Supporting Information

Imino(silyl)disilenes: Application in Versatile Bond Activation, Reversible Oxidation and Thermal Isomerization

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1. Experimental Section

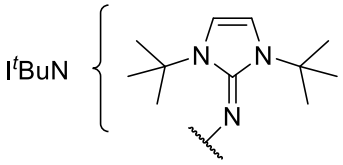
1.1 General Methods and Instrumentation

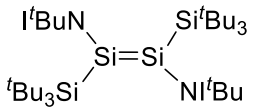
All manipulations were carried out under exclusion of water and oxygen under an atmosphere of argon 4.6 (≥99.996%) using standard Schlenk and glovebox techniques. The glassware used was heat dried under high vacuum prior to use. All solvents were refluxed over sodium/benzophenone, freshly distilled under argon and deoxygenated prior to use. PTFE-based grease (*Triboflon III* from *Freudenberg & Co. KG*) was used as sealant. Deuterated benzene (C_6D_6), toluene (Tol-d_8) and THF (THF-d_8) were obtained from Sigma-Aldrich, dried over Na/K alloy, flask-to-flask condensed, deoxygenated by three freeze-pump-thaw cycles and stored over 4 Å molecular sieves in a glovebox. All NMR samples were prepared under argon in *J. Young* PTFE valve NMR tubes. The NMR spectra were recorded on a *Bruker DRX400* (^{1}H: 400.13 MHz, ^{13}C: 100.62 MHz, ^{29}Si: 79.49 MHz), AV500 (^{1}H: 500.13 MHz), or *AV500C* (^{1}H: 500.36 MHz, ^{13}C: 125.83 MHz, ^{29}Si: 99.41 MHz) spectrometer at ambient temperature (300 K), unless otherwise stated. The ^{1}H, ^{13}C{^{1}H} and ^{29}Si{^{1}H} NMR spectroscopic chemical shifts δ are reported in ppm relative to tetramethylsilane. ^{1}H and ^{13}C{^{1}H} NMR spectra are calibrated against the residual proton and natural abundance carbon resonances of the respective deuterated solvent as internal standard (C_6D_6: δ(^{1}H) = 7.16 ppm and δ(^{13}C) = 128.1 ppm, Tol-d_8: δ(^{1}H) = 2.08 ppm and δ(^{13}C) = 20.4 ppm), THF-d_8: δ(^{1}H) = 1.73 ppm and δ(^{13}C) = 25.4 ppm).[S1] The following abbreviations are used to describe signal multiplicities: s = singlet, d = doublet, dd = doublet of doublets, dt = doublet of triplets, t = triplet, sept = septet, m = multiplet, br = broad. In some NMR spectra, signals from silicone grease (C_6D_6: δ(^{1}H) = 0.29 ppm, δ(^{13}C) = 1.4 ppm and δ(^{29}Si) = -21.8 ppm), originating from the cannulas used (*B. Braun Melsungen AG Sterican®)*, can be observed. UV-vis spectra were recorded on a *Varian, Inc. Cary 50* spectrophotometer with a Schlenk quartz cuvette. EPR spectra were recorded on a *Jeol jes-Fa200 esr* spectrometer with a spectrometer frequency of 9.267 GHz (X-band). Simulation of the EPR spectra was performed with the *Easyspin* toolbox for *Matlab*.[S2] Quantitative elemental analyses (EA) were measured with a *EURO EA (HEKAtech)* instrument equipped with a CHNS combustion analyzer at the *Laboratory for Microanalysis* at the *TUM Catalysis Research Center*. Melting Points (m.p.) were determined in sealed glass capillaries under inert gas by a *Büchi M-565* melting point apparatus. LIFDI-ESI Mass spectrometry data were acquired using an Exactive Plus Orbitrap system (ionization method: LIFDI) by Thermo Fisher Scientific. Unless otherwise stated, all commercially available chemicals were purchased from *abcr GmbH* or *Sigma-Aldrich* and used without further purification. Hydrogen (H_2) 5.0 (≥99.999%), oxygen (O_2) 5.0 (≥99.999%), carbon dioxide (CO_2) 5.0 (≥99.999%), dinitrogen monoxide (N_2O) 5.0 (≥99.999%) and carbon monoxide (CO) 4.7 (≥99.997%) were purchased from *Westfalen AG* and used as received. The compounds bis(*tert*-butyl)imidazolin-2-iminotribromosilane (I^{t}BuNSiBr$_3$)[S3], supersilyl sodium (^{t}Bu$_3$SiNa·2THF)[S4], bis(*tert*-butyl)methylsilyl sodium (^{t}Bu$_2$MeSiNa)[S5] and the functionalized trityl (fluoroaryl)borate [Ph$_3$C][B(4-(^{i}Pr$_3$Si)-C$_6$F$_4$)$_4$][S6] were prepared as described in the corresponding references.

Potassium graphite (KC_8) was synthesized following a literature reported procedure upon heating a 1:8 mixture of potassium and graphite in a thick-walled, PTFE-capped pressurize-able Schlenk flask to 500 °C until a homogenous bronze powder was obtained.[S7]

The cyclic voltammetry (CV) measurements were performed in an Ar-filled glovebox (*MBraun*, oxygen and water content < 0.1 ppm). The electrochemical three-electrode glass cell was custom made with a gold (*Alfa Aesar*, 99.999% purity) working electrode (WE), a platinum (Advent, 99.99+% purity) counter electrode (CE), and a lithium (99.9%, foil, *Rockwood Lithium*, 0.45 mm thickness) reference electrode (RE). The electrolyte in the main and the CE compartment consisted of THF (*Sigma-Aldrich*) and 0.1 M tetrabutylammonium bis(trifluoromethane)-sulfonimide (TBATFSI). For the RE compartment a solution of 0.1 M LiTFSI in THF was used. The cell compartments were separated by porous glass frits. For the separation of the RE compartment a *Vycor* 7930 frit (*Advanced Glass & Ceramics, Holden*, MA) was used in order to diminish the diffusion between the Li-ion containing RE electrolyte and the electrolyte in the main compartment. The electrodes of the cell compartments were connected *via* fused-in tungsten wires. Before the first CV was recorded, the high frequency resistance (HFR) of the glass cell setup was measured *via* Electrochemical Impedance Spectroscopy (EIS) and used for ohmic drop correction of the measured WE potential. At the end of the CVs, about 10 mg of ferrocenium hexafluorophosphate ($FcPF_6$, *Sigma-Aldrich*) were added to the electrolyte in the main compartment in order to calibrate the potential of the Li RE versus the Fc/Fc^+ couple. The CVs were recorded using a *Biologic* VMP3 potentiostat/galvanostat.

1.2 Iminodisilene I^{t}BuN(^{t}Bu$_3$Si)Si=Si(Si^{t}Bu$_3$)NI^{t}Bu (1)





1

$Si_4C_{46}H_{94}N_6$

843.64 g/mol

A solution of ^{t}Bu$_3$SiNa·2THF (833 mg, 2.27 mmol, 2.10 eq.) in *n*-hexane (10 mL) was added to a suspension of I^{t}BuNSiBr$_3$ (500 mg, 1.08 mmol, 1.00 eq.) in *n*-hexane (5 mL). The color changed to dark green. After filtration, compound **1** was obtained by crystallization from toluene at –35 °C (251 mg, 297 µmol, 55% yield). These crystals were also suitable for SC-XRD analysis.

m.p.: 161 °C (decomposition, color change to brown).

^{1}H NMR (500 MHz, C_6D_6, 300 K): δ [ppm] = 6.08 (s, 4H, C*H*-N), 1.58 – 1.50 (m*, 90H, ^{t}*Bu*).* The signal of ^{t}*Bu*N overlaps with the signal of ^{t}*Bu*$_3$Si

^{1}H NMR (500 MHz, THF-d_8, 300 K): δ [ppm] = 6.46 (s, 4H, C*H*-N), 1.61 (s, 36H, N^t*Bu*), 1.26 (s, 54H, ^{t}*Bu*$_3$Si).

^{13}C{^{1}H} NMR (126 MHz, THF-d_8, 193 K): δ [ppm] = 145.7 (*C*=N), 110.5 (*C*H-N), 57.2 (N*C*(CH$_3$)$_3$), 31.3 (Si(C(*C*H$_3$)$_3$)$_3$), 31.1 (NC(*C*H$_3$)$_3$), 21.7 (Si(*C*(CH$_3$)$_3$)$_3$).

^{29}Si{^{1}H} NMR (99 MHz, THF-d_8, 193 K): δ [ppm] = 74.3 (*Si*=Si), 23.1 (^{t}Bu$_3$*Si*).

Note: The choice of the solvent seems to be crucial for the synthesis of **1**, as performing the reaction in THF instead of hexane results in the formation of an unidentified dark purple compound instead of **1**. Unfortunately, this species is not stable above –40 °C and various trapping attempts were unsuccessful. Compound **1** is only slightly soluble in *n*-hexane, benzene and toluene, however, it shows good solubility in THF. No additional sets of signals for the *(Z)*-isomer were observed in the multinuclear NMR spectra of compound **1**. Similar to reports for disilenes **III** and **VI** the signal intensities in the ^{29}Si NMR spectrum of **1** at room temperature are very weak. Therefore, the ^{13}C and ^{29}Si NMR spectra of **1** were recorded at –80 °C.

EA: $Si_4C_{40}H_{82}N_6$ Calculated [%]: C (65.49), H (11.23), N (9.96)
Experimental [%]: C (65.02), H (11.14), N (9.59).

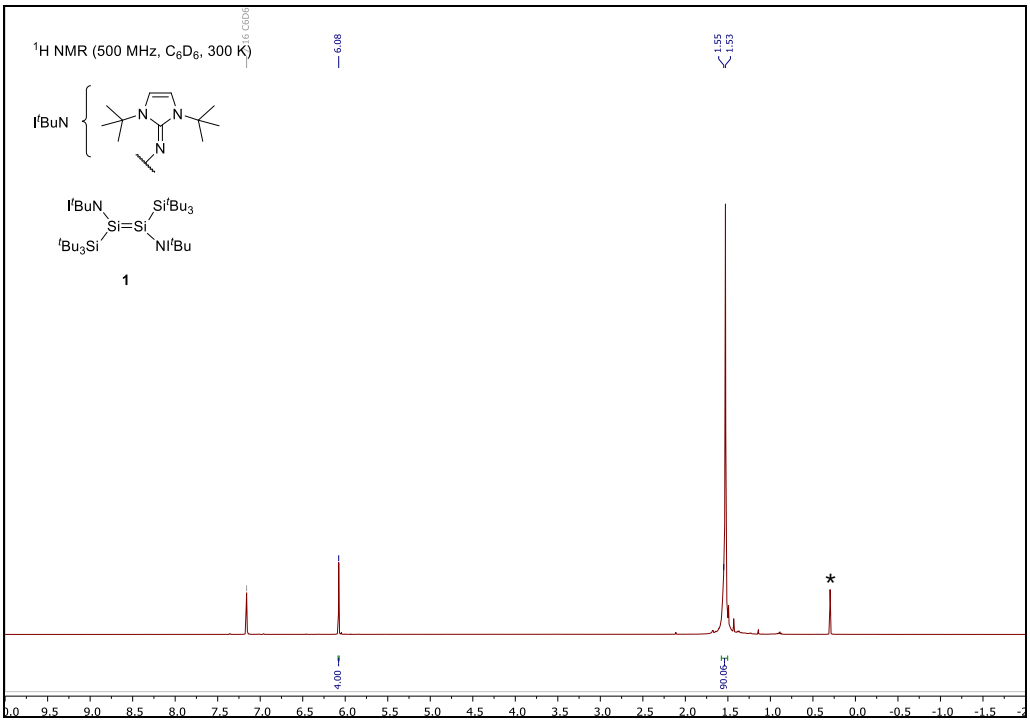


Figure S1: ^{1}H NMR spectrum (500 MHz) of compound **1** in C_6D_6 at 300 K. Signal labeled with * belongs to silicone grease.

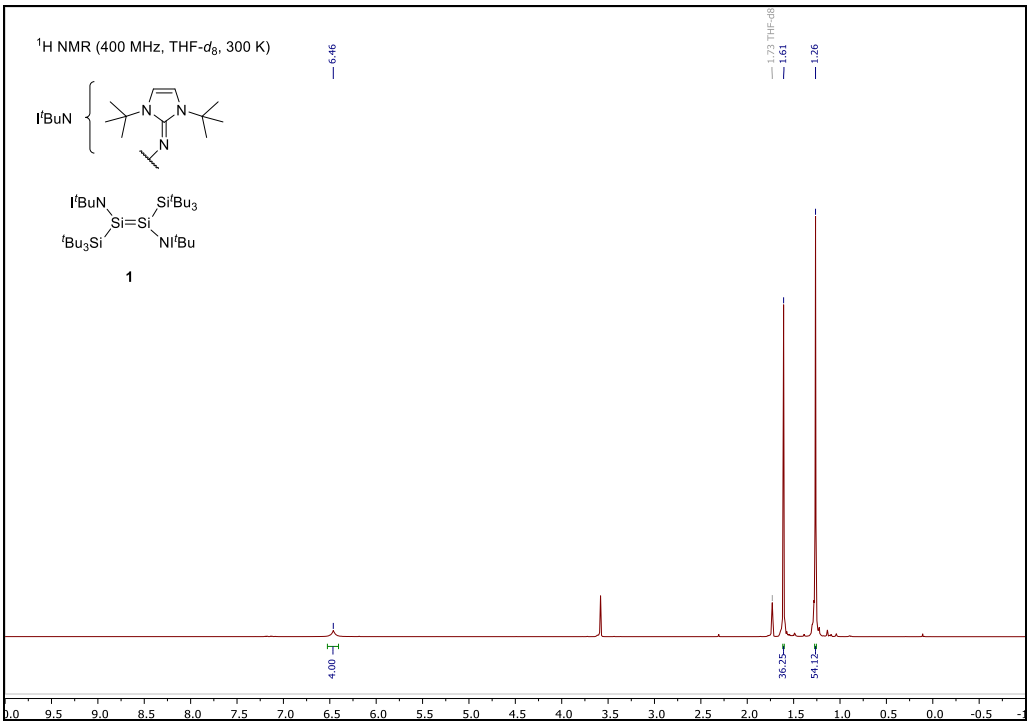


Figure S2: ^{1}H NMR spectrum (400 MHz) of compound **1** in THF-d_8 at 300 K.

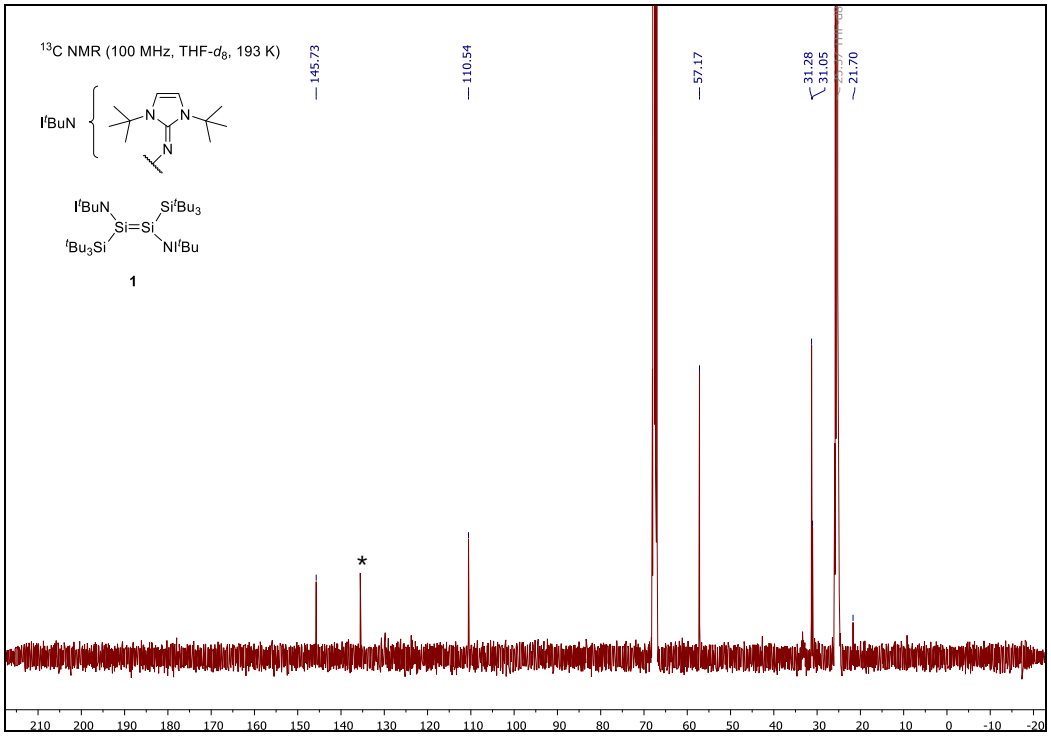


Figure S3: ^{13}C NMR spectrum (100 MHz) of compound **1** in THF-d_8 at 193 K. Signal labeled with * belongs to residual toluene.

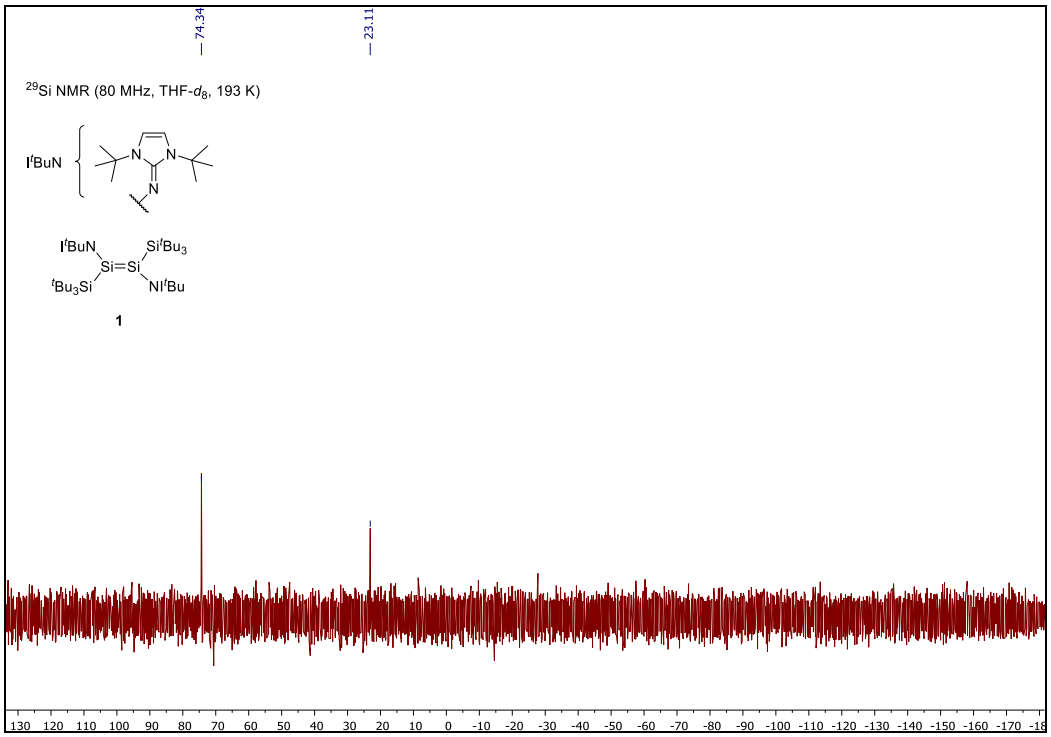


Figure S4: ^{29}Si NMR spectrum (80 MHz) of compound **1** in THF-d_8 at 193 K.

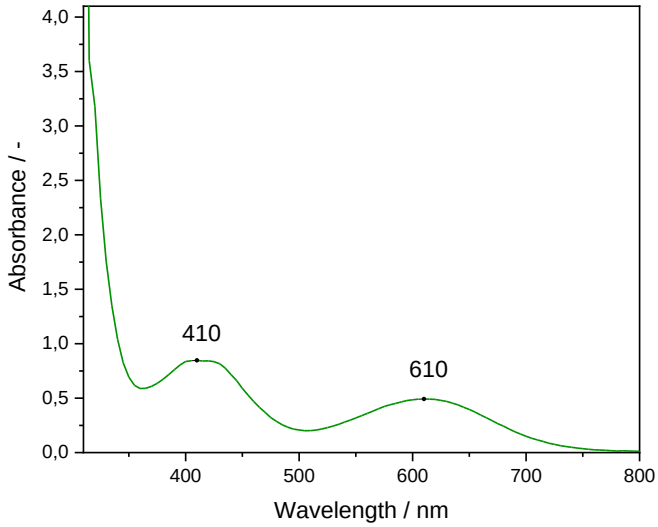
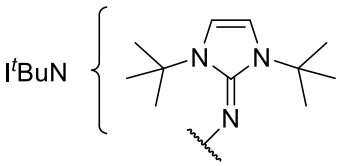
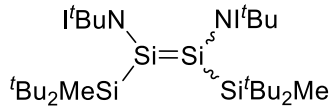


Figure S5: UV-vis spectrum of green disilene **1** in *n*-hexane (2.5×10^{-3} M), measured at room temperature (λ_{max} = 410 nm (ε = 339 L mol^{-1} cm^{-1}); 610 nm (ε = 197 L mol^{-1} cm^{-1})).

1.3 Iminodisilene I^{t}BuN(^{t}Bu$_2$MeSi)Si=Si(Si^{t}Bu$_2$Me)NI^{t}Bu (2)





2

$Si_4C_{40}H_{82}N_6$

759.48 g/mol

A solution of ^{t}Bu$_2$MeSiNa (684 mg, 3.79 mmol, 2.15 eq.) in THF (15 mL) was added dropwise to a solution of I^{t}BuNSiBr$_3$ (815 mg, 1.76 mmol, 1.00 eq.) in THF (20 mL) at room temperature. An immediate color change to deep red was observed. After stirring the mixture for 1 h, the solvent was removed under reduced pressure and the residue extracted with toluene (3 × 4 mL). The solvent was evaporated *in vacuo* and the byproduct ^{t}Bu$_2$MeSiBr was removed by sublimation in high vacuum (70 °C, 2×10^{-5} mbar). Compound **2** was obtained as crystalline deep red solid (550 mg, 724 µmol, 82%) and is stable at ambient and elevated (90 °C) temperatures in solid state and in solution (benzene, toluene, *n*-hexane, THF). Single crystals suitable for XRD analysis were obtained from cooling a concentrated solution of **2** in *n*-hexane to –35 °C. In solution, temperature-dependent *(E/Z)*-isomerization of **2** with **2-*(Z)*** as major species can be observed.

m.p.: 211 °C (decomposition, color change to brown).

2-*(Z)*:

^{1}H NMR (500 MHz, C$_6$D$_6$, 300 K): δ [ppm] = 6.04 (s, 4H, C*H*-N), 1.47 (s, 36H, ^{t}*Bu*$_2$MeSi), 1.43 (s, 36H, N^t*Bu*), 0.52 (s, 6H, ^{t}Bu$_2$*Me*Si).

^{13}C{^{1}H} NMR (126 MHz, C$_6$D$_6$, 300 K): δ [ppm] = 144.1 (*C*=N), 107.9 (*C*H-N), 54.9 (N*C*(CH$_3$)$_3$), 31.2 (Si(C(*C*H$_3$)$_3$)$_2$(CH$_3$)), 29.6 (NC(*C*H$_3$)$_3$), 21.2 (Si(*C*(CH$_3$)$_3$)$_2$(CH$_3$)), –3.9 (Si(C(CH$_3$)$_3$)$_2$(*C*H$_3$)).

^{29}Si{^{1}H} NMR (99 MHz, C$_6$D$_6$, 300 K): δ [ppm] = 67.4 (*Si*=Si), 20.4 (^{t}Bu$_2$Me*Si*).

2-*(E)*:

^{1}H NMR (500 MHz, C$_6$D$_6$, 300 K): δ [ppm] = 6.11 (s, 4H, C*H*-N), 1.59 (s, 36H, ^{t}*Bu*$_2$MeSi), 1.46 (s, 36H, N^t*Bu*), 0.18 (s, 6H, ^{t}Bu$_2$*Me*Si).

^{13}C{^{1}H} NMR (126 MHz, C$_6$D$_6$, 300 K): δ [ppm] = 144.8 (*C*=N), 108.6 (*C*H-N), 55.8 (N*C*(CH$_3$)$_3$), 31.1 (Si(C(*C*H$_3$)$_3$)$_2$(CH$_3$)), 29.9 (NC(*C*H$_3$)$_3$), 21.9 (Si(*C*(CH$_3$)$_3$)$_2$(CH$_3$)), –7.0 (Si(C(CH$_3$)$_3$)$_2$(*C*H$_3$)).

^{29}Si{^{1}H} NMR (99 MHz, C$_6$D$_6$, 300 K): δ [ppm] = 71.4 (*Si*=Si), 7.9 (^{t}Bu$_2$Me*Si*).

Note: As opposed to **1**, the best results were achieved when performing the reaction in THF.

EA:	$Si_4C_{40}H_{82}N_6$	Calculated [%]:	C (63.26), H (10.88), N (11.07)
		Experimental [%]:	C (63.08), H (10.97), N (10.79).

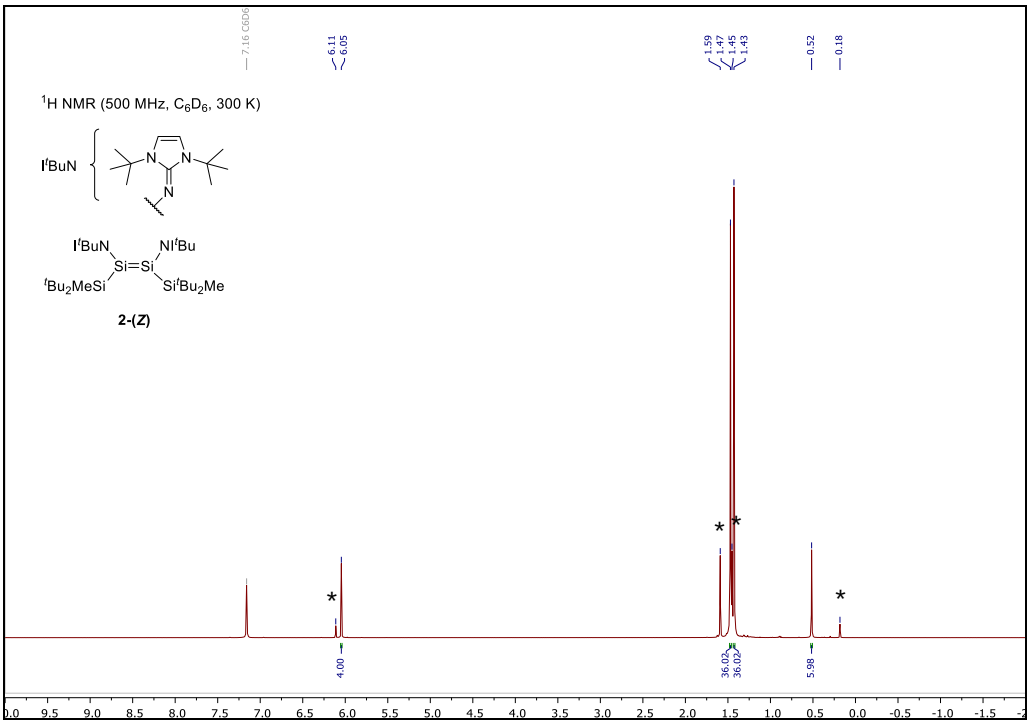


Figure S6: ^{1}H NMR spectrum (500 MHz) of compound **2-*(Z)*** in C_6D_6 at 300 K. Signals labeled with * belong to **2-*(E)***.

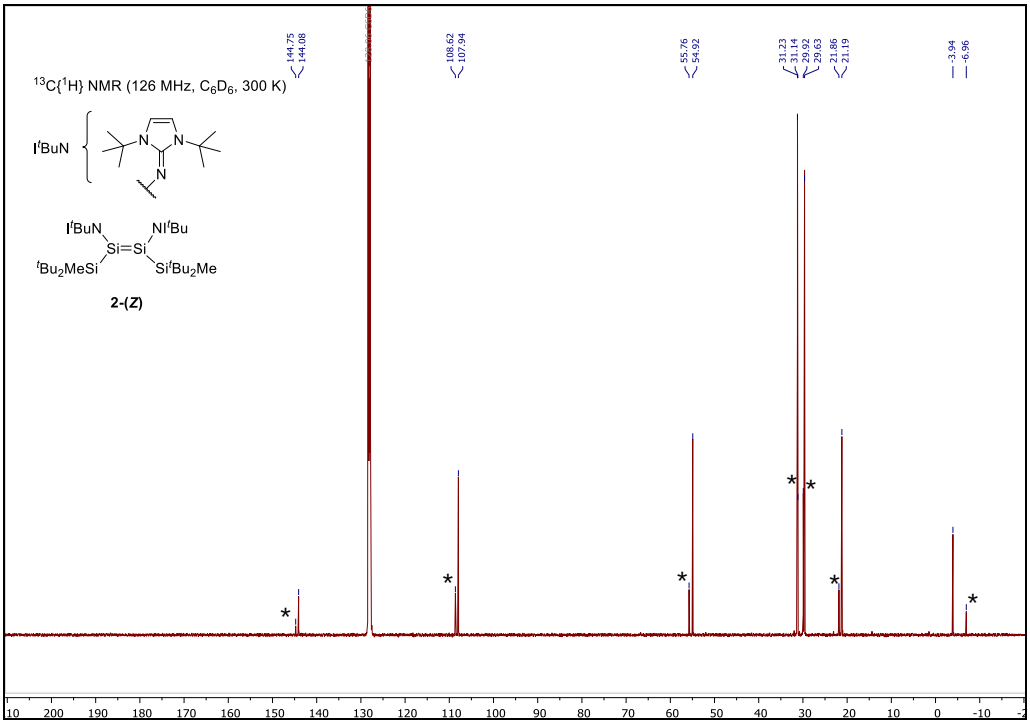


Figure S7: ^{13}C{^{1}H} spectrum (126 MHz) of compound **2-*(Z)*** in C_6D_6 at 300 K. Signals labeled with * belong to **2-*(E)***.

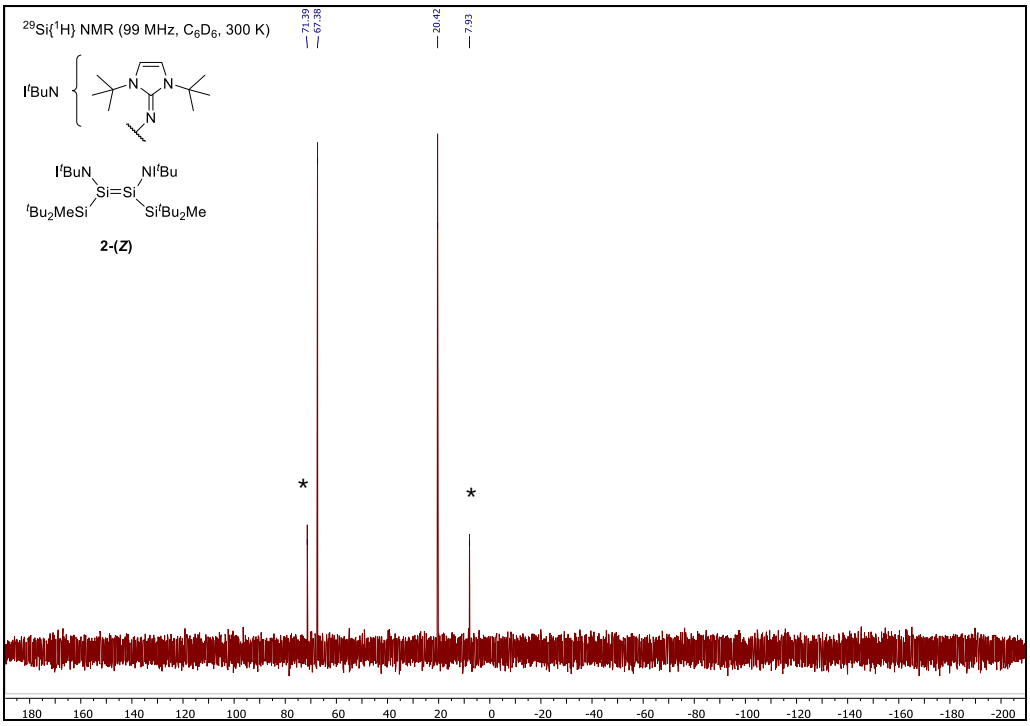


Figure S8: $^{29}Si\{^{1}H\}$ NMR spectrum (99 MHz) of compound **2-*(Z)*** in C_6D_6 at 300 K. Signals labeled with * belong to **2-*(E)***.

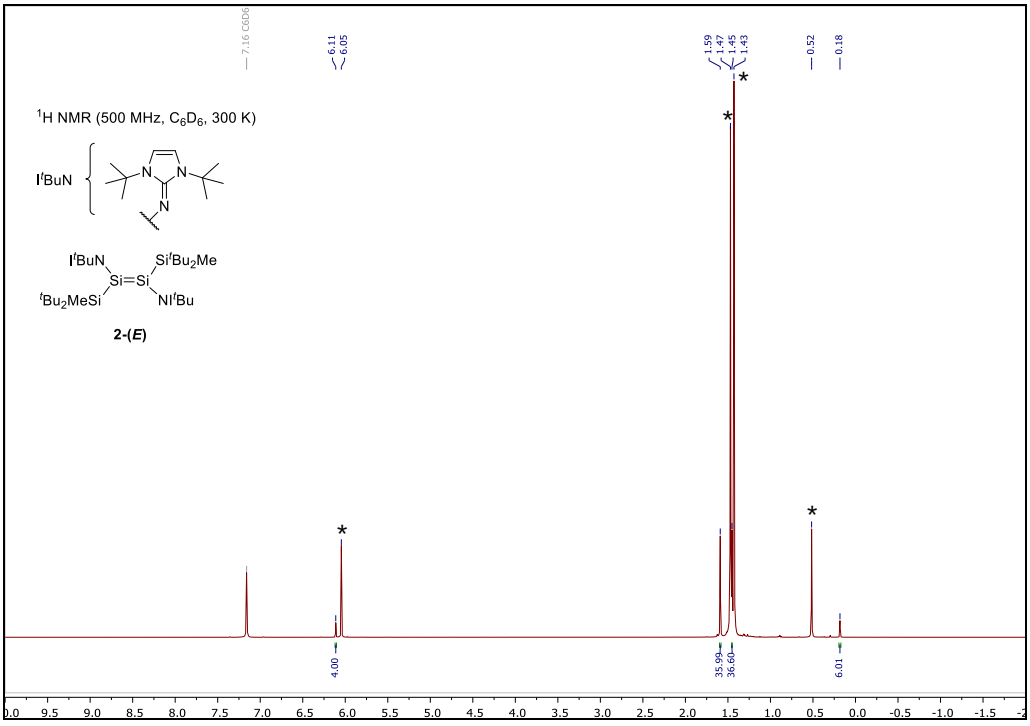


Figure S9: ^{1}H NMR spectrum (500 MHz) of compound **2-*(E)*** in C_6D_6 at 300 K. Signals labeled with * belong to **2-*(Z)***.

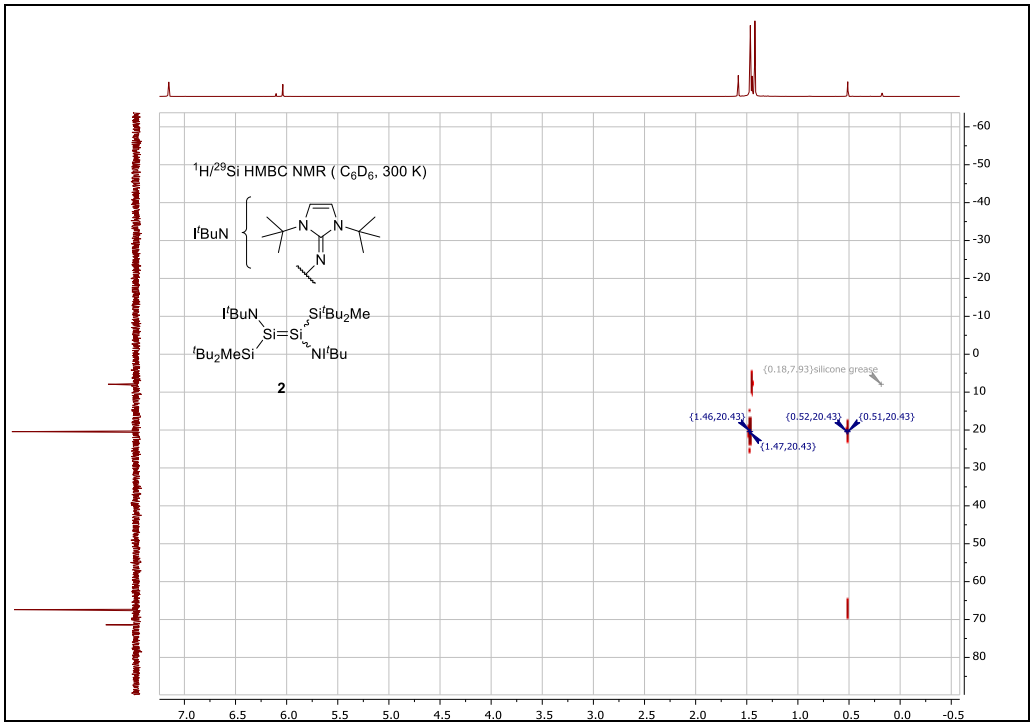


Figure S10: ^{1}H/^{29}Si HMBC NMR spectrum of disilene **2** in C_6D_6 at 300 K.

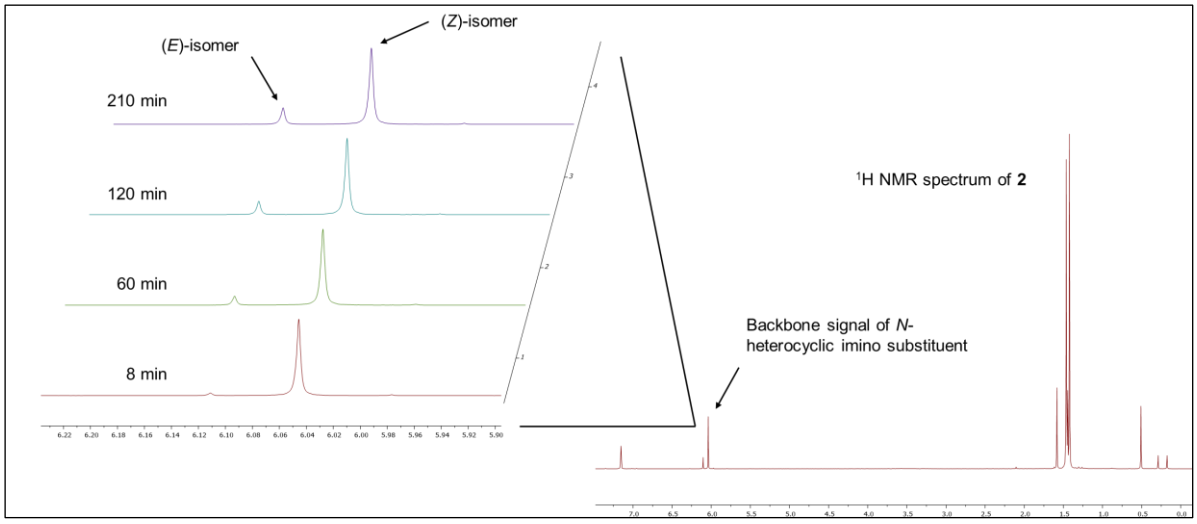


Figure S11: ^{1}H NMR kinetic studies of (*E*/*Z*)-isomerization of **2** in solution at room temperature.

Note: Crystals of **2** (5 mg) were dissolved in C_6D_6 and the isomerization process was monitored by ^{1}H NMR spectroscopy. NMR measurement 8 minutes after dissolving the crystals revealed almost no observable (*E*)-isomer. Hence, we assume that **2** adopts solely (*Z*)-configuration in the solid state. In solution the equilibrium of (*E*) and (*Z*) is reached at room temperature after 3.5 hours with a ration of (*E*):(*Z*) = 18:82. The concentration of **2**, as well as exposure to visible light have no influence on the kinetic of this isomerization reaction.

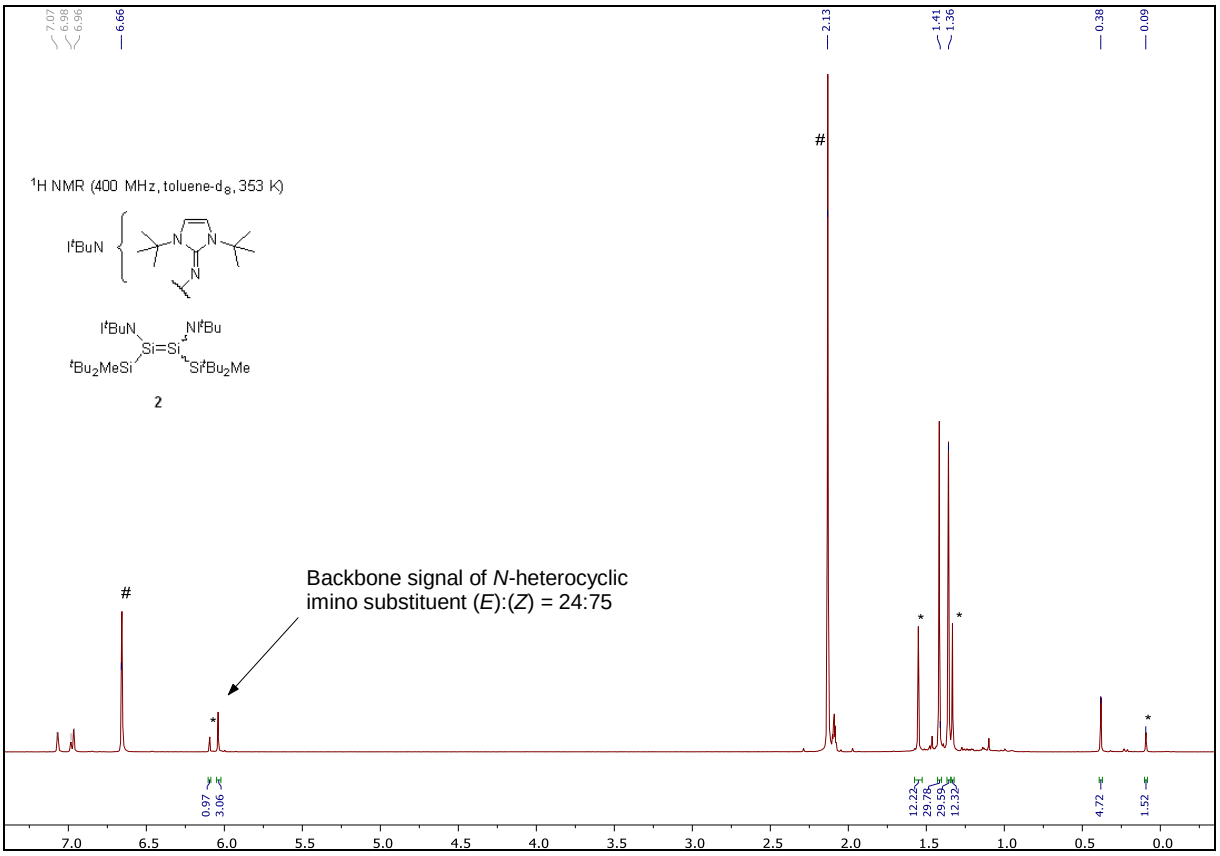


Figure S12: ^{1}H NMR spectrum (400 MHz) of compound **2** in toluene-d$_8$ at 353 K. Signals labelled with * belong to **2-*(E)***, signals labelled with # belong to mesitylene (internal standard).

Note: In a teflon-capped NMR tube, crystals of disilene **2** (11.4 mg, 15.01 µmol, 1.0 eq) were dissolved in toluene-d$_8$ (0.4 mL) and subsequently an internal standard of mesitylene (10 µL, 72.35 µmol, 4.82 eq.) was added. The sample was heated to 80°C in the NMR spectrometer. After sufficient waiting time to reach the equilibrium between the isomers, the NMR spectrum in Figure S12 was measured at 80 °C. The ratio of **2-(*E*)**:**2-(*Z*)** is 24:76.

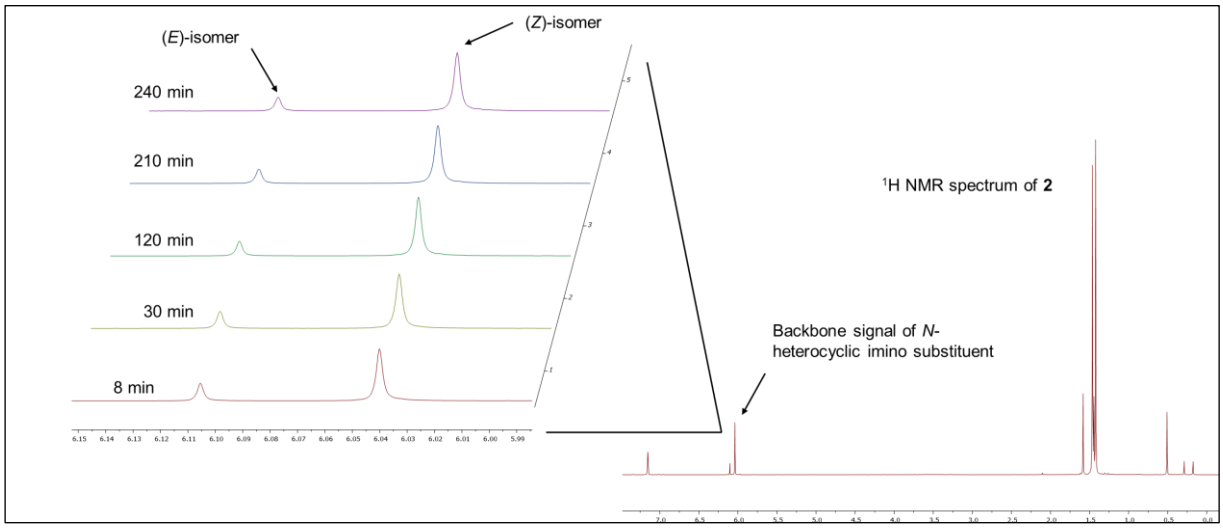


Figure S13: ^{1}H NMR kinetic studies of (*E/Z*)-isomerization of **2** after heating to 80 °C in solution at room temperature.

Note: A solution of **2** in C_6D_6 was heated to 80 °C for 6 hours. Subsequently, the (*E*/*Z*)-isomerization process was monitored at room temperature by ^{1}H NMR spectroscopy. The initially (after 8 min) observed ratio (*E*):(*Z*) = 24:76 changed within 3.5 hours to (*E*):(*Z*) = 18:82, the same value, which was previously observed from isomerization of crystalline **2** at room temperature. This process can be repeated in cycles and is fully reversible. No decomposition products were observed.

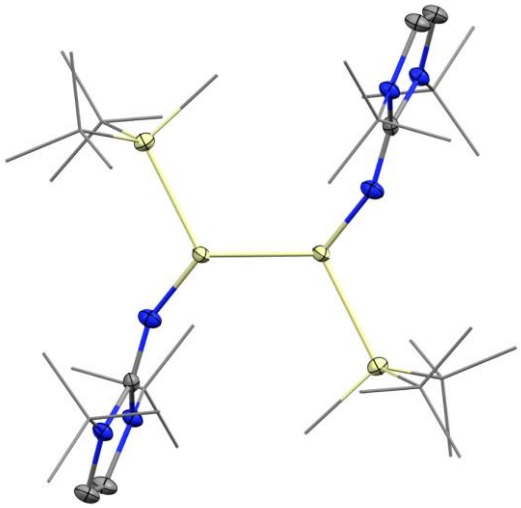


Figure S14: Solid state structure of **2-(*E*)**.

Note: This solid state structure was surprisingly obtained from a reactivity test of **2** and contains a minor, unknown, co-crystalized compound. Therefore, no satisfactory structure was obtained and structural parameters cannot be discussed. Nonetheless, this structure is an unambiguous evidence for the existence of the (*E*)-isomer of **2**.

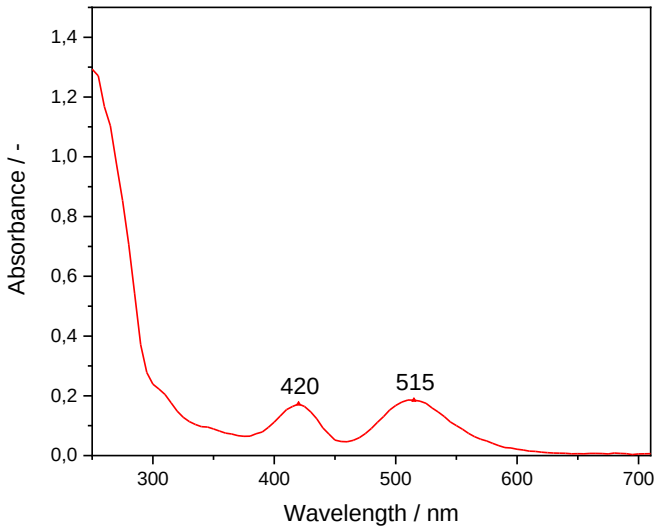


Figure S15: UV-vis spectrum of red disilene **2** in *n*-hexane (2.5×10^{-3} M), measured at room temperature (λ_{max} = 420 nm (ε = 69 L mol^{-1} cm^{-1}); 515 nm (ε = 74 L mol^{-1} cm^{-1})).

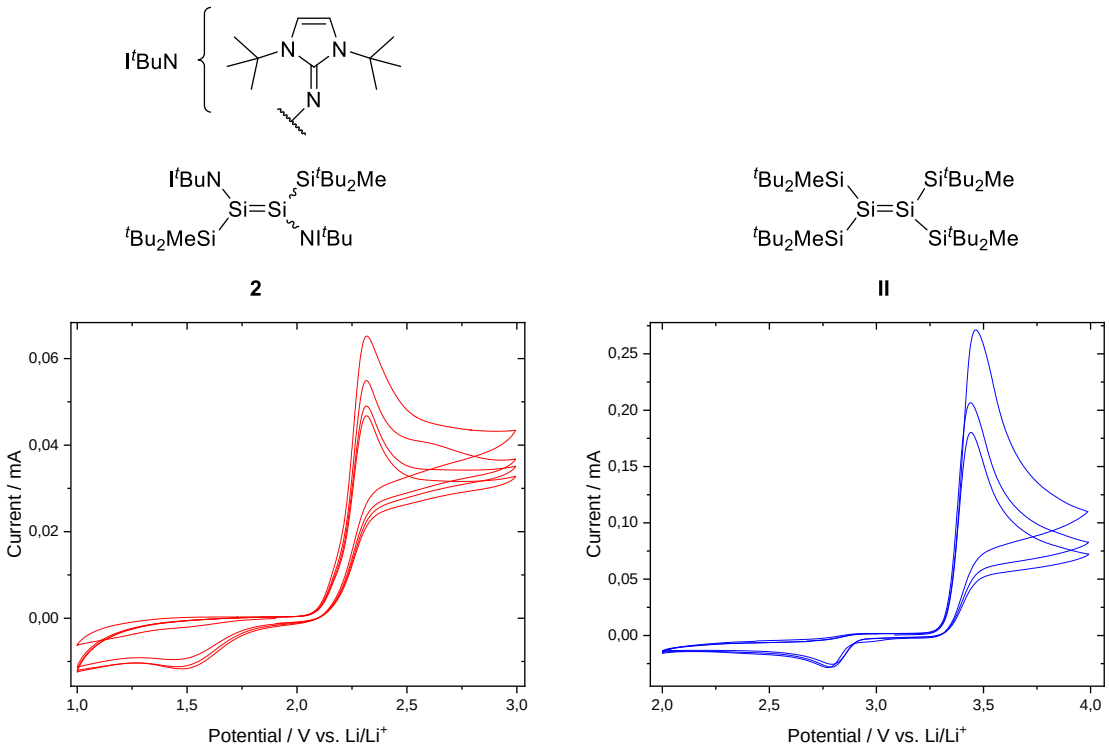
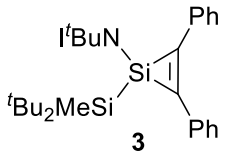


Figure S16: Cyclic voltammogram displaying the oxidation waves of **2** (left) and (^{t}Bu$_2$MeSi)$_2$Si=Si(Si^{t}Bu$_2$Me)$_2$ (**II**) (right), measured in multiple cycles in a three-electrode setup using a lithium metal reference electrode (0.1 M (*n*-Bu$_4$N)TFSI in THF at room temperature).

Note: Since the only disilene radical cation reported so far derives from one-electron oxidation of **II**, we measured the cyclic voltammograms of **II** and iminodisilene **2** under the same conditions for comparison. Apparently, the oxidation of **2** occurs at lower potentials than required for the oxidation of **II** (~1 V vs. Li/Li$^+$). This result already indicates the accessibility of a cationic species, from oxidation of **2**.

1.4 I^{t}BuN(^{t}Bu$_2$MeSi)Si-PhCCPh (3)



3

$Si_2C_{34}H_{51}N_3$

557.36 g/mol

Disilene **2** (23.2 mg, 30.6 µmol, 1.0 eq) was dissolved in C_6D_6 and diphenylacetylene (10.9 mg, 61.1 µmol, 2.0 eq) was added. The reaction mixture was heated to 90 °C for 20 minutes, during which the loss of the red color of **2** yielded a pale-yellow solution. All volatiles were removed under reduced pressure to afford a yellow powder (27.7 mg, 94% yield) Characterization by multinuclear NMR spectroscopy revealed the [2+1] cycloaddition product as the main product. A slight impurity of residual diphenylacetylene (marked with # in the NMR spectra) and a second byproduct (marked with * in the NMR spectra) from a not completely pure batch of disilene **2-(*Z*)** is contained in the NMR spectra. No attempts to separate the residues by crystallization or washing were successful. A saturated solution of the product mixture in toluene was cooled to –35 °C to give pale-yellow crystals of **3** suitable for SC-XRD analysis.

Note: Reaction at lower temperatures (50 °C) affords another product besides **3**, which we assume to be the [2+2] cycloaddition product. Unfortunately, we were not able to separate the two compounds to characterize this species unambiguously.

^{1}H NMR (500 MHz, C_6D_6, 300 K): δ [ppm] = 7.78 – 7.75 (m, 4H, Ar-*H*), 7.23 (t, *J* = 7.7 Hz, 4H, Ar-*H*), 7.08 – 7.03 (m, 2H, Ar-*H*), 5.98 (s, 2H, C*H*-N), 1.41 (s, 18H, ^{t}*Bu*N), 1.34 (s, 18H, ^{t}*Bu*$_2$MeSi), 0.42 (s, 6H, ^{t}Bu$_2$*Me*Si).

^{13}C{^{1}H} NMR (126 MHz, C_6D_6, 300 K): δ [ppm] = 166.8 (Si*C*$_2$), 138.2 (*C*=N), 128.5 (*m*-*C*$_{Ar}$), 128.1 (*p*-*C*$_{Ar}$), 126.6 (*o*-*C*$_{Ar}$), 123.7 ($^{quart.}$*C*$_{Ar}$), 107.5 (*C*H-N), 55.0 (N*C*(CH$_3$)$_3$), 30.0 (Si(C(*C*H$_3$)$_3$)$_2$(CH$_3$)), 28.9 (NC(*C*H$_3$)$_3$), 20.7 (Si(*C*(CH$_3$)$_3$)$_2$(CH$_3$)), –6.2 (Si(C(CH$_3$)$_3$)$_2$(*C*H$_3$)).

^{29}Si{^{1}H} NMR (99 MHz, C_6D_6, 195 K): δ [ppm] = 2.7 (*Si*^{t}Bu$_2$Me), –122.4 (N*Si*Si^{t}Bu$_2$Me).

LIFDI-MS:	$C_{34}H_{51}N_3Si_2$	Calculated [%]:	557.3616 m/z
		Experimental [%]:	557.3607 m/z.

Note: To prove the proposed mechanism of the (*Z*/*E*)-isomerization of **2** via the monomeric silylenes, we also tested the conversion of **2** with $B(C_6F_5)_3$, as the adduct with the monomer of **VI** was reported previously.[S8] In the reaction with BCF we obtained a green or red oily compound, depending on choice of solvent and temperature, which we were unfortunately not able to characterize.

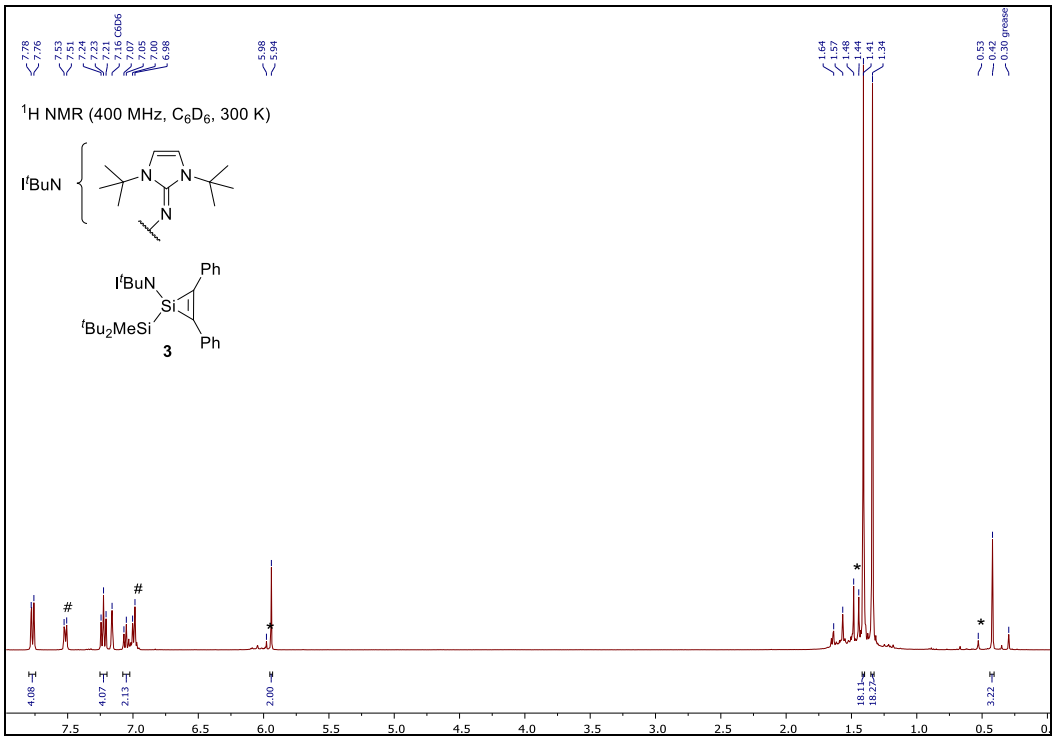


Figure S17: ^{1}H NMR spectrum (500 MHz) of compound **3** in C_6D_6 at 300 K. Signals labeled with * belong to the byproduct and signals labelled with # belong to excess diphenylacetylene.

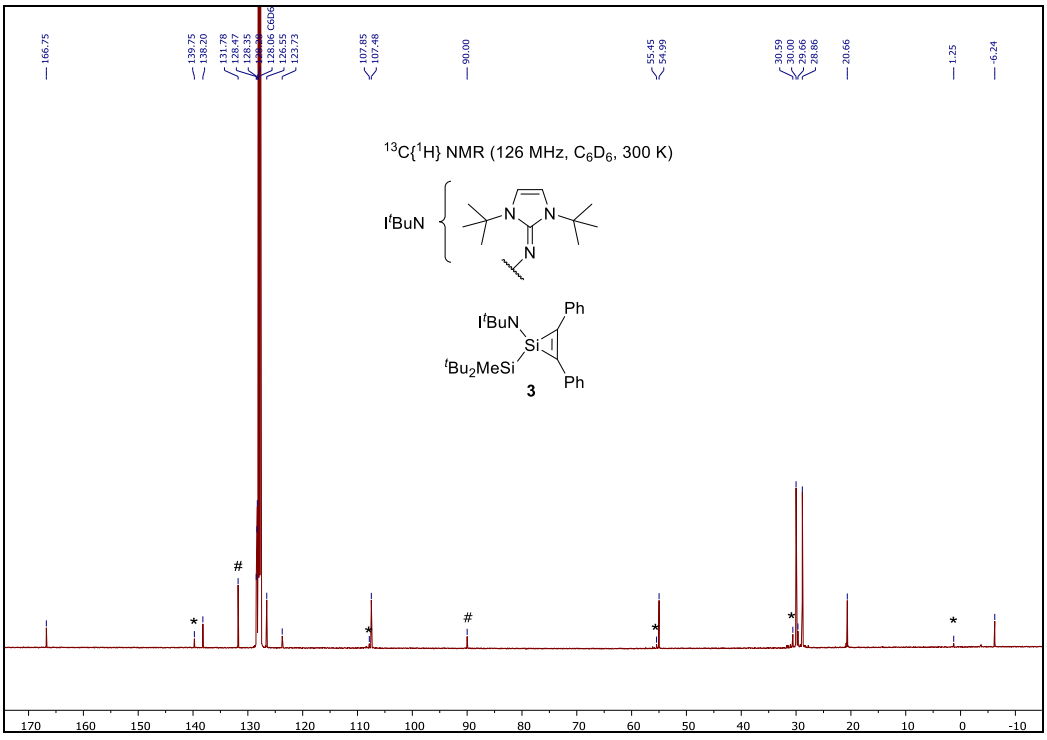


Figure S18: ^{13}C{^{1}H} spectrum (126 MHz) of compound **3** in C_6D_6 at 300 K. Signals labeled with * belong to the byproduct and signals labelled with # belong to excess diphenylacetylene. The signals corresponding to the phenyl C atoms of excess diphenylacetylene are not observable due to overlaying signals with the solvent C_6D_6.

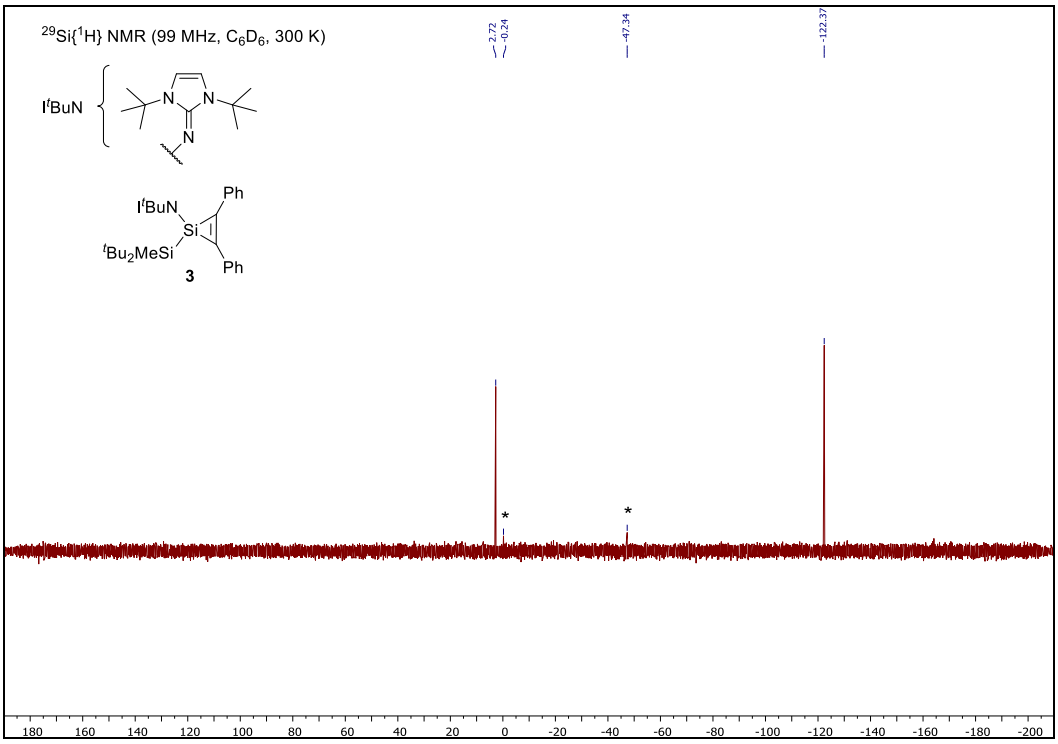


Figure S19: $^{29}Si\{^{1}H\}$ spectrum (99 MHz) of compound **3** in C_6D_6 at 300 K. Signals labeled with * belong to the byproduct.

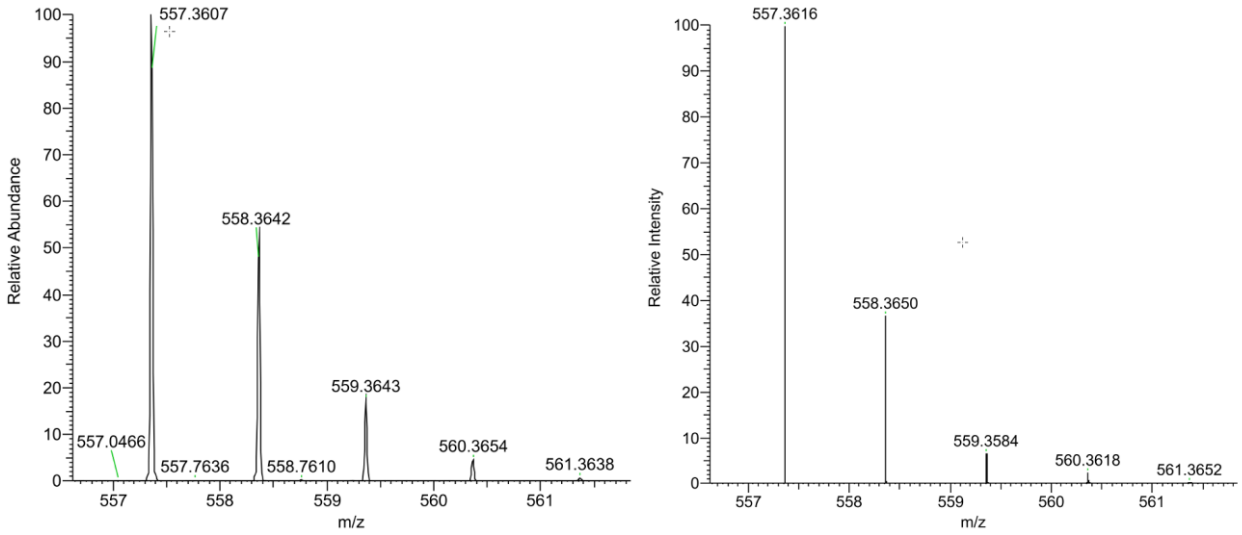
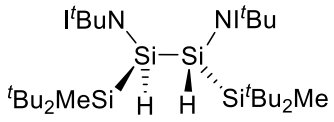


Figure S20: LIFDI-MS spectrometry (detail view with isotope pattern) of **3**. Measured (left, m/z = 557.3607) and simulated (right, m/z = 557.3616) mass spectrum.

1.5 I^{t}BuN(^{t}Bu$_2$MeSi)HSi-SiH(Si^{t}Bu$_2$Me)NI^{t}Bu (4)



4

$Si_4C_{40}H_{84}N_6$

761.49 g/mol

A toluene (8 mL) solution of disilene **1** (60.0 mg, 79.0 µmol, 1.00 eq.) in a pressurizable Schlenk flask was degassed (freeze-pump-thaw) and subsequently exposed to hydrogen gas (1 bar) at room temperature. Complete decolorization occurred within 2 hours. After concentrating the solution under reduced pressure, silane **4** was obtained by crystallization at –35 °C as colorless crystals (47.6 mg, 62.5 µmol, 79% yield). These crystals were also suitable for SC-XRD analysis.

m.p.: 195 °C (decomposition).

^{1}H NMR (500 MHz, C_6D_6, 300 K): δ [ppm] = 6.53 (s, 2H, Si*H*), 6.05 (d, 2H, ^3J = 3.3 Hz, C*H*-N), 6.03 (d, 2H, ^3J = 3.3 Hz, C*H*-N),1.49 (s, 18H, ^{t}*Bu*N), 1.45 (s, 18H, ^{t}*Bu*$_2$MeSi), 1.37 (s, 18H, *t*Bu$_2$MeSi), 1.36 (s, 18H, ^{t}*Bu*N), 0.42 (s, 6H, ^{t}Bu$_2$*Me*Si).

^{13}C{^{1}H} NMR (126 MHz, C_6D_6, 300 K): δ [ppm] = 141.7 (*C*=N), 107.5 (*C*H-N), 107.2 (*C*H-N), 55.0 (N*C*(CH$_3$)$_3$), 54.4 (N*C*(CH$_3$)$_3$), 31.0 (Si(C(*C*H$_3$)$_3$)$_2$(CH$_3$)), 30.1 (Si(C(*C*H$_3$)$_3$)$_2$(CH$_3$)), 29.9 (NC(*C*H$_3$)$_3$), 29.5 (NC(*C*H$_3$)$_3$), 21.6 (Si(*C*(CH$_3$)$_3$)$_2$(CH$_3$)), 21.5 (Si(*C*(CH$_3$)$_3$)$_2$(CH$_3$)), –4.8 (Si(C(CH$_3$)$_3$)$_2$(*C*H$_3$)).

^{29}Si{^{1}H} NMR (99 MHz, C_6D_6, 195 K): δ [ppm] = 6.1 (^{t}Bu$_2$Me*Si*), –69.1 (*Si*H).

EA:	$Si_4C_{40}H_{82}N_6$	Calculated [%]:	C (63.09), H (11.12), N (11.04)
		Experimental [%]:	C (62.69), H (11.22), N (10.62).

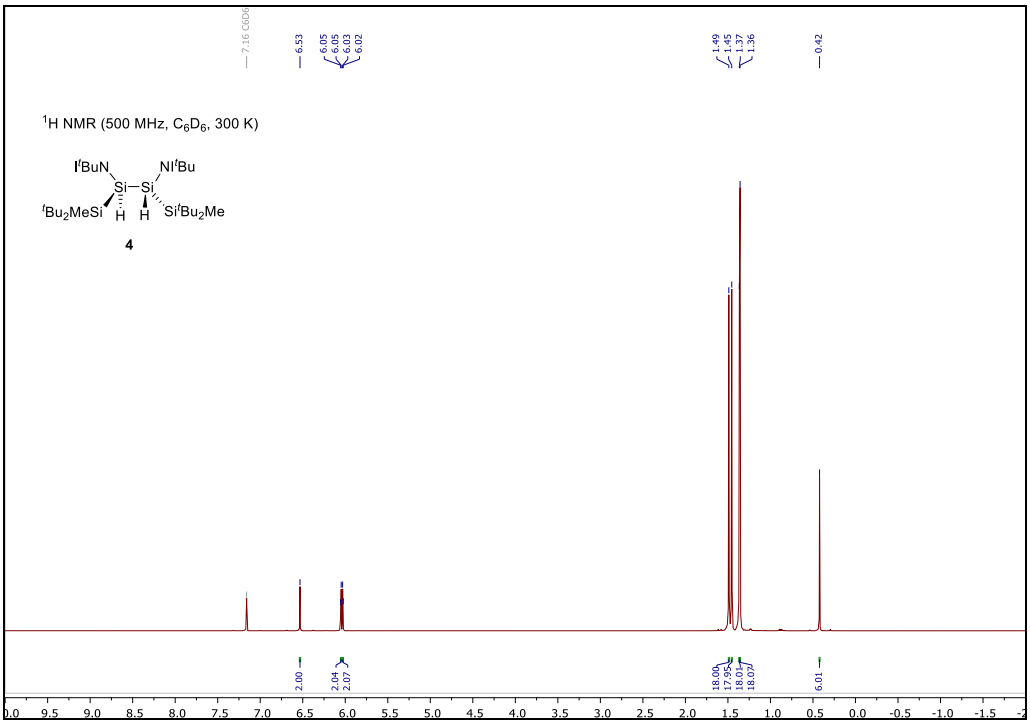


Figure S21: ^{1}H NMR spectrum (500 MHz) of compound **4** in C_6D_6 at 300 K.

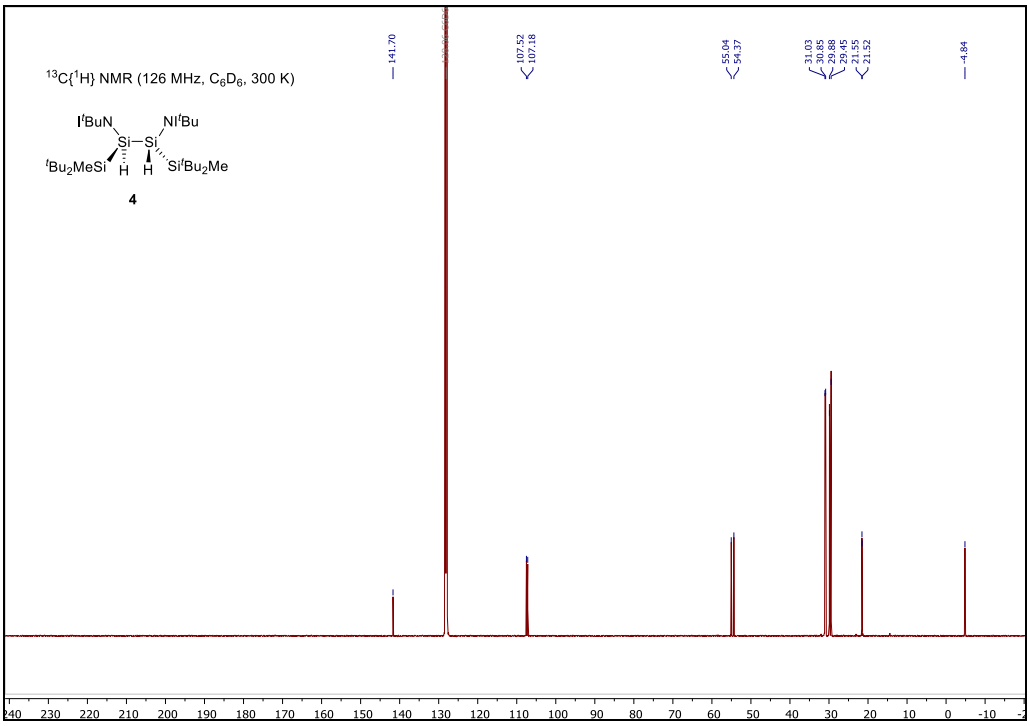


Figure S22: ^{13}C{^{1}H} spectrum (126 MHz) of compound **4** in C_6D_6 at 300 K.

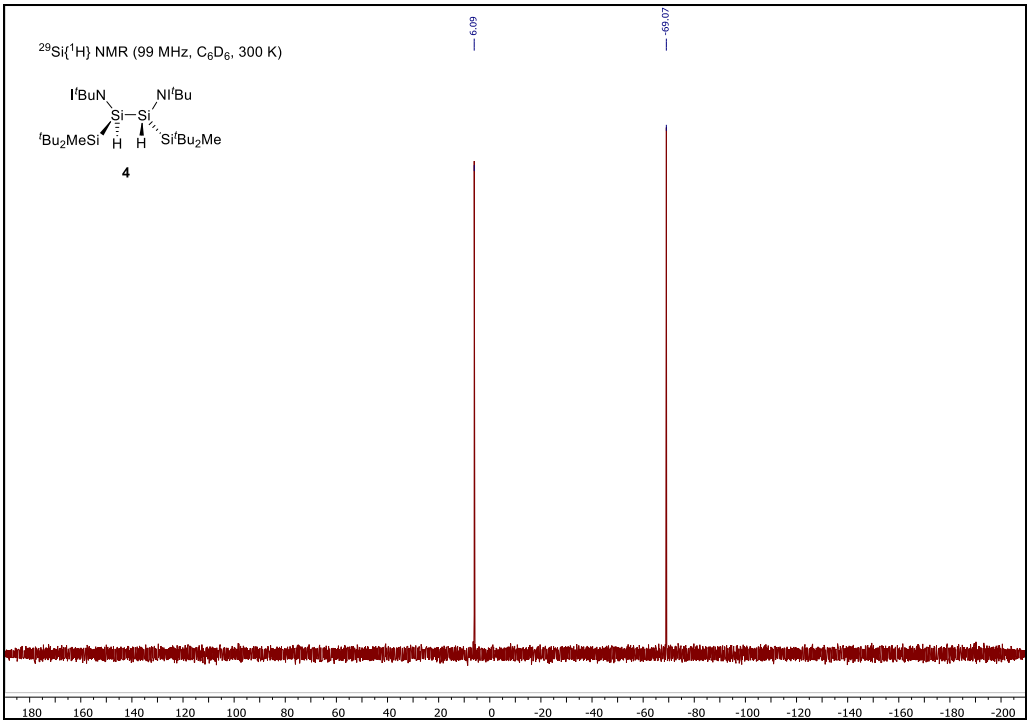
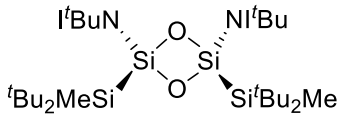


Figure S23: $^{29}Si\{^{1}H\}$ NMR spectrum (99 MHz) of compound **4** in C_6D_6 at 300 K.

1.6. Dioxadisiletane 5



5

$Si_4C_{40}H_{82}N_6O_2$

791.48 g/mol

In a pressurizeable Schlenk flask, a solution of disilene **2** (70.0 mg, 92.2 µmol) in *n*-pentane (10 mL) was cooled to –130 °C and exposed to oxygen (1.2 bar) under stirring. The deep red color rapidly vanished and the solution was allowed to warm to room temperature. After evaporation of all volatiles *in vacuo*, compound **5** was obtained from recrystallization of the residue in *n*-hexane at –35 °C as colorless crystals (61.4 mg, 76.3 µmol, 83%).

m.p.: 266 °C

^{1}H NMR (500 MHz, C_6D_6, 300 K): δ [ppm] = 5.98 (s, 4H, C*H*-N), 1.48 (s, 36H, N^t*Bu*), 1.44 (s, 36H, ^{t}*Bu*$_2$MeSi), 0.53 (s, 6H, ^{t}Bu$_2$*Me*Si).

^{13}C{^{1}H} NMR (126 MHz, C_6D_6, 300 K): δ [ppm] = 140.1 (*C*=N), 108.0 (*C*H-N), 55.7 (N*C*(CH$_3$)$_3$), 30.8 (Si(C(*C*H$_3$)$_3$)$_2$(CH$_3$)), 29.9 (NC(*C*H$_3$)$_3$), 21.1 (Si(*C*(CH$_3$)$_3$)$_2$(CH$_3$)), –3.6 (Si(C(CH$_3$)$_3$)$_2$(*C*H$_3$)).

^{29}Si{^{1}H} NMR (99 MHz, C_6D_6, 195 K): δ [ppm] = –0.2 (^{t}Bu$_2$Me*Si*), –47.3 (*Si*O).

EA:	$Si_4C_{40}H_{82}Br_2N_6$	Calculated [%]:	C (60.70), H (10.44), N (10.62)
		Experimental [%]:	C (59.66), H (10.44), N (10.18).

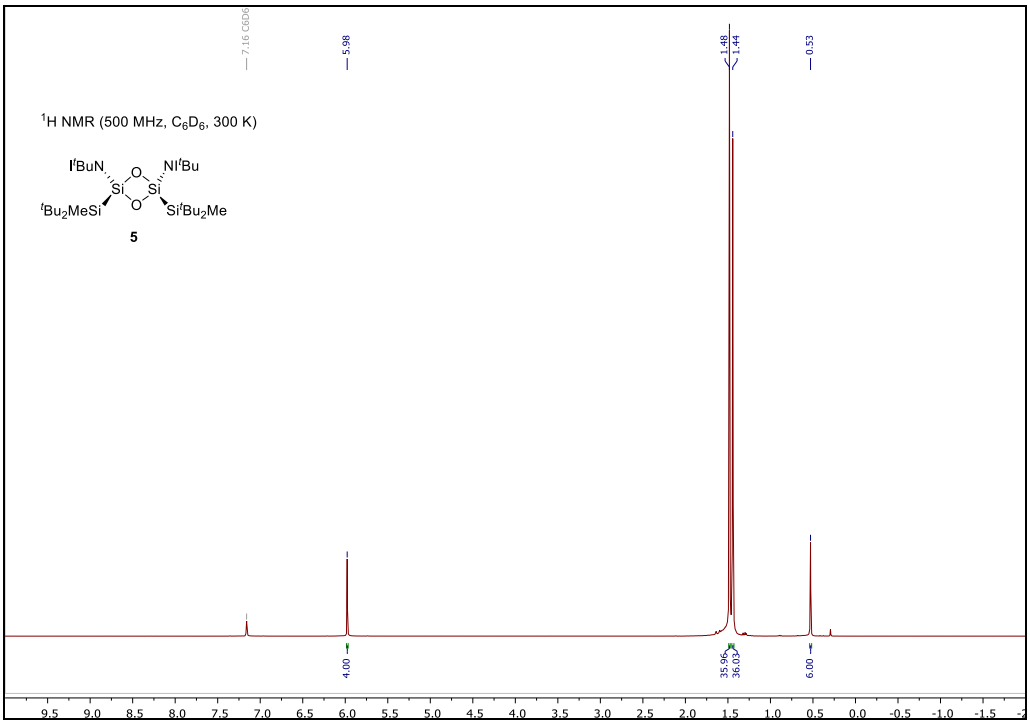


Figure S24: ^{1}H NMR spectrum (500 MHz) of compound **5** in C_6D_6 at 300 K.

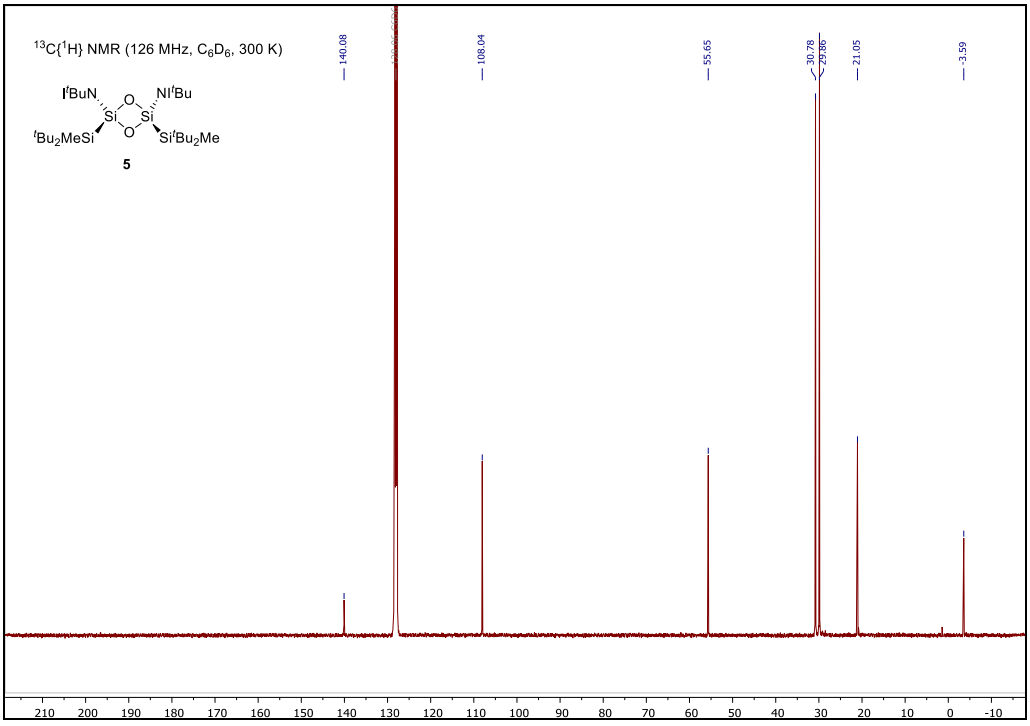


Figure S25: ^{13}C NMR spectrum (126 MHz) of compound **5** in C_6D_6 at 300 K.

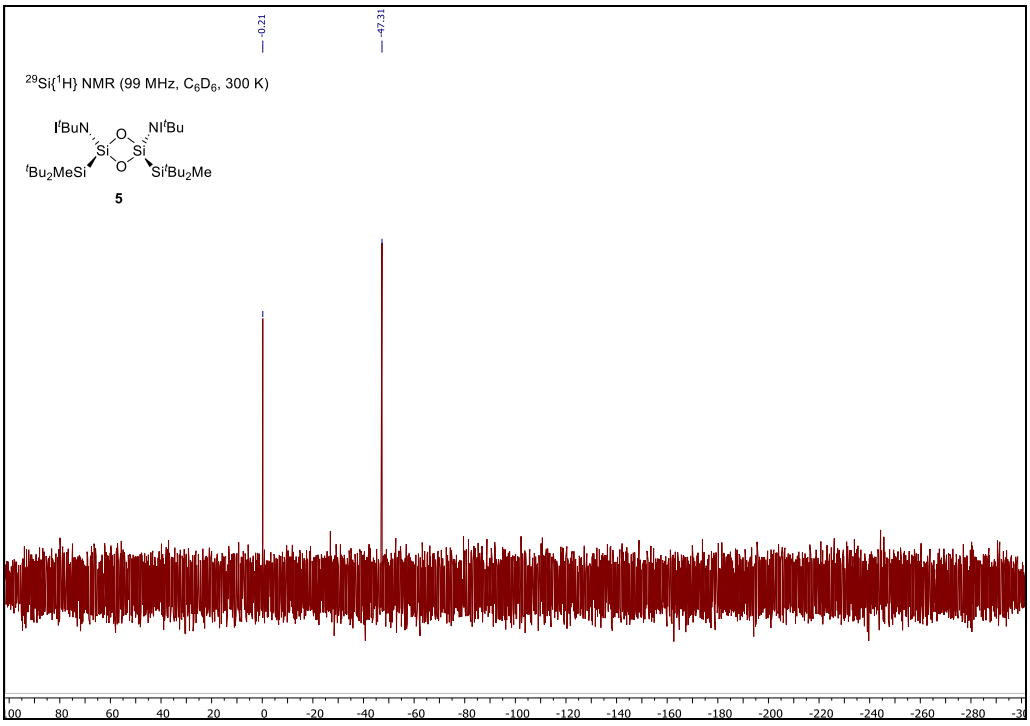
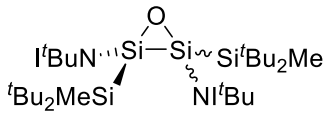


Figure S26: ^{29}Si NMR spectrum (99 MHz) of compound **5** in C_6D_6 at 300 K.

1.7. Disilaoxirane 6-*t*/*c*



6-*t*/*c*

$Si_4C_{40}H_{82}N_6O$

775.48 g/mol

An *n*-pentane (8 mL) solution of **2** (70.0 mg, 92.2 µmol) in a pressurizeable Schlenk flask was cooled to –78 °C and exposed to N_2O (1 bar) under stirring. The red solution turned yellow and was allowed to warm to ambient temperature after 20 minutes. All volatiles were removed under reduced pressure and the yellow solid residue was purified by recrystallization from *n*-hexane to give yellow crystals (57.3 mg). Multinuclear NMR spectroscopy revealed the composition of this crystals to be 25% **5** and 75% **6-*c*** (77% yield). Various separation attempts were unsuccessful. Heating of a sample of **6-*c*** in C_6D_6 to 70 °C for 16 hours lead to quantitative isomerization to **6-*t***, in agreement with the corresponding *trans*-product of **VI**.

Note: Neither the crystals of **6-*c***, nor that of **6-*t*** were suitable for SC-XRD analysis due to co-crystallization with compound **5**. Compounds **6** were identified by comparison of multinuclear NMR spectroscopic data with literature reported disilaoxiranes.[S8] Different to **VI**, selective conversion of **2** with CO_2 could not be obtained even at low temperatures (–80 °C). Although dioxadisiletane **5** was observed as the main product, at least two additional species occurred. Despite all efforts (variation of solvents and temperatures), these compounds could not be isolated and identified, but they presumably are the cycloaddition products of CO_2 with the Si=Si double bond akin to the reaction of **VI** with carbon dioxide.[S8]

6-*c*:

^{1}H NMR (500 MHz, C_6D_6, 300 K): δ [ppm] = 6.02 (d, ^3J = 3.2 Hz, 2H, C*H*-N), 6.00 (d, ^3J = 3.2 Hz, 2H, C*H*-N), 1.48 (s, 18H, N^t*Bu*), 1.47 (s, 18H, N^t*Bu*), 1.43 (s, 18H, ^{t}*Bu*$_2$MeSi), 1.41 (s, 18H, ^{t}*Bu*$_2$MeSi), 0.50 (s, 6H, ^{t}Bu$_2$*Me*Si).

6-*t*

^{1}H NMR (500 MHz, C_6D_6, 300 K): δ [ppm] = 6.08 (d, ^3J = 3.2 Hz, 2H, C*H*-N), 6.06j (d, ^3J = 3.2 Hz, 2H, C*H*-N), 1.48 (s, 18H, N^t*Bu*), 1.47 (s, 18H, N^t*Bu*), 1.43 (s, 18H, ^{t}*Bu*$_2$MeSi), 1.41 (s, 18H, ^{t}*Bu*$_2$MeSi), 0.50 (s, 6H, ^{t}Bu$_2$*Me*Si).

^{13}C{^{1}H} NMR (126 MHz, C_6D_6, 300 K): δ [ppm] = 143.1 (*C*=N), 108.4 (*C*H-N), 108.3 (*C*H-N), 55.9 (N*C*(CH$_3$)$_3$), 55.3 (N*C*(CH$_3$)$_3$), 30.9 (Si(C(*C*H$_3$)$_3$)$_2$(CH$_3$)), 30.7 (Si(C(*C*H$_3$)$_3$)$_2$(CH$_3$)), 29.5 (NC(*C*H$_3$)$_3$), 22.1 (Si(*C*(CH$_3$)$_3$)$_2$(CH$_3$)), 21.9 (Si(*C*(CH$_3$)$_3$)$_2$(CH$_3$)), –6.4 (Si(C(CH$_3$)$_3$)$_2$(*C*H$_3$)).

^{29}Si{^{1}H} NMR (99 MHz, C_6D_6, 195 K): δ [ppm] = 5.3 (^{t}Bu$_2$Me*Si*), –48.8 (*Si*O).

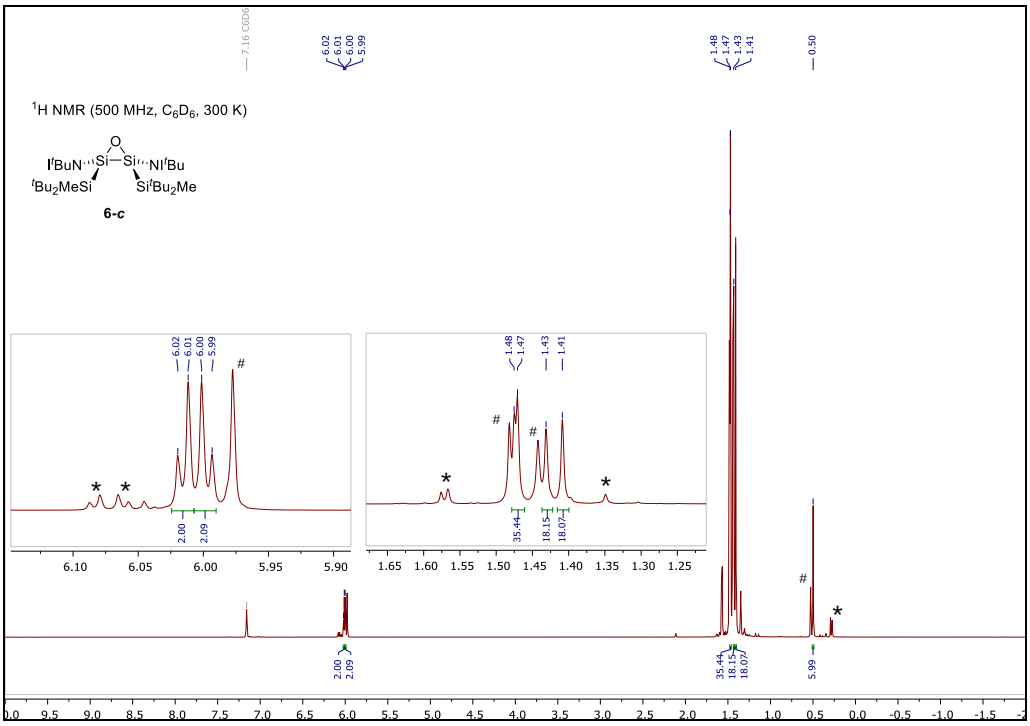


Figure S27: ^{1}H NMR spectrum (500 MHz) of compound **6-*c*** in C_6D_6 at 300 K. Signals labeled with * and # belong to compounds **6-*t*** (*) and **5** (#).

Note: Due to signal overlap for the N^{t}Bu groups (1.48 ppm and 1.47 ppm), separate integration was not possible.

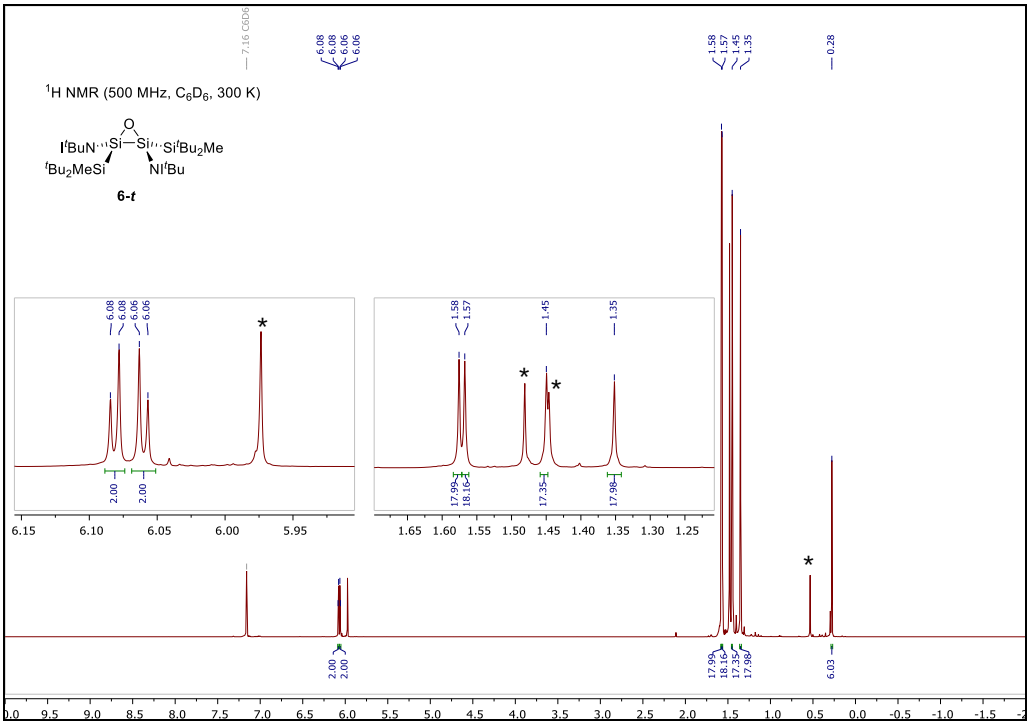


Figure S28: ^{1}H NMR spectrum (500 MHz) of compound **6-*t*** in C_6D_6 at 300 K. Signals labeled with *belong to compound **5**.

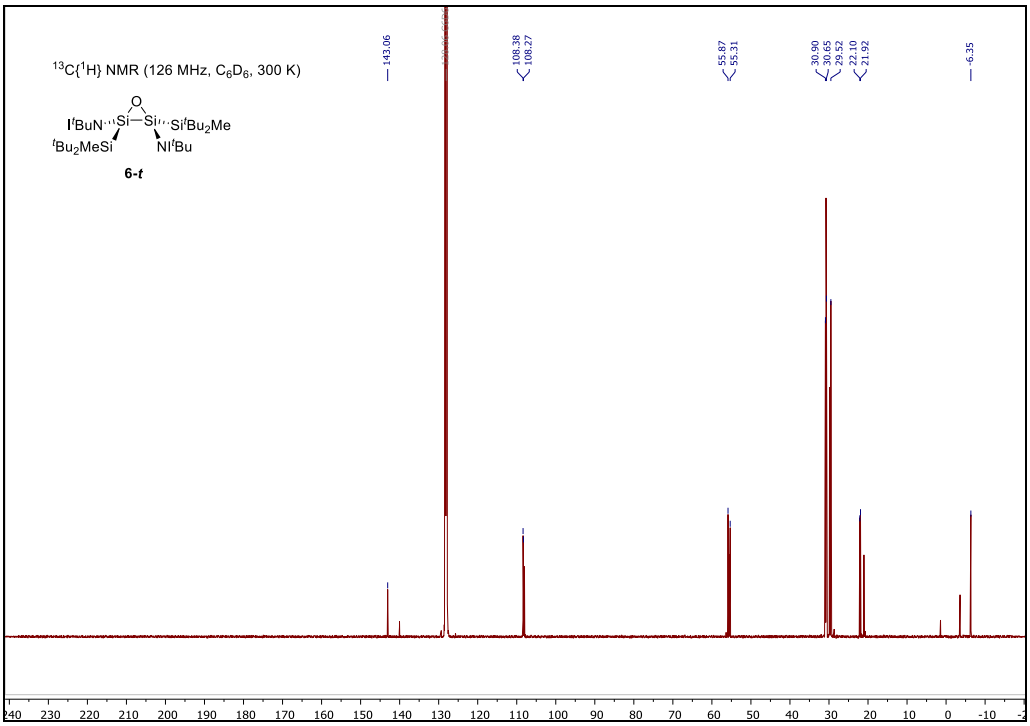


Figure S29: ^{13}C NMR spectrum (126 MHz) of compound **6-*t*** in C_6D_6 at 300 K. Unlabeled signals belong to compound **5**.

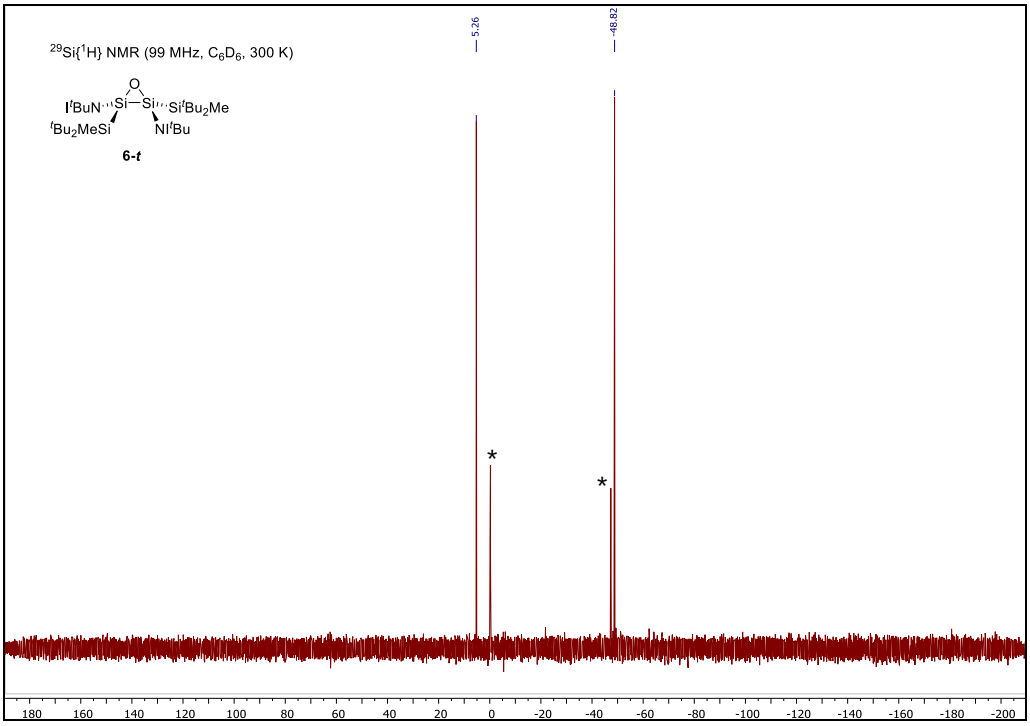


Figure S30: ^{29}Si NMR spectrum (99 MHz) of compound **6-*t*** in C_6D_6 at 300 K. Signals labelded with * belong to compound **5**.

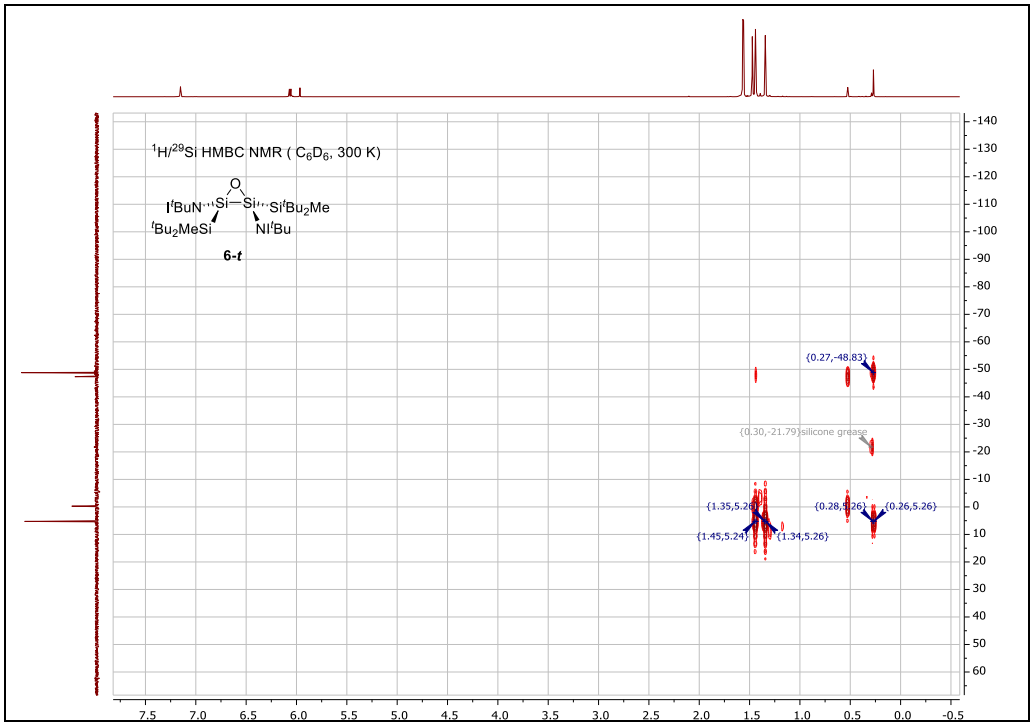
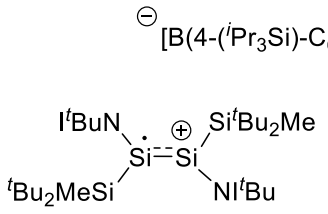


Figure S31: ^{1}H/^{29}Si HMBC NMR spectrum of mixture of compounds **6-*t*** and **5** in C_6D_6 at 300 K.

1.8. Radical Cation of I^{t}BuN(^{t}Bu$_2$MeSi)Si=Si(Si^{t}Bu$_2$Me)NI^{t}Bu 7



7

$Si_8C_{100}H_{166}N_6BF_{16}$

1991.12 g/mol

To a mixture of iminodisilene **2** (39.0 mg, 51.4 µmol, 1.00 eq.) and the functionalized trityl (fluoroaryl)borate $[Ph_3C][B(4\text{-}(^iPr_3Si)\text{-}C_6F_4)_4]$ (75.8 mg, 51.4 µmol, 1.00 eq.) toluene (4 mL) was added at room temperature. The reaction mixture turned dark green and a phase separation to a lower oily green layer and a top brown layer was observed. After evaporation of all volatile compounds *in vacuo*, the oily residue was washed with *n*-hexane (5 × 3 mL) to give radical cation **7** as extremely air and moisture sensitive green powder (67.0 mg, 33.4 µmol, 66% yield). Crystals almost suitable for SC-XRD analysis were obtained from diffusion of *n*-hexane into a difluorobenzene solution of **7** at ambient temperature.

Note: The TIPS-functionalized borate anion was used in order to facilitate crystallization. Utilization of the commercially available $B(C_6F_5)_4$ anion also provides the disilene radical cation.

EPR (toluene, 286 K) g = 2.0029.

EA:	$Si_8C_{100}H_{166}BF_{16}N_6$	Calculated [%]:	C (60.30), H (8.40), N (4.22)
		Experimental [%]:	C (59.15), H (7.93), N (3.57)

Note: Because of the extreme sensitivity of **7**, no better matching elemental analysis was obtained. The carbon value however was reproducibly low, presumably due to the formation of incombustible silicon carbides.

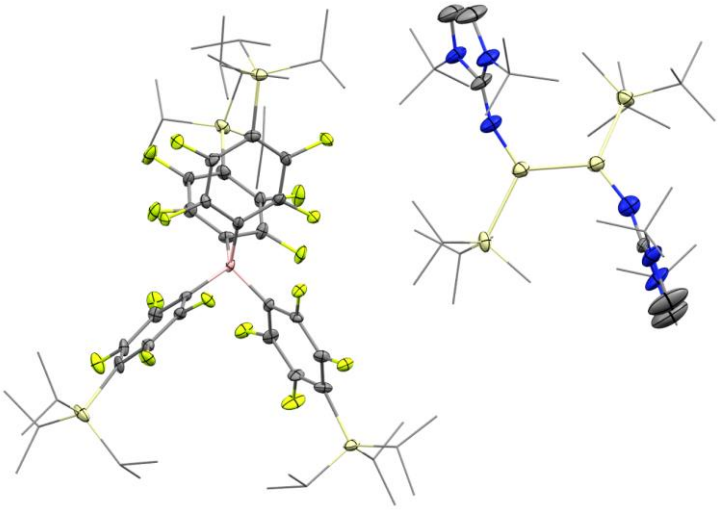


Figure S32: Solid state structure of compound **7**.

Note: Because of twinning and disorder, no satisfactory structure was obtained. Therefore, structural parameters cannot be discussed. Nonetheless, this structure reveals (*E*)-configuration of the substituents and three-coordinate silicon centers without interaction with solvent molecules or anions.

Table S1: Details for the EPR measurement of **7**.

Parameters used for the EPR measurement of 7*	
solvent	toluene
***T* [K]**	286
***v* [GHz]**	9.3109
***MW* [mT]**	0.04
***TC* [s]**	0.1
***P* [mW]**	5
***RG* [dB]**	40
***CF* [mT]**	331
***SW* [mT]**	10

*T = temperature, *v* = microwave frequency, *MW* = modulation width, *TC* = time constant, *P* = microwave power, *RG* = receiver gain, *CF* = center field, *SW* = sweep width

Table S2: Details for the simulated spectrum of **7**.

Parameters used to simulate the spectrum of 7*	
g	2.0029
$a(^{29}Si^{Central})/n$	1.897 mT/2
$a(^{14}N^{NHI\text{-}exo})/n$	0.250 mT/2
$a(^{14}N^{NHI\text{-}endo})/n$	0.133 mT/4
lwpp	0.103 mT

**a* = hyperfine coupling constants, *n* = number of equivalent nuclei, *lwpp* = linewidth peak-to-peak (Gaussian)

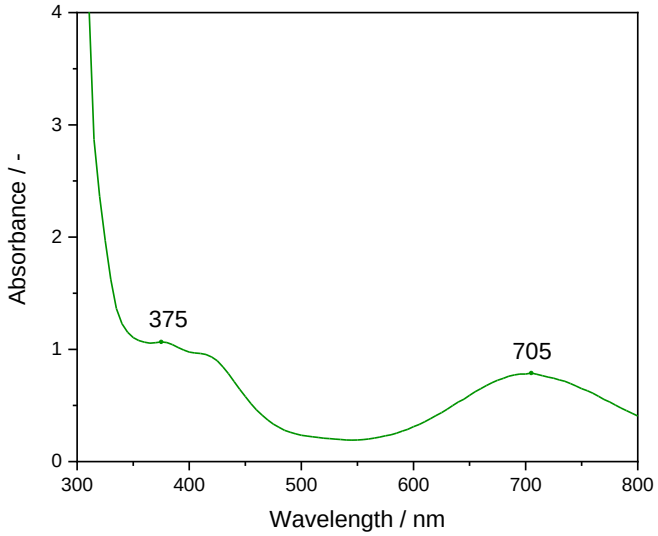
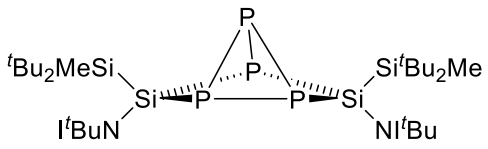


Figure S33: UV-vis spectrum of disilene radical cation **7** in 1,2-difluorobenzene, measured at room temperature.

1.9. Compound 8



8

$Si_4C_{40}H_{82}N_6P_4$

883.37 g/mol

Under exclusion of light, white phosphorus (4.89 mg, 39.5 µmol, 1.00 eq.) was added to a solution of disilene **8** (30.0 mg, 39.5 µmol, 1.00 eq.) in toluene (2 mL) at room temperature. The dark red color completely vanished within 18 hours stirring to give a slightly cloudy, pale yellow mixture. After filtration and evaporation of the solvent, compound **8** was obtained as colorless crystalline solid (32.9 mg, 37.2 µmol, 94%). Crystals suitable for SC-XRD analysis were obtained from a cooled (–35 °C) solution of **8** in a toluene / *n*-hexane (1:1) mixture.

m.p.: 218 °C (decomposition, color change to yellow).

^{1}H NMR (500 MHz, C_6D_6, 300 K): δ [ppm] = 5.86 (d, ^{3}J = 3.2 Hz, 2H, C*H*-N), 5.78 (d, ^{3}J = 3.2 Hz, 2H, C*H*-N), 1.65 (s, 18H, ^{t}*Bu*$_2$MeSi), 1.61 (s, 18H, ^{t}*Bu*$_2$MeSi), 1.35 (s, 18H, N^{t}*Bu*), 1.29 (s, 18H, N^{t}*Bu*), 0.73 (s, 6H, ^{t}Bu$_2$*Me*Si).

^{13}C{^{1}H} NMR (100 MHz, C_6D_6, 300 K): δ [ppm] = 140.7 (*C*=N), 108.8 (*C*H-N), 108.1 (*C*H-N), 55.9 (N*C*(CH$_3$)$_3$), 55.2 (N*C*(CH$_3$)$_3$), 31.8 (Si(C(*C*H$_3$)$_3$)$_2$(CH$_3$)), 31.6 (Si(C(*C*H$_3$)$_3$)$_2$(CH$_3$)), 30.6 (NC(*C*H$_3$)$_3$), 30.3 (NC(*C*H$_3$)$_3$), 23.0 (Si(*C*(CH$_3$)$_3$)$_2$(CH$_3$)), 23.0 (Si(*C*(CH$_3$)$_3$)$_2$(CH$_3$)), –1.7 (Si(C(CH$_3$)$_3$)$_2$(*C*H$_3$)).

^{29}Si{^{1}H} NMR (99 MHz, C_6D_6, 300 K): δ [ppm] = 11.9 (s, ^{t}Bu$_2$Me*Si*), –52.2 (m, *Si*P$_2$).

^{31}P{^{1}H} NMR (162 MHz, C_6D_6, 300 K): δ [ppm] = 106.6 (dt, $^{1}J_{P\text{-}P}$ = 126.9 Hz, $^{2}J_{P\text{-}P}$ = 8.5 Hz, 1P, *P*Si$_2$), –44.0 (dd, $^{1}J_{P\text{-}P}$ = 158.1 Hz, $^{2}J_{P\text{-}P}$ = 8.9 Hz, 2P, *P*SiP$_2$), –217.6 (dt, $^{1}J_{P\text{-}P}$ = 157.9 Hz, $^{1}J_{P\text{-}P}$ = 129.0 Hz, 1P, *P*P$_3$).

EA:	$Si_4C_{40}H_{82}N_6P_4$	Calculated [%]:	C (54.39), H (9.36), N (9.51)
		Experimental [%]:	C (54.14), H (9.25), N (9.35).

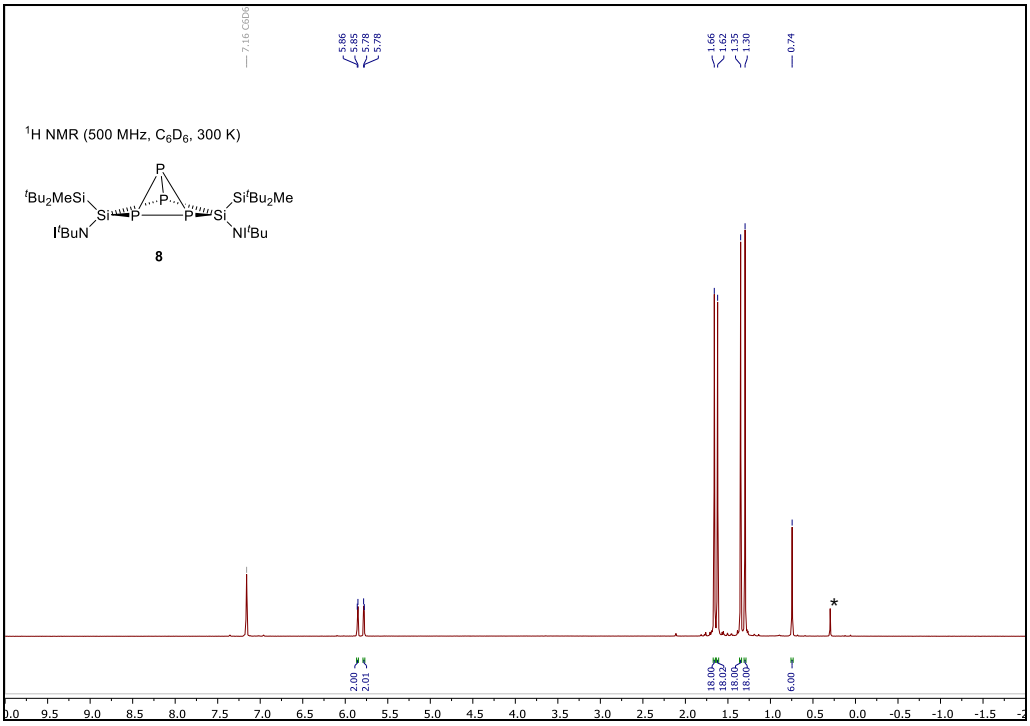


Figure S34: ^{1}H NMR spectrum (500 MHz) of compound **8** in C_6D_6 at 300 K. The signal labeled with * belongs to silicone grease.

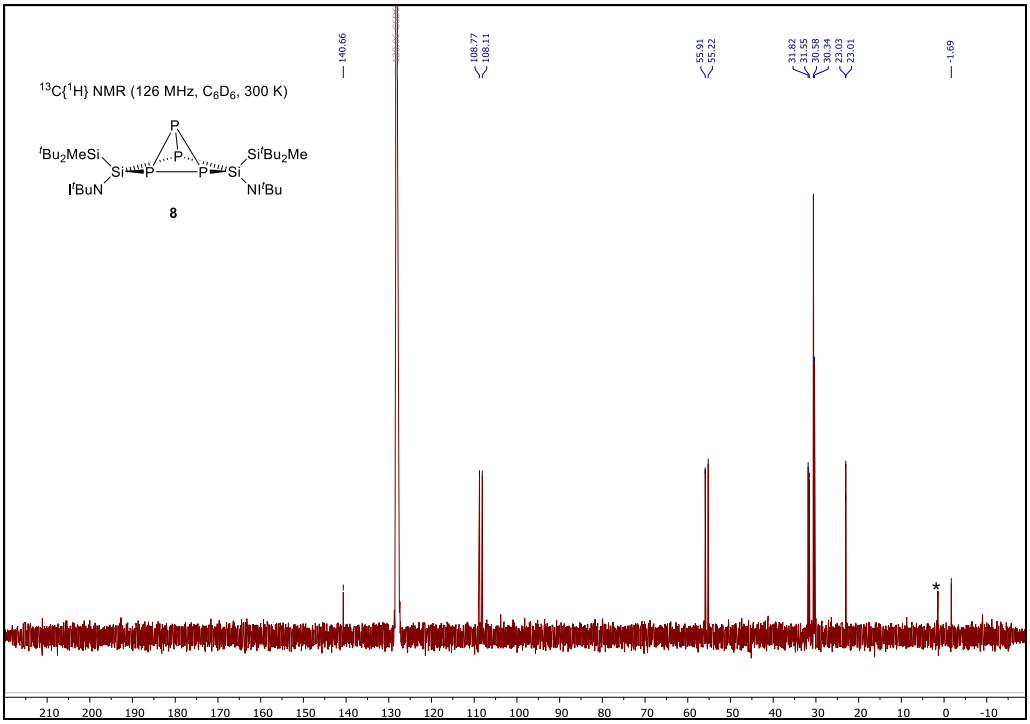


Figure S35: ^{13}C{^{1}H} spectrum (126 MHz) of compound **8** in C_6D_6 at 300 K. The signal labeled with * belongs to silicone grease.

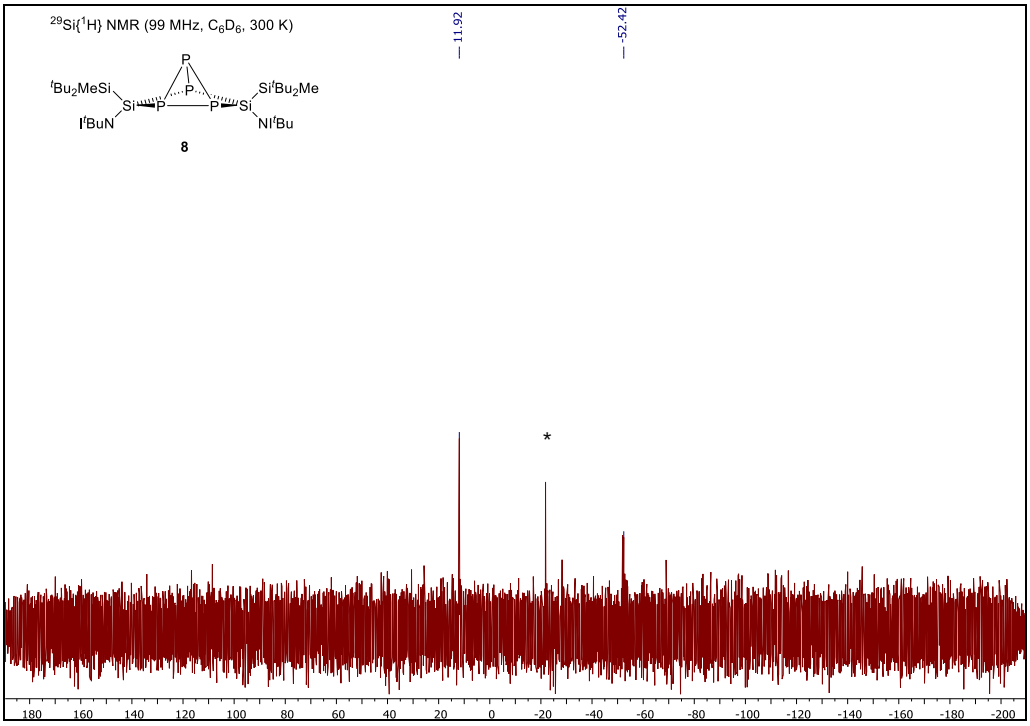


Figure S36: $^{29}Si\{^{1}H\}$ NMR spectrum (99 MHz) of compound **8** in C_6D_6 at 300 K. The signal labeled with * belongs to silicone grease.

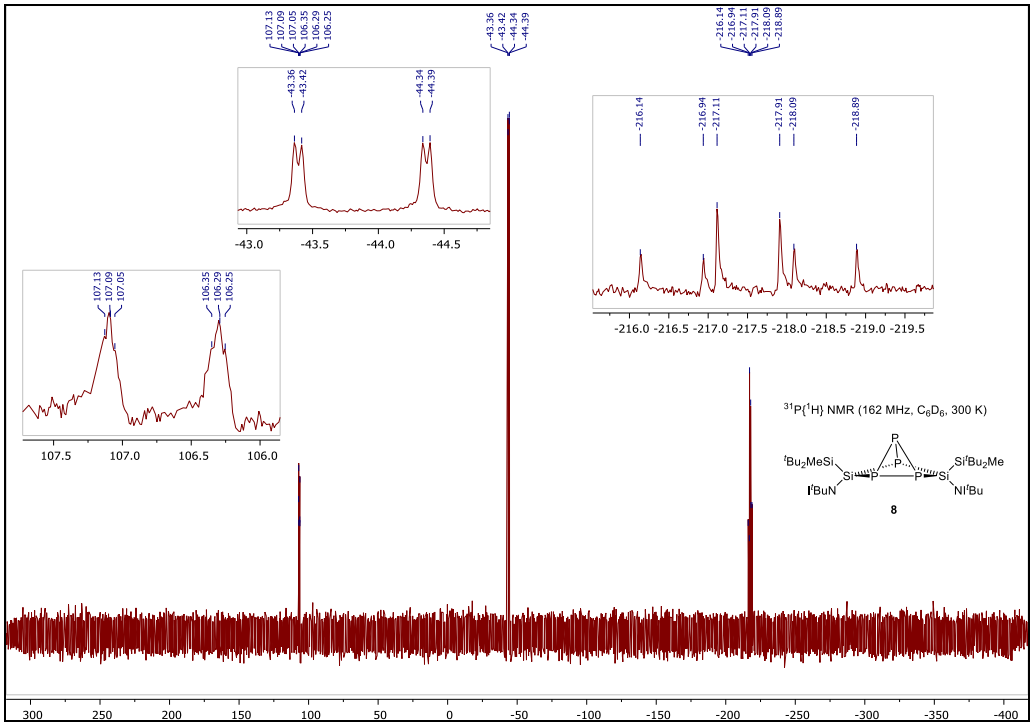


Figure S37: $^{31}P\{^{1}H\}$ spectrum (162 MHz) of compound **8** in C_6D_6 at 300 K.

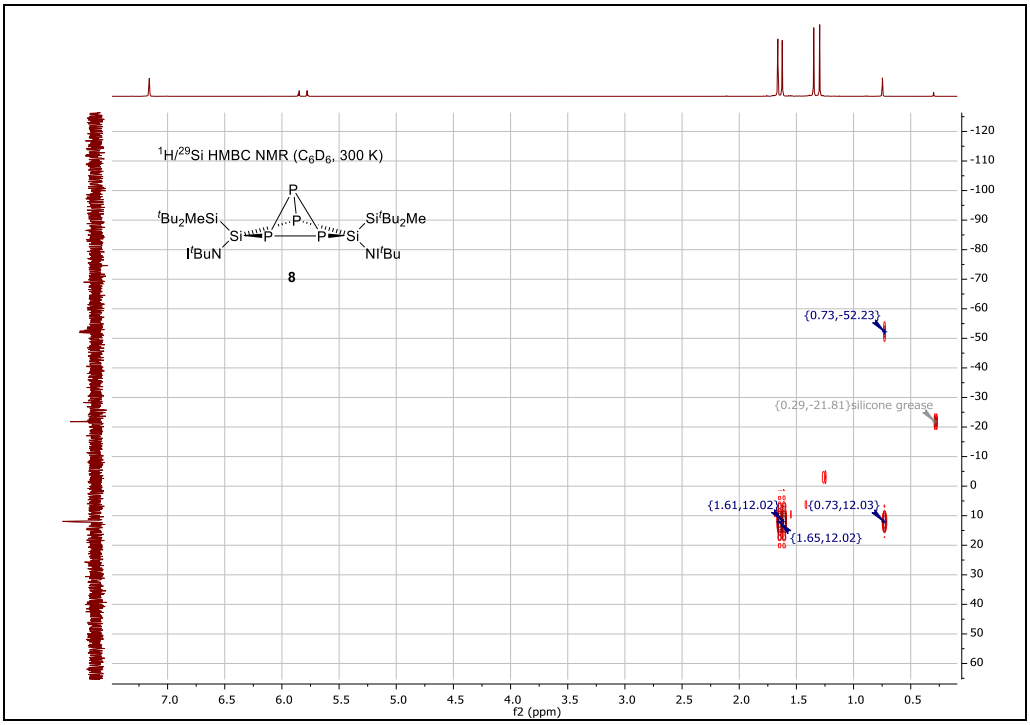
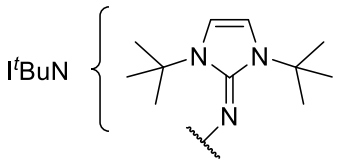
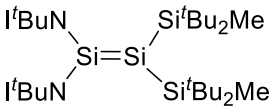


Figure S38: ^{1}H/^{29}Si HMBC NMR spectrum of compound **8** in C_6D_6 at 300 K.

1.10. Compound 9





9

$Si_4C_{40}H_{82}N_6$

759.48 g/mol

A solution of disilene I^{t}BuN(^{t}Bu$_2$MeSi)Si=Si(Si^{t}Bu$_2$Me)NI^{t}Bu (**2**) (100 mg, 132 µmol) in toluene (5 mL) was heated in a pressurizable Schlenk flask to 115 °C for 4 days. After filtration, the solution was concentrated *in vacuo* and cooled to –35 °C for crystallization. Compound **9** was obtained as purple crystals (75.4 mg, 75% yield). These crystals were also suitable for SC-XRD analysis.

Note: The crystals are only slightly soluble in *n*-hexane, however they show good solubility in toluene and benzene. Although the crystals are purple, the resulting solution is deep red.

m.p.: 65 °C (decomposition, color change to black).

^{1}H NMR (500 MHz, C_6D_6, 300 K): δ [ppm] = 6.00 (s, 4H, C*H*-N), 1.54 (s, 36H, ^{t}*Bu*N), 1.50 (s, 36H, ^{t}*Bu$_2$*MeSi), 0.36 (s, 6H, ^{t}Bu$_2$*Me*Si).

^{13}C{^{1}H} NMR (126 MHz, C_6D_6, 300 K): δ [ppm] = 139.2 (*C*=N), 108.3 (*C*H-N), 55.9 (N*C*(CH$_3$)$_3$), 31.4 (Si(C(*C*H$_3$)$_3$)$_2$(CH$_3$)), 29.5 (NC(*C*H$_3$)$_3$), 22.6 (Si(*C*(CH$_3$)$_3$)$_2$(CH$_3$)), –3.0 (Si(C(CH$_3$)$_3$)$_2$(*C*H$_3$)).

^{29}Si{^{1}H} NMR (99 MHz, C_6D_6, 300 K): δ [ppm] = 30.4 (=*Si*N$_2$), 23.0 (^{t}Bu$_2$Me*Si*), –176.1 (=*Si*Si$_2$).

EA: $Si_4C_{40}H_{82}N_6$ Calculated: C (63.26), H (10.88), N (11.07)
Experimental: C (63.12), H (10.93), N (11.05).

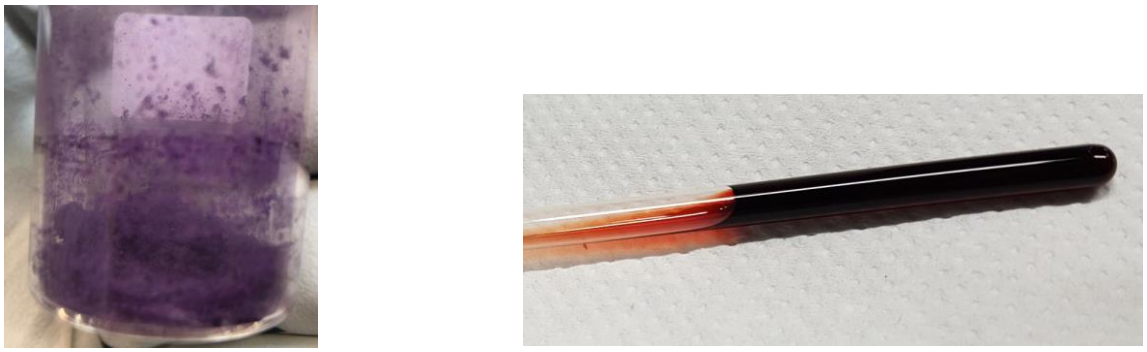


Figure S39: Dark purple solid of iminodisilene **9** (left) and red benzene solution of **9** (right).

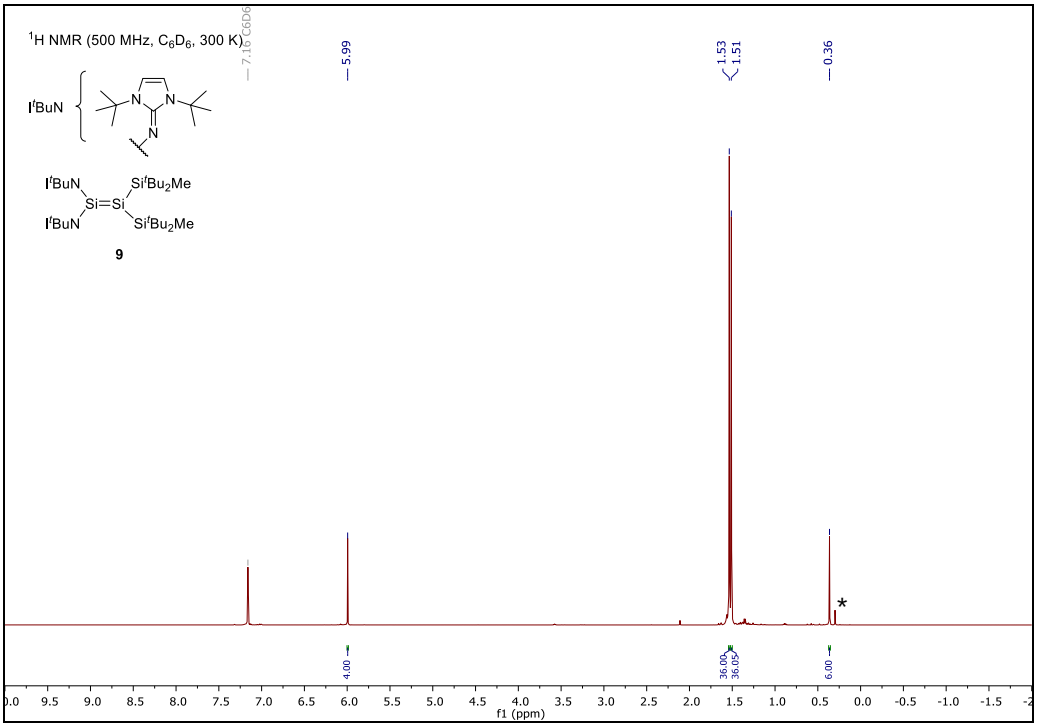


Figure S40: ^{1}H NMR spectrum (500 MHz) of compound **9** in C_6D_6 at 300 K. Signal labeled with * belongs to silicone grease.

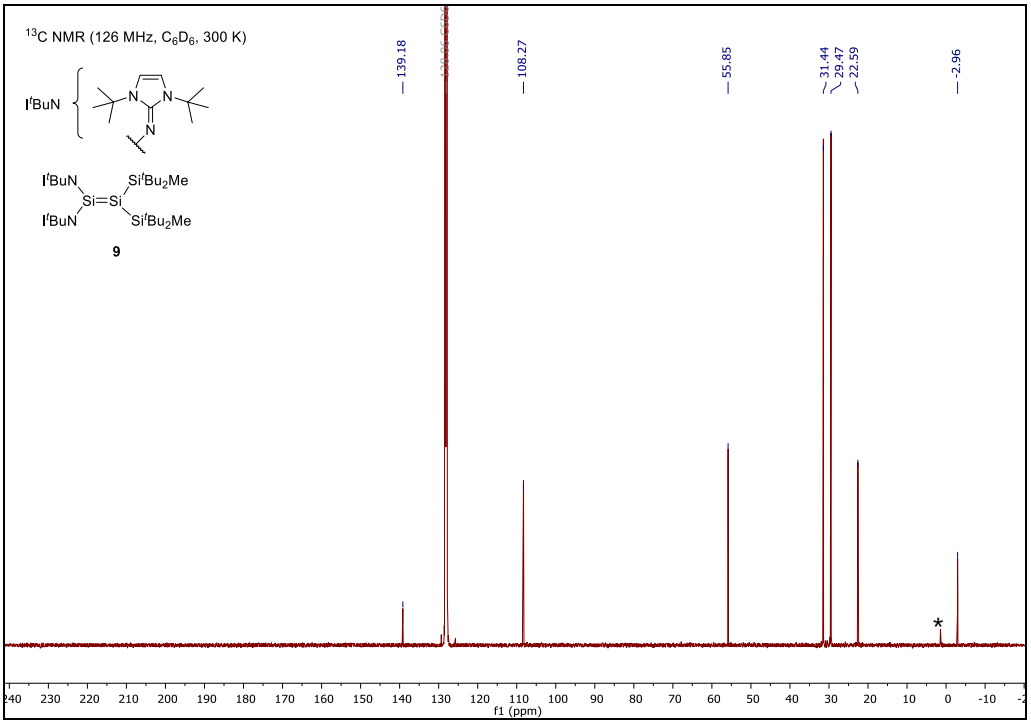


Figure S41: ^{13}C NMR spectrum (126 MHz) of compound **9** in C_6D_6 at 300 K. Signal labeled with * belongs to silicone grease.

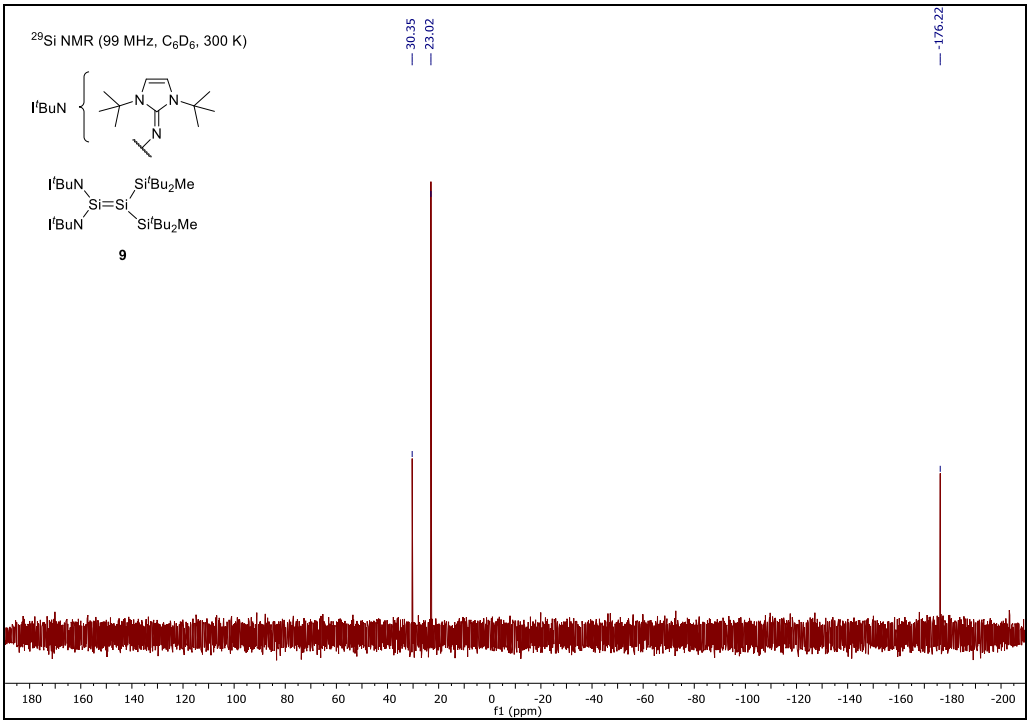


Figure S42: ^{29}Si NMR spectrum (99 MHz) of compound **9** in C_6D_6 at 300 K.

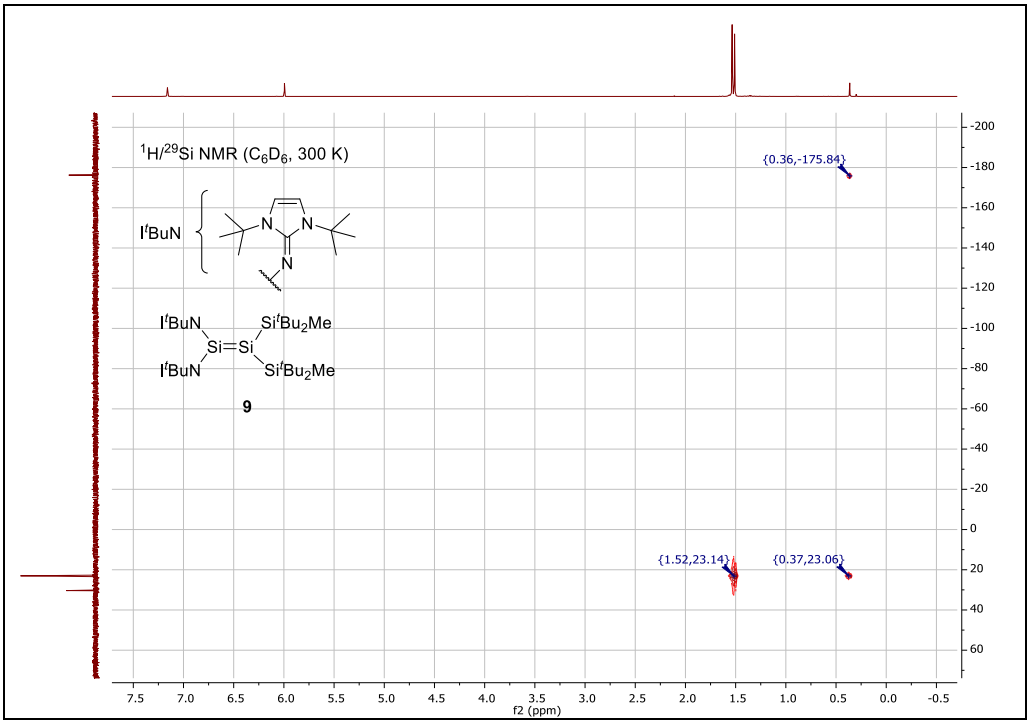


Figure S43: ^{1}H/^{29}Si HMBC NMR spectrum of compound **9** in C_6D_6 at 300 K.

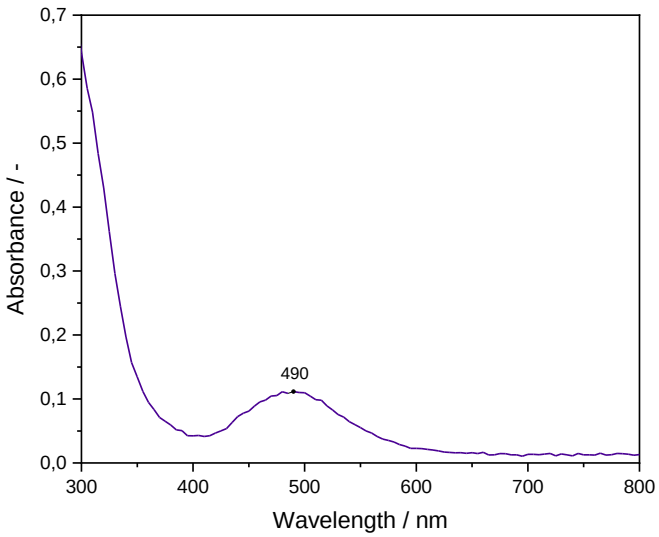


Figure S44: UV-vis spectrum of disilene **9** in toluene (2.5×10^{-3} M), measured at room temperature (λ_{max} = 490 nm (ε = 45 L mol^{-1} cm^{-1})).

2. X-ray Crystallographic Data

2.1 General Information

The X-ray intensity data of **5** were collected on an X-ray single crystal diffractometer equipped with a CMOS detector (*Bruker Photon-100*), a rotating anode (*Bruker TXS*) with MoKα radiation (λ = 0.71073 Å) and a *Helios* mirror optic by using the *APEX III* software package.[S9] The X-ray intensity data of **1**, **2-(*Z*)**, **3**, **4**, **8** and **9** were collected on an X-ray single crystal diffractometer equipped with a CMOS detector (*Bruker Photon-100*), an IMS microsource with MoKα radiation (λ = 0.71073 Å) and a *Helios* mirror optic by using the *APEX III* software package.[S9] The measurements were performed on single crystals coated with the perfluorinated ether *Fomblin® Y*. The crystal was fixed on the top of a micro sampler, transferred to the diffractometer and frozen under a stream of cold nitrogen. A matrix scan was used to determine the initial lattice parameters. Reflections were merged and corrected for Lorenz and polarization effects, scan speed, and background using *SAINT*.[S10] Absorption corrections, including odd and even ordered spherical harmonics were performed using *SADABS*.[S10] Space group assignments were based upon systematic absences, E statistics, and successful refinement of the structures. Structures were solved by direct methods with the aid of successive difference Fourier maps, and were refined against all data using the *APEX III* software in conjunction with *SHELXL-2014*[S11] and *SHELXLE*.[S12] All H atoms (except Si–H) were placed in calculated positions and refined using a riding model, with methylene and aromatic C–H distances of 0.99 and 0.95 Å, respectively, and $U_{iso}(H) = 1.2 \cdot U_{eq}(C)$. H atoms bound to Si atoms could be located in the difference Fourier maps and were allowed to refine freely. Full-matrix least-squares refinements were carried out by minimizing $\Delta w(F_o^2 - F_c^2)$[S10] with *SHELXL-97* weighting scheme.[S13] Neutral atom scattering factors for all atoms and anomalous dispersion corrections for the non-hydrogen atoms were taken from International Tables for Crystallography.[S14] The images of the crystal structures were generated by *Mercury*.[S15] The CCDC numbers - contain the supplementary crystallographic data for the structures. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre *via* https://www.ccdc.cam.ac.uk/structures/.

2.2 SC-XRD structures

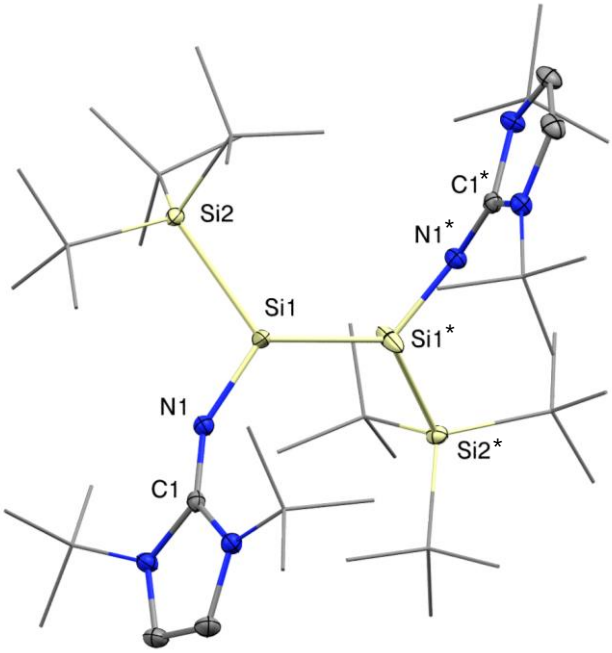


Figure S45: SC-XRD structure of disilene **1** with thermal ellipsoids drawn at the 50% probability level. Hydrogen atoms are omitted for clarity, ^{t}Bu and Me groups are simplified as wireframes. Selected bond lengths [Å] and angles [°]: Si1–Si1* 2.2534(7), Si1–Si2 2.4142(6), Si1–N1 1.682(1), N1–C1 1.285(2), N1–Si1–Si1* 122.97(5), Si2–Si1–Si1* 124.52(3), Si2–Si1–N1 110.56(4).

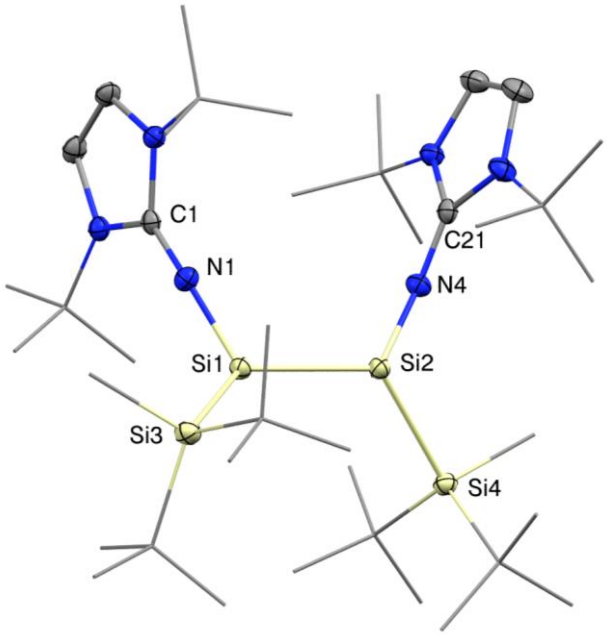


Figure S46: SC-XRD structure of disilene **2-(*Z*)** with thermal ellipsoids drawn at the 50% probability level. Hydrogen atoms are omitted for clarity, ^{t}Bu and Me groups are simplified as wireframes. Selected bond lengths [Å] and angles [°]: Si1–Si2 2.2844(7), Si1–Si3 2.3922(7), Si2–Si4 2.4001(7), Si1–N1 1.683(1), Si2–N4 1.680(1), N1–C1 1.283(2), N4–C21 1.278(2), Si3–Si1–N1 104.35(5), Si4–Si2–N4 103.84(5), Si2–Si1–Si3 121.28(2), Si2–Si1–N1 119.25(5).

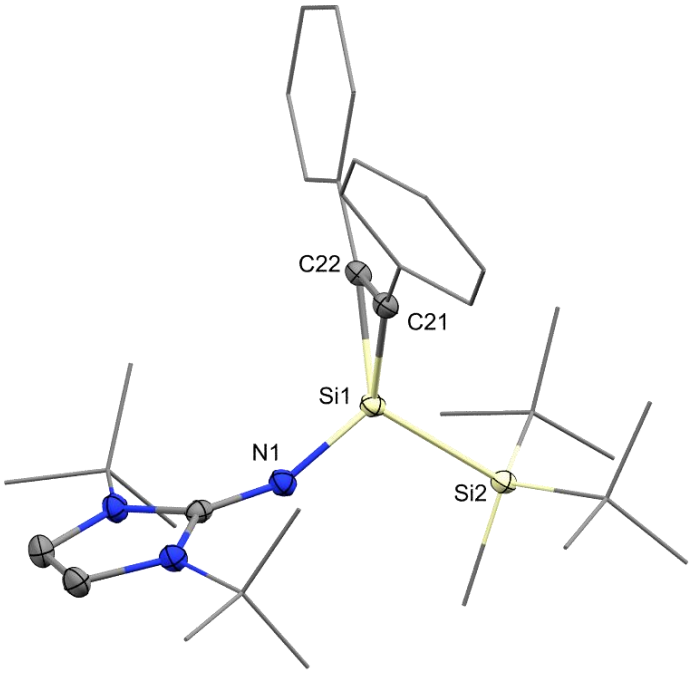


Figure S47: SC-XRD structure of **3** with thermal ellipsoids drawn at the 50% probability level. Hydrogen atoms are omitted for clarity, ^{t}Bu and Me groups are simplified as wireframes. Selected bond lengths [Å] and angles [°]: Si1–Si2 2.3606(7), Si1–N1 1.659(1), Si1–C21 1.840(2), Si1–C22 1.548(2), C21–C22 1.353(2), N1–Si1–Si2 107.59(5), N1–Si1–C21 123.22(7), N1–Si1–C22 124.66(7).

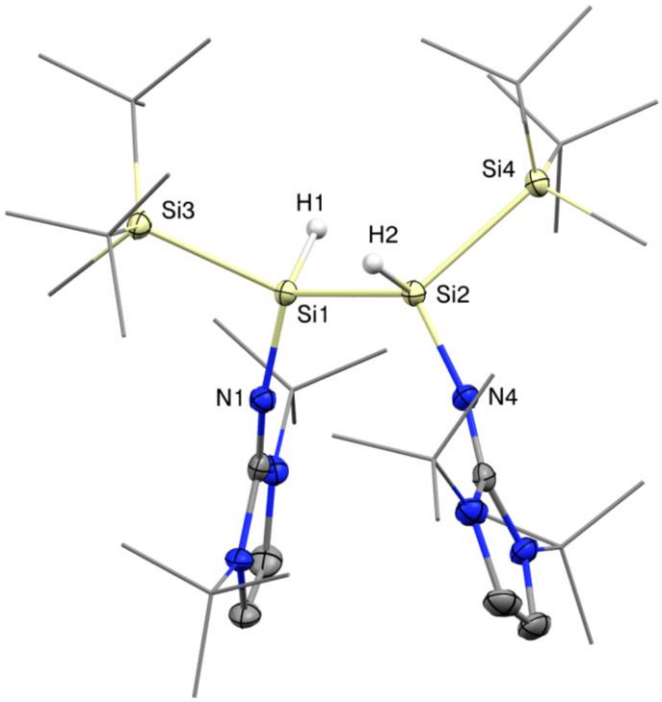


Figure S48: SC-XRD structure of hydrosilane **4** with thermal ellipsoids drawn at the 50% probability level. Hydrogen atoms are omitted for clarity, ^{t}Bu and Me groups are simplified as wireframes. Selected bond lengths [Å] and angles [°]: Si1–Si2 2.4184(6), Si1–H1 1.43(1), Si1–Si3 2.4085(6), Si1–N1 1.682(1), Si2–H2 1.42(2), H1–Si1–Si3 101.1(6), N1–Si1–H1 113.9(6), N1–Si1–Si2 111.91(4), Si2–Si1–Si3 120.40(2).

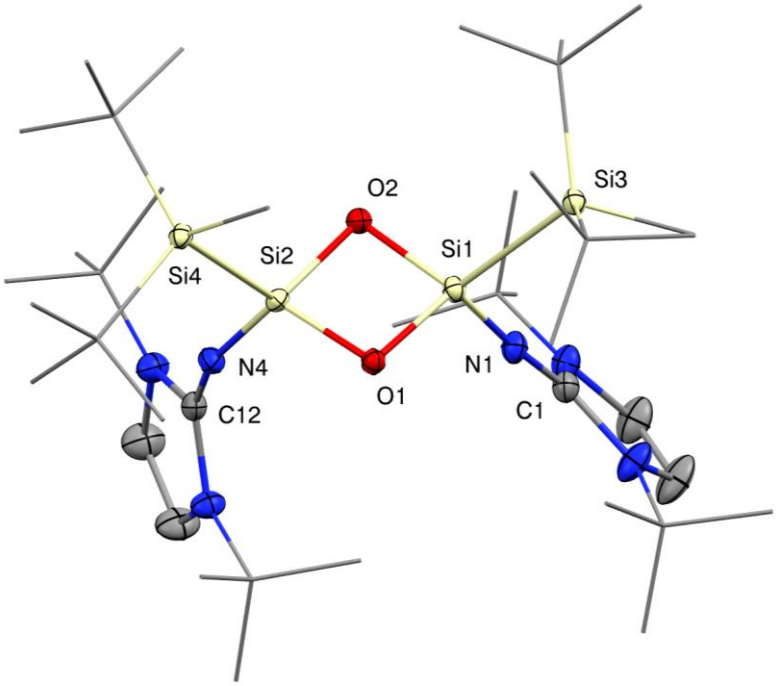


Figure S49: SC-XRD structure of compound **5** with thermal ellipsoids drawn at the 50% probability level. Hydrogen atoms are omitted for clarity, ^{t}Bu and Me groups are simplified as wireframes. Selected bond lengths [Å] and angles [°]: Si1–O1 1.686(1), Si1–O2 1.695(1), Si1–Si3 2.3897(6), Si1–N1 1.641(1), N1–C1 1.274(2), Si2–O1 1.698(1), Si2–O2 1.691(1), Si3–Si1–O1 119.63(4), Si3–Si1–O2 114.96(4), Si3–Si1–N1 106.06(5), Si1–O1–Si2 91.77(5).

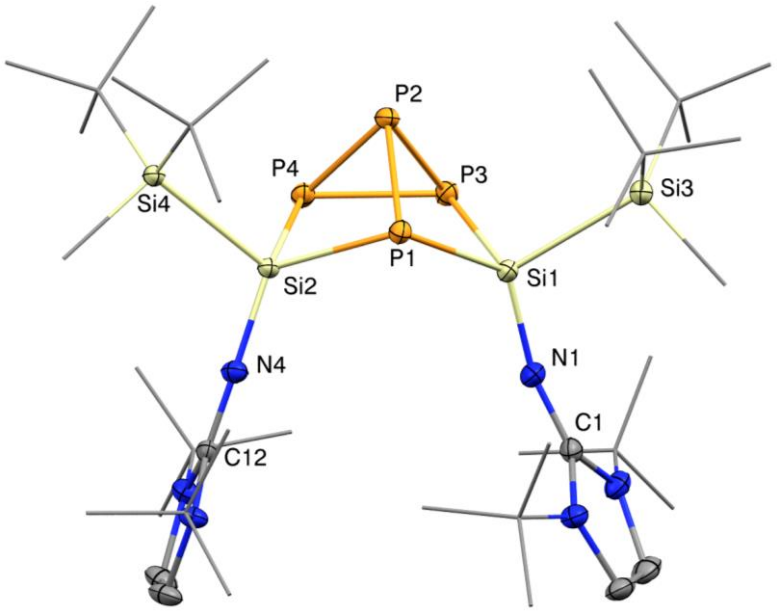


Figure S50: SC-XRD structure of compound **8** with thermal ellipsoids drawn at the 50% probability level. Hydrogen atoms are omitted for clarity, ^{t}Bu and Me groups are simplified as wireframes. Selected bond lengths [Å] and angles [°]: Si1–P1 2.2785(8), Si1–P3 2.2723(7), P1–P2 2.2937(7), P3–P2 2.2301(8), N1–Si1–Si3 109.32(4), P1–Si1–P3 94.22(2), P1–P2–P3 94.95(2), Si1–P1–Si2 106.69(2).

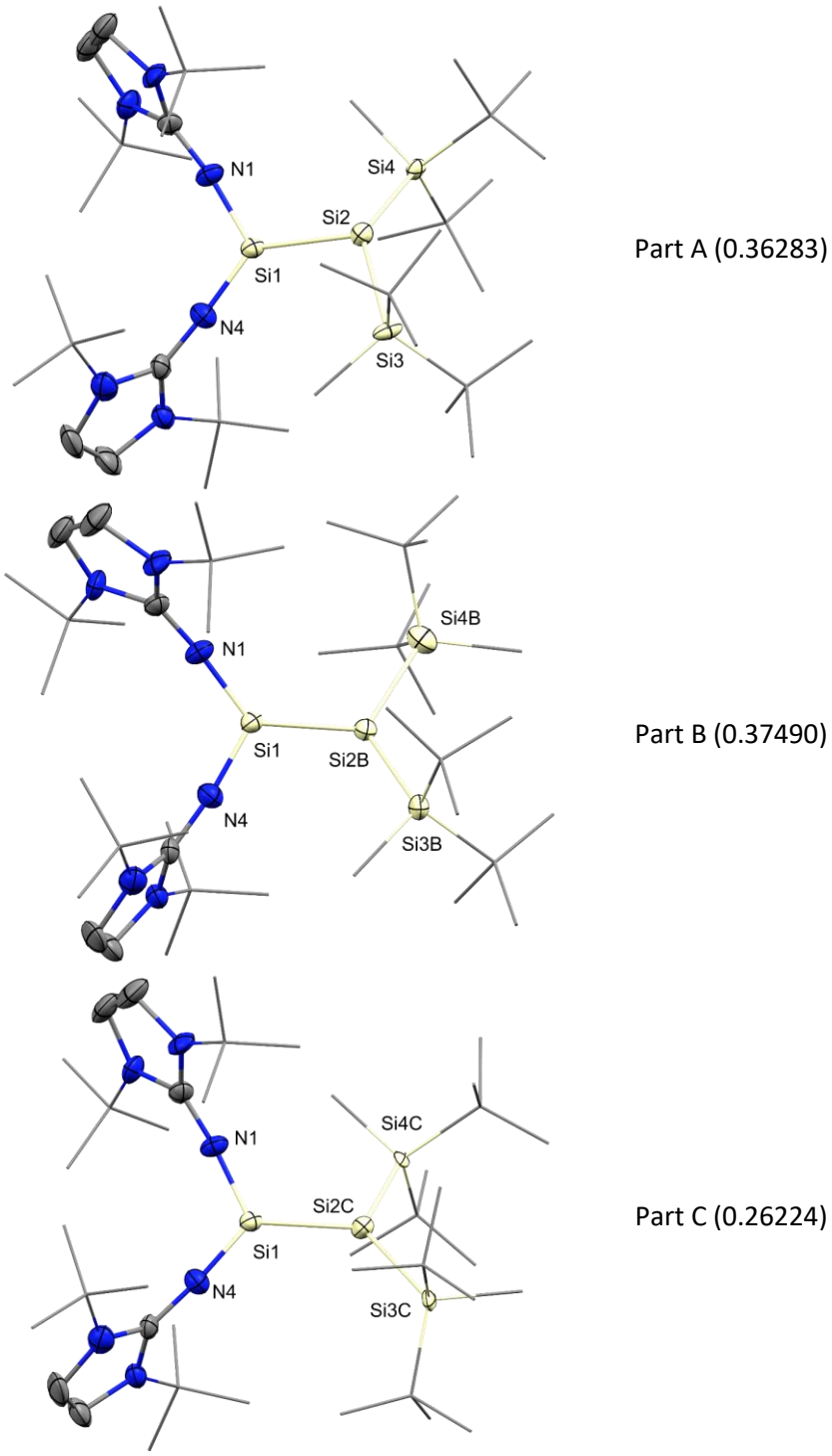


Figure S51: SC-XRD structure of disilene **9** (including the disordered silyl groups) with thermal ellipsoids drawn at the 30% probability level and occupation ratio of the disordered groups. Hydrogen atoms are omitted for clarity, ^{t}Bu and Me groups are simplified as wireframes. For more information, the full crystallographic information file is available free of charge from the Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk/structures/ (cf. CCDC-2059209). Selected bond lengths [Å] and angles [°] Part A: Si1–Si2 2.219(4), Si1–N1 1.659(4), Si1–N4 1.604(4), Si2–Si3 2.360(6), Si2–Si4 2.343(5), N1–Si1–N4 113.1(2), Si3–Si2–Si4 138.2(2), Si1–Si2–Si3 106.3(2), Si2–Si1–N1 115.4(2), θ(Silyl/NHI) 40.3/8.1, τ 46.9; Part B: Si1–Si2B 2.246(3), Si2B–Si3B 2.382(6), Si2B–Si4B 2.344(5), Si3B–Si2B–Si4B 126.3(2), Si1–Si2B–Si3B 105.0(2), Si2B–Si1–N1 130.0(2), θ(Silyl/NHI) 26.2/6.7, τ 45.2; Part C: Si1–Si2C 2.203(5), Si2C–Si3C 2.371(7), Si2C–Si4C 2.351(8), Si3C–Si2C–Si4C 126.6(3), Si1–Si2C–Si3C 124.0(3), Si2C–Si1–N1 118.2(2), θ(Silyl/NHI) 4.9/1.1, τ 41.0.

2.3 Crystal data and structural refinement parameters

Table S3: Crystal data and structural refinement parameters for compounds **1-(*E*)**, **2-(*Z*)**, **3** and **4**.

Compound #	**1-(*E*)**	**2-(*Z*)**	**3**	**4**
CCDC #	2059203	2059204	2059205	2059206
Chemical formula	$Si_4C_{46}H_{94}N_6$	$Si_4C_{40}H_{82}N_6$	$Si_2C_{34}H_{51}N_3$	$Si_4C_{40}H_{84}N_6$
Formula weight	843.62	759.47	557.96	761.49
Temperature	100(2) K	100(2) K	100(2) K	100(2) K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å	0.71073 Å
Crystal size	0.155 × 0.182 × 0.186 mm	0.185 × 0.228 × 0.254 mm	0.098 × 0.148 × 0.285 mm	0.266 × 0.333 × 0.487 mm
Crystal habit	clear dark green fragment	clear red fragment	clear colorless fragment	clear colorless fragment
Crystal system	monoclinic	triclinic	monoclinic	triclinic
Space group	C 1 2/c 1	P -1	P 21/n	P -1
Unit cell dimensions	a = 21.5194(19) Å, , α = 90°	a = 10.4102(19) Å, α = 81.153(7)°	a = 10.1287(11) Å, α = 90°	a = 10.6636(5) Å, α = 80.983(2)°
	b = 10.3978(9) Å, β = 91.393(3)°	b = 12.363(2) Å, β = 76.718(7)°	b = 19.437(2) Å, β = 95.309(4)°	b = 12.0948(6) Å, β = 83.783(2)°
	c = 23.024(2) Å, γ = 90°	c = 21.101(4) Å, γ = 65.519(7)°	c = 16.5735(18) Å, γ = 90°	c = 21.0683(11) Å, γ = 65.412(2)°
Volume	5150.2(8) $Å^3$	2400.2(8) $Å^3$	3248.9(6) $Å^3$	2437.5(2) $Å^3$
Z	8	2	4	2
Density (calculated)	1.088 g/cm^3	1.051 g/cm^3	1.141 g/cm^3	1.038 g/cm^3
Absorption coefficient	0.151 mm^{-1}	0.156 mm^{-1}	0.136 mm^{-1}	0.153 mm^{-1}
F(000)	1872	840	1216	844
Diffractometer	Bruker D8 Venture Duo IMS	Bruker D8 Venture Duo IMS	Bruker D8 Venture Duo IMS	Bruker D8 Venture Duo IMS
Radiation source	IMS microsource, Mo	IMS microsource, Mo	IMS microsource, Mo	IMS microsource, Mo
Theta range for data collection	2.17 to 26.02°	2.21 to 25.35°	2.27 to 25.35	1.96 to 25.35°
Index ranges	-26<=h<=26	-12<=h<=12	-12<=h<=12	-12<=h<=12
	-12<=k<=12	-14<=k<=14	-23<=k<=23	-14<=k<=14
	-28<=l<=28	-25<=l<=25	-19<=l<=19	-25<=l<=25
Reflections collected	79283	55819	144772	106589
Independent reflections	5073 [R(int) = 0.0311]	8777 [R(int) = 0.0309]	5953 [R(int) = 0.0606]	8902 [R(int) = 0.0274]
Coverage of independent reflections	100.0%	99.9%	99.9%	99.7%
Absorption correction	Multi-scan	Multi-Scan	Multi-scan	Multi-Scan
Max. and min. transmission	0.9770 and 0.9720	0.9610 and 0.9720	0.9870 and 0.9760	0.9600 and 0.9410
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	SHELXL-2016/6 (Sheldrick, 2016)	SHELXL-2014/7 (Sheldrick, 2014)	SHELXL-2016/6 (Sheldrick, 2016)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	$\Sigma\, w(F_o^2 - F_c^2)^2$	$\Sigma\, w(F_o^2 - F_c^2)^2$	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	5073 / 0 / 268	8777 / 0 / 477	5953 / 0 / 365	8902 / 0 / 485
Goodness-of-fit on F^2	1.061	1.040	1.122	1.046
Δ/σmax	0.001	0.001	0.018	0.001
Final R indices	4598 data; I>2σ(I):	7672 data; I>2σ(I):	5470 data; I>2σ(I):	8372 data; I>2σ(I):
	R1 = 0.0342, wR2 = 0.0834	R1 = 0.0333, wR2 = 0.0820	R1 = 0.0404, wR2 = 0.1000	R1 = 0.0281, wR2 = 0.0694
	all data:	all data:	all data:	all data:
	R1 = 0.0388, wR2 = 0.0860	R1 = 0.0403, wR2 = 0.0861	R1 = 0.0447, wR2 = 0.1026	R1 = 0.0302, wR2 = 0.0714
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0348P)^2+7.2742P]$	$w=1/[\sigma^2(F_o^2)+(0.0379P)^2+1.3913P]$	$w=1/[\sigma^2(F_o^2)+(0.0446P)^2+2.1762P]$	$w=1/[\sigma^2(F_o^2)+(0.0260P)^2+1.2312P]$
	where $P=(F_o^2+2F_c^2)/3$	where $P=(F_o^2+2F_c^2)/3$	where $P=(F_o^2+2F_c^2)/3$	where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	0.456 and -0.374 $eÅ^{-3}$	0.615 and -0.295 $eÅ^{-3}$	0.359 and -0.346 $eÅ^{-3}$	0.305 and -0.200 $eÅ^{-3}$
R.M.S. deviation from mean	0.044 $eÅ^{-3}$	0.047 $eÅ^{-3}$	0.044 $eÅ^{-3}$	0.034 $eÅ^{-3}$

Table S4: Crystal data and structural refinement parameters for compounds **5**, **8** and **9**.

Compound #	**5**	**8**	**9**
CCDC #	2059207	2059208	2059209
Chemical formula	$Si_4C_{40}H_{82}N_6O_2$	$Si_4C_{40}H_{82}N_6P_4$	$Si_4C_{40}H_{82}N_6$
Formula weight	791.47	883.35	759.47
Temperature	100(2) K	100(2) K	100(2) K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å
Crystal size	0.169 × 0.201 × 0.294 mm	0.256 × 0.319 × 0.339 mm	0.157 × 0.279 × 0.296 mm
Crystal habit	clear colorless fragment	clear colorless fragment	clear purple fragment
Crystal system	triclinic	triclinic	triclinic
Space group	P -1	P -1	P -1
Unit cell dimensions	a = 11.8823(10) Å, α = 103.907(3)° b = 12.5801(10) Å, β = 97.451(3)° c = 17.6952(13) Å, γ = 108.909(3)°	a = 10.0360(17) Å, α = 90.316(6)° b = 11.430(2) Å, β = 100.375(6)° c = 24.720(4) Å, γ = 115.781(5)°	a = 10.4607(14) Å, α = 87.804(6)° b = 12.233(2) Å, β = 84.887(5)° c = 20.302(3) Å, γ = 64.736(4)°
Volume	2366.1(3) $Å^3$	2500.4(8) $Å^3$	2340.1(6) $Å^3$
Z	2	2	2
Density (calculated)	1.111 g/cm^3	1.173 g/cm^3	1.078 g/cm^3
Absorption coefficient	0.163 mm^{-1}	0.281 mm^{-1}	0.160 mm^{-1}
F(000)	872	960	840
Diffractometer	Bruker D8 Venture	Bruker D8 Venture Duo IMS	Bruker D8 Venture Duo IMS
Radiation source	TXS rotating anode, Mo	IMS microsource, Mo	IMS microsource, Mo
Theta range for data collection	2.33 to 25.68°	2.28 to 25.68°	2.01 to 25.35
Index ranges	-14<=h<=14 -15<=k<=15 -21<=l<=21	-12<=h<=12 -13<=k<=13 -30<=l<=30	-12<=h<=12 -14<=k<=14 -24<=l<=24
Reflections collected	104064	69988	91859
Independent reflections	8998 [R(int) = 0.0373]	9439 [R(int) = 0.0232]	8579 [R(int) = 0.0507]
Coverage of independent reflections	99.9%	99.6%	99.9%
Absorption correction	Multi-Scan	Multi-Scan	Multi-scan
Max. and min. transmission	0.9730 and 0.9610	0.9320 and 0.9110	0.9750 and 0.9540
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Refinement program	SHELXL-2016/6 (Sheldrick, 2016)	SHELXL-2016/6 (Sheldrick, 2016)	SHELXL-2016/6 (Sheldrick, 2016)
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$	$\Sigma w(F_o^2 - F_c^2)^2$	$\Sigma w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	8998 / 204 / 690	9439 / 0 / 513	8579 / 1033 / 887
Goodness-of-fit on F^2	1.040	1.030	1.035
Δ/σmax	0.046	0.002	0.001
Final R indices	8093 data; I>2σ(I): R1 = 0.0320, wR2 = 0.0811 all data: R1 = 0.0368, wR2 = 0.0843	8839 data; I>2σ(I): R1 = 0.0245, wR2 = 0.0609 all data: R1 = 0.0267, wR2 = 0.0626	7492 data; I>2σ(I): R1 = 0.0583, wR2 = 0.1381 all data: R1 = 0.0694, wR2 = 0.1499
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0376P)^2+1.5234P]$ where $P=(F_o^2+2F_c^2)/3$	$w=1/[\sigma^2(F_o^2)+(0.0251P)^2+1.4676P]$ where $P=(F_o^2+2F_c^2)/3$	$w=1/[\sigma^2(F_o^2)+(0.0573P)^2+2.3265P]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	0.457 and -0.314 $eÅ^{-3}$	0.335 and -0.266 $eÅ^{-3}$	0.316 and -0.318 $eÅ^{-3}$
R.M.S. deviation from mean	0.046 $eÅ^{-3}$	0.038 $eÅ^{-3}$	0.049 $eÅ^{-3}$

3 DFT Calculations

3.1 General Information

Geometry optimizations and harmonic frequency calculations were performed using *Gaussian16*[S16] at the B3LYP-D3/def2-SVP[S17-22] level of density functional theory (abbreviated B3LYP-D3 in the following). The "ultrafine" grid option was used for numerical integrations,[S23] as being standard in *Gaussian16 Rev. B.01*. Stationary points are characterized as minima by analysis of computed Hessians. The connectivity between minima and transition states was validated by IRC calculations [S24] or displacing the geometry along the transition mode, followed by unconstrained optimization. We chose this level of density functional theory based on the well correspondence of the SC-XRD and the calculated structures (see Table S5), whereas the M06-L and M06-2X functionals in combination with the 6-31+G(d,p) split valence basis set underestimate the Si=Si bond length during geometry optimization. To reference and improve the energy values obtained at the B3LYP-D3 level, we performed single point calculations with *ORCA 4.2.21*[S25-26] on the DLPNO-CCSD(T)[S27-28]/def2-TZVPP[S22] (NormalPNO, VeryTightSCF)(abbreviated DLPNO-CCSD(T) in the following) on the B3LYP-D3 optimized geometries, which gave a well correspondence (see Figure S59 and Figure S60). Energy decomposition analysis with natural orbitals for chemical valence (EDA-NOCV) was performed with *ADF 2019*,[S29-30] employing the B3LYP-D3/TZ2P level of theory (gas phase calculations, no frozen core, Becke grid of quality "good") on B3LYP-D3 structures. To enable a comparisons between the base-stabilized disilenes published previously[S31-32] and **9**, bonding analysis was performed at the M06-2X/6-311++G(2d,2p)[S33-35] level of theory (abbreviated M06-2X in the following). The results obtained on the B3LYP-D3/def2-TZVP level of theory (usage of def2-SVP results in the appearance of non-nuclear attractors (NNA) along the Si=Si bond, as had been reported previously[S36]) correspond to the presented M06-2X ones. Natural Bond Orbital (NBO) and Natural Resonance Theory (NRT) analyses were performed using the *NBO 6.0* program [S37-38], interfaced with *Gaussian16* [S37-39]. The AIMAll [S40] and multiwfn [S41-42] programs were used for QTAIM analyses.[S43-44] Results of TD-DFT calculations were obtained with *Gaussian16* at the B3LYP-D3/def2-TZVP(SMD:*n*-hexane)[S45] level of theory. Pictures of molecular structures were generated with the *ChemCraft*,[S46] *Cylview*,[S47] *Chimera*[S48] or *GaussView* [S49] programs. All molecular orbital surfaces are depicted with an isovalue of 0.05. If not stated otherwise, reported energy values correspond to the free energy values (T = 298.15 K, p = 1 atm).

3.2 Calculated Structures

Comparison of Calculated and Experimental Structures

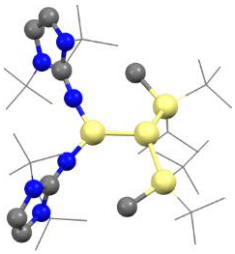
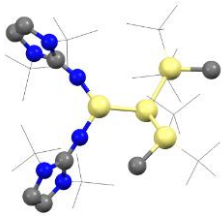
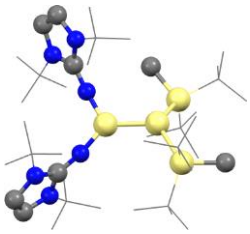
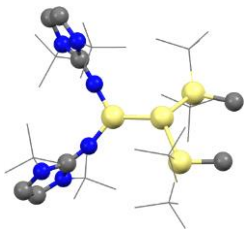
Table S5: Comparison of selected bond lengths [Å] and angles [°] for the computed and experimental structures of **1-(*E*)**, **2-(Z)** and **9**. Geometries are calculated at the B3LYP-D3/def2-SVP level of theory. Experimental data are taken from SC-XRD analyses; θ represents the bent angle, τ the twist angle as defined in the main text.

Compound	Bond/Angle [Å/°]	Exp. [Å/°]	Calc. [Å/°]	Δ(Calc.-Exp.) [Å/°]
1-(*E*)*	r(Si1=Si1′)	2.2534(7)	2.24	0.01
	r(Si1–N2)	1.682(1)	1.71	0.03
	r(Si1–Si2)	2.4142(6)	2.42	0.01
	r(N1–C1)	1.285(2)	1.28	0.00
	a(N1–Si1–Si2)	110.56(4)	111.1	0.5
	d(Si2–Si1=Si1′–Si2′)	-130.78(3)	-129.3	1.5
	d(N1–Si1=Si1′–N1′)	-165.59(7)	-163.8	1.8
	d(Si2–Si1=Si1′–N1′)	31.82(6)	33.4	1.6
	θ	12.8	12.7	0.1
	τ	40.2	40.8	0.6
2-(*Z*)	r(Si1=Si2)	2.2844(7)	2.28	0.00
	r(Si1/2–N1/4)	1.683(1)/1.680(1)	1.70	0.02
	r(Si1/2–Si3/4)	2.3922(7)/2.4001(7)	2.41	0.02/0.01
	r(N1/4–C1/21)	1.283(2)/1.278(2)	1.28	0.00
	a(Si3/4–Si1/2–N1/4)	104.35(5)/103.84(5)	104.6/104.6	0.3/0.8
	d(Si3–Si1=Si2–Si4)	83.24(3)	86.2	3.0
	d(N1–Si1=Si2–N4)	–14.32(8)	–16.3	2.0
	d(Si3–Si1=Si2–N4)	–146.60(5)	–145.1	1.5
	θ	36.3/34.7	38.3/38.3	2.0/3.6
	τ	25.5	23.3	2.2
9*[2]	r(Si1–Si2)	2.219(4)	2.24	0.02
	r(Si1–N1/4)	1.659(4)/1.604(4)	1.66	0.00/0.06
	r(Si2–Si3/Si4)	2.360(6)/2.343(5)	2.39/2.38	0.03/0.04
	a(N1–Si1–N4)	113.1(2)	110.1	3
	a(Si3–Si2–Si4)	138.2(2)	132.7	5.5
	d(N1–Si1–Si2–Si3)	152.1(2)	161.1	9
	d(N1–Si1–Si2–Si4)	-55.6(3)	-51.6	4
	d(N4–Si1–Si2–Si4)	135.3(3)	142.6	7.3
	θ(Silyl/NHI)	40.3/8.1	41.8/10.2	1.5/2.1
	τ	46.9	42.4	4.5

*the calculated structure has one negative frequency in line with thermal ellipsoids oriented out of plane
*[2]as the SC-XRD structure of **9** revealed different isomers concerning the orientation of the methyl group in Si^{t}Bu$_2$Me, only Part A is compared here; see the next page for the other isomers and corresponding discussion.

Calculated isomers for 9

Table S6: Different calculated isomers of **9** including their structural metrics.

Compound	**9**	**9^{I2}**	**9^{I3}**	**9^{I4}**
Corresponding to XRD part	A	B	C	–
Molecular structure (^{t}Bu groups depicted as wireframes)				
ΔG_{rel}*	0.0	+2.4	+1.3	+3.9
Bond length [Å], angles [°] and dihedreals [°] of the different isomers				
r(Si1–Si2)	2.24	2.26	2.23	2.26
r(Si1–N1/4)	1.66	1.67	1.67	1.67
r(Si2–Si3/Si4)	2.39/2.38	2.38/2.40	2.37	2.37/2.39
a(N1-Si1-N4)	110.1	111.3	110.9	110.6
a(Si3-Si2-Si4)	132.7	123.6	126.0	119.4
d(N1-Si1-Si2-Si3)	161.1	131.3	155.6	147.2
d(N1-Si1-Si2-Si4)	-51.6	-6.5	-54.9	-69.3
d(N4-Si1-Si2-Si4)	142.6	160.7	136.6	125.6
θ(Silyl/NHI)	41.8/10.2	44.2/9.3	31.6/8.3	34.2/10.7
τ	42.4	52.7	44.2	49.1

* obtained at the DLPNO-CCSD(T)/def2-TZVPP//B3LYP-D3/def2-SVP level of theory, referenced to **9**
Note: the calculated Isomers **9^{I2}** and **9^{I3}** show some deviation from XRD parts B and C (*trans*-bent angle), which can be compensated using a different level of theory (PBEh-3c). The results of PBEh-3c optimized structures coincide with the presented ones.

The disordered SC-XRD structure of **9** hinted towards different accessible isomers, which differ in the orientation of the methyl groups. Calculations on all parts contained in the XRD structure revealed Part A lowest in energy and the isomers **9^{I2}** and **9^{I3}**(Table S6), which are close in energy. Another possible isomer with both methyl groups pointing away from the central Si–Si bond **9^{I4}** is raised in energy. To not overcomplicate the discussion in the manuscript, only **9**, the isomer lowest in energy, is discussed there.

The calculated absorption band of **9** at 463 nm (see Table S7, next page) is decreased in comparison to the experimental value (490 nm, see Figure S44). We anticipate the connection to the different possible isomers, which agrees with the slight red shift of the HOMO→LUMO transition for the isomer **9^{I2}** (496 nm) and **9^{I3}** (511 nm)(Table S7). Interestingly, the calculated absorption band for **9^{I4}** (561 nm) (the isomer not present in the SC-XRD data) exhibits a significant red shift of the HOMO→LUMO transition, which renders this configuration unlikely to be present.

3.3 TD-DFT calculations

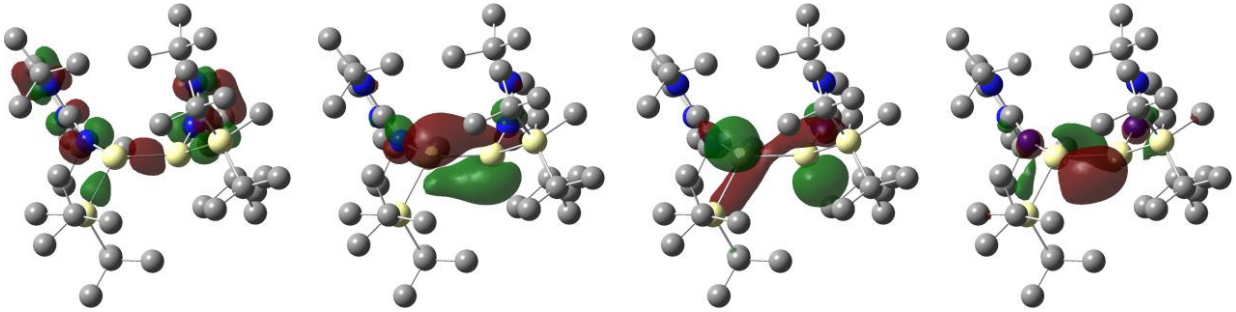
Calculated UV-vis absorption bands for 2-(*Z*), 2-(*E*) and 9

Table S7: Calculated transitions and UV-vis absorption bands using TD-DFT in Gaussian16 at the B3LYP-D3/def2-TZVP(SMD:n-hexane) level of theory for **2-(*Z*)**, **2-(*E*)** and **9** (including isomers $\mathbf{9^{I2}}$/$\mathbf{9^{I3}}$/$\mathbf{9^{I4}}$).

Compound	Wavelength [nm]	MO contributions	f	Contribution
2-(*Z*)	516	HOMO→LUMO	0.1907	92.0%
		HOMO→LUMO+1		7.0%
	438	HOMO-1→LUMO	0.0100	99.2%
	432	HOMO→LUMO	0.0689	6.6%
		HOMO→LUMO+1		90.1%
	372	HOMO-2→LUMO	0.0444	97.4%
	355	HOMO→LUMO+3	0.0101	96.3%
2-(*E*)	492	HOMO→LUMO	0.2571	98.5%
	422	HOMO→LUMO+1	0.0000	95.4%
	417	HOMO-1→LUMO	0.0000	98.0%
	374	HOMO-1→LUMO+2	0.0000	98.1%
	336	HOMO-2→LUMO	0.0207	91.8%
		HOMO→LUMO+3		4.9%
9	463	HOMO→LUMO	0.0868	96.4%
	362	HOMO→LUMO+1	0.0226	51.8%
		HOMO→LUMO+2		35.1%
		HOMO→LUMO+6		8.1%
	331	HOMO→LUMO+1	0.0155	39.0%
		HOMO→LUMO+2		32.1%
		HOMO→LUMO+5		9.5%
		HOMO→LUMO+6		8.3%
		HOMO→LUMO+10		7.4%
$\mathbf{9^{I2}}$	496	HOMO→LUMO	0.0806	97.5%
$\mathbf{9^{I3}}$	511	HOMO→LUMO	0.0711	97.3%
$\mathbf{9^{I4}}$	561	HOMO→LUMO	0.0542	98.0%
1/1'	682/661	HOMO→LUMO	0.0775/0.0971	95.0%/95.8%
		HOMO→LUMO+2		3.9%/3.7%

Orbitals involved in UV-vis transitions of 2-(*Z*), 2-(*E*) and 9

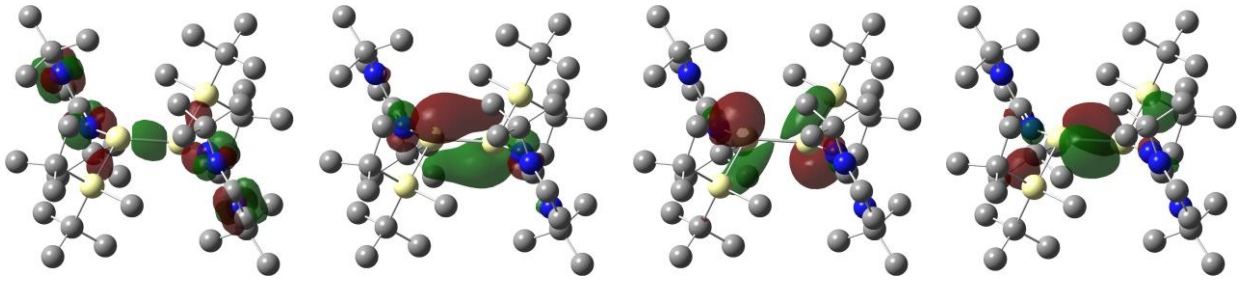
2-(*Z*):



HOMO–1 (–4.51 eV) HOMO (–3.62 eV) LUMO (–0.91 eV) LUMO+1 (0.15 eV)

Figure S52: Molecular orbitals of **2-(*Z*)**, obtained at the B3LYP-D3/def2-TZVP(SMD:n-hexane) level, isovalue 0.05.

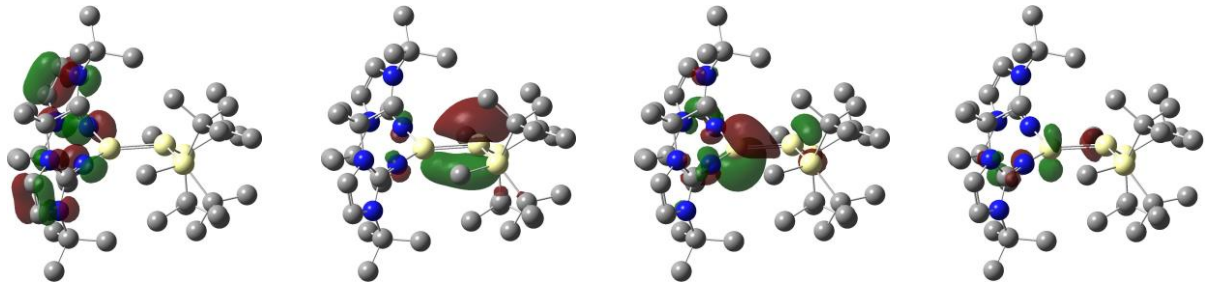
2-(*E*):



HOMO–1 (–4.50 eV) HOMO (–3.55 eV) LUMO (–0.74 eV) LUMO+1 (0.32 eV)

Figure S53: Molecular orbitals of **2-(*E*)**, obtained at the B3LYP-D3/def2-TZVP(SMD:n-hexane) level, isovalue 0.05.

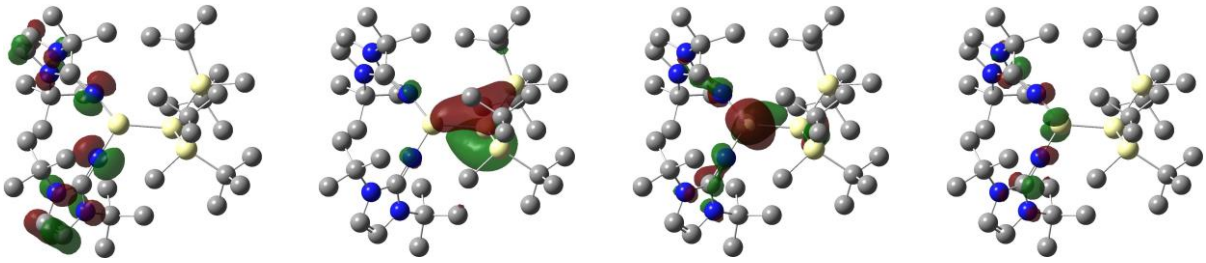
9:



HOMO–1 (–4.96 eV) HOMO (–3.75 eV) LUMO (–0.39 eV) LUMO+1 (0.56 eV)

Figure S54: Molecular orbitals of **9**, obtained at the B3LYP-D3/def2-TZVP(SMD:n-hexane) level, isovalue 0.05.

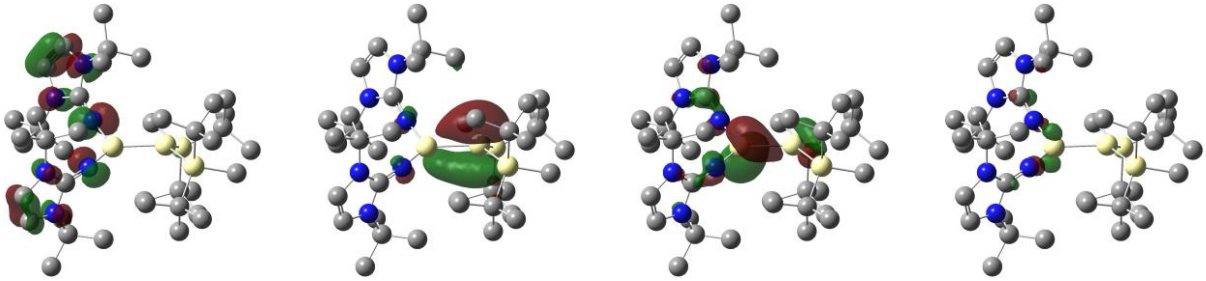
9^{I2}:



HOMO–1 (–4.95 eV) HOMO (–3.77 eV) LUMO (–0.57 eV) LUMO+1 (0.50 eV)

Figure S55: Molecular orbitals of **9^{I2}**, obtained at the B3LYP-D3/def2-TZVP(SMD:n-hexane) level, isovalue 0.05.

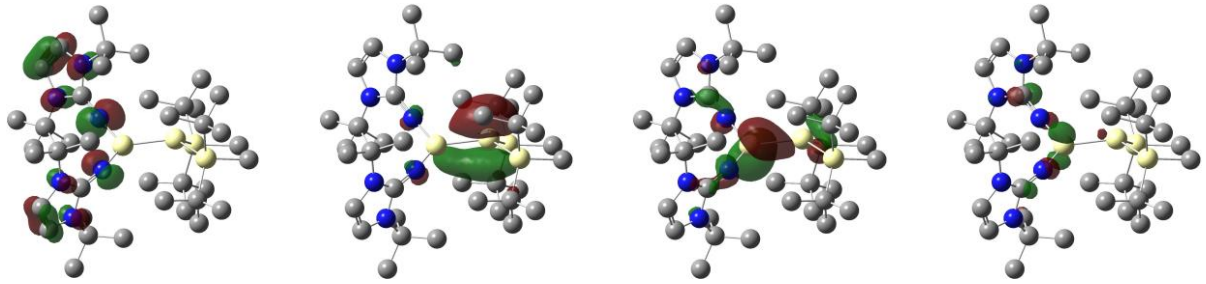
9^{I3}:



HOMO–1 (–4.93 eV) HOMO (–3.65 eV) LUMO (–0.51 eV) LUMO+1 (0.54 eV)

Figure S56: Molecular orbitals of **9^{I3}**, obtained at the B3LYP-D3/def2-TZVP(SMD:n-hexane) level, isovalue 0.05.

9^{I4}:



HOMO–1 (–4.96 eV) HOMO (–3.65 eV) LUMO (–0.70 eV) LUMO+1 (0.49 eV)

Figure S57: Molecular orbitals of **9^{I4}**, obtained at the B3LYP-D3/def2-TZVP(SMD:n-hexane) level, isovalue 0.05.

3.4 Mechanistic investigations for the 2-(*Z*)/2-(*E*) interconversion

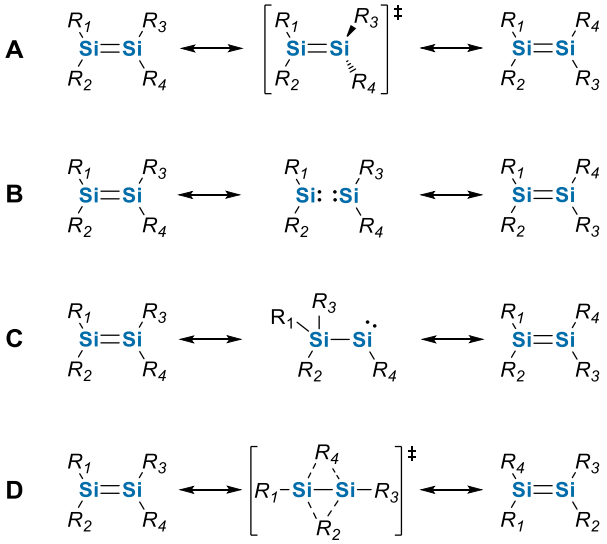


Figure S58: Possible isomerization pathways for Disilenes.

Pathway **A**:

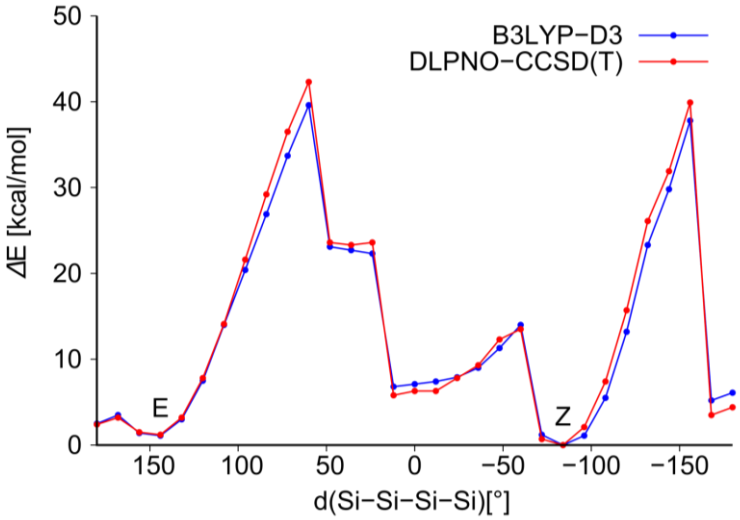


Figure S59: Relaxed PES Scan around the dihedral angle (Si3–Si1–Si2–Si4) of **2** with marked *E*/*Z* isomer.

Pathway **B**:

Table S8: Monomerization energies obtained at the DLPNO-CCSD(T)/def2-TZVPP//B3LYP-D3/def2-SVP level of theory; *** 1-(*E*)'**: optimized structure without imaginary frequency.

Compound	ΔG_{298} [kcal/mol]
2-(Z)/2-(E)	22.5
VI	7.9
1-(*E*)'*	8.8

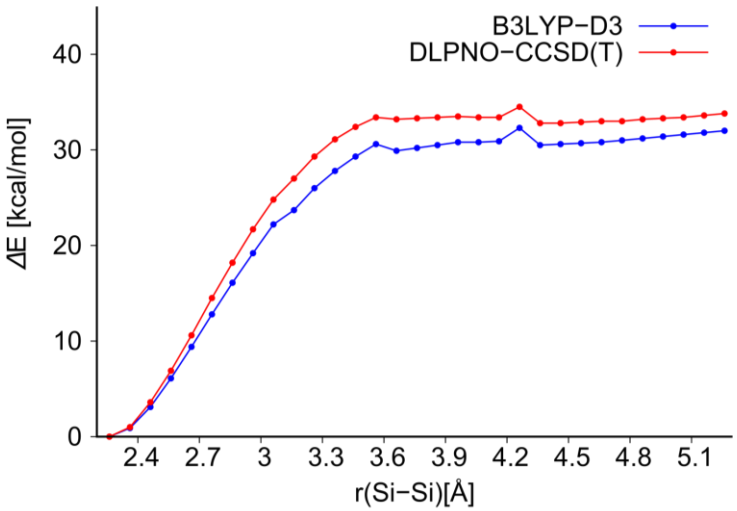
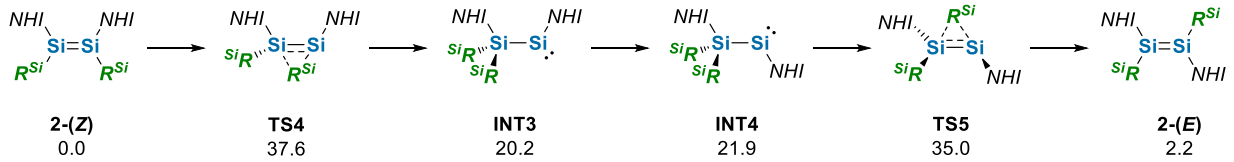


Figure S60: Relaxed PES-scan along the central Si1–Si2 bond.

Pathway **C**:



NHI = NI^{t}Bu
R^{Si} = Si^{t}Bu$_2$Me

Figure S61: Computed reaction pathway for the interconversion of **2-(*Z*)**/**2-(*E*)** via silyl-silylenes **INT3**/**INT4**.

Pathway **D**:

We have investigated the mechanistic route for the concerted dyotropic rearrangement (pathway **D**) as it had been concluded for aryl-substituted disilenes,[S50] but we couldn't determine a suitable transition state accessible in energy. We attribute this to the steric demand of the ligands as the *tert*-butyl groups of the imino and the silyl ligands do not allow to access the spatial arrangement for a concerted transition state in pathway **D**.

Energy difference between *Z*/*E* isomer for the different disilenes:

Table S9: Energy differences between the *Z*/*E* isomers for the different disilenes (**1**, **2** and **VI**) and resulting ratio at room temperature, obtained at the DLPNO-CCSD(T)/def2-TZVPP//B3LYP-D3/def2-SVP level of theory

Compound	ΔG_{298} [kcal/mol]	Z [%]	E [%]
1	-3.7	0.2	99.8
2	+2.2	97.7	2.3
VI*	+1.8*	95.3*	4.7*

*the DLPNO-CCSD(T)/def2-TZVPP//B3LYP-D3/def2-SVP level of theory does not coincide with the experimental und theoretical results reported for **VI** previously [S3]

3.5 EDA of 2-(*Z*) and 2-(*E*)

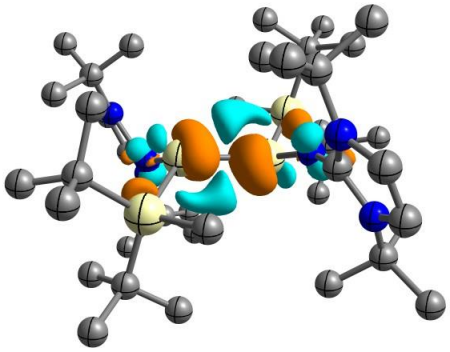
We chose to perform the EDA-NOVC of the disilenes with respect to the singlet fragments.[S51-53] We note, however, that the fragmentation into the respective triplet silylenes yields less negative ΔE_{orb} contributions, which is recommended by Zhao *et al.,*[S54] but results in a much higher preparation energy. Factors contributing to the relative stability of **2-(*Z*)** (Table S10):

- The steric energy (sum of Pauli repulsion and electrostatic attraction) is lower for **2-(*Z*)**
- The dispersion interaction for **2-(*Z*)** is roughly 3 kcal/mol higher.
- The orbital interaction (mainly the first deformation density, see Figure S62) is higher in **2-(*E*)**, presumable due to the absence of twisting and a shortened bond length in comparison to **2-(*Z*)**.
- The interaction energy of **2-(*E*)** is slightly higher, but a significantly lower preparation energy (solely connected to geometry, as the fragments are already in their "relaxed" electronic singlet configuration) leads to an overall higher dissociation energy of **2-(*Z*)**.
- The geometric preparation energy is directly linked to the interligand angle (a(Si^{Silyl}–$Si^{central}$–N^{NHI})): **2-(*E*)** (112.5 °) > **2-(*Z*)** (104.6 °) > monomer $\mathbf{2^M}$ (99.1 °). The free silylenes need less geometric distortion to form the *Z* isomer, which lowers its relative energy compared to *E*

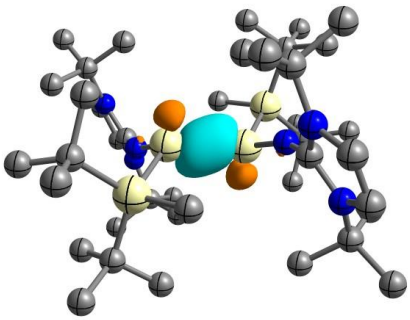
Table S10: Energy decomposition analysis of disilenes **2-(*E*)** and **2-(*Z*)**, energies in kcal/mol

Energy [kcal/mol]	2-(*E*)	2-(*Z*)
ΔE_{Pauli}	299.8	286.7
ΔE_{elstat}	–171.4	–161.0
ΔE_{steric}	128.4	125.6
ΔE_{orb}	–155.5	–148.1
ΔE_{disp}	–26.2	–29.0
ΔE_{int}	–53.3	–51.5
ΔE_{prep}	15.4	9.4
D_e	37.9	42.1

The two respective NOCV deformation densities with the highest NOCV eigenvalues are shown in Figure S62 and Figure S63. They are qualitatively equivalent for disilenes **2-(*E*)** and **2-(*Z*)**. The first deformation density $\Delta\rho_1$ shows the mutual donation from the sp-type lone pairs into the opposite p-type acceptor orbitals (π-type). The second deformation density $\Delta\rho_2$ shows further accumulation of σ-type charge density between the silicon centers.



$\Delta E_1 = -112.3$
$|v_1| = 1.36$



$\Delta E_2 = -32.2$
$|v_2| = 0.60$

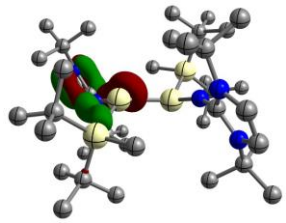
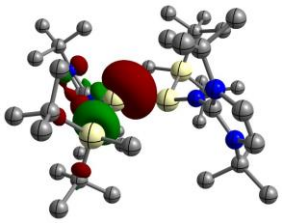
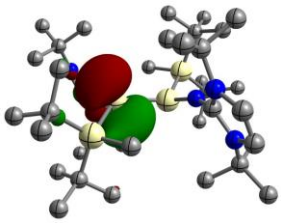
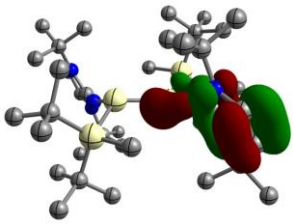
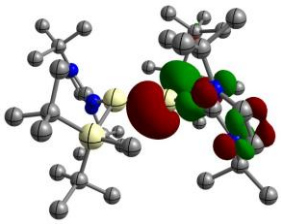
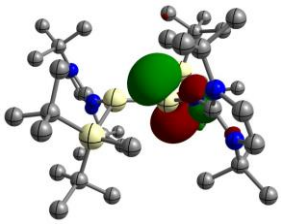
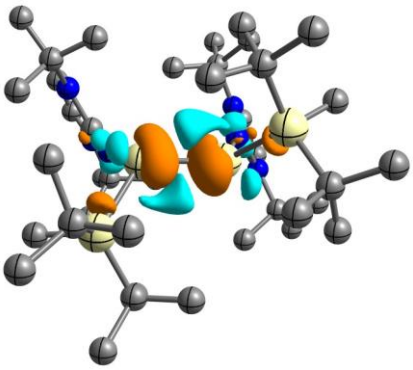
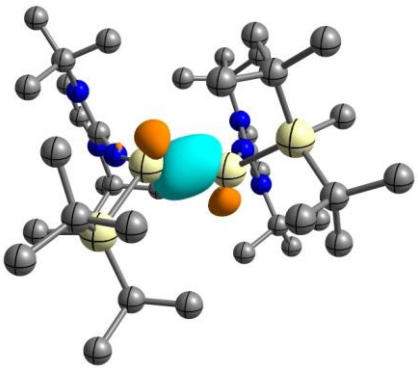
HOMO–1	HOMO	LUMO
		
		
$v_1 = -0.08$ $v_2 = -0.01$	$v_1 = -0.43$ $v_2 = -0.14$	$v_1 = 0.61$ $v_2 = 0.08$

Figure S62: First (left) and second (right) deformation densities of disilene **2-(*E*)**; charge depletion in orange, charge accumulation in light blue; orbital interaction energies Δ*E* in kcal/mol and charge eigenvalues v as quantification for the charge transfer between donor (negative values) and acceptor (positive numbers) fragments (in e) for the involved fragment orbitals; isovalue = 0.005 a_0^{-3}.

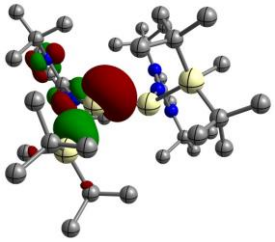


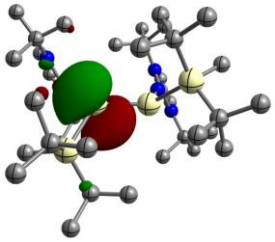
ΔE_1 = –103.7
$|v_1|$ = 1.30

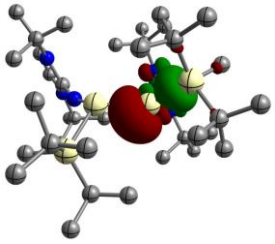


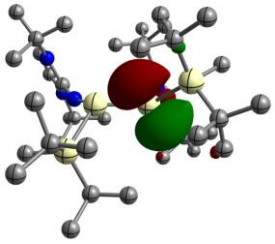
ΔE_2 = –32.8
$|v_2|$ = 0.62

HOMO	LUMO









v_1 = –0.41
v_2 = –0.15

v_1 = 0.60
v_2 = 0.10

Figure S63: First (left) and second (right) deformation densities of disilene **2-(*Z*)**; charge depletion in orange, charge accumulation in light blue; orbital interaction energies Δ*E* in kcal/mol and charge eigenvalues v as quantification for the charge transfer between donor (negative values) and acceptor (positive numbers) fragments (in e) for the involved fragment orbitals; isovalue = 0.005 a_0^{-3}.

3.6 LED of 2-(*Z*) and 2-(*E*)

To investigate the differences of the dispersion interaction for **2-(*Z*)**/**2-(*E*)** in more detail, we performed Local Energy Decomposition (LED)[S55] analysis on the DLPNO-CCSD(T)/def2-TZVPP (RIJCOSX with GridX4,[S56] NormalPNO, VeryTightSCF) level of theory with respect to two interacting silylene fragments. Since this fragmentation scheme cuts through a covalent (double) bond, the Foster-Boys orbitals corresponding to the central Si=Si double bond have similar populations on both fragments.[S57] This results in an arbitrary assignment of the electrons to either one of the fragments leading to large electrostatic and exchange interactions. The LED dispersion energy can, however, be corrected according to Lu, Neese and Bistoni:[S58] We deleted the inter-fragment strong pair dispersive contributions (dipol-dipol & cross excitations) involving the critical PNOs of the central Si=Si double bond. This resulted in an almost similar reduction of the computed dispersion energy by 13.5 kcal/mol and 13.8 kcal/mol for **2-(*E*)** and **2-(*Z*)**, respectively. The corrected LED dispersion energies align well with the dispersion energy obtained by Grimme's empirical D3 model within the EDA-NOCV at the B3LYP-D3/TZ2P//B3LYP-D3/def2-SVP level of theory (Table S11).

Table S11: Comparison of the dispersion energies obtained from EDA and LED.

ΔE_{disp} [kcal/mol]	2-(*E*)	2-(*Z*)
Grimme's D3 model	26.2	29.0
LED corrected	25.9	28.9
LED uncorrected	39.4	42.7

A recent contribution by Mata and Wuttke[S59] offers the possibility to evaluate the dispersion interactions obtained within LED analysis in a more intuitive way: a graphical representation of the dispersion interaction density (DID). The DID is mapped onto the isosurface of molecular electron density and hence gives a more intuitive visualization of London dispersion interactions. The graphical results for the dispersion interaction density of **2-(*Z*)** and **2-(*E*)** are given in Figure S64, where increased interaction is connected with red coloring and zero interaction represented in blue. As results of the Me group of Si^{t}Bu$_2$Me pointing towards the double bond, the dispersion interaction in **2-(*E*)** is dominated by interactions between the Me groups of the silyl ligand and the ^{t}Bu groups of the NHI ligand. Interaction between the ^{t}Bu groups of the NHI and the silyl group is less pronounced due to increased spatial distance. By contrast, the Me groups in **2-(*Z*)** point away from the Si=Si bond, which yields a spatial approach of the ^{t}Bu of NHI and silyl group. This yields an increased dispersion interaction between the ^{t}Bu groups of the NHI and the silyl groups of both silylene fragments in comparison to **2-(*E*)**.

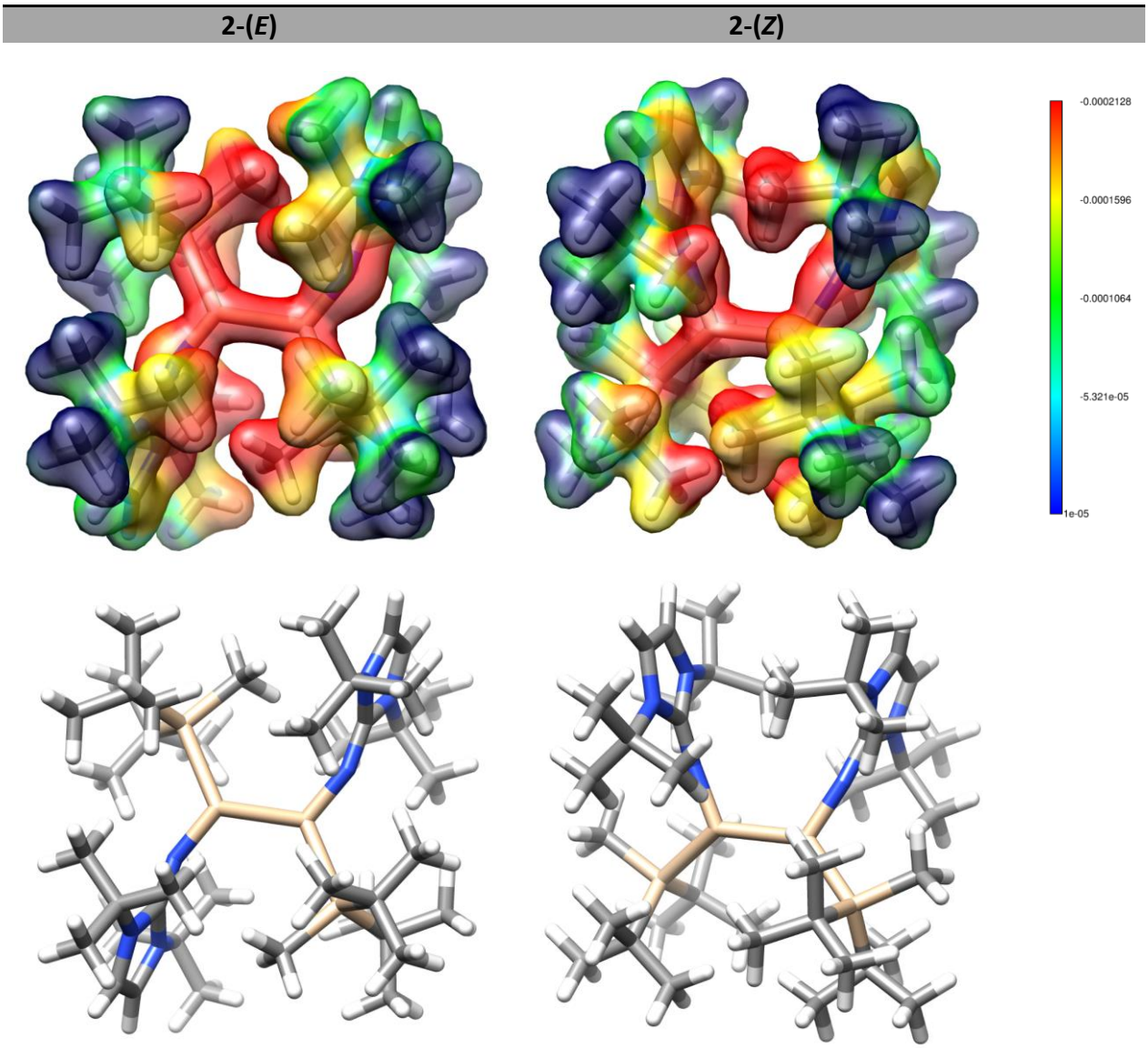


Figure S64: Projected DID plots (top) considering the monomeric silylenes as the interacting fragments and molecular structure in same orientation (bottom) for **2-(*Z*)/(*E*)**. Molecular density isosurfaces were generated at an isovalue of 0.05. DID color scheme ranges from highest value (red) to zero interaction energy (blue).

Note: As stated above LED analysis utilizes the Foster-Boys localization method. This is problematic in the case of two interaction silylene fragments as the electrons in the Foster-Boys orbitals for the Si–Si bond are assigned rather randomly to silylene fragment 1 or 2. This can be corrected for the dispersion energy term according to Lu, Neese and Bistoni[S58] but it is not possible for the projected DID plots. As a direct result, the central Si=Si bond is marked red in Figure S64. However, this is the case in a comparable manner for both isomers of disilene **2**, hence evaluation of the projected DID plots is possible on a comparative scale for the interaction between the two fragments beside the central Si=Si bond.

3.7 H_2 activation

We further investigated the H_2 activation by disilene **2-(*Z*)**. The results are summarized in Figure S65. In line with the previous report for H_2 activation by disilene **VI**,[S3] the energetically preferred pathway proceeds via a concerted transition state at the disilene via **TS2H$_2$** with the lowest barrier of 24.8 kcal/mol. Reaction of the monomeric silylene in **TS2^{M}H$_2$** or **TS2^{M}H$_2$'** is disfavored, which is in line with a reported experiment: addition of ^{t}Bu$_2$SiSiH$_2$ to disilene **VI** did not show any reaction.[S3] Hence, the pathway via **TSINT2^M** can be excluded. Moreover, the formation of a silyl-silylene via NHI or silyl migration is connected with a barrier of 37.6/34.7 kcal/mol (Figure S61, Figure S69 and Figure S70). Hence, H_2 activation via a silyl-silylene can be excluded based on the results for the isomerization reactions.

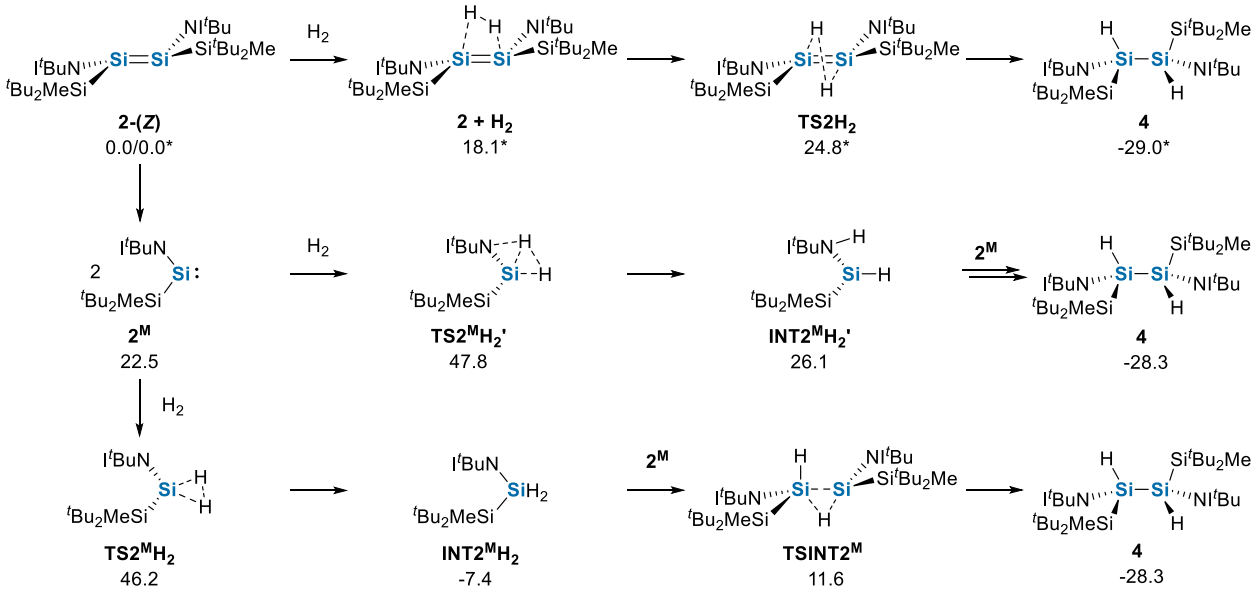


Figure S65: Calculated pathways for the H_2 activation by **2-(*Z*)**, energy values in kcal/mol. Unfortunately, we were not able to detect the transition state **TS2H$_2$** at the B3LYP-D3/ def2-SVP level of theory. However, the transition state was found using the PBEh-3c[S60] level of theory. Energy values marked with * were obtained at the DLPNO-CCSD(T)/def2-TZVPP//PBEh-3c level of theory.

Further interested in the orbital interactions involved in **TS2H$_2$**, we performed NBO calculations at the M06-2X/6-311++G(2d,2p) level of theory (Figure S66). Accordingly, the dominant interactions are π(Si1–Si2) to σ*(H–H) and σ(H–H) to π*(Si1–Si2) electron donations. However, there is a significant contribution of electron donation from σ(H–H) to σ*(Si1/2–N1/N4). As those interactions are present on both sides of the disilene, the H–H bond is not polarized according to NPA.

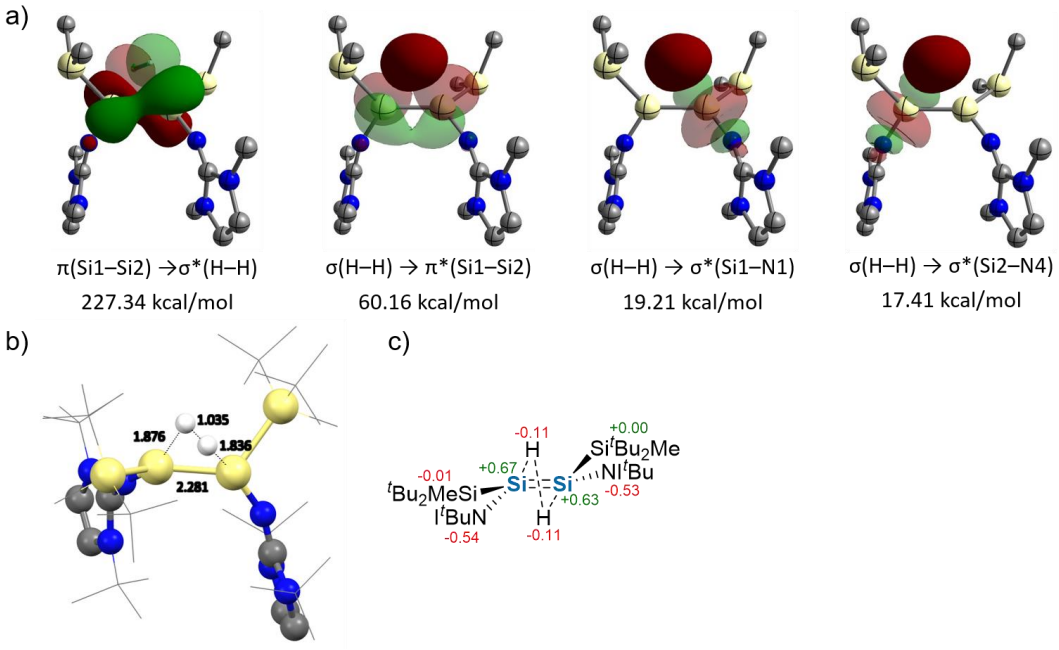
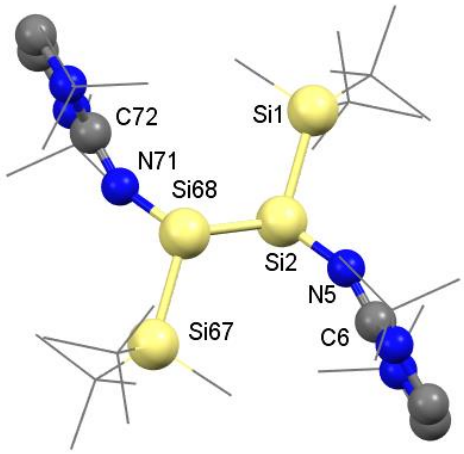


Figure S66: Selected results of the NBO analysis of **TS2H$_2$** at the M06-2X/6-311++G(2d,2p) level of theory. (a) dominant NBO interactions (occupied NBOs solid, vacant NBOs faded) and corresponding perturbative interaction energies, (b) molecular connectivity and (c) NPA group charges (red negative, green positive).

3.8 Radical cation 7

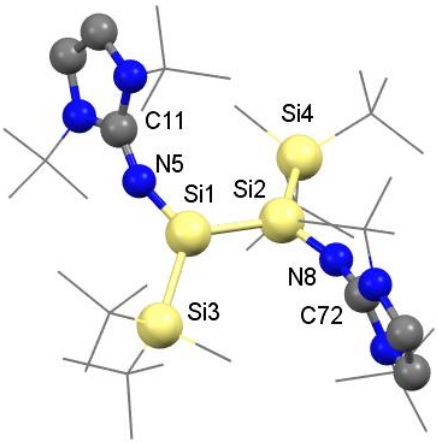
Calculated structure of 2-(*E*)



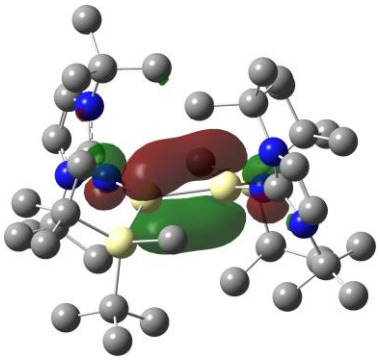
Bond/Angle	Calc. [Å/°]
r(Si2–Si68)	2.26
r(Si2/69–N5/71)	1.70
r(Si2/68–Si1/67)	2.39
r(N5/71–C6/72)	1.28
a(N5/71–Si2/68–Si1/67)	112.5
d(Si1–Si2–Si68–Si67)	180.0
d(Si1–Si2–Si68–N71)	42.2
θ	35.2
τ	0.0

Figure S67: Calculated structure of **2-(*E*)** including selected bond length and angles; obtained at the B3LYP-D3/def2-SVP level of theory.

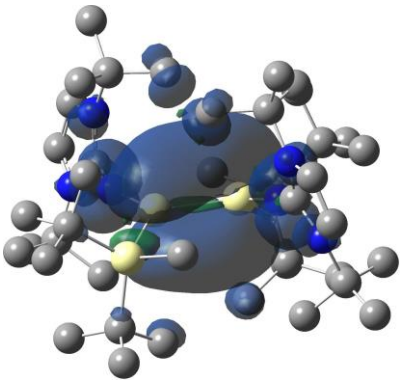
Radical Cation 7



Bond/Angle	Calc. [Å/°]
r(Si1–Si2)	2.29
r(Si1/2–N5/8)	1.65
r(Si1/2–Si3/4)	2.38
r(N5/8–C11/72)	1.30
a(N5/8–Si1/2–Si3/4)	120.1
d(Si3–Si1–Si2–Si4)	146.6
d(Si3–Si1–Si2–N8)	–27.4
θ	5.3/5.1
τ	29.2



SOMO



spin density

Figure S68: Calculated structure of **7** including selected bond length and angles, SOMO and spin density; obtained at the B3LYP-D3/def2-SVP level of theory.

3.9 Mechanistic investigations for the 2-(*Z*)/9 interconversion

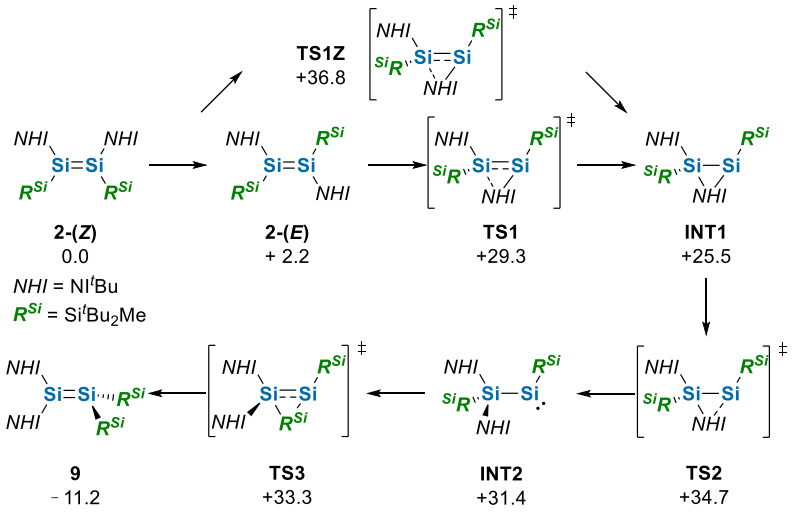


Figure S69: Computed reaction pathway for the interconversion of **2-(*Z*)**/**2-(*E*)** to **9** via initial NHI shift followed by shift of the silyl group, the alternative NHI migration starting from the Z isomer in **TS1Z** is located higher in energy.

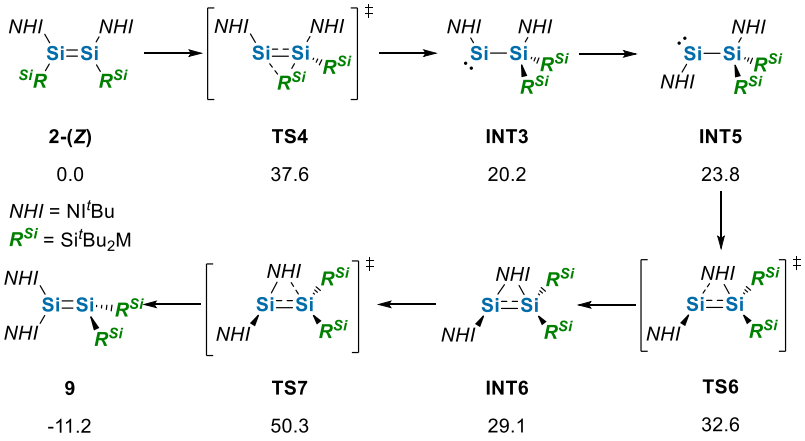


Figure S70: Computed reaction pathway for the interconversion of **2-(*Z*)**/**2-(*E*)** to **9** via initial silyl shift followed by shift of the NHI ligand.

3.10 NBO analysis

NBO analysis of disilene 9

Table S12: Selected results of the NBO analysis of **9**.

Bond	NPA charge	NBO analysis (NLMOs)			NPA analysis	
		Pol.	Hybr.	WBI	Fragment	NPA Charge [e]
σ(Si1–Si2)	+1.77 (Si1)	45% (Si1) 52% (Si2)	$sp^{0.52}$ (Si1) $sp^{2.10}$ (Si2)	1.33	**NHI**	–0.57/–0.56
π(Si1–Si2)	–0.77 (Si2)	19% (Si1) 73% (Si2)	$sp^{9.47}$ (Si1) $sp^{8.97}$ (Si2)	1.33	**$Si(NHI)_2$**	+0.64
Si1–N1	–1.26 (N1)	14% (Si1) 85% (N1)	$sp^{1.59}$ (Si1) $sp^{0.95}$ (N1)	0.65	**Si^tBu_2Me**	+0.06/+0.07
Si1–N4	–1.25 (N4)	14% (Si1) 85% (N4)	$sp^{1.59}$ (Si1) $sp^{0.95}$ (N4)	0.65	**$Si(Si^tBu_2Me)_2$**	–0.64
Si2–Si3	+1.55 (Si3)	54% (Si2) 43% (Si3)	$sp^{1.96}$ (Si2) $sp^{1.42}$ (Si3)	0.97		
Si2–Si4	+1.60 (Si4)	55% (Si2) 41% (Si4)	$sp^{1.69}$ (Si2) $sp^{1.36}$ (Si4)	0.96		
LP(N1)	–	88% (N1) 4% (Si1) 4% (C1)	p (N1) p (Si1) p (C1)	–		
LP(N4)	–	88% (N4) 5% (Si1) 4% (C12)	p (N4) p (Si1) p (C12)	–		

Pol. = polarization, Hybr. = hybridization, WBI = Wiberg bond index;
NBO analysis of the other isomers $\mathbf{9^{I2}}$/$\mathbf{9^{I3}}$ coincide with the values of **9**.

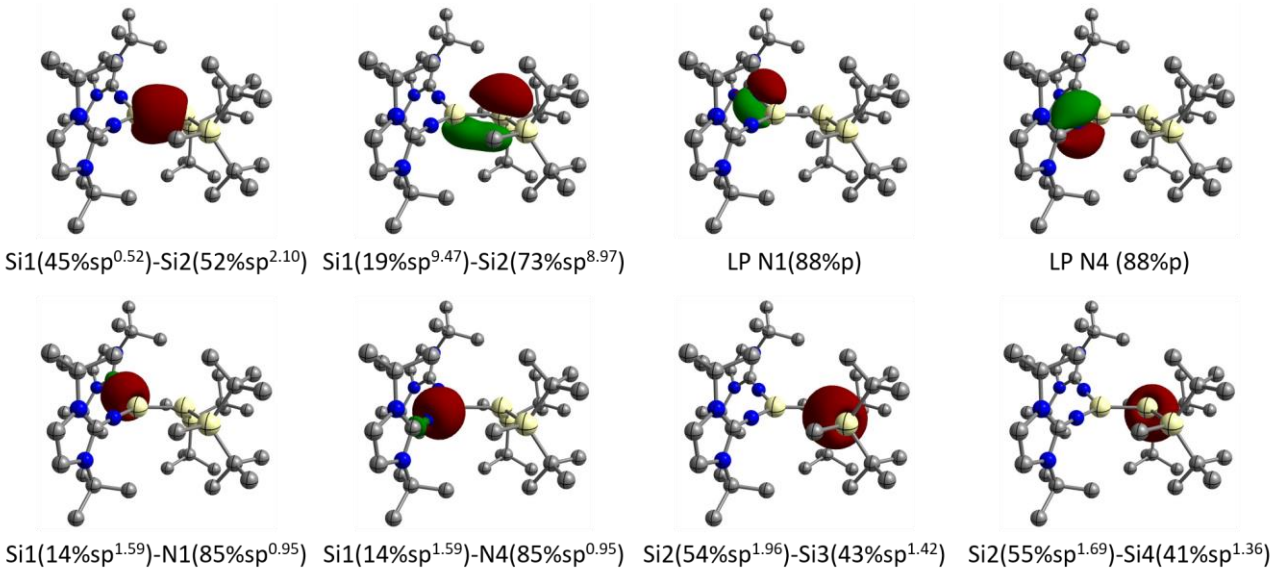


Figure S71: Selected NLMOs of **9**.

NBO analysis of disilene 2-(*Z*)

Table S13: Selected results of the NBO analysis of **2-(*Z*)**.

Bond		NBO analysis (NLMOs)			NPA analysis	
	NPA charge	Pol.	Hybr.	WBI	Fragment	NPA Charge [e]
σ(Si1–Si2)	+0.58 (Si1)	48% (Si1) 48% (Si2)	$sp^{0.98}$ (Si1) $sp^{0.96}$ (Si2)	1.43	**Si central**	+0.58/+0.61
π(Si1–Si2)	+0.61 (Si2)	47% (Si1) 46% (Si2)	$sp^{3.88}$ (Si1) $sp^{3.90}$ (Si2)	1.43	**NHI**	–0.55/–0.56
Si1–N1	–1.18 (N1)	16% (Si1) 83% (N1)	$sp^{2.77}$ (Si1) $sp^{1.15}$ (N1)	0.70	**Si^{t}Bu$_2$Me**	–0.04/–0.04
Si2–N4	–1.18 (N4)	16% (Si2) 83% (N4)	$sp^{2.82}$ (Si2) $sp^{1.15}$ (N4)	0.70	**Si(Si^{t}Bu$_2$Me)(NHI)**	–0.02/+0.02
Si1–Si3	+1.41 (Si3)	48% (Si1) 49% (Si3)	$sp^{1.43}$ (Si1) $sp^{1.59}$ (Si3)	0.90		
Si2–Si4	+1.41 (Si4)	48% (Si2) 49% (Si4)	$sp^{1.41}$ (Si2) $sp^{1.59}$ (Si4)	0.90		
LP(N1)	–	87% (N1) 4% (C1) 3% (Si1)	$sp^{14.70}$ (N1) p (C1) p (Si1)	–		
LP(N4)	–	88% (N4) 4% (C21) 3% (Si2)	$sp^{14.68}$ (N4) p (C21) p (Si2)	–		

Pol. = polarization, Hybr. = hybridization, WBI = Wiberg bond index.

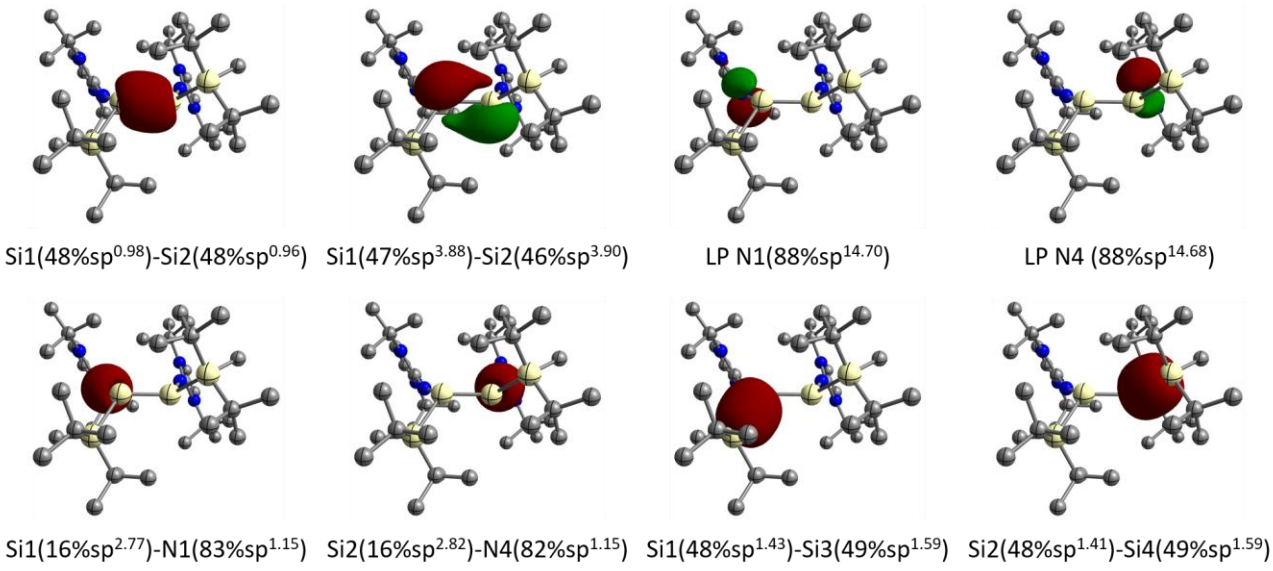


Figure S72: Selected NLMOs of **2-(*Z*)**.

NBO analysis of disilene 2-(*E*)

Table S14: Selected results of the NBO analysis of **2-(*E*)**.

Bond	NBO analysis (NLMOs)				NPA analysis	
	NPA charge	Pol.	Hybr.	WBI	Fragment	NPA Charge [e]
σ(Si1–Si2)	+0.59 (Si1)	48% (Si1) 48% (Si2)	$sp^{1.02}$ (Si1) $sp^{1.02}$ (Si2)	1.44	**Si central**	+0.59
π(Si1–Si2)	+0.59 (Si2)	46% (Si1) 46% (Si2)	$sp^{5.41}$ (Si1) $sp^{5.41}$ (Si2)	1.44	**NHI**	–0.54/–0.54
Si1–N1	–1.17 (N1)	17% (Si1) 82% (N1)	$sp^{2.65}$ (Si1) $sp^{0.99}$ (N1)	0.71	**Si^{t}Bu$_2$Me**	–0.05/–0.05
Si2–N4	–1.17 (N4)	17% (Si2) 82% (N4)	$sp^{2.65}$ (Si2) $sp^{0.99}$ (N4)	0.71	**Si(Si^{t}Bu$_2$Me)(NHI)**	0.00
Si1–Si3	+1.41 (Si3)	48% (Si1) 49% (Si3)	$sp^{1.41}$ (Si1) $sp^{1.55}$ (Si3)	0.92		
Si2–Si4	+1.41 (Si4)	48% (Si2) 49% (Si4)	$sp^{1.41}$ (Si2) $sp^{1.55}$ (Si4)	0.92		
LP(N1)	–	87% (N1) 4% (C1) 3% (Si1)	p (N1) p (C1) p (Si1)	–		
LP(N4)	–	87% (N4) 4% (C1) 3% (Si1)	p (N4) p (C1) p (Si1)	–		

Pol. = polarization, Hybr. = hybridization, WBI = Wiberg bond index.

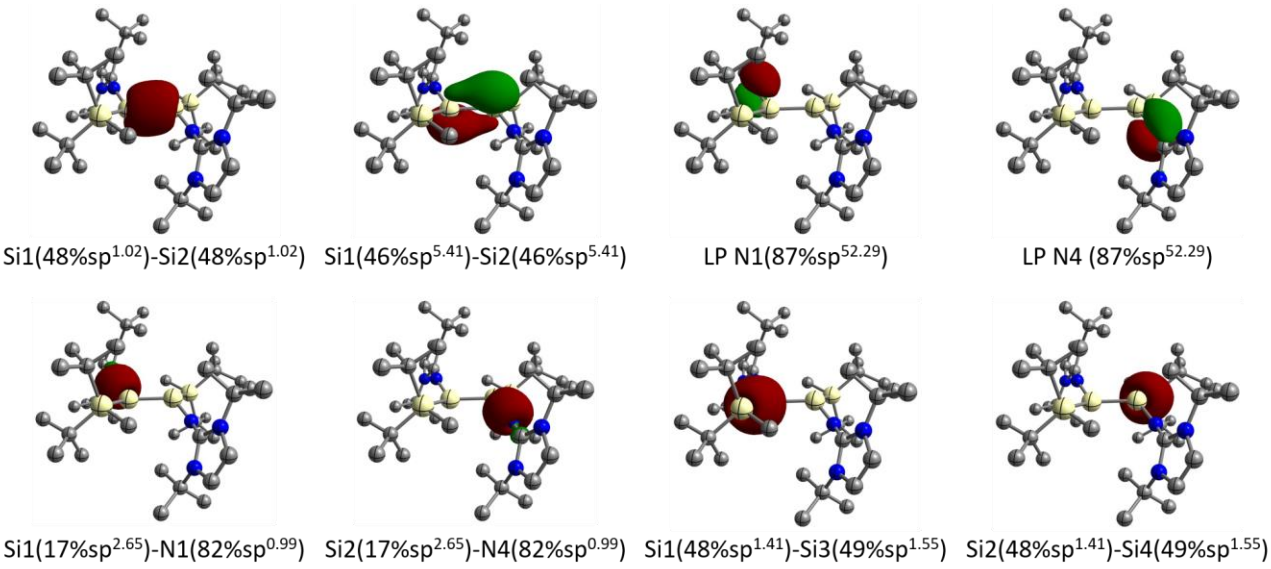


Figure S73: Selected NLMOs of **2-(*E*)**.

NBO analysis of disilene 1-(*E*)

Table S15: Selected results of the NBO analysis of **1-(*E*)**.

Bond	NBO analysis (NLMOs)				NPA analysis	
	NPA charge	Pol.	Hybr.	WBI	Fragment	NPA Charge [e]
σ(Si1–Si1')	+0.55 (Si1)	49% (Si1) 49% (Si1')	$sp^{1.09}$ (Si1) $sp^{1.09}$ (Si1')	1.54	**Si central**	+0.55/+0.55
π(Si1–Si1')	+0.55 (Si1')	45% (Si1) 45% (Si1')	$sp^{99.99}$ (Si1) $sp^{99.99}$ (Si1')	1.54	**NHI**	–0.58/–0.58
Si1–N1	–1.20 (N1)	16% (Si1) 82% (N1)	$sp^{2.28}$ (Si1) $sp^{1.26}$ (N1)	0.68	**Si^{t}Bu$_3$**	+0.04/+0.04
Si1'–N1'	–1.20 (N1')	16% (Si1') 82% (N1')	$sp^{2.28}$ (Si1') $sp^{1.26}$ (N1')	0.68	**Si(Si^{t}Bu$_3$)(NHI)**	0.00
Si1–Si2	+1.67 (Si2)	52% (Si1) 44% (Si2)	$sp^{1.21}$ (Si1) $sp^{1.38}$ (Si2)	0.89		
Si1'–Si2'	+1.67 (Si2')	52% (Si1') 44% (Si2')	$sp^{1.21}$ (Si1') $sp^{1.38}$ (Si2')	0.89		
LP(N1)	–	89% (N1) 4% (C1) 2% (Si1)	$sp^{9.92}$ (N1) p (C1) p (Si1)	–		
LP(N1')	–	89% (N1') 4% (C1') 2% (Si1')	$sp^{9.92}$ (N1') p (C1') p (Si1')	–		

Pol. = polarization, Hybr. = hybridization, WBI = Wiberg bond index.

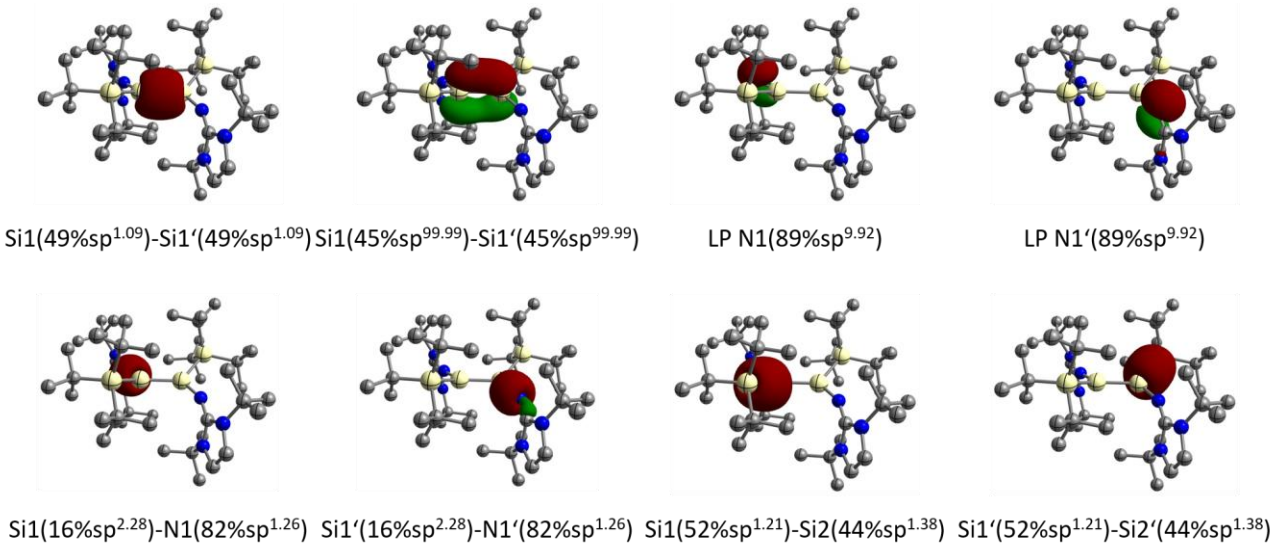


Figure S74: Selected NLMOs of **1-(*E*)**.

3.11 QTAIM analysis

QTAIM Analysis of 9

Table S16: Selected properties of the electron density distribution of the central Si–Si, Si–N and Si–Si^{Silyl} bonds in **9**: Bond path lengths $d_{A–B}$, the electron density ρ_{bcp}, the Laplacian of the electron density $\nabla^2\rho_{bcp}$, the total energy density H_{bcp}, the bond ellipticity $\varepsilon_{bcp} = \lambda_1/\lambda_2 - 1$ (derived from the two negative eigenvalues of the Hessian matrix of the electron density at the bcp with $\lambda_1 \geq \lambda_2$), delocalization index $\delta_{A,B}$.

Bond	$d_{A–B}$ [Å]	ρ_{bcp} [eÅ^{-3}]	$\nabla^2\rho_{bcp}$ [eÅ^{-5}]	H_{bcp} [E$_h$Å^{-3}]	ε_{bcp}	$\delta_{A,B}$
Si1Si2	2.24	0.59	–1.64	–0.37	0.57	1.12
Si1N1	1.66	0.93	17.16	–0.46	0.13	0.61
Si2Si4	2.38	0.54	–2.29	–0.22	0.12	0.79

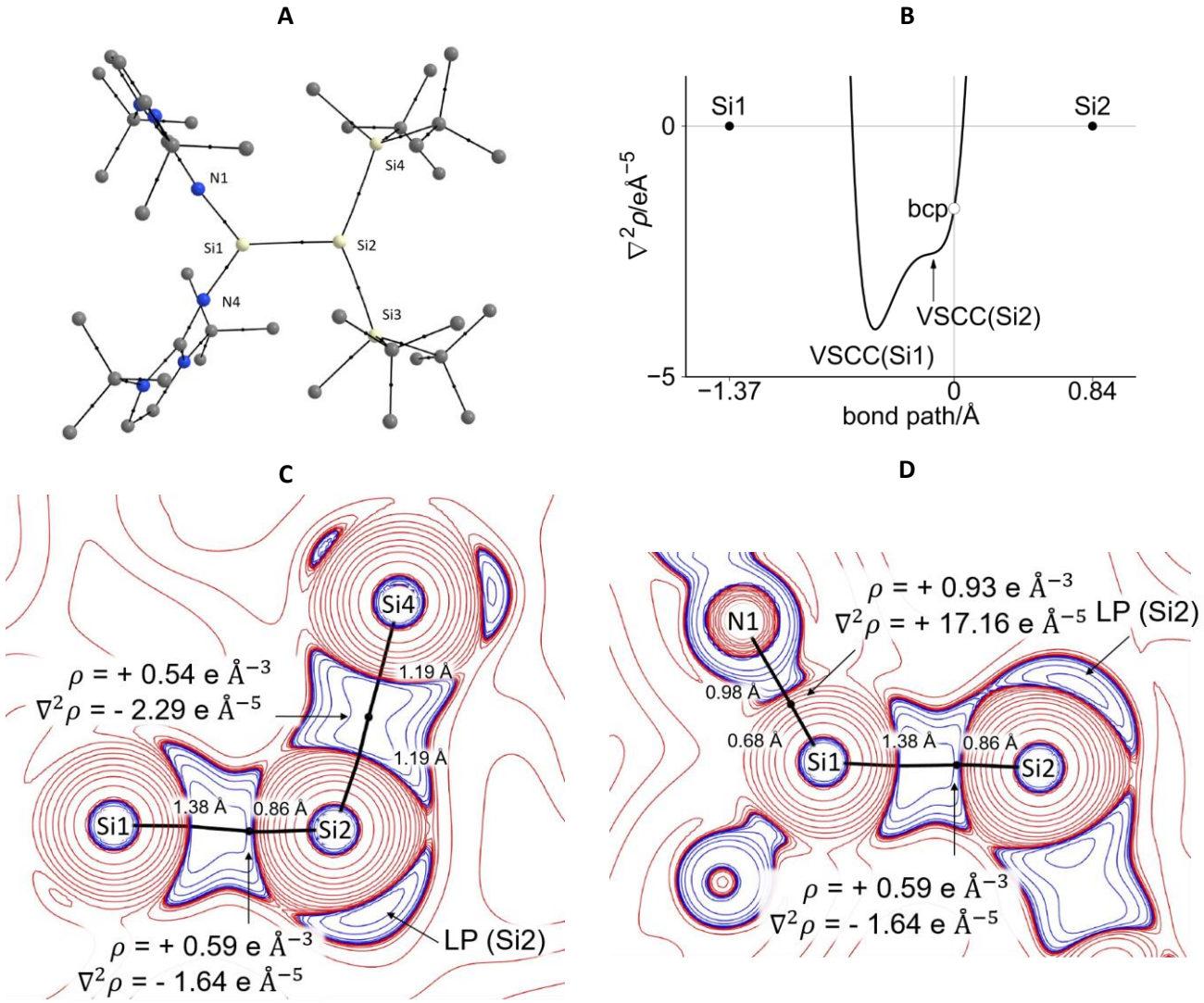


Figure S75: QTAIM Analysis of **9**. (**A**) Molecular graph (**B**) 1D Laplacian profile along the Si1–Si2 bond path (**C**, **D**) 2D plot of $\nabla^2\rho$(r); charge concentration (blue) and depletion (red), bond paths (black lines) and bond-critical points (bcps; black dots) with characteristic properties of the Si1–Si2, Si1-N1 and Si2–Si4 bonds.

QTAIM Analysis of 2-(*Z*)

Table S17: Selected properties of the electron density distribution of the central Si–Si, Si–N and Si–Si^{Silyl} bonds in **2-(*Z*)**: Bond path lengths d_{A-B}, the electron density ρ_{bcp}, the Laplacian of the electron density $\nabla^2\rho_{bcp}$, the total energy density H_{bcp}, the bond ellipticity $\varepsilon_{bcp} = \lambda_1/\lambda_2 - 1$ (derived from the two negative eigenvalues of the Hessian matrix of the electron density at the bcp with $\lambda_1 \geq \lambda_2$), delocalization index $\delta_{A,B}$.

Bond	d_{A-B} [Å]	ρ_{bcp} [eÅ^{-3}]	$\nabla^2\rho_{bcp}$ [eÅ^{-5}]	H_{bcp} [E$_h$Å^{-3}]	ε_{bcp}	$\delta_{A,B}$
Si1Si2	2.28	0.58	–2.39	–0.26	0.48	1.12
Si1N1	1.70	0.85	14.76	–0.41	0.07	0.71
Si1Si3	2.41	0.55	–2.56	–0.23	0.08	0.72

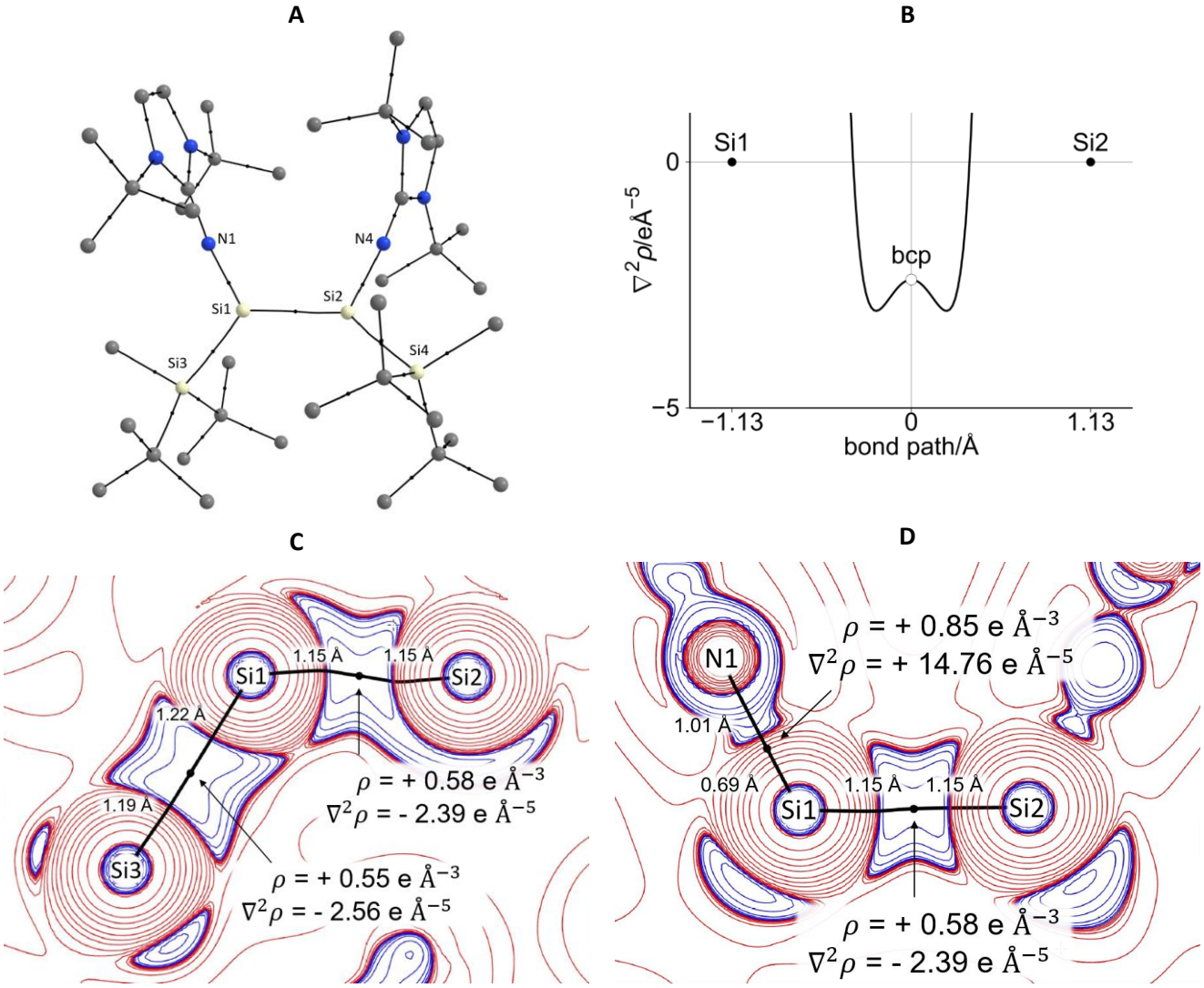


Figure S76: QTAIM Analysis of ***2-(Z)***. (**A**) Molecular graph (**B**) 1D Laplacian profile along the Si1–Si2 bond path (**C**, **D**) 2D plot of $\nabla^2\rho$(r); charge concentration (blue) and depletion (red), bond paths (black lines) and bond-critical points (bcps; black dots) with characteristic properties of the Si1–Si2, Si1-N1 and Si1–Si3 bonds.

QTAIM Analysis of 2-(*E*)

Table S18: Selected properties of the electron density distribution of the central Si–Si, Si–N and Si–Si^{Silyl} bonds in **2-(*E*)**: Bond path lengths d_{A-B}, the electron density ρ_{bcp}, the Laplacian of the electron density $\nabla^2\rho_{bcp}$, the total energy density H_{bcp}, the bond ellipticity $\varepsilon_{bcp} = \lambda_1/\lambda_2 - 1$ (derived from the two negative eigenvalues of the Hessian matrix of the electron density at the bcp with $\lambda_1 \geq \lambda_2$), delocalization index $\delta_{A,B}$.

Bond	d_{A-B} [Å]	ρ_{bcp} [eÅ^{-3}]	$\nabla^2\rho_{bcp}$ [eÅ^{-5}]	H_{bcp} [E$_h$Å^{-3}]	ε_{bcp}	$\delta_{A,B}$
Si1Si2	2.26	0.59	–2.53	–0.28	0.52	1.15
Si1N1	1.70	0.86	14.87	–0.41	0.09	0.71
Si1Si3	2.39	0.57	–2.74	–0.24	0.10	0.74

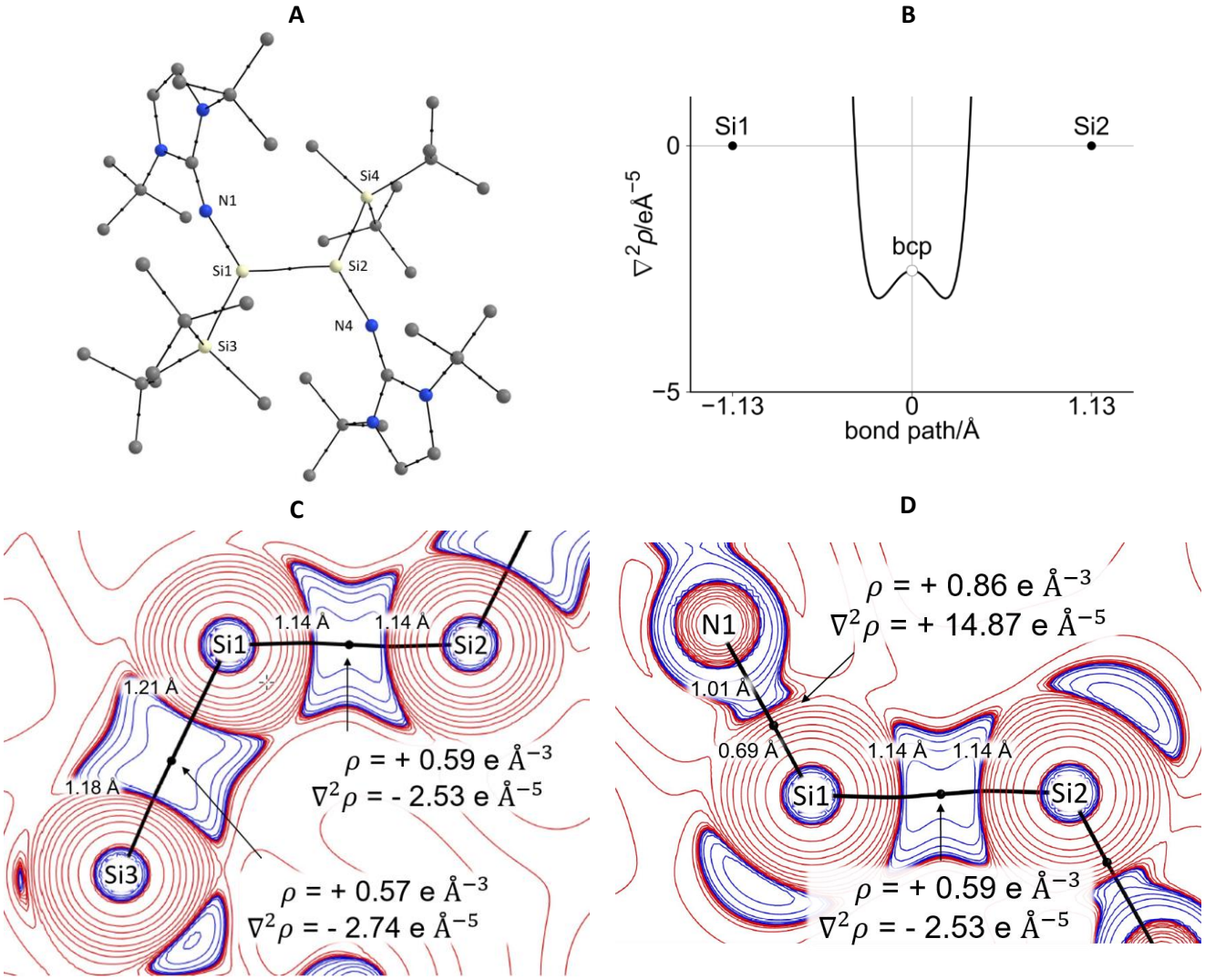
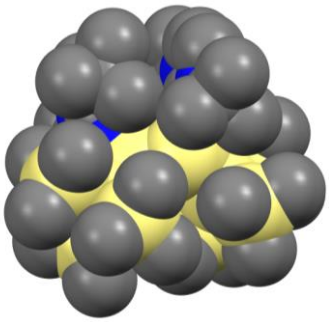
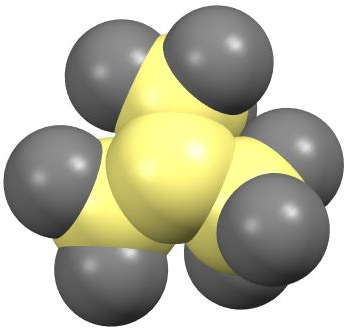


Figure S77: QTAIM Analysis of **2-(*E*)**. (**A**) Molecular graph (**B**) 1D Laplacian profile along the Si1–Si2 bond path (**C**, **D**) 2D plot of $\nabla^2\rho$(r); charge concentration (blue) and depletion (red), bond paths (black lines) and bond-critical points (bcps; black dots) with characteristic properties of the Si1–Si2, Si1-N1 and Si1–Si3 bonds.

3.12 Steric effects of the silyl ligands

VI

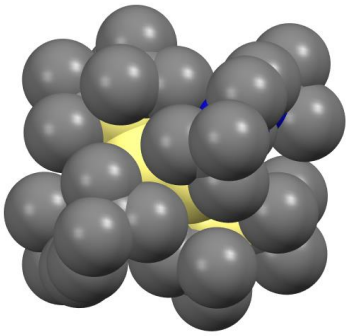


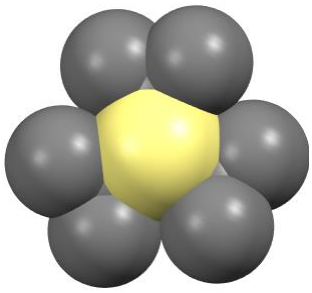


%Vbur($SiTMS_3$) = 32.3

Figure S78: Space filling diagrams of disilene **VI** and the hypersilyl ligand with $\%V_{bur}$ calculated with the SambVca 2.1 web tool using default parameters with H atoms omitted from the calculation.[S61-62]

1-(*E*)

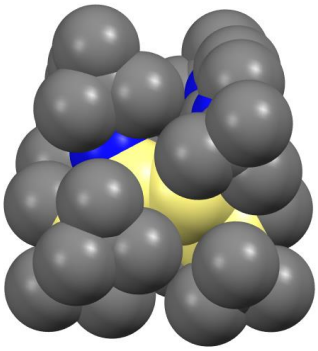


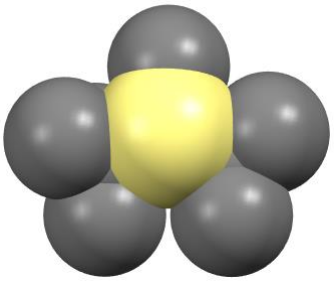


%Vbur(Si^tBu_3) = 36.6

Figure S79: Space filling diagrams of disilene **1-(*E*)** and the supersilyl ligand with $\%V_{bur}$ calculated with the SambVca 2.1 web tool using default parameters with H atoms omitted from the calculation.[S61-62]

2





%Vbur(Si^tBu_2Me) = 32.2

Figure S80: Space filling diagrams of disilene **2-(*Z*)** and the Si^tBu_2Me ligand with $\%V_{bur}$ calculated with the SambVca 2.1 web tool using default parameters with H atoms omitted from the calculation.[S61-62]

3.13 Calculated energies

Table S19. Calculated energies at the B3LYP-D3/def2-svp level of theory, values marked with * were obtained at the PBEh-3c level of theory.

Structure	E(SCF) [H/particle]
((Si^{t}Bu$_3$)(I^{t}BuN)Si)$_2$ (1-(*E*))	-3294.3965523
((Si^{t}Bu$_3$)(I^{t}BuN)Si)$_2$ (1-(*E*)')	-3294.397509
(Si^{t}Bu$_3$)(I^{t}BuN)Si (1^M)	-1647.171551
((Si^{t}Bu$_3$)(I^{t}BuN)Si)$_2$ (1-(*Z*))	-3294.392351
((Si^{t}Bu$_2$Me)(I^{t}BuN)Si)$_2$ (2-(*Z*))	-3058.721827
((Si^{t}Bu$_2$Me)(I^{t}BuN)Si)$_2$ (2^M)	-1529.323700
((Si^{t}Bu$_2$Me)(I^{t}BuN)Si)$_2$ (2-(*E*))	-3058.713479
((SiTMS$_3$)(I^{t}BuN)Si)$_2$ (VI-(*Z*))	-4802.683889
((SiTMS$_3$)(I^{t}BuN)Si) (VI^M)	-2401.311554
((SiTMS$_3$)(I^{t}BuN)Si)$_2$ (VI-(*E*))	-4802.672546
(I^{t}BuN)$_2$Si→Si(Si^{t}Bu$_2$Me)$_2$ (9)	-3058.736176
(I^{t}BuN)$_2$Si→Si(Si^{t}Bu$_2$Me)$_2$ (9^{I2})	-3058.733441
(I^{t}BuN)$_2$Si→Si(Si^{t}Bu$_2$Me)$_2$ (9^{I3})	-3058.734007
(I^{t}BuN)$_2$Si→Si(Si^{t}Bu$_2$Me)$_2$ (9^{I4})	-3058.732167
TS1	-3058.675009
TS1Z	-3058.660623
INT1	-3058.679623
TS2	-3058.669739
INT2	-3058.672044
TS3	-3058.669728
TS4	-3058.667883
INT3	-3058.693929
INT4	-3058.690227
TS5	-3058.672058
INT5	-3058.675169
TS6	-3058.674241
INT6	-3058.675169
TS7	-3058.649264
7	-3058.563135

H_2	-1.173790
2 + H_2*	-3055.876733
TS2H_2*	-3055.859669
4	-3059.960943
TS2$^M H_2$	-1530.473817
TS2$^M H_2$'	-1530.452067
INT2$^M H_2$	-1530.564253
INT2$^M H_2$'	-1530.513200
TSINT2^M	-3059.889791

3.14 Cartesian Coordinates (x,y,z) for the optimized structures

1-(*E*)

Si	0.00224	1.11969	0.00167
N	-1.44121	2.01627	0.20686
C	-2.53271	2.27287	0.82977
Si	1.78259	2.51850	-0.83996
N	-2.86447	2.14370	2.19880
C	-4.21320	2.45315	2.37229
H	-4.72466	2.35015	3.31989
C	-4.72272	2.83678	1.18613
H	-5.73758	3.13200	0.95327
N	-3.71856	2.75385	0.22692
C	-1.97417	1.78831	3.34646
C	-1.76693	0.26802	3.40428
H	-1.18780	0.00017	4.30038
H	-1.21671	-0.09649	2.52694
H	-2.73550	-0.25085	3.45072
C	-0.63571	2.53625	3.23967
H	-0.80260	3.62186	3.18094
H	-0.06003	2.22896	2.36056
H	-0.02652	2.32379	4.13068
C	-2.64105	2.23704	4.66233
H	-2.89203	3.30862	4.64824
H	-1.93335	2.06542	5.48610
H	-3.54847	1.65995	4.89384
C	-3.16053	4.89408	-0.81068
H	-3.14927	5.49402	-1.73395
H	-2.12896	4.78673	-0.45790
H	-3.73103	5.44247	-0.04426
C	-3.79569	3.51384	-1.05763
C	1.28491	4.42645	-0.67181
C	-5.27095	3.69788	-1.45690
H	-5.82042	4.35945	-0.77124
H	-5.79256	2.72998	-1.51417
H	-5.30844	4.16255	-2.45298
C	-3.10303	2.76338	-2.20286
H	-3.13179	3.38351	-3.11190
H	-3.63031	1.82337	-2.41341
H	-2.06523	2.52525	-1.96096
C	0.60881	4.71058	0.68676
H	0.34969	5.78398	0.75455
H	1.25249	4.47855	1.54527
H	-0.31721	4.13343	0.79783
C	0.27732	4.81857	-1.77105
H	-0.09674	5.84203	-1.58512
H	-0.59222	4.15089	-1.79000
H	0.72807	4.82051	-2.77257
C	2.50725	5.36015	-0.81077
H	2.16689	6.41243	-0.79699
H	3.05400	5.20948	-1.75317
H	3.22236	5.24664	0.01601
C	1.97417	2.03559	-2.75145
C	3.60096	0.64118	0.39803
H	2.73448	0.22894	0.92197
H	4.48745	0.44227	1.02816
H	3.72797	0.06585	-0.52514
C	4.71435	2.66956	-0.52626
H	4.69123	3.74770	-0.73583
H	4.90357	2.14635	-1.47516
H	5.59028	2.48117	0.12236
C	3.33890	2.79654	1.57072
H	3.34743	3.89467	1.53966
H	4.20346	2.48339	2.18490
H	2.42883	2.47757	2.10291
C	3.43805	2.15362	0.17020
C	0.59749	1.92580	-3.44564
H	0.05433	2.87723	-3.49117
H	-0.04925	1.19156	-2.94260
H	0.73718	1.57991	-4.48654
C	2.84474	3.03506	-3.54195
H	2.38289	4.02990	-3.61613
H	2.98241	2.66856	-4.57635
H	3.84694	3.16288	-3.10831
C	2.62230	0.64307	-2.84873
H	2.60452	0.28797	-3.89538
H	2.07894	-0.09729	-2.24446
H	3.67368	0.64435	-2.52695
Si	-0.00224	-1.11969	0.00167
N	1.44121	-2.01627	0.20686
C	2.53271	-2.27287	0.82977
Si	-1.78259	-2.51850	-0.83996
N	2.86447	-2.14370	2.19880
C	4.21320	-2.45315	2.37229
H	4.72466	-2.35015	3.31989
C	4.72272	-2.83678	1.18613
H	5.73758	-3.13200	0.95327
N	3.71856	-2.75385	0.22692
C	1.97417	-1.78831	3.34646
C	1.76693	-0.26802	3.40428
H	1.18780	-0.00017	4.30038
H	1.21671	0.09649	2.52694
H	2.73550	0.25085	3.45072
C	0.63571	-2.53625	3.23967
H	0.80260	-3.62186	3.18094
H	0.06003	-2.22896	2.36056
H	0.02652	-2.32379	4.13068
C	2.64105	-2.23704	4.66233
H	2.89203	-3.30862	4.64824
H	1.93335	-2.06542	5.48610
H	3.54847	-1.65995	4.89384
C	3.16053	-4.89408	-0.81068
H	3.14927	-5.49402	-1.73395
H	2.12896	-4.78673	-0.45790
H	3.73103	-5.44247	-0.04426
C	3.79569	-3.51384	-1.05763
C	-1.28491	-4.42645	-0.67181
C	5.27095	-3.69788	-1.45690
H	5.82042	-4.35945	-0.77124
H	5.79256	-2.72998	-1.51417
H	5.30844	-4.16255	-2.45298
C	3.10303	-2.76338	-2.20286
H	3.13179	-3.38351	-3.11190
H	3.63031	-1.82337	-2.41341
H	2.06523	-2.52525	-1.96096
C	-0.60881	-4.71058	0.68676
H	-0.34969	-5.78398	0.75455
H	-1.25249	-4.47855	1.54527
H	0.31721	-4.13343	0.79783
C	-0.27732	-4.81857	-1.77105
H	0.09674	-5.84203	-1.58512
H	0.59222	-4.15089	-1.79000
H	-0.72807	-4.82051	-2.77257
C	-2.50725	-5.36015	-0.81077
H	-2.16689	-6.41243	-0.79699
H	-3.05400	-5.20948	-1.75317
H	-3.22236	-5.24664	0.01601
C	-1.97417	-2.03559	-2.75145
C	-3.60096	-0.64118	0.39803
H	-2.73448	-0.22894	0.92197
H	-4.48745	-0.44227	1.02816
H	-3.72797	-0.06585	-0.52514
C	-4.71435	-2.66956	-0.52626
H	-4.69123	-3.74770	-0.73583
H	-4.90357	-2.14635	-1.47516
H	-5.59028	-2.48117	0.12236
C	-3.33890	-2.79654	1.57072
H	-3.34743	-3.89467	1.53966
H	-4.20346	-2.48339	2.18490

H	-2.42883	-2.47757	2.10291
C	-3.43805	-2.15362	0.17020
C	-0.59749	-1.92580	-3.44564
H	-0.05433	-2.87723	-3.49117
H	0.04925	-1.19156	-2.94260
H	-0.73718	-1.57991	-4.48654
C	-2.84474	-3.03506	-3.54195
H	-2.38289	-4.02990	-3.61613
H	-2.98241	-2.66856	-4.57635
H	-3.84694	-3.16288	-3.10831
C	-2.62230	-0.64307	-2.84873
H	-2.60452	-0.28797	-3.89538
H	-2.07894	0.09729	-2.24446
H	-3.67368	-0.64435	-2.52695

1-(*E*)'

Si	0.91070	-0.55548	-0.21823
N	2.44928	-0.02114	0.26540
C	3.31481	0.70254	0.87512
Si	1.02513	-2.91167	-0.85565
N	3.40289	1.02528	2.24538
C	4.45926	1.91354	2.43822
H	4.68178	2.36509	3.39578
C	5.07568	2.10957	1.25687
H	5.92351	2.74501	1.03693
N	4.40986	1.37047	0.28253
C	2.55457	0.52981	3.37246
C	1.23946	1.31970	3.42186
H	0.65167	1.02296	4.30331
H	0.62229	1.13501	2.53054
H	1.44214	2.39895	3.48860
C	2.30437	-0.97984	3.23014
H	3.25760	-1.52692	3.18774
H	1.73511	-1.21823	2.32814
H	1.73452	-1.33867	4.09956
C	3.30630	0.74407	4.70124
H	4.30263	0.27625	4.68621
H	2.72407	0.27729	5.50875
H	3.41467	1.80807	4.95830
C	5.82831	-0.31707	-0.77514
H	6.31353	-0.66060	-1.70194
H	5.14160	-1.10056	-0.43613
H	6.60335	-0.18218	-0.00411
C	5.07358	1.00423	-1.00633
C	2.86023	-3.62732	-0.67360
C	6.07824	2.10509	-1.39330
H	6.93746	2.15973	-0.70914
H	5.59126	3.09157	-1.43501
H	6.47697	1.88035	-2.39319
C	4.06419	0.88776	-2.15534
H	4.59441	0.58820	-3.07210
H	3.58311	1.85709	-2.33974
H	3.28393	0.15490	-1.94261
C	3.48447	-3.21482	0.67675
H	4.51856	-3.60249	0.74214
H	2.93600	-3.61238	1.54042
H	3.52287	-2.12388	0.78055
C	3.76743	-3.06914	-1.78861
H	4.81581	-3.36371	-1.59866
H	3.74091	-1.97368	-1.83688
H	3.50062	-3.45960	-2.78003
C	2.90046	-5.16782	-0.77607
H	3.95230	-5.50907	-0.74953
H	2.46143	-5.54494	-1.71134
H	2.38576	-5.66058	0.06056
C	0.50892	-2.84407	-2.76632
C	-1.55304	-3.23323	0.41283
H	-1.37020	-2.27695	0.91014
H	-2.23500	-3.81323	1.06152
H	-2.09793	-3.01817	-0.51240
C	-0.58042	-5.35633	-0.45862
H	0.30294	-5.97828	-0.65837
H	-1.12295	-5.22764	-1.40667
H	-1.24305	-5.93470	0.21222
C	0.34601	-4.26459	1.60231
H	1.22378	-4.92503	1.58544
H	-0.41614	-4.75643	2.23468
H	0.63302	-3.32962	2.10838
C	-0.23914	-4.00238	0.19745
C	1.23112	-1.69441	-3.50743
H	2.31860	-1.82522	-3.56156
H	1.03238	-0.71789	-3.03887
H	0.85810	-1.63537	-4.54660
C	0.79007	-4.15942	-3.52207
H	1.86492	-4.37789	-3.59949
H	0.40363	-4.08361	-4.55566
H	0.30458	-5.02969	-3.05797
C	-0.99851	-2.54121	-2.85609
H	-1.28474	-2.34183	-3.90505
H	-1.27257	-1.65177	-2.27088
H	-1.61736	-3.38044	-2.50758
Si	-0.91778	0.74866	0.24751
N	-2.49513	0.04646	0.22223
C	-3.33999	-0.71045	0.82462
Si	-0.97680	2.91452	-0.85087
N	-3.45713	-1.07503	2.18908
C	-4.48227	-2.01150	2.32442
H	-4.71134	-2.50486	3.25927
C	-5.05656	-2.19910	1.12111
H	-5.86754	-2.86644	0.85946
N	-4.39572	-1.40712	0.18832
C	-2.69156	-0.55850	3.36502
C	-1.30347	-1.21317	3.42214
H	-0.77422	-0.89444	4.33236
H	-0.69128	-0.92458	2.55859
H	-1.39359	-2.30900	3.43870
C	-2.58837	0.97459	3.31084
H	-3.58720	1.42817	3.22796
H	-1.97969	1.31818	2.46629
H	-2.11162	1.34180	4.23208
C	-3.44631	-0.91649	4.66093
H	-4.47796	-0.53308	4.65271
H	-2.92024	-0.45303	5.50782
H	-3.46820	-1.99982	4.85074
C	-5.80472	0.30767	-0.82927
H	-6.27224	0.68803	-1.75078
H	-5.12436	1.07645	-0.44648
H	-6.59428	0.14174	-0.07911
C	-5.04506	-1.00452	-1.09608
C	-2.80260	3.66407	-0.67905
C	-6.04610	-2.08998	-1.53030
H	-6.91310	-2.16670	-0.85781
H	-5.56045	-3.07559	-1.60119
H	-6.43169	-1.83026	-2.52706
C	-4.01502	-0.85372	-2.22276
H	-4.51485	-0.47092	-3.12575
H	-3.57378	-1.83015	-2.46422
H	-3.20856	-0.17512	-1.93715
C	-3.41181	3.33124	0.70055
H	-4.41897	3.78233	0.77973
H	-2.81813	3.71625	1.54024
H	-3.52007	2.24771	0.83540
C	-3.73521	3.04840	-1.74107
H	-4.77922	3.35336	-1.54296
H	-3.70416	1.95303	-1.72482
H	-3.49348	3.38197	-2.75907
C	-2.83420	5.19676	-0.86581
H	-3.88362	5.54603	-0.84635
H	-2.40476	5.51898	-1.82567
H	-2.30671	5.73211	-0.06394
C	-0.50734	2.72897	-2.76955
C	1.63414	3.30973	0.33083
H	1.46270	2.40404	0.92019
H	2.34158	3.93869	0.90269
H	2.14357	3.00930	-0.59104
C	0.64998	5.37321	-0.66261
H	-0.23495	5.98634	-0.88118
H	1.16548	5.17666	-1.61420
H	1.33347	5.99181	-0.05112
C	-0.22957	4.43399	1.49133
H	-1.10762	5.09300	1.44999
H	0.54902	4.96858	2.06688
H	-0.50329	3.53677	2.06906
C	0.31733	4.07018	0.09350
C	-1.23289	1.52097	-3.40190
H	-2.32331	1.63265	-3.42748
H	-1.00119	0.58979	-2.86510
H	-0.89378	1.39112	-4.44647
C	-0.83658	3.99196	-3.59420
H	-1.91506	4.19702	-3.64279
H	-0.49027	3.85449	-4.63566
H	-0.34145	4.89347	-3.20562
C	0.99936	2.45044	-2.90435
H	1.24857	2.20962	-3.95412
H	1.30199	1.58854	-2.29244
H	1.61678	3.31348	-2.61609

1^{M}

Si	-0.16425	-0.05497	-1.49202
Si	-2.15851	-0.00534	-0.01575
N	1.16984	-0.00510	-0.47029
N	3.20363	1.13581	0.12249
N	3.22793	-1.09539	0.13934
C	2.40850	0.00952	-0.12025
C	4.46978	0.71183	0.52896
C	4.48459	-0.63751	0.53956
C	2.81408	2.54577	-0.16033
C	1.56380	2.91657	0.65447
C	2.56621	2.71152	-1.67193
C	3.95733	3.48535	0.25517
C	2.88037	-2.51458	-0.15165
C	1.62465	-2.92069	0.63753
C	2.66606	-2.68421	-1.66794
C	4.03906	-3.42450	0.28678
C	-1.90135	-0.15419	1.94426
C	-0.71247	0.73043	2.37989
C	-1.54204	-1.59682	2.35555
C	-3.15262	0.26113	2.74686
C	-3.08430	1.69243	-0.46961
C	-2.48393	2.86800	0.33032
C	-4.60211	1.64671	-0.19629
C	-2.87341	2.03655	-1.96316
C	-3.17276	-1.56484	-0.70378
C	-2.22898	-2.78975	-0.76982
C	-4.39923	-1.93369	0.15497
C	-3.65964	-1.30880	-2.14687
H	5.26012	1.39736	0.80569
H	5.28951	-1.30114	0.82748
H	1.75377	2.79242	1.73142
H	0.71333	2.28386	0.38810
H	1.29251	3.96662	0.46623
H	2.30102	3.75610	-1.89836
H	1.75000	2.06684	-2.02239
H	3.47486	2.45394	-2.23845
H	4.18893	3.39894	1.32783
H	3.64454	4.52206	0.06457
H	4.87497	3.30591	-0.32513
H	1.39480	-3.98162	0.45532
H	0.75680	-2.32558	0.34019
H	1.78539	-2.77911	1.71723
H	2.43264	-3.73495	-1.90091
H	3.57848	-2.40188	-2.21638

H	1.83928	-2.06090	-2.03308
H	4.25006	-3.32827	1.36291
H	4.96174	-3.22431	-0.27837
H	3.75576	-4.46932	0.09445
H	-0.54698	0.62417	3.46888
H	-0.87753	1.79779	2.18450
H	0.21399	0.43504	1.86707
H	-1.31599	-1.62680	3.43780
H	-0.65019	-1.96582	1.83163
H	-2.36112	-2.30825	2.18117
H	-2.96710	0.12058	3.82879
H	-4.03807	-0.33895	2.48874
H	-3.41286	1.31941	2.60416
H	-2.67158	2.79124	1.41016
H	-2.93556	3.81901	-0.00860
H	-1.39614	2.95719	0.18262
H	-4.83776	1.40801	0.85080
H	-5.11579	0.90947	-0.83023
H	-5.05600	2.63159	-0.41757
H	-1.80958	2.19639	-2.20707
H	-3.40265	2.97708	-2.20692
H	-3.25026	1.26535	-2.64706
H	-1.83624	-3.08915	0.21015
H	-1.36579	-2.61008	-1.43569
H	-2.76942	-3.66122	-1.18511
H	-4.12251	-2.23511	1.17534
H	-4.93676	-2.78824	-0.29862
H	-5.11711	-1.10423	0.23654
H	-4.12563	-2.22754	-2.55008
H	-2.83564	-1.03852	-2.82650
H	-4.41891	-0.51581	-2.20136

1-(*Z*)

Si	1.06724	-0.56876	0.32203
Si	2.82676	-1.99457	-0.72819
Si	-1.15307	-0.53373	-0.37919
Si	-2.82049	-2.01382	0.72542
N	1.70122	0.97496	0.63531
N	2.19920	2.38501	2.53957
N	2.21542	3.33268	0.52287
N	-1.76716	1.07759	-0.47779
N	-1.98873	2.36170	-2.55199
N	-2.04043	3.46326	-0.61275
C	1.99074	2.09831	1.16898
C	2.56698	3.71934	2.68562
C	2.58114	4.29073	1.46571
C	1.98296	1.45050	3.68238
C	2.87477	0.21357	3.52015
C	0.50118	1.05502	3.75205
C	2.36501	2.14282	5.00116
C	2.14554	3.70069	-0.92160
C	1.50338	2.60298	-1.77020
C	1.27461	4.96576	-1.05716
C	3.57076	3.98704	-1.43035
C	0.99944	-2.59320	-2.94970
C	1.25715	-4.35317	-1.22000
C	3.05981	-3.98584	-2.90418
C	4.48448	-4.23414	0.28018
C	2.66477	-3.44882	1.80118
C	4.71703	-2.08014	1.48714
C	3.56773	-0.36761	-2.99395
C	5.46339	-1.65456	-2.00501
C	4.58133	0.35628	-0.83552
C	-1.90412	2.16293	-1.15173
C	-2.17361	3.71679	-2.81618
C	-2.21778	4.38013	-1.64426
C	-1.98517	1.31163	-3.61355
C	-3.09055	0.28684	-3.31662
C	-0.60068	0.64977	-3.70173
C	-2.29447	1.94882	-4.97973
C	-2.28911	3.79859	0.81971
C	-1.24196	3.13252	1.71854
C	-3.71008	3.34044	1.18139
C	-2.18850	5.32056	1.02551
C	-1.23517	-1.88407	3.20981
C	-1.03469	-3.96029	1.90700
C	-3.10397	-3.52493	3.25236
C	-4.10129	-4.60591	0.10336
C	-2.17570	-3.97184	-1.34434
C	-4.35144	-2.83817	-1.62731
C	-5.62086	-1.77227	1.63100
C	-4.01122	-0.03974	2.43860
C	-4.84110	0.00820	0.08196
H	2.80340	4.16818	3.64119
H	2.83668	5.30802	1.19407
H	2.76465	-0.45179	4.38975
H	3.93192	0.50760	3.43604
H	2.59862	-0.35125	2.62643
H	-0.12004	1.92892	3.99182
H	0.34837	0.29562	4.53313
H	0.15873	0.63381	2.80102
H	1.74115	3.02615	5.20445
H	3.42506	2.43929	5.02109
H	2.20296	1.43116	5.82361
H	0.52800	2.30740	-1.37543
H	2.12561	1.70835	-1.82330
H	1.36781	2.99374	-2.78902
H	0.26907	4.76990	-0.66644
H	1.17724	5.23515	-2.11901
H	1.69814	5.83471	-0.53316
H	3.53974	4.27584	-2.49258
H	4.20343	3.09499	-1.33372
H	4.04353	4.80853	-0.87007
H	0.20709	-2.07950	-2.38904
H	0.52163	-3.35698	-3.59083
H	1.45885	-1.85201	-3.61600
H	0.53638	-3.91245	-0.52138
H	1.92416	-5.01001	-0.64615
H	0.68389	-4.99608	-1.91150
H	2.54790	-4.75299	-3.51446
H	3.84563	-4.49959	-2.33424
H	3.54732	-3.29639	-3.60796
H	3.83138	-5.01046	-0.14085
H	5.00719	-4.69022	1.14156
H	5.25063	-3.99418	-0.47099
H	1.93422	-4.15732	1.39152
H	2.09723	-2.60712	2.22735
H	3.17740	-3.95919	2.63776
H	4.28740	-1.11627	1.78122
H	5.60831	-1.87632	0.87817
H	5.06582	-2.57966	2.40970
H	3.46414	-1.16970	-3.73789
H	4.22905	0.39981	-3.43674
H	2.57649	0.08979	-2.86136
H	5.28448	-2.55904	-2.60056
H	6.02067	-1.94988	-1.10499
H	6.13505	-1.00358	-2.59576
H	3.71874	0.97107	-0.55987
H	5.27955	0.97799	-1.42676
H	5.10124	0.09110	0.09319
H	-2.24192	4.12092	-3.81712
H	-2.32666	5.44353	-1.47653
H	-4.07303	0.78168	-3.27228
H	-2.92263	-0.21510	-2.35991
H	-3.11819	-0.48090	-4.10421
H	-0.61889	-0.16670	-4.43969
H	-0.29420	0.22007	-2.73947
H	0.15759	1.38206	-4.01460
H	-2.30672	1.15048	-5.73575
H	-1.52610	2.67515	-5.28475
H	-3.27976	2.43909	-4.99617
H	-1.47656	3.35383	2.77013
H	-0.23822	3.52292	1.50252
H	-1.22796	2.04989	1.57224
H	-4.45130	3.85121	0.54638
H	-3.93567	3.56880	2.23473
H	-3.81264	2.26323	1.03304
H	-2.98843	5.87269	0.51035
H	-1.21422	5.71400	0.69939
H	-2.29047	5.53057	2.10012
H	-1.82601	-1.03084	3.56626
H	-0.37667	-1.48504	2.65507
H	-0.84481	-2.40893	4.10205
H	-0.51081	-4.36758	2.79094
H	-0.26127	-3.54215	1.24765
H	-1.50767	-4.80736	1.39222
H	-3.74672	-2.77422	3.73448
H	-2.60009	-4.08020	4.06529
H	-3.75311	-4.23889	2.72886
H	-4.99029	-4.30402	0.67491
H	-3.44058	-5.16695	0.77871
H	-4.44075	-5.31674	-0.67298
H	-2.51806	-4.69555	-2.10751
H	-1.47175	-4.50388	-0.69633
H	-1.61771	-3.18276	-1.86873
H	-4.55993	-3.60816	-2.39269
H	-3.92650	-1.97162	-2.15026
H	-5.31950	-2.54137	-1.20194
H	-6.01897	-2.35104	0.78523
H	-6.43364	-1.10191	1.96856
H	-5.41832	-2.47296	2.45135
H	-4.82275	0.67937	2.65317
H	-3.09509	0.54121	2.25470
H	-3.86004	-0.63214	3.35175
H	-5.23570	-0.54317	-0.77958
H	-4.02162	0.64282	-0.27174
H	-5.65367	0.66802	0.43900
C	-3.38556	-3.41468	-0.57172
C	-4.39403	-0.92266	1.23190
C	-2.03732	-2.87528	2.34295
C	3.70479	-2.98795	0.75625
C	2.01903	-3.27378	-2.01134
C	4.17061	-0.87797	-1.66666

2-(*Z*)

Si	0.59845	-1.13680	0.08920
Si	0.59821	1.13690	-0.08925
Si	2.10566	2.48030	1.22038
Si	2.10624	-2.47987	-1.22037
N	-3.23332	-2.34261	-0.42442
N	-0.90941	-1.90840	-0.06686
N	-0.90979	1.90823	0.06678
N	-2.38513	2.98673	-1.53164
N	-2.38445	-2.98718	1.53164
N	-3.23378	2.34193	0.42445
C	-4.79327	-2.04912	-2.31826
H	-5.07893	-3.11216	-2.33019
H	-4.86365	-1.67426	-3.34968
H	-5.52246	-1.48884	-1.71290
C	-3.35486	-1.84173	-1.82119
C	-2.04154	-2.35905	0.31780
C	-2.04205	2.35862	-0.31783
C	-1.42928	3.38223	-2.60551
C	-2.17878	4.15436	-3.70364
H	-2.95776	3.54015	-4.18079
H	-1.45767	4.43778	-4.48391
H	-2.63609	5.07971	-3.32181
C	-0.79371	2.13711	-3.24882
H	-0.25229	1.52264	-2.51665
H	-0.07470	2.44482	-4.02372
H	-1.56312	1.51003	-3.72178
C	1.14701	4.08995	1.57591

H	0.09767	3.88538	1.82639
H	1.15114	4.75174	0.69665
H	1.60546	4.64339	2.41150
C	2.48309	1.65365	2.95644
C	3.40705	2.54099	3.81353
H	3.03197	3.57210	3.91648
H	4.42618	2.59138	3.40056
H	3.49337	2.12233	4.83354
C	3.11864	0.25940	2.82563
H	3.21205	-0.21337	3.82107
H	4.12749	0.29613	2.38957
H	2.49868	-0.40431	2.20213
C	1.12924	1.49904	3.68273
H	1.28034	1.01541	4.66578
H	0.43078	0.86913	3.10880
H	0.64058	2.46876	3.86650
C	3.68165	3.02514	0.19982
C	4.38450	4.22511	0.86890
H	4.78018	3.98127	1.86509
H	3.71259	5.09123	0.97830
H	5.24051	4.55267	0.24971
C	4.68676	1.87302	0.04374
H	5.52467	2.17655	-0.61131
H	4.22251	0.98820	-0.41323
H	5.12210	1.56727	1.00726
C	3.22751	3.47006	-1.20687
H	4.10269	3.79195	-1.80143
H	2.53161	4.32257	-1.16914
H	2.73211	2.65784	-1.76118
C	2.48350	-1.65320	-2.95647
C	1.12965	-1.49919	-3.68289
H	1.28064	-1.01555	-4.66595
H	0.43090	-0.86954	-3.10904
H	0.64139	-2.46911	-3.86665
C	3.40790	-2.54024	-3.81339
H	3.03323	-3.57150	-3.91630
H	4.42701	-2.59019	-3.40033
H	3.49414	-2.12163	-4.83344
C	3.11847	-0.25869	-2.82574
H	3.21181	0.21400	-3.82123
H	4.12729	-0.29497	-2.38956
H	2.49817	0.40487	-2.20241
C	1.14798	-4.08976	-1.57581
H	1.60656	-4.64315	-2.41136
H	0.09859	-3.88546	-1.82631
H	1.15226	-4.75150	-0.69651
C	3.68238	-3.02433	-0.19980
C	4.38540	-4.22424	-0.86883
H	4.78093	-3.98046	-1.86509
H	3.71365	-5.09050	-0.97805
H	5.24153	-4.55156	-0.24968
C	4.68732	-1.87203	-0.04386
H	5.52532	-2.17541	0.61114
H	4.22297	-0.98725	0.41310
H	5.12254	-1.56627	-1.00743
C	3.22840	-3.46923	1.20694
H	4.10366	-3.79095	1.80146
H	2.53261	-4.32184	1.16931
H	2.73292	-2.65703	1.76122
C	-2.39528	-2.63081	-2.72822
H	-1.35899	-2.47277	-2.41347
H	-2.49892	-2.29308	-3.77092
H	-2.61885	-3.70839	-2.68551
C	-3.03055	-0.34197	-1.86368
H	-3.73546	0.23047	-1.24439
H	-3.11099	0.02570	-2.89701
H	-2.01588	-0.14681	-1.50187
C	-4.25328	-2.92529	0.32203
H	-5.27266	-3.01106	-0.03177
C	-3.73874	-3.31770	1.50773
H	-4.24672	-3.79459	2.33574
C	-1.42849	-3.38243	2.60550
C	-0.35807	-4.31097	2.00604
H	-0.82768	-5.21295	1.58344
H	0.35709	-4.61888	2.78370
H	0.19750	-3.80990	1.20819
C	-2.17787	-4.15426	3.70393
H	-2.95673	-3.53989	4.18105
H	-1.45665	-4.43753	4.48415
H	-2.63528	-5.07967	3.32238
C	-0.79281	-2.13715	3.24841
H	-0.25146	-1.52289	2.51601
H	-0.07371	-2.44468	4.02330
H	-1.56214	-1.50993	3.72130
C	-3.35516	1.84093	1.82119
C	-4.79351	2.04829	2.31844
H	-5.07915	3.11134	2.33051
H	-4.86378	1.67334	3.34983
H	-5.52278	1.48809	1.71311
C	-2.39546	2.62993	2.72816
H	-1.35921	2.47191	2.41328
H	-2.49898	2.29212	3.77085
H	-2.61903	3.70752	2.68555
C	-3.03086	0.34116	1.86352
H	-3.73586	-0.23121	1.24426
H	-3.11119	-0.02658	2.89683
H	-2.01624	0.14602	1.50157
C	-4.25387	2.92452	-0.32190
H	-5.27323	3.01014	0.03198
C	-3.73946	3.31709	-1.50760
H	-4.24756	3.79395	-2.33555
C	-0.35877	4.31059	-2.00594
H	-0.82831	5.21247	-1.58305
H	0.35628	4.61870	-2.78362
H	0.19690	3.80931	-1.20830

2^{M}

Si	-0.44834	-0.00218	1.50966
Si	-2.19936	-0.00860	-0.21346
N	2.99191	-1.08491	-0.03526
N	0.90946	-0.00850	0.51123
N	2.94693	1.14431	-0.04646
C	3.75444	-3.41288	-0.36241
H	4.11596	-3.21458	-1.38276
H	3.42198	-4.46039	-0.32653
H	4.59367	-3.30673	0.34196
C	2.56839	-2.51122	0.01444
C	2.15612	0.01435	0.19173
C	-3.21190	-1.67714	-0.04803
C	-2.29863	-2.81930	-0.54112
H	-2.82098	-3.79081	-0.45717
H	-1.37623	-2.89665	0.05778
H	-2.00204	-2.69591	-1.59483
C	-4.49291	-1.66846	-0.90250
H	-4.28875	-1.43292	-1.95998
H	-5.22932	-0.93863	-0.53223
H	-4.98053	-2.66168	-0.87681
C	-3.58728	-1.97139	1.41898
H	-4.10965	-2.94410	1.49171
H	-4.25675	-1.21019	1.84484
H	-2.69964	-2.02964	2.07091
C	-1.50091	0.06123	-1.98735
H	-2.25419	-0.22793	-2.73918
H	-0.63157	-0.60452	-2.09604
H	-1.16113	1.08020	-2.23070
C	-3.28650	1.60366	0.02123
C	-4.18250	1.87664	-1.20308
H	-4.91788	1.07635	-1.37221
H	-3.59290	1.98765	-2.12730
H	-4.74869	2.81718	-1.06193
C	-4.16245	1.51550	1.28444
H	-4.67246	2.48011	1.46756
H	-3.57097	1.28055	2.18515
H	-4.94729	0.74933	1.18922
C	-2.32084	2.79813	0.18130
H	-2.88963	3.74008	0.29642
H	-1.66307	2.92226	-0.69312
H	-1.67749	2.70137	1.07330
C	1.43750	-2.73682	-1.00499
H	0.58502	-2.08155	-0.80042
H	1.09176	-3.78094	-0.96420
H	1.79621	-2.52832	-2.02515
C	2.12293	-2.87193	1.44413
H	2.94560	-2.69792	2.15513
H	1.84169	-3.93549	1.49189
H	1.26256	-2.27413	1.76710
C	4.25566	-0.62121	-0.40365
H	5.08587	-1.28108	-0.61946
C	4.22845	0.72833	-0.41025
H	5.03159	1.41891	-0.63235
C	2.46557	2.55277	-0.01236
C	1.31652	2.71774	-1.02346
H	1.67453	2.51197	-2.04435
H	0.92840	3.74717	-0.99051
H	0.49578	2.02800	-0.80333
C	3.60974	3.49673	-0.41441
H	4.45860	3.43779	0.28393
H	3.23395	4.52988	-0.39252
H	3.97068	3.29648	-1.43459
C	2.01993	2.91567	1.41667
H	1.18968	2.28631	1.75838
H	1.69258	3.96640	1.45199
H	2.85684	2.78824	2.12090

2-(*E*)

Si	0.05228	3.02412	0.41630
Si	0.73796	0.82650	-0.22483
N	4.34729	-0.18464	-1.10511
N	4.13357	-0.83346	1.01404
N	2.38263	0.54533	0.08051
C	3.48726	-0.09550	0.00578
C	5.47297	-0.92823	-0.76297
H	6.27742	-1.14056	-1.45519
C	4.11197	0.45857	-2.42852
C	3.79012	-0.94141	2.46201
C	2.27938	3.31341	2.24493
H	2.58716	2.31773	1.89541
H	2.63669	3.44232	3.28405
H	2.81110	4.05066	1.62606
C	4.64045	0.08333	3.23649
H	5.71648	-0.09814	3.08749
H	4.42612	0.02314	4.31515
H	4.41063	1.10413	2.89681
C	0.08346	2.55124	3.20207
H	0.19815	1.49040	2.92933
H	-0.99611	2.74796	3.29607
H	0.53105	2.69435	4.20304
C	0.29417	3.70197	-2.35899
H	0.45460	4.45500	-3.15354
H	-0.71730	3.28925	-2.50096
H	1.00907	2.88201	-2.52980
C	1.90628	4.88983	-0.85507
H	2.13542	5.54892	-1.71335
H	2.65794	4.08714	-0.85002
H	2.05124	5.48751	0.05728
C	-0.51246	5.53890	-0.87686
H	-0.26037	6.29678	-1.64219
H	-0.47864	6.04064	0.10204
H	-1.55391	5.22976	-1.05776
C	0.39701	4.94679	2.56858
H	0.89904	5.68632	1.92638
H	0.71858	5.14991	3.60751

H	-0.68740	5.13998	2.52157
C	5.34619	-1.31489	0.52341
H	6.02875	-1.90271	1.12491
C	0.46830	4.34978	-0.96973
C	3.95793	1.97581	-2.23197
H	4.87910	2.40437	-1.80681
H	3.13216	2.19327	-1.54862
H	3.75688	2.46743	-3.19602
C	0.74931	3.49757	2.17978
C	2.86531	-0.15151	-3.09311
H	2.68936	0.32470	-4.07024
H	1.96322	-0.01293	-2.48210
H	3.00819	-1.23013	-3.25807
C	2.30307	-0.68360	2.73322
H	2.03464	0.36404	2.58445
H	2.08850	-0.94976	3.77944
H	1.65197	-1.28382	2.08714
C	5.31879	0.20777	-3.34692
H	5.13213	0.70461	-4.31006
H	5.46806	-0.86349	-3.55113
H	6.24834	0.62623	-2.93170
C	-1.84361	2.98914	0.56297
H	-2.22025	3.93583	0.98270
H	-2.17408	2.17126	1.21517
H	-2.32605	2.84001	-0.41302
C	4.11453	-2.37202	2.93835
H	5.18621	-2.61137	2.88148
H	3.56112	-3.11600	2.34556
H	3.81561	-2.48065	3.99120
Si	-0.05228	-3.02409	-0.41618
Si	-0.73795	-0.82647	0.22501
N	-4.34747	0.18455	1.10491
N	-4.13354	0.83338	-1.01421
N	-2.38257	-0.54520	-0.08045
C	-3.48728	0.09548	-0.00586
C	-5.47320	0.92800	0.76261
H	-6.27775	1.14025	1.45473
C	-4.11227	-0.45860	2.42837
C	-3.78988	0.94147	-2.46212
C	-2.27953	-3.31368	-2.24456
H	-2.58745	-2.31807	-1.89497
H	-2.63695	-3.44263	-3.28363
H	-2.81105	-4.05104	-1.62563
C	-4.64004	-0.08325	-3.23681
H	-5.71611	0.09813	-3.08795
H	-4.42556	-0.02295	-4.31543
H	-4.41020	-1.10407	-2.89718
C	-0.08386	-2.55107	-3.20192
H	-0.19873	-1.49027	-2.92912
H	0.99573	-2.74759	-3.29605
H	-0.53154	-2.69423	-4.20285
C	-0.29409	-3.70194	2.35914
H	-0.45443	-4.45499	3.15369
H	0.71731	-3.28907	2.50114
H	-1.00912	-2.88209	2.52991
C	-1.90596	-4.89013	0.85521
H	-2.13499	-5.54922	1.71351
H	-2.65777	-4.08759	0.85010
H	-2.05078	-5.48788	-0.05711
C	0.51290	-5.53874	0.87704
H	0.26094	-6.29666	1.64238
H	0.47918	-6.04051	-0.10185
H	1.55429	-5.22940	1.05795
C	-0.39692	-4.94671	-2.56851
H	-0.89876	-5.68637	-1.92630
H	-0.71857	-5.14983	-3.60742
H	0.68753	-5.13972	-2.52163
C	-5.34628	1.31467	-0.52375
H	-6.02881	1.90244	-1.12534
C	-0.46808	-4.34980	0.96988
C	-3.95815	-1.97585	2.23190
H	-4.87925	-2.40446	1.80666
H	-3.13229	-2.19329	1.54865
H	-3.75719	-2.46742	3.19599
C	-0.74942	-3.49757	-2.17959
C	-2.86570	0.15155	3.09308
H	-2.68987	-0.32459	4.07026
H	-1.96353	0.01294	2.48220
H	-3.00862	1.23018	3.25794
C	-2.30279	0.68378	-2.73316
H	-2.03430	-0.36385	-2.58439
H	-2.08812	0.94997	-3.77936
H	-1.65179	1.28401	-2.08701
C	-5.31920	-0.20782	3.34662
H	-5.13263	-0.70461	4.30981
H	-5.46853	0.86345	3.55077
H	-6.24868	-0.62633	2.93131
C	1.84360	-2.98899	-0.56302
H	2.22027	-3.93565	-0.98279
H	2.17396	-2.17108	-1.21524
H	2.32613	-2.83984	0.41293
C	-4.11432	2.37210	-2.93837
H	-5.18600	2.61142	-2.88153
H	-3.56097	3.11606	-2.34550
H	-3.81535	2.48083	-3.99120

VI-(*Z*)

Si	1.05832	-0.23598	0.41858
Si	2.54892	-1.83172	-0.60475
Si	1.56272	-3.10937	-2.35667
Si	3.46287	-3.19529	1.14187
Si	4.38169	-0.75581	-1.71373
Si	-1.14468	-0.07580	-0.29496
Si	-2.73315	-1.64269	0.62197
Si	-1.78921	-3.04231	2.30399
Si	-3.70425	-2.89207	-1.17851
Si	-4.51589	-0.54854	1.77502
N	1.92737	1.20788	0.46697
N	2.99495	2.75720	1.95478
N	2.45921	3.49819	-0.07730
N	-1.82715	1.48366	-0.23877
N	-2.62893	2.97674	-1.97668
N	-2.08962	3.85785	-0.00018
C	2.39749	2.35804	0.74326
C	3.40954	4.08228	1.85132
C	3.08638	4.53036	0.62005
C	3.23672	1.86471	3.12378
C	4.17629	0.72129	2.70109
C	1.90259	1.32585	3.67143
C	3.92198	2.66355	4.24435
C	2.06857	3.66780	-1.50654
C	1.25974	2.48332	-2.04112
C	1.18692	4.92713	-1.62701
C	3.35407	3.82262	-2.34231
C	0.72546	-1.94270	-3.59555
C	0.27110	-4.35832	-1.75467
C	2.89121	-4.10080	-3.29121
C	3.22851	-5.04404	0.77253
C	2.65275	-2.80867	2.81329
C	5.32578	-2.90013	1.38373
C	3.87244	-0.05969	-3.41056
C	5.77121	-2.00753	-2.08198
C	5.20235	0.64651	-0.73482
C	-2.13835	2.63741	-0.69978
C	-2.85888	4.35082	-2.02791
C	-2.53844	4.88274	-0.82945
C	-2.99871	2.01474	-3.05573
C	-4.05628	1.03222	-2.52232
C	-1.74666	1.28381	-3.56712
C	-3.61661	2.78014	-4.23803
C	-1.82652	3.99749	1.46241
C	-0.42008	3.48822	1.79964
C	-2.88677	3.19944	2.23337
C	-1.91554	5.47777	1.86249
C	-0.91710	-2.00015	3.62800
C	-0.53567	-4.28356	1.61367
C	-3.14409	-4.05151	3.18017
C	-3.65331	-4.76016	-0.83710
C	-2.82358	-2.56553	-2.82633
C	-5.52520	-2.42028	-1.46034
C	-5.95583	-1.73926	2.14348
C	-3.91871	0.06414	3.47596
C	-5.27415	0.89791	0.80725
H	3.89778	4.61546	2.65679
H	3.25476	5.50882	0.18524
H	4.36096	0.04784	3.55139
H	5.14121	1.12872	2.36456
H	3.74847	0.13656	1.87966
H	1.26219	2.15531	4.00607
H	2.09352	0.66750	4.53275
H	1.35056	0.74777	2.92084
H	3.29925	3.50268	4.59062
H	4.90547	3.05040	3.93716
H	4.08361	1.99416	5.10159
H	0.34312	2.32476	-1.46504
H	1.82885	1.55085	-2.02510
H	0.98342	2.70596	-3.08178
H	0.27037	4.81037	-1.03151
H	0.89031	5.07056	-2.67686
H	1.70487	5.84207	-1.30348
H	3.10165	3.97136	-3.40359
H	3.97548	2.91918	-2.26016
H	3.95388	4.68425	-2.01115
H	0.01286	-1.28518	-3.07551
H	0.17579	-2.52143	-4.35712
H	1.45873	-1.30629	-4.11128
H	-0.53126	-3.86554	-1.18982
H	0.71857	-5.12706	-1.10761
H	-0.18451	-4.86402	-2.62315
H	2.40778	-4.74870	-4.04288
H	3.47341	-4.74646	-2.61421
H	3.59543	-3.44078	-3.82120
H	2.16200	-5.31534	0.74928
H	3.71626	-5.65290	1.55330
H	3.67203	-5.31881	-0.19819
H	1.57435	-3.00634	2.80772
H	2.79248	-1.75371	3.09118
H	3.11309	-3.43331	3.59865
H	5.56443	-1.82898	1.47858
H	5.91556	-3.31022	0.55065
H	5.65361	-3.40272	2.31012
H	3.68990	-0.87714	-4.12564
H	4.69991	0.55259	-3.80917
H	2.97091	0.56737	-3.37748
H	5.39233	-2.98516	-2.41465
H	6.40323	-2.17005	-1.19674
H	6.41522	-1.60426	-2.88294
H	4.49076	1.43079	-0.44703
H	5.99480	1.10092	-1.35454
H	5.67242	0.26219	0.18241
H	-3.21368	4.85917	-2.91472
H	-2.57029	5.92041	-0.52367
H	-4.94795	1.58069	-2.18454
H	-3.68080	0.44870	-1.67555
H	-4.35733	0.33372	-3.31682
H	-2.02359	0.56787	-4.35572
H	-1.24026	0.72411	-2.76952
H	-1.02952	2.00284	-3.98909
H	-3.88079	2.05469	-5.02090
H	-2.90963	3.49888	-4.67969
H	-4.53720	3.31141	-3.95289
H	-0.25557	3.55797	2.88492
H	0.34569	4.09699	1.30135
H	-0.28880	2.44516	1.49566

H	-3.89925	3.56155	1.99764
H	-2.72409	3.29544	3.31768
H	-2.82292	2.14090	1.96522
H	-2.92171	5.89436	1.70357
H	-1.18151	6.09345	1.31982
H	-1.68915	5.56129	2.93535
H	-1.63329	-1.39857	4.20569
H	-0.18784	-1.31639	3.16706
H	-0.38025	-2.66017	4.33051
H	-0.06446	-4.83675	2.44367
H	0.25906	-3.77797	1.04854
H	-1.01446	-5.01429	0.94577
H	-3.81487	-3.40336	3.76550
H	-2.67595	-4.76634	3.87902
H	-3.75886	-4.62732	2.47029
H	-4.15730	-5.01028	0.11029
H	-2.61788	-5.13006	-0.78077
H	-4.16395	-5.30770	-1.64805
H	-3.36932	-3.07352	-3.64048
H	-1.79226	-2.93716	-2.82500
H	-2.78585	-1.49145	-3.05714
H	-5.88281	-2.89690	-2.38944
H	-5.65573	-1.33221	-1.56731
H	-6.16938	-2.76264	-0.63710
H	-6.55878	-1.93480	1.24477
H	-6.61871	-1.27648	2.89566
H	-5.61571	-2.70572	2.54393
H	-4.62382	0.81388	3.87403
H	-2.91740	0.51597	3.44854
H	-3.88924	-0.77817	4.18573
H	-5.84371	0.52274	-0.05685
H	-4.51305	1.59599	0.43683
H	-5.97278	1.45150	1.45813

VI^{M}

Si	0.11660	0.08250	-1.78402
Si	-1.68449	0.02313	-0.10458
Si	-3.17587	-1.60761	-0.95576
Si	-2.80517	2.10702	-0.27770
Si	-1.29873	-0.47036	2.18098
N	1.51134	0.04103	-0.86059
N	3.51042	1.07912	-0.02567
N	3.43752	-1.14849	-0.06138
C	2.69777	-0.00374	-0.37344
C	4.71495	0.59175	0.48346
C	4.67150	-0.75769	0.46074
C	3.15788	2.51220	-0.22142
C	1.89304	2.84525	0.58952
C	2.95765	2.79125	-1.72327
C	4.30702	3.39613	0.28799
C	2.98915	-2.54842	-0.29703
C	2.79440	-2.77889	-1.80754
C	4.06374	-3.52229	0.21084
C	1.69003	-2.80782	0.48590
C	-2.22451	-3.23832	-1.19066
C	-3.85784	-1.06490	-2.64333
C	-4.64471	-1.93162	0.20600
C	-4.61306	1.98801	0.29497
C	-2.79286	2.70276	-2.08171
C	-1.93898	3.43389	0.77332
C	-1.33523	-2.34285	2.51686
C	-2.66441	0.28473	3.26979
C	0.37472	0.21683	2.75616
H	5.51137	1.23644	0.83188
H	5.42458	-1.46401	0.78525
H	1.60946	3.89636	0.42736
H	2.08010	2.69848	1.66380
H	1.04991	2.20713	0.30353
H	3.87595	2.54993	-2.28123
H	2.72770	3.85673	-1.87890
H	2.13617	2.19788	-2.14207
H	5.23865	3.22724	-0.27320
H	4.50126	3.24047	1.36009
H	4.02454	4.45003	0.15176
H	3.73851	-2.59967	-2.34546
H	2.03010	-2.11236	-2.22497
H	2.48233	-3.81867	-1.99143
H	5.01456	-3.40897	-0.33177
H	3.70991	-4.55039	0.04718
H	4.25004	-3.40213	1.28894
H	1.34643	-3.83976	0.31668
H	0.89086	-2.12463	0.18010
H	1.86102	-2.67148	1.56453
H	-1.38622	-3.10342	-1.89487
H	-2.88142	-4.02920	-1.59238
H	-1.80748	-3.59371	-0.23466
H	-3.04046	-0.81522	-3.33939
H	-4.49894	-0.17394	-2.54330
H	-4.46352	-1.86792	-3.09791
H	-5.31731	-2.69434	-0.22380
H	-5.23048	-1.01371	0.37102
H	-4.30837	-2.29479	1.19012
H	-5.19030	1.31391	-0.35825
H	-5.09354	2.98152	0.26489
H	-4.68412	1.60408	1.32490
H	-3.27560	1.97136	-2.74896
H	-1.76273	2.85132	-2.44571
H	-3.33094	3.66187	-2.17783
H	-0.91311	3.61267	0.41585
H	-1.87765	3.14237	1.83406
H	-2.49038	4.38836	0.71559
H	-2.33340	-2.75938	2.30886
H	-1.10541	-2.53674	3.57897
H	-0.60775	-2.89655	1.90660
H	-3.65229	-0.11522	2.98827
H	-2.70704	1.38128	3.17533
H	-2.49004	0.04233	4.33269
H	1.19604	-0.15526	2.12439
H	0.57820	-0.07133	3.80193
H	0.38137	1.31637	2.69742

VI-(*E*)

Si	1.02228	0.07008	-0.27891
N	2.00523	1.24443	0.42263
C	2.88265	1.94116	1.03231
Si	2.35206	-1.92462	-0.65089
N	3.04571	2.07490	2.42650
C	4.10423	2.93739	2.69110
H	4.42812	3.19054	3.69204
C	4.61740	3.34815	1.51382
H	5.44645	4.02123	1.33011
N	3.89781	2.74592	0.48342
C	2.18109	1.44622	3.46471
C	0.73303	1.92266	3.28295
H	0.10177	1.52324	4.09187
H	0.30897	1.57202	2.33323
H	0.68080	3.02094	3.31083
C	2.28149	-0.08444	3.36962
H	3.30809	-0.41713	3.57935
H	1.99671	-0.44320	2.37470
H	1.61058	-0.54915	4.10678
C	2.66086	1.87455	4.86124
H	3.69701	1.55990	5.05922
H	2.01972	1.38942	5.61140
H	2.58037	2.96205	5.01053
C	5.68544	2.90497	-1.19473
H	5.90968	3.10212	-2.25378
H	5.98189	1.87176	-0.96386
H	6.31090	3.58345	-0.59627
C	4.17835	3.10737	-0.93626
C	3.79035	4.58419	-1.14361
H	4.36321	5.25213	-0.48226
H	2.72083	4.72777	-0.93235
H	3.98540	4.88608	-2.18435
C	3.39277	2.24808	-1.93008
H	3.71225	2.51645	-2.94845
H	2.31777	2.42343	-1.85185
H	3.57358	1.17845	-1.78317
C	5.21127	-0.70783	1.21421
H	6.31124	-0.71397	1.30563
H	4.79282	-1.14566	2.13271
H	4.87987	0.33797	1.15458
C	5.60412	-0.97800	-1.81682
H	6.67915	-0.88141	-1.58576
H	5.23021	0.01537	-2.09771
H	5.50919	-1.63177	-2.69744
C	5.47110	-3.44801	-0.08478
H	6.56681	-3.35482	0.01307
H	5.26237	-4.09659	-0.95010
H	5.09412	-3.95233	0.81872
C	-0.24057	-4.07417	0.34338
H	-0.76195	-3.12043	0.48710
H	-0.63350	-4.80696	1.06848
H	-0.48367	-4.43698	-0.66775
C	2.39297	-5.47077	-0.18475
H	3.49192	-5.47223	-0.16887
H	2.06572	-5.63941	-1.22322
H	2.04155	-6.32710	0.41754
C	2.12181	-3.72963	2.33786
H	3.21716	-3.68141	2.45100
H	1.76009	-4.60456	2.90512
H	1.69804	-2.82476	2.79630
C	2.49990	-0.74411	-3.96855
H	3.54304	-0.42042	-3.83573
H	1.84435	0.08242	-3.65035
H	2.33028	-0.91812	-5.04525
C	3.27345	-3.70677	-3.57279
H	4.33025	-3.46949	-3.37325
H	3.16182	-3.85978	-4.66021
H	3.04666	-4.66027	-3.07076
C	0.33207	-2.81082	-3.40941
H	0.23122	-2.99830	-4.49228
H	-0.35320	-1.99261	-3.14224
H	0.00523	-3.71519	-2.87292
Si	-1.18254	0.21639	0.45131
N	-2.17649	-1.14976	0.45392
C	-2.95948	-2.04642	0.91547
Si	-2.32642	2.05556	-0.62188
N	-3.20071	-2.39202	2.26222
C	-4.12651	-3.43169	2.31344
H	-4.48122	-3.86649	3.23851
C	-4.47124	-3.75217	1.04933
H	-5.16868	-4.50626	0.70273
N	-3.77372	-2.91995	0.17883
C	-2.50257	-1.82186	3.45045
C	-0.98812	-2.05766	3.32349
H	-0.48153	-1.71477	4.23833
H	-0.55498	-1.51080	2.47689
H	-0.77735	-3.12849	3.19185
C	-2.83157	-0.32590	3.59405
H	-3.91381	-0.18199	3.72765
H	-2.51075	0.24942	2.71649
H	-2.31238	0.08850	4.47209
C	-2.98958	-2.53746	4.72227
H	-4.07028	-2.40569	4.88395
H	-2.47153	-2.09972	5.58770
H	-2.75702	-3.61301	4.70591
C	-5.47485	-2.70582	-1.57588
H	-5.66190	-2.70868	-2.66054
H	-5.74815	-1.71741	-1.18017
H	-6.14127	-3.45298	-1.11898
C	-3.98910	-3.00670	-1.29342

C	-3.63364	-4.43429	-1.75260
H	-4.26000	-5.19709	-1.26611
H	-2.58175	-4.65667	-1.52304
H	-3.78022	-4.52505	-2.83967
C	-3.11781	-2.01787	-2.07350
H	-3.32434	-2.15062	-3.14634
H	-2.05275	-2.19610	-1.89872
H	-3.32477	-0.97876	-1.80415
C	-5.23709	0.72042	1.00846
H	-6.33909	0.69463	1.06488
H	-4.85671	1.11730	1.96203
H	-4.87209	-0.31113	0.90511
C	-5.46661	1.12241	-2.03505
H	-6.55259	0.98811	-1.89021
H	-5.04279	0.15268	-2.32818
H	-5.32437	1.81713	-2.87739
C	-5.52052	3.51261	-0.18100
H	-6.61718	3.38874	-0.15499
H	-5.27727	4.20852	-0.99944
H	-5.21108	3.98002	0.76712
C	0.16037	4.27199	0.50672
H	0.71522	3.33040	0.60737
H	0.49986	4.97063	1.29048
H	0.41985	4.71041	-0.47054
C	-2.50043	5.60755	-0.05422
H	-3.59918	5.58845	-0.02880
H	-2.18716	5.80934	-1.09122
H	-2.15966	6.45476	0.56658
C	-2.26571	3.75276	2.39560
H	-3.36585	3.72913	2.46435
H	-1.90186	4.56969	3.04230
H	-1.88498	2.80088	2.79589
C	-2.19999	0.82766	-3.95328
H	-3.25528	0.51951	-3.92085
H	-1.58755	-0.00923	-3.58368
H	-1.92784	1.01083	-5.00711
C	-2.95500	3.80187	-3.60680
H	-4.02939	3.60361	-3.46685
H	-2.77441	3.93653	-4.68747
H	-2.72462	4.75473	-3.10440
C	-0.05899	2.84771	-3.20110
H	0.14870	2.99494	-4.27476
H	0.57429	2.02387	-2.83853
H	0.23135	3.76341	-2.66313
Si	2.11263	-2.32072	-2.98294
Si	4.71013	-1.71843	-0.30846
Si	1.63370	-3.87059	0.50697
Si	-1.87427	2.38939	-2.92694
Si	-4.69649	1.81836	-0.43987
Si	-1.71503	4.00197	0.59256

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Si	0.67119	0.05210	0.01991
Si	-1.48825	-0.33036	0.46372
C	2.57923	-2.14240	0.41574
N	1.81781	-1.13235	0.23850
C	3.68262	-3.90731	1.32957
H	3.96074	-4.65086	2.06506
N	2.75736	-2.89626	1.58201
Si	-2.66937	1.72441	0.73315
C	-1.46980	3.20188	0.61723
H	-0.51414	2.98967	1.10877
H	-1.91505	4.08619	1.10222
H	-1.25280	3.46092	-0.42704
C	-4.12264	2.13856	-0.51485
C	-3.57386	1.99612	-1.94725
H	-2.79886	2.74644	-2.16242
H	-4.38383	2.14225	-2.68612
H	-3.13152	1.00801	-2.12488
C	-4.62253	3.59056	-0.35867
H	-5.09777	3.77746	0.61339
H	-5.37796	3.80965	-1.13681
H	-3.80974	4.32388	-0.48238
C	-5.31028	1.17812	-0.33367
H	-5.00737	0.12587	-0.42657
H	-6.08247	1.36746	-1.10281
H	-5.79366	1.29947	0.64841
C	4.09795	-3.79654	0.04837
H	4.78827	-4.42943	-0.49456
N	3.44075	-2.71248	-0.52858
C	0.63553	-2.75742	2.87096
H	0.36869	-3.78895	2.59676
H	0.16361	-2.06762	2.15931
H	0.20757	-2.54749	3.86341
C	2.54338	-1.15776	3.33139
H	2.15295	-0.94375	4.33796
H	2.12615	-0.41971	2.63988
H	3.63804	-1.03888	3.34808
C	2.16061	-2.58978	2.91882
C	4.35887	-0.68095	-1.58168
H	5.26047	-0.74974	-0.95270
H	3.62934	-0.03780	-1.07541
H	4.63637	-0.20803	-2.53592
C	2.54190	-2.03198	-2.74234
H	2.16360	-3.04592	-2.94163
H	2.79814	-1.56128	-3.70357
H	1.73806	-1.45094	-2.28046
C	4.85401	-2.93593	-2.54450
H	4.50154	-3.96027	-2.74036
H	5.79110	-2.98386	-1.96968
H	5.08363	-2.47265	-3.51503
C	3.78480	-2.08791	-1.83855
C	2.72947	-3.56411	3.96282
H	2.46760	-4.60901	3.73714
H	2.29064	-3.32019	4.94090
H	3.82311	-3.48037	4.05737
C	-3.24356	1.69530	2.61963
C	-1.97387	1.78662	3.49435
H	-2.24405	1.69979	4.56364
H	-1.45048	2.74739	3.36819
H	-1.26186	0.97774	3.26235
C	-4.15480	2.88761	2.96816
H	-4.33747	2.91849	4.05885
H	-5.13901	2.81166	2.48136
H	-3.71176	3.85676	2.68643
C	-3.97927	0.39357	2.98764
H	-3.34324	-0.48975	2.81910
H	-4.90804	0.25837	2.41273
H	-4.25713	0.40140	4.05856
C	1.85076	2.70811	-0.38306
N	1.40680	1.52114	-0.22500
C	2.43854	4.70550	-1.29254
H	2.52749	5.48742	-2.03574
N	1.85465	3.46763	-1.55634
Si	-1.98051	-2.32593	-0.72937
C	-0.42618	-3.43120	-0.67709
H	0.34234	-3.07152	-1.37248
H	-0.69528	-4.45838	-0.97212
H	0.02435	-3.46945	0.32051
C	-3.35478	-3.32684	0.24959
C	-2.76201	-3.70395	1.62441
H	-1.90545	-4.39013	1.53052
H	-3.52548	-4.21494	2.24035
H	-2.41950	-2.81599	2.17953
C	-3.75178	-4.62629	-0.47778
H	-4.27280	-4.42963	-1.42699
H	-4.44283	-5.21669	0.15281
H	-2.88392	-5.26956	-0.69559
C	-4.62260	-2.48811	0.48660
H	-4.39810	-1.55730	1.02474
H	-5.34757	-3.05267	1.10280
H	-5.13174	-2.22245	-0.45114
C	2.80585	4.73311	0.00818
H	3.26043	5.54308	0.56428
N	2.45957	3.51227	0.58468
C	-0.09647	2.65766	-2.85063
H	-0.67429	3.56975	-2.64019
H	-0.33152	1.91156	-2.08259
H	-0.42541	2.26060	-3.82289
C	2.22498	1.74080	-3.28809
H	1.92723	1.39861	-4.29100
H	2.06442	0.91938	-2.58375
H	3.30014	1.97802	-3.30398
C	1.40446	2.98101	-2.89365
C	3.87128	1.84825	1.73335
H	4.74561	2.17157	1.14655
H	3.39103	1.01255	1.21084
H	4.22332	1.48806	2.71185
C	1.67820	2.61701	2.77006
H	1.00728	3.47569	2.92054
H	2.01102	2.26099	3.75685
H	1.10290	1.81446	2.29752
C	3.63085	4.15887	2.66204
H	2.98359	5.03666	2.81190
H	4.54380	4.47334	2.13418
H	3.93117	3.79450	3.65510
C	2.89746	3.02673	1.92644
C	1.64111	4.07842	-3.94228
H	1.07102	4.99257	-3.71702
H	1.29767	3.70776	-4.91884
H	2.70702	4.33573	-4.03924
C	-2.38024	-2.14665	-2.65022
C	-1.43580	-1.09223	-3.26063
H	-1.61646	-1.00117	-4.34857
H	-0.37655	-1.36557	-3.12664
H	-1.56722	-0.10088	-2.80691
C	-2.12470	-3.47734	-3.39237
H	-2.36795	-3.35983	-4.46535
H	-2.73846	-4.30588	-3.01086
H	-1.06985	-3.78739	-3.33343
C	-3.83955	-1.72232	-2.89746
H	-4.11568	-0.81773	-2.33783
H	-4.54964	-2.51572	-2.61819
H	-4.00195	-1.50552	-3.97007

9^{I2}

Si	-0.43941	0.04075	0.03744
N	-1.35182	-1.34025	-0.17774
N	-2.67624	-2.75838	-1.59731
N	-3.18245	-2.71612	0.56508
N	-1.41024	1.38189	0.23980
N	-3.20399	2.91653	-0.16455
N	-2.15482	3.08063	1.78876
C	-2.30810	-2.17497	-0.38027
C	-3.74589	-3.62320	-1.38340
H	-4.20569	-4.20215	-2.17356
C	-4.05533	-3.59684	-0.06840
H	-4.82413	-4.14869	0.45654
C	-1.99481	-2.54027	-2.90952
C	-0.52277	-2.94832	-2.78136
H	0.00111	-2.79145	-3.73587
H	-0.43522	-4.00868	-2.50208
H	-0.02360	-2.35172	-2.01480
C	-2.66155	-3.40789	-3.98731
H	-2.14373	-3.23230	-4.94123
H	-3.72166	-3.14893	-4.13306
H	-2.58183	-4.48179	-3.76045
C	-2.12113	-1.06589	-3.32194
H	-1.60350	-0.89894	-4.27836
H	-1.66894	-0.40527	-2.57664
H	-3.17741	-0.78494	-3.44171
C	-3.26231	-2.30723	1.99741

C	-4.30165	-3.17711	2.72157
H	-4.32025	-2.88672	3.78187
H	-4.04585	-4.24663	2.67297
H	-5.31730	-3.03272	2.32314
C	-3.71018	-0.83707	2.06758
H	-3.80028	-0.52085	3.11753
H	-4.69122	-0.71454	1.58322
H	-2.99399	-0.17547	1.56846
C	-1.89949	-2.51729	2.67563
H	-1.96113	-2.23377	3.73719
H	-1.11759	-1.91620	2.20562
H	-1.59716	-3.57400	2.61417
C	-2.16459	2.35636	0.58870
C	-3.79112	3.95124	0.55653
H	-4.60832	4.55085	0.17712
C	-3.15184	4.05132	1.74253
H	-3.33350	4.75202	2.54659
C	-3.71423	2.36815	-1.45262
C	-2.60039	2.40594	-2.51158
H	-2.26846	3.44137	-2.68137
H	-2.97171	1.99563	-3.46277
H	-1.73484	1.81834	-2.19309
C	-4.88416	3.23018	-1.95228
H	-5.22820	2.82634	-2.91547
H	-4.58218	4.27545	-2.11907
H	-5.73997	3.21053	-1.26069
C	-4.22503	0.93578	-1.21204
H	-4.65307	0.52548	-2.13869
H	-5.01081	0.93963	-0.44094
H	-3.41615	0.27708	-0.88003
C	-1.19165	2.90638	2.92048
C	-1.56924	3.86559	4.06123
H	-0.86902	3.70495	4.89327
H	-2.58608	3.67990	4.44087
H	-1.48426	4.92089	3.76110
C	0.22420	3.24425	2.43689
H	0.93209	3.18942	3.27777
H	0.25785	4.26272	2.02060
H	0.56971	2.52987	1.68021
C	-1.26426	1.46889	3.46217
H	-0.57580	1.36110	4.31358
H	-0.96670	0.73583	2.70556
H	-2.28354	1.23504	3.80368
Si	1.77011	0.26489	0.44878
Si	2.36184	1.90430	-1.17194
Si	3.05734	-1.72164	0.85918
C	0.96040	3.18751	-1.35878
H	1.36660	4.10960	-1.80681
H	0.49736	3.44755	-0.39884
H	0.16605	2.81701	-2.01928
C	2.64052	1.22129	-2.99623
C	1.42509	0.35577	-3.38287
H	0.48427	0.93076	-3.36751
H	1.29358	-0.49698	-2.70434
H	1.54790	-0.04053	-4.40872
C	2.74084	2.35907	-4.03416
H	2.82402	1.93296	-5.05204
H	3.61881	3.00061	-3.88231
H	1.84796	3.00461	-4.02669
C	3.90855	0.35342	-3.06607
H	4.01363	-0.10689	-4.06671
H	3.87759	-0.46375	-2.33034
H	4.82179	0.94080	-2.88060
C	3.88440	2.92685	-0.46499
C	4.49333	3.87496	-1.51460
H	5.25149	4.52660	-1.04090
H	3.74111	4.53512	-1.97620
H	5.00192	3.32545	-2.32136
C	4.99251	2.00689	0.07201
H	5.83950	2.60652	0.45586
H	5.39153	1.32717	-0.69559
H	4.62480	1.39243	0.90719
C	3.36794	3.77482	0.71696
H	4.20772	4.32328	1.18363
H	2.90933	3.14469	1.49470
H	2.62316	4.52315	0.40363
C	4.90039	-1.46548	0.43689
H	5.47435	-2.35435	0.74538
H	5.33263	-0.59859	0.95077
H	5.05670	-1.32282	-0.64233
C	2.57136	-3.37583	-0.07509
C	3.54257	-4.54185	0.20608
H	3.27019	-5.40940	-0.42456
H	3.51122	-4.88112	1.24994
H	4.58645	-4.28647	-0.03427
C	1.14757	-3.82472	0.29972
H	0.82932	-4.67520	-0.33244
H	0.40690	-3.02259	0.17458
H	1.09736	-4.16646	1.34590
C	2.65298	-3.07478	-1.58512
H	2.27893	-3.93312	-2.17304
H	3.69110	-2.89023	-1.90417
H	2.06486	-2.19205	-1.86534
C	2.99562	-1.87908	2.82378
C	3.71086	-0.64819	3.42299
H	3.63001	-0.66458	4.52634
H	3.26402	0.29584	3.07016
H	4.78451	-0.63020	3.17765
C	3.71319	-3.14529	3.32924
H	3.79612	-3.11940	4.43218
H	4.73512	-3.24221	2.92819
H	3.16141	-4.06190	3.07191
C	1.54905	-1.89363	3.35061
H	1.54337	-1.93264	4.45667
H	0.98520	-2.76694	2.99168
H	1.00114	-0.98709	3.04829

9^{I3}

Si	-0.49104	0.03707	0.01752
Si	1.72083	0.06561	0.32070
C	-1.98611	2.46782	0.70423
N	-1.36989	1.42848	0.28233
C	-2.76287	4.19209	1.96779
H	-2.86741	4.85079	2.81972
N	-1.91108	3.08972	1.95761
C	-3.37639	4.27027	0.76636
H	-4.09113	5.00527	0.41918
N	-2.91694	3.21966	-0.02149
C	0.44265	2.88879	2.69419
H	0.62199	3.93801	2.41253
H	0.72828	2.23433	1.86068
H	1.10020	2.63885	3.54094
C	-1.30088	1.22653	3.48730
H	-0.67391	0.95116	4.34836
H	-1.06218	0.53581	2.67284
H	-2.35719	1.09246	3.76444
C	-1.02567	2.68804	3.09448
C	-4.15719	1.46323	-1.22324
H	-4.97155	1.52276	-0.48424
H	-3.45341	0.68767	-0.90143
H	-4.58847	1.16600	-2.19085
C	-2.32603	2.79600	-2.39149
H	-1.85039	3.78510	-2.47335
H	-2.72840	2.51837	-3.37766
H	-1.55651	2.06948	-2.11674
C	-4.49723	3.87075	-1.80697
H	-4.05709	4.87551	-1.89915
H	-5.36129	3.91963	-1.12716
H	-4.87272	3.58028	-2.79885
C	-3.46069	2.83119	-1.35328
C	-1.33278	3.57271	4.31415
H	-1.10280	4.63242	4.12705
H	-0.69753	3.24339	5.14872
H	-2.38177	3.48382	4.63706
C	2.73886	-2.12558	2.76781
C	-2.44498	-2.08316	-0.50447
N	-1.50074	-1.26810	-0.20685
C	-3.84854	-3.46146	-1.64435
H	-4.27253	-3.99960	-2.48207
N	-2.76355	-2.59680	-1.76588
Si	2.52005	1.83158	-1.03994
C	1.27577	3.27405	-0.92587
H	0.24362	2.94387	-1.09026
H	1.51901	4.04321	-1.67662
H	1.31608	3.74595	0.06609
C	4.20740	2.56714	-0.34353
C	4.19036	2.48254	1.19623
H	3.29245	2.95332	1.62881
H	5.07407	2.99922	1.61629
H	4.21103	1.44242	1.55320
C	4.34219	4.05692	-0.73123
H	4.31923	4.21879	-1.81923
H	5.30736	4.45273	-0.36302
H	3.54868	4.67537	-0.28473
C	5.44938	1.81895	-0.86214
H	5.39785	0.73841	-0.67061
H	6.35943	2.19836	-0.36033
H	5.59691	1.96051	-1.94348
C	-4.21452	-3.50241	-0.34380
H	-5.00275	-4.08202	0.11918
N	-3.36545	-2.66245	0.37165
C	-0.57939	-2.56100	-2.92670
H	-0.42201	-3.61892	-2.67219
H	-0.10693	-1.95002	-2.15195
H	-0.07366	-2.35190	-3.88131
C	-2.30098	-0.75900	-3.35517
H	-1.78594	-0.48546	-4.28834
H	-1.90547	-0.12446	-2.55604
H	-3.37400	-0.54366	-3.46927
C	-2.07607	-2.24731	-3.04526
C	-3.91397	-0.81011	1.89995
H	-4.85983	-0.63650	1.36330
H	-3.14585	-0.16079	1.46493
H	-4.05545	-0.52302	2.95291
C	-2.20223	-2.57524	2.55455
H	-1.94026	-3.64229	2.48507
H	-2.30883	-2.31105	3.61769
H	-1.37479	-1.99649	2.13705
C	-4.62720	-3.14632	2.44165
H	-4.40456	-4.22254	2.37846
H	-5.60979	-2.95622	1.98375
H	-4.70335	-2.88434	3.50684
C	-3.51620	-2.29485	1.80873
C	-2.66608	-3.08541	-4.18945
H	-2.52934	-4.16431	-4.01991
H	-2.13825	-2.82516	-5.11814
H	-3.73559	-2.87957	-4.34924
C	2.62474	1.38139	-2.94996
C	1.19075	1.13105	-3.45838
H	1.20912	0.82349	-4.52108
H	0.56168	2.03306	-3.39019
H	0.69398	0.33029	-2.88815
C	3.23445	2.53276	-3.77357
H	3.20078	2.28894	-4.85230
H	4.28936	2.71448	-3.51905
H	2.68750	3.48021	-3.63939
C	3.44738	0.10200	-3.18262
H	3.04149	-0.74086	-2.60723
H	4.50285	0.22190	-2.89837
H	3.42663	-0.18170	-4.25208
Si	2.87335	-1.94925	0.80891
C	4.72422	-1.68823	0.43799
H	5.10096	-0.76168	0.89342
H	4.90399	-1.62662	-0.64612

H	5.32461	-2.52299	0.83563
C	2.36426	-3.57468	-0.15971
C	2.50314	-3.27489	-1.66489
H	1.92585	-2.39039	-1.96084
H	2.14292	-4.13256	-2.26290
H	3.55207	-3.09738	-1.95061
C	3.28873	-4.76959	0.15359
H	3.02949	-5.62209	-0.50244
H	3.19533	-5.12160	1.18935
H	4.34979	-4.53478	-0.02789
C	0.90919	-3.96986	0.15286
H	0.79646	-4.31103	1.19415
H	0.58698	-4.80589	-0.49671
H	0.20817	-3.13708	-0.00376
C	1.27551	-2.10973	3.24442
H	0.70092	-2.96350	2.85712
H	0.76328	-1.18566	2.93365
H	1.23075	-2.15946	4.34914
C	3.41017	-3.41348	3.28213
H	4.44082	-3.53278	2.91002
H	2.84372	-4.31378	3.00098
H	3.46153	-3.39881	4.38708
C	3.45789	-0.91767	3.40646
H	3.35993	-0.96009	4.50769
H	3.02320	0.03699	3.06944
H	4.53533	-0.90253	3.17765

g^{I4}

Si	-0.34254	-0.04358	0.00577
Si	1.81531	0.46976	0.43370
C	-2.43105	1.85894	0.82759
N	-1.52880	1.06151	0.39017
C	-3.71241	3.18535	2.15695
H	-4.04225	3.70090	3.04910
N	-2.60168	2.34585	2.12940
C	-4.24341	3.23272	0.91513
H	-5.09999	3.79533	0.56696
N	-3.47498	2.42143	0.08630
C	-0.30625	2.52968	3.05554
H	-0.30676	3.59979	2.80141
H	0.18608	1.97197	2.24802
H	0.30153	2.38801	3.96256
C	-1.75712	0.52097	3.58185
H	-1.10977	0.28740	4.44010
H	-1.38710	-0.04550	2.72215
H	-2.77869	0.18143	3.80957
C	-1.73655	2.03398	3.31031
C	-4.09098	0.57249	-1.42417
H	-4.93719	0.31278	-0.76949
H	-3.22557	-0.02733	-1.12398
H	-4.35869	0.30675	-2.45776
C	-2.61228	2.48366	-2.22923
H	-2.45651	3.57256	-2.19232
H	-2.81421	2.19442	-3.27173
H	-1.68646	1.99998	-1.90764
C	-5.03699	2.85679	-1.78128
H	-4.88691	3.94550	-1.72115
H	-5.92973	2.58541	-1.19758
H	-5.23999	2.60814	-2.83307
C	-3.79086	2.08016	-1.32951
C	-2.29235	2.75360	4.54993
H	-2.26634	3.84810	4.43769
H	-1.65936	2.49616	5.41103
H	-3.32046	2.44022	4.78882
C	2.95620	-1.55390	2.96471
C	-1.77678	-2.46534	-0.79426
N	-1.01677	-1.52704	-0.35373
C	-2.82114	-3.95390	-2.16033
H	-3.08090	-4.47384	-3.07312
N	-1.90446	-2.90738	-2.11525
Si	2.61688	2.19805	-0.98404
C	4.50131	2.30323	-0.71575
H	4.75666	2.29686	0.35325
H	4.89757	3.23415	-1.15307
H	5.02199	1.45862	-1.19066
C	2.39310	1.93949	-2.92201
C	3.34284	2.85079	-3.72734
H	3.16002	3.92051	-3.55570
H	3.21053	2.66752	-4.81058
H	4.40018	2.64989	-3.49406
C	0.94417	2.19456	-3.36444
H	0.23596	1.58358	-2.78290
H	0.80879	1.92461	-4.42920
H	0.64921	3.24935	-3.25600
C	2.74146	0.47918	-3.25721
H	3.75392	0.19909	-2.92476
H	2.69451	0.31363	-4.35067
H	2.03630	-0.21139	-2.77840
C	-3.26849	-4.17884	-0.90520
H	-3.97487	-4.92359	-0.56207
N	-2.63820	-3.27715	-0.05249
C	0.35720	-2.52207	-3.01864
H	0.61750	-3.57308	-2.82516
H	0.65829	-1.93108	-2.14921
H	0.93336	-2.17248	-3.88770
C	-1.52744	-0.90714	-3.52872
H	-0.95089	-0.50197	-4.37353
H	-1.31168	-0.28818	-2.65206
H	-2.59946	-0.81757	-3.75904
C	-1.14559	-2.37646	-3.28720
C	-3.68586	-1.72305	1.53970
H	-4.60566	-1.70841	0.93456
H	-3.04481	-0.89636	1.21430
H	-3.96068	-1.55686	2.59189
C	-1.69093	-3.14505	2.23059
H	-1.20558	-4.12665	2.11664
H	-1.93220	-2.99621	3.29395
H	-0.97485	-2.37798	1.92818
C	-3.91955	-4.19447	1.85437
H	-3.47090	-5.19152	1.72630
H	-4.88803	-4.16738	1.33241
H	-4.11997	-4.05421	2.92639
C	-2.97292	-3.07821	1.38704
C	-1.50439	-3.18590	-4.54257
H	-1.23545	-4.24794	-4.43814
H	-0.93284	-2.78101	-5.39004
H	-2.57262	-3.10879	-4.79727
C	1.90564	3.91965	-0.36079
C	2.37202	5.09357	-1.24384
H	2.06179	6.05323	-0.78901
H	1.92709	5.05807	-2.25007
H	3.46741	5.12934	-1.35899
C	0.36772	3.92795	-0.31377
H	0.00160	4.87733	0.12195
H	-0.02862	3.10929	0.29782
H	-0.07993	3.83719	-1.31338
C	2.44205	4.14980	1.06884
H	3.53584	4.28112	1.08241
H	2.19589	3.31081	1.73784
H	1.99804	5.06785	1.49808
Si	3.27008	-1.32406	1.02999
C	5.07210	-0.71702	0.89017
H	5.19962	0.28873	1.31309
H	5.40342	-0.68293	-0.15832
H	5.74488	-1.39918	1.43581
C	3.21267	-3.00669	0.02772
C	3.43814	-2.65629	-1.45575
H	2.72893	-1.90177	-1.81117
H	3.32496	-3.55749	-2.08711
H	4.45143	-2.26073	-1.63267
C	4.32860	-3.98990	0.43835
H	4.31677	-4.86789	-0.23520
H	4.21015	-4.36877	1.46203
H	5.33047	-3.53810	0.36055
C	1.84709	-3.69863	0.19216
H	1.70575	-4.07670	1.21746
H	1.76887	-4.56959	-0.48636
H	1.00755	-3.02454	-0.03283
C	1.47001	-1.79766	3.27686
H	1.10140	-2.73281	2.83158
H	0.84114	-0.97245	2.90882
H	1.31143	-1.87129	4.36996
C	3.77407	-2.71901	3.55366
H	4.84595	-2.65367	3.30605
H	3.40660	-3.69657	3.20695
H	3.69370	-2.71827	4.65714
C	3.38966	-0.25275	3.67456
H	3.16174	-0.31846	4.75548
H	2.86051	0.62636	3.27190
H	4.47208	-0.07016	3.58196

TS1

Si	0.19532	-3.12108	-0.59793
Si	-0.99459	-1.05949	-1.19155
N	-4.11018	0.38236	0.07370
N	-3.11542	0.73640	2.03819
N	-1.70660	-0.23674	0.36221
C	-2.86531	0.22119	0.74834
C	-4.98602	1.07647	0.90566
H	-5.96880	1.39746	0.59019
C	-4.58350	-0.21505	-1.22082
C	-2.28336	0.48919	3.25047
C	-2.26276	-3.97392	0.66725
H	-2.47911	-2.92466	0.91692
H	-2.79517	-4.60900	1.40126
H	-2.70178	-4.17843	-0.32198
C	-1.94023	-1.00462	3.31557
H	-2.86023	-1.60700	3.37177
H	-1.32863	-1.21992	4.20365
H	-1.39077	-1.30252	2.41880
C	-0.21081	-3.94708	2.10517
H	-0.24184	-2.87424	2.32968
H	0.83105	-4.28198	2.22976
H	-0.81581	-4.46258	2.87502
C	0.95281	-2.91144	-3.33997
H	1.01578	-3.32218	-4.36562
H	1.97838	-2.63854	-3.04175
H	0.35000	-1.98890	-3.39523
C	-1.05732	-4.33950	-2.91790
H	-0.97975	-4.73503	-3.94886
H	-1.73381	-3.47016	-2.94551
H	-1.53582	-5.12109	-2.30689
C	1.25238	-5.19273	-2.40456
H	1.35886	-5.56480	-3.44175
H	0.86278	-6.02522	-1.80375
H	2.26658	-4.96202	-2.04011
C	-0.53376	-5.77166	0.45554
H	-0.96765	-6.11270	-0.49589
H	-1.01904	-6.35586	1.26100
H	0.53427	-6.04308	0.45828
C	-4.38619	1.29292	2.09074
H	-4.76686	1.82687	2.95144
C	0.33512	-3.95372	-2.38206
C	-4.34093	-1.73155	-1.19850
H	-4.81701	-2.18643	-0.31643
H	-3.26859	-1.96373	-1.18848
H	-4.76163	-2.19257	-2.10514
C	-0.75089	-4.26620	0.69686
C	-3.88814	0.46159	-2.40889
H	-4.25350	0.03207	-3.35453
H	-2.80358	0.28841	-2.37182
H	-4.09814	1.54255	-2.41555

C	-1.03201	1.36780	3.19669
H	-0.43162	1.14435	2.30982
H	-0.40524	1.20559	4.08468
H	-1.31730	2.42838	3.16600
C	-6.10104	0.00475	-1.37427
H	-6.41836	-0.47498	-2.31105
H	-6.36672	1.07000	-1.45097
H	-6.67497	-0.45333	-0.55447
C	2.00180	-3.03802	0.02300
H	2.65113	-2.53582	-0.70832
H	2.40881	-4.04862	0.19800
H	2.07972	-2.47638	0.96274
C	-3.07492	0.85801	4.51713
H	-4.00665	0.27946	4.60500
H	-3.31413	1.93134	4.56517
H	-2.45070	0.62426	5.39204
Si	-0.28938	2.97742	-0.81084
Si	0.30081	0.65748	-0.34777
N	3.48976	-0.24457	1.92268
N	3.93483	-0.16259	-0.25448
N	1.75043	0.61591	0.51351
C	2.92834	0.11262	0.68936
C	4.78369	-0.71259	1.73063
H	5.41054	-1.06999	2.53674
C	2.84303	-0.06386	3.25238
C	4.05339	0.21972	-1.69697
C	1.16484	3.77332	-3.25353
H	1.96186	3.05223	-3.02287
H	1.14345	3.88725	-4.35308
H	1.46208	4.74583	-2.83643
C	4.84551	1.53796	-1.77849
H	5.84166	1.43060	-1.32215
H	4.97787	1.84243	-2.82845
H	4.30888	2.33978	-1.25118
C	-0.59820	2.03312	-3.53365
H	0.12886	1.21918	-3.39914
H	-1.57662	1.63748	-3.23231
H	-0.65156	2.25482	-4.61595
C	0.43688	4.17973	1.67299
H	1.04283	4.89873	2.25498
H	-0.62179	4.41461	1.86370
H	0.64033	3.18144	2.07735
C	2.30748	4.00477	0.03486
H	2.88152	4.73163	0.63973
H	2.56583	2.99548	0.38617
H	2.65522	4.10467	-1.00305
C	0.48465	5.71317	-0.28212
H	1.03467	6.43510	0.34993
H	0.78553	5.90254	-1.32215
H	-0.58665	5.95574	-0.19168
C	-1.25319	4.39962	-3.11438
H	-1.07760	5.34786	-2.58460
H	-1.20504	4.61611	-4.19773
H	-2.28277	4.07790	-2.89512
C	5.05654	-0.65657	0.41302
H	5.96359	-0.94290	-0.10305
C	0.79643	4.27389	0.17863
C	2.52539	1.42744	3.44507
H	3.45288	2.02055	3.41728
H	1.86428	1.78599	2.65155
H	2.03608	1.59220	4.41685
C	-0.21876	3.30854	-2.75588
C	1.58697	-0.94195	3.32411
H	1.06379	-0.77808	4.27714
H	0.89722	-0.71728	2.50592
H	1.86050	-2.00486	3.26259
C	2.69850	0.39632	-2.38369
H	2.17101	1.27524	-2.00432
H	2.86457	0.55824	-3.45858
H	2.05988	-0.48686	-2.26944
C	3.80495	-0.50477	4.36673
H	3.29981	-0.36312	5.33327
H	4.07140	-1.56961	4.28670
H	4.72652	0.09666	4.38319
C	-2.08925	3.24044	-0.26744
H	-2.39185	4.29329	-0.38342
H	-2.77145	2.61979	-0.86405
H	-2.22902	2.95400	0.78398
C	4.80238	-0.90353	-2.44408
H	5.85128	-1.00355	-2.13178
H	4.29979	-1.87124	-2.29890
H	4.80930	-0.67781	-3.52022

INT1

Si	1.74080	-2.63881	-0.66408
Si	-0.30512	-1.44950	-1.31412
N	-3.68699	-1.56181	0.20373
N	-2.90189	-0.76953	2.12691
N	-1.29745	-0.86599	0.32533
C	-2.50962	-1.07373	0.81770
C	-4.74616	-1.40760	1.09219
H	-5.77059	-1.62702	0.82938
C	-3.88634	-2.32112	-1.08696
C	-2.00105	-0.67280	3.32009
C	0.02452	-4.57427	0.62728
H	-0.65755	-3.75666	0.90400
H	-0.12545	-5.39530	1.35469
H	-0.28967	-4.94775	-0.36032
C	-0.99215	-1.82429	3.24982
H	-1.51577	-2.79282	3.25437
H	-0.31368	-1.79271	4.11330
H	-0.40076	-1.76219	2.33279
C	1.85760	-3.59398	2.03103
H	1.34304	-2.65885	2.28076
H	2.93859	-3.40894	2.13014
H	1.58025	-4.33991	2.79998
C	2.27180	-2.07161	-3.41078
H	2.55733	-2.38789	-4.43209
H	2.99321	-1.29958	-3.10034
H	1.27658	-1.60060	-3.48614
C	1.27351	-4.32469	-2.99232
H	1.54326	-4.62158	-4.02406
H	0.24770	-3.92340	-3.02007
H	1.25938	-5.24334	-2.38555
C	3.69584	-3.88105	-2.47764
H	3.97307	-4.15564	-3.51367
H	3.78783	-4.79043	-1.86882
H	4.45109	-3.16154	-2.12223
C	2.39275	-5.33240	0.34889
H	2.15620	-5.82623	-0.60476
H	2.25740	-6.08747	1.14713
H	3.46147	-5.06490	0.33667
C	-4.27520	-0.92146	2.25439
H	-4.82235	-0.65529	3.14864
C	2.27485	-3.28399	-2.45352
C	-2.99327	-3.56972	-1.06781
H	-3.21076	-4.18493	-0.18090
H	-1.93110	-3.29640	-1.06986
H	-3.17457	-4.17382	-1.96978
C	1.49332	-4.11252	0.62500
C	-3.61151	-1.41583	-2.29065
H	-3.74908	-1.98359	-3.22339
H	-2.57348	-1.05979	-2.28300
H	-4.30622	-0.56204	-2.30009
C	-1.33486	0.69964	3.34576
H	-0.70159	0.85308	2.46749
H	-0.70599	0.80158	4.23992
H	-2.09965	1.48821	3.37190
C	-5.34680	-2.80191	-1.19208
H	-5.44384	-3.36013	-2.13385
H	-6.06402	-1.96819	-1.23507
H	-5.62800	-3.48352	-0.37522
C	3.25653	-1.66724	-0.02866
H	3.56242	-0.89052	-0.74297
H	4.11844	-2.33609	0.13606
H	3.03586	-1.16048	0.91955
C	-2.82162	-0.83263	4.61237
H	-3.36017	-1.79122	4.64768
H	-3.53874	-0.01089	4.76000
H	-2.12299	-0.80925	5.46126
Si	-1.77533	2.40215	-0.80467
Si	-0.21905	0.59418	-0.28172
N	3.12792	1.48863	1.86604
N	3.31479	1.79649	-0.32952
N	1.10237	1.21675	0.61402
C	2.36641	1.46921	0.67549
C	4.44928	1.80858	1.58858
H	5.21964	1.86201	2.34603
C	2.59239	1.32468	3.24262
C	3.18142	2.14571	-1.77798
C	-0.98556	3.85943	-3.26021
H	0.07259	3.63098	-3.07613
H	-1.10522	3.96679	-4.35416
H	-1.19790	4.84282	-2.81826
C	3.28626	3.67691	-1.92032
H	4.24176	4.05303	-1.52438
H	3.21802	3.96647	-2.98057
H	2.47126	4.17053	-1.37400
C	-1.65450	1.47757	-3.55806
H	-0.63018	1.10346	-3.42550
H	-2.33050	0.65876	-3.28310
H	-1.80326	1.67582	-4.63608
C	-1.59542	3.78130	1.68353
H	-1.37880	4.69334	2.27029
H	-2.62516	3.47463	1.92436
H	-0.91544	2.99808	2.03540
C	0.05046	4.53851	-0.01878
H	0.24242	5.43718	0.59728
H	0.77040	3.76562	0.28652
H	0.26073	4.81288	-1.06147
C	-2.37621	5.18063	-0.21726
H	-2.20008	6.07108	0.41492
H	-2.25648	5.50032	-1.26189
H	-3.42876	4.88718	-0.07411
C	-3.38320	3.19928	-3.05442
H	-3.68274	4.09997	-2.49730
H	-3.47998	3.43272	-4.13101
H	-4.11390	2.40742	-2.82953
C	4.56246	1.99600	0.26257
H	5.44459	2.24973	-0.31099
C	-1.39864	4.05613	0.18216
C	1.59042	2.45970	3.51059
H	2.10608	3.43173	3.46497
H	0.79630	2.46079	2.75983
H	1.13887	2.35370	4.50862
C	-1.93441	2.75672	-2.74596
C	1.97315	-0.07264	3.37272
H	1.49629	-0.19091	4.35659
H	1.22841	-0.24116	2.59221
H	2.75322	-0.84176	3.27563
C	1.86619	1.67176	-2.38053
H	1.01407	2.17631	-1.91769
H	1.85334	1.92046	-3.45125
H	1.73462	0.58981	-2.27990
C	3.72725	1.43528	4.27473
H	3.29481	1.28831	5.27541
H	4.49598	0.66117	4.12955
H	4.20771	2.42521	4.26556
C	-3.49715	1.84247	-0.21337
H	-4.23727	2.65075	-0.32171
H	-3.85218	0.97822	-0.78951
H	-3.47298	1.54194	0.84357
C	4.32421	1.46579	-2.56345
H	5.31555	1.87234	-2.31896

H	4.33842	0.38331	-2.37425
H	4.16747	1.62388	-3.64058

TS2

Si	-3.41609	-0.53467	-0.50286
Si	-1.44159	0.41949	-1.59832
N	0.13573	4.00961	0.29759
N	0.87852	3.12079	2.20081
N	0.15193	1.57268	0.47992
C	0.36775	2.76197	0.93401
C	0.54745	5.03840	1.13858
H	0.52591	6.08063	0.85159
C	-0.68491	4.27603	-0.92585
C	1.00524	2.21916	3.38108
C	-3.35509	1.37503	1.67888
H	-2.32945	1.64457	1.39367
H	-3.46219	1.58107	2.76029
H	-4.04441	2.04832	1.14757
C	-0.37999	1.63208	3.68936
H	-1.09864	2.44280	3.88471
H	-0.33584	0.98401	4.57640
H	-0.74968	1.04293	2.84565
C	-2.62280	-0.97037	2.15246
H	-1.60470	-0.83751	1.76122
H	-2.85846	-2.04502	2.09684
H	-2.61127	-0.69251	3.22187
C	-4.55199	-0.21502	-3.11062
H	-5.39847	0.06200	-3.76687
H	-4.32533	-1.27617	-3.31050
H	-3.67896	0.37923	-3.42384
C	-5.22023	1.53138	-1.44841
H	-6.00631	1.86158	-2.15345
H	-4.32833	2.14859	-1.63974
H	-5.57906	1.76069	-0.43258
C	-6.20408	-0.77703	-1.33575
H	-7.01358	-0.46497	-2.02246
H	-6.57558	-0.63062	-0.31237
H	-6.05392	-1.85802	-1.48640
C	-5.05588	-0.44702	1.90606
H	-5.82265	0.22242	1.48747
H	-5.08961	-0.32978	3.00579
H	-5.35148	-1.48470	1.68135
C	0.99892	4.50226	2.28810
H	1.42866	5.00779	3.14250
C	-4.92431	0.03230	-1.63238
C	-2.10975	3.75712	-0.68582
H	-2.54847	4.23811	0.20200
H	-2.12019	2.67458	-0.52083
H	-2.74686	3.96796	-1.55676
C	-3.64561	-0.10843	1.38924
C	-0.03441	3.64259	-2.15884
H	-0.70748	3.71851	-3.02517
H	0.17125	2.58302	-1.99682
H	0.90788	4.15587	-2.40220
C	2.04920	1.14203	3.08305
H	1.73637	0.51519	2.24400
H	2.19773	0.49403	3.95788
H	3.01032	1.61328	2.83408
C	-0.77907	5.79124	-1.18362
H	-1.35420	5.94115	-2.10881
H	0.21086	6.24793	-1.33419
H	-1.30466	6.32523	-0.37805
C	-3.42818	-2.43897	-0.62029
H	-4.29448	-2.84479	-0.07184
H	-2.51439	-2.87457	-0.19743
H	-3.51700	-2.76807	-1.66726
C	1.48102	3.01693	4.60684
H	0.76304	3.79532	4.90513
H	2.46615	3.47992	4.44249
H	1.58060	2.31933	5.45106
Si	2.72246	0.54751	-1.42972
Si	0.53270	0.07547	-0.34466
N	0.45251	-3.34359	1.91834
N	-0.16718	-3.59192	-0.22170
N	0.71970	-1.40480	0.53868
C	0.38349	-2.63432	0.69451
C	-0.10333	-4.60719	1.76833
H	-0.23347	-5.29753	2.59134
C	1.10914	-2.87934	3.17144
C	0.04894	-3.72205	-1.70109
C	3.08629	-1.04121	-3.86811
H	2.39348	-1.78979	-3.45800
H	3.01554	-1.10301	-4.97010
H	4.10575	-1.34862	-3.59535
C	1.47386	-4.25169	-1.93920
H	1.61695	-5.21297	-1.42177
H	1.65837	-4.40413	-3.01417
H	2.21668	-3.54229	-1.56011
C	1.39792	0.78736	-4.01024
H	0.57399	0.13500	-3.68956
H	1.11104	1.81650	-3.75311
H	1.45052	0.73293	-5.11387
C	4.42863	0.05467	0.80700
H	5.25327	-0.49827	1.29428
H	4.67281	1.12623	0.86684
H	3.52699	-0.11778	1.40181
C	4.03093	-1.95032	-0.61251
H	4.86729	-2.44757	-0.08569
H	3.10376	-2.20987	-0.08480
H	3.98688	-2.38175	-1.62201
C	5.56853	-0.13383	-1.38708
H	6.41001	-0.60981	-0.84924
H	5.57890	-0.53179	-2.41164
H	5.79026	0.94392	-1.43990
C	3.81105	1.35522	-3.98731
H	4.82841	1.15765	-3.62317
H	3.83380	1.25634	-5.08891
H	3.57379	2.40670	-3.76289
C	-0.47159	-4.76149	0.48554
H	-0.96293	-5.60961	0.02851
C	4.24953	-0.42820	-0.64351
C	2.54950	-2.44911	2.85605
H	3.12511	-3.29799	2.45566
H	2.55585	-1.65003	2.11231
H	3.04803	-2.08812	3.76861
C	2.75565	0.39068	-3.40024
C	0.29146	-1.73112	3.76908
H	0.77523	-1.34546	4.67940
H	0.20135	-0.92035	3.04519
H	-0.71928	-2.07635	4.03083
C	-0.14336	-2.40056	-2.44125
H	0.61084	-1.66704	-2.15028
H	-0.04251	-2.56459	-3.52334
H	-1.15008	-1.99372	-2.25404
C	1.16648	-4.02557	4.19514
H	1.68890	-3.65961	5.09117
H	0.16520	-4.35413	4.51249
H	1.72505	-4.89409	3.81424
C	3.10985	2.36940	-1.01732
H	4.16479	2.59979	-1.23631
H	2.48861	3.06302	-1.59513
H	2.92994	2.57747	0.04773
C	-0.96657	-4.72724	-2.28492
H	-0.75693	-5.76388	-1.98681
H	-1.99500	-4.47392	-1.99416
H	-0.90152	-4.69419	-3.38209

INT2

Si	-3.53314	0.06838	-0.51530
Si	-1.43111	0.29958	-1.75977
N	0.89244	3.78337	-0.17097
N	1.70230	3.26218	1.84205
N	0.77229	1.44672	0.57310
C	1.07860	2.68390	0.71047
C	1.45311	4.92879	0.39410
H	1.51262	5.87566	-0.12621
C	-0.00183	3.82916	-1.36166
C	1.78263	2.63257	3.19006
C	-2.93600	1.73297	1.78775
H	-1.87609	1.73903	1.49400
H	-2.97240	1.88279	2.88304
H	-3.42623	2.60188	1.32350
C	0.34819	2.37166	3.68303
H	-0.20153	3.32260	3.76545
H	0.35987	1.88955	4.67212
H	-0.19083	1.72044	2.98676
C	-2.83066	-0.73109	2.10079
H	-1.79184	-0.76623	1.75228
H	-3.27957	-1.72293	1.93784
H	-2.80984	-0.56016	3.19207
C	-4.58625	1.09242	-3.00838
H	-5.41751	1.55354	-3.57469
H	-4.43758	0.07591	-3.40910
H	-3.66961	1.65845	-3.23403
C	-5.03151	2.54380	-1.02216
H	-5.76990	3.08878	-1.63975
H	-4.07986	3.08841	-1.10152
H	-5.36979	2.61711	0.02203
C	-6.29444	0.40675	-1.33498
H	-7.06624	0.99776	-1.86303
H	-6.61073	0.32618	-0.28531
H	-6.31208	-0.60472	-1.76919
C	-5.05376	0.38757	1.95002
H	-5.65728	1.22479	1.57001
H	-5.04168	0.47283	3.05303
H	-5.58123	-0.54888	1.70587
C	1.93431	4.61402	1.61209
H	2.46573	5.24965	2.30853
C	-4.91554	1.08389	-1.50139
C	-1.36956	3.24499	-0.98881
H	-1.83535	3.82014	-0.17516
H	-1.27689	2.21697	-0.59695
H	-2.03847	3.25631	-1.85900
C	-3.61029	0.40075	1.41124
C	0.62542	3.08019	-2.54012
H	-0.06486	3.05985	-3.39617
H	0.85094	2.04435	-2.27480
H	1.56119	3.56779	-2.84895
C	2.61053	1.34522	3.11459
H	2.14094	0.62720	2.43990
H	2.69887	0.89073	4.11273
H	3.62136	1.56611	2.74167
C	-0.23585	5.28766	-1.79698
H	-0.92869	5.28597	-2.65103
H	0.69253	5.77385	-2.13156
H	-0.68787	5.89183	-0.99641
C	-4.01990	-1.76554	-0.73985
H	-4.98158	-1.96900	-0.24188
H	-3.25989	-2.41923	-0.29280
H	-4.12909	-2.02792	-1.80409
C	2.47690	3.58823	4.17424
H	1.90924	4.51785	4.32952
H	3.49740	3.84151	3.84754
H	2.55459	3.08457	5.14883
Si	2.74973	-0.14847	-1.60827
Si	0.57993	0.00448	-0.36014
N	-0.19414	-2.97018	2.29285
N	-0.93068	-3.43732	0.22780
N	0.46181	-1.43862	0.57631
C	-0.14255	-2.49750	0.96258
C	-1.02374	-4.08239	2.36484
H	-1.28021	-4.56836	3.29733

C	0.61507	-2.45023	3.43161
C	-0.74474	-3.84046	-1.20214
C	2.67489	-2.19378	-3.70014
H	1.84480	-2.67299	-3.16333
H	2.55761	-2.44336	-4.77128
H	3.60658	-2.66910	-3.36028
C	0.56998	-4.63126	-1.32096
H	0.54436	-5.51468	-0.66420
H	0.72917	-4.97104	-2.35624
H	1.42129	-4.00765	-1.02907
C	1.46341	-0.06513	-4.20949
H	0.51272	-0.38934	-3.76216
H	1.47092	1.03506	-4.18673
H	1.44745	-0.36234	-5.27499
C	4.28628	-0.55096	0.73043
H	4.95234	-1.15862	1.37107
H	4.75441	0.43856	0.61527
H	3.34703	-0.40813	1.27481
C	3.55276	-2.67867	-0.34743
H	4.26456	-3.21410	0.30889
H	2.57689	-2.67202	0.15283
H	3.46339	-3.26735	-1.27097
C	5.41153	-1.34569	-1.34384
H	6.14261	-1.85797	-0.69031
H	5.35273	-1.92812	-2.27511
H	5.83525	-0.35873	-1.58762
C	3.94367	-0.11161	-4.24923
H	4.89027	-0.49135	-3.84132
H	3.90588	-0.40754	-5.31457
H	3.98532	0.98796	-4.22228
C	-1.46403	-4.36992	1.12600
H	-2.15314	-5.14700	0.82213
C	4.05301	-1.25024	-0.62119
C	2.10434	-2.50663	3.05629
H	2.40221	-3.53720	2.80829
H	2.30740	-1.87115	2.19141
H	2.72065	-2.15681	3.89863
C	2.70102	-0.66368	-3.51386
C	0.18721	-1.01694	3.76429
H	0.83999	-0.60404	4.54642
H	0.25788	-0.38099	2.87748
H	-0.84740	-0.99469	4.13206
C	-0.70969	-2.62679	-2.13163
H	0.17059	-2.00859	-1.94542
H	-0.67085	-2.95152	-3.18080
H	-1.63032	-2.02711	-2.01844
C	0.39360	-3.32916	4.67288
H	1.00799	-2.92941	5.49280
H	-0.65392	-3.31454	5.01057
H	0.70158	-4.37234	4.50370
C	3.54104	1.59203	-1.55657
H	4.63508	1.50632	-1.65140
H	3.19479	2.23407	-2.37553
H	3.32232	2.10540	-0.60922
C	-1.91457	-4.74042	-1.64688
H	-1.89718	-5.72429	-1.15757
H	-2.88705	-4.26520	-1.45887
H	-1.82619	-4.92059	-2.72810

TS3

Si	-3.41611	-0.01090	-1.04426
Si	-1.26374	-1.10300	-1.41918
N	3.61640	-0.57425	-2.33790
N	4.32424	0.35682	-0.44374
N	1.95912	-0.18707	-0.64270
C	3.15799	-0.14407	-1.07035
C	4.98236	-0.34902	-2.45131
H	5.55526	-0.60243	-3.33378
C	2.76792	-1.17353	-3.40427
C	4.55302	0.90468	0.92467
C	-4.07602	-1.24426	-3.62626
H	-3.05652	-1.65625	-3.68929
H	-4.44980	-1.11742	-4.65998
H	-4.70542	-2.00513	-3.14338
C	5.21102	2.29365	0.79092
H	6.19113	2.25127	0.29365
H	5.36560	2.72929	1.78987
H	4.56215	2.96905	0.21469
C	-3.22247	1.10041	-3.66205
H	-2.16496	0.78525	-3.68705
H	-3.26086	2.11388	-3.23353
H	-3.55934	1.17553	-4.71294
C	-3.85899	-1.21802	1.47825
H	-4.48368	-1.78539	2.19333
H	-3.58356	-0.27323	1.96593
H	-2.93675	-1.79049	1.32705
C	-5.06408	-2.33443	-0.41930
H	-5.62520	-2.90901	0.34112
H	-4.21455	-2.95651	-0.73998
H	-5.73185	-2.20804	-1.28522
C	-5.87349	-0.14587	0.49775
H	-6.50595	-0.69939	1.21712
H	-6.49485	0.06676	-0.38347
H	-5.61664	0.81629	0.96792
C	-5.55788	0.64047	-2.90730
H	-6.26868	-0.08359	-2.48127
H	-5.87724	0.83033	-3.94957
H	-5.66864	1.58777	-2.35513
C	5.41154	0.21224	-1.30387
H	6.41524	0.51673	-1.03129
C	-4.61905	-0.97990	0.16145
C	1.67695	-0.17072	-3.81070
H	2.13148	0.76028	-4.18542
H	1.04205	0.07182	-2.95474
H	1.04333	-0.59737	-4.60297
C	-4.11231	0.10786	-2.88509
C	2.15713	-2.47914	-2.88093
H	1.50726	-2.93588	-3.64228
H	1.54959	-2.28514	-1.99466
H	2.95001	-3.19659	-2.61763
C	3.26363	1.06511	1.72736
H	2.55829	1.75331	1.25415
H	3.52331	1.46144	2.72054
H	2.75107	0.11211	1.86466
C	3.62359	-1.48910	-4.64105
H	2.97138	-1.93108	-5.40820
H	4.41632	-2.22028	-4.42086
H	4.07976	-0.58514	-5.07333
C	-3.34817	1.76936	-0.36989
H	-4.32036	2.27785	-0.47834
H	-2.58912	2.37705	-0.87807
H	-3.08482	1.76303	0.69741
C	5.49063	-0.05833	1.68213
H	6.46355	-0.16854	1.18035
H	5.03395	-1.05598	1.75922
H	5.67779	0.31824	2.69960
Si	0.61159	-2.49369	1.31028
Si	0.38310	-0.16304	-0.01798
N	-0.24466	3.56065	-0.12100
N	-0.94354	3.15800	1.95504
N	0.06764	1.30962	0.80017
C	-0.32154	2.53182	0.85164
C	-0.83435	4.71960	0.38225
H	-0.94901	5.62497	-0.19838
C	0.48831	3.51644	-1.41803
C	-0.99777	2.60170	3.33380
C	-1.76560	-4.06062	0.48541
H	-2.05049	-3.27667	-0.23836
H	-2.17320	-5.01034	0.09219
H	-2.27728	-3.85200	1.43547
C	0.44809	2.43634	3.83634
H	0.93257	3.42317	3.90640
H	0.46434	1.96632	4.83115
H	1.03038	1.81554	3.14896
C	0.34475	-4.51124	-0.74920
H	0.08637	-3.75845	-1.50694
H	1.43927	-4.62458	-0.72853
H	-0.07789	-5.47408	-1.09130
C	0.95281	-0.94239	3.66597
H	0.71382	-0.72019	4.72265
H	2.04965	-0.92092	3.57718
H	0.55483	-0.12793	3.05389
C	-1.10596	-2.36746	3.66260
H	-1.21492	-2.18722	4.74871
H	-1.70551	-1.60659	3.14574
H	-1.55621	-3.34950	3.45188
C	1.15683	-3.37334	4.06401
H	1.10520	-3.12351	5.14071
H	0.75289	-4.38671	3.95175
H	2.22358	-3.40211	3.79196
C	0.06977	-5.32605	1.58706
H	-0.44601	-5.22580	2.55258
H	-0.28207	-6.27068	1.13301
H	1.14665	-5.44473	1.78439
C	-1.25089	4.47640	1.64006
H	-1.77408	5.13990	2.31624
C	0.37756	-2.30919	3.25983
C	1.95000	3.12074	-1.16369
H	2.42360	3.84823	-0.48647
H	2.01516	2.12479	-0.72183
H	2.51205	3.10721	-2.11017
C	-0.24037	-4.15244	0.63180
C	-0.21229	2.54495	-2.37552
H	0.36529	2.43251	-3.30394
H	-0.33260	1.55380	-1.92175
H	-1.21127	2.91968	-2.63395
C	-1.78634	1.28424	3.32349
H	-1.41008	0.60975	2.55012
H	-1.71420	0.78281	4.29956
H	-2.84821	1.48887	3.11940
C	0.48167	4.90718	-2.07694
H	1.03171	4.83876	-3.02681
H	-0.53589	5.25414	-2.31182
H	0.98378	5.66298	-1.45442
C	2.47978	-2.80037	1.07151
H	2.75245	-3.80460	1.43523
H	2.77518	-2.72069	0.01751
H	3.06919	-2.06495	1.63666
C	-1.72791	3.57669	4.27199
H	-1.19153	4.53026	4.38905
H	-2.75420	3.78263	3.93105
H	-1.79449	3.11159	5.26663

TS4

Si	0.88182	-0.53344	-1.54099
Si	-0.97490	0.09795	-0.26812
Si	-2.62678	1.46894	-1.53521
Si	-0.81239	-2.91809	-1.26679
N	4.50610	-0.23233	0.40791
N	2.36209	-0.31806	-0.69490
N	-1.03165	0.49606	1.37157
N	-0.10901	1.70706	3.24518
N	3.94198	1.52371	-0.86876
N	-2.13646	0.80669	3.49408
C	4.75229	-1.68228	0.67228
C	3.47414	0.25772	-0.43128
C	-1.08141	0.94559	2.57101
C	1.34076	1.76979	2.87860
C	-4.45565	0.92782	-1.40890
H	-4.71951	0.52182	-0.42368
H	-4.71005	0.16990	-2.16215
H	-5.09792	1.80419	-1.59402

C	-2.59325	3.25900	-0.71979
C	-2.22404	1.49773	-3.45905
C	0.28424	-3.99487	-0.03840
C	-0.41226	-3.49936	-3.04535
H	-0.58530	-4.58352	-3.16195
H	0.63236	-3.27859	-3.30363
H	-1.04842	-2.97411	-3.77539
C	-2.73548	-3.37321	-1.07468
C	5.49856	0.74059	0.52356
H	6.35233	0.63447	1.18101
C	5.15766	1.79755	-0.23942
H	5.67059	2.74551	-0.33748
C	3.43990	2.28772	-2.05025
C	-3.20402	-0.23399	3.41587
C	-1.81803	1.50163	4.65778
H	-2.50172	1.59867	5.49142
C	-0.59566	2.05177	4.50433
H	-0.06146	2.70218	5.18485
C	-4.07217	-0.01175	2.17095
H	-4.59375	0.95436	2.23207
H	-3.46481	-0.01402	1.26373
H	-4.82286	-0.81160	2.08826
C	-4.11307	-0.14420	4.65127
H	-4.91298	-0.89170	4.54702
H	-3.57527	-0.36568	5.58508
H	-4.58930	0.84476	4.73708
C	-2.51358	-1.60838	3.40070
H	-1.94023	-1.75217	4.33017
H	-3.25554	-2.41628	3.31765
H	-1.82289	-1.68672	2.55391
C	3.62744	-2.25711	1.53931
H	3.66384	-1.83056	2.55188
H	2.65336	-2.03396	1.10371
H	3.73389	-3.34816	1.62282
C	6.07642	-1.85935	1.43229
H	6.07253	-1.31783	2.39110
H	6.20475	-2.92853	1.65664
H	6.94777	-1.53717	0.84287
C	4.86508	-2.40367	-0.68438
H	3.95955	-2.25918	-1.28529
H	5.72326	-2.00703	-1.25003
H	5.01311	-3.48422	-0.53649
C	1.53781	2.48988	1.54430
H	1.12619	3.50910	1.58138
H	2.61011	2.54885	1.31024
H	1.05788	1.93847	0.73323
C	2.11503	2.53909	3.96049
H	3.16947	2.59299	3.65344
H	1.74808	3.57118	4.07367
H	2.08030	2.03631	4.93852
C	1.88987	0.34011	2.79143
H	2.96086	0.37072	2.55098
H	1.75257	-0.19146	3.74637
H	1.39147	-0.22139	1.99368
C	4.39974	3.45025	-2.36060
H	5.41070	3.09844	-2.61517
H	4.00864	3.99904	-3.22952
H	4.46817	4.16454	-1.52591
C	3.40725	1.36321	-3.28242
H	4.40822	0.94258	-3.46748
H	2.70019	0.53261	-3.16069
H	3.09956	1.93537	-4.17122
C	2.06033	2.89076	-1.75608
H	1.32831	2.12363	-1.48310
H	2.12061	3.61262	-0.92980
H	1.68185	3.41555	-2.64514
C	-3.04663	-4.81367	-1.53926
H	-2.57963	-5.58424	-0.91462
H	-4.13959	-4.98134	-1.49449
H	-2.74000	-4.98976	-2.58160
C	-3.21215	-3.19379	0.37178
H	-3.03830	-2.16740	0.71939
H	-4.29871	-3.38870	0.45159
H	-2.70679	-3.87505	1.07278
C	-3.55316	-2.43317	-1.96944
H	-3.31755	-2.56936	-3.03584
H	-4.63616	-2.62153	-1.84503
H	-3.36982	-1.38508	-1.71345
C	-0.21043	-5.44546	0.12444
H	0.50851	-6.01290	0.74571
H	-1.18555	-5.50558	0.62902
H	-0.29037	-5.97143	-0.84022
C	0.31359	-3.34048	1.35566
H	1.03694	-3.85373	2.01572
H	0.59008	-2.27734	1.31723
H	-0.66955	-3.39898	1.84469
C	1.70331	-4.06821	-0.63114
H	2.12088	-3.07469	-0.83397
H	2.38811	-4.58173	0.06739
H	1.71592	-4.63430	-1.57565
C	-1.15877	3.75779	-0.48939
H	-0.59028	3.85476	-1.42459
H	-1.16968	4.75278	-0.00564
H	-0.60564	3.08127	0.17089
C	-3.33852	4.29164	-1.58770
H	-3.40261	5.25406	-1.04619
H	-2.81842	4.49143	-2.53630
H	-4.37011	3.98551	-1.82411
C	-3.30198	3.18267	0.64892
H	-4.36048	2.89405	0.55492
H	-2.81589	2.46867	1.32589
H	-3.27688	4.17318	1.14036
C	-3.40313	2.10612	-4.25197
H	-3.58654	3.16132	-4.00879
H	-3.18117	2.05671	-5.33418
H	-4.34295	1.55548	-4.09228
C	-2.02425	0.05713	-3.97014
H	-1.75596	0.07369	-5.04278
H	-1.21037	-0.46720	-3.44464
H	-2.93980	-0.54246	-3.87641
C	-0.94913	2.29868	-3.77534
H	-1.03139	3.35717	-3.48461
H	-0.07161	1.87003	-3.27247
H	-0.74697	2.27395	-4.86219

INT3

Si	-1.48683	0.16532	-1.58643
Si	0.89253	-0.04100	-0.50490
Si	1.58442	-2.37890	-1.13786
Si	1.81612	1.80385	-1.92349
N	-4.75779	1.45168	0.14059
N	-2.78259	0.23094	-0.51559
N	1.33615	0.21162	1.15094
N	0.61573	-0.25529	3.42361
N	-4.93702	-0.75828	-0.05187
N	2.81216	-0.32879	2.99068
C	-4.24101	2.84618	0.08113
C	-4.02922	0.30044	-0.18612
C	1.55463	-0.08419	2.37296
C	-0.73549	0.38107	3.46009
C	3.41263	-2.66876	-1.60400
H	4.11977	-2.21158	-0.90157
H	3.64133	-2.29220	-2.61040
H	3.59953	-3.75549	-1.60395
C	1.29960	-3.57559	0.40222
C	0.60718	-2.98102	-2.73457
C	1.15419	3.49709	-1.16710
C	1.02754	1.68573	-3.65935
H	1.16675	2.63891	-4.19496
H	-0.04884	1.46500	-3.62434
H	1.50689	0.89666	-4.25728
C	3.74539	1.90321	-2.30870
C	-6.06351	1.08876	0.46567
H	-6.81619	1.80434	0.76981
C	-6.17234	-0.25126	0.34789
H	-7.03439	-0.87824	0.53429
C	-4.67384	-2.17599	-0.42234
C	4.11923	0.19798	2.49932
C	2.60789	-0.69623	4.31921
H	3.40874	-1.02783	4.96802
C	1.28689	-0.65360	4.57898
H	0.77399	-0.94050	5.48820
C	4.46004	-0.39358	1.12784
H	4.61428	-1.47809	1.20678
H	3.65409	-0.20777	0.41402
H	5.38476	0.05883	0.74083
C	5.24242	-0.19566	3.47253
H	6.20008	0.14494	3.05219
H	5.13013	0.27634	4.45974
H	5.30295	-1.28736	3.60185
C	4.01348	1.73150	2.45009
H	3.77600	2.12496	3.45125
H	4.96148	2.17976	2.11595
H	3.21953	2.03840	1.76099
C	-3.05864	2.97347	1.05288
H	-3.40923	2.81549	2.08405
H	-2.28510	2.23059	0.83934
H	-2.60868	3.97484	0.98713
C	-5.33777	3.82716	0.52528
H	-5.67110	3.63549	1.55666
H	-4.92389	4.84552	0.49442
H	-6.21145	3.80447	-0.14362
C	-3.85233	3.18521	-1.36984
H	-3.08850	2.50373	-1.75919
H	-4.73688	3.11655	-2.02227
H	-3.45614	4.21034	-1.42506
C	-1.66629	-0.27104	2.43688
H	-1.81443	-1.33437	2.67324
H	-2.64805	0.22448	2.44616
H	-1.26829	-0.18978	1.42277
C	-1.35878	0.20253	4.85470
H	-2.36723	0.64130	4.84047
H	-1.46473	-0.86016	5.12216
H	-0.78444	0.71433	5.64132
C	-0.56146	1.88640	3.19099
H	-1.51392	2.41490	3.33329
H	0.17813	2.31173	3.88758
H	-0.21490	2.06434	2.16660
C	-5.90420	-3.03574	-0.09107
H	-6.78765	-2.74535	-0.67941
H	-5.67304	-4.08173	-0.33936
H	-6.15708	-2.99537	0.97955
C	-4.41366	-2.26120	-1.93833
H	-5.30203	-1.92227	-2.49419
H	-3.56434	-1.63796	-2.24335
H	-4.19621	-3.30051	-2.22863
C	-3.48689	-2.70334	0.39639
H	-2.59121	-2.09779	0.23915
H	-3.72419	-2.68263	1.47128
H	-3.26340	-3.74153	0.10954
C	4.00865	2.71764	-3.59531
H	3.63734	3.75019	-3.53816
H	5.09862	2.77305	-3.77593
H	3.56056	2.24852	-4.48395
C	4.55433	2.53212	-1.16191
H	4.36715	2.03471	-0.20369
H	5.63818	2.45253	-1.36940
H	4.32944	3.60154	-1.03290
C	4.26292	0.47746	-2.55544
H	3.69136	-0.03879	-3.34382
H	5.32102	0.49816	-2.87779
H	4.20635	-0.13612	-1.65076
C	1.65162	4.71968	-1.96325
H	1.18135	5.64023	-1.56859

H	2.73978	4.85677	-1.88339
H	1.39467	4.65896	-3.03281
C	1.55445	3.67210	0.30918
H	1.06929	4.57114	0.73449
H	1.25367	2.80673	0.91600
H	2.63882	3.80273	0.43158
C	-0.38127	3.48093	-1.24894
H	-0.81061	2.65561	-0.66160
H	-0.80213	4.41477	-0.83143
H	-0.74904	3.39109	-2.28218
C	-0.01414	-3.25236	1.12734
H	-0.88368	-3.38114	0.47112
H	-0.15476	-3.92407	1.99549
H	-0.02615	-2.22336	1.50624
C	1.27252	-5.05744	-0.02279
H	1.19833	-5.69794	0.87611
H	0.41008	-5.29957	-0.66072
H	2.18696	-5.35994	-0.55761
C	2.46111	-3.40643	1.40081
H	3.42783	-3.71012	0.96914
H	2.55785	-2.37585	1.75906
H	2.28737	-4.04279	2.28877
C	1.24396	-4.24430	-3.35611
H	1.24649	-5.10821	-2.67855
H	0.67241	-4.53871	-4.25622
H	2.28093	-4.06764	-3.68011
C	0.68424	-1.86693	-3.79739
H	0.23865	-2.21244	-4.74904
H	0.13111	-0.96688	-3.49701
H	1.72437	-1.57073	-4.01293
C	-0.86989	-3.27677	-2.42628
H	-0.99378	-4.14541	-1.76195
H	-1.37127	-2.42152	-1.94487
H	-1.43025	-3.48755	-3.35575

INT4

Si	0.36858	0.58330	2.49912
Si	0.70257	0.42698	0.00503
N	4.04720	-1.77724	-0.07687
N	2.54400	-2.96210	-1.21912
N	1.81123	-0.83421	-0.37196
C	2.70146	-1.72814	-0.53318
C	4.62326	-2.99081	-0.44894
H	5.63936	-3.25873	-0.18295
C	4.91536	-0.71826	0.50786
C	1.34423	-3.36688	-1.99727
C	3.71590	-3.70506	-1.14205
H	3.82023	-4.69583	-1.56491
C	1.20721	1.93981	3.67803
C	0.62986	-1.22137	3.23994
C	-1.49751	0.93667	2.64281
H	-1.87585	0.67952	3.64537
H	-2.06639	0.36805	1.89478
H	-1.70284	2.00567	2.47835
Si	1.39116	2.44778	-1.32588
Si	-1.39999	-0.25514	-1.30623
N	-5.04221	0.37946	0.06207
N	-4.67090	-1.81906	0.10436
N	-2.78748	-0.37105	-0.35431
C	-4.03603	-0.58469	-0.10109
C	-6.23698	-0.26256	0.38269
H	-7.15194	0.27197	0.60237
C	-4.93099	1.81823	-0.31117
C	-4.09280	-3.15707	-0.20831
C	-6.01207	-1.59197	0.41346
H	-6.70102	-2.38657	0.66839
C	2.84908	3.44204	-0.57902
C	2.04841	1.94935	-3.11657
C	-0.10929	3.71635	-1.40984
H	3.81465	3.02592	-0.90122
H	2.81300	4.48630	-0.92859
H	2.85248	3.45803	0.51790
C	-6.25179	2.53851	0.00606
H	-6.50886	2.46977	1.07422
H	-6.13312	3.60363	-0.24015
H	-7.09275	2.15479	-0.59085
C	-4.67629	1.91230	-1.82761
H	-3.75950	1.38622	-2.11886
H	-5.51857	1.46430	-2.37816
H	-4.58045	2.96452	-2.13519
C	-3.81939	2.48658	0.51098
H	-4.05490	2.42945	1.58408
H	-2.85503	2.00020	0.35433
H	-3.72587	3.54501	0.22664
C	-3.72827	-3.21182	-1.70474
H	-2.96985	-2.46337	-1.96939
H	-3.33259	-4.20767	-1.95911
H	-4.62232	-3.02759	-2.32101
C	-5.13390	-4.25126	0.07818
H	-6.02279	-4.16132	-0.56421
H	-4.67427	-5.22874	-0.12798
H	-5.45116	-4.25023	1.13220
C	-2.87130	-3.40932	0.68296
H	-2.42003	-4.38426	0.44582
H	-2.11598	-2.63594	0.53927
H	-3.16352	-3.40874	1.74379
C	1.12409	-2.36499	-3.14221
H	0.23114	-2.63583	-3.72561
H	0.97296	-1.35519	-2.75143
H	1.99761	-2.35467	-3.81253
C	0.12816	-3.43778	-1.06451
H	-0.05042	-2.46534	-0.59501
H	-0.77150	-3.72492	-1.62648
H	0.29548	-4.17208	-0.26163
C	1.55672	-4.76246	-2.60691
H	2.39897	-4.78272	-3.31490
H	1.71860	-5.53105	-1.83550
H	0.64991	-5.03746	-3.16523
C	6.01680	-0.36845	-0.51571
H	6.65447	0.43892	-0.12341
H	6.66343	-1.23080	-0.73579
H	5.56800	-0.02980	-1.46044
C	4.13279	0.55116	0.82947
H	3.69757	0.98571	-0.07090
H	3.32265	0.35934	1.53762
H	4.81900	1.28784	1.27312
C	5.55597	-1.25283	1.80419
H	6.19049	-2.13323	1.62384
H	6.19216	-0.47401	2.25194
H	4.78287	-1.53010	2.53295
C	-0.33535	-2.15836	2.49811
H	-0.12998	-2.17278	1.42032
H	-0.22918	-3.19725	2.86433
H	-1.38509	-1.86533	2.64109
C	0.28680	-1.28381	4.74139
H	0.31514	-2.33524	5.08475
H	1.00560	-0.72674	5.35992
H	-0.72171	-0.89922	4.96188
C	2.06081	-1.75130	3.04482
H	2.80625	-1.14255	3.57571
H	2.14267	-2.78151	3.44044
H	2.34106	-1.78497	1.98568
C	0.34954	2.15110	4.94784
H	0.26421	1.24945	5.56850
H	0.81414	2.93450	5.57605
H	-0.66867	2.49374	4.71046
C	1.25606	3.29014	2.94723
H	1.74246	4.05572	3.58058
H	1.81848	3.22785	2.00782
H	0.24891	3.66131	2.70900
C	2.63451	1.57273	4.12336
H	3.31600	1.43135	3.27373
H	3.05539	2.38450	4.74584
H	2.65975	0.65685	4.73216
C	-0.42269	4.13958	0.03731
H	0.42450	4.66025	0.50784
H	-1.28677	4.83000	0.05890
H	-0.68091	3.27713	0.67006
C	-1.37724	3.09549	-2.01109
H	-1.69752	2.20185	-1.45459
H	-2.21891	3.80982	-1.96085
H	-1.25590	2.80066	-3.06155
C	0.22105	4.98544	-2.22085
H	0.30034	4.77774	-3.29783
H	-0.58841	5.72902	-2.09613
H	1.15649	5.46934	-1.89973
C	2.69105	3.16193	-3.82645
H	3.10999	2.84021	-4.79842
H	1.97208	3.96485	-4.03674
H	3.52035	3.59732	-3.24743
C	3.15122	0.88077	-2.96890
H	2.78678	-0.03547	-2.49306
H	3.55010	0.61130	-3.96470
H	4.00163	1.25271	-2.37631
C	0.93358	1.39410	-4.02207
H	0.34148	0.59969	-3.54177
H	0.23100	2.18333	-4.33070
H	1.36732	0.97150	-4.94747

TS5

Si	-0.23959	-0.95841	2.42350
Si	0.53622	-0.07749	0.24501
N	4.49932	-0.43346	-0.28287
N	3.47042	-1.75926	-1.74362
N	2.09359	-0.65098	-0.09481
C	3.22262	-0.91481	-0.63683
C	5.44092	-0.89921	-1.19665
H	6.48313	-0.60448	-1.16179
C	4.95181	0.36403	0.89510
C	2.49262	-2.69134	-2.37745
C	4.81992	-1.71179	-2.07385
H	5.24267	-2.23967	-2.91838
C	-0.17928	0.31902	3.90709
C	0.57951	-2.69637	2.84784
C	-2.08525	-1.33935	2.15543
H	-2.48898	-1.90685	3.01031
H	-2.24755	-1.93254	1.24672
H	-2.67371	-0.42037	2.04691
Si	0.62087	2.79297	-0.49432
Si	-1.00125	0.39645	-1.51667
N	-4.79736	-0.19239	-0.11298
N	-3.95471	-1.98064	-1.15006
N	-2.55153	-0.02208	-0.96432
C	-3.64274	-0.66015	-0.76620
C	-5.75570	-1.20332	-0.09525
H	-6.71619	-1.09635	0.39271
C	-5.07727	1.24244	0.16809
C	-3.12213	-2.85229	-2.02325
C	-5.24694	-2.28543	-0.72009
H	-5.70006	-3.25895	-0.85430
C	1.84451	3.37260	0.87265
C	1.65419	2.99969	-2.17942
C	-0.80982	4.16455	-0.36977
H	2.84423	2.95166	0.71278
H	1.94714	4.46975	0.84730
H	1.52319	3.08881	1.88465
C	-6.45745	1.38701	0.82751
H	-6.52342	0.81397	1.76538
H	-6.61600	2.44759	1.07216
H	-7.27545	1.07627	0.16042
C	-5.08570	2.00142	-1.17247
H	-4.14061	1.86009	-1.70996

H	-5.90543	1.62965	-1.80760
H	-5.23230	3.07942	-1.00682
C	-4.02550	1.79414	1.14176
H	-4.13267	1.31567	2.12726
H	-3.01267	1.60717	0.77367
H	-4.15708	2.87833	1.26898
C	-2.88417	-2.15642	-3.37757
H	-2.33191	-1.21495	-3.26718
H	-2.30302	-2.81602	-4.04095
H	-3.84670	-1.93539	-3.86491
C	-3.86447	-4.17267	-2.29174
H	-4.81417	-4.01343	-2.82426
H	-3.22968	-4.80673	-2.92762
H	-4.06337	-4.72961	-1.36351
C	-1.79921	-3.19210	-1.31818
H	-1.17633	-3.82236	-1.97010
H	-1.22366	-2.29456	-1.06490
H	-1.99395	-3.74599	-0.38872
C	1.40102	-1.89913	-3.10622
H	0.68244	-2.58732	-3.57743
H	0.84247	-1.25563	-2.41732
H	1.83923	-1.26225	-3.88892
C	1.89737	-3.59362	-1.28732
H	1.36113	-2.99460	-0.54710
H	1.19498	-4.31630	-1.72839
H	2.69284	-4.15110	-0.76903
C	3.21079	-3.58173	-3.40533
H	3.63803	-2.99759	-4.23445
H	4.00570	-4.18859	-2.94592
H	2.47263	-4.27250	-3.83806
C	5.46355	1.72842	0.39767
H	5.80545	2.33911	1.24720
H	6.30741	1.61547	-0.30004
H	4.66799	2.27766	-0.12352
C	3.84183	0.56170	1.92717
H	2.99449	1.11671	1.52542
H	3.47091	-0.39886	2.29600
H	4.25619	1.12632	2.77590
C	6.09406	-0.40809	1.59132
H	6.98165	-0.52492	0.95315
H	6.40794	0.13627	2.49473
H	5.75045	-1.40959	1.89225
C	-0.01191	-3.74370	1.88164
H	0.09449	-3.45097	0.82917
H	0.50574	-4.71296	2.00633
H	-1.08247	-3.91818	2.06916
C	0.24182	-3.14810	4.28241
H	0.60604	-4.18030	4.44368
H	0.72299	-2.51514	5.04297
H	-0.84233	-3.15271	4.47905
C	2.11087	-2.68677	2.69050
H	2.58789	-1.98850	3.39541
H	2.52183	-3.69164	2.90358
H	2.41639	-2.40173	1.67480
C	-1.09075	-0.11188	5.07592
H	-0.74958	-1.02983	5.57219
H	-1.10734	0.68448	5.84351
H	-2.13173	-0.26911	4.75260
C	-0.71302	1.66096	3.37811
H	-0.69789	2.42827	4.17435
H	-0.11114	2.04220	2.54431
H	-1.75266	1.58094	3.02549
C	1.25098	0.53111	4.43055
H	1.91965	0.90096	3.64099
H	1.25540	1.28278	5.24184
H	1.69044	-0.39205	4.84026
C	-1.29475	4.24631	1.09078
H	-0.49319	4.54521	1.78368
H	-2.10027	4.99979	1.17974
H	-1.70297	3.29209	1.44291
C	-2.01873	3.85027	-1.26340
H	-2.47116	2.88742	-1.00197
H	-2.79849	4.62670	-1.14249
H	-1.75711	3.80680	-2.32985
C	-0.26957	5.55725	-0.75822
H	0.00897	5.61939	-1.81969
H	-1.05422	6.31834	-0.58634
H	0.60379	5.85845	-0.15876
C	2.65521	4.17228	-2.07337
H	3.21370	4.26813	-3.02379
H	2.16856	5.13931	-1.88522
H	3.40121	4.01606	-1.27934
C	2.47092	1.72170	-2.44102
H	1.82738	0.84347	-2.57929
H	3.07547	1.83684	-3.36069
H	3.16860	1.49989	-1.62216
C	0.74656	3.24111	-3.40023
H	-0.00615	2.44566	-3.50922
H	0.22009	4.20571	-3.34769
H	1.35692	3.25786	-4.32301

INT5

Si	-0.58533	-0.92857	2.46830
Si	-0.78698	-0.34535	0.06134
N	-2.50845	2.87922	-1.44229
N	-4.07745	2.05199	-0.07422
N	-1.91997	0.97068	-0.03247
C	-2.71460	1.86763	-0.46471
C	-3.72302	3.50800	-1.71943
H	-3.84184	4.22201	-2.52488
C	-1.20962	3.43053	-1.92152
C	-4.61818	1.71442	1.27707
C	-4.66167	3.02061	-0.88694
H	-5.71863	3.25407	-0.85778
C	-2.21844	-0.85594	3.44886
C	0.56597	0.41756	3.31432
C	0.04970	-2.75584	2.78009
Si	-1.67017	-1.93138	-1.65147
Si	1.32203	0.29052	-1.31580
N	5.06210	-0.35240	-0.41084
N	4.64545	1.78973	0.03578
N	2.75354	0.36159	-0.42913
C	4.02216	0.57835	-0.29421
C	6.27235	0.28149	-0.13652
H	7.22036	-0.24024	-0.12166
C	4.92474	-1.75061	-0.90805
C	3.99794	3.13177	0.01475
C	6.02100	1.57956	0.13094
H	6.71793	2.35782	0.41288
C	-3.54363	-2.46501	-1.39902
C	-1.70390	-0.85230	-3.22390
C	-0.50810	-3.45619	-2.11515
H	-2.61201	0.16471	3.52672
H	-2.02447	-1.22076	4.47098
H	-3.00039	-1.49098	3.01354
H	-0.68921	-0.64770	-3.59792
H	-2.19247	0.11148	-3.02511
H	-2.26942	-1.35898	-4.02332
C	4.40594	-1.72315	-2.35806
H	5.11306	-1.18033	-3.00485
H	4.30101	-2.75000	-2.74074
H	3.42851	-1.23134	-2.43121
C	3.97882	-2.51908	0.02146
H	4.40469	-2.58340	1.03442
H	3.01444	-2.01337	0.09108
H	3.81242	-3.53953	-0.35427
C	6.29524	-2.44512	-0.89404
H	6.16005	-3.48246	-1.23300
H	7.01385	-1.96556	-1.57586
H	6.72818	-2.48014	0.11738
C	3.52897	3.42931	-1.42282
H	3.07933	4.43314	-1.47614
H	4.38630	3.39923	-2.11349
H	2.78685	2.69775	-1.76826
C	5.01940	4.20505	0.42569
H	5.85129	4.28851	-0.28967
H	4.50847	5.17844	0.45124
H	5.42747	4.01675	1.43049
C	2.83957	3.16860	1.02123
H	2.34152	4.14915	0.98842
H	2.09779	2.39715	0.80941
H	3.21563	3.00272	2.04122
C	-0.18202	3.40508	-0.78173
H	-0.55101	3.96939	0.08854
H	0.02697	2.38584	-0.44272
H	0.75677	3.85823	-1.12271
C	-1.39272	4.90866	-2.32541
H	-0.40566	5.32964	-2.56739
H	-2.01980	5.02668	-3.22121
H	-1.82912	5.50226	-1.50786
C	-0.72635	2.64759	-3.14897
H	0.20861	3.07822	-3.54064
H	-0.52417	1.60166	-2.89983
H	-1.48812	2.67850	-3.94371
C	-3.70217	2.36998	2.32455
H	-2.67864	1.99266	2.22309
H	-3.68561	3.46234	2.18278
H	-4.05854	2.15657	3.34414
C	-4.69425	0.19702	1.46279
H	-4.98264	-0.04406	2.49628
H	-5.43948	-0.23872	0.78428
H	-3.72433	-0.25740	1.25364
C	-6.03719	2.28359	1.43699
H	-6.72536	1.88398	0.67616
H	-6.42105	1.98014	2.42225
H	-6.05754	3.38282	1.39636
C	0.13691	1.81462	2.82342
H	0.15445	1.90599	1.72961
H	-0.88192	2.06510	3.15531
H	0.81074	2.58893	3.23423
C	0.42250	0.41701	4.85143
H	0.72651	-0.53323	5.31098
H	1.06637	1.20667	5.28300
H	-0.60860	0.63166	5.17330
C	2.04353	0.18156	2.95186
H	2.20704	0.14072	1.86519
H	2.67148	0.99928	3.35198
H	2.42617	-0.75361	3.38887
C	0.49032	-2.99636	4.23706
H	-0.29719	-2.74187	4.96418
H	0.73116	-4.06647	4.38154
H	1.39289	-2.42556	4.50105
C	-1.11908	-3.71396	2.47715
H	-1.93653	-3.61496	3.20777
H	-1.54570	-3.54170	1.48118
H	-0.77390	-4.76394	2.51202
C	1.22687	-3.09255	1.85692
H	0.97658	-2.92332	0.80160
H	2.11028	-2.48486	2.08806
H	1.51927	-4.15505	1.95628
C	-3.99471	-3.54671	-2.40094
H	-5.08097	-3.72408	-2.28881
H	-3.82480	-3.24566	-3.44694
H	-3.49354	-4.51229	-2.23798
C	-3.80598	-2.99143	0.02263
H	-4.88588	-3.17785	0.17326
H	-3.28447	-3.94286	0.20755
H	-3.48440	-2.28220	0.79687
C	-4.41098	-1.21433	-1.66252
H	-4.08247	-0.33797	-1.09317
H	-4.40450	-0.93590	-2.72732
H	-5.46306	-1.41817	-1.38911
C	-0.79406	-3.94258	-3.55420
H	-0.10219	-4.76788	-3.80771

H	-1.81373	-4.32730	-3.68427
H	-0.63462	-3.14855	-4.29967
C	-0.67567	-4.64574	-1.15279
H	-1.69669	-5.05609	-1.16987
H	0.00871	-5.46693	-1.43775
H	-0.44342	-4.37801	-0.11436
C	0.96223	-3.00162	-2.08803
H	1.15109	-2.17014	-2.78652
H	1.28486	-2.68436	-1.08705
H	1.63197	-3.83018	-2.38684

TS6

Si	-0.34550	-1.91588	2.03366
Si	-0.85003	-0.47254	0.05716
N	-1.39575	3.54590	-0.63867
N	-2.24233	2.73187	1.26034
N	-0.60891	1.34633	0.08581
C	-1.31430	2.43501	0.23832
C	-2.48042	4.33359	-0.25563
H	-2.82891	5.17106	-0.84444
C	-0.39945	4.05015	-1.64948
C	-2.21583	2.27042	2.68853
C	-2.99590	3.84273	0.88433
H	-3.85997	4.18149	1.44155
C	-1.41586	-1.66896	3.59379
C	1.50854	-1.71218	2.65471
C	-0.69667	-3.77620	1.50660
Si	-2.82373	-0.77525	-1.41041
Si	0.81000	0.34973	-1.46900
N	4.29402	-1.08030	-0.95230
N	4.45072	0.74925	0.34785
N	2.33407	0.30767	-0.70656
C	3.55408	0.02653	-0.47615
C	5.56560	-1.04662	-0.37545
H	6.28892	-1.84287	-0.50027
C	3.93821	-1.88564	-2.15726
C	4.35090	2.22432	0.56424
C	5.66190	0.05312	0.39932
H	6.48283	0.35134	1.04007
C	-4.61007	-0.68331	-0.58332
C	-2.76120	0.76690	-2.52237
C	-2.62298	-2.26836	-2.68905
H	-1.17781	-0.72606	4.10472
H	-1.20542	-2.49058	4.29736
H	-2.49254	-1.68191	3.37940
H	-1.89651	0.72358	-3.19869
H	-2.68771	1.69542	-1.94495
H	-3.67554	0.82061	-3.13543
C	3.74075	-0.93830	-3.35721
H	4.64770	-0.33313	-3.51439
H	3.54915	-1.52200	-4.27119
H	2.89161	-0.25887	-3.20609
C	2.68136	-2.73581	-1.90346
H	2.87532	-3.48057	-1.11902
H	1.82514	-2.12910	-1.58898
H	2.39827	-3.26956	-2.82358
C	5.09196	-2.84782	-2.48732
H	4.80372	-3.45496	-3.35780
H	6.01770	-2.31244	-2.74620
H	5.29928	-3.53848	-1.65551
C	4.34204	2.90583	-0.81803
H	4.26414	3.99916	-0.71281
H	5.27348	2.67267	-1.35828
H	3.49545	2.55348	-1.41953
C	5.57665	2.71233	1.35314
H	6.51433	2.59090	0.79085
H	5.45450	3.78507	1.56379
H	5.66882	2.18967	2.31792
C	3.09736	2.58599	1.37689
H	3.00407	3.68163	1.43278
H	2.18857	2.18077	0.92370
H	3.17828	2.19647	2.40104
C	1.01094	3.90074	-1.07212
H	1.10580	4.46339	-0.13077
H	1.25674	2.85465	-0.87451
H	1.74885	4.29177	-1.78729
C	-0.63479	5.55587	-1.89053
H	0.17071	5.92457	-2.54172
H	-1.58337	5.75926	-2.40950
H	-0.60488	6.13596	-0.95564
C	-0.54731	3.32701	-2.99383
H	0.14078	3.77429	-3.72854
H	-0.29384	2.26330	-2.90140
H	-1.57469	3.42345	-3.37523
C	-0.77470	1.94924	3.09050
H	-0.35899	1.14425	2.48581
H	-0.12764	2.83030	2.95911
H	-0.74430	1.64992	4.14817
C	-3.14232	1.06541	2.86860
H	-3.11894	0.71464	3.90994
H	-4.17864	1.33054	2.61665
H	-2.83280	0.24025	2.21885
C	-2.70670	3.40945	3.60561
H	-3.77560	3.63139	3.47367
H	-2.57156	3.09417	4.65069
H	-2.13088	4.33371	3.44850
C	1.88839	-0.22582	2.72202
H	1.72623	0.27779	1.76244
H	1.33139	0.31006	3.50413
H	2.96195	-0.12578	2.96301
C	1.69958	-2.30084	4.06930
H	1.47541	-3.37441	4.12999
H	2.75415	-2.17113	4.37679
H	1.08097	-1.78485	4.82018
C	2.48667	-2.39731	1.68582
H	2.34578	-2.03689	0.66194
H	3.53031	-2.16800	1.96859
H	2.38354	-3.49226	1.68559
C	-0.16614	-4.78559	2.54488
H	-0.55752	-4.59673	3.55704
H	-0.48450	-5.80605	2.26095
H	0.93158	-4.79597	2.60142
C	-2.22365	-3.95667	1.42792
H	-2.70871	-3.83158	2.40820
H	-2.68470	-3.24159	0.73868
H	-2.47443	-4.97073	1.06586
C	-0.07812	-4.12090	0.14073
H	-0.37929	-3.41271	-0.64098
H	1.01845	-4.12134	0.16997
H	-0.40002	-5.12681	-0.18712
C	-5.73597	-1.07241	-1.56221
H	-6.71882	-0.89160	-1.08762
H	-5.71127	-0.47554	-2.48742
H	-5.70403	-2.13607	-1.84138
C	-4.74389	-1.56792	0.66764
H	-5.72068	-1.39495	1.15711
H	-4.69292	-2.63856	0.41904
H	-3.96199	-1.36302	1.41244
C	-4.83620	0.79289	-0.18968
H	-3.99378	1.21538	0.36962
H	-4.99001	1.43186	-1.07200
H	-5.73914	0.88663	0.44223
C	-3.46733	-1.99870	-3.95733
H	-3.31517	-2.82548	-4.67598
H	-4.54502	-1.94424	-3.75603
H	-3.16962	-1.07168	-4.46936
C	-3.05461	-3.62853	-2.11200
H	-4.10537	-3.62874	-1.78242
H	-2.95542	-4.41662	-2.88167
H	-2.43969	-3.93531	-1.25905
C	-1.15306	-2.35697	-3.15124
H	-0.80448	-1.41851	-3.60989
H	-0.46156	-2.58636	-2.33022
H	-1.04318	-3.15685	-3.90739

INT6

Si	-0.42191	-2.02423	1.95503
Si	-0.90486	-0.49574	0.06048
N	-1.05317	3.60289	-0.52826
N	-1.90467	2.75228	1.35040
N	-0.40286	1.31419	0.08661
C	-1.01871	2.45873	0.29936
C	-2.09971	4.41948	-0.09807
H	-2.41763	5.29366	-0.64928
C	-0.06775	4.10710	-1.55419
C	-1.84134	2.28138	2.77935
C	-2.61965	3.90555	1.02893
H	-3.45696	4.25746	1.61825
C	-1.42354	-1.75095	3.55587
C	1.46193	-2.00353	2.51695
C	-0.94961	-3.81988	1.35375
Si	-2.94073	-0.50922	-1.33025
Si	0.73030	0.45702	-1.39851
N	4.08227	-1.25226	-1.12356
N	4.46364	0.42435	0.32968
N	2.28008	0.30647	-0.65656
C	3.46720	-0.12602	-0.52151
C	5.36869	-1.39437	-0.59888
H	6.00424	-2.24260	-0.82171
C	3.61334	-1.90347	-2.38089
C	4.52254	1.87409	0.67981
C	5.60040	-0.38516	0.26564
H	6.46852	-0.22907	0.89480
C	-4.68635	-0.33125	-0.43358
C	-2.78558	1.08468	-2.35777
C	-2.89683	-1.93833	-2.69269
H	-1.08224	-0.85962	4.10020
H	-1.27845	-2.62019	4.21754
H	-2.50115	-1.64871	3.37141
H	-1.94052	1.01254	-3.05595
H	-2.63368	1.97717	-1.74032
H	-3.70717	1.23455	-2.94340
C	3.45807	-0.83084	-3.47715
H	4.40733	-0.28807	-3.61129
H	3.18975	-1.30554	-4.43404
H	2.67185	-0.10485	-3.23009
C	2.29551	-2.66321	-2.15059
H	2.45587	-3.50815	-1.46622
H	1.51554	-2.02357	-1.72206
H	1.91899	-3.06054	-3.10557
C	4.66332	-2.92393	-2.85234
H	4.28926	-3.41602	-3.76203
H	5.62324	-2.44705	-3.10118
H	4.83870	-3.70834	-2.10006
C	4.61478	2.67206	-0.63563
H	4.64041	3.75532	-0.43805
H	5.53129	2.39492	-1.18062
H	3.75304	2.45483	-1.27821
C	5.77811	2.14919	1.52326
H	6.70866	1.98680	0.95951
H	5.76591	3.20219	1.84164
H	5.79667	1.52346	2.42919
C	3.29987	2.30484	1.50877
H	3.32896	3.39613	1.65584
H	2.36321	2.03704	1.01201
H	3.31814	1.82667	2.49791
C	1.35456	3.84418	-1.05029
H	1.52234	4.34306	-0.08352
H	1.55978	2.77754	-0.92631
H	2.08131	4.23898	-1.77495
C	-0.21927	5.63700	-1.69171
H	0.58700	5.99855	-2.34572

H	-1.16803	5.93033	-2.16494
H	-0.12516	6.15217	-0.72357
C	-0.32529	3.47835	-2.92970
H	0.35388	3.92767	-3.67132
H	-0.13802	2.39566	-2.90883
H	-1.36210	3.66159	-3.24960
C	-0.43425	1.77458	3.09176
H	-0.17153	0.91362	2.48031
H	0.31884	2.55484	2.90403
H	-0.37854	1.48438	4.15070
C	-2.90141	1.20408	3.02276
H	-2.85177	0.84569	4.06087
H	-3.91082	1.60056	2.84287
H	-2.74356	0.35128	2.35407
C	-2.11657	3.47528	3.71822
H	-3.15408	3.83413	3.66120
H	-1.94741	3.14758	4.75449
H	-1.43966	4.31690	3.50844
C	1.97473	-0.56279	2.66172
H	1.82556	0.01677	1.74374
H	1.49812	-0.03650	3.50131
H	3.06088	-0.57429	2.86265
C	1.64131	-2.69253	3.88765
H	1.33181	-3.74610	3.89247
H	2.71100	-2.66696	4.16742
H	1.08839	-2.17529	4.68740
C	2.34731	-2.70957	1.47639
H	2.21370	-2.27368	0.48122
H	3.41426	-2.59220	1.73938
H	2.14488	-3.78868	1.41279
C	-0.47718	-4.91994	2.32598
H	-0.81495	-4.74574	3.35989
H	-0.89571	-5.89339	2.00924
H	0.61638	-5.02992	2.33920
C	-2.48847	-3.86562	1.32095
H	-2.93030	-3.73986	2.32143
H	-2.90807	-3.08691	0.67545
H	-2.83688	-4.83881	0.92888
C	-0.40653	-4.15205	-0.04760
H	-0.67196	-3.38804	-0.78886
H	0.68692	-4.24302	-0.05872
H	-0.82177	-5.11305	-0.40375
C	-5.87128	-0.58505	-1.38671
H	-6.82100	-0.36079	-0.86554
H	-5.83533	0.05818	-2.28003
H	-5.92703	-1.63129	-1.72193
C	-4.84075	-1.26723	0.77686
H	-5.78608	-1.05249	1.30957
H	-4.87327	-2.32495	0.47582
H	-4.02143	-1.15336	1.50117
C	-4.78751	1.13312	0.04442
H	-3.89616	1.45585	0.59348
H	-4.91865	1.83039	-0.79651
H	-5.65957	1.25909	0.71304
C	-3.75807	-1.53478	-3.91323
H	-3.69401	-2.32977	-4.67932
H	-4.82145	-1.40888	-3.67142
H	-3.40399	-0.60680	-4.38621
C	-3.41276	-3.29223	-2.17258
H	-4.44881	-3.23272	-1.80403
H	-3.39981	-4.04114	-2.98628
H	-2.79434	-3.69169	-1.36117
C	-1.45316	-2.11086	-3.20975
H	-1.04313	-1.17501	-3.61973
H	-0.75875	-2.44094	-2.42710
H	-1.43041	-2.86842	-4.01547

TS7

Si	-0.87650	0.58555	-1.06391
Si	1.24078	-0.63135	-0.43232
Si	3.12029	0.65592	-1.29076
Si	1.59870	-2.65093	0.90204
N	-4.32062	-0.85666	0.55325
N	-2.21029	-0.28805	-0.40260
N	-0.27246	1.55504	0.31681
N	0.08987	3.15038	2.08584
N	-4.00721	-1.45942	-1.56830
N	-0.89987	3.93804	0.25276
C	-4.08347	-0.33192	1.92471
C	-3.37588	-0.80501	-0.49004
C	-0.35459	2.75144	0.81459
C	0.71868	2.28321	3.11681
C	4.92673	0.44950	-0.54158
C	3.06454	0.24448	-3.20972
C	2.67978	2.49390	-1.09882
C	0.30831	-3.92480	0.14558
C	1.69618	-2.74486	2.85618
C	3.29508	-3.24589	0.26375
C	-5.46115	-1.52030	0.11885
H	-6.32273	-1.69972	0.74967
C	-5.27531	-1.87905	-1.17169
H	-5.95550	-2.41095	-1.82424
C	-3.48664	-1.53181	-2.96251
C	-1.62300	4.12441	-1.04782
C	-0.73813	4.98372	1.15965
H	-1.06063	5.99565	0.96019
C	-0.12649	4.51165	2.26138
H	0.16947	5.05015	3.15147
H	4.12144	-2.77535	0.81514
H	3.37704	-4.33702	0.39758
H	2.85238	2.83821	-0.06863
H	1.62276	2.66239	-1.32886
H	3.29303	3.11115	-1.77545
H	3.43146	-3.03360	-0.80675
C	2.14153	1.94937	2.65313
H	2.68578	1.38104	3.41984
H	2.11754	1.35725	1.73147
H	2.69789	2.87882	2.45532
C	0.80385	3.03609	4.45625
H	1.21521	2.34997	5.21061
H	1.47516	3.90665	4.40885
H	-0.18663	3.36589	4.80512
C	-0.14764	1.03345	3.33659
H	-0.23260	0.44387	2.41935
H	0.28633	0.41017	4.13063
H	-1.16200	1.33070	3.64222
C	-2.90995	3.27995	-1.05235
H	-3.57646	3.60307	-0.23791
H	-3.43862	3.40505	-2.00958
H	-2.71440	2.20894	-0.92506
C	-2.04826	5.59843	-1.19804
H	-2.73993	5.92061	-0.40515
H	-1.18470	6.28009	-1.22456
H	-2.57804	5.70216	-2.15558
C	-0.69554	3.79964	-2.23096
H	-0.42651	2.73387	-2.25552
H	-1.21104	4.02562	-3.17732
H	0.21850	4.41040	-2.17566
C	-3.73864	1.16778	1.86041
H	-3.64571	1.57119	2.88109
H	-2.79238	1.32522	1.33297
H	-4.53432	1.72303	1.33983
C	-2.93371	-1.12325	2.56813
H	-2.03142	-1.02973	1.95435
H	-2.71989	-0.73914	3.57718
H	-3.19590	-2.18937	2.64899
C	-5.35355	-0.50909	2.77002
H	-6.20898	0.03914	2.34551
H	-5.63062	-1.56812	2.88520
H	-5.16449	-0.10722	3.77617
C	-3.42030	-0.11133	-3.55296
H	-3.09911	-0.15499	-4.60581
H	-4.41195	0.36678	-3.50970
H	-2.69502	0.51302	-3.00954
C	-2.10586	-2.21079	-2.98325
H	-1.35870	-1.63848	-2.42336
H	-2.16576	-3.21694	-2.54453
H	-1.75278	-2.30232	-4.02187
C	-4.44128	-2.37857	-3.82124
H	-5.43697	-1.91915	-3.91381
H	-4.02210	-2.45963	-4.83450
H	-4.55356	-3.39884	-3.42285
C	2.53050	-1.55689	3.36160
H	3.57315	-1.60563	3.01132
H	2.11436	-0.60162	3.02956
H	2.56034	-1.55025	4.46744
C	2.40470	-4.03726	3.31699
H	2.48652	-4.03674	4.42014
H	1.86396	-4.94995	3.03374
H	3.42839	-4.11395	2.91860
C	0.29706	-2.68504	3.49488
H	-0.27417	-1.80777	3.16383
H	-0.30152	-3.57847	3.26319
H	0.38285	-2.62835	4.59612
C	0.58602	-4.04884	-1.36863
H	-0.14933	-4.73203	-1.83197
H	0.49910	-3.08051	-1.88575
H	1.58731	-4.45663	-1.57870
C	0.46572	-5.32707	0.76709
H	0.17066	-5.34893	1.82661
H	-0.19084	-6.04196	0.23717
H	1.49397	-5.71639	0.69155
C	-1.14301	-3.45694	0.34674
H	-1.31568	-2.45278	-0.06037
H	-1.84211	-4.14832	-0.15992
H	-1.42629	-3.43488	1.40798
C	3.09411	-1.27729	-3.45532
H	4.01338	-1.75150	-3.08052
H	2.23737	-1.78173	-2.97684
H	3.03207	-1.49277	-4.53821
C	4.23514	0.90373	-3.96614
H	4.26418	1.99494	-3.81350
H	5.21458	0.49591	-3.67727
H	4.12167	0.73251	-5.05298
C	1.75184	0.80924	-3.79537
H	0.85283	0.41297	-3.29777
H	1.70579	1.90701	-3.71574
H	1.68225	0.55702	-4.87026
C	5.76714	1.70493	-0.87068
H	6.78370	1.58934	-0.45064
H	5.88025	1.87181	-1.95178
H	5.33877	2.61907	-0.43238
C	4.83498	0.33982	0.99094
H	5.84131	0.19653	1.42687
H	4.41556	1.25092	1.44156
H	4.20750	-0.50321	1.30826
C	5.67743	-0.78272	-1.08133
H	5.87285	-0.71260	-2.16098
H	6.66015	-0.87092	-0.58187
H	5.13737	-1.71984	-0.89892

7

Si	-0.83653	-0.77956	-0.02245
Si	0.83608	0.77963	-0.02124
Si	-0.37308	-3.03574	-0.61142
Si	0.37311	3.03542	-0.61212
N	-2.39435	-0.29656	0.24806
N	-3.63109	1.03120	1.84983
N	-4.39021	0.92521	-0.23394
N	2.39404	0.29569	0.24699
N	3.63063	-1.03055	1.85038
N	4.39068	-0.92522	-0.23312

C	-3.36805	0.49133	0.59657
C	-4.78103	1.81510	1.76252
H	-5.18254	2.37050	2.59966
C	-5.24098	1.75123	0.49368
H	-6.10130	2.24398	0.05973
C	-2.90591	0.72526	3.12776
C	-1.50541	1.35365	3.09391
H	-0.91278	0.98463	2.24750
H	-0.96001	1.10596	4.01710
H	-1.56898	2.44863	3.01999
C	-3.68065	1.32967	4.30980
H	-3.14844	1.07835	5.23811
H	-4.69848	0.91967	4.38815
H	-3.73715	2.42685	4.25364
C	-2.83594	-0.79854	3.32634
H	-2.24931	-1.28494	2.54156
H	-3.84553	-1.23652	3.32192
H	-2.36681	-1.02301	4.29572
C	-4.67949	0.38712	-1.60486
C	-5.93759	1.06637	-2.16473
H	-5.81406	2.15695	-2.24777
H	-6.83169	0.84972	-1.56198
H	-6.12173	0.67594	-3.17565
C	-4.93633	-1.12408	-1.47832
H	-5.14443	-1.55584	-2.46849
H	-5.80606	-1.31123	-0.82995
H	-4.06845	-1.63697	-1.04848
C	-3.50772	0.68547	-2.55225
H	-3.36126	1.77075	-2.65874
H	-3.72456	0.27341	-3.54882
H	-2.57546	0.23744	-2.19482
C	1.48151	-3.25339	-0.27783
H	2.08097	-2.65177	-0.97498
H	1.76635	-4.30904	-0.41337
H	1.76225	-2.95689	0.74130
C	-1.38104	-4.22727	0.53779
C	-0.81315	-4.09747	1.96748
H	0.23680	-4.42414	2.02975
H	-1.39366	-4.72943	2.66263
H	-0.86690	-3.06387	2.34635
C	-2.88200	-3.87355	0.56964
H	-3.05836	-2.84567	0.91984
H	-3.41289	-4.55639	1.25687
H	-3.35663	-3.97397	-0.41677
C	-1.21100	-5.68817	0.07171
H	-1.67777	-5.86880	-0.90834
H	-1.69644	-6.37075	0.79187
H	-0.15233	-5.98766	0.00408
C	-0.65158	-3.23777	-2.52937
C	-2.13652	-3.42963	-2.88431
H	-2.25845	-3.47795	-3.98115
H	-2.75721	-2.59669	-2.52285
H	-2.54887	-4.36294	-2.47260
C	0.15594	-4.45573	-3.03050
H	-0.00597	-4.58744	-4.11529
H	-0.14327	-5.39474	-2.54182
H	1.23896	-4.32609	-2.87850
C	-0.13307	-1.98131	-3.25972
H	0.91212	-1.74775	-3.00693
H	-0.73655	-1.08782	-3.03307
H	-0.17825	-2.13463	-4.35273
C	3.36788	-0.49147	0.59664
C	5.24181	-1.75003	0.49543
H	6.10262	-2.24252	0.06212
C	4.78131	-1.81348	1.76408
H	5.18275	-2.36825	2.60168
C	2.90510	-0.72393	3.12795
C	2.83561	0.79994	3.32582
H	3.84537	1.23754	3.32166
H	2.36614	1.02502	4.29490
H	2.24950	1.28629	2.54063
C	1.50446	-1.35206	3.09396
H	0.91257	-0.98415	2.24657
H	0.95836	-1.10299	4.01635
H	1.56795	-2.44714	3.02158
C	3.67924	-1.32808	4.31053
H	3.73617	-2.42521	4.25452
H	3.14614	-1.07708	5.23843
H	4.69688	-0.91771	4.38957
C	4.68022	-0.38771	-1.60422
C	3.50895	-0.68722	-2.55187
H	3.72621	-0.27634	-3.54884
H	2.57651	-0.23887	-2.19530
H	3.36268	-1.77265	-2.65713
C	4.93629	1.12370	-1.47853
H	5.80581	1.31169	-0.83014
H	4.06806	1.63647	-1.04925
H	5.14438	1.55495	-2.46894
C	5.93889	-1.06661	-2.16317
H	6.12327	-0.67659	-3.17422
H	5.81601	-2.15730	-2.24564
H	6.83263	-0.84915	-1.56018
C	-1.48156	3.25296	-0.27888
H	-1.76709	4.30824	-0.41572
H	-1.76208	2.95756	0.74064
H	-2.08075	2.65009	-0.97521
C	1.38080	4.22740	0.53678
C	1.21061	5.68809	0.07005
H	1.69598	6.37109	0.78985
H	0.15188	5.98738	0.00236
H	1.67729	5.86831	-0.91011
C	0.81283	4.09816	1.96646
H	1.39328	4.73043	2.66140
H	0.86653	3.06473	2.34576
H	-0.23711	4.42488	2.02845
C	2.88180	3.87382	0.56879
H	3.35649	3.97436	-0.41757
H	3.05829	2.84593	0.91895
H	3.41258	4.55665	1.25613
C	0.65193	3.23664	-2.53011
C	-0.15621	4.45393	-3.03192
H	0.14220	5.39333	-2.54349
H	-1.23920	4.32364	-2.88025
H	0.00599	4.58535	-4.11670
C	0.13429	1.97955	-3.25997
H	0.17955	2.13242	-4.35305
H	-0.91080	1.74550	-3.00721
H	0.73829	1.08656	-3.03281
C	2.13681	3.42916	-2.88489
H	2.25889	3.47716	-3.98173
H	2.75781	2.59665	-2.52302
H	2.54863	4.36281	-2.47345

H_2

H	0.00000	0.00000	0.38037
H	0.00000	0.00000	-0.38037

$2 + H_2$

Si	-0.72824	-1.06653	-0.10212
Si	-0.55307	1.18013	0.14076
Si	-2.24357	-2.44136	1.14052
Si	-1.84078	2.74045	-1.14811
N	0.68722	-1.95898	-0.19631
N	2.11820	-2.98752	-1.79880
N	2.98290	-2.50652	0.16522
N	1.03374	1.77435	0.11033
N	3.37857	2.06189	-0.03716
N	2.44369	2.59905	1.88462
C	1.80666	-2.42123	-0.56631
C	3.43340	-3.41047	-1.79438
C	3.95833	-3.11921	-0.60120
C	1.16887	-3.20072	-2.90619
C	1.88418	-3.90036	-4.06226
C	0.03129	-4.10733	-2.43774
C	0.63797	-1.86586	-3.42930
C	3.24924	-2.16477	1.57385
C	4.48640	-1.26332	1.63349
C	2.09872	-1.42029	2.23512
C	3.49727	-3.46495	2.34476
C	-1.23874	-4.04408	1.34569
C	-2.61134	-1.80684	2.93578
C	-3.52958	-2.79109	3.66829
C	-1.28561	-1.73202	3.69782
C	-3.23866	-0.41387	2.97003
C	-3.85265	-2.93558	0.15677
C	-3.54774	-2.93276	-1.34375
C	-5.05729	-2.02287	0.40247
C	-4.26195	-4.36313	0.54726
C	2.15137	2.10239	0.61594
C	4.36759	2.53002	0.80679
C	3.80206	2.84887	1.97461
C	3.56192	1.79606	-1.47580
C	5.05193	1.82991	-1.81350
C	3.03083	0.41305	-1.83935
C	2.85190	2.87863	-2.28625
C	1.46571	2.95740	2.93000
C	2.19290	3.61299	4.10525
C	0.46282	3.97234	2.38180
C	0.75865	1.71162	3.45986
C	-0.72976	4.28517	-1.18074
C	-3.50773	3.34744	-0.33926
C	-3.35923	3.31959	1.18475
C	-3.76217	4.80431	-0.75619
C	-4.75116	2.54341	-0.72836
C	-2.03152	2.16486	-2.98811
C	-0.62387	1.99090	-3.56666
C	-2.76549	3.22578	-3.81453
C	-2.76536	0.83162	-3.12453
H	-3.01854	0.04262	-0.36187
H	-3.03307	0.37633	0.31554
H	4.95603	-3.29669	-0.24318
H	3.90627	-3.87686	-2.63740
H	1.16970	-4.04709	-4.87158
H	2.26293	-4.88556	-3.78601
H	2.70625	-3.30550	-4.46354
H	-0.66766	-4.28564	-3.25596
H	-0.52000	-3.66095	-1.61580
H	0.41851	-5.07181	-2.10550
H	-0.04344	-2.04199	-4.26287
H	1.45470	-1.24029	-3.79064
H	0.09181	-1.30453	-2.67433
H	4.70471	-1.00579	2.67020
H	4.31311	-0.33389	1.09094
H	5.38007	-1.73767	1.22620
H	2.41292	-1.15830	3.24702
H	1.20261	-2.02748	2.31212
H	1.84136	-0.50165	1.71358
H	3.69599	-3.24977	3.39536
H	4.35099	-4.02194	1.95624
H	2.62217	-4.11379	2.29326
H	-1.70835	-4.73470	2.04870
H	-0.23104	-3.83158	1.70199
H	-1.12724	-4.57103	0.39717
H	-3.65370	-2.48320	4.71215
H	-3.12760	-3.80629	3.68200
H	-4.52800	-2.83693	3.23207
H	-1.45941	-1.38932	4.72377
H	-0.59718	-1.02439	3.23268
H	-0.78291	-2.69888	3.76330
H	-3.41749	-0.10474	4.00570
H	-4.19591	-0.36332	2.44980
H	-2.57323	0.32568	2.51884

H	-4.41899	-3.27974	-1.91011
H	-2.71809	-3.59559	-1.59671
H	-3.29144	-1.93830	-1.71357
H	-5.90752	-2.36223	-0.19881
H	-4.86824	-0.98598	0.12787
H	-5.38319	-2.03277	1.44299
H	-5.16515	-4.65449	0.00028
H	-4.48638	-4.46232	1.61007
H	-3.49181	-5.09618	0.30512
H	5.40467	2.57380	0.53347
H	4.27632	3.21532	2.86462
H	5.17244	1.58260	-2.86775
H	5.62036	1.09378	-1.24211
H	5.49719	2.81455	-1.66319
H	3.15861	0.24664	-2.91007
H	1.97630	0.30775	-1.60119
H	3.58552	-0.36522	-1.31590
H	3.02337	2.72482	-3.35267
H	3.22164	3.87092	-2.02285
H	1.78024	2.84881	-2.11341
H	1.45478	3.87668	4.86189
H	2.70547	4.53282	3.81985
H	2.90992	2.94128	4.57976
H	-0.21963	4.28395	3.17361
H	-0.13495	3.56092	1.57435
H	0.97554	4.85893	2.00590
H	0.05708	1.98972	4.24773
H	1.47766	1.00931	3.88257
H	0.18963	1.19405	2.68873
H	-1.03727	4.98783	-1.95754
H	0.31237	4.02638	-1.35354
H	-0.76473	4.82206	-0.23183
H	-4.24528	3.75138	1.66293
H	-2.49728	3.89847	1.52479
H	-3.23832	2.30708	1.57204
H	-4.69963	5.15729	-0.31305
H	-3.85507	4.92401	-1.83646
H	-2.97651	5.47978	-0.41780
H	-5.63133	2.95437	-0.22239
H	-4.68726	1.49304	-0.45075
H	-4.95336	2.58871	-1.79927
H	-0.68099	1.63044	-4.59969
H	-0.03801	1.26265	-3.00057
H	-0.06469	2.92813	-3.58399
H	-2.77610	2.93962	-4.87182
H	-2.28856	4.20629	-3.75537
H	-3.80595	3.34513	-3.50920
H	-2.82173	0.53608	-4.17794
H	-3.78789	0.87009	-2.74610
H	-2.24123	0.03724	-2.58826

$TS2H_2$

Si	1.12894	-0.50489	0.09652
Si	-1.13130	-0.75207	-0.08804
Si	2.45228	-1.60733	1.75567
Si	-2.10124	-2.13608	-1.77569
N	1.98576	0.88893	-0.28523
N	2.98322	2.42013	-1.79426
N	2.00815	3.27444	-0.01297
N	-2.22481	0.50526	0.16229
N	-2.77339	2.81874	0.06800
N	-3.37670	1.70944	1.87102
C	2.28182	2.06740	-0.65057
C	3.15369	3.78987	-1.82928
C	2.56706	4.30870	-0.74772
C	3.61194	1.46507	-2.72436
C	4.28856	2.23192	-3.86008
C	4.67718	0.66536	-1.97533
C	2.55971	0.54582	-3.34276
C	1.53309	3.50885	1.36596
C	0.66296	4.77085	1.38526
C	0.68007	2.36653	1.90533
C	2.75228	3.70627	2.27001
C	3.82394	-0.35530	2.16705
C	1.56812	-2.02805	3.42800
C	2.51540	-2.77777	4.37028
C	1.18583	-0.70299	4.09445
C	0.29537	-2.85812	3.25678
C	3.35883	-3.12566	0.95092
C	3.73861	-2.78153	-0.49204
C	2.48637	-4.38053	0.92993
C	4.65901	-3.43671	1.70300
C	-2.72781	1.56305	0.65831
C	-3.43672	3.69168	0.91240
C	-3.79596	3.01943	2.01153
C	-2.46981	3.09684	-1.35111
C	-2.67937	4.58420	-1.63253
C	-1.01744	2.76343	-1.68348
C	-3.42644	2.29096	-2.22692
C	-3.62980	0.62263	2.83376
C	-4.45889	1.15978	3.99973
C	-4.42727	-0.49644	2.16143
C	-2.30492	0.10523	3.38919
C	-3.85048	-1.43812	-2.06721
C	-2.40532	-3.93724	-1.11605
C	-3.35346	-3.81542	0.08361
C	-3.08430	-4.79317	-2.19127
C	-1.15668	-4.68518	-0.64671
C	-1.19012	-2.01275	-3.47661
C	-0.90442	-0.53092	-3.73646
C	-2.06937	-2.52793	-4.62111
C	0.13377	-2.77544	-3.47534
H	0.53619	-2.24457	-0.27795
H	-0.23051	-2.26992	0.41742
H	2.48625	5.34058	-0.46164
H	3.65351	4.30114	-2.62991
H	4.73135	1.51210	-4.54758
H	5.09638	2.87598	-3.50972
H	3.58041	2.83331	-4.43269
H	5.13473	-0.07090	-2.63742
H	4.24369	0.13641	-1.13070
H	5.46434	1.32327	-1.60345
H	3.02300	-0.08612	-4.10167
H	1.77351	1.12777	-3.82515
H	2.09647	-0.10589	-2.60825
H	0.28731	4.92951	2.39577
H	-0.20026	4.66498	0.72742
H	1.20196	5.67596	1.10641
H	0.22706	2.69224	2.84310
H	1.26638	1.47968	2.11913
H	-0.12454	2.09367	1.22597
H	2.44161	3.87869	3.30149
H	3.35381	4.56008	1.95415
H	3.39099	2.82296	2.25434
H	4.46115	-0.69670	2.98516
H	3.41286	0.61284	2.45172
H	4.46389	-0.18064	1.30085
H	2.05089	-2.89181	5.35581
H	3.46192	-2.25461	4.52197
H	2.74430	-3.78198	4.01154
H	0.66927	-0.89128	5.04212
H	0.50938	-0.11737	3.47122
H	2.05507	-0.08219	4.32005
H	-0.18139	-3.02022	4.23009
H	0.49027	-3.84087	2.82672
H	-0.42794	-2.36333	2.60805
H	4.29082	-3.61199	-0.94548
H	4.38424	-1.90353	-0.54922
H	2.86275	-2.59345	-1.11565
H	3.00089	-5.19178	0.40345
H	1.53912	-4.21202	0.41600
H	2.26156	-4.74576	1.93316
H	5.17025	-4.28194	1.22944
H	4.49450	-3.70834	2.74530
H	5.35406	-2.59562	1.68830
H	-3.58380	4.73083	0.68717
H	-4.30231	3.38526	2.88441
H	-2.40560	4.78163	-2.66841
H	-2.04722	5.21651	-1.00593
H	-3.71802	4.89474	-1.51172
H	-0.83132	2.96631	-2.73916
H	-0.77678	1.72141	-1.50078
H	-0.32972	3.37765	-1.10516
H	-3.23193	2.48937	-3.28199
H	-4.46412	2.55620	-2.01792
H	-3.30368	1.22599	-2.05248
H	-4.64994	0.34214	4.69383
H	-5.42825	1.54435	3.67890
H	-3.93757	1.93864	4.55851
H	-4.64051	-1.28414	2.88499
H	-3.88520	-0.94208	1.33226
H	-5.37890	-0.11891	1.78424
H	-2.48402	-0.67150	4.13389
H	-1.74787	0.91020	3.87114
H	-1.67479	-0.32434	2.61432
H	-4.53420	-2.20515	-2.43539
H	-3.84525	-0.63998	-2.80970
H	-4.27736	-1.02142	-1.15497
H	-3.57109	-4.80624	0.49683
H	-4.31017	-3.36031	-0.17942
H	-2.91019	-3.22279	0.88807
H	-3.41441	-5.74392	-1.75902
H	-2.40124	-5.03812	-3.00578
H	-3.96456	-4.31899	-2.62880
H	-1.42089	-5.71030	-0.36481
H	-0.70936	-4.21591	0.22814
H	-0.38508	-4.74937	-1.41470
H	-0.41067	-0.40324	-4.70644
H	-0.24802	-0.10537	-2.97704
H	-1.81563	0.07172	-3.75834
H	-1.56632	-2.36875	-5.58122
H	-3.02822	-2.00875	-4.67314
H	-2.27781	-3.59443	-4.54528
H	0.68348	-2.59396	-4.40558
H	-0.01644	-3.85384	-3.39756
H	0.77626	-2.47019	-2.64596

4

Si	0.70430	1.19957	-0.19655
Si	0.70735	-1.19779	0.19596
Si	2.02592	2.63659	1.22065
Si	2.03206	-2.63224	-1.22084
N	-0.87701	1.82619	-0.20342
N	-2.31978	2.87945	-1.86073
N	-3.18408	2.36402	0.12541
N	-0.87226	-1.82885	0.20303
N	-3.17834	-2.37154	-0.12483
N	-2.31222	-2.88485	1.86106
C	-1.98622	2.30589	-0.61448
C	-3.66619	3.23824	-1.85961
C	-4.18811	2.92964	-0.65335
C	-1.37047	3.16023	-2.97199
C	-2.09022	3.92659	-4.09393
C	-0.22344	4.04494	-2.45194
C	-0.84982	1.83593	-3.55088
C	-3.30788	2.03154	1.57125
C	-4.75572	2.25370	2.03419
C	-2.94412	0.55927	1.80836
C	-2.37977	2.96427	2.36521
C	1.07929	4.28656	1.35991
C	2.24123	1.97415	3.04430
C	2.70568	3.09351	3.99940

C	0.86597	1.47782	3.53487
C	3.23977	0.80500	3.11250
C	3.70554	3.04299	0.30554
C	3.37408	3.88052	-0.94901
C	4.42590	1.76029	-0.14603
C	4.65955	3.86184	1.19634
C	-1.98035	-2.31067	0.61461
C	-4.18089	-2.93916	0.65438
C	-3.65787	-3.24648	1.86049
C	-3.30337	-2.03964	-1.57069
C	-4.75088	-2.26516	-2.03312
C	-2.94306	-0.56658	-1.80827
C	-2.37342	-2.97050	-2.36470
C	-1.36200	-3.16298	2.97221
C	-2.07947	-3.93097	4.09449
C	-0.21283	-4.04486	2.45209
C	-0.84460	-1.83721	3.55066
C	1.08967	-4.28460	-1.35988
C	3.71294	-3.03418	-0.30624
C	3.38380	-3.87223	0.94860
C	4.66874	-3.85092	-1.19706
C	4.43025	-1.74965	0.14495
C	2.24500	-1.96906	-3.04455
C	0.86859	-1.47567	-3.53472
C	2.71177	-3.08719	-3.99997
C	3.24095	-0.79769	-3.11270
H	1.38267	1.35711	-1.53859
H	1.38598	-1.35237	1.53824
H	-5.20567	3.05763	-0.30744
H	-4.16445	3.67205	-2.71670
H	-1.36676	4.12458	-4.89821
H	-2.48014	4.89616	-3.74868
H	-2.91551	3.34377	-4.53032
H	0.47713	4.27642	-3.26846
H	0.33783	3.54887	-1.65587
H	-0.62241	4.99137	-2.05486
H	-0.08428	2.02655	-4.31842
H	-1.67163	1.26841	-4.01212
H	-0.39834	1.21484	-2.77353
H	-4.82509	1.98476	3.09835
H	-5.46420	1.61521	1.48403
H	-5.06965	3.30416	1.93702
H	-3.00152	0.33200	2.88290
H	-1.93280	0.34070	1.45429
H	-3.64243	-0.10564	1.28060
H	-2.43899	2.74022	3.44145
H	-2.66406	4.01686	2.20923
H	-1.34605	2.82825	2.03331
H	1.75833	5.09538	1.67643
H	0.27067	4.22010	2.10169
H	0.62334	4.57766	0.40259
H	2.74752	2.70913	5.03584
H	2.01398	3.95093	3.99930
H	3.70787	3.47198	3.75362
H	0.95561	1.04011	4.54662
H	0.44493	0.70147	2.88088
H	0.13110	2.29349	3.59928
H	3.28739	0.40226	4.14153
H	4.26054	1.11204	2.83761
H	2.94369	-0.02520	2.45410
H	4.30268	4.11381	-1.50238
H	2.89489	4.83948	-0.69620
H	2.70877	3.34250	-1.64134
H	5.33609	2.01134	-0.72244
H	3.79262	1.14176	-0.79833
H	4.74084	1.13478	0.70083
H	5.54821	4.17206	0.61534
H	5.02491	3.27931	2.05582
H	4.18907	4.77956	1.58558
H	-5.19823	-3.06963	0.30876
H	-4.15485	-3.68141	2.71776
H	-4.82120	-1.99662	-3.09732
H	-5.46059	-1.62814	-1.48285
H	-5.06245	-3.31630	-1.93565
H	-3.00149	-0.33969	-2.88283
H	-1.93211	-0.34554	-1.45470
H	-3.64269	0.09680	-1.28031
H	-2.43321	-2.74667	-3.44096
H	-2.65554	-4.02367	-2.20861
H	-1.33996	-2.83226	-2.03292
H	-1.35527	-4.12697	4.89859
H	-2.46702	-4.90160	3.74952
H	-2.90612	-3.35020	4.53105
H	0.48856	-4.27429	3.26847
H	0.34689	-3.54758	1.65569
H	-0.60947	-4.99244	2.05540
H	-0.07807	-2.02560	4.31776
H	-1.66768	-1.27186	4.01230
H	-0.39530	-1.21501	2.77292
H	1.77071	-5.09146	-1.67713
H	0.28051	-4.21993	-2.10122
H	0.63502	-4.57736	-0.40244
H	4.31311	-4.10322	1.50175
H	2.90681	-4.83237	0.69615
H	2.71743	-3.33561	1.64101
H	5.55831	-4.15885	-0.61621
H	5.03245	-3.26771	-2.05678
H	4.20039	-4.76987	-1.58595
H	5.34099	-1.99839	0.72147
H	3.79546	-1.13243	0.79703
H	4.74370	-1.12363	-0.70208
H	0.95707	-1.03762	-4.54642
H	0.44604	-0.70031	-2.88052
H	0.13543	-2.29286	-3.59904
H	2.75308	-2.70241	-5.03627
H	2.02170	-3.94595	-4.00029
H	3.71464	-3.46384	-3.75410
H	3.28730	-0.39439	-4.14157
H	4.26249	-1.10263	-2.83836
H	2.94331	0.03159	-2.45386

TS2^{M}H$_2$

Si	-2.29558	-0.04618	-0.24063
N	3.07022	-1.13389	-0.04465
N	1.00939	0.00896	0.52972
N	3.06655	1.09066	-0.04728
C	3.78578	-3.47152	-0.41541
H	4.09987	-3.27024	-1.45087
H	3.43830	-4.51386	-0.36887
H	4.66107	-3.38570	0.24633
C	2.63482	-2.55224	0.02508
C	2.24260	-0.02203	0.19345
C	-3.61542	-1.48789	-0.10157
C	-3.09226	-2.71761	-0.87479
H	-3.79509	-3.56324	-0.75996
H	-2.10849	-3.05493	-0.50914
H	-2.99570	-2.51539	-1.95348
C	-4.96995	-1.09366	-0.72409
H	-4.86985	-0.77504	-1.77461
H	-5.46735	-0.28467	-0.16964
H	-5.65498	-1.96165	-0.71158
C	-3.84421	-1.88563	1.37191
H	-4.58623	-2.70350	1.43440
H	-4.22734	-1.04967	1.97596
H	-2.92362	-2.24928	1.85475
C	-1.60508	-0.01867	-2.01045
H	-2.41987	0.02869	-2.75209
H	-1.00749	-0.91997	-2.21257
H	-0.95393	0.85476	-2.16686
C	-3.06038	1.72833	0.10318
C	-3.97382	2.18457	-1.05488
H	-4.85484	1.54242	-1.18595
H	-3.43400	2.21496	-2.01516
H	-4.34506	3.20801	-0.85997
C	-3.84973	1.73848	1.42498
H	-4.18779	2.76412	1.66320
H	-3.23189	1.39119	2.26998
H	-4.74866	1.10498	1.38069
C	-1.91778	2.75731	0.21578
H	-2.33315	3.76229	0.41629
H	-1.33181	2.82904	-0.71256
H	-1.22056	2.52618	1.03705
C	1.45086	-2.77230	-0.93636
H	0.59826	-2.13290	-0.68205
H	1.12240	-3.82236	-0.89451
H	1.75473	-2.54439	-1.97015
C	2.26714	-2.90142	1.47885
H	3.14694	-2.78385	2.13079
H	1.92295	-3.94539	1.54505
H	1.47237	-2.25162	1.86199
C	4.34248	-0.69412	-0.40553
H	5.16309	-1.36648	-0.62047
C	4.33796	0.65688	-0.41088
H	5.15363	1.33299	-0.63319
C	2.60234	2.50374	-0.03383
C	1.52364	2.67453	-1.11768
H	1.94958	2.47598	-2.11379
H	1.12547	3.70070	-1.10545
H	0.69936	1.97462	-0.94376
C	3.77842	3.44001	-0.35091
H	4.58593	3.35205	0.39226
H	3.41527	4.47783	-0.32712
H	4.19444	3.25858	-1.35353
C	2.06109	2.86148	1.36240
H	1.21378	2.22326	1.63399
H	1.72918	3.91115	1.37764
H	2.84929	2.73460	2.12102
Si	-0.46310	-0.26468	1.31795
H	-0.97738	-1.75986	0.61965
H	-0.61368	-1.79181	1.70388

TS2^{M}H$_2$'

Si	-0.52268	0.23550	1.57235
Si	-2.21436	-0.09160	-0.19693
N	3.12988	-0.90066	-0.15476
N	0.98733	-0.15485	0.61004
N	2.79800	1.30096	-0.12339
C	4.17851	-3.10840	-0.52454
H	4.38626	-2.89734	-1.58444
H	4.00647	-4.19032	-0.42892
H	5.07055	-2.86081	0.07061
C	2.92706	-2.36728	-0.02600
C	2.17276	0.07726	0.17070
C	-3.11667	-1.82403	0.00352
C	-2.15640	-2.93176	-0.47843
H	-2.63692	-3.92215	-0.37115
H	-1.22686	-2.95979	0.10966
H	-1.88175	-2.81468	-1.53874
C	-4.39575	-1.89952	-0.85317
H	-4.20466	-1.66664	-1.91359
H	-5.17724	-1.21413	-0.49263
H	-4.81948	-2.92082	-0.81458
C	-3.48767	-2.10872	1.47342
H	-3.97922	-3.09625	1.55841
H	-4.18419	-1.36262	1.88333
H	-2.60195	-2.13260	2.12822
C	-1.42761	-0.07179	-1.93428
H	-2.11357	-0.47714	-2.69671
H	-0.50205	-0.66760	-1.94710
H	-1.16168	0.95321	-2.23624
C	-3.44400	1.43234	-0.11337
C	-4.33054	1.53644	-1.37107

H	-5.00974	0.68022	-1.48397
H	-3.72891	1.60866	-2.29169
H	-4.95856	2.44614	-1.32000
C	-4.33535	1.35434	1.14038
H	-4.94064	2.27481	1.24126
H	-3.74067	1.25045	2.06352
H	-5.03952	0.50940	1.09657
C	-2.60515	2.72552	-0.02982
H	-3.27022	3.60643	0.04291
H	-1.97795	2.86918	-0.92330
H	-1.94632	2.74415	0.85474
C	1.73460	-2.80220	-0.89918
H	0.81339	-2.27988	-0.62222
H	1.56493	-3.88499	-0.79797
H	1.94044	-2.58044	-1.95793
C	2.71826	-2.72996	1.45712
H	3.60838	-2.45231	2.04284
H	2.55708	-3.81382	1.56337
H	1.85726	-2.21243	1.89513
C	4.28389	-0.27858	-0.62648
H	5.16451	-0.82333	-0.94147
C	4.08327	1.05582	-0.60795
H	4.76376	1.84361	-0.90377
C	2.19234	2.64522	0.05835
C	0.91844	2.74348	-0.79603
H	1.16302	2.63069	-1.86362
H	0.43118	3.71842	-0.64770
H	0.20176	1.95842	-0.53674
C	3.17553	3.72806	-0.41521
H	4.10236	3.73272	0.17818
H	2.69825	4.71092	-0.29134
H	3.43219	3.61532	-1.47948
C	1.89615	2.88178	1.55024
H	1.16644	2.16310	1.95070
H	1.48619	3.89312	1.69783
H	2.82118	2.79148	2.14099
H	-0.42364	-1.55572	1.74037
H	0.31210	-1.29546	1.17816

H	-3.57795	1.93914	-2.21401
H	-4.65656	2.89689	-1.17732
C	-4.09131	1.69541	1.23221
H	-4.54665	2.69325	1.37374
H	-3.49124	1.47818	2.13150
H	-4.91602	0.96737	1.19205
C	-2.22146	2.83155	0.01519
H	-2.75352	3.79654	0.10916
H	-1.60415	2.89241	-0.89437
H	-1.54279	2.74758	0.87835
C	1.34465	-2.78689	-0.87809
H	0.51679	-2.13200	-0.58995
H	1.01329	-3.83159	-0.77623
H	1.58207	-2.59780	-1.93674
C	2.28651	-2.83223	1.48314
H	3.18598	-2.65452	2.09335
H	1.98979	-3.88606	1.60165
H	1.47641	-2.20259	1.86734
C	4.23719	-0.67343	-0.61111
H	5.02656	-1.34583	-0.92191
C	4.24141	0.67805	-0.59277
H	5.03435	1.35424	-0.88616
C	2.57539	2.52551	0.03368
C	1.38407	2.77534	-0.90739
H	1.68309	2.61442	-1.95515
H	1.02246	3.80967	-0.80153
H	0.56178	2.09233	-0.67169
C	3.72613	3.46298	-0.36245
H	4.60775	3.32734	0.28276
H	3.38643	4.50269	-0.24827
H	4.02782	3.32704	-1.41220
C	2.19771	2.80834	1.49958
H	1.36572	2.17579	1.82802
H	1.90018	3.86258	1.61193
H	3.05986	2.61953	2.15850
Si	-0.48879	-0.10814	1.37978
H	-0.62455	-1.38547	2.17051
H	-0.68096	0.97716	2.40858

H	-5.26016	0.37783	-1.18536
H	-4.17570	1.45195	-2.09382
H	-5.40325	2.13767	-1.00716
C	-4.44497	1.12672	1.37204
H	-5.12839	1.97988	1.54439
H	-3.76412	1.07194	2.23852
H	-5.06206	0.21459	1.36993
C	-2.97908	2.68355	0.07697
H	-3.73057	3.48920	0.18025
H	-2.41855	2.88361	-0.85149
H	-2.27379	2.77071	0.91817
C	2.19165	-2.82008	-1.22590
H	1.16194	-2.43859	-1.24604
H	2.12222	-3.91796	-1.21541
H	2.68417	-2.51166	-2.16065
C	2.33644	-2.72956	1.32678
H	2.95845	-2.39786	2.17211
H	2.23658	-3.82412	1.37950
H	1.33846	-2.29340	1.45949
C	4.41494	-0.19883	-0.17884
H	5.35947	-0.71631	-0.28020
C	4.17563	1.12850	-0.13353
H	4.88206	1.94601	-0.17820
C	2.16725	2.69847	-0.06367
C	0.87395	2.67124	-0.89290
H	1.04935	2.23236	-1.88668
H	0.51990	3.70405	-1.02482
H	0.07387	2.11226	-0.39981
C	3.14612	3.66778	-0.75312
H	4.05709	3.84386	-0.16221
H	2.64693	4.64064	-0.86236
H	3.43049	3.31641	-1.75711
C	1.90783	3.17150	1.37417
H	1.18545	2.50874	1.87702
H	1.48867	4.18990	1.35933
H	2.84746	3.19135	1.94954
H	-0.52420	-1.06050	2.04714
H	0.70403	-1.12430	-0.10038

$INT2^{M}H_2$

Si	-2.25837	-0.00577	-0.22214
N	3.00178	-1.11260	-0.14010
N	1.01198	0.01093	0.63208
N	3.01079	1.11063	-0.10677
C	3.71357	-3.45773	-0.46754
H	3.96665	-3.29540	-1.52638
H	3.38008	-4.50034	-0.36208
H	4.62366	-3.33733	0.13969
C	2.58088	-2.53169	0.00231
C	2.20489	-0.00176	0.18629
C	-3.35141	-1.61415	-0.04190
C	-2.47830	-2.81602	-0.46363
H	-3.04975	-3.75636	-0.35388
H	-1.57592	-2.91085	0.16111
H	-2.15532	-2.75051	-1.51473
C	-4.59338	-1.56713	-0.95256
H	-4.33656	-1.35899	-2.00431
H	-5.31513	-0.80343	-0.62442
H	-5.11968	-2.53967	-0.93046
C	-3.80799	-1.84041	1.41409
H	-4.37871	-2.78496	1.48919
H	-4.46351	-1.03639	1.77905
H	-2.95591	-1.91993	2.10729
C	-1.47672	-0.01781	-1.95781
H	-2.23676	-0.17799	-2.74006
H	-0.71682	-0.80746	-2.05209
H	-0.97714	0.94146	-2.16350
C	-3.24019	1.67343	-0.05101
C	-4.15025	1.91806	-1.27255
H	-4.93512	1.15528	-1.37595

$INT2^{M}H_2$'

Si	-0.50578	0.36161	1.45928
Si	-2.28782	-0.06169	-0.14608
N	3.19089	-0.85602	-0.07101
N	0.89792	-0.17001	0.17187
N	2.79863	1.32816	-0.02638
C	4.38438	-3.02116	-0.06676
H	4.91184	-2.80649	-1.00844
H	4.23913	-4.10913	-0.01043
H	5.02316	-2.72785	0.77940
C	3.00625	-2.34254	-0.00656
C	2.18994	0.09449	0.03925
C	-2.96082	-1.90856	-0.04897
C	-1.79590	-2.83042	-0.47135
H	-2.10373	-3.89196	-0.41888
H	-0.92946	-2.71617	0.20155
H	-1.46390	-2.63955	-1.50533
C	-4.15028	-2.16463	-0.99264
H	-3.93843	-1.86513	-2.03212
H	-5.05233	-1.62530	-0.66604
H	-4.40710	-3.24136	-1.00817
C	-3.37408	-2.29295	1.38484
H	-3.66497	-3.36019	1.42815
H	-4.23629	-1.70847	1.73909
H	-2.55007	-2.14445	2.10005
C	-1.63821	0.14416	-1.93972
H	-2.34838	-0.25820	-2.68101
H	-0.67131	-0.36273	-2.08245
H	-1.48017	1.20814	-2.17561
C	-3.67815	1.30621	0.04864
C	-4.67884	1.30891	-1.12366

$TSINT2^{M}$

Si	-1.13786	-0.30846	0.63060
Si	0.59654	1.19504	0.12998
Si	-3.25051	0.42994	1.47741
Si	1.10560	2.84575	-1.58068
N	-1.40959	-1.73314	-0.26694
N	-1.22603	-3.54767	-1.79372
N	-0.40840	-3.90930	0.24608
N	2.03865	0.36428	0.46340
N	3.75455	-1.29061	-0.01050
N	3.90042	-0.11230	1.87713
C	-1.03574	-2.92774	-0.54855
C	-0.72341	-4.84253	-1.75337
C	-0.22382	-5.06211	-0.51765
C	-2.05533	-2.97502	-2.89236
C	-2.04232	-3.92815	-4.09685
C	-3.50002	-2.82158	-2.38440
C	-1.47537	-1.62365	-3.33733
C	-0.03940	-3.78877	1.68898
C	0.46636	-5.14665	2.20514
C	1.08562	-2.75690	1.87169
C	-1.28544	-3.40747	2.50643
C	-4.16514	-1.20824	1.82249
C	-3.00030	1.30980	3.20252
C	-4.29472	1.22483	4.03968
C	-1.88270	0.57026	3.96917
C	-2.59488	2.78752	3.05310
C	-4.35046	1.40684	0.19419
C	-4.57113	0.47569	-1.01584
C	-3.66227	2.68440	-0.30727
C	-5.71889	1.77926	0.79755

C	3.11958	-0.25884	0.71313
C	4.87977	-1.71828	0.69635
C	4.96236	-1.00957	1.84321
C	3.44095	-1.68834	-1.41108
C	4.34774	-2.85192	-1.84076
C	1.98232	-2.15421	-1.53472
C	3.70770	-0.47975	-2.31602
C	3.58979	0.83825	2.97743
C	4.66114	0.72529	4.07310
C	3.60631	2.27644	2.42815
C	2.22086	0.48774	3.59306
C	2.99522	2.96352	-1.85675
C	0.62249	4.59830	-0.83391
C	1.52903	4.84187	0.39385
C	0.86636	5.73355	-1.84831
C	-0.84161	4.67507	-0.36883
C	0.30385	2.43330	-3.31492
C	0.79558	1.02931	-3.72263
C	0.75078	3.42352	-4.40920
C	-1.23431	2.41140	-3.25290
H	-0.93020	0.96173	-0.47848
H	0.10184	2.10106	1.23339
H	0.26321	-5.95107	-0.13938
H	-0.73803	-5.51224	-2.60385
H	-2.63098	-3.47514	-4.90777
H	-2.49818	-4.90226	-3.86344
H	-1.02171	-4.09291	-4.47619
H	-4.13434	-2.37350	-3.16487
H	-3.52457	-2.17423	-1.50043
H	-3.91805	-3.80504	-2.11681
H	-2.08388	-1.20285	-4.15249
H	-0.44715	-1.75062	-3.70624
H	-1.46026	-0.91065	-2.50670
H	0.71020	-5.04236	3.27221
H	1.38408	-5.46942	1.69073
H	-0.29492	-5.93613	2.11136
H	1.32083	-2.64980	2.94169
H	0.80540	-1.76543	1.49382
H	2.00179	-3.07229	1.35199
H	-1.03434	-3.36906	3.57725
H	-2.08619	-4.14853	2.35920
H	-1.67468	-2.42763	2.21618
H	-5.24677	-1.03737	1.94457
H	-3.79831	-1.68692	2.74303
H	-4.01518	-1.91759	0.99475
H	-4.13911	1.70506	5.02376
H	-4.59696	0.18297	4.23109
H	-5.14277	1.73534	3.55984
H	-1.78886	0.98100	4.99175
H	-0.90528	0.67736	3.47489
H	-2.08677	-0.50913	4.06960
H	-2.36011	3.22087	4.04313
H	-3.40266	3.39561	2.61771
H	-1.70101	2.90771	2.42118
H	-5.17666	0.99020	-1.78483
H	-5.10476	-0.44820	-0.74307
H	-3.61781	0.18679	-1.48539
H	-4.26020	3.15273	-1.11120
H	-2.66958	2.46581	-0.72054
H	-3.53514	3.43568	0.48430
H	-6.36544	2.22651	0.01968
H	-5.62350	2.52395	1.60297
H	-6.25677	0.90773	1.20430
H	5.53625	-2.50225	0.34199
H	5.69997	-1.08781	2.63198
H	4.06002	-3.15863	-2.85704
H	4.22900	-3.72651	-1.18256
H	5.41022	-2.56728	-1.87068
H	1.74222	-2.34366	-2.59133
H	1.28361	-1.40499	-1.15317
H	1.81779	-3.08760	-0.98092
H	3.50671	-0.72819	-3.36908
H	4.75465	-0.15118	-2.22375
H	3.05890	0.34913	-2.02392
H	4.42188	1.44101	4.87303
H	5.66511	0.97206	3.69478
H	4.68645	-0.27888	4.52334
H	3.37664	2.99293	3.23172
H	2.86719	2.40409	1.63140
H	4.60017	2.51824	2.01963
H	1.97660	1.19750	4.39850
H	2.24602	-0.52629	4.02174
H	1.42256	0.52125	2.84323
H	3.28952	4.00174	-2.07752
H	3.33041	2.34366	-2.69989
H	3.54675	2.63579	-0.96223
H	1.30345	5.82974	0.83701
H	2.59978	4.83799	0.13654
H	1.36777	4.09134	1.18239
H	0.74514	6.71424	-1.35136
H	0.14448	5.70412	-2.67784
H	1.87864	5.71298	-2.28260
H	-1.04342	5.66048	0.09182
H	-1.07639	3.90971	0.38267
H	-1.55101	4.55642	-1.20045
H	0.26900	0.69015	-4.63355
H	0.61474	0.27551	-2.94236
H	1.87133	1.02230	-3.94966
H	0.40985	3.06973	-5.40045
H	1.84743	3.52369	-4.45818
H	0.32929	4.42762	-4.26286
H	-1.65203	2.13700	-4.23974
H	-1.65587	3.39115	-2.98226
H	-1.60638	1.67488	-2.52509

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