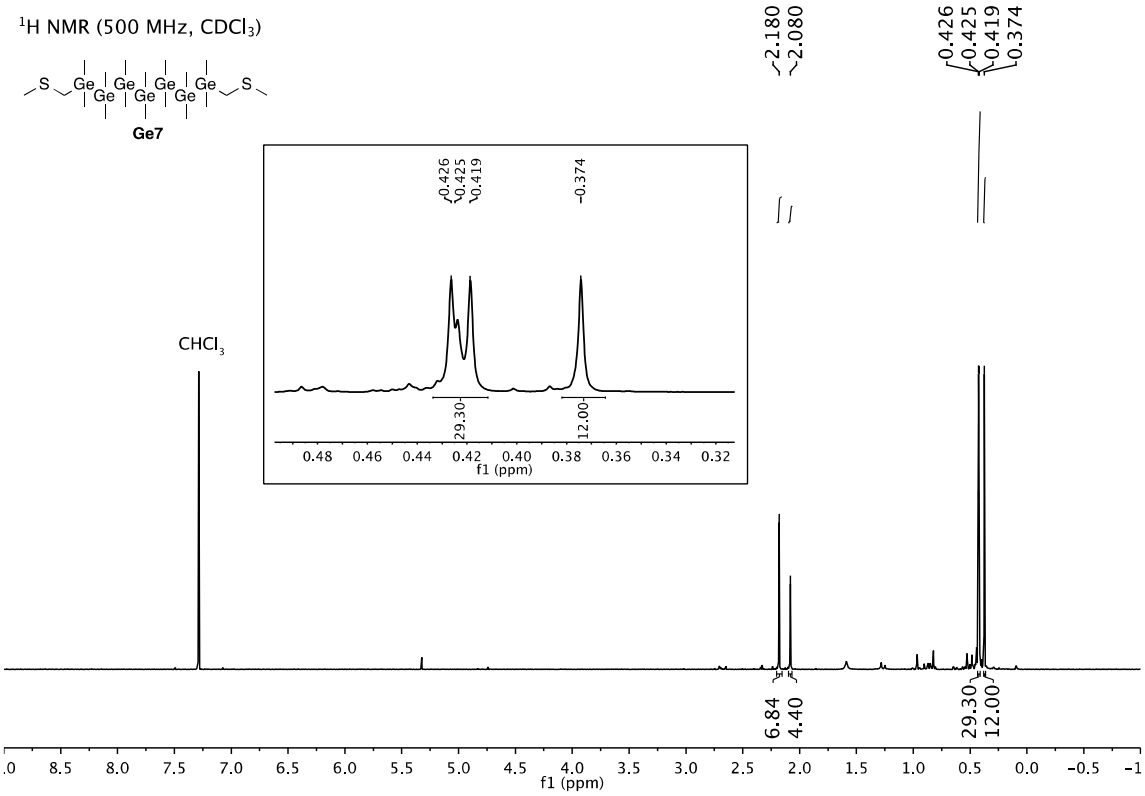
Ge4

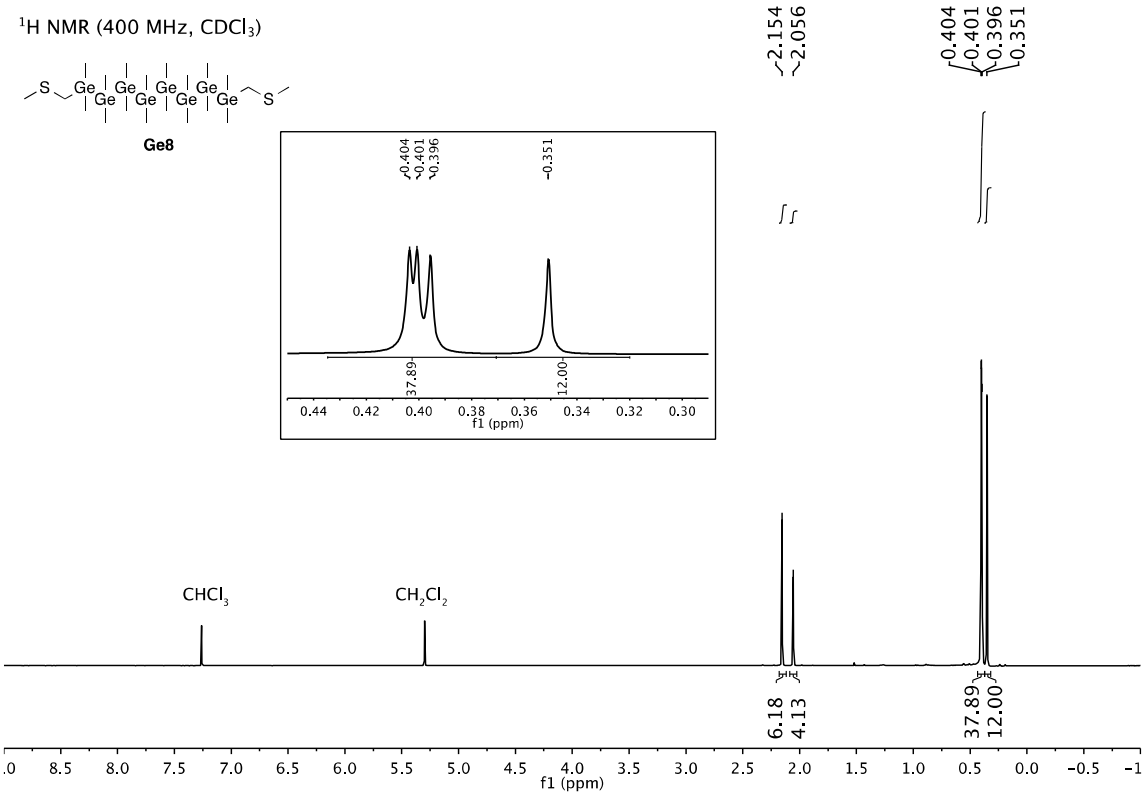
^{1}H NMR (300 MHz, $CDCl_3$)

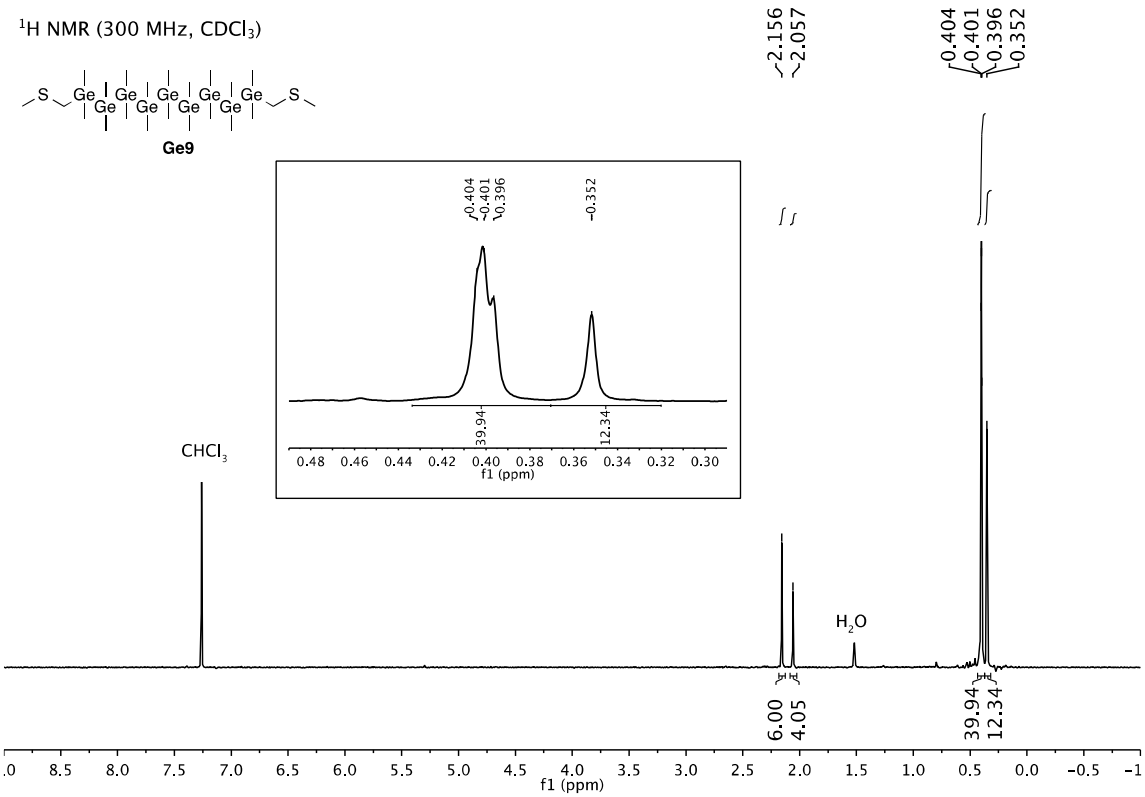


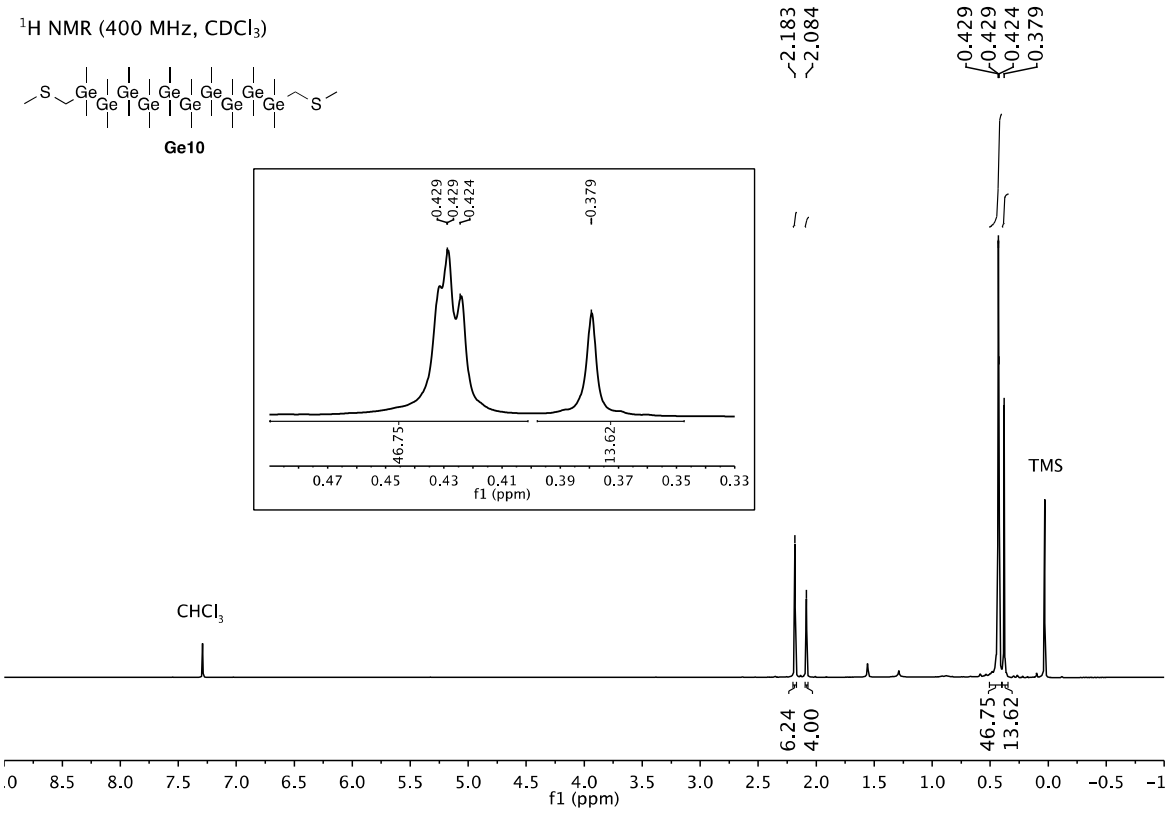
Ge5


^{1}H NMR (300 MHz, $CDCl_3$)
Ge6
2.155
2.056
0.405
0.397
0.352
$CHCl_3$
H_2O
TMS
6.00
4.14
23.24
11.30
f1 (ppm)


^{1}H NMR (500 MHz, $CDCl_3$)
Ge7
2.180
2.080
0.426
0.425
0.419
0.374
$CHCl_3$
6.84
4.40
29.30
12.00
f1 (ppm)


1H NMR (400 MHz, CDCl3)
Ge8
2.154
2.056
0.404
0.401
0.396
0.351
CHCl3
CH2Cl2
6.18
4.13
37.89
12.00
f1 (ppm)


1H NMR (300 MHz, CDCl3)
Ge9
2.156
2.057
0.404
0.401
0.396
0.352
CHCl3
H2O
6.00
4.05
39.94
12.34
f1 (ppm)


1H NMR (400 MHz, CDCl3)
Ge10
2.183
2.084
0.429
0.429
0.424
0.379
TMS
CHCl3
6.24
4.00
46.75
13.62
f1 (ppm)

Cyclic Voltammetry Measurements

CV measurements were conducted in a 0.1 M tetrabutylammonium hexafluorophosphate ($TBAPF_6$) solution in dichloromethane at room temperature in an ambient atmosphere, with a scanning rate of 0.1 V/s. A 0.5 mM concentration was used for **Si1**-**Si10** and **Ge1**-**Ge10**. A glassy carbon working electrode, Pt wire counter electrode, and Ag/AgCl reference electrode were used in a 3-electrode setup. The experiments were calibrated with the standard ferrocene(Fc)/ferrocenium(Fc^+) redox system and an assumption that the HOMO energy of Fc is 4.8 eV below vacuum. The HOMO energies are determined from the onset of the first oxidation by CV vs. Fc^+/Fc and the equation E_{HOMO}= -(4.80 V + E_{onset}^{ox}).[1]

Table ST1. Cyclic voltammetry-derived onset oxidation energies and HOMO levels for **Si1**-**Si10** and **Ge1**-**Ge10** vs. the Fc^+/Fc redox system.

	Si*n*		**Ge*n***	
n	E_{onset} (V)	E_{HOMO} (eV)	E_{onset} (V)	E_{HOMO} (eV)
1	0.681	-5.48	0.542	-5.34
2	0.627	-5.43	0.496	-5.30
3	0.646	-5.36	0.456	-5.26
4	0.558	-5.35	0.443	-5.24
5	0.554	-5.35	0.417	-5.22
6	0.503	-5.30	0.374	-5.17
7	0.429	-5.23	0.325	-5.13
8	0.385	-5.19	0.293	-5.09
9	0.343	-5.14	0.255	-5.05
10	0.301	-5.10	0.200	-5.00

UV-Vis Absorption Spectroscopy

Absorption spectra were taken on a Shimadzu UV-1800 spectrophotometer. A 1-cm quartz cuvette was charged with 2 mL of hexanes and a background spectrum was recorded. A second 1-cm quartz cuvette was charged with 2 mL of the **Si1**-**Si10** and **Ge1**-**Ge10** 25-100 μM solutions in hexanes and an absorption spectrum recorded.

Table ST2. Absorption peak maxima for the **Si***n* and **Ge***n* series. No discernable absorbance peak observed for the *n*=1-3 oligomers.

	Si*n*	**Ge***n*
n	λ_{max} (nm)	λ_{max} (nm)
1	—	—
2	—	—
3	—	—
4	236	231
5	252	246
6	261	256
7	269	263
8	274	272
9	277	272
10	280	273

IV. STM Break-Junction Experimental Details

We use a home-built modified Scanning Tunneling Microscope (STM) to measure single molecule conductance. We use a 0.25 mm diameter gold wire (99.998%, Alfa Aesar) as the STM tip and a 100 nm thick gold (99.999%, Alfa Aesar) layer evaporated on mica as the substrate. A commercially available single-axis piezoelectric positioner (Nano-P15, Mad City Labs) is used to achieve sub-angstrom level control of the tip-substrate distance. The STM is controlled using a custom written program in IgorPro (Wavemetrics, Inc.) and operates in ambient conditions at room temperature. The gold substrate is UV/Ozone cleaned for 20 minutes immediately before use. After we collect at least a thousand traces to ensure that the gold is clean, we introduce our molecules dissolved in 1,2,4-trichlorobenzene (Sigma-Aldrich or Alfa Aesar, 99% purity). The solvent concentrations for the oligogermanes are as follows: 1mM for **Ge1-Ge6**, 0.1mM for **Ge7-Ge10**.

We form a Au-Au atomic contact between the tip and the substrate with a conductance of at least $5G_0$, then withdraw the tip. After the gold point contact breaks, a target molecule can bridge the gap. The conductance (G=I/V) of the junction is measured as a function of junction elongation to generate a conductance versus displacement trace. We repeat this process thousands of time for each molecule studied. Conductance traces are used to make 1D conductance histograms (Figure 2a) without any data selection. We record the current as a function of tip/substrate displacement with an applied bias of 225 mV for **Ge1-6**, 500 mV for **Ge7**, **Ge8** and 630 mV for **Ge9**, **Ge10**. The tip is withdrawn at a speed of about 19 nm/s and the data is collected at a 40 kHz acquisition rate.

V. Computational Chemistry

General Methods

All DFT calculations were carried out with Jaguar (version 8.3, Schrodinger, LLC, New York, NY, 2014). We used a B3LYP functional for all molecules, a 6-31G** basis set for light atoms, and a LACVP** basis set for Au and Ge atoms.[8] Our methods for performing the tunnel coupling calculations that follow were detailed in a previous article.[2]

Table ST3: *Relative Energies for A-A, O-A, and O-O Configurations with Fixed Dihedrals for [Au-**Ge4**-Au]$^{2+}$*

Dihedral Config.		A-A		O-A		O-O	
Au-Au Distance (Å)	Elongation (Å)	Total Energy (Hartrees)	Rel. Energy (kcal/mol)	Total Energy (Hartrees)	Rel. Energy (kcal/mol)	Total Energy (Hartrees)	Rel. Energy (kcal/mol)
13.63	-0.5	-1559.729281	0	-1559.728029	0.79	-1559.728681	0.38
14.13	0	-1559.730233	0	-1559.729832	0.25	-1559.729431	0.50
14.63	0.5	-1559.730155	0	-1559.730946	-0.50	-1559.729973	0.11
15.13	1	-1559.727664	0	-1559.731526	-2.42	-1559.730192	-1.59
15.63	1.5	-1559.722568	0	-1559.729939	-4.63	-1559.731194	-5.41
16.13	2	-1559.714388	0	-1559.725892	-7.22	-1559.732183	-11.17
16.63	2.5	-1559.703548	0	-1559.718352	-9.29	-1559.729651	-16.38
17.13	3	-1559.690465	0	-1559.708242	-11.15	-1559.723845	-20.95

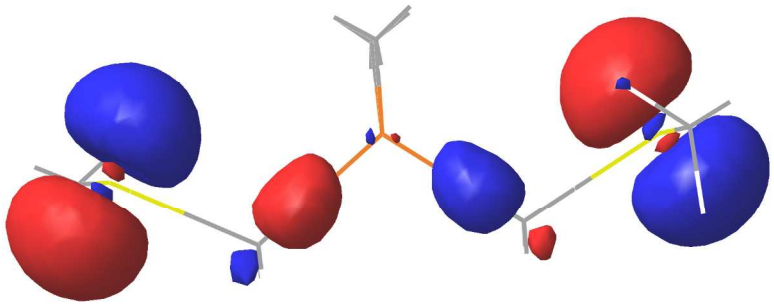
Table ST4: *Values for Lowest Energy Geometries without Dihedral Constraint for Au-**Ge4**-Au (Figure 4c)*

[Au-**Ge4**-Au]$^{2+}$								Au-**Ge4**-Au
Au-Au Distance (Å)	Elongation (Å)	Dihedral Config.	Total Energy (Hartrees)	Ge-Ge-Ge-Ge Dihedral	Me-S-CH_2-$GeMe_2$-(ω_1)	Me-S-CH_2-$GeMe_2$-(ω_2)	Au-S bond length (Å)	Relative Tunnel Coupling Squared
13.63	-0.5	A-A	-1559.729079	-165.7	-166.1	175.0	2.35	0.89
14.13	0	A-A	-1559.730187	-173.7	-179.8	-173.8	2.34	1.00
14.63	0.5	O-A	-1559.731097	172.5	86.2	179.9	2.35	1.02
15.13	1	O-A	-1559.731613	-172.6	85.8	-175.7	2.35	0.91
15.63	1.5	O-O	-1559.731606	173.8	87.0	-87.1	2.35	1.50
16.13	2	O-O	-1559.732427	-171.9	86.9	-87.1	2.36	1.43
16.63	2.5	O-O	-1559.729651	-170.1	93.0	-93.0	2.38	1.52
17.13	3	O-O	-1559.724291	-173.4	88.5	-88.5	2.41	1.67

*Calculation details of HOMO for **Si1** and **Ge1***

Me-S-CH_2-Si(Ge)Me_2- dihedral constrained to 92˚ to ensure coplanarity of S lone pair with C-Si(Ge) bond.

Geometry Optimization for **Si1**:
B3LYP - LACVP**



HOMO surface of **Si1** with isovalue = 0.06.
HOMO energy: -5.56 eV

Total Energy: -1324.191135 hartrees

Final geometry:

	angstroms		
atom	x	y	z
S1	2.6853210000	-3.1211970000	-3.4387330000
C2	1.7412840000	-3.7691170000	-1.9857670000
Si3	0.0473020000	-2.9376120000	-1.6865870000
C4	-0.6578750000	-3.7148050000	-0.0898610000
S5	-2.3527540000	-3.1402420000	0.3786170000
C6	-3.3840740000	-4.4003410000	-0.4479660000
C7	3.6917590000	-1.8216450000	-2.6430690000
H8	2.3934750000	-3.7263900000	-1.1056630000
H9	1.5860850000	-4.8344530000	-2.1927970000
C10	-1.0703930000	-3.2837780000	-3.1675840000
C11	0.2343790000	-1.0775510000	-1.4265250000
H12	-0.0155520000	-3.4415980000	0.7555420000
H13	-0.6631320000	-4.8106130000	-0.1207080000
H14	-4.4226610000	-4.1568840000	-0.2121630000
H15	-3.2567380000	-4.3846320000	-1.5324590000
H16	-3.1610750000	-5.3993820000	-0.0630850000
H17	4.3137410000	-1.3846210000	-3.4277160000
H18	3.0719290000	-1.0353920000	-2.2069560000

H19	4.3428710000	-2.2488970000	-1.8753070000
H20	-0.7363110000	-0.6302640000	-1.1897100000
H21	0.9168270000	-0.8456190000	-0.6014570000
H22	0.6158450000	-0.5921610000	-2.3306370000
H23	-2.0454910000	-2.8017840000	-3.0433480000
H24	-0.6162690000	-2.8912040000	-4.0830320000
H25	-1.2368440000	-4.3567680000	-3.3133250000

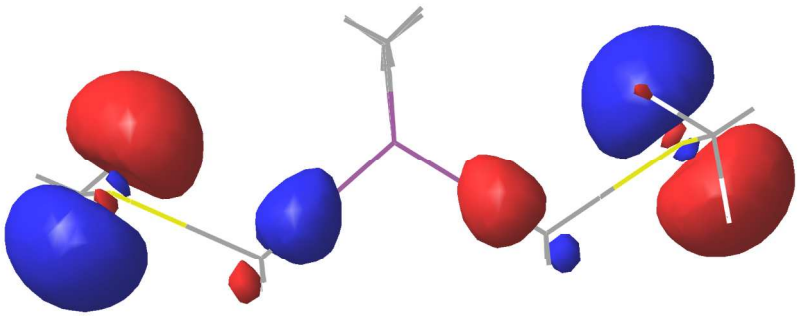
special geometric constraints coord value target

Si3-C2-S1-C7	92.00009	92.00000
Si3-C4-S5-C6	91.99955	92.00000

nuclear repulsion energy..... 730.324814434 hartrees

Geometry Optimization for **Ge1**:

B3LYP - LACVP**



HOMO surface of **Ge1** with isovalue = 0.06.
HOMO energy: -5.49 eV

Total Energy: -1038.445872 hartrees

Final geometry:
angstroms

atom	x	y	z
S1	2.7550330769	-3.1358441316	-3.4556561006
C2	1.8301648289	-3.8002997913	-2.0048241919
Ge	0.0544770218	-2.9451860612	-1.6755194804
C4	-0.6980965299	-3.7506000917	-0.0086988416
S5	-2.3819452929	-3.1539978089	0.4500636294
C6	-3.4213540767	-4.4021304703	-0.3837647038
C7	3.7539428762	-1.8357123748	-2.6524192859
H8	2.4801268219	-3.7541575265	-1.1246803963

H9	1.6744166111	-4.8636941321	-2.2151398232
C10	-1.1096625624	-3.3103488412	-3.2252066734
C11	0.2445913463	-1.0017093166	-1.3972349884
H12	-0.0506528709	-3.4840546142	0.8333546530
H13	-0.7133179631	-4.8448274599	-0.0490094456
H14	-4.4599795430	-4.1393337270	-0.1689064998
H15	-3.2741684617	-4.3963275707	-1.4664445507
H16	-3.2217868245	-5.4020857746	0.0118640058
H17	4.3572461043	-1.3737915485	-3.4376469730
H18	3.1274983457	-1.0674978452	-2.1928038900
H19	4.4225517285	-2.2666074764	-1.9017350938
H20	-0.7256982227	-0.5650008452	-1.1439935346
H21	0.9389413097	-0.7810664403	-0.5805379468
H22	0.6129486851	-0.5152922989	-2.3051295929
H23	-2.0805435498	-2.8214336414	-3.1030882873
H24	-0.6457832749	-2.9274415212	-4.1386912286
H25	-1.2771112259	-4.3841204690	-3.3546686366

special geometric constraints	coord	value	target
Ge-C2-S1-C7	92.00120	92.00000	
Ge-C4-S5-C6	92.00008	92.00000	

nuclear repulsion energy..... 555.861300940 hartrees

*Structure Details for **Ge1-Ge10** from Fig. 1*

Ge1

Total energy: -1038.450270 hartrees

final geometry:

	angstroms		
atom	x	y	z
C1	4.4705307028	-0.0239080197	-1.5726875056
S2	3.3424475393	1.3473213878	-1.1430689480
C3	1.9992426835	0.4303213075	-0.3112552386
Ge	0.5359210224	1.6382331753	0.3176964078
C5	-0.7784223648	0.3994642588	1.1744793862
S6	-2.2313362143	1.2857128149	1.8382283703
C7	-3.1913670857	-0.1083001583	2.5255766625
C8	1.2310808961	2.9183739940	1.6436158557
C9	-0.2934614040	2.5597472354	-1.2130055051
H10	5.3297690664	0.4152127603	-2.0858626836

H11	4.8205830453	-0.5409425040	-0.6748122836
H12	3.9841531226	-0.7377282740	-2.2434474500
H13	2.4021486095	-0.1112186830	0.5526303803
H14	1.5728857967	-0.3066364974	-1.0019065084
H15	-0.2743517333	-0.1410937901	1.9841716784
H16	-1.1035604558	-0.3362448662	0.4295515496
H17	-4.1026856639	0.3114954266	2.9588683225
H18	-3.4669198001	-0.8199605379	1.7422221137
H19	-2.6303092183	-0.6228567423	3.3107317603
H20	0.4226448909	3.5406028867	2.0375580934
H21	1.6965623873	2.3946571159	2.4838445036
H22	1.9839133685	3.5698271791	1.1910810556
H23	-1.1254145037	3.1863508230	-0.8796099538
H24	0.4380063641	3.1931878938	-1.7225465446
H25	-0.6814518422	1.8384024410	-1.9383080764

special geometric constraints	coord	value	target
	Ge-C5-S6-C7	-179.99783	180.00000
	C3-Ge-C5-S6	-179.99846	180.00000
	S2-C3-Ge-C5	-180.00144	180.00000
	C1-S2-C3-Ge	-179.99896	180.00000

nuclear repulsion energy..... 546.612493311 hartrees

Ge2

Total energy: -1122.073797 hartrees

Final geometry:

angstroms

atom	x	y	z
C1	-4.7467281361	2.8079097270	-1.7090443155
S2	-3.5735754190	1.4695871607	-1.2948574349
Ge3	1.3785969069	2.7727382092	0.2626570803
C4	2.9185672943	1.6006601208	0.7894634935
S5	4.4003120816	2.5723694241	1.2402422381
C6	5.5730796515	1.2334138541	1.6535513060
C7	0.9303987470	3.9574789569	1.7870618231
C8	1.9207682875	3.8747007594	-1.2930411537
Ge9	-0.5517717153	1.2704140720	-0.3177668513
C10	-2.0920243604	2.4419808105	-0.8448915494
C11	-0.1034233230	0.0853016709	-1.8418356485
C12	-1.0937774404	0.1687332862	1.2381404619
H13	-5.6872672197	2.3323899181	-1.9988916730
H14	-4.9279911559	3.4536075411	-0.8451958389
H15	-4.3800477895	3.4072177705	-2.5471239996

H16	3.1570528899	0.9342343438	-0.0472532982
H17	2.6142547161	0.9795436157	1.6396226870
H18	6.5138863821	1.7084485934	1.9433245282
H19	5.2063933084	0.6339764530	2.4915447758
H20	5.7538537166	0.5879146260	0.7894583093
H21	1.7936172008	4.5738081903	2.0549659487
H22	0.6441273183	3.3748046809	2.6673870445
H23	0.0987512464	4.6215028226	1.5327604510
H24	1.1076230786	4.5384539793	-1.6020169661
H25	2.7890618086	4.4894500413	-1.0382329348
H26	2.1899389168	3.2456254864	-2.1463860633
H27	-2.3305630386	3.1087444199	-0.0084485127
H28	-1.7880303528	3.0627515566	-1.6953955199
H29	-0.9668059578	-0.5306531513	-2.1100534320
H30	0.1835505835	0.6677201051	-2.7220905931
H31	0.7277866286	-0.5790720661	-1.5870232926
H32	-1.3640610649	0.7980404179	2.0909531532
H33	-1.9613259690	-0.4469958494	0.9831695181
H34	-0.2801606163	-0.4940417468	1.5479208777

special geometric constraints	coord	value	target
C1-S2-C10-Ge9	-179.98263	180.00000	
S2-C10-Ge9-Ge3	-179.98761	180.00000	
C4-Ge3-Ge9-C10	-179.99312	180.00000	
S5-C4-Ge3-Ge9	-179.98823	180.00000	
Ge3-C4-S5-C6	-180.00575	180.00000	

nuclear repulsion energy..... 766.966532199 hartrees

Ge3

Total energy: -1205.699272 hartrees

Final geometry:

	angstroms		
atom	x	y	z
S1	9.3386050739	2.2522155937	-7.6645362272
C2	9.3662456320	4.0321248013	-7.2503317347
C3	7.7898238930	1.7389068126	-6.8405732191
Ge4	7.4019032888	-0.2168075359	-7.0767454028
C5	7.2460655767	-0.6045982701	-9.0134904131
C6	8.9012438616	-1.2610129999	-6.3101358557
Ge7	5.2451292973	-0.6406641127	-5.8583301045
C8	3.8321498393	0.5381129693	-6.6333409484
C9	5.4791242097	-0.1126237756	-3.9470390394
Ge10	4.4380213579	-3.0192830030	-5.9398494172

C11	4.0649520946	-3.6103466599	-7.7938538065
C12	5.7231636255	-4.2661080376	-5.0913895004
C13	2.7228789704	-3.0508416439	-4.8967409669
S14	1.9668249583	-4.7138567340	-4.8364818154
C15	0.4749477102	-4.3684922135	-3.8387301733
H16	10.2675961108	4.4543154445	-7.7020575250
H17	8.4913283764	4.5448487425	-7.6600207643
H18	9.4084890105	4.1832611482	-6.1679377837
H19	7.8562038504	1.9547123769	-5.7680442826
H20	6.9499215792	2.3129705036	-7.2484437827
H21	7.0530996639	-1.6680646459	-9.1839004664
H22	6.4292859646	-0.0340723684	-9.4648495326
H23	8.1726370491	-0.3351229623	-9.5291590989
H24	9.0168257301	-1.0577793497	-5.2416341852
H25	8.7329990896	-2.3348121733	-6.4359701950
H26	9.8392342074	-0.9981155980	-6.8082336014
H27	2.8886619543	0.4172612979	-6.0918719991
H28	4.1272021594	1.5899682483	-6.5664095897
H29	3.6522425365	0.3021786206	-7.6860554365
H30	6.2435700889	-0.7229567246	-3.4577993312
H31	5.7814657617	0.9365001209	-3.8704143486
H32	4.5419709304	-0.2349246688	-3.3950016899
H33	3.6403532743	-4.6186925119	-7.7914833479
H34	3.3496514266	-2.9430638413	-8.2831737053
H35	4.9816545740	-3.6233796756	-8.3910614762
H36	6.6661682957	-4.2907273691	-5.6457507436
H37	5.3096667625	-5.2788087016	-5.0690868575
H38	5.9412968667	-3.9667575178	-4.0622401081
H39	2.9278666506	-2.7044856195	-3.8772841493
H40	2.0213414426	-2.3458777781	-5.3573703308
H41	-0.0692266509	-5.3107963494	-3.7354231122
H42	0.7435518197	-4.0036862346	-2.8432504802
H43	-0.1707979132	-3.6393724383	-4.3363524863

special geometric constraints coord value target

Ge10-C13-S14-C15	179.99734	180.00000
Ge7-Ge10-C13-S14	-180.00643	180.00000
Ge4-Ge7-Ge10-C13	-180.00537	180.00000
C3-Ge4-Ge7-Ge10	180.00709	180.00000
S1-C3-Ge4-Ge7	-180.01036	180.00000
C2-S1-C3-Ge4	-179.99945	180.00000

nuclear repulsion energy..... 1012.910452145 hartrees

Ge4
Total energy: -1289.324892 hartrees

Final geometry:

	angstroms		
atom	x	y	z
S1	10.1367142928	1.9697579868	-7.9826824037
C2	10.5555682985	3.7418424862	-7.8264908324
C3	8.4995651739	1.9360339048	-7.1697632628
Ge4	7.6915410286	0.0973403910	-7.1448135678
C5	7.4935355327	-0.5298944367	-9.0147717630
C6	8.9171432804	-1.1176911761	-6.1697879094
Ge7	5.4666564619	0.3236108033	-5.9840031893
C8	4.3637287232	1.6497163346	-6.9875341481
C9	5.7817301647	1.0650603141	-4.1582266493
Ge10	4.2141325572	-1.8475490565	-5.8050044485
C11	3.8981893611	-2.5894066193	-7.6304129347
C12	5.3164901753	-3.1741174950	-4.8012550349
Ge13	1.9895374936	-1.6190318069	-4.6438113323
C14	0.7644910794	-0.4042031119	-5.6198409240
C15	2.1879941770	-0.9902529367	-2.7743542212
C16	1.1799031599	-3.4570540209	-4.6172836514
S17	-0.4572033577	-3.4886169068	-3.8040974177
C18	-0.8776638744	-5.2604854013	-3.9588274322
H19	11.5289810118	3.8860654134	-8.3023127127
H20	9.8165713369	4.3670779291	-8.3355215381
H21	10.6277364837	4.0376406949	-6.7760589855
H22	8.5958495367	2.2900739737	-6.1369493913
H23	7.8151507927	2.6116822232	-7.6955463017
H24	7.0917219944	-1.5471505876	-9.0447157863
H25	6.8177457898	0.1191929866	-9.5791078320
H26	8.4646047738	-0.5276477476	-9.5189144900
H27	9.0444537931	-0.7991599344	-5.1311357239
H28	8.5309811314	-2.1414212944	-6.1664590406
H29	9.9023718848	-1.1223435279	-6.6456210604
H30	3.4090776936	1.8222916308	-6.4809339967
H31	4.8862483195	2.6088255010	-7.0601349143
H32	4.1507169771	1.3015624317	-8.0022425619
H33	6.3820705103	0.3816972424	-3.5509350927
H34	6.3109256924	2.0214514452	-4.2170177299
H35	4.8330126144	1.2348322641	-3.6396745955
H36	3.3682979862	-3.5453826244	-7.5711764304
H37	3.2982411055	-1.9058455446	-8.2378491277
H38	4.8467048893	-2.7600719377	-8.1490201638
H39	6.2706717325	-3.3479215868	-5.3083099330
H40	4.7931762011	-4.1327208384	-4.7276175383

H41	5.5304741689	-2.8254822017	-3.7869248196
H42	0.6362934734	-0.7242058683	-6.6579368865
H43	1.1515084909	0.6191913930	-5.6249684740
H44	-0.2204601214	-0.3979998947	-5.1434619169
H45	2.5877488226	0.0278537760	-2.7453772793
H46	2.8655738165	-1.6375739796	-2.2101263719
H47	1.2173212068	-0.9941707490	-2.2694634968
H48	1.0832084067	-3.8118644208	-5.6497926972
H49	1.8636851509	-4.1329439829	-4.0910205901
H50	-1.8554763840	-5.4017753707	-3.4912107456
H51	-0.9409906741	-5.5593263451	-5.0089770473
H52	-0.1442160961	-5.8853569203	-3.4413990071

special geometric constraints	coord	value	target
	Ge13-C16-S17-C18	-180.00100	180.00000
	Ge10-Ge13-C16-S17	180.00513	180.00000
	Ge7-Ge10-Ge13-C16	-179.98589	180.00000
	Ge4-Ge7-Ge10-Ge13	-180.00139	180.00000
	C3-Ge4-Ge7-Ge10	180.00260	180.00000
	S1-C3-Ge4-Ge7	-179.99713	180.00000
	C2-S1-C3-Ge4	-179.99999	180.00000

nuclear repulsion energy..... 1278.963713076 hartrees

Ge5

Total energy: -1372.950311 hartrees

Final geometry:

	angstroms		
atom	x	y	z
Ge1	2.9612153489	11.9184684643	3.0505542755
Ge2	3.2047856926	14.4114550502	2.7815223132
C3	4.4307493593	14.7405543434	1.2408063734
C4	4.1064212740	15.1126744188	4.4188035959
Ge5	1.0373602600	15.6404404610	2.4165960902
C6	0.1416829310	14.9360013618	0.7802857478
C7	-0.1798629100	15.3112270748	3.9613469004
Ge8	1.4192138369	18.1158838438	2.1635701234
C9	2.6403495669	18.4525477247	0.6205941606
C10	2.3175847934	18.8261929681	3.7985617620
Ge11	-0.6739220761	19.4674314345	1.7914348847
C12	-1.6093861892	18.9618320014	0.1191808155
C13	-1.9326348730	19.3405838512	3.3168835224

C14	-0.0516338190	21.3705943444	1.6301224560
S15	-1.4250425377	22.5442963581	1.3521556008
C16	-0.5048231075	24.1208443477	1.2597215424
C17	4.8290885196	11.2307470489	3.3213126503
S18	4.8917187037	9.4171642058	3.5413847721
C19	6.6899213505	9.1678992451	3.7533995013
C20	2.1978558383	11.0574825431	1.4372392727
C21	1.8735205528	11.4353902625	4.6350052881
H22	4.6547085314	15.8071321364	1.1431119177
H23	5.3772292217	14.2087752429	1.3813438302
H24	3.9870926979	14.4004716051	0.3007110326
H25	4.3321623896	16.1780632179	4.3125364419
H26	3.4760242664	14.9870250280	5.3037447370
H27	5.0487430290	14.5843384131	4.5956501398
H28	-0.8151328100	15.4414905276	0.6156329458
H29	0.7616679002	15.0870973433	-0.1079308637
H30	-0.0541235841	13.8635577708	0.8783775669
H31	-1.1391540719	15.8168000980	3.8119954497
H32	-0.3756271980	14.2406142722	4.0777454352
H33	0.2551631431	15.6793442729	4.8948246324
H34	2.8119085399	19.5260841263	0.4924103614
H35	3.6107091487	17.9729007469	0.7806489891
H36	2.2198734139	18.0628399838	-0.3108639101
H37	2.4869334172	19.9038207176	3.7073036959
H38	1.7109223745	18.6527588121	4.6919410905
H39	3.2881398311	18.3440605815	3.9496890530
H40	-2.4541073993	19.6336698870	-0.0605289005
H41	-0.9379316085	19.0246183718	-0.7420084067
H42	-1.9902199685	17.9378532869	0.1794100566
H43	-2.7793811787	20.0170890017	3.1666272523
H44	-2.3191965688	18.3222079913	3.4202883143
H45	-1.4427269954	19.6150928237	4.2555432853
H46	0.6588775430	21.4355949361	0.7980058793
H47	0.4807015043	21.6417436505	2.5491314820
H48	-1.2380312512	24.9130274512	1.0877566110
H49	0.0225228420	24.3237324671	2.1961975693
H50	0.2079338697	24.1119068161	0.4301710520
H51	5.4342207118	11.5146532601	2.4525388401
H52	5.2563363618	11.7210912735	4.2036814883
H53	6.8526215605	8.0967909570	3.8979103892
H54	7.2392802203	9.4927980570	2.8652232284
H55	7.0601873345	9.7039016797	4.6319438949
H56	2.2001977888	9.9693260821	1.5517883577
H57	1.1670119887	11.3843683168	1.2710119831
H58	2.7809616700	11.3050079497	0.5455235679
H59	1.8735077709	10.3505889156	4.7779317673

H60	2.2738957003	11.8961914262	5.5426621618
H61	0.8379493691	11.7670769526	4.5136929313

special geometric constraints coord value target

Ge11-C14-S15-C16	179.99733	180.00000
Ge8-Ge11-C14-S15	-179.99809	180.00000
Ge5-Ge8-Ge11-C14	180.00582	180.00000
Ge2-Ge5-Ge8-Ge11	-180.00753	180.00000
Ge1-Ge2-Ge5-Ge8	180.00251	180.00000
Ge5-Ge2-Ge1-C17	180.00097	180.00000
Ge2-Ge1-C17-S18	180.00000	180.00000
Ge1-C17-S18-C19	180.00000	180.00000

nuclear repulsion energy..... 1562.138843648 hartrees

Ge6

Total energy: -1456.576094 hartrees

Final geometry:

angstroms

atom	x	y	z
Ge1	5.8583622461	11.7484660045	3.2238177265
Ge2	3.5573308502	12.7173631109	2.8781830165
Ge3	3.5425775501	15.2247436501	2.6425989847
C4	4.6948395837	15.7387607377	1.0975057943
C5	4.3414007889	16.0351593197	4.2808774053
Ge6	1.2158751762	16.1405608077	2.2990199795
C7	0.4182517656	15.3305307715	0.6600016800
C8	0.0633687387	15.6250301667	3.8432602896
Ge9	1.2006807251	18.6479430657	2.0632873524
C10	2.3349309338	19.1901875576	0.5131363333
C11	1.9821206783	19.4872488029	3.6967791979
Ge12	-1.0997982822	19.6182670446	1.7175104122
C13	-1.9473826742	18.9614674740	0.0504481687
C14	-2.3013241797	19.2615423708	3.2532447952
C15	-0.8354870311	21.6035454652	1.5615367869
S16	-2.4037523491	22.5060270574	1.3035333395
C17	-1.7921197718	24.2262288428	1.2108134088
C18	5.5965543131	9.7628502619	3.3800427438
S19	7.1663356784	8.8622059966	3.6381981017
C20	6.5560566337	7.1418195468	3.7310234654
C21	7.0593243309	12.1066428826	1.6879982511
C22	6.7056973357	12.4068179487	4.8904316901
C23	2.7763752911	11.8793305280	1.2437817166
C24	2.4222753074	12.1747450992	4.4275962551

H25	4.7553573132	16.8276374487	1.0054961093
H26	5.7110793673	15.3534266872	1.2278424042
H27	4.3003500816	15.3413924584	0.1579635306
H28	4.4051230669	17.1232783214	4.1824616691
H29	3.7423905106	15.8103419660	5.1679325402
H30	5.3524929780	15.6509730362	4.4488923079
H31	-0.5929449601	15.7143169519	0.4917220449
H32	1.0176875673	15.5562653499	-0.2265261198
H33	0.3550864721	14.2423085492	0.7577140911
H34	-0.9528042724	16.0106068948	3.7132953392
H35	0.0028220606	14.5360290288	3.9338024189
H36	0.4578363615	16.0211480094	4.7833142735
H37	2.3334792185	20.2786294221	0.3964621524
H38	3.3706370980	18.8679324024	0.6579925324
H39	1.9706118882	18.7488738001	-0.4189643158
H40	1.9796542414	20.5783602196	3.6084964264
H41	1.4137863123	19.2183269241	4.5917701829
H42	3.0170173829	19.1630091424	3.8429759394
H43	-2.8980508396	19.4758419513	-0.1195902728
H44	-1.3049308394	19.1427540808	-0.8160894289
H45	-2.1429620983	17.8864397171	0.1092386316
H46	-3.2567775901	19.7764779782	3.1146455391
H47	-2.4988210384	18.1899679268	3.3538220367
H48	-1.8594937687	19.6146840792	4.1895005005
H49	-0.1577556248	21.8004332583	0.7230451864
H50	-0.3522249344	21.9639307604	2.4768237525
H51	-2.6621645777	24.8701584910	1.0574344385
H52	-1.2952481510	24.5175736144	2.1406765909
H53	-1.1040701911	24.3541317488	0.3702021378
H54	5.1137150329	9.4015368970	2.4647657740
H55	4.9190738179	9.5649786325	4.2186554332
H56	7.4260976143	6.4989981117	3.8878984733
H57	5.8656252069	7.0142141823	4.5696211242
H58	6.0625190892	6.8488262777	2.8000028529
H59	8.0157956370	11.5937342495	1.8271355219
H60	6.6183290834	11.7518487444	0.7519787264
H61	7.2547088230	13.1784657254	1.5866773798
H62	7.6570575951	11.8936353948	5.0602529867
H63	6.8999811535	13.4819960824	4.8312587420
H64	6.0638071315	12.2249969369	5.7572791157
H65	1.7415860972	12.2038989267	1.0974128578
H66	3.3451597209	12.1489185958	0.3492623796
H67	2.7785911582	10.7880996932	1.3311354673
H68	1.3866216499	12.4970285822	4.2822383244
H69	2.4236553799	11.0862423981	4.5440819253
H70	2.7860969711	12.6159319369	5.3599738483

special geometric constraints	coord	value	target
	Ge12-C15-S16-C17	-180.00092	180.00000
	Ge9-Ge12-C15-S16	180.00709	180.00000
	Ge6-Ge9-Ge12-C15	179.99950	180.00000
	Ge3-Ge6-Ge9-Ge12	179.99953	180.00000
	Ge2-Ge3-Ge6-Ge9	180.00242	180.00000
	Ge1-Ge2-Ge3-Ge6	179.99880	180.00000
	Ge3-Ge2-Ge1-C18	180.00000	180.00000
	Ge2-Ge1-C18-S19	-180.00000	180.00000
	Ge1-C18-S19-C20	180.00000	180.00000

nuclear repulsion energy..... 1860.850066980 hartrees

Ge7

Total energy: -1540.201593 hartrees

Final geometry:

angstroms

atom	x	y	z
Ge1	4.9552945202	11.5365103001	3.4739332309
Ge2	4.8446803088	9.0543804513	3.8316357116
Ge3	2.7155108453	12.6305289463	3.1030003020
Ge4	2.9262426292	15.1206822332	2.7534385774
C5	4.1148787778	15.4418638171	1.1846535090
C6	3.8117655698	15.9270847178	4.3522919547
Ge7	0.7462702953	16.3299160679	2.3720224839
C8	-0.1648283051	15.6155053732	0.7497143891
C9	-0.4730027223	16.0504981198	3.9227647068
Ge10	1.1162727627	18.7950995402	2.0407103435
C11	2.2836223925	19.0830483931	0.4491817273
C12	2.0377363856	19.5967914697	3.6184930200
Ge13	-0.9900579183	20.1166917633	1.6488675705
C14	-1.9319264809	19.5617996825	-0.0058058931
C15	-2.2464666772	20.0359380453	3.1795379253
C16	-0.3691063718	22.0118346693	1.4233671902
S17	-1.7382448123	23.1839524426	1.1188759199
C18	-0.8060268701	24.7480685782	0.9734690152
C19	6.7557165411	8.5058893013	4.0910499626
S20	6.9591808371	6.7097943233	4.3763076151
C21	8.7737674143	6.6203912284	4.5586672896
C22	4.1188416806	8.0986105774	2.2538932269

C23	3.8109922911	8.5521357395	5.4471760462
C24	6.1220025711	11.8377373437	1.8809989439
C25	5.8786156298	12.3280357140	5.0549119296
C26	1.8707617401	11.7910118309	1.5065070776
C27	1.5302330216	12.2792138503	4.6652085774
H28	4.2953089837	16.5149167252	1.0477992825
H29	5.0814418604	14.9552645373	1.3205566125
H30	3.6648241370	15.0512562064	0.2674680527
H31	3.9655982812	17.0009968366	4.2108578538
H32	3.2062779292	15.7870703938	5.2516840225
H33	4.7896872516	15.4689048718	4.5272963072
H34	-1.1398510737	16.0957469651	0.6213966388
H35	0.4284918940	15.8052870959	-0.1486110692
H36	-0.3266788209	14.5359297408	0.8272438928
H37	-1.4261592693	16.5636831083	3.7630855113
H38	-0.6818560193	14.9861390526	4.0675649344
H39	-0.0293433806	16.4370920163	4.8438132190
H40	2.4321736904	20.1529201640	0.2724346534
H41	3.2659594850	18.6239796504	0.5949114564
H42	1.8382722270	18.6490417117	-0.4506701916
H43	2.2098701395	20.6659126199	3.4577554075
H44	1.4399598552	19.4825104380	4.5271063015
H45	3.0080110467	19.1211377012	3.7891585332
H46	-2.7621733717	20.2430163788	-0.2166298410
H47	-1.2588806420	19.5737217386	-0.8676793265
H48	-2.3361282509	18.5498711968	0.0951920165
H49	-3.0866790034	20.7185357034	3.0183947848
H50	-2.6456044563	19.0244066650	3.3022304153
H51	-1.7532334507	20.3221142597	4.1125938457
H52	0.3367492135	22.0454241680	0.5852338621
H53	0.1701424923	22.3106879336	2.3294932660
H54	-1.5332508145	25.5330253459	0.7505662466
H55	-0.2987177852	24.9886616933	1.9124165196
H56	-0.0750452702	24.7010668748	0.1607572582
H57	7.1603079157	9.0606408576	4.9456204565
H58	7.3229025603	8.8012447102	3.2006102941
H59	9.0277349312	5.5783580515	4.7671948082
H60	9.2728161069	6.9283331177	3.6352042356
H61	9.1167125121	7.2456284921	5.3877594850
H62	4.2052607143	7.0171894786	2.3943085629
H63	3.0630929897	8.3416231696	2.1003704058
H64	4.6640080357	8.3661312967	1.3444736690
H65	3.8845536847	7.4748637652	5.6242230110
H66	4.1903238371	9.0670035052	6.3343063557
H67	2.7537321017	8.8094124626	5.3311317082
H68	6.2705482397	12.9054696216	1.6979753356

H69	7.1059734305	11.3812623221	2.0316630540
H70	5.6807445749	11.3993064785	0.9806133463
H71	6.0332513569	13.4022569369	4.9193492507
H72	5.2947533077	12.1825739190	5.9686355150
H73	6.8583448481	11.8612926470	5.2008749896
H74	0.8729599709	12.2043960527	1.3293926191
H75	2.4746133122	11.9614975934	0.6112519673
H76	1.7690221428	10.7101350793	1.6460196385
H77	0.5272390958	12.6803453497	4.4883851025
H78	1.4386590965	11.2041916012	4.8513422324
H79	1.9257442596	12.7485403020	5.5694028987

special geometric constraints	coord	value	target
Ge13-C16-S17-C18		179.96241	180.00000
Ge10-Ge13-C16-S17		179.89724	180.00000
Ge7-Ge10-Ge13-C16		-179.93956	180.00000
Ge4-Ge7-Ge10-Ge13		179.98550	180.00000
Ge3-Ge4-Ge7-Ge10		-179.99463	180.00000
Ge1-Ge3-Ge4-Ge7		-179.97469	180.00000
Ge2-Ge1-Ge3-Ge4		179.99999	180.00000
Ge3-Ge1-Ge2-C19		180.00000	180.00000
Ge1-Ge2-C19-S20		180.00000	180.00000
Ge2-C19-S20-C21		180.00000	180.00000

nuclear repulsion energy..... 2173.770807278 hartrees

Ge8

Total energy: -1623.827251 hartrees

Final geometry:

	angstroms		
atom	x	y	z
Ge1	5.3777948879	11.9855277233	2.9735981222
Ge2	5.2900335693	9.4869254362	3.2877551466
Ge3	3.0714693574	13.0017279397	2.7968569895
Ge4	3.1360518633	15.5057757286	2.4815266248
C5	4.1668496044	15.9336299172	0.8276484392
C6	4.1003532190	16.3370245953	4.0178633732
Ge7	0.8308212734	16.5241209941	2.3045820806
C8	-0.1455372389	15.7154135156	0.7643665282
C9	-0.2135454791	16.1168910996	3.9548202776
Ge10	0.9249761522	19.0223909416	1.9905106300
C11	1.9513535808	19.4612574407	0.3354295626
C12	1.8839328499	19.8645235588	3.5256753947
Ge13	-1.3380781152	20.1178412744	1.8047195752

C14	-2.3614279664	19.4713871229	0.2349921893
C15	-2.4247999872	19.8781468270	3.4452319094
C16	-0.9655873879	22.0773074602	1.5646147665
S17	-2.4890240941	23.0751266355	1.4067586045
C18	-1.7761333067	24.7466583142	1.2101176491
Ge19	7.5578906039	8.4012885385	3.4724733975
C20	7.1961999864	6.4398076972	3.7129741859
S21	8.7256766251	5.4510962895	3.8699951266
C22	8.0231701205	3.7752655298	4.0672440661
C23	8.5789345454	9.0529909361	5.0415987340
C24	8.6427444405	8.6464507987	1.8315291037
C25	4.3331529356	8.6419167126	1.7530063240
C26	4.2661905706	9.0448557405	4.9435103745
C27	6.4215954722	12.3943584544	1.3233625398
C28	6.3535160003	12.7955152175	4.5137997865
C29	2.1072938345	12.1707939115	1.2604327927
C30	2.0407417042	12.5730615419	4.4505503434
H31	4.2429752773	17.0163877521	0.6878410940
H32	5.1817636731	15.5286568787	0.8885888291
H33	3.6870756752	15.5110656163	-0.0597877421
H34	4.1780925095	17.4207182008	3.8859928145
H35	3.5812405855	16.1477923454	4.9618929256
H36	5.1141017403	15.9334208727	4.1026125514
H37	-1.1444875581	16.1522668312	0.6672133207
H38	0.3886005131	15.8803578231	-0.1756847569
H39	-0.2607719099	14.6359379359	0.9031334087
H40	-1.2141688311	16.5571218974	3.8980684259
H41	-0.3267250078	15.0359633258	4.0838878330
H42	0.2805716946	16.5139863992	4.8461725174
H43	1.9894554121	20.5444307631	0.1810333059
H44	2.9799669159	19.0947708945	0.4072377619
H45	1.4921757723	19.0088766531	-0.5482342016
H46	1.9232520171	20.9521132256	3.4062865788
H47	1.3847232593	19.6454935989	4.4740138855
H48	2.9120296515	19.4953399400	3.5914815396
H49	-3.2941207853	20.0342451998	0.1322368392
H50	-1.7875954692	19.5963927674	-0.6878383800
H51	-2.6089899874	18.4107671972	0.3398735066
H52	-3.3575327675	20.4451399704	3.3686482878
H53	-2.6741740740	18.8237712816	3.5981623032
H54	-1.8860170689	20.2312229075	4.3293634016
H55	-0.3489122374	22.2073438531	0.6677557604
H56	-0.3856413918	22.4294051069	2.4256114666
H57	-2.6115177962	25.4436207047	1.1044302452
H58	-1.1881641109	25.0291632094	2.0880548533
H59	-1.1512517605	24.8045589909	0.3143195003

H60	6.6178052782	6.0842267730	2.8524051979
H61	6.5808882730	6.3063696592	4.6102742892
H62	8.8625888559	3.0852900887	4.1859839901
H63	7.3885166383	3.7170376997	4.9561299771
H64	7.4475396069	3.4838390693	3.1840688645
H65	9.5141155379	8.4942287711	5.1443425314
H66	8.8218868224	10.1146410727	4.9360897202
H67	8.0059507300	8.9260019868	5.9647323683
H68	9.5779498225	8.0834747670	1.9074166744
H69	8.1051212142	8.2915341239	0.9474772449
H70	8.8875094761	9.7019526825	1.6790556490
H71	4.2967212209	7.5543182934	1.8726539921
H72	3.3041475105	9.0083948211	1.6872206898
H73	4.8316868165	8.8620072199	0.8046472563
H74	4.2308007476	7.9615117386	5.0973931047
H75	4.7252334776	9.4978409771	5.8269942577
H76	3.2366517020	9.4090200405	4.8729390821
H77	6.5340733486	13.4753992492	1.1948251873
H78	7.4225306467	11.9548090332	1.3797625831
H79	5.9276685376	11.9974041846	0.4319131576
H80	6.4674784500	13.8751761502	4.3750426505
H81	5.8196665195	12.6299565016	5.4540013203
H82	7.3530840227	12.3599142627	4.6109708968
H83	1.0931871690	12.5736280349	1.1765252330
H84	2.6257494505	12.3612765990	0.3164171243
H85	2.0305604763	11.0870029672	1.3915114135
H86	1.0255728353	12.9774777157	4.3895761944
H87	1.9652391652	11.4902187495	4.5901811906
H88	2.5201607584	12.9958176907	5.3381649522

special geometric constraints	coord	value	target
Ge13-C16-S17-C18	-179.99915	180.00000	
Ge10-Ge13-C16-S17	180.00518	180.00000	
Ge7-Ge10-Ge13-C16	180.00000	180.00000	
Ge4-Ge7-Ge10-Ge13	180.00067	180.00000	
Ge3-Ge4-Ge7-Ge10	-179.99782	180.00000	
Ge1-Ge3-Ge4-Ge7	180.00110	180.00000	
Ge2-Ge1-Ge3-Ge4	180.00000	180.00000	
Ge3-Ge1-Ge2-Ge19	180.00000	180.00000	
Ge1-Ge2-Ge19-C20	180.00000	180.00000	
Ge2-Ge19-C20-S21	180.00000	180.00000	
Ge19-C20-S21-C22	-180.00000	180.00000	

nuclear repulsion energy..... 2496.798643715 hartrees

Ge9
Total energy: -1707.452732 hartrees

Final geometry

	angstroms		
atom	x	y	z
Ge1	1.7370981997	7.2115188479	1.8309602044
Ge2	3.6984684152	5.8423367184	2.6346675858
Ge3	-0.2069931276	5.8059934566	1.0369613835
Ge4	-2.1575048043	7.2339214925	0.2939160484
C5	-1.5623706660	8.4508125546	-1.1709586222
C6	-2.7360881182	8.3848871561	1.8222539138
Ge7	-4.1501270419	5.9096125981	-0.5177067600
C8	-3.6192938477	4.7542000210	-2.0547457827
C9	-4.8008600088	4.7076971345	0.9346399701
Ge10	-6.0320226155	7.4248779126	-1.2320160795
C11	-5.4135649009	8.6361770096	-2.6934831578
C12	-6.5858534810	8.5817548724	0.2978810425
Ge13	-8.0862282365	6.2222561286	-2.0656533530
C14	-7.7145942105	5.1430756086	-3.6867476865
C15	-8.9132038767	5.0740740591	-0.6772454038
C16	-9.3820712483	7.6801254696	-2.5496911180
S17	-10.9711160685	7.0399021923	-3.1890814469
C18	-11.8564170868	8.6062724103	-3.5090020444
Ge19	5.6095895838	7.3024374176	3.3926167850
Ge20	7.6222750485	6.0190831772	4.2016167020
C21	8.9713464721	7.4160426234	4.7163990437
S22	10.5363929969	6.7016769744	5.3340059782
C23	11.4842497440	8.2256925538	5.6807045882
C24	8.4078959869	4.8767808369	2.7841803416
C25	7.2170292885	4.9104475744	5.7942503518
C26	5.0063607882	8.4875464664	4.8822224216
C27	6.2049601069	8.4873639261	1.8986249652
C28	4.3284977083	4.6427178563	1.1715483320
C29	3.1361748000	4.6795269475	4.1561074360
C30	2.3431871784	8.3863257051	0.3396445687
C31	1.1340819966	8.3946190970	3.3204453569
C32	0.3876914000	4.6415123493	-0.4701781290
C33	-0.7989432544	4.6090020843	2.5170585000
H34	-2.3832265898	9.0986692444	-1.4931588372
H35	-0.7395820214	9.0899589649	-0.8353696250
H36	-1.2173900599	7.8846334612	-2.0407505958
H37	-3.5623977714	9.0390696742	1.5264730965
H38	-3.0722804186	7.7807876871	2.6700835343
H39	-1.9118711070	9.0180423480	2.1647730934
H40	-4.4726838705	4.1700672922	-2.4128392266

H41	-3.2428678189	5.3502047535	-2.8907251537
H42	-2.8322689200	4.0543979176	-1.7569569297
H43	-5.6629746615	4.1235580428	0.5971006082
H44	-4.0155888994	4.0077865080	1.2366968170
H45	-5.1042375917	5.2779338032	1.8173400821
H46	-6.2296078719	9.2829972738	-3.0299655417
H47	-4.5991954820	9.2787995766	-2.3464078208
H48	-5.0525979153	8.0676440471	-3.5547178346
H49	-7.4169794276	9.2329278584	0.0083382872
H50	-6.9081885665	7.9815959613	1.1537381734
H51	-5.7578394190	9.2186888950	0.6243887743
H52	-8.6432802266	4.7262334781	-4.0880118052
H53	-7.2532506905	5.7542555799	-4.4680829038
H54	-7.0353491095	4.3164521126	-3.4581639808
H55	-9.8589122957	4.6600183431	-1.0403091082
H56	-8.2518176604	4.2436904300	-0.4125629611
H57	-9.1215726675	5.6455426919	0.2321379321
H58	-8.9157280160	8.3228925735	-3.3058089831
H59	-9.5682431538	8.2905060227	-1.6580958817
H60	-12.8425409604	8.3462339855	-3.9015056429
H61	-11.9849330487	9.1775858428	-2.5853752837
H62	-11.3298717046	9.2150663086	-4.2493910865
H63	8.5314773780	8.0564065842	5.4898341275
H64	9.1772798724	8.0414887967	3.8395742545
H65	12.4556104295	7.9196020619	6.0777024677
H66	11.6430262729	8.8061180404	4.7673364117
H67	10.9767863231	8.8440549206	6.4266982224
H68	9.3385683157	4.4216210986	3.1359781746
H69	7.7175359027	4.0761187460	2.5022469256
H70	8.6352438458	5.4601681503	1.8868652037
H71	8.1318922347	4.4525811575	6.1816701970
H72	6.7772781460	5.5154541417	6.5923973105
H73	6.5109682724	4.1128403552	5.5447371760
H74	5.8340648669	9.1075167017	5.2412909271
H75	4.2060472049	9.1550522196	4.5474953111
H76	4.6292788255	7.9038249631	5.7266304539
H77	7.0492533937	9.1093065866	2.2134558424
H78	6.5208280706	7.9032959120	1.0291001116
H79	5.3956059691	9.1531054864	1.5828271709
H80	5.1776476733	4.0384664724	1.5054788312
H81	3.5300581813	3.9620069292	0.8612278966
H82	4.6444610972	5.2153938978	0.2949111987
H83	3.9751628274	4.0699230488	4.5060563042
H84	2.7746139725	5.2733343213	5.0002178924
H85	2.3327395450	4.0031358167	3.8494882087
H86	1.5267687380	9.0291671596	-0.0034541803

H87	3.1680279205	9.0286194230	0.6622894855
H88	2.6894978609	7.7945967423	-0.5124457859
H89	0.3136806564	9.0420379531	2.9969675544
H90	0.7849585810	7.8078273126	4.1744654346
H91	1.9533926542	9.0345584909	3.6626673768
H92	-0.4383597586	4.0185838429	-0.8274648880
H93	0.7516067340	5.2361484388	-1.3132693805
H94	1.1972795009	3.9781040680	-0.1502595940
H95	-1.6223745946	3.9673013478	2.1890567698
H96	0.0224554943	3.9647314828	2.8448852223
H97	-1.1421460183	5.1847443569	3.3811073472

special geometric constraints	coord	value	target
	Ge20-C21-S22-C23	179.69581	180.00000
	Ge19-Ge20-C21-S22	-179.74630	180.00000
	Ge2-Ge19-Ge20-C21	179.48210	180.00000
	Ge1-Ge2-Ge19-Ge20	-179.66217	180.00000
	Ge3-Ge1-Ge2-Ge19	179.49033	180.00000
	Ge2-Ge1-Ge3-Ge4	178.72881	180.00000
	Ge1-Ge3-Ge4-Ge7	-179.99997	180.00000
	Ge3-Ge4-Ge7-Ge10	-180.00000	180.00000
	Ge4-Ge7-Ge10-Ge13	179.99999	180.00000
	Ge7-Ge10-Ge13-C16	-180.00000	180.00000
	Ge10-Ge13-C16-S17	179.99999	180.00000
	Ge13-C16-S17-C18	-180.00000	180.00000

nuclear repulsion energy..... 2831.333234048 hartrees

Ge10

Total energy: -1791.078564 hartrees

Final geometry:

	angstroms		
atom	x	y	z
Ge1	1.6742828802	7.7948621872	1.4534153277
Ge2	3.6762197650	6.4449513735	2.2066395480
Ge3	-0.2925314145	6.3082529853	0.8659883817
Ge4	-2.3362865035	7.5929761315	0.1020956081
C5	-1.8704553564	8.6868004909	-1.5007295053
C6	-2.9041861670	8.8510928710	1.5418978577
Ge7	-4.2855039288	6.0806680488	-0.4771330193
C8	-3.7568096235	4.8206115870	-1.9297778855
C9	-4.7872423598	4.9816275642	1.1107623354
Ge10	-6.3134857477	7.3790824447	-1.2363228771

C11	-5.8644511720	8.4733616958	-2.8453632436
C12	-6.8980356482	8.6394859510	0.1981404365
Ge13	-8.2997940922	5.9343140491	-1.8313993200
C14	-7.9251153577	4.7109811028	-3.3462709909
C15	-8.9601710475	4.8789137628	-0.2880038484
C16	-9.7405848828	7.2197703658	-2.3906435855
S17	-11.2919848408	6.3804098006	-2.8709145621
C18	-12.3319922370	7.8201906142	-3.3024570591
Ge19	5.6940749007	7.8489048856	2.8158868552
Ge20	7.6358011068	6.4095193195	3.5535124662
Ge21	9.7156598958	7.6945415389	4.1902719908
C22	11.0544329949	6.2914155882	4.7211255877
S23	12.6621083678	6.9977522699	5.2288893698
C24	13.5869836889	5.4717660399	5.6258188428
C25	9.4233922917	8.9018607384	5.7355305598
C26	10.4596488067	8.7359524398	2.6759417289
C27	8.1421197562	5.1449704697	2.0928753605
C28	7.1089604818	5.3078093910	5.1338820627
C29	5.2287110643	9.1079173303	4.2919661743
C30	6.2641895181	8.9434762160	1.2484066132
C31	4.1918029547	5.1813850423	0.7515086385
C32	3.1627231513	5.3447164078	3.7892761272
C33	2.1818846111	8.8885279325	-0.1368669442
C34	1.1480122189	9.0548847219	2.9087144568
C35	0.2511581619	5.0451227445	-0.5786713860
C36	-0.7783103266	5.2078076379	2.4568432068
H37	-2.7348607662	9.2666576703	-1.8385703604
H38	-1.0621450258	9.3874417752	-1.2693267929
H39	-1.5425306362	8.0540704481	-2.3305165000
H40	-3.7749708288	9.4336454600	1.2260148458
H41	-3.1705977364	8.3125858332	2.4557061502
H42	-2.0979572879	9.5505270208	1.7833182931
H43	-4.5926319922	4.1656073449	-2.1961109581
H44	-3.4490313640	5.3599744830	-2.8297287680
H45	-2.9214648234	4.1907727975	-1.6092731632
H46	-5.6338748589	4.3282415707	0.8767171560
H47	-3.9494468933	4.3510765852	1.4247873421
H48	-5.0713112715	5.6135844492	1.9570620108
H49	-6.7461606151	9.0172571484	-3.1993553918
H50	-5.0865637810	9.2068805317	-2.6121795824
H51	-5.5025721653	7.8446943865	-3.6641016694
H52	-7.7943715401	9.1863600693	-0.1117298579
H53	-7.1295753424	8.1060333269	1.1245923952
H54	-6.1142616484	9.3715400154	0.4156898713
H55	-8.8395601214	4.1886875192	-3.6436661360
H56	-7.5512192595	5.2603716969	-4.2150838206

H57	-7.1757578310	3.9636030262	-3.0682659473
H58	-9.8849069009	4.3584757110	-0.5552336176
H59	-8.2208947757	4.1328717469	0.0191322747
H60	-9.1700801353	5.5229922457	0.5708009799
H61	-9.3696739466	7.8126874956	-3.2346397630
H62	-9.9384550048	7.9051380732	-1.5584505952
H63	-13.3069594425	7.4338725290	-3.6109013140
H64	-12.4688791010	8.4789186846	-2.4401094657
H65	-11.8966335771	8.3851068953	-4.1316991367
H66	11.2049362130	5.6146391086	3.8721384538
H67	10.6356264776	5.7061647315	5.5479059972
H68	14.5864976076	5.7742253959	5.9489846236
H69	13.1046293586	4.9195538068	6.4374543937
H70	13.6790054276	4.8277519312	4.7465480471
H71	10.3718447030	9.3484196553	6.0492778315
H72	8.7314005927	9.7085547015	5.4752673360
H73	9.0066386284	8.3583427617	6.5884037675
H74	11.4180562757	9.1812842158	2.9597345318
H75	10.6275590814	8.0989151227	1.8027575898
H76	9.7781867228	9.5407256593	2.3838280446
H77	8.9994983341	4.5338507341	2.3928556329
H78	7.3130919476	4.4705749767	1.8574163488
H79	8.4117091019	5.6819895381	1.1788768276
H80	7.9515819561	4.6983996509	5.4762150168
H81	6.7859153107	5.9382941278	5.9673142388
H82	6.2855825494	4.6329884983	4.8805884138
H83	6.0984165959	9.7091838019	4.5757137371
H84	4.4315460940	9.7905236892	3.9809842595
H85	4.8856761949	8.5687656560	5.1796437938
H86	7.1446487796	9.5448054376	1.4967116677
H87	6.5171011828	8.3100967456	0.3933188673
H88	5.4643040065	9.6244819959	0.9410077986
H89	5.0374961557	4.5595752452	1.0604049279
H90	3.3573060240	4.5186691286	0.5016894638
H91	4.4802559332	5.7190290574	-0.1561386862
H92	4.0004703657	4.7202027500	4.1139222645
H93	2.8647725147	5.9763326339	4.6308511531
H94	2.3231329141	4.6859147082	3.5463308904
H95	1.3437178731	9.5135111403	-0.4603535542
H96	3.0237966924	9.5468078550	0.0997737324
H97	2.4751011109	8.2535829698	-0.9778676611
H98	0.3090611312	9.6825589093	2.5926670933
H99	0.8462463153	8.5153006399	3.8110320452
H100	1.9829974822	9.7122693760	3.1710211238
H101	-0.5726475777	4.3699754114	-0.8303047152
H102	0.5387605035	5.5821378002	-1.4868658489

H103	1.1033594692	4.4363489620	-0.2607024001
H104	-1.6091084096	4.5353157793	2.2215595589
H105	0.0710598591	4.5974255451	2.7792455826
H106	-1.0806258087	5.8385577349	3.2974827822

special geometric constraints coord value target

Ge13-C16-S17-C18	179.99388	180.00000
Ge10-Ge13-C16-S17	-179.98975	180.00000
Ge7-Ge10-Ge13-C16	-179.99920	180.00000
Ge3-Ge4-Ge7-Ge10	179.99780	180.00000
Ge4-Ge7-Ge10-Ge13	-179.99003	180.00000
Ge1-Ge3-Ge4-Ge7	-179.98082	180.00000
Ge2-Ge1-Ge3-Ge4	-179.99999	180.00000
Ge3-Ge1-Ge2-Ge19	179.99999	180.00000
Ge1-Ge2-Ge19-Ge20	-179.99999	180.00000
Ge2-Ge19-Ge20-Ge21	180.00000	180.00000
Ge19-Ge20-Ge21-C22	-180.00000	180.00000
Ge20-Ge21-C22-S23	180.00000	180.00000
Ge21-C22-S23-C24	-180.00000	180.00000

nuclear repulsion energy..... 3171.831122076 hartrees

References

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