

Supporting Information

Tetrasilane-Bridged Bicyclo[4.1.0]heptasil-1(6)-ene

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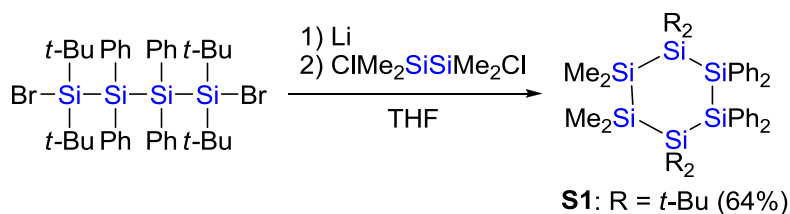
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1. Experimental Details

Reactions. All experiments were performed under a nitrogen or argon atmosphere unless otherwise noted. Lithium powder (Kanto) and sodium (Kanto) were purchased and used without further purification. Tetrahydrofuran (THF) was distilled from sodium benzophenone ketyl. Benzene was distilled from calcium hydride. Toluene, hexane, and benzene-*d*₆ used in a glovebox were dried over a potassium mirror, degassed by freeze–pump–thaw cycles, distilled in a vacuum line, and stored in the glovebox. Hydrogen chloride was generated by the addition of concentrated sulfuric acid to sodium chloride and dried by concentrated sulfuric acid. Aluminum chloride (Kanto) was purified by sublimation under reduced pressure. 1,4-Dibromo-1,1,4,4-tetra-*tert*-butyl-2,2,3,3-tetraphenyltetrasilane^{S1} and 1,2-dichloro-1,1,2,2-tetramethyldisilane^{S2} were prepared according to the reported procedures.

Measurements. ¹H (600 MHz), ¹³C (151 MHz), and ²⁹Si (119 MHz) NMR spectra were measured with a JEOL JNM-ECA600 spectrometer. IR spectra were recorded on a Shimadzu FTIR-8700 spectrophotometer. UV–visible spectra were measured on a JASCO V-570 spectrophotometer with a 1 mm quartz cell filled with argon. Mass spectra were recorded on a Shimadzu GCMS-QP2010 SE mass spectrometer. High-resolution mass spectra (APCI) were recorded on a Bruker Daltonics solariX Fourier transform ion cyclotron resonance mass spectrometer. Elemental analyses were performed in the Research and Analytical Center for Giant Molecules, Graduate School of Science, Tohoku University, Japan. All melting points except for **1** were measured on a Yazawa BY-2 micro melting point apparatus and were uncorrected. The melting point of **1** was measured under an argon atmosphere in a sealed tube on a Yanaco MP-J3 micro melting point apparatus and was uncorrected.

Synthesis of 1,1,4,4-Tetra-*tert*-butyl-2,2,3,3-tetramethyl-5,5,6,6-tetraphenylcyclohexasilane (S1).

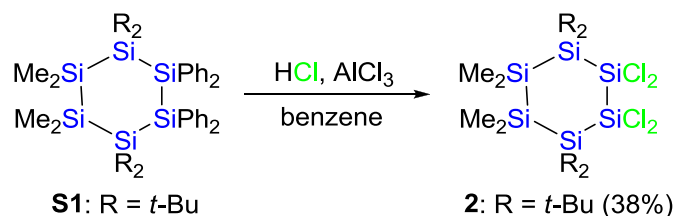


A mixture of 1,4-dibromo-1,1,4,4-tetra-*tert*-butyl-2,2,3,3-tetraphenyltetrasilane (6.00 g, 7.42 mmol) and lithium powder (0.526 g, 75.8 mmol) in THF (180 mL) was stirred at room temperature for 5 h. The mixture was added to a solution of 1,2-dichloro-1,1,2,2-tetramethyldisilane (3.05 g, 16.3 mmol) in THF (20 mL). After the mixture was stirred at room temperature overnight, the volatile

materials were removed under reduced pressure, and the residue was passed through a short column of silica gel (eluent: chloroform). The eluate was evaporated, and the residue was separated by column chromatography of silica gel with hexane–chloroform (10:1) ($R_f = 0.33$) to give **S1** (3.66 g, 64%) as colorless crystals.

S1. Mp: 284–285 °C. ^1H NMR (600 MHz, CDCl_3): δ 0.63 (s, 12H), 1.05 (s, 36H), 7.07 (t, 8H, $J = 7.2$ Hz), 7.17 (t, 4H, $J = 7.2$ Hz), 7.56 (d, 8H, $J = 7.2$ Hz). ^{13}C NMR (151 MHz, CDCl_3): δ 0.9, 25.7, 32.7, 127.1, 128.4, 136.2, 138.3. ^{29}Si NMR (119 MHz, CDCl_3): δ -39.4, -30.1, -8.2. IR (KBr): 3050, 2850, 1460, 1430, 1360, 1090, 840, 810, 790, 740, 700 cm^{-1} . MS (EI, 70 eV): m/z 764 (M^+ , 0.2), 707 (10), 549 (9), 259 (11), 197 (26), 135 (72), 73 (100). HRMS (APCI): found 764.39309 (M^+), calcd for $\text{C}_{44}\text{H}_{68}\text{Si}_6$ 764.39311.

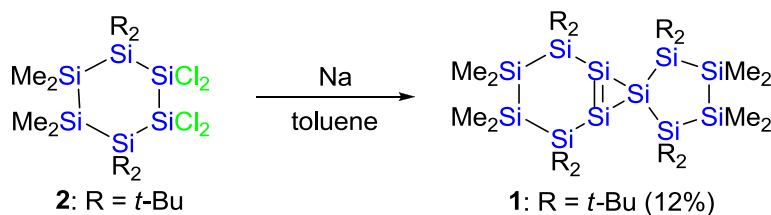
Synthesis of 1,1,4,4-Tetra-*tert*-butyl-2,2,3,3-tetrachloro-5,5,6,6-tetramethylcyclohexasilane (2).



Hydrogen chloride was passed through a mixture of **S1** (1.30 g, 1.70 mmol) and aluminum chloride (0.340 g, 2.55 mmol) in benzene (80 mL) at 35 °C for 2 h. The reaction was monitored by ^1H NMR spectroscopy. The solvent was removed under reduced pressure. Hexane was added, and insoluble materials were filtered off. The solvent of the filtrate was removed under reduced pressure, and the residue was washed with hexane to give **2** (0.387 g, 38%) as colorless crystals.

2. Mp: 228–230 °C. ^1H NMR (600 MHz, CDCl_3): δ 0.46 (s, 12H), 1.31 (s, 36H). ^{13}C NMR (151 MHz, CDCl_3): δ -0.7, 25.1, 31.7. ^{29}Si NMR (119 MHz, CDCl_3): δ -39.8, -4.9, 19.6. IR (KBr): 2860, 1460, 1390, 1360, 1240, 1180, 1010, 940, 840, 810, 790, 730, 680, 640, 580, 550, 520 cm^{-1} . MS (EI, 70 eV): m/z 598 ($\text{M}^+(\text{}^{35}\text{Cl}_3\text{}^{37}\text{Cl})$, 4), 596 ($\text{M}^+(\text{}^{35}\text{Cl}_4)$, 2), 541 ($\text{}^{35}\text{Cl}_3\text{}^{37}\text{Cl}$, 15), 539 ($\text{}^{35}\text{Cl}_4$, 9), 73 (100). HRMS (APCI): found 596.11196 ($\text{M}^+(\text{}^{35}\text{Cl}_4)$), 598.10899 ($\text{M}^+(\text{}^{35}\text{Cl}_3\text{}^{37}\text{Cl})$), calcd for $\text{C}_{20}\text{H}_{48}\text{}^{35}\text{Cl}_4\text{Si}_6$ 596.11202, $\text{C}_{20}\text{H}_{48}\text{}^{35}\text{Cl}_3\text{}^{37}\text{ClSi}_6$ 598.10904. Anal. Found: C, 39.92; H, 8.28. Calcd for $\text{C}_{20}\text{H}_{48}\text{Cl}_4\text{Si}_6$: C, 40.11; H, 8.08.

Synthesis of Spiro[2,2,5,5-tetra-*tert*-butyl-3,3,4,4-tetramethylbicyclo[4.1.0]heptasil-1(6)-ene-7,5'-1',1',4',4'-tetra-*tert*-butyl-2',2',3',3'-tetramethylcyclopentasilane] (1).



In a glovebox under an argon atmosphere, a mixture of **2** (0.210 g, 0.35 mmol) and sodium dispersion (32.6 mg, 1.42 mmol) in toluene (12 mL) was refluxed for 4 h. The color of the mixture changed from colorless to deep red-brown. The solvent was removed under reduced pressure. The residue was dissolved in hexane, and the mixture was filtered. The solvent of the filtrate was removed under reduced pressure. The residue was separated by column chromatography of silica gel with hexane ($R_f = 0.88$), followed by recrystallization from toluene–hexane at $-30\text{ }^\circ\text{C}$ to give **1** (18.0 mg, 12%) as red-orange crystals.

1. Mp (under an argon atmosphere in a sealed tube): $238\text{ }^\circ\text{C}$ (decomp.). ^1H NMR (600 MHz, C_6D_6): δ 0.49 (s, 12H), 0.55 (s, 12H), 1.31 (s, 36H), 1.40 (s, 36H). ^{13}C NMR (151 MHz, C_6D_6): δ -0.8 , 0.5 , 24.4 , 25.4 , 32.3 , 32.6 . ^{29}Si NMR (119 MHz, C_6D_6): δ -85.4 , -41.1 , -31.5 , -11.9 , 15.0 , 147.1 . UV–visible (hexane): λ_{max} 468 (ϵ 2200), 328 (sh, 11000), 297 (36000), 249 nm (sh, 39000). HRMS (APCI): found 884.49695 (M^+), calcd for $\text{C}_{40}\text{H}_{96}\text{Si}_{11}$ 884.49685. Anal. Found: C, 54.24; H, 10.87. Calcd for $\text{C}_{40}\text{H}_{96}\text{Si}_{11}$: C, 54.21; H, 10.92.

2. Spectral Data

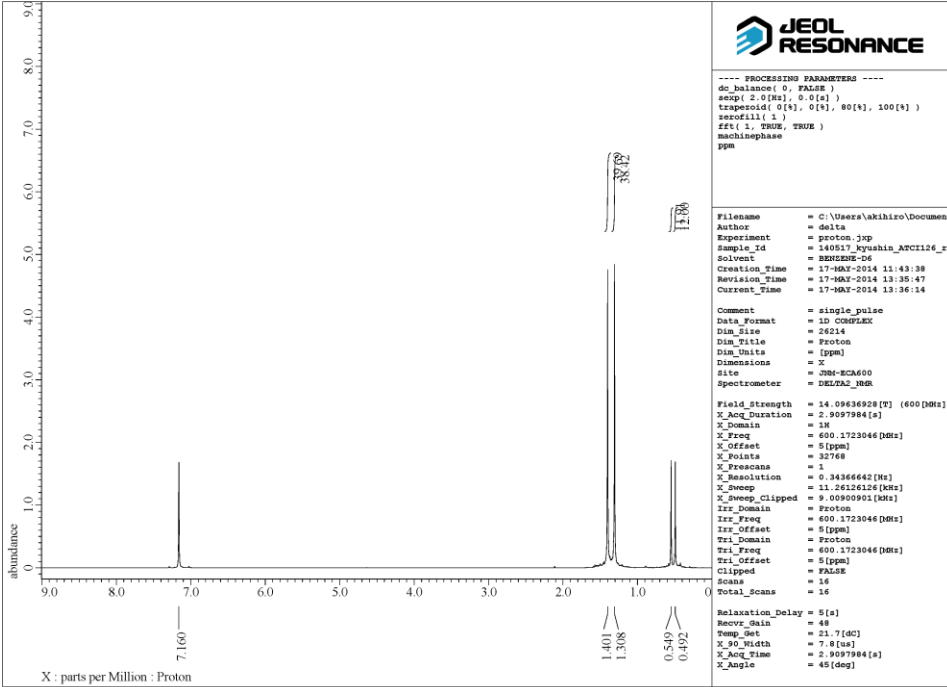


Figure S1. ^1H NMR spectrum of **1** in C_6D_6 at room temperature.

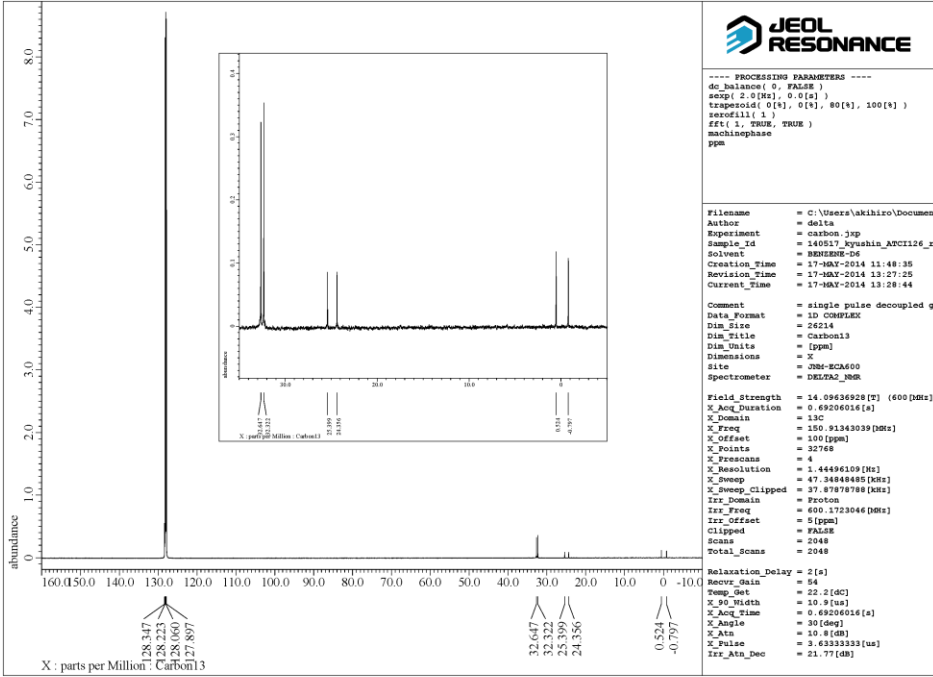


Figure S2. ^{13}C NMR spectrum of **1** in C_6D_6 at room temperature.

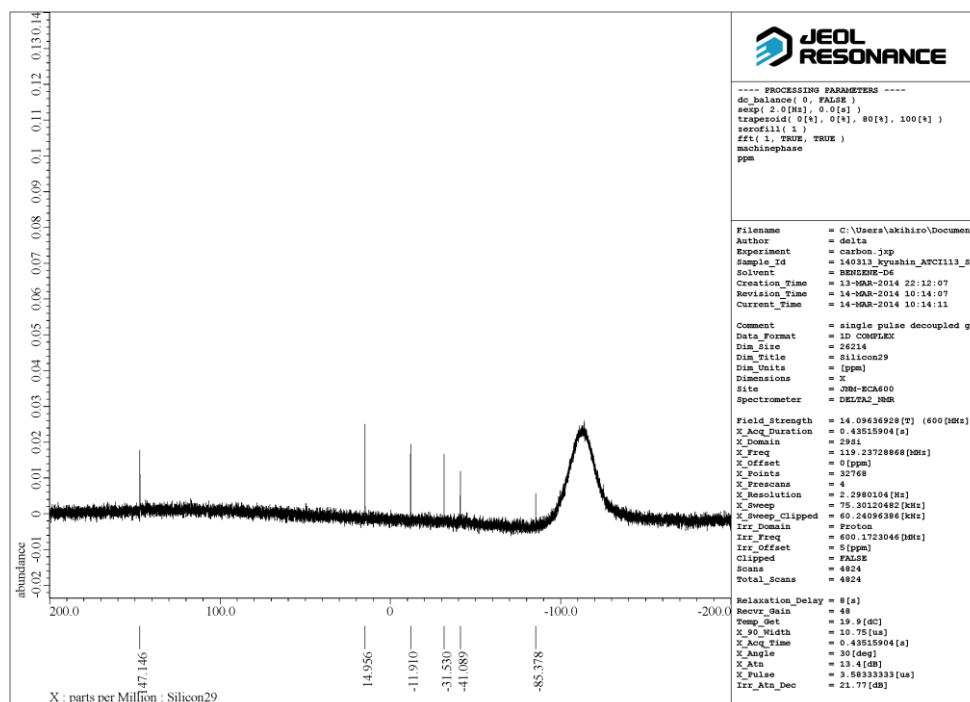


Figure S3. ^{29}Si NMR spectrum of **1** in C_6D_6 at room temperature.

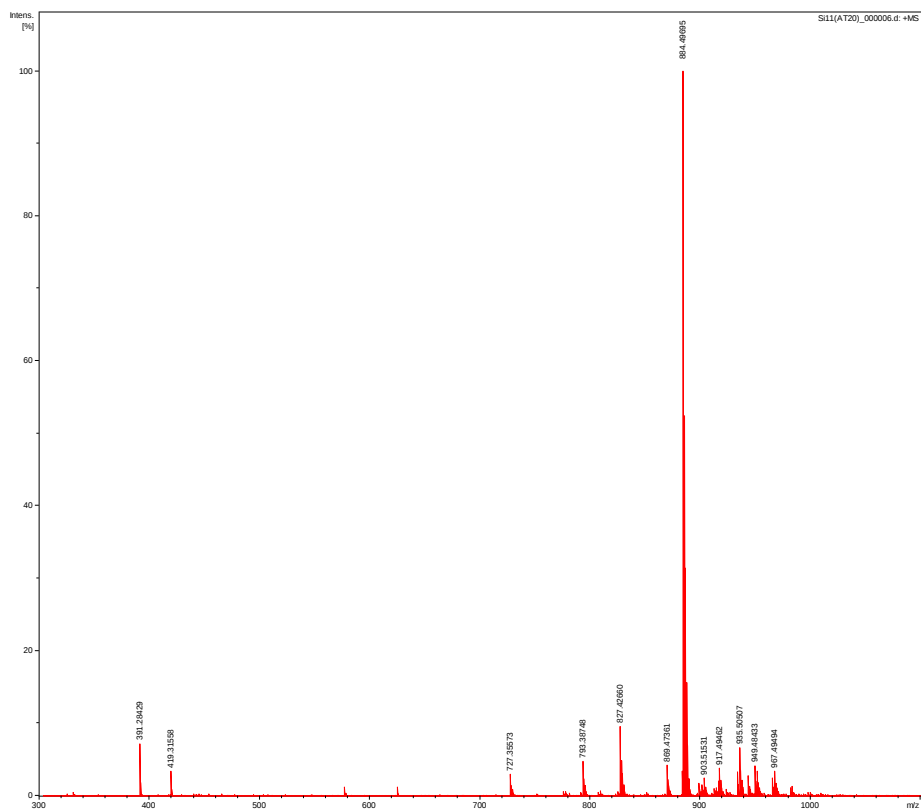


Figure S4. High-resolution mass spectrum of **1** (APCI).

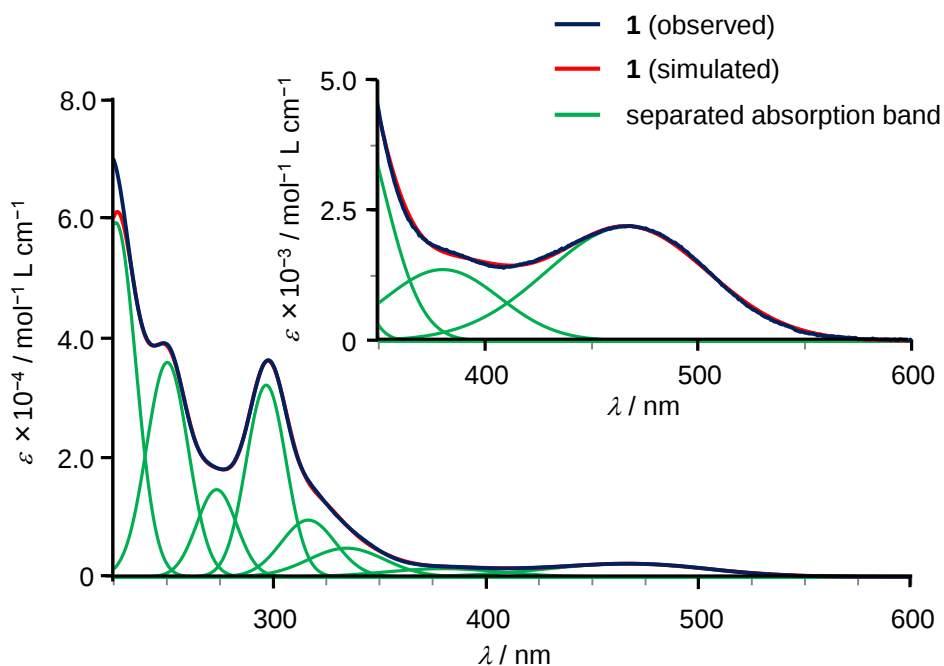


Figure S5. Observed (blue) and simulated (red) UV–visible spectra of **1** in hexane at room temperature. The observed absorption was analyzed by curve fitting with the green absorption bands.

Table S1. Absorption Maxima and Extinction Coefficients Used in the Curve Fitting in Figure S5

λ / nm	$\varepsilon / \text{mol}^{-1} \text{ L cm}^{-1}$	FWHM / nm ^a
466	2200	89
380	1370	63
335	4800	42
317	9500	30
297	32100	22
273	14600	22
250	35900	23
226	59300	22

^aFull width at half maximum.

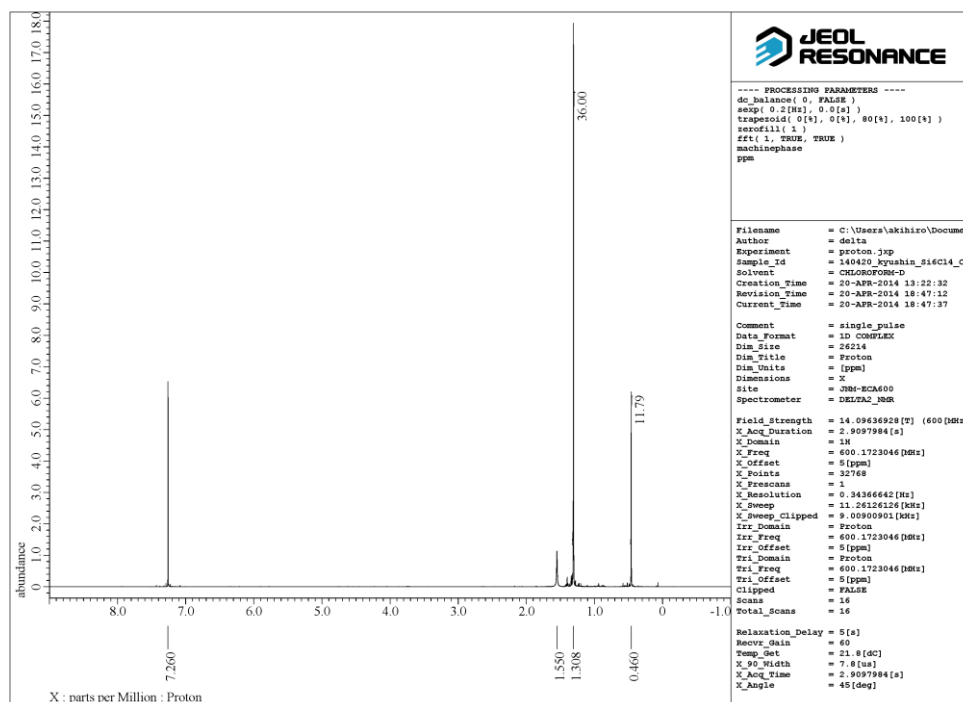


Figure S6. ^1H NMR spectrum of 2 in CDCl_3 at room temperature.

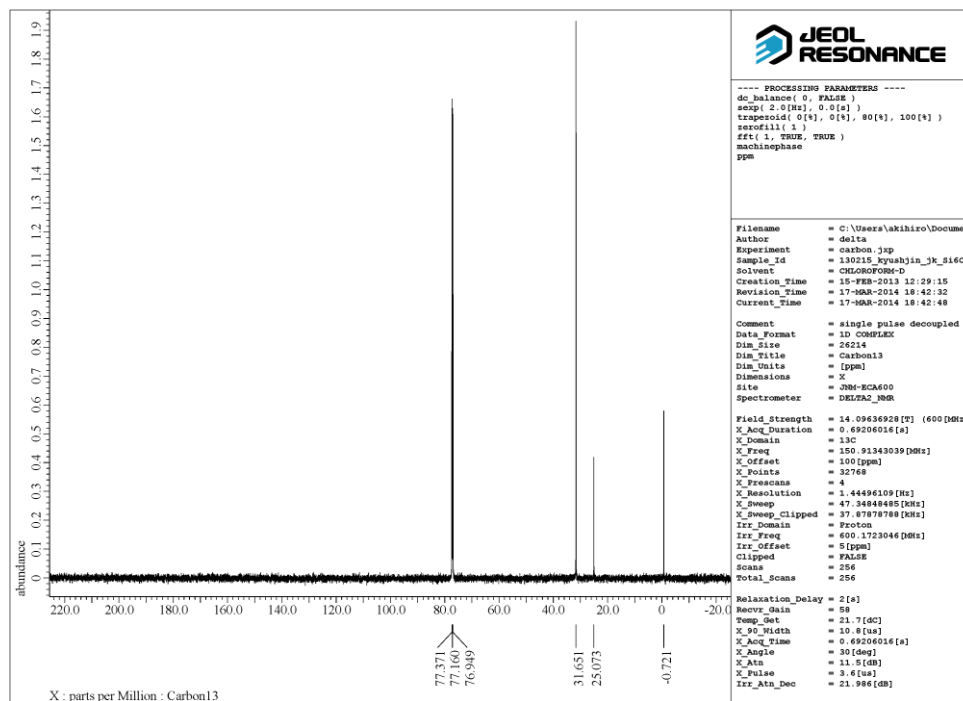


Figure S7. ^{13}C NMR spectrum of 2 in CDCl_3 at room temperature.

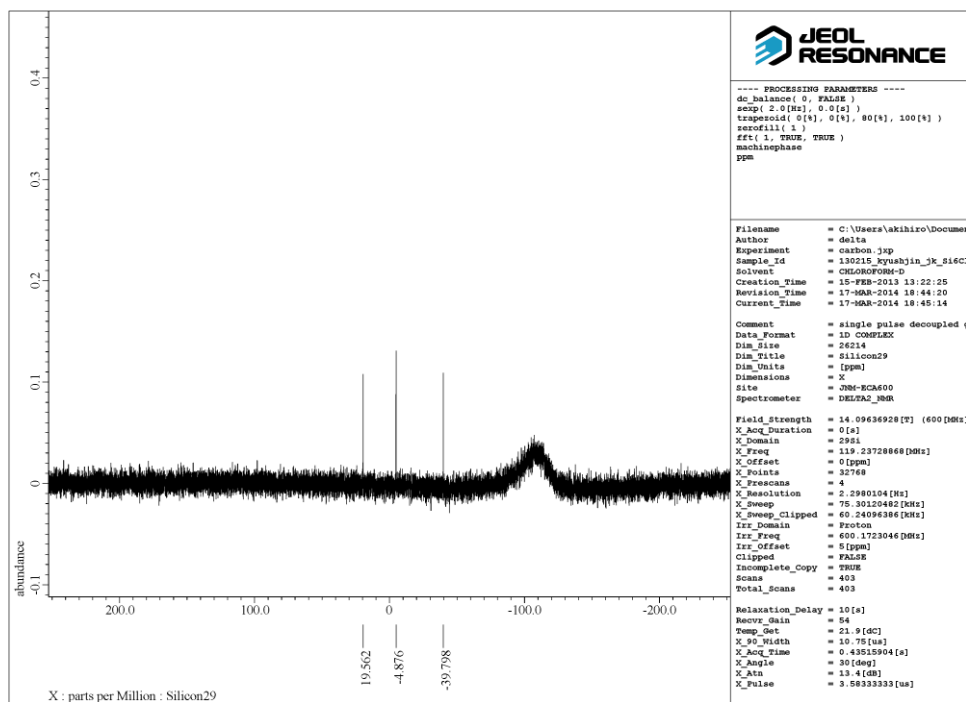


Figure S8. ^{29}Si NMR spectrum of **2** in CDCl_3 at room temperature.

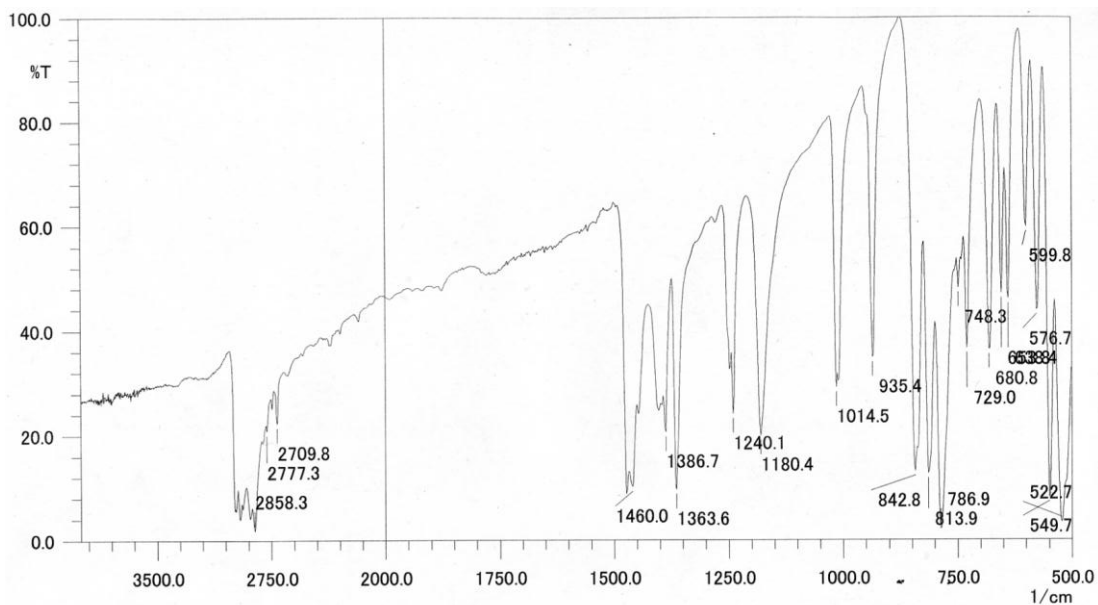


Figure S9. IR spectrum of **2** (KBr).

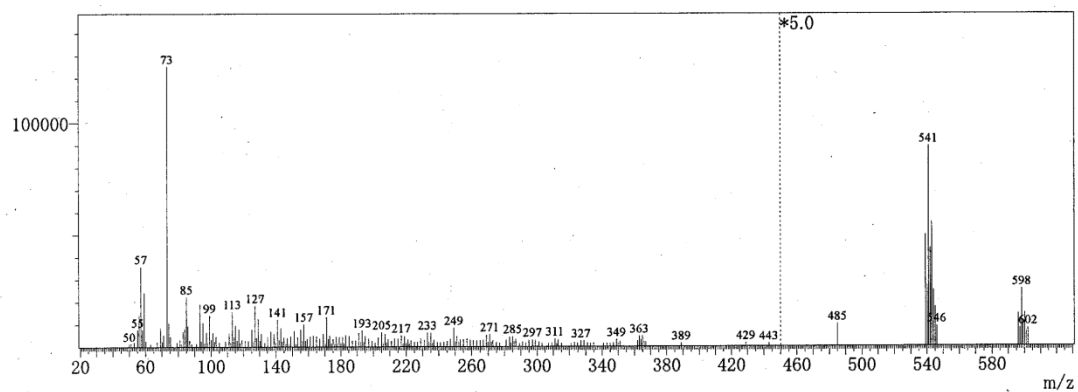


Figure S10. Mass spectrum of **2** (EI, 70 eV).

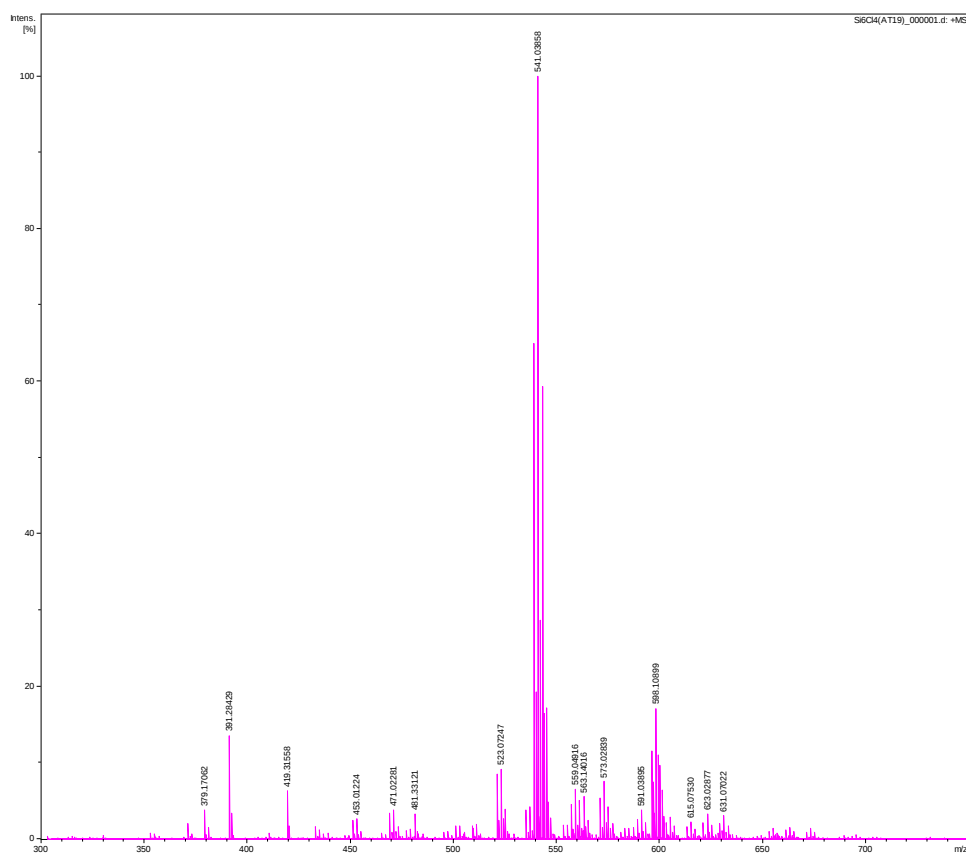


Figure S11. High-resolution mass spectrum of **2** (APCI).

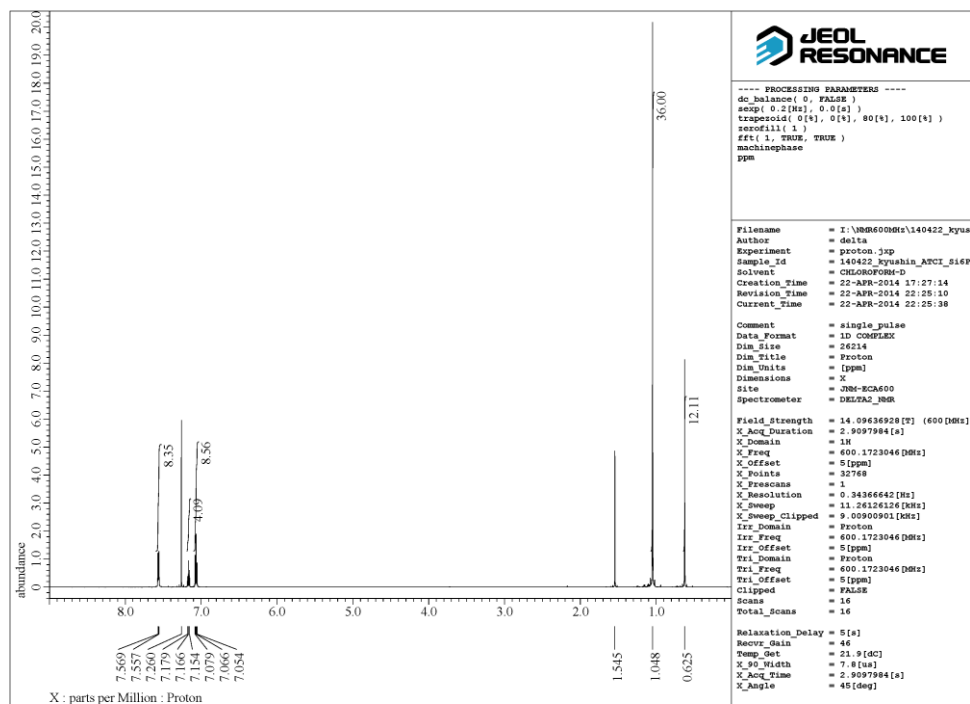


Figure S12. ^1H NMR spectrum of S1 in CDCl_3 at room temperature.

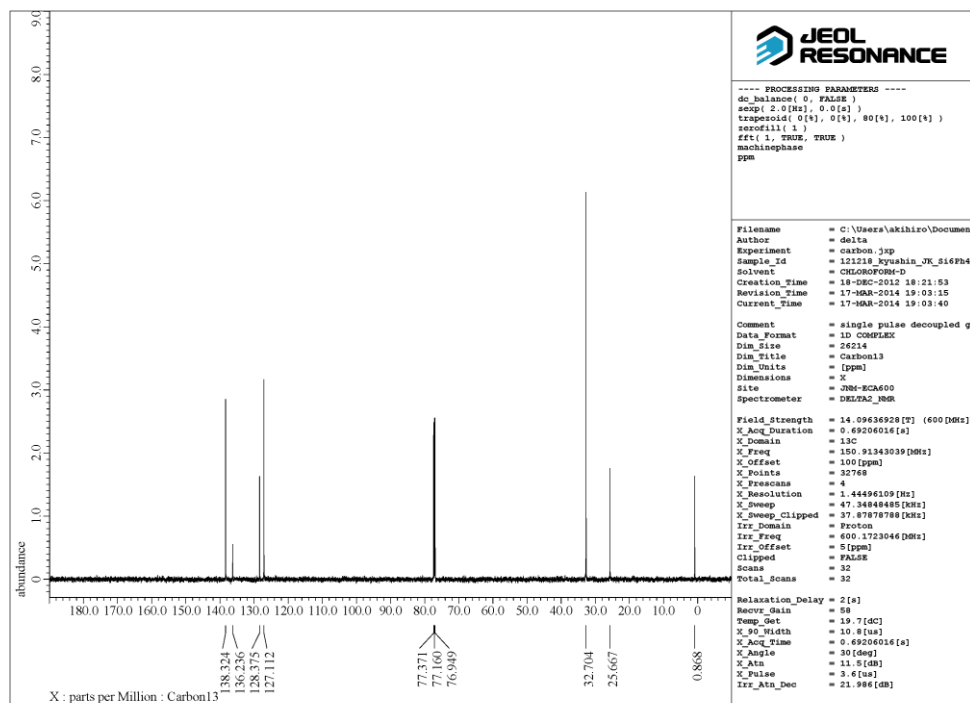


Figure S13. ^{13}C NMR spectrum of S1 in CDCl_3 at room temperature.

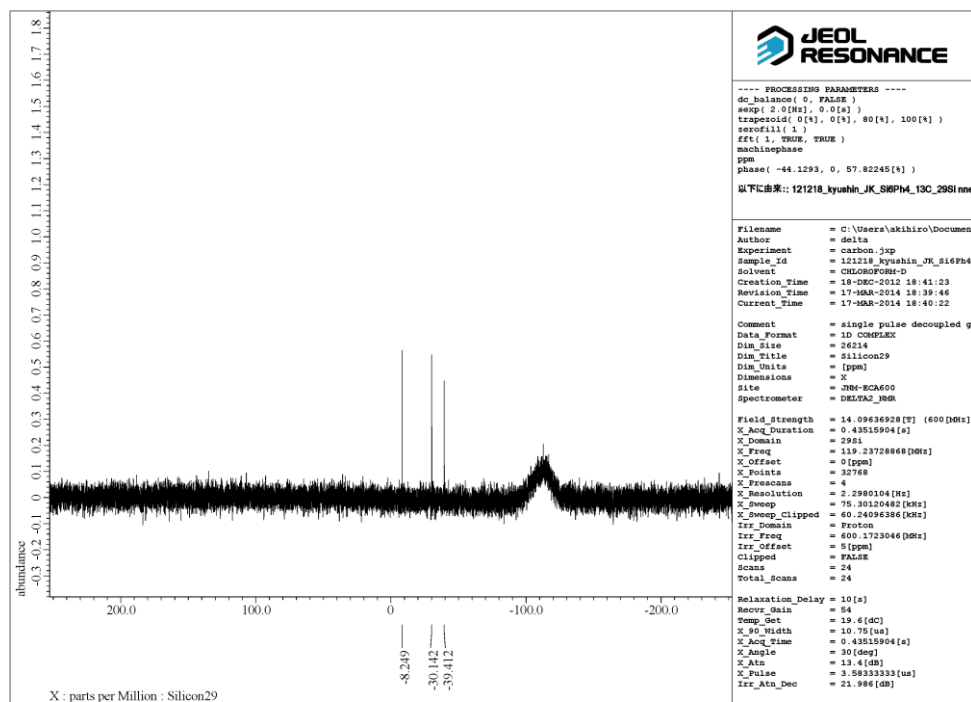


Figure S14. ^{29}Si NMR spectrum of **S1** in CDCl_3 at room temperature.

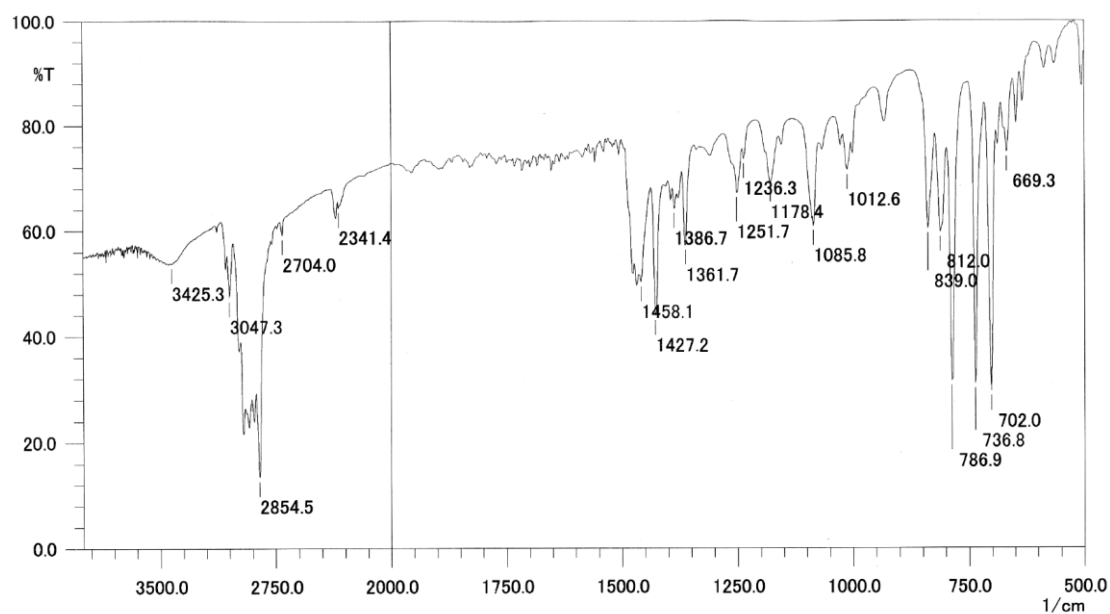


Figure S15. IR spectrum of **S1** (KBr).

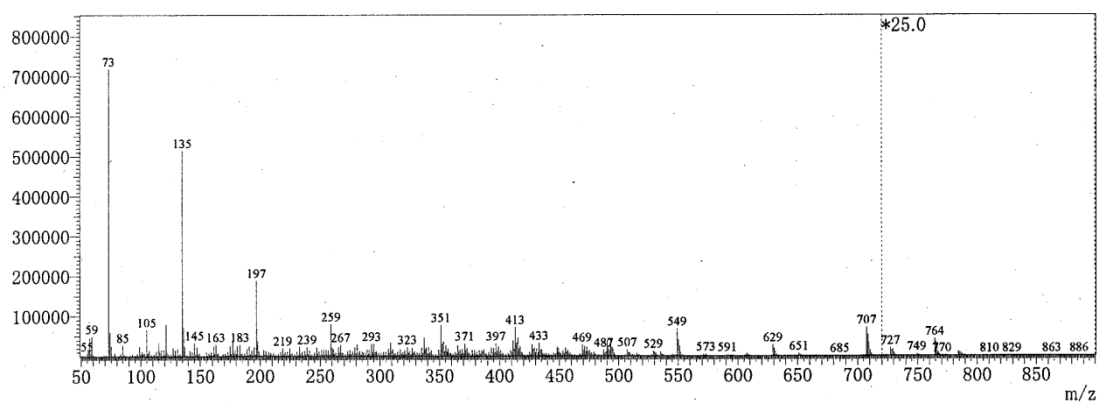


Figure S16. Mass spectrum of S1 (EI, 70 eV).

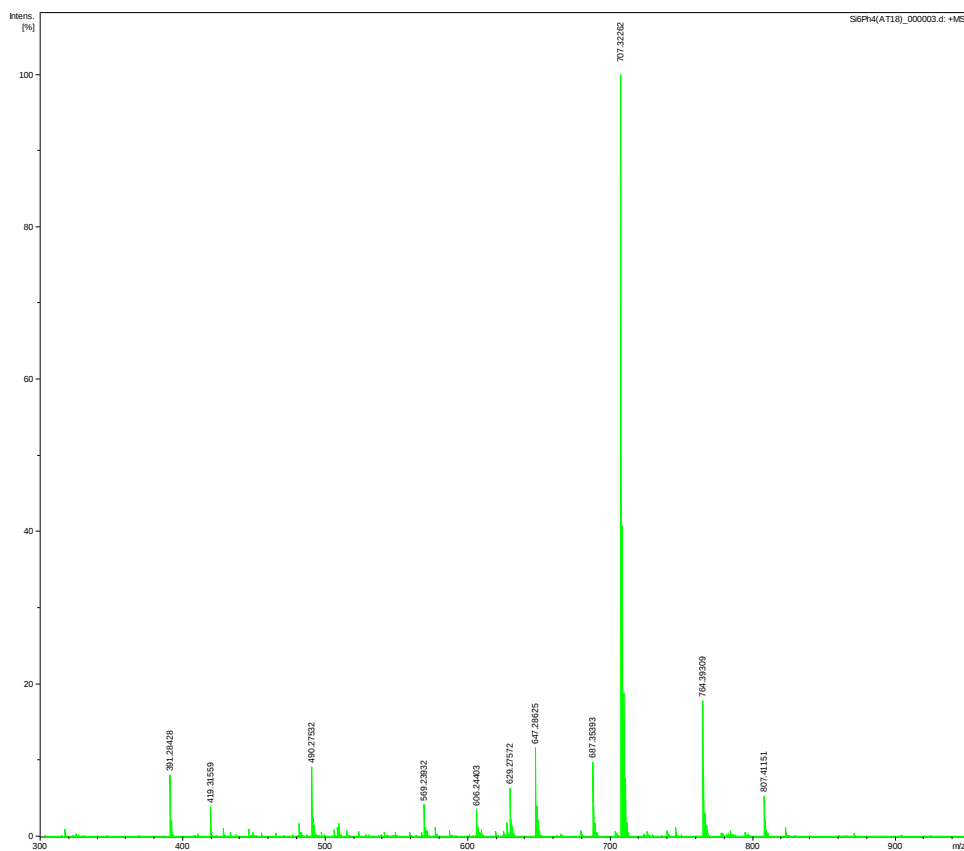


Figure S17. High-resolution mass spectrum of S1 (APCI).

3. X-ray Crystallographic Analysis

Red-orange crystals of **1** were obtained by recrystallization from toluene–hexane at $-30\text{ }^{\circ}\text{C}$ in a glovebox under an argon atmosphere. Colorless crystals of **2** were grown by slow evaporation of a hexane solution at room temperature in air. Intensity data were collected on a Rigaku R-Axis IV⁺⁺ imaging plate diffractometer using graphite-monochromated Mo $K\alpha$ radiation. The data were corrected for Lorentz and polarization effects. An empirical absorption correction based on multi-scan was also applied. The structures were solved by a direct method using SHELXS-97^{S3,S4} and refined by the full-matrix least-squares method on F^2 for all reflections using SHELXL-97.^{S3,S4} Non-hydrogen atoms were refined anisotropically. All hydrogen atoms were generated by AFIX instructions and were not refined. All calculations were carried out using Yadokari-XG 2009.^{S5}

Crystal data for **1** (183 K): $\text{C}_{40}\text{H}_{96}\text{Si}_{11}$, fw 886.16, triclinic, space group $P\bar{1}$, red-orange crystal, $a = 12.0612(16)$, $b = 14.318(2)$, $c = 18.484(2)$ Å, $\alpha = 101.875(3)$, $\beta = 97.825(2)$, $\gamma = 111.173(3)^{\circ}$, $V = 2834.4(7)$ Å³, $Z = 2$, $D_{\text{calcd}} = 1.038\text{ g cm}^{-3}$, $R_1 = 0.049$ (all data), $wR_2 = 0.136$ (all data), GOF = 1.14.

Crystal data for **2** (173 K): $\text{C}_{20}\text{H}_{48}\text{Cl}_4\text{Si}_6$, fw 598.92, monoclinic, space group $P2_1/n$, colorless crystal, $a = 9.1903(5)$, $b = 21.5113(11)$, $c = 16.6086(10)$ Å, $\beta = 96.6520(8)^{\circ}$, $V = 3261.3(3)$ Å³, $Z = 4$, $D_{\text{calcd}} = 1.220\text{ g cm}^{-3}$, $R_1 = 0.044$ (all data), $wR_2 = 0.083$ (all data), GOF = 1.28.

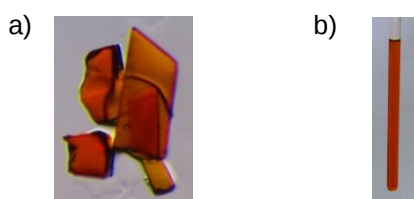


Figure S18. Photographs of **1**: a) crystals and b) a C_6D_6 solution.

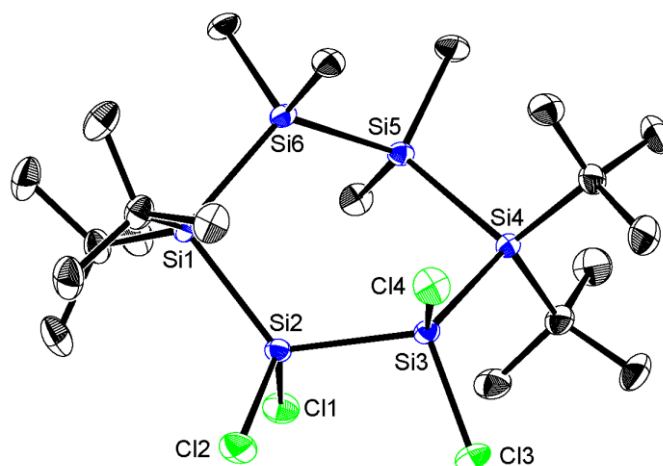
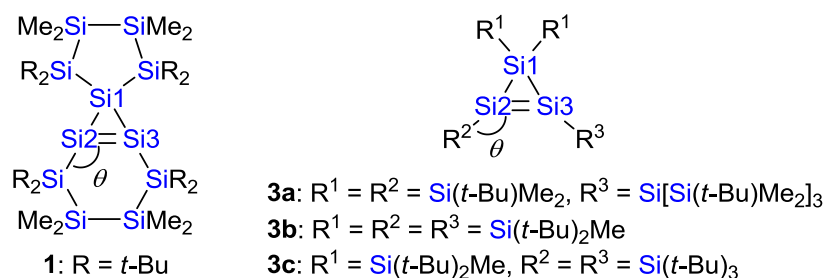


Figure S19. Molecular structure of **2**. Thermal ellipsoids are drawn at the 50% probability level. Hydrogen atoms are omitted for clarity. Selected bond lengths (Å), bond angles (deg), and dihedral angles (deg): Si1–Si2 2.3813(7), Si1–Si6 2.3963(7), Si2–Si3 2.3738(7), Si2–Cl1 2.0815(7), Si2–Cl2 2.0748(7), Si3–Si4 2.3958(7), Si3–Cl3 2.0756(7), Si3–Cl4 2.0785(7), Si4–Si5 2.4036(7), Si5–Si6 2.3835(8); Si2–Si1–Si6 101.83(3), Si1–Si2–Si3 119.68(3), Si2–Si3–Si4 117.08(3), Si3–Si4–Si5 103.17(3), Si4–Si5–Si6 115.94(3), Si1–Si6–Si5 116.62(3); Si1–Si2–Si3–Si4 –61.84(4).

Table S2. Structural Parameters of 1 and 3a–c



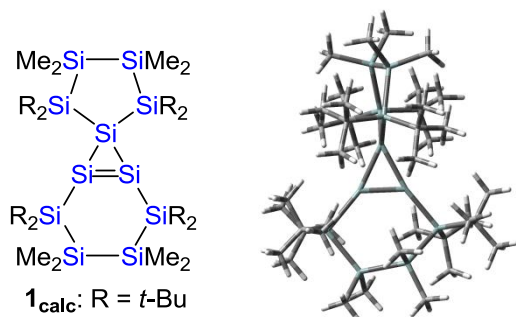
	1	3a^a	3b^b	3c^c
$d(\text{Si1}–\text{Si2}) / \text{\AA}$	2.3526(8)	2.327(2)	2.364(3)	2.3762(8)
$d(\text{Si1}–\text{Si3}) / \text{\AA}$	2.3744(7)	2.339(2)	2.352(3)	2.3694(8)
$d(\text{Si2}=\text{Si3}) / \text{\AA}$	2.1473(8)	2.132(2)	2.138(2)	2.1612(8)
$\Sigma \text{ Si2} / ^\circ$	359.2	356.7	357.5	360.0
$\Sigma \text{ Si3} / ^\circ$	360.0	360.0	358.1	359.8
$\theta / ^\circ$	128.35(3)	147.04(8)	146.4(2)	144.74(4)
	131.73(3)	147.34(6)	146.3(2)	145.00(3)
$\varphi(\text{Si}–\text{Si}=\text{Si}–\text{Si}) / ^\circ$	6.50(7)	21.4(2)	31.9(2)	4.84(5)

^aRef S6. ^bRef S7. ^cRef S8.

4. Theoretical Calculations

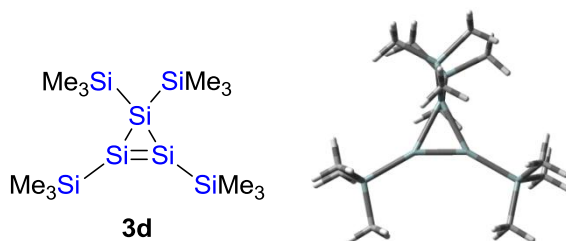
All theoretical calculations were performed using Gaussian 09^{S9} on a Fujitsu PRIMERGY RX300 system of the Research Center for Computational Science, Japan. The geometries were optimized at the B3LYP/6-31G(d) level. It was confirmed by frequency calculations that the optimized structures have no imaginary frequency except for **5a'**–**c'**, which are the transition states of the inversion of the folded structures of **5a**–**c**. The results are summarized in Tables S3 and S4. The energy levels and lobes of the selected molecular orbitals of **1_{calc}**, **3d**, and **5d** are shown in Figures S20 and S21, respectively. The GIAO calculations of **1_{calc}**, **3d**, and **5d** were performed at the B3LYP/6-311+G(2d,p) level, and the results are summarized in Tables S5 and S6. The TD-DFT calculation of **1_{calc}** was performed at the B3LYP/6-31+G(2d,p) level, and the results are summarized in Table S7. Strain energies were calculated at the B3LYP/6-311++G(3df,2p)//B3LYP/6-31+G(d) level by using the homodesmotic reactions in Figure S22. The results are summarized in Figure S22 and Table S8.

Table S3. Atomic Coordinates of the Optimized Structures of 1_{calc}, 3d, 4a–c, 5a–d, and 5a'–c'



Si	2.72119200	0.14620700	-2.00777900	H	-4.40851100	-5.03376600	0.86519500
Si	-2.74116900	-2.54886800	-0.06466000	H	-5.05938000	-3.62259100	1.70887200
Si	1.31912700	-0.04266000	0.00719500	C	-5.61290000	-0.81474300	1.43062300
Si	-4.61677300	-0.97550500	-0.20127700	H	-6.41516300	-0.08370800	1.26679400
Si	4.97381700	0.33151000	-1.14473200	H	-5.03437900	-0.47655300	2.29282700
Si	2.76793300	-0.18825600	1.97652400	H	-6.09356800	-1.76161700	1.70005800
Si	-0.76841000	1.09480600	0.08058300	C	-2.64289900	-2.68327000	-2.93470700
Si	-2.58186500	2.61513600	0.25900800	H	-2.49713900	-3.26555500	-3.85647700
Si	-0.86837700	-1.04609900	0.02359100	H	-1.86898900	-1.90977200	-2.91054300
Si	4.95829300	-0.59277400	1.04815900	H	-3.61092900	-2.18161700	-3.01761600
Si	-4.12757800	1.23715700	-1.01084000	C	1.97659300	-2.93205200	2.29996500
C	2.25949600	1.76090300	-3.04618800	H	1.70979300	-3.77979500	2.94900300
C	-2.85539200	-3.63032700	1.57744100	H	2.85047000	-3.23461300	1.71408100
C	-2.57058200	-3.62074800	-1.71046800	H	1.14615600	-2.77168000	1.60495300
C	-2.21609000	4.34149600	-0.61366600	C	3.43195400	-1.53931400	-4.31534200
C	2.76734900	1.56144600	2.89914500	H	4.48541000	-1.32358800	-4.11399700
C	2.21858600	2.97475600	-2.09375100	H	3.07643000	-0.81969300	-5.06010900
H	3.18104600	3.15272000	-1.60516700	H	3.38519300	-2.53343300	-4.78556500
H	1.46013800	2.85269200	-1.31386800	C	1.34487400	2.05587000	3.23536600
H	1.96741100	3.88489900	-2.65887200	H	1.40102100	3.04235900	3.72109900
C	2.25218800	-1.67929100	3.15833000	H	0.81332000	1.38742800	3.91819100
C	-5.95858400	-1.64027200	-1.40738000	H	0.73334400	2.16804600	2.33409900
H	-6.30417800	-2.63342300	-1.09566500	C	-1.21551800	-4.36115600	-1.76192200
H	-5.63021100	-1.71393300	-2.44811100	H	-1.10859800	-4.86441500	-2.73429800
H	-6.82861700	-0.97219300	-1.38106900	H	-1.12940900	-5.12872800	-0.98899400
C	2.56179800	-1.52992200	-3.03952000	H	-0.36552800	-3.68116100	-1.65209400
C	3.40597300	2.61400600	1.96917200	C	-2.68746300	-2.71005200	2.80425400
H	2.86593100	2.70382400	1.01943200	H	-3.44350600	-1.92034500	2.84102100
H	4.45297000	2.38953000	1.74485000	H	-1.70407200	-2.23096900	2.82490100
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H	-3.49347000	1.94895500	-3.36109900	H	-1.77300000	-5.19111500	2.63536100
C	-3.11954900	2.81543500	2.15032600	C	1.10513800	-1.80563900	-3.46142100
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H	-4.69638700	-4.22996500	-1.77995200	H	0.74962800	-1.10004600	-4.21709400
H	-3.62357500	-5.44864500	-1.06974700	H	0.41871200	-1.75508600	-2.61172600
H	-3.61918400	-5.17706700	-2.81215300	C	6.30000100	-0.57164400	-2.19791300
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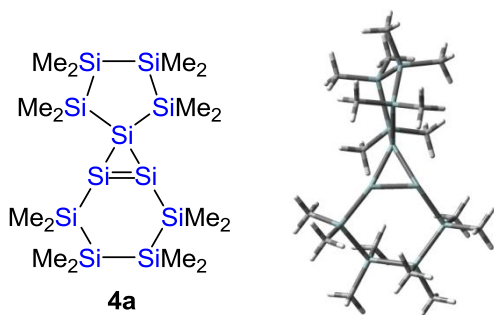
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H	5.03611100	2.78951500	-0.42528000	C	5.38969500	-2.45431000	0.89273200
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C	0.97741500	-1.35777700	3.96555700	H	4.65013700	-3.02337000	0.32266500
H	0.15108200	-1.03418500	3.32340500	H	5.49437000	-2.93002200	1.87413300
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H	0.64334200	-2.25367500	4.51047800	H	-3.27189500	1.59030000	3.94150200
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H	4.59899900	1.13872800	4.06151100	H	-3.27086600	0.63392600	2.45115200
H	3.09970300	0.90003900	4.97381400	C	6.40628400	0.13412900	2.07616700
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C	-0.89804500	4.95645900	-0.09212700	H	6.35122700	1.22036500	2.19689600
H	-0.04051600	4.30469900	-0.29121500	H	7.35915000	-0.09580800	1.58215000
H	-0.91825700	5.16262900	0.98071800	C	3.01843100	-2.69659800	-2.13648800
H	-0.70764800	5.91120900	-0.60498700	H	2.42209700	-2.76801900	-1.21879800
C	3.37881700	-2.02799500	4.15773800	H	4.07087400	-2.60883600	-1.84917800
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H	4.30094600	-2.33668300	3.65449200	C	-2.36268200	3.94905500	2.87459600
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Si	0.18186600	1.99603800	2.33649800	H	0.08809800	4.43805800	1.77019400
C	1.87554400	2.08487900	3.20380200	C	-1.17345600	2.06874700	3.67422800
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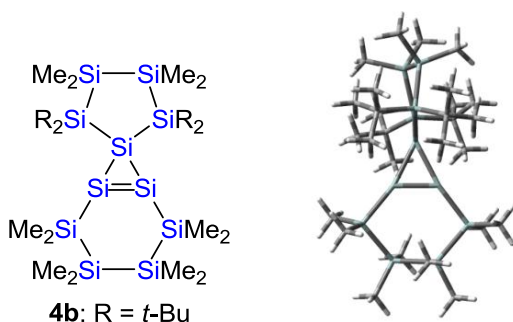
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C	-1.87554400	-2.08487900	3.20380200	H	3.69479500	-0.37208300	-4.63010100
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Si	-4.37127000	-0.95322700	-1.19918200	C	-5.49196400	-0.82008500	-2.74456500
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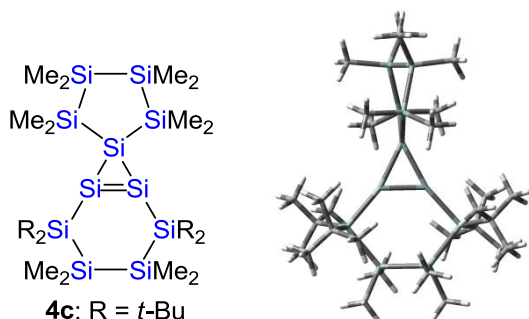
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C	0.75842100	3.07410100	-2.46665000	H	5.58041200	-1.37714900	-2.33616800
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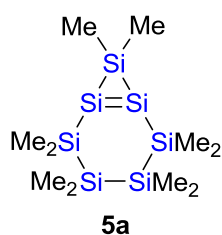
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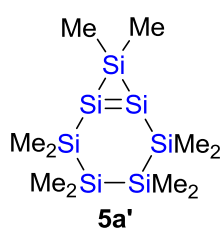
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Si	-1.86860200	-0.00003800	0.00010300	Si	0.23692200	-1.07062500	0.01560500
Si	3.86308600	1.13379800	0.42213800	Si	2.01245900	-2.62489500	0.08180700

Si	0.23703200	1.07048100	-0.01541600	H	-2.21833600	1.94943500	-3.07521100
Si	-5.42751500	0.51346800	1.07230400	H	-3.86674100	1.68987200	-3.67557700
Si	3.86314000	-1.13365000	-0.42189300	C	0.73521600	-3.85408900	2.39805800
C	5.49694700	1.87927400	-0.26415500	H	0.82220200	-4.21950000	3.43217700
H	5.66363700	2.88651500	0.13710900	H	-0.01511200	-3.05461900	2.39538600
H	5.51222000	1.95109600	-1.35682800	H	0.34514300	-4.67778600	1.79387500
H	6.35162500	1.26161400	0.03910900	C	2.55957800	-2.22857800	2.87099600
C	4.14942400	-1.03573900	-2.31252200	H	3.56575800	-1.86355100	2.64220900
H	5.00595800	-0.38086000	-2.51596300	H	1.87635600	-1.37161000	2.84729400
H	3.28910600	-0.63332600	-2.85402500	H	2.57725700	-2.60868500	3.90314400
H	4.38609300	-2.01862200	-2.73490700	C	3.13002900	-4.50524700	2.00132800
C	4.14898700	1.03597300	2.31282300	H	4.12625700	-4.21210200	1.65056000
H	5.00542000	0.38104000	2.51651700	H	3.23443600	-4.82729200	3.04805500
H	3.28848500	0.63361900	2.85408100	H	2.81476100	-5.38225000	1.42628500
H	4.38559300	2.01884800	2.73524800	C	3.10140200	-4.73133200	-1.59522500
C	-6.84210700	0.11815200	-2.19544900	H	3.49013700	-5.24801800	-0.71206700
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H	-6.77449900	1.19938700	-2.35951400	H	3.88202900	-4.05285700	-1.95486600
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C	-5.62635900	-2.40796800	-0.88098300	H	0.52786500	-5.72657500	-1.73419800
H	-6.58053900	-2.65963500	-0.40235500	H	1.02500500	-5.63451800	-0.04266500
H	-4.82465400	-2.84235300	-0.27229100	H	-0.24973500	-4.56308300	-0.65152200
H	-5.60470400	-2.90446900	-1.85869200	C	1.29391300	-3.32506100	-2.61863900
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H	5.66359700	-2.88639000	-0.13697200	H	0.31183600	-2.85368700	-2.49809900
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H	-6.81405800	0.37173000	3.17685800	H	3.88181500	4.05315500	1.95478100
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H	-7.82260500	0.09173800	1.74983400	C	0.70948200	5.03224300	0.89988800
C	2.11090600	-3.34827500	1.90966700	H	1.02501200	5.63441000	0.04196400
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C	-2.65243700	1.32099800	3.20361300	H	0.34489700	4.67744200	-1.79434600
H	-3.26528700	1.30890400	4.11343800	H	0.82221100	4.21894500	-3.43251700
H	-1.61620700	1.10799500	3.49315000	H	-0.01506400	3.05413600	-2.39562800
H	-2.68095300	2.33516900	2.79052700	C	3.12991900	4.50514000	-2.00156000
C	-3.23908900	-1.68352800	2.77558800	H	3.23438600	4.82694600	-3.04835200
H	-2.21808200	-1.94967700	3.07485500	H	2.81457400	5.38227000	-1.42674700
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C	-2.65234100	-1.32124100	-3.20332800	H	3.56596300	1.86347000	-2.64203700
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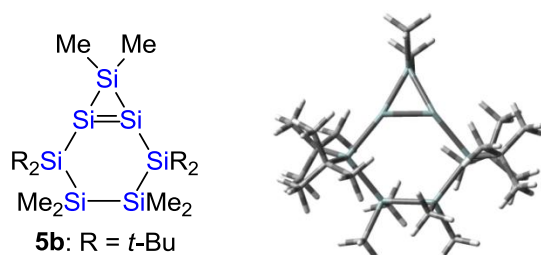


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Si	-1.56542200	-1.20989300	-0.69878800	H	-0.81107400	-3.64762600	1.87262700
Si	0.33088000	-2.45341200	-0.02332600	H	0.94026400	-3.58852000	2.13070900
Si	-1.61211900	0.98249000	-0.81523900	H	-0.05391600	-2.15865300	2.46348600
Si	2.17908400	-0.98184600	-0.28117300	C	2.51118700	-0.76728200	-2.15154700
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H	0.11184400	3.66094100	-2.63471700	H	2.76534600	-1.72758600	-2.61635900
H	1.75433200	3.69429400	-1.96735900	H	1.63381700	-0.36768900	-2.67231200
H	1.15305000	2.23455100	-2.77159300	C	3.74282000	-1.76758600	0.50044300
C	-0.34997900	3.95440200	0.59027400	H	3.96531700	-2.74057800	0.04520100
H	0.49484100	4.62881700	0.77948200	H	4.61928600	-1.12512800	0.35117100
H	-1.12089100	4.52339200	0.05769300	H	3.62544400	-1.92430400	1.57896200
H	-0.76325900	3.65279000	1.55876700	C	3.48494300	2.08464900	0.81256700
C	-5.07555500	-0.19872100	-0.82313200	H	3.36080300	3.06304900	1.29300200
H	-5.65329800	-1.07571500	-0.50454500	H	4.22702700	1.52345700	1.39376300
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C	-3.84549100	0.01411300	1.98988900	H	1.89648100	0.28835600	3.10723600
H	-4.45492500	0.90295000	2.19817400	H	1.11497800	1.87425200	3.04284200
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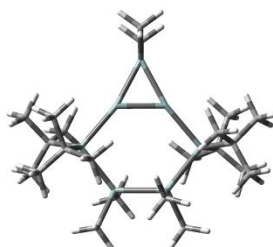
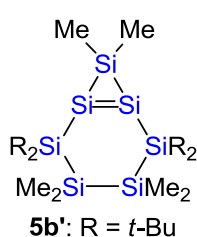
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Si	2.04737300	1.07626600	0.51555800	H	-5.39472300	1.00089400	1.46764100
Si	-1.56105300	-1.07669500	0.08064800	H	-5.40123900	-0.76687800	1.59421500
Si	0.29474800	-2.52168100	0.20979600	H	-4.16436600	0.17813500	2.45032200
Si	-1.56106200	1.07668200	-0.08043900	C	-4.74997700	-0.11453300	-1.52913800

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H	-4.16409900	-0.17826200	-2.45044200	H	2.02916300	1.86556000	2.90915600
C	0.54500200	-3.13730700	1.99698300	H	0.94320500	0.48031100	2.70870100
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H	3.88622700	-2.05490300	0.93715000	H	1.45955600	3.73966600	-2.06843300
C	1.91358400	-0.89395600	-2.41364700	H	0.63119100	2.30532200	-2.70303600
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Si	1.12504400	-1.88444700	0.85056300	H	-1.29828300	-4.39015200	1.05809500
Si	-1.09149700	1.56844100	-0.65391100	H	-2.03208700	-3.18467800	2.12565800
Si	-2.58369500	-0.17498000	-0.06411300	C	1.90348900	-3.62895400	0.63828500
Si	1.07745900	1.55715000	-0.59676000	H	2.90485800	-3.66117100	1.08476000
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C	3.35840000	-0.77665300	-1.81638100	H	1.99648100	-3.93454300	-0.40901400
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C	0.02091500	4.94661500	-1.58708900	H	0.32102300	-2.44037800	3.15113000
H	-0.86595500	5.58699000	-1.49625500	H	1.95862600	-1.78815900	3.23741900
H	0.90728100	5.58375800	-1.47252900	H	0.57874600	-0.69564400	3.03849700
H	0.03340900	4.51696500	-2.59266900	C	-3.27806400	-0.28870200	-2.85379500
C	-0.01268500	4.45923200	1.43752400	H	-2.53607100	-1.07894300	-2.99956500
H	0.87660200	5.09284800	1.55084900	H	-4.03706300	-0.40208200	-3.64219600
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H	-0.02858400	3.74244800	2.26408700	C	-4.70287900	-1.70292000	-1.35181100
C	-3.95452100	-0.35590200	-1.46670800	H	-5.45581200	-1.78124000	-2.15023400
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H	1.87556200	-2.36950100	-2.17163400	H	2.44652200	0.66403100	2.84979400
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H	4.69719800	0.95406600	-2.14638500	H	-1.87189900	-0.95071600	2.86411300
H	4.26917800	0.05815700	-3.60755000	H	-1.32611300	0.70496600	2.54974500
H	3.09001000	1.14435500	-2.85775600	H	-2.58223000	0.39518500	3.75963800
C	4.51251700	-1.78144400	-1.60719600	C	-4.48468400	-0.67186900	2.08485000
H	4.86357600	-2.15286300	-2.58142300	H	-4.81075200	-0.46660200	3.11539100
H	5.37439800	-1.32450900	-1.10923800	H	-5.35479600	-0.52185700	1.43726300
H	4.20660100	-2.65408900	-1.01867000	H	-4.20685300	-1.73106400	2.03628000
C	4.95345200	1.37156800	0.55104500	C	-3.79258500	1.72530000	1.78121300
H	5.61532700	1.79115200	1.32337400	H	-4.59033500	1.94371100	1.06631800
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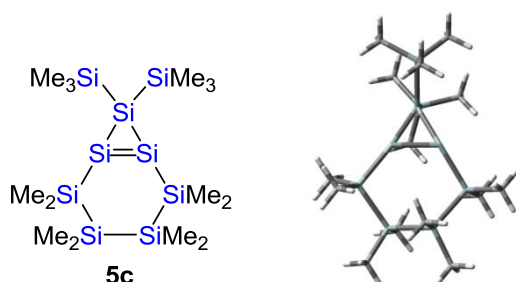


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Si	-1.13225100	-1.97162000	-0.65036200	H	1.97558200	-2.99475600	2.42076000
Si	1.08197300	1.60018100	0.35272500	H	0.61319300	-1.89984600	2.70351700
Si	2.60386100	-0.17963400	0.02523400	C	-0.99599000	-2.00938000	-2.55989600
Si	-1.07334300	1.60234800	0.24292100	H	-0.32103800	-2.82002400	-2.86156400
Si	1.12156300	-2.09537400	0.21470700	H	-1.96694400	-2.20685300	-3.02730300
C	0.05690500	4.67776900	-1.47496900	H	-0.60265200	-1.07847800	-2.97680600
H	-0.81965100	5.33551000	-1.53936500	C	-1.91802300	-3.66765000	-0.20155600
H	0.95059400	5.31477400	-1.50205200	H	-2.90572800	-3.76456600	-0.66885100
H	0.06869800	4.03426300	-2.35976300	H	-1.29767400	-4.49217100	-0.57484100
C	-0.03782700	4.88633200	1.58298700	H	-2.04647300	-3.81012500	0.87632200
H	0.85035000	5.53136600	1.57535000	C	-3.96626100	0.22927500	-1.30744500
H	-0.92142200	5.53362300	1.51069300	C	-3.34478900	-0.50180700	1.85719400
H	-0.07401600	4.36197100	2.54217000	C	-3.27619600	0.85598900	-2.53968500
C	3.34186100	0.02167200	-1.78954000	H	-2.51012200	0.20488100	-2.96974500
C	3.96503400	-0.18196400	1.44526100	H	-4.02328400	1.04839200	-3.32416500
C	1.89450200	-3.59317400	-0.70881100	H	-2.80172100	1.81431800	-2.29815200
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H	1.27842900	-4.48905100	-0.56114500	H	-5.46189300	-0.78494000	-2.52522900
H	1.99106300	-3.43256800	-1.78780100	H	-4.04226400	-1.78569700	-2.20650700

H	-5.24892900	-1.53183200	-0.93854600
C	-5.00374200	1.24795500	-0.78856200
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H	-5.62608100	0.83867900	0.01362700
H	-4.53122800	2.16545200	-0.41832600
C	4.69290300	-1.54401200	1.51925100
H	5.44743100	-1.52020800	2.31955100
H	4.00845900	-2.36814200	1.74742900
H	5.21527500	-1.79221800	0.58971800
C	5.01836900	0.92517400	1.22427100
H	4.56062800	1.91761000	1.13673300
H	5.70601300	0.95674600	2.08250800
H	5.62768000	0.75227100	0.33118800
C	3.29085300	0.08598800	2.80890800
H	2.52346500	-0.65439000	3.05245400
H	4.04615900	0.05069300	3.60820200
H	2.82174100	1.07601800	2.84434000
C	2.23181600	-0.27428400	-2.81789500
H	1.88787600	-1.31203800	-2.76738800
H	1.36263900	0.37833000	-2.67504500
H	2.61041000	-0.10486200	-3.83691300
C	4.51164800	-0.95501600	-2.03861000

H	4.84450000	-0.87666900	-3.08435600
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C	-4.49831800	-1.52743800	1.81908500
H	-4.83377500	-1.74904400	2.84322100
H	-5.36891900	-1.15212200	1.27081000
H	-4.19631500	-2.47744900	1.36346000
C	-3.85675500	0.80357000	2.50471100
H	-4.66447900	1.27202500	1.93599600
H	-4.24632100	0.58770500	3.51077500
H	-3.05418700	1.54176000	2.61567800
C	-2.22760000	-1.05761100	2.76369300
H	-1.86083500	-2.03053600	2.42227800
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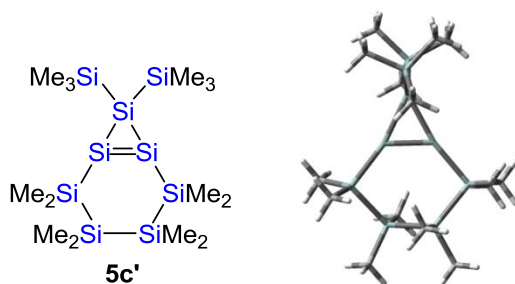
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Si	0.31075400	1.28987000	-0.72990200
Si	-1.54793700	2.43747300	0.17682800
Si	0.25582400	-0.87895900	-0.96042400
Si	-3.43628500	1.09287100	-0.35267000
C	-2.11494900	-2.99379900	-2.37636100
H	-1.31551600	-3.54655300	-2.88289700
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H	-2.59562500	4.69963200	-0.17941200
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H	-2.16452800	3.18244300	2.49303700
H	-1.20969600	1.69087900	2.57204800
C	-3.66437600	1.09023700	-2.25054100
H	-4.51739400	0.46623100	-2.54437400
H	-3.85264900	2.10416000	-2.62432400
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H	-5.90299000	1.28525700	0.15792400
H	-4.94997900	1.90694300	1.51448400
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H	-3.62424400	-0.55830800	2.86276700
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H	3.95341000	-2.55337600	1.87359000	C	5.30355800	1.50531500	-0.97495900
H	5.16156600	-1.26546700	1.75352300	H	5.72761400	1.20577500	-0.00899100
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H	0.57756600	-0.16707300	3.20277500	H	4.84631600	2.49318500	-0.84658000
H	0.98760500	-1.84353200	2.80748000	C	3.41334900	0.78621100	-3.31889000
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H	4.36064000	1.73010900	2.35918400	H	4.24953900	0.89575400	-4.02173100
H	2.71537600	2.11478700	2.88274300	$E = -3164.38497427$ hartree			
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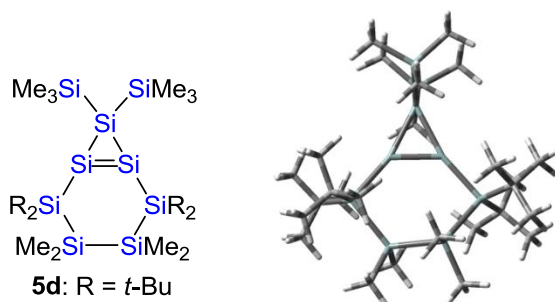


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Si	1.63256700	-2.46717400	0.59754100	H	2.34663500	4.74163600	0.20025000
Si	-0.20455900	1.03782400	-0.26781000	H	0.60059100	4.70499100	-0.09954800
Si	3.37760000	-1.14304500	-0.34567900	H	1.25876600	3.98899800	1.38149300
C	1.89363400	-2.82539700	2.45189900	C	1.89389900	2.82459700	-2.45241900
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H	2.34686400	-4.74137700	-0.20157500	Si	-3.57962100	-0.47872800	-1.95135900
H	0.60082000	-4.70498600	0.09825500	C	-2.44181500	1.17903500	3.29983100
H	1.25892700	-3.98836200	-1.38251400	H	-1.65077300	0.46797100	3.56333000
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H	5.13959900	-2.94728600	-0.16652200	H	-3.01167800	1.40495600	4.21040500
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H	4.02604300	-0.66026200	-2.73433000	H	-4.51890300	2.69072300	1.18224800
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C	3.23832600	1.25072300	2.24879900	H	-5.09232200	-1.53986600	1.86374400
H	4.02529200	0.66072200	2.73479000	H	-3.66386200	-1.87171400	2.85337400
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C	-4.94076400	-1.75538600	-1.56806100

H	-5.65238700	-1.37874200	-0.82370000
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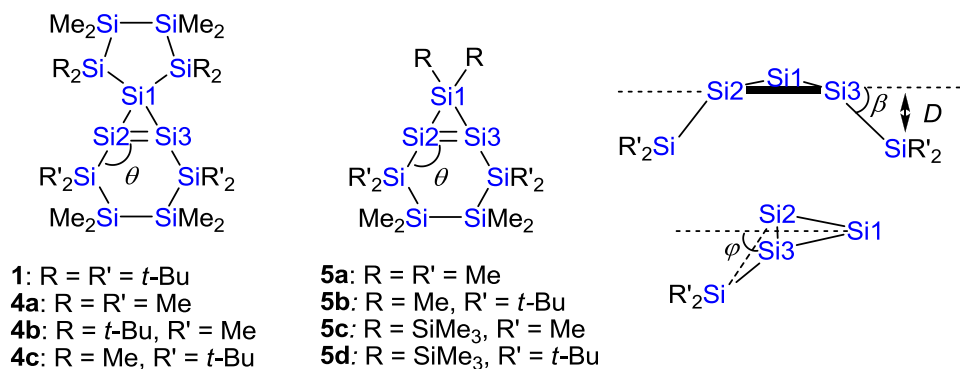
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Si	-1.16751500	-2.62337000	-0.00247800
Si	0.61208200	1.06792400	-0.02224900
Si	-3.01597100	-1.11477800	0.45596500
C	-0.91832200	3.95862200	-1.42601100
C	-1.25079400	3.40482800	1.81042100
C	-0.93572600	-3.95433100	1.42918100
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C	-3.29008800	-0.95557400	2.34395300
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C	-2.24634700	4.68604100	-1.73448000
H	-2.09153700	5.42238000	-2.53707200
H	-2.63768100	5.22814500	-0.86784900
H	-3.02523700	3.99607100	-2.07556400
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H	-4.13625500	0.31248500	-2.54380300
H	-2.41141300	0.53433000	-2.86161600
H	-3.49497100	1.93463100	-2.81038900
C	-1.71345700	2.32148500	2.80600300
H	-1.72330800	2.73326000	3.82604800
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C	-0.43175000	3.25757500	-2.71266500
H	-1.12215600	2.48321200	-3.05873400
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C	0.14259400	5.00983900	-1.03902800
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H	-5.50590400	-1.25684000	0.08486900
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H	-1.72181300	-2.73085200	-3.82618100
H	-1.03980300	-1.45354000	-2.80677600
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H	0.52048300	-4.71037100	-1.64466400
H	0.86481700	-3.10453300	-2.30131800
H	0.04127800	-4.31326700	-3.29849000
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H	-2.36338800	-4.92945600	-2.90087900

H	-3.26938100	-4.26798600	-1.53394500	H	3.42734300	-0.11088200	4.43959000
H	-1.95365400	-5.42211800	-1.25643100	H	2.10003800	0.64343500	3.53553900
C	-2.26680600	-4.67745300	1.73464500	C	5.27665100	1.35304500	-2.01796800
H	-2.11661800	-5.41306600	2.53878000	H	4.79619400	2.33444000	-1.93138400
H	-2.65702800	-5.21971300	0.86760700	H	5.98886800	1.25815900	-1.18990200
H	-3.04482100	-3.98480100	2.07231200	H	5.85261600	1.34502000	-2.95258500
Si	4.00049500	0.04499800	2.00299800	C	4.92778900	-1.71210100	-2.15554000
C	4.93200900	1.69892400	2.15453100	H	5.62292900	-1.86490500	-1.32182600
H	5.62537700	1.85255900	1.31948600	H	4.23528600	-2.56161600	-2.16897600
H	4.23969600	2.54855100	2.17045800	H	5.51098600	-1.74288500	-3.08520600
H	5.51722500	1.72850000	3.08296600	C	2.84862400	0.13666200	-3.50323700
C	5.27992900	-1.36607800	2.01335600	H	2.09443500	-0.65803000	-3.53327000
H	4.79917400	-2.34735800	1.92716500	H	2.31420300	1.09313200	-3.47494500
H	5.99038400	-1.27071800	1.18384100	H	3.41986400	0.09665300	-4.43971800
H	5.85787300	-1.35873400	2.94675600				
C	2.85467300	-0.15076400	3.50397800				
H	2.32083100	-1.10757100	3.47602300				

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Table S4. Structural Parameters of 1, 1_{calc}, 4a–c, 5a–d, and 5a'–c'



structural parameter	observed	calculated			
	1	1_{calc}	4a	4b	4c
$d(\text{Si1-Si2}) / \text{\AA}$	2.3526(8)	2.407	2.344	2.366	2.362
$d(\text{Si1-Si3}) / \text{\AA}$	2.3744(7)	2.378	2.373	2.380	2.362
$d(\text{Si2=Si3}) / \text{\AA}$	2.1473(8)	2.144	2.183	2.144	2.141
$\Sigma \text{ Si2} / ^\circ$	359.2	359.8	339.6	357.2	359.9
$\Sigma \text{ Si3} / ^\circ$	360.0	359.7	324.0	351.8	359.9
$\theta / ^\circ$	128.35(3)	131.4	128.7	129.8	131.2
bent angle $\beta / ^{\circ a}$	131.73(3)	127.3	121.2	126.0	131.2
	4.1 ^b	2.1 ^b	27.3 ^c	8.3 ^c	1.1 ^b
fold angle $\varphi / ^{\circ d}$	0.9 ^b	2.4 ^b	37.2 ^c	13.8 ^c	1.1 ^b
	5.2	2.8	36.0	10.8	1.4
	1.3	3.0	45.1	17.1	1.4

structural parameter	calculated						
	5a	5a'^e	5b	5b'^e	5c	5c'^e	5d
$d(\text{Si1-Si2}) / \text{\AA}$	2.326	2.330	2.325	2.327	2.344	2.364	2.365
$d(\text{Si1-Si3}) / \text{\AA}$	2.333	2.330	2.330	2.331	2.378	2.364	2.365
$d(\text{Si2=Si3}) / \text{\AA}$	2.196	2.159	2.170	2.158	2.182	2.144	2.139
$\Sigma \text{ Si2} / ^\circ$	334.1	360.0	348.5	358.4	340.6	360.0	359.9
$\Sigma \text{ Si3} / ^\circ$	328.0	360.0	343.3	353.2	323.9	360.0	359.9
$\theta / ^\circ$	126.3	128.0	130.3	130.8	129.7	128.6	131.2
bent angle $\beta / ^{\circ a}$	123.8	128.0	128.3	129.5	120.2	128.6	131.2
	30.9 ^c	0.5 ^b	18.8 ^c	6.1 ^c	26.7 ^c	0.9 ^b	1.6 ^b
fold angle $\varphi / ^{\circ d}$	35.1 ^c	0.5 ^b	23.2 ^c	13.3 ^c	36.7 ^c	0.9 ^b	1.5 ^b
	39.6	0.7	25.0	8.0	35.8	1.2	2.2
	43.7	0.7	30.1	17.4	43.8	1.2	2.0

^aA bent angle β is defined as $\sin \beta = D/d(\text{Si2-SiR}'_2)$ or $D/d(\text{Si3-SiR}'_2)$, where D is the distance between the silicon atom (SiR'_2) and the Si1–Si2–Si3 plane. ^btrans-Bent geometry. ^ccis-Bent geometry. ^dA fold angle φ is defined as the angle between the Si1–Si2–Si3 plane and the $\text{R}'_2\text{Si-Si2-Si3}$ plane.

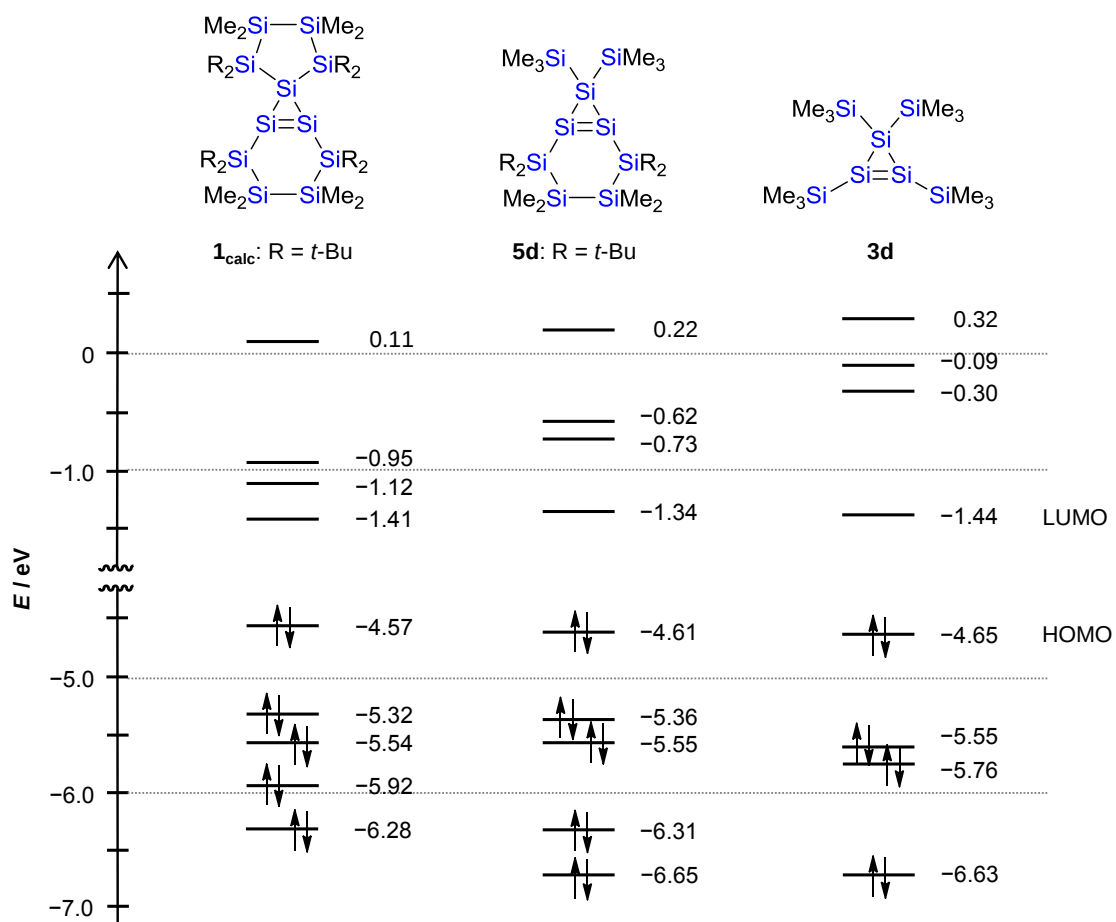


Figure S20. Energy levels of the selected molecular orbitals of 1_{calc} , 3d , and 5d .

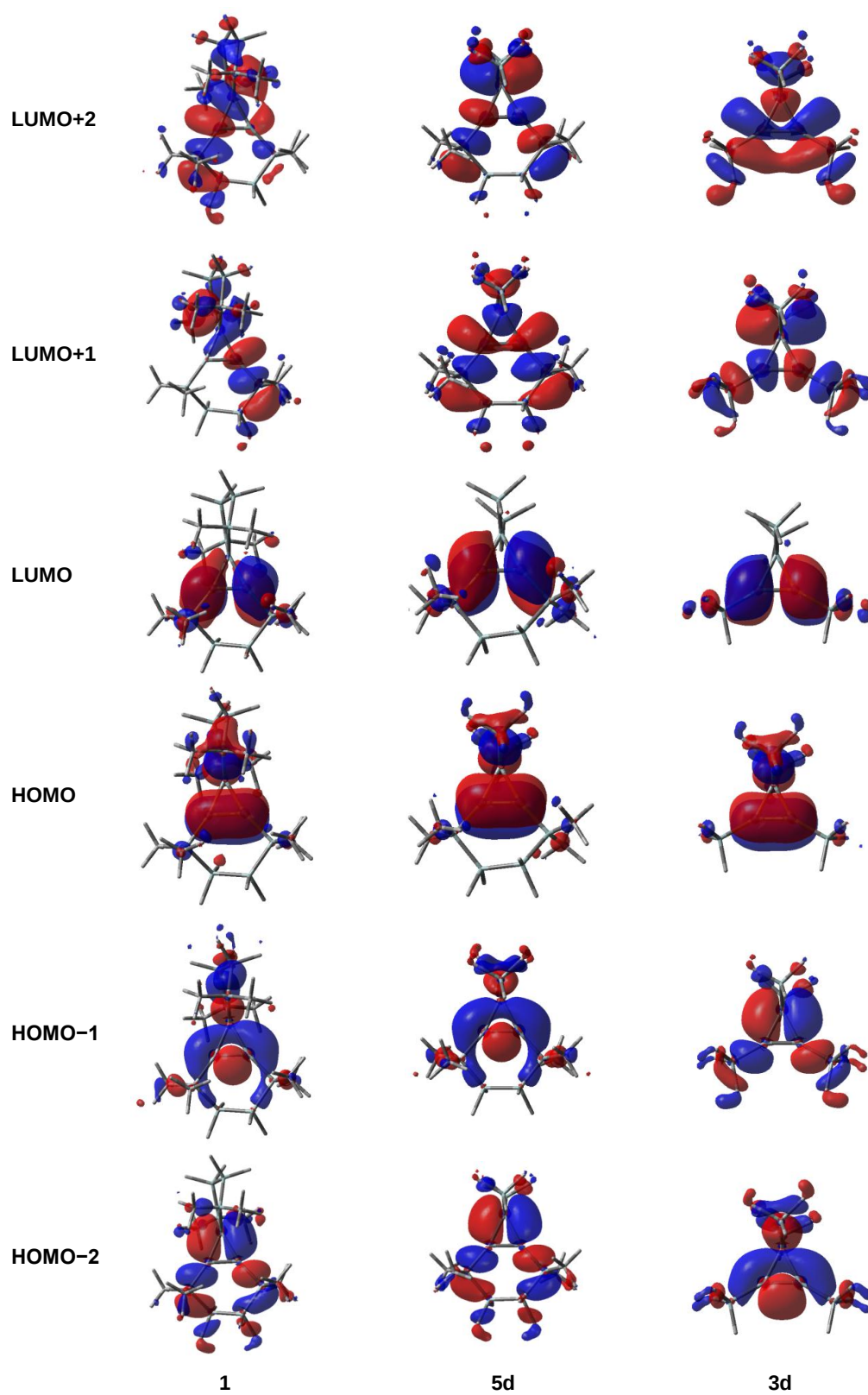
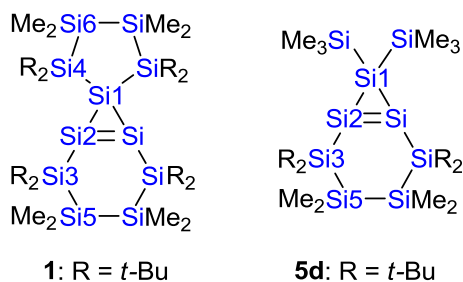
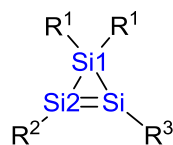


Figure S21. Selected molecular orbitals of **1_{calc}**, **3d**, and **5d**.

Table S5. Calculated and Reported ^{29}Si Chemical Shifts of **1**, **1_{calc}**, **3a–d**, and **5d**



nucleus	$\delta(\mathbf{1}, \text{obsd}) / \text{ppm}$	$\delta(\mathbf{1}_{\text{calc}}) / \text{ppm}$	$\delta(\mathbf{5d}, \text{calcd}) / \text{ppm}$
Si1	−85.4	−54.2	−74.8
Si2	147.1	205.7	169.3
Si3	15.0	25.8	14.0
Si4	−11.9	−3.8	—
Si5	−31.5	−20.7	−21.1
Si6	−41.1	−32.2	—
SiMe ₃	—	—	−7.2



- 3a:** R¹ = R² = Si(*t*-Bu)Me₂, R³ = Si[Si(*t*-Bu)Me₂]₃
3b: R¹ = R² = R³ = Si(*t*-Bu)₂Me
3c: R¹ = Si(*t*-Bu)₂Me, R² = R³ = Si(*t*-Bu)₃
3d: R¹ = R² = R³ = SiMe₃

nucleus	$\delta(\mathbf{3a}, \text{obsd}) / \text{ppm}^a$	$\delta(\mathbf{3b}, \text{obsd}) / \text{ppm}^b$	$\delta(\mathbf{3c}, \text{obsd}) / \text{ppm}^c$	$\delta(\mathbf{3d}, \text{calcd}) / \text{ppm}^d$
Si1	−117.2	−127.3	−115.1	−105.2
Si2	81.9, 99.8	97.7	97.4	102.9
SiR ₃	0.4, 6.4, 14.0	7.9, 27.1	11.5, 39.6	−7.8, 2.1

^aRef S10. ^bRef S7. ^cRef S8. ^dCalculated by assuming the C₂ symmetry.

Table S6. Magnetic Shielding Tensors of ^{29}Si Nuclei of 1_{calc} , 3d, and 5d Calculated by the GIAO Method

SCF GIAO Magnetic shielding tensor (ppm) of 1_{calc} :

Si1	Isotropic =	384.0002	Anisotropy =	263.2167
XX=	251.1094	YX=	6.4184	ZX= 24.3152
XY=	4.5447	YY=	342.2826	ZY= 23.0651
XZ=	6.4205	YZ=	-14.1316	ZZ= 558.6086
Eigenvalues:	250.0439	342.4787	559.4780	
Si2	Isotropic =	122.1632	Anisotropy =	593.5168
XX=	-349.0369	YX=	379.9701	ZX= 51.4083
XY=	-47.8695	YY=	199.3146	ZY= -20.4758
XZ=	15.2167	YZ=	27.7210	ZZ= 516.2119
Eigenvalues:	-396.4606	245.1091	517.8410	
Si2'	Isotropic =	126.1707	Anisotropy =	584.9515
XX=	-358.9774	YX=	-369.5085	ZX= 8.9630
XY=	73.3282	YY=	221.4849	ZY= -29.7411
XZ=	11.5596	YZ=	37.0184	ZZ= 516.0047
Eigenvalues:	-394.7044	257.0781	516.1384	
Si3	Isotropic =	298.2367	Anisotropy =	40.8857
XX=	287.9127	YX=	20.9063	ZX= -1.3234
XY=	16.6121	YY=	281.9876	ZY= 9.3476
XZ=	-2.8147	YZ=	1.5412	ZZ= 324.8099
Eigenvalues:	265.4511	303.7652	325.4938	
Si3'	Isotropic =	309.7945	Anisotropy =	80.9536
XX=	301.0445	YX=	-7.1582	ZX= -9.4396
XY=	-0.5716	YY=	295.1140	ZY= -29.5038
XZ=	-27.6797	YZ=	-55.5715	ZZ= 333.2251
Eigenvalues:	262.6881	302.9319	363.7636	
Si4	Isotropic =	332.1261	Anisotropy =	58.3342
XX=	309.1007	YX=	-2.9584	ZX= 0.4149
XY=	-6.7358	YY=	370.2782	ZY= -12.7076
XZ=	3.0518	YZ=	4.1886	ZZ= 316.9995
Eigenvalues:	308.4825	316.8803	371.0156	
Si4'	Isotropic =	335.2267	Anisotropy =	62.8578
XX=	314.1550	YX=	10.3973	ZX= -1.7473
XY=	13.9275	YY=	373.8951	ZY= -14.2515
XZ=	-4.2619	YZ=	0.8920	ZZ= 317.6301
Eigenvalues:	311.2761	317.2722	377.1319	
Si5	Isotropic =	347.3769	Anisotropy =	13.0240
XX=	352.1909	YX=	-5.7218	ZX= 0.3123
XY=	-2.9312	YY=	346.6365	ZY= -9.5565
XZ=	-2.6431	YZ=	-8.1329	ZZ= 343.3034
Eigenvalues:	335.1665	350.9047	356.0596	
Si5'	Isotropic =	353.6344	Anisotropy =	17.8384
XX=	360.8695	YX=	2.3100	ZX= 2.9776
XY=	3.9556	YY=	337.9709	ZY= -9.4452
XZ=	3.6661	YZ=	-5.5791	ZZ= 362.0628
Eigenvalues:	335.2153	360.1613	365.5267	

Si6 Isotropic = 362.3683 Anisotropy = 25.4675
 XX= 360.4420 YX= -8.3473 ZX= 4.2095
 XY= -10.2734 YY= 369.8366 ZY= 7.9289
 XZ= -2.0661 YZ= 14.1611 ZZ= 356.8264
 Eigenvalues: 347.6564 360.1019 379.3467
 Si6' Isotropic = 361.7404 Anisotropy = 24.1477
 XX= 363.0736 YX= 7.5669 ZX= -1.4730
 XY= 11.8846 YY= 367.5130 ZY= 6.7170
 XZ= 3.9077 YZ= 10.7115 ZZ= 354.6344
 Eigenvalues: 349.1704 358.2119 377.8388

SCF GIAO Magnetic shielding tensor (ppm) of **3d**:

Si1 Isotropic = 435.0835 Anisotropy = 275.9627
 XX= 374.9675 YX= 27.0908 ZX= 0.0000
 XY= 23.2372 YY= 616.4644 ZY= 0.0000
 XZ= 0.0000 YZ= 0.0000 ZZ= 313.8185
 Eigenvalues: 313.8185 372.3733 619.0586
 Si2 Isotropic = 226.9128 Anisotropy = 428.6101
 XX= 286.6274 YX= 16.0158 ZX= 166.9635
 XY= 17.3634 YY= 511.4021 ZY= -11.8882
 XZ= -293.5830 YZ= 27.9641 ZZ= -117.2909
 Eigenvalues: -127.1534 295.2390 512.6529
 Si2' Isotropic = 226.9128 Anisotropy = 428.6101
 XX= 286.6274 YX= 16.0158 ZX= -166.9635
 XY= 17.3634 YY= 511.4021 ZY= 11.8882
 XZ= 293.5830 YZ= -27.9641 ZZ= -117.2909
 Eigenvalues: -127.1534 295.2390 512.6529
 Si7 (SiMe₃) Isotropic = 327.7003 Anisotropy = 11.9264
 XX= 325.7176 YX= -1.2130 ZX= -9.0162
 XY= 0.5808 YY= 326.1226 ZY= 0.2743
 XZ= -4.1720 YZ= -1.4059 ZZ= 331.2608
 Eigenvalues: 321.2678 326.1819 335.6513
 Si7' (SiMe₃) Isotropic = 327.7003 Anisotropy = 11.9264
 XX= 325.7176 YX= -1.2130 ZX= 9.0162
 XY= 0.5808 YY= 326.1226 ZY= -0.2743
 XZ= 4.1720 YZ= 1.4059 ZZ= 331.2608
 Eigenvalues: 321.2678 326.1819 335.6513
 Si8 (SiMe₃) Isotropic = 337.6136 Anisotropy = 10.0143
 XX= 339.4010 YX= -2.4969 ZX= 0.4327
 XY= -4.9010 YY= 338.5589 ZY= -8.0906
 XZ= -3.5632 YZ= -4.4995 ZZ= 334.8811
 Eigenvalues: 328.9738 339.5773 344.2898
 Si8' (SiMe₃) Isotropic = 337.6136 Anisotropy = 10.0143
 XX= 339.4010 YX= -2.4969 ZX= -0.4327
 XY= -4.9010 YY= 338.5589 ZY= 8.0906
 XZ= 3.5632 YZ= 4.4995 ZZ= 334.8811
 Eigenvalues: 328.9738 339.5773 344.2898

SCF GIAO Magnetic shielding tensor (ppm) of **5d**:

Si1 Isotropic = 404.6402 Anisotropy = 241.0314

XX= 278.2326 YX= 0.1976 ZX= -0.2573
 XY= 0.2229 YY= 370.3801 ZY= -0.9083
 XZ= 0.1624 YZ= 4.8512 ZZ= 565.3079
 Eigenvalues: 278.2321 370.3607 565.3278
 Si2 Isotropic = 160.5391 Anisotropy = 600.1941
 XX= -340.0849 YX= -369.5905 ZX= 1.3373
 XY= 99.3038 YY= 261.1909 ZY= 1.7890
 XZ= -11.0156 YZ= 8.8675 ZZ= 560.5112
 Eigenvalues: -369.0773 290.0260 560.6684
 Si2' Isotropic = 160.4570 Anisotropy = 600.2076
 XX= -339.2353 YX= 371.6791 ZX= -1.1725
 XY= -97.0774 YY= 260.1563 ZY= 1.5217
 XZ= 10.9603 YZ= 8.5044 ZZ= 560.4502
 Eigenvalues: -369.2043 289.9800 560.5955
 Si3 Isotropic = 315.8245 Anisotropy = 76.9343
 XX= 292.6751 YX= -15.5587 ZX= -8.9702
 XY= -6.5333 YY= 291.1470 ZY= -7.9934
 XZ= -11.7462 YZ= -19.5945 ZZ= 363.6515
 Eigenvalues: 277.4218 302.9378 367.1141
 Si3' Isotropic = 315.7702 Anisotropy = 76.8115
 XX= 292.6882 YX= 15.5853 ZX= 9.0470
 XY= 6.5404 YY= 291.1500 ZY= -8.1470
 XZ= 11.6231 YZ= -19.7003 ZZ= 363.4725
 Eigenvalues: 277.3751 302.9577 366.9779
 Si5 Isotropic = 350.9826 Anisotropy = 23.4172
 XX= 358.1691 YX= -0.2870 ZX= 6.7665
 XY= -0.0741 YY= 342.7367 ZY= -11.0273
 XZ= 11.4444 YZ= -9.7841 ZZ= 352.0420
 Eigenvalues: 334.8815 351.4722 366.5940
 Si5' Isotropic = 350.9799 Anisotropy = 23.1538
 XX= 358.0004 YX= 0.2110 ZX= -6.7475
 XY= 0.0778 YY= 342.7392 ZY= -10.9339
 XZ= -11.2998 YZ= -9.4901 ZZ= 352.2002
 Eigenvalues: 335.1148 351.4092 366.4158
 Si7 (SiMe₃) Isotropic = 337.0704 Anisotropy = 12.0879
 XX= 336.6406 YX= 0.8571 ZX= 6.4153
 XY= -0.5497 YY= 337.1749 ZY= -1.7929
 XZ= 8.9223 YZ= -3.5445 ZZ= 337.3958
 Eigenvalues: 328.8696 337.2126 345.1290
 Si7' (SiMe₃) Isotropic = 337.0786 Anisotropy = 12.0353
 XX= 336.6095 YX= -0.9021 ZX= -6.4353
 XY= 0.5355 YY= 337.2147 ZY= -1.7492
 XZ= -8.8685 YZ= -3.5915 ZZ= 337.4116
 Eigenvalues: 328.8706 337.2631 345.1021

Table S7. Transition Energies, Wavelengths, and Oscillator Strengths of the Transitions of

1_{calc}^a

Excited State 1:	Singlet-A	245 -> 251	-0.19745	
2.5860 eV	479.45 nm	f=0.0017	245 -> 253	0.10285
245 -> 247	0.69396	Excited State 12:	Singlet-A	
Excited State 2:	Singlet-A	4.0254 eV	308.00 nm	f=0.1168
2.6485 eV	468.12 nm	f=0.0271	242 -> 247	0.47390
245 -> 246	0.61839	242 -> 248	0.17729	
245 -> 248	0.27640	243 -> 247	0.21373	
Excited State 3:	Singlet-A	243 -> 248	0.19996	
2.7658 eV	448.28 nm	f=0.0133	245 -> 249	0.14829
245 -> 246	-0.27230	245 -> 250	-0.31277	
245 -> 248	0.63337	Excited State 13:	Singlet-A	
Excited State 4:	Singlet-A	4.0433 eV	306.64 nm	f=0.1516
2.8921 eV	428.71 nm	f=0.0004	242 -> 247	0.43895
244 -> 246	0.68015	242 -> 248	0.15776	
245 -> 247	0.10223	243 -> 247	-0.19249	
245 -> 248	0.11197	243 -> 248	-0.22154	
Excited State 5:	Singlet-A	245 -> 249	-0.15862	
3.2060 eV	386.73 nm	f=0.0018	245 -> 250	0.32352
243 -> 246	0.69981	245 -> 252	-0.10164	
Excited State 6:	Singlet-A	Excited State 14:	Singlet-A	
3.3304 eV	372.28 nm	f=0.0036	4.0599 eV	305.39 nm
243 -> 247	-0.10493	f=0.0311	245 -> 250	0.11230
244 -> 247	0.66666	245 -> 251	0.30818	
244 -> 248	0.17026	245 -> 252	0.50104	
Excited State 7:	Singlet-A	245 -> 255	-0.18258	
3.5242 eV	351.81 nm	f=0.0070	245 -> 256	-0.12013
243 -> 247	0.15023	245 -> 259	0.15172	
244 -> 247	-0.14801	Excited State 15:	Singlet-A	
244 -> 248	0.65814	4.1041 eV	302.10 nm	f=0.0025
Excited State 8:	Singlet-A	241 -> 246	0.66141	
3.7242 eV	332.92 nm	f=0.0764	245 -> 251	-0.13328
243 -> 247	0.53235	245 -> 252	0.13784	
243 -> 248	-0.35200	Excited State 16:	Singlet-A	
245 -> 246	0.10668	4.1144 eV	301.34 nm	f=0.0566
245 -> 249	0.11622	241 -> 246	0.19536	
245 -> 250	0.18198	245 -> 249	0.14320	
Excited State 9:	Singlet-A	245 -> 251	0.53281	
3.8125 eV	325.20 nm	f=0.0219	245 -> 252	-0.27793
243 -> 248	0.37826	245 -> 253	-0.10242	
245 -> 249	0.36166	245 -> 255	0.10588	
245 -> 250	0.44816	245 -> 262	0.10782	
Excited State 10:	Singlet-A	Excited State 17:	Singlet-A	
3.9489 eV	313.97 nm	f=0.0042	4.2958 eV	288.62 nm
242 -> 246	0.68357	f=0.0077	245 -> 251	0.15482
Excited State 11:	Singlet-A	245 -> 252	-0.11568	
3.9661 eV	312.61 nm	f=0.0896	245 -> 253	0.58266
243 -> 247	-0.21457	245 -> 254	-0.28566	
243 -> 248	-0.26141	245 -> 257	-0.10008	
245 -> 249	0.50713	Excited State 18:	Singlet-A	
245 -> 250	-0.16470	4.3119 eV	287.54 nm	f=0.0021

242 -> 247	-0.24665	239 -> 246	-0.29205
242 -> 248	0.64774	240 -> 246	-0.25861
Excited State 19:	Singlet-A	245 -> 252	-0.14341
4.3407 eV	285.63 nm f=0.0042	245 -> 257	0.33625
245 -> 253	-0.10687	245 -> 258	0.23208
245 -> 255	-0.21687	245 -> 259	0.30112
245 -> 256	0.59353	245 -> 262	-0.12299
245 -> 261	0.11670	Excited State 23:	Singlet-A
Excited State 20:	Singlet-A	4.3976 eV	281.94 nm f=0.0289
4.3697 eV	283.74 nm f=0.0034	239 -> 246	-0.29296
239 -> 246	-0.19701	240 -> 246	-0.27515
240 -> 246	-0.15665	245 -> 252	0.26401
245 -> 252	-0.10831	245 -> 255	0.35432
245 -> 253	0.12836	245 -> 256	0.12511
245 -> 254	0.44822	245 -> 259	-0.23972
245 -> 255	-0.31590	245 -> 261	0.12082
245 -> 257	-0.22760	Excited State 24:	Singlet-A
245 -> 262	0.10765	4.4555 eV	278.27 nm f=0.0179
Excited State 21:	Singlet-A	239 -> 246	-0.12162
4.3719 eV	283.59 nm f=0.0347	239 -> 247	0.32131
239 -> 246	0.21159	240 -> 247	0.36379
240 -> 246	0.17668	240 -> 248	0.14119
245 -> 253	0.29671	241 -> 247	0.39951
245 -> 254	0.41541	245 -> 255	-0.17418
245 -> 255	0.21167	Excited State 25:	Singlet-A
245 -> 256	0.15333	4.4753 eV	277.04 nm f=0.0018
245 -> 257	0.16830	239 -> 246	-0.43053
245 -> 258	0.13903	240 -> 246	0.52230
Excited State 22:	Singlet-A	241 -> 247	-0.15590
4.3919 eV	282.30 nm f=0.0087		

^aThe 245th orbital is the HOMO, and the 246th orbital is the LUMO.

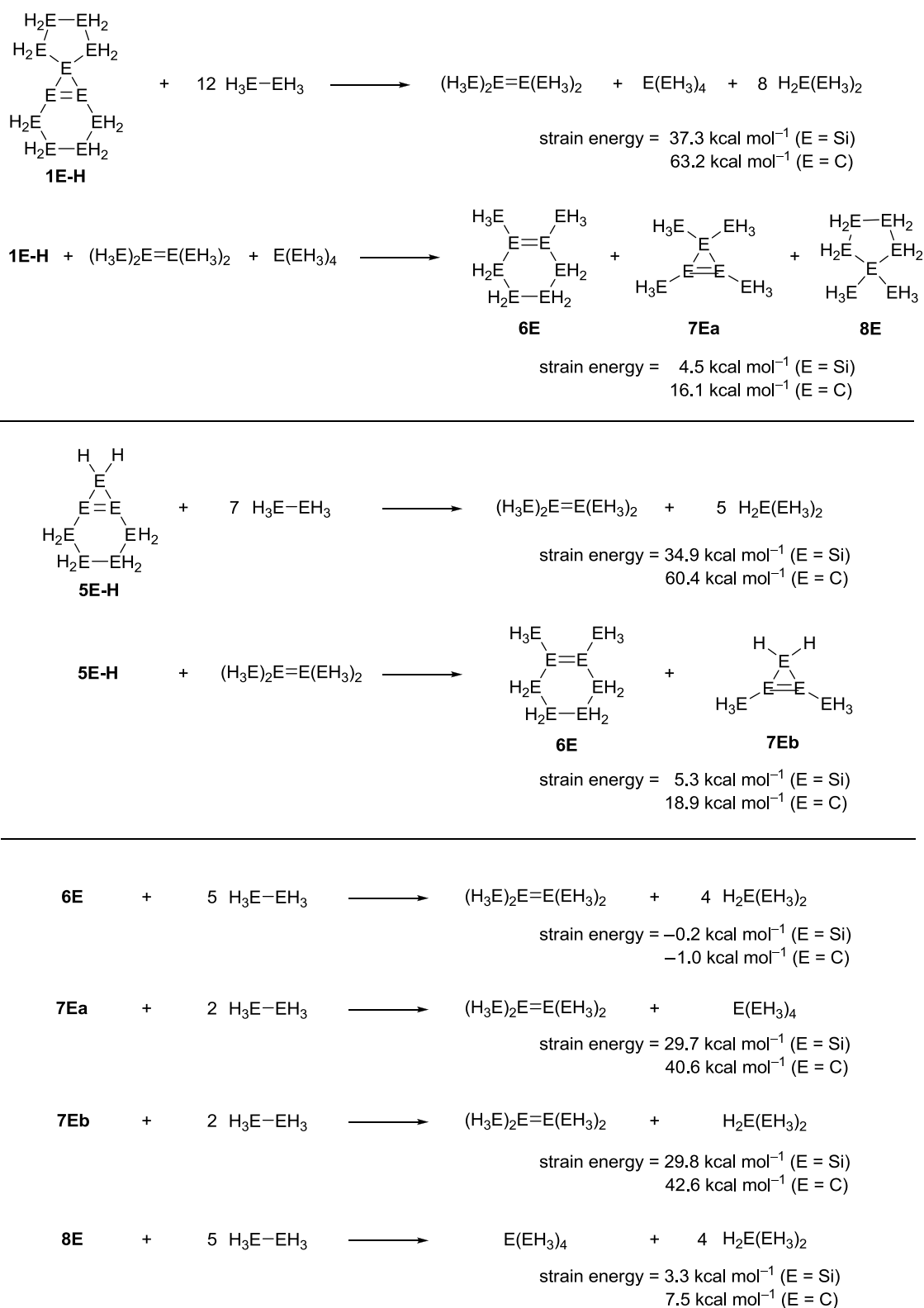
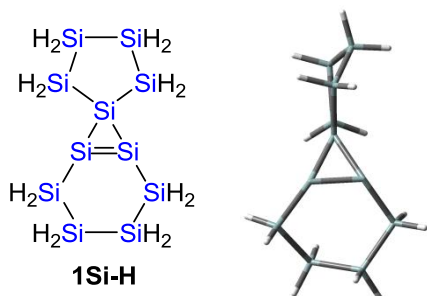
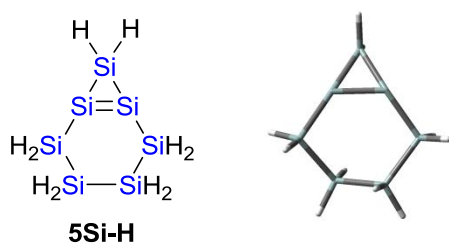


Figure S22. Strain energies of bicyclo[4.1.0]heptasil-1(6)-ene and related compounds.

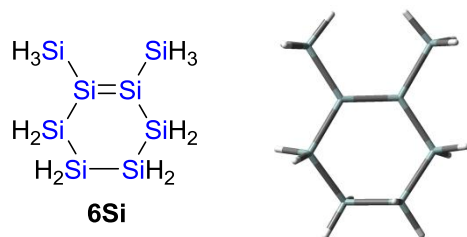
Table S8. Atomic Coordinates of the Optimized Structures



Si	3.01458200	-0.53596000	1.74387400	H	4.77298600	-2.03522000	-0.45043200
Si	-2.69002700	2.10935100	1.14351400	H	6.14104800	-0.50287500	0.81727300
Si	1.11280300	-0.04270700	0.41176900	H	2.81971000	-1.76776000	2.55711000
Si	-3.97035100	1.34234100	-0.68842500	H	3.28080000	0.59894700	2.67615500
Si	4.79822700	-0.69175000	0.19820600	H	-2.21506700	3.51085600	0.96757800
Si	1.93126600	0.83071200	-1.64963700	H	-3.48882500	2.04598500	2.40038800
Si	-0.76485600	-1.46602900	0.64101800	H	-3.19562600	1.61675100	-1.93293800
Si	-2.43775200	-2.27177500	-0.81046300	H	-5.25816700	2.09252700	-0.78682000
Si	-0.90620800	0.59539400	1.37062600	H	-5.41097800	-1.35704100	-1.56913700
Si	4.28347600	0.95385500	-1.41869900	H	-4.98808500	-1.27561100	0.79625800
Si	-4.39626700	-0.97918100	-0.54072800	H	-1.92166800	-2.13738100	-2.20408800
H	1.31483100	2.15195200	-1.96510600	H	-2.72221900	-3.71815800	-0.58368100
H	1.56769200	-0.10564200	-2.75336500	$E = -3194.35079386$ hartree			
H	5.00981100	0.76683300	-2.70690400				
H	4.64525000	2.29633600	-0.87707600				

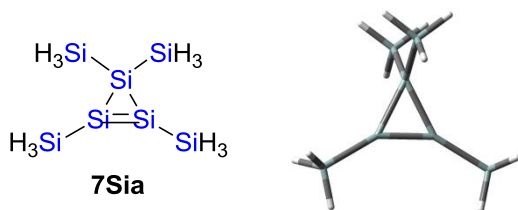


Si	-0.48834700	-2.41339600	-0.34436000	H	-3.44816600	-1.80984700	0.76627900
Si	3.10597700	-0.01209900	0.61369500	H	-3.61335900	1.67353500	0.26824500
Si	-2.13002200	-1.10738500	0.74349300	H	-2.57437300	0.83888100	-1.73246400
Si	1.40878300	1.15603000	-0.47125300	H	-0.38730800	2.78827100	1.51906600
Si	-0.50282800	2.41005600	0.08053900	H	-0.60793200	3.67142800	-0.70750900
Si	1.39759200	-1.03017800	-0.57900700	H	4.47508200	0.02620200	0.03250200
Si	-2.38143800	1.01903900	-0.26418600	H	3.23591600	-0.11654800	2.09873100
H	-0.17069700	-3.66415400	0.40142500	$E = -2032.62149908$ hartree			
H	-0.94754600	-2.79529800	-1.71025200				
H	-1.69766700	-0.92141500	2.15908100				



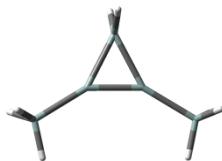
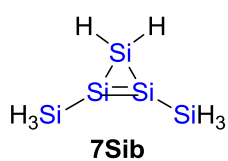
Si	1.05201400	2.31938400	-0.11755500	H	0.89336700	3.51025600	0.76827700
Si	2.91769300	1.04187400	0.54878900	H	1.27829700	2.84233000	-1.49703800
Si	1.05202600	-2.31940700	0.11764600	Si	-2.95362100	-2.29698500	0.09127000
Si	2.91763600	-1.04188900	-0.54887800	H	-3.01619600	-3.21085200	-1.08251900
Si	-0.94597600	-1.08511900	0.07165700	H	-3.04301100	-3.13079600	1.32160700
Si	-0.94596100	1.08504600	-0.07158800	H	-4.11884100	-1.37606100	0.04798200
H	0.89336800	-3.51034700	-0.76809300	Si	-2.95351500	2.29707300	-0.09132600
H	1.27839700	-2.84224600	1.49715500	H	-4.11882700	1.37631100	-0.04711300
H	2.85198800	-0.81960400	-2.02160800	H	-3.01556300	3.21165100	1.08193700
H	4.17195200	-1.79655700	-0.26015300	H	-3.04323600	3.13015600	-1.32213300
H	4.17199800	1.79651700	0.25995800				
H	2.85217500	0.81957700	2.02152400				

$E = -2324.59447315$ hartree



Si	1.12884400	-0.00025900	-0.00002200	Si	2.45044900	-0.00055500	1.95732900
Si	-0.95117900	1.06835300	-0.00003200	H	3.33057500	-1.20362600	2.01280900
Si	-0.95163100	-1.06800700	-0.00000300	H	3.33162800	1.20176500	2.01241600
Si	2.45066200	-0.00056000	-1.95722400	H	1.57893100	0.00002100	3.16425100
H	3.33161600	-1.20305700	-2.01199700	Si	-2.13861500	3.09237900	-0.00003200
H	1.57935700	-0.00111700	-3.16429800	H	-3.59539900	2.79831000	0.00016200
H	3.33102500	1.20233800	-2.01269900	H	-1.79052600	3.88396000	1.20942000
Si	-2.14024400	-3.09134100	-0.00003700	H	-1.79083900	3.88379900	-1.20968000
H	-1.79259100	-3.88314000	1.20940000				
H	-3.59685700	-2.79642700	0.00018100				
H	-1.79295000	-3.88295600	-1.20969700				

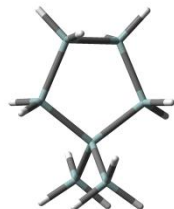
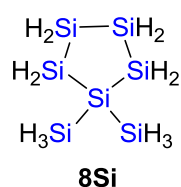
$E = -2033.82138177$ hartree



Si	0.00002200	2.15445700	0.00001100
Si	1.07205200	0.10392000	0.00000400
Si	-1.07207200	0.10395200	-0.00001700
Si	-3.08519200	-1.10564400	-0.00000200
H	-3.88153300	-0.76736800	-1.20934000
H	-2.77943800	-2.56031000	-0.00013200
H	-3.88140200	-0.76756000	1.20947600
Si	3.08518600	-1.10565300	0.00000000

H	2.77946100	-2.56032400	-0.00008700
H	3.88149200	-0.76739200	-1.20936500
H	3.88141800	-0.76752300	1.20945100
H	0.00002300	3.03799700	1.20314400
H	0.00003100	3.03802400	-1.20310100

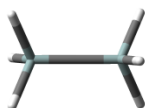
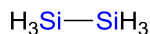
$E = -1452.35885267$ hartree



Si	-0.40794700	1.67840300	0.88911800
Si	-2.58650300	1.17148200	0.11868400
Si	-0.40512600	-1.63389800	-0.96055400
Si	-2.57020100	-1.17577700	-0.12855200
Si	1.03175800	0.00332100	-0.00139800
Si	2.31237000	-0.95628800	1.73098800
H	3.22489400	-2.00400400	1.19520300
H	3.13562700	0.07961700	2.41378900
H	1.42085800	-1.58611400	2.74382600
Si	2.44528900	0.91507000	-1.65391600
H	3.34744400	1.94548500	-1.06939000
H	3.28478300	-0.14838300	-2.27158700
H	1.63641900	1.55531800	-2.72755700

H	0.04974000	-3.01799500	-0.64373800
H	-0.40249000	-1.49264200	-2.44630200
H	-2.72195600	-1.81097500	1.21275800
H	-3.65604700	-1.69000700	-1.01017600
H	-2.79090900	1.80210500	-1.21782000
H	-3.65465400	1.66730800	1.03189700
H	-0.37755000	1.62147600	2.38001600
H	0.02889200	3.04642400	0.48790600

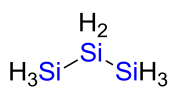
$E = -2035.10375757$ hartree



Si	1.17622500	-0.00000700	-0.00001500
H	1.69835000	-1.37996100	0.19833400
H	1.69840500	0.51821700	-1.29416900
H	1.69851900	0.86170500	1.09591200
Si	-1.17622500	0.00000700	0.00001500

H	-1.69835000	1.37997300	-0.19824600
H	-1.69851900	-0.86163600	-1.09596700
H	-1.69840400	-0.51829900	1.29413700

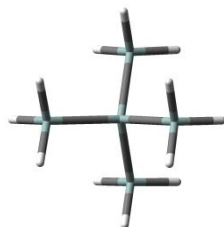
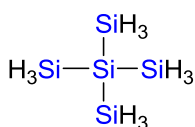
$E = -582.646423133$ hartree



Si	0.00000000	0.88370000	0.00000000
H	0.00000000	1.76838900	1.20134900
H	0.00000000	1.76838900	-1.20134900
Si	1.96389100	-0.41647500	0.00000000
H	2.00985700	-1.28760100	-1.20641300
H	3.17329800	0.45156600	0.00000000
H	2.00985600	-1.28760100	1.20641300

Si	-1.96389100	-0.41647500	0.00000000
H	-2.00985600	-1.28760100	1.20641300
H	-3.17329800	0.45156600	0.00000000
H	-2.00985700	-1.28760100	-1.20641300

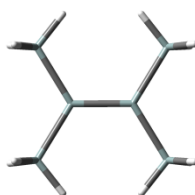
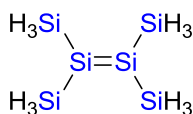
$E = -873.375717760$ hartree



Si	-0.00008400	-0.00003200	0.00010800
Si	1.08567200	-1.97283900	0.70891100
H	0.34121600	-3.17607400	0.24521600
H	2.46759900	-2.03655000	0.15833700
H	1.17100800	-2.01898900	2.19465200
Si	-0.12156000	0.02759700	-2.35729800
H	-0.88013400	-1.15230600	-2.85662300
H	-0.80817300	1.26051400	-2.83202700
H	1.24279900	-0.00720400	-2.95244400
Si	1.21710600	1.87979800	0.74719600

H	0.55224900	3.14006600	0.31519100
H	1.31174300	1.88620900	2.23311200
H	2.59788900	1.86464800	0.19032400
Si	-2.18119500	0.06545900	0.90117000
H	-2.97024400	-1.11362000	0.44928000
H	-2.13378900	0.05444900	2.38931000
H	-2.89131100	1.29909700	0.46444900

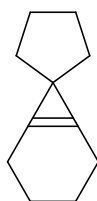
$E = -1454.83818402$ hartree



Si	-1.08347700	0.00004800	0.09368200
Si	1.08404000	0.00001400	-0.09383700
Si	-2.30339200	-1.99974400	-0.01507400
H	-3.10747300	-2.06096600	-1.26697700
H	-1.38734000	-3.16869100	0.02658500
H	-3.24681800	-2.08602100	1.13368700
Si	-2.30332700	1.99986100	-0.01530100
H	-3.10661700	2.06153100	-1.26768800
H	-3.24747000	2.08578100	1.13289900
H	-1.38723000	3.16874000	0.02731700

Si	2.30303900	-2.00030600	0.01513100
H	3.24692700	-2.08688600	-1.13323100
H	3.10655100	-2.06242400	1.26735500
H	1.38621300	-3.16862600	-0.02721600
Si	2.30330800	2.00014500	0.01535500
H	1.38663800	3.16857600	-0.02722000
H	3.10643300	2.06207000	1.26783600
H	3.24753400	2.08664600	-1.13272700

$E = -1744.32344011$ hartree



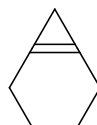
1C-H



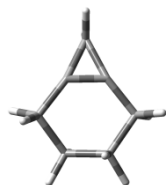
H	-1.10848900	-1.43769000	-1.47556900
H	-1.23594800	0.26381000	-1.91541000
H	-3.59673100	-0.21373400	-1.69964300
H	-3.29964300	-1.46864000	-0.49262800
H	-3.10892800	1.55950100	-0.04655700
H	-4.09492000	0.41395300	0.87423500
H	-1.65490500	1.06986800	1.89119300
H	-2.09156900	-0.64420700	1.82776300
H	1.49600300	-2.44657700	0.15944800
H	2.14919000	-1.63013000	1.57188700
H	2.57408000	-0.94283500	-1.38588300
H	3.81404700	-1.23566500	-0.16867800
H	3.76016000	1.16145300	-0.71960700
H	3.23804100	0.93952400	0.94816900
H	1.47357300	1.64821400	-1.47106300

H	1.68666900	2.55234400	0.02079500
C	0.53325100	0.71613200	0.20559400
C	0.58839200	-0.52807100	0.60066500
C	-0.78245200	-0.03536700	0.19988100
C	-1.47094300	-0.46283000	-1.12514600
C	-2.98614700	-0.46962200	-0.82579700
C	-3.14565100	0.53015600	0.33804500
C	-1.91249500	0.25013600	1.21210500
C	1.63267900	1.53420200	-0.38760900
C	2.94991500	0.76007300	-0.09738500
C	2.83420900	-0.76809300	-0.33162200
C	1.75913600	-1.45824900	0.55819500

$E = -428.850065083$ hartree



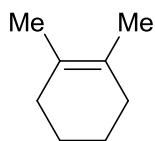
5C-H



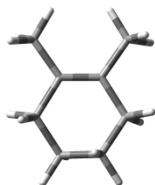
H	0.00076100	2.42143000	0.47597100
H	0.47775000	1.98962100	-1.15964700
H	1.31001500	0.66327200	1.47677200
H	2.36875500	1.28053500	0.21118500
H	2.42625000	-1.17967400	0.20192100
H	1.68329000	-0.61347800	-1.29141400
H	0.26006900	-1.91558500	1.11014300
H	0.29500200	-2.46631400	-0.55915800
H	-3.06335900	-0.08621100	-0.48187500
H	-2.50074400	0.06110300	1.24657000

C	-0.91433200	0.61523800	-0.28475300
C	-2.20436900	-0.01947800	0.19101100
C	-0.89606300	-0.68333100	-0.18448800
C	0.27945500	-1.56390600	0.06648000
C	1.53452700	-0.68583500	-0.20478000
C	1.42748000	0.74354000	0.38623100
C	0.23033800	1.56798900	-0.17478000

$E = -272.753692970$ hartree



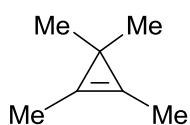
6C



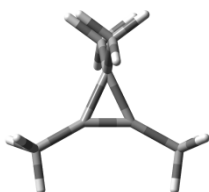
H	0.05572700	2.42791300	-0.54756900
H	-1.46868200	1.60692800	-0.80284800
H	1.28109900	0.84082200	-1.90856500
H	-0.17853200	1.24068900	-2.81566400
H	0.17853200	-1.24068900	-2.81566400
H	-1.28109900	-0.84082200	-1.90856500
H	-0.05572700	-2.42791300	-0.54756900
H	1.46868200	-1.60692800	-0.80284800
H	0.28971700	2.28040500	1.96692600
H	-1.43269200	1.96765400	1.78665000
H	-0.44988300	0.89833000	2.79243700
H	0.44988300	-0.89833000	2.79243700

H	-0.28971700	-2.28040500	1.96692600
H	1.43269200	-1.96765400	1.78665000
C	-0.18558500	0.64862900	0.62737300
C	0.18558500	-0.64862900	0.62737300
C	0.38903300	-1.42785600	-0.66296700
C	-0.18558500	-0.74240200	-1.90782200
C	0.18558500	0.74240200	-1.90782200
C	-0.38903300	1.42785600	-0.66296700
C	-0.45265000	1.47488400	1.86485500
C	0.45265000	-1.47488400	1.86485500

$E = -313.386290052$ hartree



7Ca



H	2.21215400	-0.88434700	-1.31896300
H	0.92967800	-0.00009100	-2.17153300
H	2.21257700	0.88343200	-1.31884500
H	-1.10272800	-2.54871700	0.88153600
H	-2.46071600	-1.81352800	0.00080300
H	-1.10393100	-2.54783300	-0.88249000
H	2.21238900	-0.88427800	1.31870300
H	2.21277700	0.88350300	1.31864700
H	0.93002500	-0.00008100	2.17150100
H	-2.45995900	1.81447600	0.00005500
H	-1.10222300	2.54881500	0.88189200

H	-1.10231200	2.54852200	-0.88213900
C	-0.65673800	0.65171300	0.00009300
C	-0.65699200	-0.65149100	0.00015300
C	0.71036400	-0.00015600	0.00000700
C	1.55943600	-0.00030500	-1.27383800
C	1.55964500	-0.00024800	1.27371100
C	-1.37226300	1.95225300	-0.00001000
C	-1.37307500	-1.95174400	0.00002300

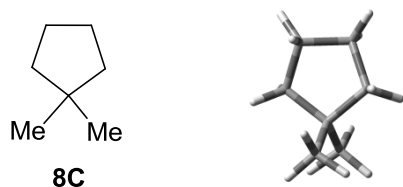
$E = -273.994543311$ hartree



H	-0.88177300	-0.37407100	2.55017000
H	-0.00033800	-1.74678800	1.83965300
H	0.88197200	-0.37449700	2.54992700
H	-0.00033800	-1.74678800	-1.83965300
H	-0.88177300	-0.37407100	-2.55017000
H	0.88197200	-0.37449700	-2.54992700
H	0.91480500	2.00986600	0.00000000
H	-0.91424400	2.01016100	0.00000000

C	-0.00005700	-0.65724600	1.95948500
C	-0.00005700	0.03676500	0.65006700
C	0.00018200	1.40274300	0.00000000
C	-0.00005700	0.03676500	-0.65006700
C	-0.00005700	-0.65724600	-1.95948500

$E = -195.336415899$ hartree



H	0.76327500	1.30559300	2.24806300
H	1.58615300	-0.26266300	2.14796500
H	1.92953400	0.99555400	0.94810100
H	-0.76327500	-1.30559300	2.24806300
H	-1.58615300	0.26266300	2.14796500
H	-1.92953400	-0.99555400	0.94810100
H	-0.24809600	2.11823900	0.03118200
H	-1.63589400	1.09001900	-0.31913300
H	1.02832900	1.13876000	-1.82179300
H	-0.59855000	1.20668600	-2.51024800
H	-1.02832900	-1.13876000	-1.82179300
H	0.59855000	-1.20668600	-2.51024800

H	1.63589400	-1.09001900	-0.31913300
H	0.24809600	-2.11823900	0.03118200
C	0.00000000	0.00000000	0.66198400
C	-1.13350000	-0.54117700	1.55215200
C	1.13350000	0.54117700	1.55215200
C	-0.53762700	1.11371400	-0.30127100
C	0.53762700	-1.11371400	-0.30127100
C	0.00000000	-0.76846800	-1.70256300
C	0.00000000	0.76846800	-1.70256300

$E = -275.277083366$ hartree



H	0.00000000	1.02175400	1.16529700
H	-0.88486500	-0.51087700	1.16529700
H	0.88486500	-0.51087700	1.16529700
H	0.00000000	-1.02175400	-1.16529700
H	-0.88486500	0.51087700	-1.16529700

H	0.88486500	0.51087700	-1.16529700
C	0.00000000	0.00000000	-0.76628800
C	0.00000000	0.00000000	0.76628800

$E = -79.8614329409$ hartree



H	0.87848900	0.00000000	1.24749100
H	-0.87848900	0.00000000	1.24749100
H	-0.88548100	1.32312700	-0.90772700
H	0.00000000	2.17804800	0.36760800
H	0.88548100	1.32312700	-0.90772700
H	0.88548100	-1.32312700	-0.90772700
H	0.00000000	-2.17804800	0.36760800

H	-0.88548100	-1.32312700	-0.90772700
C	0.00000000	-1.27829500	-0.26007500
C	0.00000000	0.00000000	0.58693500
C	0.00000000	1.27829500	-0.26007500

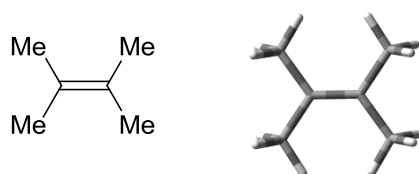
$E = -119.188237131$ hartree



H	1.53661800	-0.28279500	-1.53661800
H	1.53661800	-1.53661800	-0.28279500
H	0.28279500	-1.53661800	-1.53661800
H	1.53661800	1.53661800	0.28279500
H	0.28279500	1.53661800	1.53661800
H	1.53661800	0.28279500	1.53661800
H	-1.53661800	-0.28279500	1.53661800
H	-1.53661800	-1.53661800	0.28279500
H	-0.28279500	-1.53661800	1.53661800
H	-0.28279500	1.53661800	-1.53661800

H	-1.53661800	0.28279500	-1.53661800
H	-1.53661800	1.53661800	-0.28279500
C	0.00000000	0.00000000	0.00000000
C	-0.88978200	-0.88978200	0.88978200
C	0.88978200	0.88978200	0.88978200
C	0.88978200	-0.88978200	-0.88978200
C	-0.88978200	0.88978200	-0.88978200

$E = -197.843267770$ hartree



H	0.87975200	-2.19191100	1.26224400
H	-0.00032700	-0.96735700	2.18382200
H	-0.87956500	-2.19228800	1.26208100
H	0.87975100	-2.19191300	-1.26224300
H	-0.87956500	-2.19228700	-1.26208200
H	-0.00032400	-0.96735900	-2.18382200
H	0.87956500	2.19228800	1.26208100
H	-0.87975200	2.19191100	1.26224400
H	0.00032700	0.96735700	2.18382200
H	0.00032400	0.96735900	-2.18382200

H	-0.87975100	2.19191300	-1.26224300
H	0.87956500	2.19228700	-1.26208200
C	-0.00014100	-0.67590900	0.00000000
C	0.00014100	0.67590900	0.00000000
C	0.00000000	1.53204200	-1.25032300
C	0.00000000	1.53204100	1.25032300
C	0.00000000	-1.53204200	-1.25032300
C	0.00000000	-1.53204100	1.25032300

$E = -235.938858830$ hartree

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