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Supporting Information

Intercepting the Disilene-Silylsilylene Equilibrium

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1 Crystal Structure of Disilene 6

The solid-state structure of **6** is shown in Figure S1. The structural features of **6** are broadly similar to those of **3**. The heavily pyramidalized geometry around Si2 again indicates the presence of an electron lone pair (sum of angles at Si2 = 297.66(3)°). The marginally lower level of pyramidalization at Si2 in **6** compared to **3** (296.15(5)), together with its shorter Si1–Si2 bond distance (2.3225(6) vs. 2.3575(8) Å) is consistent with the reduced electron donating capability of 4-PPy compared to ^{Me}tPr. The N1–Si1 bond (1.8839(14) Å) is considerably shorter than that of the only other 4-PPy coordinated silicon center, a 4-PPy-stabilised bromosilylene (1.939(2) Å) reported by Tamao.^[1]

Figure S1 – Crystal structure of **6**. Selected bond lengths (Å) and angles (°): Si1-Si2 2.3225(6), Si1-N1 1.8839(14), Si1-C1 1.9076(16), Si2-Si3 2.3502(6), Si2-Si4 2.3594(7), N2-C27 1.336(2); N1-Si1-Si2 103.70(5), N1-Si1-C1 106.91(7), C1-Si1-Si2 124.15(5), Si1-Si2-Si3 105.43(2), Si1-Si2-Si4 91.87(2), Si3-Si2-Si4 100.36(2).

2 Experimental Details

General Considerations

All manipulations were carried out under an argon atmosphere using standard Schlenk or glovebox techniques. Solvents were obtained from an Inert solvent purification system and stored over 4 Å molecular sieves. C₆D₆ and THF-d₈ were dried over potassium then distilled under argon and stored over 4 Å molecular sieves. Ambient temperature NMR spectra were recorded on Bruker PRO 500 MHz or AVA 500 MHz spectrometers. Variable temperature NMR spectra were recorded on Bruker AVA 400 or AVA 600 MHz spectrometers. ¹H and ¹³C spectra were referenced to residual solvent signals.^[2] ²⁹Si NMR were referenced to an external standard of tetramethylsilane. UV/Vis spectra were acquired under argon in hexane on a Varian Cary 300 UV-visible Spectrophotometer. Cp*SiHCl₂,^[3] Ar*SiHCl₂,^[4] (THF)_nKSi(SiMe₃)₃,^[5] and ^{Me}iPr^[6] were prepared according to literature procedures. All other reagents were used as supplied.

Preparation of silane 1

Tris(trimethylsilyl)pentamethylcyclopentadienylchlorosilane [(Cp*)(Si(SiMe₃))SiHCl]

A solution of Cp*SiHCl₂ (1.15 g, 4.9 mmol) in C₆H₆ (10 mL) was added over 10 seconds to KSi(SiMe₃)₃·THF_n (2.0 g, 4.9 mmol, n = 1.67) in C₆H₆ (40 mL) at room temperature giving a yellow/orange mixture which was stirred for 2 hours at room temperature. The volatiles were removed under reduced pressure and the resulting waxy solid was extracted with warm (45 °C) hexane (50 mL). The filtrate was concentrated and cooled to afford colourless, block-shaped crystals of silane **1** (1.35 g, 62%) of excellent purity for further synthetic work. Samples of higher purity could be obtained by dissolution of **1** in hexane, filtration through celite and multiple recrystallisations.

¹H NMR (500.2 MHz, C₆D₆, 300 K): δ (ppm) 5.43 (s, 1H, Si-H, ¹J_{H-Si} = 200 Hz, ²J_{H-Si} = 13 Hz), 1.79 (br s, 15H, Cp*-CH₃), 0.27 (s, 27H, Si(SiMe₃)₃).

¹³C{¹H} NMR (125.8 MHz, C₆D₆, 300 K): δ (ppm) 136.0 (br s, Cp* C-Me) 11.7 (br s, Cp* -CH₃), 2.4 (s, Si(SiMe₃)₃, ¹J_{C-Si} = 45 Hz).

²⁹Si{¹H} NMR (99.4 MHz, C₆D₆, 300 K): δ (ppm) 20.2 (s, Si-H), - 8.8 (s, Si(SiMe₃)₃), - 126.1 (s, Si(SiMe₃)₃)

Melting Point: 174-176 °C

Elemental Analysis: Despite repeated attempts compound **1** proved unsuitable for combustion analysis. Found (%): C, 50.95 H, 10.63. Calc. for C₁₉H₄₅Si₅: C, 51.00; H, 9.69.

Mass Peak Analysis: Calculated mass for C₁₉H₄₃ClSi₅ for most abundant isotopes: 446.18942 Da;
Observed mass peak: 446.18894 Da.

Preparation of silane 2

Tris(trimethylsilyl)2,6-bis(2,4,6-trimethylphenyl)phenylchlorosilane [(Ar*)(Si(SiMe₃))SiHCl]

Potassium tris(trimethylsilyl)silyl was prepared *in situ* by the addition of THF (15 mL) to tetrakis(trimethylsilyl)silane (2 g, 6.23 mmol) and potassium *tert*-butoxide (0.76 g, 6.77 mmol). The reaction was stirred for 16 hours before removal of the volatiles and extraction with warm hexane (40 °C, 50 mL) to remove excess potassium *tert*-butoxide. The hexane was removed *in vacuo* and the anion was dissolved in THF (20 mL). The solution was added dropwise over 1 minute to a solution of terphenyldichlorosilane (2.6 g, 6.23 mmol) in THF (50 mL) at – 78 °C. The reaction was allowed to warm to room temperature and stirred for a total of 18 hours.

The volatiles were removed *in vacuo* and the product was extracted with hot diethyl ether (3 × 90 mL). Concentration of the resultant solution afforded pure silane **2** as colourless, block-shaped crystals suitable for X-ray diffraction containing 0.33 equivalents of diethyl ether (confirmed by elemental analysis, ¹H and ¹³C NMR) (1.92 g, 4.00 mmol, 64%).

¹H NMR (500.2 MHz, C₆D₆, 300 K): δ (ppm) 7.16 (t, *J*_{H-H} = 7.5 Hz, 1H, *p*-H), 6.88 (s, 2H, Mes-H), 6.85 (s, 2H, Mes-H), 6.83 (d, *J*_{H-H} = 7.5 Hz, 2H, *m*-H), 5.39 (s, *J*_{H-Si} = 215, 13 Hz, 1H, Si-H), 2.24 (s, 6H, Mes-CH₃), 2.19 (s, 6H, Mes-CH₃), 2.14 (s, 6H, Mes-CH₃), 0.18 (s, 27H, Si(SiCH₃)₃).

¹³C{¹H} NMR (125.8 MHz, C₆D₆, 300 K): δ (ppm) 149.8 (s, Ar C-Mes), 140.8 (s, Mes-CCH₃), 136.6 (s, Mes-CCH₃), 135.4 (br s, Mes-CCH₃), 133.4 (s, Ar C-Si), 131.0 (s, *p*-Ar), 129.4 (s *m*-Ar), 128.4 (s, Mes *m*-CH), 128.3 (s, Mes *m*-CH), 21.9 (s, Mes-CH₃), 21.9 (br s, Mes-CH₃), 20.8 (s, Mes-CH₃), 2.60 (s, SiMe₃, ¹*J*_{C-Si} = 45 Hz)

²⁹Si{¹H} NMR (99.4 MHz, C₆D₆, 300 K): δ (ppm) – 7.53 (s, Si-H), – 8.72 (s, SiMe₃), – 117.6 (s, Si(SiMe₃)₃).

Melting Point: 249–251 °C

Elemental Analysis: Found (%): C, 63.19; H, 8.62. Calc. for C₃₃H₅₃ClSi₅·¹/₃C₄H₁₀O: C, 63.35; H, 8.54.

Mass Peak Analysis: Calculated mass for $\text{C}_{33}\text{H}_{53}\text{ClSi}_5$ for most abundant isotopes: 624.26767 Da;
Observed mass peak: 624.26739 Da.

Preparation of disilene **3**

Zwitterion [⁺I^{Me}iPr)(Cp*)SiH-Si⁻(SiMe₃)₂]

THF (40 mL) was added to a flask charged with **1** (1.44 g, 3.22 mmol), KO^tBu (0.38 g, 3.37 mmol) and I^{Me}iPr (0.60 g, 3.33 mmol) and the resultant red/orange mixture was stirred for 16 hours. The volatiles were removed and the orange solid was extracted with benzene (1 × 50 mL, 2 × 10 mL). Removal of the volatiles and washing with diethyl ether (4 × 10 mL) gave pure disilene **3** as a bright orange powder (882 mg, 1.70 mmol, 53%). Orange, block-shaped single crystals suitable for X-ray diffraction could be grown from a concentrated solution in benzene at room temperature or diethyl ether at – 20 °C.

¹H NMR (500.2 MHz, C₆D₆, 300 K): δ (ppm) 5.83 (sept, 1H, I^{Me}iPr CHMe₂, ³J_{H-H} = 6.8 Hz), 5.71 (s, 1H, Si-H, ¹J_{H-Si} = 165 Hz), 5.06 (sept, 1H, I^{Me}iPr CHMe₂, ³J_{H-H} = 6.8 Hz), 2.41 (s, 3H, Cp*), 1.95 (s, 3H, Cp*), 1.67 (s, 3H, Cp*), 1.60 (s, 3H, Cp*), 1.56 (d, 3H, I^{Me}iPr CHMeMe × 1, ³J_{H-H} = 6.8 Hz), 1.54 (s, 3H, Cp*), 1.40 (s, 3H, I^{Me}iPr Me), 1.36 (s, 3H, I^{Me}iPr Me), 1.05 (d, 3H, I^{Me}iPr CHMeMe × 2, ³J_{H-H} = 6.8 Hz), 0.95 (d, 3H, I^{Me}iPr CHMeMe × 1, ³J_{H-H} = 6.8 Hz), 0.59 (s, 18H, SiMe₃ × 2).

¹³C{¹H} NMR (125.8 MHz, C₆D₆, 300 K): δ (ppm) 156.1 (s, I^{Me}iPr C-Si), 141.4 (s, Cp* C-CH₃), 140.8 (s, Cp* C-CH₃), 132.6 (s, Cp* C-CH₃), 132.3 (s, Cp* C-CH₃), 127.1 (s, I^{Me}iPr C-CH₃), 126.9 (s, I^{Me}iPr C-CH₃), 56.4 (s, Cp* C-Si), 52.3 (s, I^{Me}iPr C(CH₃)₂), 51.2 (s, I^{Me}iPr C(CH₃)₂), 22.5 (s, I^{Me}iPr C(CH₃)₂), 21.9 (s, I^{Me}iPr C(CH₃)₂), 21.5 (s, I^{Me}iPr C(CH₃)₂), 20.5 (s, I^{Me}iPr C(CH₃)₂), 18.6 (s, Cp*-CH₃), 13.6 (s, Cp*-CH₃), 11.9 (s, Cp*-CH₃), 11.8 (s, Cp*-CH₃), 11.4 (s, Cp*-CH₃), 9.8 (s, I^{Me}iPr C-CH₃), 9.7 (s, I^{Me}iPr C-CH₃), 6.3 (s, Si(CH₃)₃).

²⁹Si{¹H} NMR (99.4 MHz, C₆D₆, 300 K): δ (ppm) – 5.1 (s, Si-H), – 13.0 (s, Si(SiMe₃)₂), – 202.2 (Si(SiMe₃)₂).

Melting point: 170 – 172 °C (dp)

Elemental Analysis: Found (%): C, 62.09; H, 10.27; N, 5.26. Calculated for $\text{C}_{27}\text{H}_{54}\text{N}_2\text{Si}_4$: C, 62.47; H, 10.49; N, 5.40.

Mass Peak Analysis: Calculated mass for $\text{C}_{27}\text{H}_{54}\text{N}_2\text{Si}_4$ for most abundant isotopes: 518.33587 Da;
Observed mass peak: 518.33740 Da.

UV-vis: (λ_{max} , ϵ): 444 nm, 494 $\text{dm}^3 \text{mol}^{-1} \text{cm}^{-1}$

Preparation of silylsilylene **5**

NHC-stabilised silylsilylene

THF (50 mL) was added to a flask containing silane **2** (650 mg, 1.00 mmol), potassium *tert*-butoxide (131 mg, 1.17 mmol) and $\text{I}^{\text{Me}}\text{iPr}$ (180 mg, 1.00 mmol). The mixture was heated to 50 °C for 16 h at which point complete conversion was confirmed by ^1H NMR spectroscopy. Removal of the volatiles afforded a red oily solid which was extracted with pentane (2×30 mL) and concentrated to afford pure silylsilylene **5** as red, block-shaped, extremely sensitive crystals suitable for X-ray diffraction (283 mg, 0.41 mmol, 41%). An analytically pure sample was obtained by recrystallisation from pentane at -20 °C.

^1H NMR (500.2 MHz, C_6D_6 , 300 K): δ (ppm) 7.33 (br, 1H, $\text{I}^{\text{Me}}\text{iPr}$, CHMe_2), 7.20 (t, 1H, $p\text{-Ar-H}$, $^3J_{\text{H-H}} = 7.5$ Hz), 7.10 (s, 1H, Mes-H), 6.96 – 6.94 (m, 2H, Mes-H and $m\text{-Ar-H}$), 6.91 (d, 1H, $m\text{-Ar-H}$, $^3J_{\text{H-H}} = 7.5$ Hz), 6.88 (s, 1H, Mes-H), 6.42 (s, 1H, Mes-H), 5.48 (br, 1H, $\text{I}^{\text{Me}}\text{iPr}$, CHMe_2), 3.91 (s, 1H, Si-H , $^1J_{\text{H-Si}} = 155$ Hz), 2.81 (s, 3H, Mes-CH_3), 2.36 (s, 3H, Mes-CH_3), 2.28 (s, 3H, Mes-CH_3), 2.27 (s, 3H, Mes-CH_3), 2.22 (s, 3H, Mes-CH_3), 1.68 (br, 3H, $\text{I}^{\text{Me}}\text{iPr}$, CH_3), 1.61 (br, 3H, $\text{I}^{\text{Me}}\text{iPr}$, CH_3), 1.54 (s, 3H, Mes-CH_3), 1.06 (br, 6H, $\text{I}^{\text{Me}}\text{iPr}$, CH_3), 0.99 (br, 6H, $\text{I}^{\text{Me}}\text{iPr}$, CH_3), 0.35 (s, 9H, $\text{Si(CH}_3)_3$), 0.32 (s, 9H, $\text{Si(CH}_3)_3$).

$^{13}\text{C}\{^1\text{H}\}$ NMR (125.8 MHz, C_6D_6 , 300 K): δ (ppm) 172.2 (s, $\text{I}^{\text{Me}}\text{iPr}$, C-Si , $^1J_{\text{C-Si}} = 25$ Hz), 149.9 (s, Ar $m\text{-C-Mes}$), 148.7 (s, Ar $m\text{-C-Mes}$), 143.8 (s, Mes *ipso*-C-Ar), 141.7 (s, Mes *ipso*-C-Ar), 141.1 (s, Ar C-Si), 137.9 (s, Mes *o*-C-CH₃), 136.0 (s, Mes *p*-C-CH₃), 135.5 (s, Mes *o*-C-CH₃), 135.2 (s, Mes *o*-C-CH₃), 135.1 (s, Mes *o*-C-CH₃), 134.3 (s, Mes *p*-C-CH₃), 129.6 (s, Mes C-H), 128.9 (s, Ar $m\text{-C-H}$), 127.9 (s, Mes C-H), 127.8 (s, Mes C-H), 127.6 (s, Ar *p*-C-H), 127.5 (s, Ar $m\text{-C-H}$), 127.0 (s, Mes C-H), 126.2 (br s, $\text{I}^{\text{Me}}\text{iPr}$, C-CH₃), 125.4 (br s, $\text{I}^{\text{Me}}\text{iPr}$, C-CH₃), 54.3 (s, $\text{I}^{\text{Me}}\text{iPr}$, CMe₂), 51.8 (s, $\text{I}^{\text{Me}}\text{iPr}$, CMe₂), 25.3 (s, Mes-CH₃), 22.9 (br s, $\text{I}^{\text{Me}}\text{iPr}$, CH₃), 22.5 (s, Mes-CH₃), 21.5 (br s, $\text{I}^{\text{Me}}\text{iPr}$, CH₃), 21.5 (s, Mes-CH₃), 21.4 (s, Mes-CH₃), 21.0 (s, Mes-CH₃), 21.0 (br s, $\text{I}^{\text{Me}}\text{iPr}$, CH₃), 20.8 (s, Mes-CH₃), 19.8 (br s, $\text{I}^{\text{Me}}\text{iPr}$, CH₃), 9.8 (s, $\text{I}^{\text{Me}}\text{iPr}$, CH₃ $\times 2$), 5.0 (s, $\text{Si(CH}_3)_3$, $^1J_{\text{C-Si}} = 41$ Hz, $^2J_{\text{C-Si}} = 10$ Hz), 2.4 (s, $\text{Si(CH}_3)_3$, $^1J_{\text{C-Si}} = 43$ Hz).

$^{29}\text{Si}\{^1\text{H}\}$ NMR (99.4 MHz, C_6D_6 , 300 K): δ (ppm) – 11.8 (s, $\underline{\text{Si}}\text{Me}_3$), – 13.8 (s, $\underline{\text{Si}}\text{Me}_3$), – 68.8 (s, $\underline{\text{Si}}\text{H}$), – 121.4 ($\underline{\text{Si}}(\text{SiMe}_3)(\text{I}^{\text{Me}}\text{iPr})$).

Melting Point: 100-103 °C

Elemental Analysis: Found: C, 70.67; H, 9.18; N, 4.04. Calc. for: $\text{C}_{41}\text{H}_{64}\text{N}_2\text{Si}_4$ C, 70.62; H, 9.25; N, 4.02.

Mass Peak Analysis: Calculated mass for $\text{C}_{41}\text{H}_{64}\text{N}_2\text{Si}_4$ for most abundant isotopes: 696.41412 Da;
Observed mass peak: 696.41267 Da.

UV-vis: (λ_{max} , ϵ): 470 nm, 862 $\text{dm}^3 \text{mol}^{-1} \text{cm}^{-1}$

Preparation of disilene 6

Ar* 4-Pyrrolidinopyridine Disilene

THF (50 mL) was added at $-70\text{ }^{\circ}\text{C}$ to a flask containing silane **2** (1000 mg, 1.54 mmol), potassium *tert*-butoxide (215 mg, 1.91 mmol) and 4-pyrrolidinopyridine (228 mg, 1.54 mmol). The resultant red mixture was warmed to $-10\text{ }^{\circ}\text{C}$ and then slowly warmed to ambient temperature over 4 hours at which point complete consumption of **2** was confirmed by ^1H NMR spectroscopy. Removal of the volatiles afforded a red solid which was extracted with toluene ($2 \times 80\text{ mL}$) and concentrated to give disilene **6** as a deep red solid in $> 90\%$ (judged by NMR) purity (395 mg, 0.59 mmol, 39%). An analytically pure sample was obtained by recrystallisation from toluene at $-20\text{ }^{\circ}\text{C}$.

^1H NMR (500.2 MHz, C_6D_6 , 300 K): δ (ppm) 8.12-8.11 (m, 2H, Py C-H), 7.22 (t, 1H, $^1J_{\text{H-H}} = 7.6\text{ Hz}$, Ar *p*-C-H), 7.06 (s, 2H, Mes-H), 6.92 (d, 2H, $^1J_{\text{H-H}} = 7.6\text{ Hz}$, Ar *m*-C-H), 6.70 (s, 2H, Mes-H), 5.85 (s, 1H, Si-H, $^1J_{\text{H-Si}} = 189\text{ Hz}$), 5.46-5.44 (m, 2H, Py C-H), 2.54 (s, 6H, Mes-CH₃ $\times 2$), 2.32-2.20 (m, 4H, Py C-H₂), 2.26 (s, 6H, Mes-CH₃ $\times 2$), 1.96 (s, 6H, Mes-CH₃ $\times 2$), 1.07-1.02 (m, 4H, Py C-H₂ $\times 2$), 0.41 (s, 18H, Si(CH₃)₃ $\times 2$).

$^{13}\text{C}\{^1\text{H}\}$ NMR (125.8 MHz, C_6D_6 , 300 K): δ (ppm) 152.7 (s, Py-C-N(CH₂CH₂)₂), 148.5 (s, Ar *m*-C-Mes), 147.2 (s, Py-C-H), 140.9 (s, Mes *ipso*-C-Ar), 138.5 (s, Ar C-Si), 136.5 (s, Mes *o*-C-CH₃), 136.3 (s, Mes *p*-C-CH₃), 135.9 (s, Mes *o*-C-CH₃), 129.4 (s, Ar *p*-C-H), 128.9 (s, Ar *m*-C-H), 128.4 (s, Mes-C-H), 128.2 (s, Mes-C-H), 105.8 (s, Py-C-H), 46.7 (Py-CH₂ $\times 2$), 24.2 (Py-CH₂ $\times 2$), 22.9 (s, Mes-CH₃ $\times 2$), 22.1 (s, Mes-CH₃ $\times 2$), 20.9 (s, Mes-CH₃ $\times 2$), 6.28 (s, Si(CH₃)₃, $^1J_{\text{C-Si}} = 40\text{ Hz}$).

$^{29}\text{Si}\{^1\text{H}\}$ NMR (99.4 MHz, C_6D_6 , 300 K): δ (ppm) 34.6 (s, Si-H), -5.92 (s, Si(SiMe₃)₂), -184.0 (Si(SiMe₃)₂).

Elemental Analysis: Found: C, 70.23; H, 8.63; N, 4.09. Calc. for: C₄₁H₆₄N₂Si₄ C, 70.42; H, 8.49; N, 4.21.

Mass Peak Analysis: Calculated mass for $\text{C}_{39}\text{H}_{56}\text{N}_2\text{Si}_4$ for most abundant isotopes: 664.35152 Da;
Observed mass peak: 664.35346 Da.

Preparation of a mixture of **4** and **5** and conversion of **4** to **5**

THF (15 mL) was added at ambient temperature to a flask containing silane **2** (230 mg, 0.35 mmol), MeI^tPr (69 mg, 0.38 mmol) and KO^tBu (39 mg, 0.35 mmol). After stirring for one hour, the volatiles were removed from a reaction aliquot (**Aq-1**, 0.5 mL) which was then redissolved in C_6D_6 for ^1H NMR measurement. The reaction mixture was then heated at 50 °C for 16 hours after which a second aliquot (**Aq-2**, 0.5 mL) was taken. The volatiles were removed from the aliquot and the sample was redissolved in C_6D_6 for ^1H NMR.

By ^1H NMR, a mixture of **4** and **5** is observed when the sample is kept at room temperature, but heating leads to complete consumption of **4**. The reaction is complete within 3 hours at 55 °C, here we show the slower, cleaner conversion at 50 °C.

Figure S2 shows the ^1H NMR from 5.7 – 3.9 ppm of **Aq-1** and **Aq-2** which includes the Si-H resonances as well as some $\text{CH}(\text{CH}_3)_2$ resonances, and shows the complete consumption of **4** in this time.

Figure S2 – Expansion of ^1H NMR (500.2 MHz, C_6D_6 , 300 K) showing the Si-H and some $\text{CH}(\text{CH}_3)_2$ resonances from a mixture of **4** and **5** after 1 hour at room temperature and after 16 hours at 50 °C.

Conversion of 6 to 4 and 5

A sample of **6** (15 mg, 22 μmol) along with MeI/Pr (7 mg, 38 μmol) and mesitylene (25 μL , 21.6 mg, 0.18 mmol) was dissolved in $\text{THF-}d_8$ in a Young's NMR tube. The sample was loaded into a preheated NMR spectrometer at 55 $^\circ\text{C}$. The first ^1H spectrum was collected after 12 minutes. The sample was maintained at 55 $^\circ\text{C}$ in the spectrometer and further ^1H spectra were recorded every 5 minutes thereafter.

Figure S3 shows the three spectra and clear consumption of **6**. Initially, a mixture of **4** and **5** is obtained. Over time, **4** is consumed and the concentration of **5** increases. Figure S4 shows a plot of the concentrations of **6**, **4** and **5** as calculated from integration against mesitylene as the internal standard.

Figure S3 – Expansion of the ^1H NMR (600.8 MHz, $\text{THF-}d_8$, 328 K) of a sample of **6** being heated in the presence of MeI/Pr after 12, 37 and 87 minutes.

Figure S4 – Plot of the concentration of **6**, **4** and **5** when **6** is heated to 55 °C in the presence of ^{Me}I^{Pr}. Concentrations calculated from integration against mesitylene as an internal standard.

Base dissociation from disilene **6**

A sample of **6** was dissolved in THF-*d*₈ in an NMR tube along with mesitylene (20 μ L, 0.14 mmol) as an internal standard. The sample was slowly heated in the NMR spectrometer and spectra were recorded at 278 K, 298 K, 318 K and 333 K. The sample was then cooled and spectra were recorded at the same temperatures.

Concentrations were calculated by calibrating integrals against the mesitylene internal standard.

Temp (K)	Mesitylene (mmol)	Uncoordinated 4-Ppy (μ mol)	Coordinated 4-PPy (μ mol)	Uncoordinated 4-Ppy (%)	Coordinated 4-Ppy (%)
278	0.144	1.28	3.61	26.1	73.9
298	0.144	1.30	3.79	25.5	74.5
318	0.144	1.52	3.50	30.3	69.7
333	0.144	1.61	3.11	34.0	66.0
318	0.144	1.55	3.73	29.4	70.6
298	0.144	1.29	3.81	25.3	74.7
278	0.144	1.27	3.62	26.0	74.0

3 Computational Details

3.1 Computational Details

Geometry optimizations and harmonic frequency calculations were performed using the Gaussian16 program package^[7] employing the M06-L density functional^[8] and the 'fine' grid option in combination with the 6-31+G(d,p) basis set.^[9] For improved computational efficiency the density fitting approximation was used for these calculations (the 'auto' keyword was used for the automatic generation of a fitting basis set). Stationary points were characterized as minima or first order saddle points by eigenvalue analysis of the computed Hessians. Connectivities between minima and transition states implied in Figures and Schemes were validated either by intrinsic-reaction-coordinate (IRC) following calculations^[10] or by displacing the transition state geometries along both directions of the transition mode, followed by unconstrained optimizations to the respective minima. Single-point calculations were conducted on the optimized geometries using the M06-2X functional^[11] in combination with the 6-311++G(2d,2p) basis set^[12], and the 'ultrafine' grid option.^[13] The SMD polarizable continuum model^[14] was employed to account for solvent effects (THF), SMD-M06-2X/6-311++G(2d,2p)//RI-M06-L/6-31+G(d,p). The wave functions used for bonding analysis were obtained at the M06-2X/6-311++G(2d,2p)//RI-M06-L/6-31+G(d,p) level of theory. Natural bond orbital (NBO) calculations were performed using the NBO 6.0.18 program^[15] interfaced with Gaussian09.^[16] The AIMAll^[17] and multiwfn^[18] programs were used for QTAIM analyses.^[19] Unscaled zero-point vibrational, thermal and entropic corrections were obtained from computed Hessian matrices computed at the RI-M06-L/6-31+G(d,p) level using standard procedures as implemented in Gaussian16 to obtain free energy values at standard conditions (T = 298.15 K, p = 1 atm). Pictures of molecular structures were generated with the Cylview^[20] and ChemCraft^[21] programs.

3.2 Structural metrics of the computed and the X-RAY structure of **3**

Table S1. Selected metrics of the computed and the X-RAY structure of **3**. Hydrogen atoms and NHC methyl/*iso*-propyl groups are omitted in the computed structure.

computed structure		exp. X-RAY	
Si1-Si2	2.31 Å	Si1-Si2	2.36 Å
Si1-H1	1.50 Å	Si1-H1	1.48 Å
Si1-C1	1.95 Å	Si1-C1	1.95 Å
Si1-C12	1.97 Å	Si1-C12	1.95 Å
Si2-Si3	2.36 Å	Si2-Si3	2.36 Å
Si2-Si4	2.37 Å	Si2-Si4	2.36 Å
C1-Si1-Si2	111°	C1-Si1-Si2	110°
C1-Si1-Si2-Si3	-160°	C1-Si1-Si2-Si3	-170°
$\Sigma 4(\text{Si2})$	286°	$\Sigma 4(\text{Si2})$	297°

3.3 Structural metrics of the computed and the X-RAY structure of **5**

Table S2. Selected metrics of the computed and the X-RAY structure of **5**. Hydrogen atoms and NHC methyl/*iso*-propyl groups are omitted in the computed structure.

			<div style="display: flex; justify-content: space-around; align-items: center;"> </div>	
			computed structure	exp. X-RAY
Si1–Si2	2.36 Å	2.39 Å		
Si1–Si3	2.33 Å	2.34 Å		
Si1–C1	1.96 Å	1.98 Å		
Si2–Si4	2.35 Å	2.36 Å		
Si2–H1	1.49 Å	1.39 Å		
Si2–C12	1.92 Å	1.93 Å		
C1–Si1–Si2	102°	102°		
C1–Si1–Si2–Si4	–116°	–117°		
Σ4(Si1)	319°	317°		

3.4 Structural metrics of the computed and the X-RAY structure of 6

Table S3. Selected metrics of the computed and the X-RAY structure of **6**. Hydrogen atoms are omitted in the computed structure.

computed structure		exp. X-RAY	
Si1-Si2	2.29 Å	Si1-Si2	2.32 Å
Si1-H1	1.49 Å	Si1-H1	1.44 Å
Si1-N1	1.94 Å	Si1-N1	1.88 Å
Si1-C1	1.91 Å	Si1-C1	1.91 Å
Si2-Si3	2.34 Å	Si2-Si3	2.35 Å
Si2-Si4	2.35 Å	Si2-Si4	2.36 Å
N1-Si1-Si2	103°	N1-Si1-Si2	104°
N1-Si1-Si2-Si4	94°	N1-Si1-Si2-Si4	79°
$\Sigma 4(\text{Si2})$	303°	$\Sigma 4(\text{Si2})$	298°

3.5 QTAIM analysis of **3**

Figure S5. QTAIM analysis of **3**. (a) Molecular graph; (b) 2D plot of $\nabla^2\rho(r)$; charge concentration (blue) and depletion (red), bond paths (black lines), and bcps (blue dots).

Table S4. Selected properties of the electron density distribution in **3**; atom numbering as displayed in Figure S5. The electron density ρ_{bcp} is given in $\text{e}\text{\AA}^{-3}$, the Laplacian of the electron density $\nabla^2\rho_{\text{bcp}}$ in $\text{e}\text{\AA}^{-5}$, the total energy density H_{bcp} in $\text{E}_h\text{\AA}^{-3}$. $\varepsilon_{\text{bcp}} = \lambda_1/\lambda_2 - 1$ is the bond ellipticity derived from the two negative eigenvalues of the Hessian matrix of the electron density at the bcp, with $\lambda_1 \geq \lambda_2$. The delocalization index $\delta_{\text{A,B}}$ represents the number of electrons shared between two atoms A and B.

	ρ_{bcp}	$\nabla^2\rho_{\text{bcp}}$	H_{bcp}	ε_{bcp}	$\delta_{\text{A,B}}$
Si1–Si2	0.54	−1.69	−0.05	0.11	0.85
Si1–H1	0.79	3.01	−0.08	0.04	0.55
Si1–C1	0.64	3.89	−0.05	0.05	0.46
Si1–C12	0.68	1.12	−0.07	0.07	0.51
Si2–Si3	0.55	−2.43	−0.04	0.05	0.80
Si2–Si4	0.54	−2.29	−0.04	0.06	0.81

3.6 NBO analysis of **3**

Table S5. Selected results of the NBO analysis of **3**; wave functions computed at the M06-2X/6-311++G(2d,2p)//RI-M06-L/6-31+G(d,p) level of DFT.

Bond	NBO analysis (NLMOs) ^[a]		
	pol. [%]	hybr.	WBI
C1–Si1	76% (C1)	sp ^{1.35} (C1)	0.66
	22% (Si1)	sp ^{3.08} (Si1)	
Si1–Si2	55% (Si1)	sp ^{1.07} (Si1)	1.04
	41% (Si2)	sp ^{4.47} (Si2)	
Si2–Si3	47% (Si2)	sp ^{4.69} (Si2)	0.95
	48% (Si3)	sp ^{1.53} (Si3)	
Si2–Si4	45% (Si2)	sp ^{5.55} (Si2)	0.96
	50% (Si4)	sp ^{1.43} (Si4)	
LP(Si2)	91% (Si2)	sp ^{0.79} (Si2)	
	2% (Si1)	sp ^{22.8} (Si1)	

^[a] pol. = polarization, hybr. = hybridization, WBI = Wiberg bond index.

Table S6. Fragment charges obtained from NPA analysis of **3**; wave functions computed at the M06-2X/6-311++G(2d,2p)//RI-M06-L/6-31+G(d,p) level of DFT.

Fragment	NPA charge/e
NHC	0.38
NHC→Si(H)Cp*	0.66
Si(SiMe ₃) ₂	–0.66

3.7 Evaluation of Haaland's Definition of Dative Bonds

Figure S6. Computed homolysis and heterolysis of bonds in A^{Cp*} (cf. 3); ΔG^{298} in kcal mol⁻¹ (M06-2X/6-311++G(2d,2p)//RI-M06-L/6-31+G(d,p)).

3.8 QTAIM analysis of **4**

Figure S7. QTAIM analysis of **4**. (a) Molecular graph; (b) 2D plot of $\nabla^2\rho(r)$; charge concentration (blue) and depletion (red), bond paths (black lines), and bcps (blue dots).

Table S7. Selected properties of the electron density distribution in **4**; atom numbering as displayed in Figure S7. The electron density ρ_{bcp} is given in $\text{e}\text{\AA}^{-3}$, the Laplacian of the electron density $\nabla^2\rho_{\text{bcp}}$ in $\text{e}\text{\AA}^{-5}$, the total energy density H_{bcp} in $\text{E}_\text{h}\text{\AA}^{-3}$. $\epsilon_{\text{bcp}} = \lambda_1/\lambda_2 - 1$ is the bond ellipticity derived from the two negative eigenvalues of the Hessian matrix of the electron density at the bcp, with $\lambda_1 \geq \lambda_2$. The delocalization index $\delta_{\text{A,B}}$ represents the number of electrons shared between two atoms A and B.

	ρ_{bcp}	$\nabla^2\rho_{\text{bcp}}$	H_{bcp}	ϵ_{bcp}	$\delta_{\text{A,B}}$
Si1–Si2	0.53	–1.85	–0.05	0.15	0.86
Si1–H1	0.80	3.27	–0.08	0.04	0.55
Si1–C1	0.66	4.58	–0.06	0.10	0.47
Si1–C12	0.72	2.66	–0.07	0.03	0.52
Si2–Si3	0.54	–2.32	–0.04	0.10	0.82
Si2–Si4	0.55	–2.39	–0.04	0.06	0.81

3.9 NBO analysis of **4**

Table S8. Selected results of the NBO analysis of **4**; wave functions computed at the M06-2X/6-311++G(2d,2p)//RI-M06-L/6-31+G(d,p) level of DFT.

Bond	NBO analysis (NLMOs) ^[a]		
	pol. [%]	hybr.	WBI
C1–Si1	75% (C1) 23% (Si1)	sp ^{1.32} (C1) sp ^{3.42} (Si1)	0.68
Si1–Si2	55% (Si1) 41% (Si2)	sp ^{1.20} (Si1) sp ^{4.47} (Si2)	1.04
Si2–Si3	47% (Si2) 49% (Si3)	sp ^{4.67} (Si2) sp ^{1.51} (Si3)	0.97
Si2–Si4	45% (Si2) 50% (Si4)	sp ^{5.37} (Si2) sp ^{1.43} (Si4)	0.98
LP(Si2)	90% (Si2) 2% (Si1)	sp ^{0.79} (Si2) p (Si1)	

^[a] pol. = polarization, hybr. = hybridization, WBI = Wiberg bond index.

Table S9. Fragment charges obtained from NPA analysis of **4**; wave functions computed at the M06-2X/6-311++G(2d,2p)//RI-M06-L/6-31+G(d,p) level of DFT.

Fragment	NPA charge/e
NHC	0.38
NHC→Si(H)Cp*	0.65
Si(SiMe ₃) ₂	–0.65

3.10 QTAIM analysis of **6**

Figure S8. QTAIM analysis of **6**. (a) Molecular graph; (b) 2D plot of $\nabla^2\rho(r)$; charge concentration (blue) and depletion (red), bond paths (black lines), and bcps (blue dots).

Table S10. Selected properties of the electron density distribution in **6**; atom numbering as displayed in Figure S8. The electron density ρ_{bcp} is given in $\text{e}\text{\AA}^{-3}$, the Laplacian of the electron density $\nabla^2\rho_{\text{bcp}}$ in $\text{e}\text{\AA}^{-5}$, the total energy density H_{bcp} in $\text{E}_\text{h}\text{\AA}^{-3}$. $\epsilon_{\text{bcp}} = \lambda_1/\lambda_2 - 1$ is the bond ellipticity derived from the two negative eigenvalues of the Hessian matrix of the electron density at the bcp, with $\lambda_1 \geq \lambda_2$. The delocalization index $\delta_{\text{A,B}}$ represents the number of electrons shared between two atoms A and B.

	ρ_{bcp}	$\nabla^2\rho_{\text{bcp}}$	H_{bcp}	ϵ_{bcp}	$\delta_{\text{A,B}}$
Si1–Si2	0.55	−1.67	−0.05	0.21	0.93
Si1–H1	0.81	3.02	−0.08	0.05	0.54
Si1–N1	0.55	5.56	−0.03	0.06	0.37
Si1–C1	0.76	2.89	−0.07	0.10	0.55
Si2–Si3	0.58	−2.69	−0.04	0.07	0.82
Si2–Si4	0.57	−2.52	−0.04	0.06	0.81

3.11 NBO analysis of **6**

Table S11. Selected results of the NBO analysis of **6**; wave functions computed at the M06-2X/6-311++G(2d,2p)//RI-M06-L/6-31+G(d,p) level of DFT.

Bond	NBO analysis (NLMOs) ^[a]		
	pol. [%]	hybr.	WBI
N1–Si1	86% (N1)	sp ^{2.38} (N1)	0.38
	12% (Si1)	sp ^{3.69} (Si1)	
Si1–Si2	54% (Si1)	sp ^{0.98} (Si1)	1.15
	43% (Si2)	sp ^{4.72} (Si2)	
Si2–Si3	48% (Si2)	sp ^{4.41} (Si2)	0.96
	47% (Si3)	sp ^{1.59} (Si3)	
Si2–Si4	49% (Si2)	sp ^{3.76} (Si2)	0.97
	47% (Si4)	sp ^{1.62} (Si4)	
LP(Si2)	87% (Si2)	sp ^{0.97} (Si2)	
	5% (Si1)	p (Si1)	

^[a] pol. = polarization, hybr. = hybridization, WBI = Wiberg bond index.

Table S12. Fragment charges obtained from NPA analysis of **6**; wave functions computed at the M06-2X/6-311++G(2d,2p)//RI-M06-L/6-31+G(d,p) level of DFT.

Fragment	NPA charge/e
4-PPy	0.20
4-PPY→Si(H)Ar*	0.63
Si(SiMe ₃) ₂	–0.63

3.12 Additional Information on the Reaction Mechanism

Scheme S1. Computed reaction path for the disilene/silylsilylene isomerization of $\mathbf{A}^{\text{Ar}*}$ to $\mathbf{D}^{\text{Ar}*}$; ΔG^{298} in kcal mol⁻¹ (SMD-M06-2X/6-311++G(2d,2p)//RI-M06-L/6-31+G(d,p)).

Scheme S2. Computed reaction path for the disilene/silylsilylene isomerization of $\mathbf{E}^{\text{Ar}*}$ to $\mathbf{D}^{\text{Ar}*}$; ΔG^{298} in kcal mol⁻¹ (SMD-M06-2X/6-311++G(2d,2p)//RI-M06-L/6-31+G(d,p)).

Scheme S3. Computed reaction path for the disilene/silylsilylene isomerization of A^{Cp^*} to D^{Cp^*} ; ΔG^{298} in kcal mol⁻¹ (SMD-M06-2X/6-311++G(2d,2p)//RI-M06-L/6-31+G(d,p)).

Scheme S4. Computed reaction path for the NHC-assisted Si-Si bond cleavage in A^{Ar^*} ; ΔG^{298} in kcal mol⁻¹ (SMD-M06-2X/6-311++G(2d,2p)//RI-M06-L/6-31+G(d,p)).

Scheme S5. Computed reaction path for the hydride migration in A^{Ar^*} ; ΔG^{298} in kcal mol⁻¹ (SMD-M06-2X/6-311++G(2d,2p)//RI-M06-L/6-31+G(d,p)).

Scheme S6. Computed reaction path for the hydride migration in $\mathbf{C}^{\text{Ar}*}$; ΔG^{298} in kcal mol⁻¹ (SMD-M06-2X/6-311++G(2d,2p)//RI-M06-L/6-31+G(d,p)).

Scheme S7. Computed reaction path for the hydride migration in $\mathbf{B}^{\text{Ar}*}$; ΔG^{298} in kcal mol⁻¹ (SMD-M06-2X/6-311++G(2d,2p)//RI-M06-L/6-31+G(d,p)).

4 Crystallographic Details

Silane 1

Tris(trimethylsilyl)pentamethylcyclopentadienyl chlorosilane [(Cp*)(Si(SiMe₃))SiHCl]

Experimental

Single colourless block-shaped crystals of **1** were recrystallised from hexane by slow cooling. A suitable crystal (0.52×0.29×0.23) mm³ was selected and mounted on a MITIGEN holder in Paratone oil on a Rigaku Oxford Diffraction SuperNova diffractometer. The crystal was kept at $T = 120.0$ K during data collection. Using **Olex2**^[22], the structure was solved with the **ShelXS**^[23] structure solution program, using the Direct Methods solution method. The model was refined with version 2014/7 of **ShelXL**^[24] using Least Squares minimisation.

Crystal Data

C₅₇H₁₂₉Cl₃Si₁₅, $M_r = 1342.29$, orthorhombic, Cmc2₁ (No. 36), $a = 44.9370(12)$ Å, $b = 12.5333(2)$ Å, $c = 14.5469(3)$ Å, $\alpha = \beta = \gamma = 90^\circ$, $V = 8193.0(3)$ Å³, $T = 120.0$ K, $Z = 4$, $Z' = 0.5$, $\mu(\text{MoK}\alpha) = 0.362$, 73400 reflections measured, 10189 unique ($R_{\text{int}} = 0.0811$) which were used in all calculations. The final wR_2 was 0.1746 (all data) and R_1 was 0.0816 ($I > 2(I)$).

Plot

Hydrogen atoms (other than H1), disorder and second independent molecule omitted for clarity. Thermal ellipsoids set to 50%.

Formula	C ₅₇ H ₁₂₉ Cl ₃ Si ₁₅
$D_{\text{calc.}}/\text{g cm}^{-3}$	1.088
μ/mm^{-1}	0.362
Formula Weight	1342.29
Colour	colourless
Shape	block
Size/mm ³	0.52×0.29×0.23
T/K	120.0
Crystal System	orthorhombic
Flack Parameter	0.05(8)
Hooft Parameter	-0.06(4)
Space Group	Cmc2 ₁
$a/\text{\AA}$	44.9370(12)
$b/\text{\AA}$	12.5333(2)
$c/\text{\AA}$	14.5469(3)
α°	90
β°	90
γ°	90
$V/\text{\AA}^3$	8193.0(3)
Z	4
Z'	0.5
Wavelength/Å	0.71073
Radiation type	MoK α
$\theta_{\text{min}}^\circ$	3.121
$\theta_{\text{max}}^\circ$	29.686
Measured Refl.	73400
Independent Refl.	10189
Reflections Used	9272
R_{int}	0.0811
Parameters	540
Restraints	263
Largest Peak	0.606
Deepest Hole	-0.693
GooF	1.120
wR_2 (all data)	0.1746
wR_2	0.1706
R_1 (all data)	0.0887
R_1	0.0816

Silane 2

Tris(trimethylsilyl)2,6-bis(2,4,6-trimethylphenyl)phenylchlorosilane [(Ar*)(Si(SiMe₃))SiHCl]

Experimental

Single colourless block-shaped crystals of **2** were recrystallised from hexane by slow cooling. A suitable crystal 0.17×0.13×0.08 mm³ was selected and mounted on a MITIGEN holder in Paratone oil on a Rigaku Oxford Diffraction SuperNova diffractometer. The crystal was kept at a steady $T = 120.0$ K during data collection. The structure was solved with the **ShelXT**^[24] structure solution program using the Intrinsic Phasing solution method and by using **Olex2**^[22] as the graphical interface. The model was refined with version 2018/3 of **ShelXL**^[24] using Least Squares minimisation.

Crystal Data

C₃₃H₅₃ClSi₅, $M_r = 625.65$, monoclinic, $P2_1/c$ (No. 14), $a = 16.7147(2)$ Å, $b = 11.49900(10)$ Å, $c = 19.04910(10)$ Å, $\beta = 90.0000(10)^\circ$, $\alpha = \gamma = 90^\circ$, $V = 3661.28(6)$ Å³, $T = 120.0$ K, $Z = 4$, $Z' = 1$, $\mu(\text{CuK}\alpha) = 2.632$, 57789 reflections measured, 7613 unique ($R_{\text{int}} = 0.0735$) which were used in all calculations. The final wR_2 was 0.2024 (all data) and R_I was 0.0807 ($I > 2(I)$).

Plot

Hydrogen atoms (other than H1) and disorder omitted for clarity. Thermal ellipsoids set to 50%.

Formula	C ₃₃ H ₅₃ ClSi ₅
$D_{\text{calc.}}/\text{g cm}^{-3}$	1.135
μ/mm^{-1}	2.632
Formula Weight	625.65
Colour	colourless
Shape	block
Size/mm ³	0.17×0.13×0.08
T/K	120.0
Crystal System	monoclinic
Space Group	$P2_1/c$
$a/\text{\AA}$	16.7147(2)
$b/\text{\AA}$	11.49900(10)
$c/\text{\AA}$	19.04910(10)
α°	90
β°	90.0000(10)
γ°	90
$V/\text{\AA}^3$	3661.28(6)
Z	4
Z'	1
Wavelength/Å	1.54184
Radiation type	CuK α
$\theta_{\text{min}}^\circ$	4.491
$\theta_{\text{max}}^\circ$	76.070
Measured Refl.	57789
Independent Refl.	7613
Reflections with $I > 2(I)$	7338
R_{int}	0.0735
Parameters	508
Restraints	4
Largest Peak	0.458
Deepest Hole	-0.553
GooF	1.232
wR_2 (all data)	0.2024
wR_2	0.2013
R_I (all data)	0.0825
R_I	0.0807

Disilene 3

Zwitterion [⁽⁺⁾1^{Me}iPr)(Cp*)SiH-Si⁻(SiMe₃)₂]

Experimental

Single pale orange block-shaped crystals of **3** were recrystallised from diethyl ether by slow cooling. A suitable crystal (0.20×0.07×0.04) mm³ was selected and mounted on a MITIGEN holder in Paratone oil on a Rigaku Oxford Diffraction SuperNova diffractometer. The crystal was kept at $T = 120.0$ K during data collection. Using **Olex2**^[22], the structure was solved with the **ShelXS**^[23] structure solution program, using the Direct Methods solution method. The model was refined with version 2014/7 of **ShelXL**^[24] using Least Squares minimisation.

Crystal Data

C₂₇H₅₄N₂Si₄, $M_r = 519.08$, monoclinic, P2₁/c (No. 14), $a = 11.32508(20)$ Å, $b = 16.0662(3)$ Å, $c = 18.3367(3)$ Å, $\beta = 103.2283(16)^\circ$, $\alpha = \gamma = 90^\circ$, $V = 3247.86(10)$ Å³, $T = 120.0$ K, $Z = 4$, $Z' = 1$, $\mu(\text{CuK}\alpha) = 1.809$, 26957 reflections measured, 6729 unique ($R_{\text{int}} = 0.0889$) which were used in all calculations. The final wR_2 was 0.1551 (all data) and R_I was 0.0558 ($I > 2(I)$).

Plot

Hydrogen atoms (other than H1) and disorder omitted for clarity. Thermal ellipsoids set to 50%.

Formula	C ₂₇ H ₅₄ N ₂ Si ₄
$D_{\text{calc.}}/\text{g cm}^{-3}$	1.062
μ/mm^{-1}	1.809
Formula Weight	519.08
Colour	pale orange
Shape	block
Size/mm ³	0.20×0.07×0.04
T/K	120.0
Crystal System	monoclinic
Space Group	P2 ₁ /c
$a/\text{\AA}$	11.32508(20)
$b/\text{\AA}$	16.0662(3)
$c/\text{\AA}$	18.3367(3)
α°	90
β°	103.2283(16)
γ°	90
$V/\text{\AA}^3$	3247.86(10)
Z	4
Z'	1
Wavelength/Å	1.54184
Radiation type	CuK α
$\theta_{\text{min}}^\circ$	3.701
$\theta_{\text{max}}^\circ$	76.052
Measured Refl.	26957
Independent Refl.	6729
Reflections Used	5415
R_{int}	0.0889
Parameters	319
Restraints	0
Largest Peak	0.502
Deepest Hole	-0.581
GooF	1.038
wR_2 (all data)	0.1551
wR_2	0.1430
R_I (all data)	0.0710
R_I	0.0558

Silylsilylene 5

NHC-stabilised silylsilylene

Experimental

Single dark orange block-shaped crystals of **1** were recrystallised from pentane by slow cooling. A suitable crystal (0.42×0.36×0.24) mm³ was selected and mounted on a MITIGEN holder in Paratone oil on a Rigaku Oxford Diffraction SuperNova diffractometer. The crystal was kept at $T = 120.0$ K during data collection. Using **Olex2**^[22], the structure was solved with the **ShelXS**^[23] structure solution program, using the Direct Methods solution method. The model was refined with version 2017/1 of **ShelXL**^[24] using Least Squares minimisation.

Crystal Data

C₄₁H₆₄N₂Si₄, $M_r = 697.30$, monoclinic, $P2_1/n$ (No. 14), $a = 12.3461(4)$ Å, $b = 18.7939(8)$ Å, $c = 18.9399(6)$ Å, $\beta = 104.669(3)^\circ$, $\alpha = \gamma = 90^\circ$, $V = 4251.4(3)$ Å³, $T = 120.0$ K, $Z = 4$, $Z' = 1$, $\mu(\text{MoK}\alpha) = 0.168$, 52088 reflections measured, 21719 unique ($R_{\text{int}} = 0.0642$) which were used in all calculations. The final wR_2 was 0.1466 (all data) and R_1 was 0.0608 ($I > 2(I)$).

Plot

Hydrogen atoms (other than H1) and disorder omitted for clarity. Thermal ellipsoids set to 50%.

Formula	C ₄₁ H ₆₄ N ₂ Si ₄
$D_{\text{calc.}}/\text{g cm}^{-3}$	1.089
μ/mm^{-1}	0.168
Formula Weight	697.30
Colour	dark orange
Shape	block
Size/mm ³	0.42×0.36×0.24
T/K	120.0
Crystal System	monoclinic
Space Group	$P2_1/n$
$a/\text{\AA}$	12.3461(4)
$b/\text{\AA}$	18.7939(8)
$c/\text{\AA}$	18.9399(6)
α°	90
β°	104.669(3)
γ°	90
$V/\text{\AA}^3$	4251.4(3)
Z	4
Z'	1
Wavelength/Å	0.71073
Radiation type	MoK α
$\theta_{\text{min}}/^\circ$	2.808
$\theta_{\text{max}}/^\circ$	29.725
Measured Refl.	52088
Independent Refl.	21719
Reflections Used	12023
R_{int}	0.0642
Parameters	447
Restraints	0
Largest Peak	0.465
Deepest Hole	-0.594
GooF	0.919
wR_2 (all data)	0.1466
wR_2	0.1360
R_1 (all data)	0.1169
R_1	0.0608

Electron Density Plot Showing the Location of H1 in 5

H1 was identified from a difference Fourier map and freely refined. The above electron density plot was produced using PLATON and shows the electron density associated with H1. Note that this was produced using the untwinned HKLF4 format reflection file, since PLATON cannot correctly produce a difference map using twinned data. Hence the values of R1 and wR2 etc as stated on the map are not the same as those in the deposited CIF. However, the position of H1 is without question.

Disilene 6

Ar* 4-Pyrrolidinopyridine Disilene

Experimental

Single dark red block-shaped crystals of **6** were recrystallised from toluene by slow evaporation. A suitable crystal $0.16 \times 0.09 \times 0.07 \text{ mm}^3$ was selected and mounted on a MITIGEN holder in Paratone oil on a Rigaku Oxford Diffraction SuperNova diffractometer. The crystal was kept at a steady $T = 120.0 \text{ K}$ during data collection. The structure was solved with the **ShelXS**^[23] structure solution program using the Direct Methods solution method and by using **Olex2**^[22] as the graphical interface. The model was refined with version 2018/3 of **ShelXL**^[24] using Least Squares minimisation.

Crystal Data

$\text{C}_{39}\text{H}_{56}\text{N}_2\text{Si}_4$, $M_r = 665.21$, monoclinic, $P2_1/c$ (No. 14), $a = 15.89104(14) \text{ \AA}$, $b = 16.29426(12) \text{ \AA}$, $c = 15.02549(12) \text{ \AA}$, $\beta = 95.5918(8)^\circ$, $\alpha = \gamma = 90^\circ$, $V = 3872.08(5) \text{ \AA}^3$, $T = 120.0 \text{ K}$, $Z = 4$, $Z' = 1$, $\mu(\text{CuK}\alpha) = 1.629$, 41474 reflections measured, 8017 unique ($R_{\text{int}} = 0.0750$) which were used in all calculations. The final wR_2 was 0.1363 (all data) and R_I was 0.0489 ($I > 2(I)$).

Plot

Hydrogen atoms (other than H1) and disorder omitted for clarity. Thermal ellipsoids set to 50%.

Formula	$\text{C}_{39}\text{H}_{56}\text{N}_2\text{Si}_4$
$D_{\text{calc.}} / \text{g cm}^{-3}$	1.141
μ / mm^{-1}	1.629
Formula Weight	665.21
Colour	dark red
Shape	block
Size/ mm^3	$0.16 \times 0.09 \times 0.07$
T / K	120.0
Crystal System	monoclinic
Space Group	$P2_1/c$
$a / \text{\AA}$	15.89104(14)
$b / \text{\AA}$	16.29426(12)
$c / \text{\AA}$	15.02549(12)
α°	90
β°	95.5918(8)
γ°	90
$V / \text{\AA}^3$	3872.08(5)
Z	4
Z'	1
Wavelength/ $\text{\AA}$	1.54178
Radiation type	$\text{CuK}\alpha$
$\theta_{\text{min}}^\circ$	3.895
$\theta_{\text{max}}^\circ$	76.331
Measured Refl.	41474
Independent Refl.	8017
Reflections with $I > 2(I)$	6815
R_{int}	0.0750
Parameters	441
Restraints	35
Largest Peak	0.302
Deepest Hole	-0.399
GooF	1.056
wR_2 (all data)	0.1363
wR_2	0.1320
R_I (all data)	0.0564
R_I	0.0489

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6 NMR Spectra

Silane 1

Tris(trimethylsilyl)pentamethylcyclopentadienylchlorosilane
[(Cp*)(Si(SiMe₃))SiHCl]

¹H NMR (500.2 MHz, C₆D₆, 300 K)

¹³C NMR (125.8 MHz, C₆D₆, 300 K)

^{29}Si NMR (99.4 MHz, C_6D_6 , 300 K)

Silane 2

Tris(trimethylsilyl)2,6-bis(2,4,6-trimethylphenyl)phenylchlorosilane
[(Ar*)(Si(SiMe₃))SiHCl]

¹H NMR (500.2 MHz, C₆D₆, 300 K)

¹H Expansions

^{13}C NMR (125.8 MHz, C_6D_6 , 300 K)

^{13}C Expansions

^{29}Si NMR (99.4 MHz, C_6D_6 , 300 K)

Disilene 3

Zwitterion $[(^+I^{Me}iPr)(Cp^*)SiH-Si^-(SiMe_3)_2]$

1H NMR (500.2 MHz, C_6D_6 , 300 K)

1H Expansions

^{13}C NMR (125.8 MHz, C_6D_6 , 300 K)

^{13}C Expansions

^{29}Si NMR (99.4 MHz, C_6D_6 , 300 K)

Silylsilylene 5

NHC-stabilised silylsilylene

^1H NMR (500.2 MHz, C_6D_6 , 300 K)

^1H Expansions

^{13}C NMR (125.8 MHz, C_6D_6 , 300 K)

^{13}C Expansions

^{29}Si NMR (99.4 MHz, C_6D_6 , 300 K)

^1H - ^{29}Si HMQC

^1H - ^{29}Si HMBC

^1H - ^{29}Si HMBC Expansion

Disilene 6

Ar* 4-Pyrrolidinopyridine Disilene

^1H NMR (500.2 MHz, C_6D_6 , 300 K)

^1H Expansions

^{13}C NMR (125.8 MHz, C_6D_6 , 300 K)

¹³C Expansions

^{29}Si NMR (99.4 MHz, C_6D_6 , 300 K)

7 Cartesian Coordinates for Quantum Chemical Calculations

Cartesian coordinates

Compound (point group): total energy/Hartree (RI-M06-L/6-31+G(d,p))

A^{Ar} (C ₁): E _{tot} = -2868.32769250				C	-4.67529	-1.38774	-2.42281	C	-2.29244	2.37422	0.75201
Si	0.14959	-0.00717	-0.32648	H	-5.66629	-1.11203	-0.53611	C	-2.56247	2.25841	-0.58530
H	-0.62450	0.07700	-1.59771	H	-3.39950	-1.79441	-4.10494	C	-2.77378	3.42286	1.68550
Si	2.12677	1.18523	-0.07918	C	2.52551	-2.23773	0.54262	H	-3.10881	3.02412	2.64488
Si	2.37881	1.59542	-2.38955	C	3.14985	-2.40024	-0.71509	H	-3.62071	3.95092	1.24344
Si	1.48972	3.39630	0.45980	C	3.30314	-1.84694	1.64365	H	-1.99450	4.16473	1.89187
N	-1.37349	0.48333	2.17931	C	4.50135	-2.09370	-0.85426	C	-3.44001	3.11579	-1.42037
N	-2.19755	1.57057	0.48872	C	4.65650	-1.55258	1.46227	H	-2.96854	3.39312	-2.36704
C	-1.20169	0.71995	0.85128	C	5.27281	-1.64232	0.21835	H	-3.65984	4.04371	-0.88925
C	-2.50962	1.13974	2.63804	H	4.96768	-2.22239	-1.83091	H	-4.39583	2.63701	-1.65615
C	-3.03642	1.81054	1.56872	H	5.23851	-1.22193	2.32231	C	-0.95575	0.99591	2.44054
C	-3.03901	1.08797	4.02252	C	2.72046	-1.65051	3.00879	H	-0.26747	0.16097	2.27310
H	-2.97692	0.08965	4.46300	H	3.42607	-1.94957	3.79011	C	-2.12974	0.49799	3.26707
H	-4.09323	1.37549	4.02097	H	2.50232	-0.58576	3.16701	H	-2.80237	1.30100	3.58285
H	-2.51911	1.77969	4.69395	H	1.79437	-2.21424	3.15390	H	-1.74705	0.02398	4.17557
C	-4.30821	2.57294	1.51038	C	2.39377	-2.94804	-1.88809	H	-2.70700	-0.24488	2.71292
H	-4.16714	3.65583	1.58149	H	1.93027	-3.91459	-1.65255	C	-0.16184	2.08989	3.12812
H	-4.95006	2.27458	2.34305	H	1.57767	-2.28766	-2.19607	H	0.71456	2.37213	2.54034
H	-4.85843	2.36747	0.58714	H	3.05074	-3.08080	-2.75159	H	0.20885	1.69381	4.07757
C	0.83850	2.15505	-3.36246	C	6.70579	-1.25309	0.02572	H	-0.75863	2.97887	3.35099
H	0.07099	1.37052	-3.35804	H	6.78018	-0.25492	-0.42238	C	-1.79331	0.67599	-2.44074
H	1.09840	2.34727	-4.41180	H	7.24868	-1.22424	0.97445	H	-1.33928	-0.31049	-2.34336
H	0.38115	3.06638	-2.96378	H	7.22827	-1.94232	-0.64519	C	-3.18072	0.47721	-3.03186
C	2.98448	0.10359	-3.39181	C	-3.80329	-1.76638	1.24849	H	-3.85923	0.00863	-2.31379
H	3.83654	-0.39534	-2.91939	H	-4.66754	-1.17359	1.56640	H	-3.09726	-0.19215	-3.89281
H	3.29381	0.43324	-4.39164	H	-3.96983	-2.79442	1.59433	H	-3.63161	1.40585	-3.39061
H	2.19669	-0.64522	-3.52956	H	-2.92403	-1.40309	1.78057	C	-0.88713	1.54200	-3.29812
C	3.71654	2.91839	-2.63302	C	-5.85423	-0.98097	-3.25239	H	-1.26865	2.56321	-3.40349
H	3.47508	3.87114	-2.15132	H	-5.78433	0.07483	-3.54399	H	-0.80744	1.11080	-4.30019
H	3.87334	3.11700	-3.70040	H	-5.91859	-1.56018	-4.17805	H	0.11942	1.59611	-2.87305
H	4.66943	2.57757	-2.21288	H	-6.79516	-1.10345	-2.70863	C	-0.40093	-2.39457	0.02666
C	3.11715	4.20539	1.00983	C	-1.07961	-2.46771	-2.98442	C	-1.44252	-2.55604	-1.03337
H	3.53149	3.70128	1.88923	H	-0.35719	-1.64101	-3.00076	C	-2.67470	-2.50945	-0.44524
H	2.96946	5.26379	1.25938	H	-0.57723	-3.31261	-2.50338	C	-2.51263	-2.41952	1.00230
H	3.87851	4.15197	0.22396	H	-1.28943	-2.73434	-4.02329	C	-1.18043	-2.38676	1.30247
C	0.84184	4.62442	-0.84551	C	-2.55065	3.74898	-0.68337	C	0.72496	-3.42725	0.00065
H	1.55707	4.75000	-1.66510	H	-3.62435	3.91494	-0.57020	H	1.28357	-3.40910	-0.94161
H	0.70833	5.60829	-0.37586	H	-2.02084	4.22405	0.14778	H	0.32054	-4.43949	0.12808
H	-0.11089	4.34472	-1.30006	H	-2.24614	4.25881	-1.60133	H	1.44127	-3.24576	0.80844
C	0.34643	3.63195	1.96846	C	-3.07987	1.57066	-1.83351	C	-1.11500	-2.83168	-2.45975
H	-0.62152	3.12102	1.91493	H	-2.78914	0.52504	-1.94776	H	-0.33988	-2.15873	-2.85317
H	0.14541	4.70252	2.10692	H	-4.13474	1.60368	-1.53760	H	-1.99345	-2.74859	-3.10840
H	0.85275	3.28563	2.87607	H	-2.98449	2.06148	-2.80721	H	-0.71850	-3.84854	-2.58793
C	0.01558	-1.89412	0.08880	C	0.10782	0.55675	4.16615	C	-4.01150	-2.60537	-1.09993
C	1.08834	-2.64306	0.64880	H	-0.64270	0.68254	4.95060	H	-3.93941	-2.63666	-2.19107
C	-1.23828	-2.55457	-0.05961	H	0.96087	0.04385	4.61858	H	-4.65932	-1.75877	-0.83378
C	0.85736	-3.92077	1.17851	H	0.44119	1.54239	3.83389	H	-4.55213	-3.50736	-0.78553
C	-1.42273	-3.84681	0.45384	C	-0.93679	-1.62810	3.45134	C	-3.66993	-2.46408	1.94317
C	-0.39605	-4.51483	1.10991	H	-1.84075	-1.53325	4.06086	H	-4.37047	-1.63222	1.78440
H	1.69841	-4.46289	1.60788	H	-1.15492	-2.28245	2.60490	H	-3.35304	-2.43343	2.98968
H	-2.38717	-4.33216	0.31384	H	-0.18204	-2.12240	4.06952	H	-4.25607	-3.38235	1.81034
H	-0.55857	-5.50907	1.51841					C	-0.52510	-2.47129	2.63669
C	-2.19949	2.27615	-0.82395	A^{Cp*} (C ₁): E _{tot} = -2328.81078619				H	-0.14211	-3.48419	2.82547
H	-1.14997	2.21685	-1.14874	Si	0.39553	-0.61416	-0.23717	H	-1.21431	-2.23473	3.45350
C	-0.40048	-0.27846	3.00305	H	0.56889	-0.55544	-1.72476	H	0.34618	-1.80471	2.71500
H	0.44172	-0.44730	2.32194	Si	2.19145	0.04324	1.06439	C	3.58056	-1.63248	-1.90389
C	-2.39883	-2.03211	-0.85475	Si	3.86069	-1.17597	-0.08125	H	2.71307	-2.28750	-2.04385
C	-3.62595	-1.70853	-0.24012	Si	2.49873	2.05249	-0.15245	H	4.45608	-2.16208	-2.30064
C	-2.33407	-2.07324	-2.26704	N	-1.40041	1.36389	1.07039	H	3.41573	-0.74676	-2.52452
C	-4.73054	-1.37585	-1.03085	N	-1.83389	1.17353	-1.04516	C	4.30321	-2.80131	0.79446
C	-3.46708	-1.75360	-3.01806	C	-1.09598	0.63298	-0.03654	H	4.43990	-2.65230	1.87054

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	H	2.31303	4.24091	1.20052	H	-2.69150	-2.16852	-2.57624	C	1.10711	4.83796	0.69802
C	4.08741	2.99076	-1.34415	H	-3.66320	-1.10993	-1.54717	H	0.84573	5.60227	-0.04324	
H	4.75287	2.89899	-0.47889	C	-3.19290	-1.94920	1.01944	H	1.55405	5.34740	1.55606	
H	4.24376	3.98186	-1.78559	H	-3.79976	-1.03757	0.95170	H	0.16002	4.38926	1.01731	
H	4.41395	2.25342	-2.08652	H	-3.74557	-2.73566	0.49280	C	-3.15303	1.00839	-1.32139	
C	1.22722	2.91033	-2.41612	H	-3.14996	-2.23113	2.07435	C	-4.19397	1.23207	-0.40307	
H	1.51287	2.20900	-3.20550					C	-5.17009	0.24961	-0.22261	
H	1.34025	3.92232	-2.82397	D^{Ar} (C ₁): E _{tot} = -2868.33737992				H	-5.96688	0.42511	0.50102	
H	0.16308	2.76019	-2.20407	Si	-0.48303	-1.47041	-0.11088	C	-5.15458	-0.94301	-0.94883	
C	-2.96611	0.90477	2.78513	Si	-0.51727	0.78405	0.58625	C	-4.14556	-1.11949	-1.89672	
H	-3.44311	1.51260	2.00930	H	0.85644	1.19546	0.99538	H	-4.12566	-2.03389	-2.48968	
H	-3.16718	1.37508	3.75515	Si	-1.29565	-3.00114	1.45127	C	-3.15254	-0.16062	-2.10740	
H	-3.45826	-0.07162	2.78176	Si	-1.57413	1.30462	2.62472	C	-4.29094	2.54186	0.31976	
C	-0.41673	-0.57214	3.67124	N	2.02890	-2.53661	-1.13912	H	-3.33333	2.83644	0.75967	
H	-0.85326	-1.55541	3.46588	N	2.47278	-1.41764	0.66295	H	-5.03963	2.51129	1.11658	
H	-0.63440	-0.33019	4.71772	C	1.43327	-1.86702	-0.10340	H	-4.56842	3.35078	-0.36709	
H	0.67078	-0.65820	3.56954	C	3.41173	-2.47209	-1.04133	C	-6.18100	-2.00717	-0.70446	
C	-0.35571	2.42277	3.07129	C	3.69298	-1.76748	0.09690	H	-5.91745	-2.61470	0.17032	
H	0.73880	2.42583	2.99513	C	1.25481	-3.22051	-2.20027	H	-6.26458	-2.68892	-1.55564	
H	-0.60770	2.63283	4.11728	H	0.22476	-3.16973	-1.82071	H	-7.17025	-1.58070	-0.51170	
H	-0.73428	3.25620	2.46995	C	1.28535	-2.44510	-3.50566	C	-2.13255	-0.35386	-3.18950	
				H	0.87049	-1.44276	-3.36515	H	-2.30166	0.34120	-4.02207	
				H	0.67084	-2.96122	-4.24952	H	-2.16560	-1.37399	-3.58358	
				H	2.29407	-2.34757	-3.91941	H	-1.11703	-0.17378	-2.81777	
				C	1.65305	-4.68007	-2.34366	C	-3.15616	-3.15320	1.14133	
				H	2.59115	-4.81486	-2.88982	H	-3.66319	-2.18872	1.26621	
				H	0.87605	-5.20557	-2.90618	H	-3.62804	-3.87163	1.82259	
				H	1.74303	-5.16638	-1.36796	H	-3.35006	-3.47387	0.11144	
				C	2.27930	-0.96316	2.05815	C	-0.48907	-4.65596	0.97944	
				H	1.20237	-0.76382	2.10640	H	-0.67404	-4.90257	-0.07250	
				C	2.59052	-2.10530	3.01493	H	-0.88428	-5.47920	1.58628	
				H	2.02928	-3.00545	2.74608	H	0.59864	-4.63499	1.12455	
				H	2.30756	-1.81799	4.03271	C	-1.09525	-2.86064	3.33588	
				H	3.65654	-2.35648	3.02781	H	-0.05744	-2.70641	3.64991	
				C	3.03601	0.31013	2.39382	H	-1.44629	-3.78661	3.80997	
				H	4.09903	0.12859	2.57893	H	-1.68576	-2.03876	3.75329	
				H	2.62042	0.73311	3.31292	C	-1.70388	3.16387	2.97155	
				H	2.93710	1.06056	1.60479	H	-0.69918	3.58581	3.08720	
				C	4.36498	-3.07105	-2.00938	H	-2.23789	3.33307	3.91459	
				H	4.46233	-4.15482	-1.88521	H	-2.21252	3.74404	2.19682	
				H	5.35722	-2.63729	-1.86802	C	-3.22279	0.45387	2.95892	
				H	4.07852	-2.88660	-3.04833	H	-4.01828	0.76812	2.27912	
				C	5.02049	-1.37915	0.63261	H	-3.55184	0.65371	3.98559	
				H	5.16921	-0.29390	0.60001	H	-3.12210	-0.63092	2.84874	
				H	5.81039	-1.83949	0.03537	C	-0.35524	0.69638	3.94358	
				H	5.17371	-1.69827	1.66842	H	-0.10821	-0.36543	3.85073	
				C	-0.85353	1.99337	-0.86722	H	-0.77581	0.84716	4.94517	
				C	0.15255	2.90217	-1.28711	H	0.57679	1.26962	3.88767	
				C	-0.11784	3.85583	-2.27756					
				H	0.67622	4.53930	-2.57506	D^{Cp*} (C ₁): E _{tot} = -2328.80737879				
				C	-1.36215	3.92126	-2.89173	Si	-0.69848	0.09011	-1.11318	
				H	-1.56007	4.66817	-3.65621	Si	1.09414	-0.30075	0.37329	
				C	-2.33632	2.99472	-2.54054	H	0.53321	-0.96562	1.59941	
				H	-3.30198	2.99407	-3.04457	Si	-1.13850	2.34350	-1.58833	
				C	-2.09396	2.03412	-1.55279	Si	2.40305	1.53875	1.02737	
				C	1.56224	2.85846	-0.79385	N	-3.28269	-1.09589	-0.42991	
				C	2.44406	1.89466	-1.31729	N	-2.54073	-0.07725	1.32952	
				C	3.78187	1.90082	-0.91346	C	-2.24511	-0.32263	0.01697	
				H	4.45823	1.15543	-1.33558	C	-4.19266	-1.34578	0.58684	
				C	4.27118	2.83024	0.00591	C	-3.72642	-0.70023	1.69825	
				C	3.37763	3.77341	0.51858	C	-3.33612	-1.64427	-1.80426	
				H	3.73317	4.50550	1.24380	H	-2.55483	-1.07158	-2.32255	
				C	2.03607	3.80766	0.12880	C	-2.90464	-3.10045	-1.81232	
				C	1.95775	0.86069	-2.28621	H	-1.89856	-3.19774	-1.39270	
				H	1.13998	0.26332	-1.85697	H	-2.87838	-3.47271	-2.84055	
				H	2.76283	0.17358	-2.56813	H	-3.58233	-3.74497	-1.24281	
				H	1.55039	1.31092	-3.20024	C	-4.66853	-1.38721	-2.48722	
				C	5.69684	2.78637	0.46785	H	-5.45175	-2.08619	-2.18047	
				H	5.78471	2.28920	1.44297	H	-4.53924	-1.50670	-3.56652	
				H	6.11742	3.78919	0.58854	H	-5.02150	-0.36777	-2.30683	
				H	6.33219	2.23748	-0.23402	C	-1.79678	0.90305	2.14500	

H	-0.92392	1.12974	1.51955	Si	-3.10848	1.01768	2.59810	H	0.20739	4.19932	-0.70884
C	-2.60465	2.18148	2.31244	Si	-2.05520	3.22812	-0.16775	H	-0.94701	4.52383	-2.01388
H	-2.96978	2.54667	1.34849	N	1.18733	0.64365	-0.54767	H	-0.21727	2.92389	-1.85888
H	-1.97044	2.95766	2.75276	N	5.22223	1.20217	-1.38504	C	-2.75877	4.79152	0.64030
H	-3.46435	2.04704	2.97645	C	-0.66099	-1.67613	0.03110	H	-3.66309	4.57145	1.21844
C	-1.31683	0.33245	3.46907	C	-1.75772	-2.39495	-0.52603	H	-3.03044	5.53501	-0.11893
H	-2.11876	0.25894	4.20902	C	-1.88580	-3.77083	-0.31158	H	-2.03931	5.25507	1.32306
H	-0.55616	0.99938	3.88429	H	-2.73060	-4.29113	-0.75898	C	-3.39406	2.58634	-1.34702
H	-0.86026	-0.65169	3.33805	C	-0.95514	-4.47161	0.44527	H	-3.08885	1.65621	-1.84134
C	-5.42350	-2.16433	0.45018	H	-1.07238	-5.53881	0.61442	H	-3.60311	3.32655	-2.13107
H	-6.22103	-1.63481	-0.08118	C	0.14365	-3.79450	0.95628	H	-4.33488	2.37967	-0.82634
H	-5.80683	-2.42414	1.43911	H	0.90698	-4.33240	1.51651	C	6.19155	1.66231	-0.39018
H	-5.24465	-3.10237	-0.08214	C	0.31033	-2.41841	0.75191	C	5.87120	0.63233	-2.56441
C	-4.30762	-0.69374	3.06421	C	-2.80573	-1.74710	-1.37508	C	7.33043	1.03131	-2.39415
H	-3.70838	-1.28120	3.76780	C	-2.53017	-1.36118	-2.70114	H	8.01189	0.33973	-2.89401
H	-5.30864	-1.12891	3.04228	C	-3.53224	-0.75165	-3.46131	H	7.49751	2.02729	-2.81932
H	-4.40431	0.31221	3.48220	H	-3.29961	-0.43735	-4.47906	C	7.50556	1.06860	-0.87886
C	-0.24709	2.77510	-3.20272	C	-4.80857	-0.52046	-2.95332	H	7.61777	0.05030	-0.48684
H	0.83944	2.83474	-3.07318	C	-5.08463	-0.97093	-1.66134	H	8.37401	1.64604	-0.55497
H	-0.57979	3.74783	-3.58454	H	-6.08155	-0.82451	-1.24572	H	5.74400	-0.46255	-2.57404
H	-0.43886	2.02196	-3.97359	C	-4.11680	-1.59265	-0.87214	H	5.42351	1.02595	-3.48418
C	-3.00256	2.39904	-1.95892	C	-1.19692	-1.60158	-3.35052	H	5.90994	1.30671	0.60713
H	-3.26044	1.70435	-2.76672	H	-0.45338	-1.99250	-2.65068	H	6.22109	2.76120	-0.35935
H	-3.31464	3.40180	-2.27423	H	-0.80415	-0.67635	-3.78893	H	3.89554	2.10208	0.79197
H	-3.60963	2.12344	-1.08710	H	-1.28744	-2.32591	-4.16849	H	1.49248	1.63516	1.23260
C	-0.79073	3.82032	-0.44400	C	-5.83718	0.22376	-3.74701	H	1.02134	-0.23385	-2.41031
H	-1.28320	3.75119	0.53042	H	-5.84619	1.28405	-3.46633	H	3.38918	0.09447	-3.02226
H	-1.15518	4.73622	-0.92754	H	-6.84567	-0.16222	-3.57094	NHC (C₁): E_{tot} = -540.653444746			
H	0.27955	3.95558	-0.25816	H	-5.63510	0.17442	-4.82071	N	1.05899	-0.07752	-0.15884
C	4.01460	1.15432	1.93866	C	-4.49553	-2.10383	0.48588	N	-1.05899	-0.07752	-0.15884
H	3.90918	0.31854	2.63856	H	-4.53737	-3.19897	0.50696	C	0.00000	-0.93942	-0.13214
H	4.34533	2.03305	2.50557	H	-5.47693	-1.72833	0.78679	C	0.68196	1.26635	-0.16658
H	4.81114	0.88970	1.23722	H	-3.77332	-1.80773	1.25062	C	-0.68196	1.26635	-0.16658
C	2.83188	2.55297	-0.50741	C	1.60354	-1.85206	1.24904	C	1.64301	2.39467	-0.20504
H	3.56515	2.01910	-1.12230	C	1.71024	-1.24976	2.51816	H	2.33753	2.38285	0.64365
H	3.25845	3.52730	-0.24170	C	2.96088	-0.80954	2.95959	H	1.11027	3.34871	-0.17455
H	1.95296	2.73581	-1.13522	H	3.03212	-0.34681	3.94385	H	2.25317	2.39298	-1.11660
C	1.39880	2.61587	2.22247	C	4.11510	-0.96211	2.19044	C	-1.64300	2.39467	-0.20504
H	0.40175	2.86898	1.84954	C	3.99411	-1.58477	0.94841	H	-2.25317	2.39299	-1.11659
H	1.92406	3.56062	2.40780	H	4.88408	-1.72151	0.32939	H	-1.11027	3.34871	-0.17454
H	1.28456	2.11437	3.19022	C	2.76267	-2.04252	0.46972	H	-2.33753	2.38285	0.64366
C	2.23729	-1.67585	-0.42388	C	0.51192	-1.10199	3.40038	C	2.45329	-0.53051	-0.05825
C	3.09664	-0.96101	-1.42408	H	-0.15146	-0.30628	3.03707	H	3.06849	0.27809	-0.47498
C	3.20776	-2.12445	0.62418	H	0.80037	-0.84137	4.42217	C	2.67298	-1.78724	-0.87996
C	4.38148	-0.94405	-0.96506	H	-0.08442	-2.01968	3.43149	H	2.04787	-2.59910	-0.50063
C	4.45264	-1.67818	0.29410	C	5.44078	-0.47191	2.69136	H	3.72341	-2.08954	-0.82725
C	1.39296	-2.81374	-0.99911	H	5.44864	0.61895	2.81502	H	2.40659	-1.62633	-1.92779
H	0.75231	-3.26502	-0.23053	H	6.25388	-0.73783	2.00804	C	2.82852	-0.73483	1.40341
H	0.73588	-2.45621	-1.79981	H	5.68420	-0.89294	3.67249	H	2.66605	0.17414	1.99124
H	2.03954	-3.60366	-1.40346	C	2.70179	-2.76793	-0.84377	H	3.88034	-1.02191	1.50009
C	2.56310	-0.35683	-2.67616	H	2.66373	-3.85444	-0.69815	H	2.21076	-1.52967	1.83363
H	1.90589	-1.04855	-3.21734	H	3.58083	-2.54645	-1.45775	C	-2.45329	-0.53051	-0.05825
H	1.95339	0.54109	-2.48993	H	1.80596	-2.50947	-1.41927	H	-3.06849	0.27810	-0.47497
H	3.36744	-0.05687	-3.35532	C	1.71249	0.26161	-1.73197	C	-2.67299	-1.78723	-0.87997
C	2.81722	-2.95654	1.79370	C	3.02970	0.45611	-2.06583	H	-2.40660	-1.62632	-1.92780
H	2.06118	-2.46250	2.41963	C	3.89803	1.08570	-1.14097	H	-3.72341	-2.08954	-0.82725
H	2.37859	-3.91589	1.48607	C	3.31041	1.56670	0.05249	H	-2.04787	-2.59909	-0.50064
H	3.67424	-3.18495	2.43396	C	1.98855	1.30923	0.31620	C	-2.82851	-0.73484	1.40341
C	5.56714	-0.27922	-1.57767	C	-2.88580	-0.69039	3.40262	H	-2.21075	-1.52967	1.83362
H	6.39243	-0.98440	-1.73769	H	-2.39968	-1.42827	2.75396	H	-3.88033	-1.02192	1.50010
H	5.33217	0.17931	-2.54260	H	-3.85507	-1.10132	3.71125	H	-2.66604	0.17414	1.99125
H	5.96624	0.51494	-0.93043	H	-2.26612	-0.60108	4.30201	4-PPy (C₁): E_{tot} = -459.648314801			
C	5.72596	-1.86499	1.04685	C	-3.37946	2.21209	4.04576	N	-3.37475	-0.00001	0.00007
H	6.46008	-2.43831	0.46629	H	-2.52075	2.21488	4.72504	N	0.83614	0.00000	-0.00015
H	6.20420	-0.90485	1.28320	H	-4.26749	1.93236	4.62581	C	-2.65606	1.12882	-0.07592
H	5.57320	-2.39106	1.99336	H	-3.52263	3.24167	3.69975	C	-1.27109	1.19582	-0.08239
E^{Ar} (C₁): E_{tot} = -2787.30282188				C	-4.73792	1.05752	1.63007	C	-0.52710	0.00000	-0.00007
Si	-0.66590	0.22937	-0.14096	H	-5.03679	2.09798	1.45573	C	-1.27108	-1.19582	0.08233
H	-1.05797	0.47716	-1.55619	H	-5.54826	0.57348	2.19051	C	-2.65605	-1.12883	0.07599
Si	-1.20617	1.76811	1.46819	H	-4.65986	0.57759	0.65025				
				C	-0.61861	3.77049	-1.28727				

C	1.64380	-1.21181	0.00357	H	0.46893	1.35257	2.87833	H	-2.32520	-3.61626	-2.13879
C	1.64380	1.21182	-0.00363	H	1.88554	2.35716	2.52863	H	-2.23726	-1.93821	-2.69613
C	3.04661	0.70104	0.30115	H	2.03277	0.93270	3.55124	C	2.32724	-0.43265	-0.61833
H	3.82716	1.34857	-0.10546	C	2.95307	2.18870	-0.12172	C	1.85819	-1.52098	0.27699
H	3.19323	0.64501	1.38592	H	4.05054	2.17312	-0.13870	C	1.51984	-0.98127	1.49000
C	3.04665	-0.70104	-0.30099	H	2.65537	2.98004	0.57141	C	1.82786	0.44121	1.47489
H	3.19343	-0.64501	-1.38575	H	2.64283	2.49167	-1.13038	C	2.35759	0.77038	0.25667
H	3.82714	-1.34857	0.10573					C	3.60258	-0.72936	-1.40352
H	1.59437	1.71552	-0.98314	S2 (C ₁): E _{tot} = -1107.95228166				H	3.47935	-1.60221	-2.05532
H	1.27887	1.92465	0.74648	Si	0.00000	1.65932	-0.00010	H	4.44214	-0.93851	-0.72627
H	1.27900	-1.92470	-0.74653	Si	1.71825	0.07043	-0.00427	H	3.88682	0.11328	-2.04287
H	1.59420	-1.71542	0.98313	Si	-1.71824	0.07042	0.00423	C	1.91791	-2.96303	-0.09288
H	-0.77543	-2.15836	0.16161	C	2.08319	-0.69493	1.70961	H	1.54528	-3.14933	-1.10920
H	-3.23153	-2.05220	0.14021	H	2.29664	0.08835	2.44624	H	1.34482	-3.59383	0.59567
H	-3.23156	2.05218	-0.14009	H	2.95242	-1.36760	1.67146	H	2.95250	-3.33588	-0.07820
H	-0.77546	2.15836	-0.16174	H	1.22958	-1.26930	2.08684	C	0.96587	-1.67278	2.69026
				C	3.39195	0.84008	-0.50896	H	0.91422	-2.75769	2.55497
S1 (C ₁): E _{tot} = -1220.62511026				H	3.35597	1.22948	-1.53298	H	-0.04727	-1.32339	2.94614
Si	0.92411	-0.17681	-1.77285	H	4.20775	0.10538	-0.45596	H	1.57832	-1.49106	3.58316
H	0.72012	-1.42530	-2.55534	H	3.65131	1.68049	0.14532	C	1.61209	1.32248	2.65939
N	-1.13853	1.25608	-0.32902	C	1.56629	-1.44362	-1.16475	H	0.54564	1.42244	2.91520
N	-1.53491	-0.88068	-0.29646	H	0.71834	-2.08179	-0.88928	H	2.00946	2.33050	2.50424
C	-0.65729	0.05526	-0.73962	H	2.47493	-2.06196	-1.13117	H	2.09944	0.92095	3.55742
C	-2.31298	1.07995	0.37928	H	1.41038	-1.13349	-2.20495	C	2.94900	2.06344	-0.18253
C	-2.56780	-0.27181	0.39393	C	-2.08338	-0.69502	-1.70958	H	4.04347	1.99889	-0.26382
C	-3.09423	2.16927	1.01273	H	-2.29684	0.08823	-2.44624	H	2.72830	2.88288	0.51000
H	-2.58417	2.58236	1.88881	H	-2.95267	-1.36760	-1.67129	H	2.59434	2.35560	-1.18252
H	-4.05865	1.78652	1.34925	H	-1.22986	-1.26949	-2.08685				
H	-3.29511	2.99655	0.32752	C	-1.56618	-1.44354	1.16480	S4 (C ₁): E _{tot} = -1107.88950805			
C	-3.70668	-0.98572	1.02008	H	-0.71821	-2.08172	0.88939	Si	-0.00021	-1.59335	-0.00380
H	-4.17060	-1.70281	0.33786	H	-2.47481	-2.06192	1.13129	Si	-1.78276	-0.02387	-0.01250
H	-4.47752	-0.27051	1.31055	H	-1.41028	-1.13331	2.20497	Si	1.78261	-0.02407	0.01199
H	-3.40921	-1.53038	1.92116	C	-3.39187	0.84011	0.50908	C	-1.95939	0.49603	1.80437
C	-0.55783	2.54934	-0.78489	H	-3.35575	1.22961	1.53306	H	-2.10270	-0.36144	2.46961
H	0.41788	2.25725	-1.19270	H	-4.20768	0.10540	0.45626	H	-2.84313	1.13616	1.91043
C	-0.31407	3.53009	0.34595	H	-3.65134	1.68046	-0.14524	H	-1.09584	1.06165	2.16637
H	-1.23176	4.00494	0.69945					C	-3.40747	-0.83950	-0.52139
H	0.33509	4.32842	-0.02268	S3 (C ₁): E _{tot} = -1220.81401303				H	-3.39470	-1.16141	-1.56735
H	0.18816	3.05439	1.19174	Si	0.91213	-0.07065	-2.04792	H	-4.24586	-0.14306	-0.40343
C	-1.39440	3.11970	-1.91825	H	0.66881	-1.52732	-2.40634	H	-3.62038	-1.72343	0.08765
H	-1.48428	2.40729	-2.74309	N	-1.06928	1.27816	-0.33785	C	-1.59321	1.52800	-1.07879
H	-0.92014	4.02566	-2.30337	N	-1.51545	-0.83687	-0.34590	H	-0.70863	2.11815	-0.82317
H	-2.40151	3.39172	-1.58935	C	-0.62867	0.08228	-0.82293	H	-2.47122	2.17205	-0.95000
C	-1.41768	-2.32161	-0.64969	C	-2.21192	1.11272	0.42974	H	-1.52895	1.27996	-2.14322
H	-0.37455	-2.41811	-0.96474	C	-2.49971	-0.22506	0.41970	C	1.96139	0.50395	-1.80227
C	-1.63146	-3.25174	0.53164	C	-2.91545	2.19970	1.15452	H	2.10504	-0.35057	-2.47122
H	-1.11892	-2.89756	1.42898	H	-2.33667	2.56535	2.00980	H	2.84554	1.14414	-1.90444
H	-1.21940	-4.23172	0.27763	H	-3.86769	1.83099	1.54158	H	1.09852	1.07163	-2.16271
H	-2.68679	-3.40373	0.76554	H	-3.13422	3.06168	0.51743	C	1.59250	1.52326	1.08492
C	-2.31997	-2.63682	-1.83111	C	-3.61175	-0.93257	1.10112	H	0.70885	2.11542	0.83064
H	-3.37682	-2.50875	-1.57768	H	-4.12277	-1.63748	0.43846	H	2.47127	2.16709	0.96018
H	-2.17869	-3.67688	-2.13519	H	-4.35639	-0.21029	1.44299	H	1.52655	1.27070	2.14818
H	-2.09500	-1.99857	-2.68966	H	-3.27492	-1.49531	1.97862	C	3.40663	-0.84206	0.51929
C	2.47125	-0.33675	-0.62178	C	-0.49268	2.56659	-0.78348	H	3.39266	-1.16787	1.56402
C	1.98717	-1.46365	0.21586	H	0.44227	2.26712	-1.27030	H	4.24527	-0.14533	0.40486
C	1.58657	-0.94631	1.43116	C	-0.16022	3.50978	0.35774	H	3.62004	-1.72376	-0.09280
C	1.83990	0.48329	1.45973	H	-1.04129	4.00724	0.77327				
C	2.40478	0.86318	0.27187	H	0.50291	4.29363	-0.01994	S5 (C ₁): E _{tot} = -540.400408180			
C	3.73630	-0.54604	-1.44192	H	0.36535	2.98944	1.16156	N	1.08345	-0.06779	0.16146
H	3.65893	-1.41586	-2.10133	C	-1.38120	3.19163	-1.84701	N	-1.08344	-0.06780	-0.16147
H	4.58757	-0.71415	-0.77349	H	-1.50757	2.50633	-2.68997	C	0.00001	-0.81210	-0.00001
H	3.96499	0.32309	-2.06519	H	-0.91839	4.10853	-2.22294	C	0.67932	1.27114	0.09831
C	2.10559	-2.89972	-0.17104	H	-2.37113	3.45457	-1.45916	C	-0.67933	1.27114	-0.09831
H	1.86962	-3.07662	-1.22667	C	-1.44791	-2.26689	-0.70644	C	1.63760	2.38784	0.25798
H	1.45043	-3.54147	0.42583	H	-0.43469	-2.37053	-1.10172	H	2.14106	2.35494	1.22940
H	3.12953	-3.26516	-0.02038	C	-1.58564	-3.20037	0.48392	H	1.11294	3.34197	0.19488
C	1.03516	-1.68658	2.59759	H	-0.99844	-2.84523	1.33445	H	2.40971	2.38601	-0.51721
H	0.95978	-2.76101	2.41488	H	-1.19704	-4.18292	0.20057	C	-1.63763	2.38782	-0.25798
H	0.03893	-1.31622	2.87876	H	-2.62122	-3.34463	0.80316	H	-2.14121	2.35482	-1.22933
H	1.66348	-1.55271	3.48575	C	-2.42948	-2.57299	-1.82676	H	-1.11295	3.34195	-0.19505
C	1.54446	1.32626	2.65265	H	-3.46909	-2.42281	-1.51447	H	-2.40964	2.38608	0.51731

C	2.47420	-0.58100	0.28936	H	-1.90397	1.15663	2.59132	H	-1.96992	-0.81154	-3.46478
H	2.96805	0.11876	0.97318	C	-1.76045	3.51370	0.33578	H	-2.50189	0.65011	-2.62579
C	3.15370	-0.55241	-1.06951	H	-0.77279	3.43831	0.80584	H	-0.88889	-0.03552	-2.31858
H	2.66304	-1.24442	-1.76043	H	-2.35553	4.23717	0.90889	C	5.41222	0.44495	1.29523
H	4.19586	-0.86181	-0.96595	H	-1.60846	3.92044	-0.67011	H	5.64316	1.46893	-0.57869
H	3.14405	0.44402	-1.51773	S7 (C ₁): E _{tot} = -1760.33832343				H	4.10008	1.34514	-2.39900
C	2.43225	-1.96672	0.90084					H	4.35647	-0.35256	-2.78340
H	1.95627	-1.96639	1.88412	Si	0.27522	-0.21909	1.22936	H	2.73818	0.19712	-2.41407
H	3.44738	-2.35042	1.01562	H	1.48485	0.69246	1.25382	H	4.94778	-0.79748	2.99019
H	1.89424	-2.66449	0.24836	N	-2.01056	1.63007	0.83591	H	1.92792	-1.89509	2.50050
C	-2.47419	-0.58103	-0.28937	N	-0.41391	2.17064	-0.51832	H	2.65167	-3.14755	1.50350
H	-2.96804	0.11869	-0.97324	C	-0.80053	1.21185	0.36981	H	3.46646	-2.61139	2.98834
C	-2.43221	-1.96678	-0.90079	C	-2.35898	2.85162	0.27944	C	-5.91397	-1.86584	0.13514
H	-1.95620	-1.96649	-1.88405	C	-1.35140	3.19171	-0.58409	C	6.51958	1.18338	1.98576
H	-3.44733	-2.35049	-1.01557	C	-3.57967	3.63025	0.60621	H	-6.36063	-0.90062	-0.12615
H	-1.89421	-2.66451	-0.24825	H	-4.49493	3.17464	0.21598	H	-6.42971	-2.62686	-0.46240
C	-3.15372	-0.55239	1.06948	H	-3.50188	4.62873	0.17082	H	-6.14797	-2.07236	1.18418
H	-2.66305	-1.24435	1.76045	H	-3.71202	3.75573	1.68545	H	7.05335	1.84351	1.29648
H	-4.19587	-0.86181	0.96592	C	-1.25043	4.39540	-1.44650	H	6.13966	1.80149	2.80726
H	-3.14409	0.44407	1.51765	H	-0.26443	4.86564	-1.39137	H	7.25147	0.49609	2.42345
S6 (C ₁): E _{tot} = -1788.11758820				H	-1.98414	5.14034	-1.13042	S8 (C ₁): E _{tot} = -1648.63547644			
				H	-1.44729	4.17321	-2.50109				
Si	0.41076	0.44245	0.26867	C	-2.73691	0.90062	1.90674	Si	0.82486	-1.06082	-0.64959
H	0.32320	0.20343	1.75397	H	-2.36168	-0.12636	1.81138	N	-2.02942	-0.50937	-0.61145
Si	-1.44413	0.33637	-1.12373	C	-4.24621	0.89060	1.72185	N	-1.02799	1.24420	0.16604
Si	-2.33218	-1.66006	-0.24411	H	-4.72619	1.79332	2.11015	C	-0.78588	0.02006	-0.39285
Si	-2.61392	1.81559	0.27078	H	-4.65442	0.04062	2.27645	C	-3.02224	0.35069	-0.16301
C	1.96641	-0.65396	-0.30597	H	-4.52802	0.75504	0.67497	C	-2.39040	1.46496	0.31527
C	2.83718	-0.81000	0.89052	C	-2.31947	1.44650	3.26107	C	-4.47888	0.06663	-0.20261
C	3.91465	0.02132	0.76342	H	-1.24107	1.32588	3.40399	H	-4.90649	0.18584	-1.20388
C	3.85219	0.69105	-0.52862	H	-2.83158	0.90032	4.05845	H	-5.00827	0.74988	0.46470
C	2.73255	0.27440	-1.19194	H	-2.57680	2.50754	3.35974	H	-4.70874	-0.94982	0.12913
C	1.49142	-1.94442	-0.96636	C	0.89472	2.12254	-1.20736	C	-3.00179	2.67169	0.92687
H	0.92834	-2.57253	-0.26493	H	1.21654	1.08436	-1.05931	H	-2.86149	2.70339	2.01298
H	2.34185	-2.53485	-1.34042	C	0.78479	2.39292	-2.70095	H	-4.07676	2.67921	0.73506
H	0.82360	-1.73397	-1.81090	H	-0.05821	1.86291	-3.15279	H	-2.59789	3.60346	0.52068
C	2.51161	-1.73240	2.01083	H	1.69887	2.04141	-3.18709	C	-2.23408	-1.83700	-1.23422
H	1.55225	-1.47630	2.48330	H	0.69236	3.45703	-2.93307	H	-1.24403	-2.05199	-1.66255
H	3.27987	-1.71759	2.79099	C	1.89701	3.03321	-0.51711	C	-3.25804	-1.80800	-2.35735
H	2.41519	-2.77289	1.66727	H	1.59798	4.08572	-0.57321	H	-4.29298	-1.83139	-2.00516
C	5.00103	0.27382	1.75450	H	2.87404	2.93651	-1.00048	H	-3.11440	-2.69524	-2.97996
H	4.89311	-0.34490	2.65076	H	2.01614	2.75201	0.53280	H	-3.12706	-0.93073	-2.99735
H	5.01681	1.32209	2.08445	C	0.78633	-1.33247	-0.27506	C	-2.50858	-2.89535	-0.18117
H	5.99605	0.07180	1.33380	C	-0.21193	-2.07144	-0.96013	H	-1.64172	-3.00238	0.47920
C	4.86177	1.69339	-0.97700	C	2.13708	-1.59915	-0.63712	H	-2.68360	-3.86159	-0.66326
H	4.90145	2.56356	-0.30633	C	0.11479	-2.97715	-1.97430	H	-3.38527	-2.66120	0.43248
H	4.64436	2.06951	-1.98149	C	-1.65951	-1.94252	-0.62170	C	0.05376	2.19606	0.47599
H	5.87865	1.27635	-0.99683	C	2.44162	-2.52417	-1.64395	H	0.95482	1.57716	0.38755
C	2.28018	0.62621	-2.56463	C	3.28373	-0.91313	0.02267	C	0.10790	3.29170	-0.57733
H	2.34443	-0.23582	-3.24508	C	1.44144	-3.21040	-2.32208	H	0.27213	2.86889	-1.57288
H	2.87970	1.43177	-3.00165	H	-0.68784	-3.51235	-2.48050	H	0.92875	3.98045	-0.35861
H	1.22664	0.93941	-2.57603	C	-2.20704	-2.72592	0.41565	H	-0.81514	3.87997	-0.60567
C	-1.74263	-2.27738	1.45819	C	-2.50047	-1.12056	-1.39301	C	-0.00491	2.73825	1.89504
H	-0.68443	-2.56602	1.43735	H	3.48782	-2.70098	-1.89064	H	-0.76514	3.51266	2.02686
H	-2.32029	-3.15707	1.77478	C	4.04146	0.03849	-0.68380	H	0.96231	3.19181	2.13289
H	-1.84303	-1.50619	2.23036	C	3.63288	-1.22598	1.35378	H	-0.18346	1.94180	2.62365
C	-2.04258	-3.13864	-1.41041	H	1.69149	-3.92493	-3.10221	Si	2.64683	0.21440	-1.39700
H	-2.47100	-2.94394	-2.40000	C	-3.58224	-2.67258	0.65398	Si	1.25039	-1.29773	1.65767
H	-2.51185	-0.40863	-1.01205	C	-1.32585	-3.60474	1.25005	C	1.96690	-3.01754	1.99062
H	-0.97771	-3.34999	-1.55524	C	-3.87274	-1.10182	-1.12871	H	1.27153	-3.80129	1.67191
C	-4.23325	-1.58117	-0.09882	C	-1.93872	-0.28254	-2.50396	H	2.17976	-3.16478	3.05636
H	-4.56274	-0.88553	0.68163	C	5.07767	0.71458	-0.02991	H	2.90056	-3.17512	1.43971
H	-4.64137	-2.57117	0.14696	C	3.78864	0.32791	-2.13670	C	4.06949	-1.02604	-1.21811
H	-4.69188	-1.25520	-1.03950	C	4.68740	-0.54668	1.96176	H	3.83305	-1.98664	-1.68673
C	-4.36381	2.16833	-0.39404	C	2.88789	-2.27601	2.12307	H	4.29714	-1.22389	-0.16430
H	-4.31774	2.56023	-1.41618	C	-4.43572	-1.87905	-0.11610	H	4.98438	-0.63957	-1.68254
H	-4.88108	2.90973	0.22983	H	-3.99990	-3.27898	1.45828	C	3.30347	1.80792	-0.58312
H	-4.98271	1.26494	-0.41994	H	-0.74862	-4.30118	0.63141	H	4.31875	2.00172	-0.95184
C	-2.86649	1.32778	2.09503	H	-0.59671	-2.99987	1.80581	H	2.70431	2.68957	-0.83085
H	-3.44618	0.40205	2.18914	H	-1.91008	-4.18531	1.96894	H	3.36202	1.73354	0.50830
H	-3.39902	2.11199	2.65057	H	-4.51815	-0.45882	-1.72951	C	2.47932	0.63062	-3.23816

H	1.66615	1.34013	-3.42895	H	-5.50780	2.85451	-3.11898	C	1.26987	-0.03178	1.80042
H	2.26900	-0.26810	-3.82625	H	-6.52685	1.81304	-2.11278	C	-1.16836	-0.08402	1.82698
H	3.40223	1.07898	-3.62537	H	-5.49546	3.03633	-1.37077	C	1.26341	0.28178	3.16348
C	-0.36312	-1.17675	2.65752	C	-3.91971	-2.24014	-0.81940	C	-1.14385	0.23122	3.19040
H	-0.83178	-0.18882	2.57620	H	-4.99829	-2.34868	-0.67312	C	0.06316	0.44100	3.85059
H	-0.17227	-1.36290	3.72137	H	-3.57994	-3.06376	-1.45533	H	2.21352	0.38457	3.68506
H	-1.10711	-1.90987	2.32658	H	-3.43596	-2.38228	0.15006	H	-2.08499	0.29446	3.73388
C	2.45903	-0.08390	2.48203	C	2.81680	-0.49120	-3.13717	H	0.06944	0.69516	4.90726
H	2.13619	0.96025	2.40411	H	3.55369	0.21851	-3.52388	C	-2.46923	-0.42808	1.18267
H	3.45842	-0.14691	2.03695	H	2.56103	-1.19193	-3.94081	C	-2.79315	-1.78648	0.99076
H	2.56330	-0.31622	3.54983	H	1.90083	0.06665	-2.91176	C	-3.39313	0.56590	0.81177
S9 (C ₁): E _{tot} = -2868.32363640				C	2.25701	-3.77258	0.69371	C	-4.02238	-2.12108	0.42004
Si	0.38226	-0.51964	0.42635	H	1.28923	-3.97950	0.22847	C	-4.60431	0.18931	0.22872
Si	1.46531	1.54250	0.16087	H	2.79225	-4.72314	0.79894	C	-4.93843	-1.14889	0.01762
Si	1.01885	3.67181	-0.77420	H	2.07176	-3.39089	1.70620	H	-4.26566	-3.17438	0.27823
Si	2.96862	1.80926	1.95395	C	6.55838	-1.28495	0.12026	H	-5.30725	0.96730	-0.06840
C	-0.79083	4.11401	-1.10639	H	7.13961	-0.73883	-0.62802	C	2.56784	-0.33464	1.12727
H	-1.38860	3.27132	-1.46604	H	6.51408	-0.65741	1.01976	C	2.97326	-1.68228	1.03275
H	-0.85100	4.90908	-1.85936	H	7.11593	-2.18698	0.39164	C	3.40940	0.68085	0.63843
H	-1.26955	4.49769	-0.19857	C	-1.34306	-0.55494	1.26046	C	4.18208	-1.98905	0.05660
C	1.96944	3.72577	-2.40725	N	-1.79850	-1.70608	1.86622	C	4.61278	0.33151	0.02186
H	3.03481	3.53323	-2.23676	N	-2.22202	0.41808	1.64987	C	5.01652	-0.99702	-0.11259
H	1.87609	4.70260	-2.89649	C	-2.94359	-1.44397	2.60495	H	4.48088	-3.03459	0.32709
H	1.61526	2.96173	-3.10765	C	-1.00801	-2.95359	1.87746	H	5.24993	1.12440	-0.36935
C	1.67312	5.07122	0.32074	C	-3.19953	-0.10655	2.48805	C	3.00654	2.11698	0.73795
H	1.08157	5.17431	1.23746	C	-2.04966	1.82520	1.24367	H	2.70208	2.39448	1.75287
H	1.61329	6.02717	-0.21346	C	-3.74460	-2.47443	3.31335	H	3.81544	2.78298	0.42522
H	2.71613	4.92606	0.62010	H	-0.03216	-2.60200	1.50334	H	2.14066	2.31186	0.09114
C	4.57267	2.48274	1.20857	C	-0.78882	-3.47941	3.28734	C	6.32307	-1.34638	-0.75868
H	4.95603	1.78948	0.45138	C	-1.52475	-4.01628	0.92405	H	7.12879	-1.41277	-0.01805
H	5.34889	2.60783	1.97287	C	-4.29335	0.66414	3.12928	H	6.27611	-2.31429	-1.26610
H	4.43302	3.45207	0.71750	H	-1.47125	1.74707	0.31125	H	6.62374	-0.59338	-1.49251
C	2.40830	2.98537	3.32746	C	-1.21383	2.56203	2.27876	C	2.13780	-2.77681	1.62717
H	2.13024	3.97290	2.94589	C	-3.36086	2.53231	0.93899	H	2.04630	-2.66451	2.71416
H	3.21983	3.12819	4.05066	H	-3.81700	-3.39831	2.73130	H	1.11419	-2.76742	1.23756
H	1.55000	2.58955	3.88111	H	-4.76331	-2.11231	3.46971	H	2.56799	-3.76050	1.42124
C	3.35713	0.14369	2.74825	H	-3.33380	-2.73886	4.29407	C	-3.06577	2.01366	0.99494
H	2.47085	-0.29006	3.22474	H	-1.65282	-0.01734	3.68790	H	-3.90100	2.65349	0.69754
H	4.14144	0.24677	3.50858	H	0.04530	-4.18716	3.26597	H	-2.79719	2.25632	2.02878
H	3.69750	-0.57900	1.99791	H	-0.52313	-2.67257	3.97730	H	-2.19662	2.28396	0.38140
C	0.05499	-1.46270	-1.22068	H	-2.54322	-4.34063	1.16823	C	-1.83699	-2.87435	1.38359
C	-1.18886	-1.56455	-1.90847	H	-1.51039	-3.66640	-0.11238	H	-0.97919	-2.92177	0.69721
C	1.11687	-2.29645	-1.67512	H	-0.87737	-4.89673	0.98997	H	-1.41612	-2.71758	2.38291
C	-1.37450	-2.56084	-2.88156	H	-3.91852	1.54086	3.66769	H	-2.32258	-3.85401	1.36062
C	0.90461	-3.26456	-2.65910	H	-4.80286	0.03282	3.86049	C	-6.22658	-1.53136	-0.64538
C	-0.35130	-3.42989	-3.23705	H	-5.04272	1.01805	2.41367	H	-6.98868	-0.75628	-0.52681
H	-2.33356	-2.61668	-3.39550	H	-1.74552	2.64391	3.23439	H	-6.08647	-1.68273	-1.72251
H	1.74150	-3.88670	-2.97244	H	-0.26571	2.04547	2.45975	H	-6.62757	-2.46647	-0.24345
H	-0.51655	-4.19543	-3.99070	H	-0.98392	3.57658	1.93520	Si	-0.04654	-2.17389	-2.14533
C	2.52049	-2.09464	-1.19881	H	-4.06214	1.86625	0.43169	C	1.09238	-3.55916	-1.56590
C	3.05988	-2.78360	-0.09806	H	-3.83579	2.94103	1.83540	C	-1.79891	-2.84842	-2.31224
C	3.33834	-1.20197	-1.92349	H	-3.16145	3.36923	0.26362	C	0.52614	-1.58649	-3.84062
C	4.37830	-2.53190	0.28990	H	2.45948	1.06988	-0.85555	H	2.09143	-3.18454	-1.32037
C	4.64476	-0.96532	-1.49278	S10 (C ₁): E _{tot} = -2327.60963866				H	1.19689	-4.30291	-2.36430
C	5.18120	-1.60640	-0.37545	Si	0.04179	-0.26863	-0.78530	H	0.70352	-4.07892	-0.68454
H	4.77811	-3.05938	1.15693	Si	-0.15138	1.62811	-1.80472	H	-2.14099	-3.34795	-1.40111
H	5.25686	-0.24941	-2.04203	Si	-0.12039	3.79801	-0.94890	H	-1.83639	-3.58089	-3.12754
C	-2.29319	-0.55665	-1.82313	C	1.35868	4.73275	-1.65733	H	-2.51637	-2.05231	-2.53607
C	-3.59494	-0.89405	-1.39539	H	2.30937	4.28024	-1.35963	H	-0.12735	-0.80622	-4.24202
C	-2.08354	0.71107	-2.41556	H	1.35706	5.77057	-1.30385	H	0.51600	-2.42520	-4.54638
C	-4.62928	0.03999	-1.51659	H	1.33227	4.75598	-2.75105	H	1.54228	-1.18300	-3.80870
C	-3.14753	1.61056	-2.52358	C	-0.02164	3.77943	0.94335	H	-0.12187	1.53311	-3.29053
C	-4.43215	1.30007	-2.07873	H	-0.90791	4.25011	1.38172	S11 (C ₁): E _{tot} = -2327.59662990			
H	-5.62750	-2.24187	-1.17895	H	0.85616	4.33809	1.28529	Si	-0.53271	-0.18634	-1.18990
H	-2.96956	2.57318	-3.00384	H	0.05343	2.77011	1.36306	Si	0.61662	1.55561	-0.03709
C	-0.75714	1.07888	-3.00867	C	-1.67866	4.71288	-1.49391	Si	1.14026	1.71976	2.25724
H	-0.41102	0.31664	-3.71714	H	-1.76179	4.75280	-2.58428	Si	2.35072	2.30620	-1.45582
H	-0.81040	2.03879	-3.53120	H	-1.65989	5.74524	-1.12560	C	2.99265	1.45076	2.52926
H	0.02253	1.15255	-2.23900	H	-2.58704	4.23868	-1.11026	H	3.39743	0.62087	1.94115
C	-5.54740	2.29515	-2.17931	C	0.04458	-0.16291	1.10541	H	3.20514	1.24933	3.58570

H	3.55199	2.34810	2.24559					C	3.58270	-1.45532	2.02247
C	0.15795	0.55976	3.39548	TS ^{Ar*} (C ₁): E _{tot} = -2327.58816756				H	2.83117	-2.24539	2.08218
H	-0.66723	1.10288	3.86741	Si	0.00678	0.40438	-0.12893	H	3.26606	-0.65389	2.70276
H	0.79898	0.18058	4.19944	H	1.02705	1.05536	-0.99708	H	4.52232	-1.85057	2.42054
H	-0.27956	-0.30248	2.87964	Si	-1.94623	1.34819	0.47043	C	6.35401	1.24119	-1.15965
C	0.74011	3.48916	2.78823	Si	-1.38563	3.35539	-0.68949	H	7.03026	1.25446	-0.30102
H	1.29282	4.22588	2.19587	Si	0.53736	1.27030	2.09172	H	6.07618	2.27860	-1.37679
H	0.99284	3.65302	3.84246	C	-1.68173	2.95044	-2.51630	H	6.91777	0.87939	-2.02589
H	-0.32674	3.70434	2.66442	H	-0.86825	2.32951	-2.90827	H	2.84744	-3.77641	-0.17785
C	2.18935	4.16839	-1.71687	H	-1.72583	3.86480	-3.11919				
H	1.22192	4.42731	-2.15780	H	-2.61763	2.40382	-2.67926	TS ^{Cp*} (C ₁): E _{tot} = -1788.05728811			
H	2.97296	4.53914	-2.38787	C	0.36282	4.05801	-0.52879	Si	0.29496	0.27054	-0.75005
H	2.27609	4.71666	-0.77301	H	0.57075	4.41167	0.48670	H	1.27526	0.69475	-1.78630
C	4.07356	1.96148	-0.76403	H	0.46775	4.92221	-1.19595	Si	-1.65971	-0.43806	-1.65109
H	4.30573	2.60419	0.09025	H	1.13921	3.33590	-0.79945	Si	-2.96095	-1.34407	0.13688
H	4.83058	2.15147	-1.53438	C	-2.56788	4.74128	-0.18292	Si	-0.93787	2.31502	-0.29858
H	4.18444	0.92307	-0.43505	H	-3.61360	4.45555	-0.33541	C	-3.07061	-0.35186	1.74359
C	2.21227	1.44808	-3.13126	H	-2.38340	5.65233	-0.76424	H	-2.10145	-0.23977	2.23722
H	2.28892	0.35896	-3.03013	H	-2.45520	4.99841	0.87596	H	-3.74104	-0.87258	2.43818
H	3.01242	1.78164	-3.80313	C	0.44129	-0.20456	3.26288	H	-3.48650	0.64843	1.58454
H	1.25528	1.65938	-3.61837	H	1.00118	-0.01071	4.18560	C	-2.40209	-3.09718	0.57774
C	-0.99629	-1.37578	0.23005	H	0.82324	-1.13131	2.83212	H	-2.22177	-3.72202	-0.30279
C	-0.07366	-2.32120	0.72856	H	-0.60494	-0.37571	3.53821	H	-3.18262	-3.58726	1.17163
C	-2.30975	-1.35043	0.73030	C	2.27250	2.00370	1.97054	H	-1.48365	-3.09575	1.17279
C	-0.45471	-3.18387	1.75786	H	2.96774	1.39741	1.38421	C	-4.72787	-1.47013	-0.52180
C	-2.66976	-2.21099	1.77163	H	2.68836	2.13511	2.97761	H	-5.13164	-0.48668	-0.78605
C	-1.74428	-3.11792	2.28759	H	2.22471	2.99101	1.50068	H	-5.39580	-1.91076	0.22757
H	0.25168	-3.91717	2.14117	C	-0.49162	2.64523	2.90821	H	-4.78081	-2.09068	-1.42178
H	-3.68305	-2.17586	2.16948	H	-1.50967	2.34704	3.17131	C	-2.74562	2.42377	-0.87099
H	-2.03290	-3.78844	3.09261	H	-0.54778	3.55975	2.30999	H	-3.13479	3.39260	-0.53012
C	-3.28800	-0.41530	0.09544	H	0.02875	2.90258	3.84091	H	-3.40037	1.65606	-0.44581
C	-3.95279	-0.80708	-1.08575	C	0.31382	-1.47753	-0.15166	H	-2.85167	2.39015	-1.95833
C	-3.53877	0.86008	0.64522	C	-0.77488	-2.38758	-0.13263	C	-0.98824	2.71777	1.54543
C	-4.84836	0.07943	-1.68895	C	1.62758	-2.01106	-0.19522	H	-1.59781	2.00473	2.10720
C	-4.43266	1.71732	0.00478	C	1.82814	-3.39590	-0.14316	H	-1.45114	3.70547	1.66133
C	-5.10217	1.34595	-1.16359	C	-0.53972	-3.76675	-0.08372	H	-0.00092	2.75890	2.01090
H	-5.35763	-0.22982	-2.60122	H	-1.39394	-4.44107	-0.07554	C	-0.02051	3.67806	-1.22309
H	-4.61026	2.70368	0.43252	C	0.75348	-4.27352	-0.06877	H	-0.02939	3.49026	-2.30112
C	1.27074	-2.29590	0.09261	H	0.92286	-5.34650	-0.02930	H	1.02648	3.75863	-0.91512
C	1.37741	-2.46188	-1.31416	C	-2.19348	-1.93930	-0.22376	H	-0.50132	4.64765	-1.04653
C	2.43501	-1.99642	0.83693	C	-3.04726	-2.04937	0.88951	C	1.41838	-0.40064	0.69724
C	2.59381	-2.17267	-1.94617	C	-2.68803	-1.42037	-1.43657	C	1.96909	-1.62491	0.02860
C	3.62526	-1.72618	0.15897	C	-4.36585	-1.60371	0.78529	C	2.58342	0.53637	0.74575
C	3.72137	-1.76963	-1.23483	H	-5.01335	-1.67177	1.65895	C	3.25246	-1.36797	-0.36055
H	2.65836	-2.29127	-3.02799	C	-4.00851	-0.96684	-1.49214	C	3.63213	-0.03326	0.08489
H	4.50809	-1.46168	0.74189	H	-4.38323	-0.55824	-2.43087	C	0.66475	-0.63773	1.99636
C	2.43553	-1.99841	2.37117	C	-4.86337	-1.04049	-0.38959	H	0.25993	0.29244	2.41078
H	2.37109	-3.02044	2.72736	C	2.83551	-1.15767	-0.39716	H	-0.17708	-1.32492	1.84959
H	3.35716	-1.56124	2.72953	C	3.76936	-0.93174	0.62784	H	1.32777	-1.08134	2.74898
H	1.58843	-1.45422	2.76154	C	3.08853	-0.64871	-1.69332	C	2.53817	1.87976	1.38295
C	4.99263	-1.41367	-1.94327	C	4.22437	0.12482	-1.91458	H	2.09840	1.84328	2.38826
H	5.34529	-2.23372	-2.57742	H	4.40615	0.51449	-2.91603	H	3.53826	2.30991	1.48275
H	4.84841	-0.54602	-2.59815	C	4.90506	-0.15581	0.35791	H	1.94043	2.60072	0.80733
H	5.79071	-1.16479	-1.23878	H	5.61835	0.02253	1.16291	C	1.19233	-2.88221	-0.12502
C	0.30120	-3.12620	-2.13596	C	5.14511	0.39591	-0.89615	H	0.21674	-2.70899	-0.60466
H	-0.64661	-3.21887	-1.60224	C	-1.82148	-1.32843	-2.65773	H	1.72618	-3.62219	-0.72731
H	0.11394	-2.59354	-3.07322	H	-1.09647	-0.50522	-2.58201	H	0.97252	-3.34903	0.84532
H	0.62729	-4.13986	-2.39898	H	-2.42156	-1.14408	-3.55288	C	4.17698	-2.26186	-1.11210
C	-2.84223	1.29837	1.89570	H	-1.23332	-2.23905	-2.81454	H	3.70806	-3.21173	-1.38113
H	-3.12733	2.31599	2.17615	C	-2.54730	-2.60320	2.19102	H	4.52386	-1.79099	-2.04035
H	-3.05654	0.63500	2.74134	H	-2.42273	-3.69173	2.15379	H	5.07777	-2.49320	-0.53015
H	-1.75479	1.27822	1.76538	H	-3.24026	-2.37790	3.00582	C	4.96994	0.55908	-0.19642
C	-3.68264	-2.14067	-1.71565	H	-1.56577	-2.19262	2.45123	H	5.78218	-0.08288	0.16583
H	-2.68841	-2.15453	-2.18432	C	-6.25985	-0.50243	-0.45583	H	5.13479	0.68480	-1.27410
H	-3.69564	-2.95461	-0.98341	H	-6.61958	-0.43472	-1.48622	H	5.09470	1.54155	0.26579
H	-4.41498	-2.36431	-2.49536	H	-6.31193	0.50534	-0.02637				
C	-6.06991	2.28070	-1.82348	H	-6.96109	-1.12427	0.10855	TS-S1 (C ₁): E _{tot} = -3408.96915168			
H	-6.95682	2.44337	-1.20087	C	2.16429	-0.94967	-2.83621	Si	1.05276	0.13460	0.08405
H	-5.62280	3.26482	-1.99700	H	2.60790	-0.64695	-3.78816	H	1.24255	-1.34314	-0.06039
H	-6.41058	1.89266	-2.78682	H	1.20669	-0.42229	-2.73759	Si	-1.41384	-0.02620	0.43923
H	-0.44168	2.60747	-0.58211	H	1.91980	-0.21629	-2.89233	Si	-1.20756	-0.61291	2.18442

Si	-2.02894	1.83408	1.79567	H	-0.18224	0.71942	-3.98039	Si	-0.03928	0.08157	-0.40269
N	3.20189	1.55143	1.64545	H	-0.94476	-0.17346	-2.66788	H	1.04740	0.12617	-1.62918
N	3.41823	-0.59642	1.88369	H	-1.92959	0.42140	-4.02090	Si	1.89713	1.11250	-0.21645
C	2.79634	0.35456	1.10187	C	-4.24468	4.35150	-2.12817	Si	2.15461	2.51438	-2.04813
C	4.03432	1.35533	2.73881	H	-4.70337	4.32382	-1.13074	Si	3.36583	1.80843	1.49487
C	4.14527	0.00507	2.90884	H	-4.23285	5.40046	-2.44128	N	-1.56514	0.12527	2.19460
C	4.70096	2.41974	3.53057	H	-4.90534	3.80358	-2.80657	N	-2.34444	1.55461	0.76219
H	5.29775	3.08633	2.89886	C	5.48919	-0.06532	-1.12018	C	-1.42049	0.57287	0.91670
H	5.38669	1.96291	4.24714	H	6.48143	-0.40736	-0.81006	C	-2.60154	0.80495	2.82861
H	4.00043	3.04589	4.09162	H	5.62564	0.70491	-1.88609	C	-3.08558	1.71252	1.92605
C	4.83682	-0.70958	4.01422	H	5.02015	0.43611	-0.26276	C	-3.09481	0.51844	4.19968
H	4.27249	-1.58665	4.34276	C	5.02657	-5.01780	-1.72260	H	-3.05556	-0.54939	4.43050
H	4.92882	-0.04780	4.87884	H	5.06785	-5.51726	-2.69706	H	-4.13908	0.82712	4.29156
H	5.84504	-1.04774	3.75124	H	6.04523	-4.98817	-1.32492	H	-2.52902	1.04368	4.97677
C	0.00523	-1.09620	3.56211	H	4.43055	-5.66188	-1.06582	C	-4.20436	2.66999	2.10231
H	0.93230	-0.65552	3.18031	C	1.15020	-2.06252	-2.87602	H	-3.91110	3.70034	1.87747
H	0.26880	-1.94582	4.20630	H	0.44260	-1.76999	-2.08538	H	-4.54238	2.65305	3.14050
C	-0.46522	-0.34061	4.19993	H	1.07272	-1.29555	-3.65358	H	-5.06390	2.42766	1.46769
C	-0.72347	-3.32283	1.49992	H	0.81102	-3.01346	-3.29832	C	2.42805	4.32791	-1.56515
H	0.00500	-3.29168	0.68067	C	2.55384	-2.89570	2.32198	H	1.57350	4.73540	-1.01350
H	-1.63710	-3.78856	1.11421	H	2.79984	-2.89517	3.39007	H	2.57217	4.94721	-2.45891
H	-0.33194	-3.98691	2.28079	H	1.52780	-2.55527	2.20802	H	3.31491	4.45955	-0.93508
C	-2.81168	-2.01170	3.12517	H	2.60978	-3.92862	1.96166	C	0.67001	2.45884	-3.21788
H	-3.57088	-2.44940	2.46697	C	4.93072	-2.56019	1.60447	H	0.50413	1.44625	-3.60077
H	-3.24824	-1.13041	3.60471	H	5.65744	-1.85215	1.19496	H	0.83520	3.12181	-4.07614
H	-2.59756	-2.74352	3.91503	H	5.21931	-2.81209	2.62804	H	-0.25428	2.77249	-2.71980
C	-2.70235	1.51647	3.55198	H	4.99550	-3.47845	1.01550	C	3.66839	1.98228	-3.05735
H	-2.04198	0.91637	4.18366	C	2.66145	3.98333	1.95118	H	4.57172	1.93348	-2.43809
H	-3.68457	1.03155	3.55540	H	3.60401	4.43790	2.26776	H	3.87079	2.66681	-3.89027
C	-0.49601	2.89879	2.09548	H	2.08534	4.75933	1.43945	H	3.51094	0.98004	-3.47293
H	-0.07398	3.24490	1.14670	H	2.09138	3.68809	2.83486	C	5.07402	2.15565	0.76088
H	0.27998	2.31413	2.60328	C	3.90037	3.15584	-0.08416	H	5.52402	1.23684	0.36879
H	-0.72982	3.77931	2.71027	H	4.90264	3.24543	0.35313	H	5.75317	2.56583	1.51789
C	-3.37817	2.97396	1.07140	H	3.92609	2.38730	-0.86229	H	5.02836	2.87433	-0.06463
H	-3.73066	2.64401	0.09100	H	3.65942	4.11110	-0.56239	C	2.69643	3.43110	2.21715
H	-3.00088	3.99518	0.94420	N	-4.89964	-1.03331	0.53040	H	1.71978	3.28003	2.69171
H	-4.24430	3.02413	1.74418	C	-5.70104	-2.10600	0.14195	H	2.56500	4.19542	1.44442
C	1.62590	0.87362	-1.63233	C	-4.92197	-2.88750	-0.66402	H	3.37554	3.83685	2.97768
C	1.10771	2.07329	-2.19875	N	-3.67688	-2.26172	-0.73134	C	3.61622	0.64667	2.96382
C	2.77289	0.32056	-2.27113	C	-3.64845	-1.10442	-0.00565	H	2.67413	0.39778	3.46212
C	1.80928	2.74919	-3.21013	H	-2.82574	2.49255	4.04009	H	4.26246	1.12714	3.70845
C	3.42301	0.99833	-3.31453	C	-5.27426	-4.16751	-1.32741	H	4.09111	-0.29121	2.66276
C	2.97858	2.23629	-3.75392	H	-4.73487	-5.02132	-0.90363	C	-0.34046	-1.80705	-0.38655
H	1.38545	3.67091	-3.60584	H	-5.06692	-4.15559	-2.40254	C	0.68195	-2.78359	-0.22864
H	4.28218	0.52697	-3.78917	H	-6.34206	-4.36561	-1.20636	C	-1.67685	-2.28431	-0.53443
H	3.50109	2.76583	-4.54655	C	-7.10044	-2.33477	0.57940	C	0.35422	-4.13431	-0.05749
C	3.50348	-2.03144	1.51834	H	-7.73995	-1.45997	0.42164	C	-1.96819	-3.64431	-0.36046
H	3.19013	-2.05487	0.46956	H	-7.16862	-2.59962	1.64046	C	-0.96697	-4.56761	-0.08422
C	2.87036	2.82502	0.98740	H	-7.53755	-3.15944	0.01091	H	1.16244	-4.85170	0.07727
H	1.90697	2.61232	0.50141	C	-2.59592	-2.59996	-1.68039	H	-2.99773	-3.97777	-0.48192
C	3.31300	-1.04616	-2.00360	H	-1.75480	-1.98505	-1.32642	H	-1.20709	-5.61867	0.05396
C	4.64823	-1.22083	-1.58268	C	-5.33966	0.17208	1.24901	C	-2.33785	2.43531	-0.43237
C	2.54867	-2.18370	-2.35204	H	-4.39649	0.67993	1.46663	H	-1.84488	1.81173	-1.19370
C	5.18834	-2.50850	-1.52893	C	-2.98718	-2.14920	-3.07663	C	-0.56428	-0.76439	2.83284
C	3.11244	-3.45477	-2.22621	H	-3.81301	-2.73920	-3.47782	H	0.23225	-0.81564	2.08054
C	4.43720	-3.64326	-1.82724	H	-2.13799	-2.24102	-3.76094	C	-2.81768	-1.44538	-1.02107
H	6.22180	-2.62801	-1.20250	H	-3.29497	-1.09177	-3.06585	C	-3.99084	-1.27778	-0.25380
H	2.50358	-4.32245	-2.48174	C	-2.18481	-4.06585	-1.66833	C	-2.81333	-0.98635	-2.36306
C	-0.27204	2.61957	-1.98717	H	-2.83055	-4.68498	-2.29798	C	-5.09699	-0.62511	-0.80722
C	-1.33257	1.93734	-2.62683	H	-2.17610	-4.48739	-0.66164	C	-3.94261	-0.34347	-2.87422
C	-0.51188	3.90855	-1.47474	H	-1.16825	-4.15196	-2.06407	C	-5.09937	-0.15156	-2.11762
C	-2.60629	2.50521	-2.65322	C	-6.03464	-0.11574	2.56960	H	-5.99097	-0.50103	-0.19399
C	-1.80125	4.44663	-1.52760	H	-7.06672	-0.45330	2.43988	H	-3.92493	-0.01153	-3.91237
C	-2.86777	3.76129	-2.10489	H	-6.07013	0.80604	3.15898	C	2.13371	-2.45329	-0.34999
H	-3.41143	1.96200	-3.14970	H	-5.49081	-0.86547	3.15176	C	2.67945	-2.27620	-1.64001
H	-1.96836	5.44278	-1.11559	C	-6.16123	1.06196	0.32733	C	2.98069	-2.39135	0.76889
C	0.59035	4.77984	-0.94589	H	-7.11231	0.59172	0.05386	C	4.03188	-1.96931	-1.77526
H	0.81746	5.59268	-1.64703	H	-5.60800	1.27840	-0.59217	C	4.33397	-2.08348	0.58927
H	0.30712	5.25115	0.00255	H	-6.38770	2.01312	0.81902	C	4.87854	-1.84930	-0.67149
H	1.51720	4.22468	-0.79624					H	4.43730	-1.81787	-2.77573
C	-1.08785	0.65993	-3.36601					H	4.98233	-2.03328	1.46466

TS-S2 (C₁): E_{tot} = -2868.26607548

C	2.46263	-2.61424	2.15893	H	-6.61760	-2.11509	0.90292	H	-4.15821	1.64536	-0.68010
H	3.27060	-2.89463	2.84151	C	-2.40574	-2.59714	-1.72560	C	-2.18847	4.18905	-1.65517
H	2.01621	-1.69645	2.56262	H	-2.85744	-3.56883	-1.50866	H	-2.62843	4.48646	-0.69776
H	1.69300	-3.39125	2.19598	H	-1.35509	-2.63551	-1.41814	H	-2.84370	4.56984	-2.44703
C	1.82752	-2.38890	-2.86807	H	-2.39684	-2.46239	-2.81390	H	-1.22691	4.70296	-1.75300
H	1.16462	-3.26048	-2.83358	C	2.36158	-0.47685	-1.21724	C	-1.30399	1.91324	-3.51582
H	1.18146	-1.50761	-2.97758	C	2.62185	-1.85183	-1.04086	H	-0.32338	2.37227	-3.67029
H	2.44497	-2.45961	-3.76784	C	3.83669	-2.25155	-0.48121	H	-1.97534	2.27412	-4.30367
C	6.32582	-1.50173	-0.84873	H	4.02839	-3.31687	-0.35175	H	-1.18050	0.83359	-3.64404
H	6.44504	-0.58051	-1.43076	C	4.79861	-1.33099	-0.06507	C	0.94178	-1.56330	0.25554
H	6.82554	-1.35621	0.11328	C	4.53270	0.02345	-0.26699	C	2.29191	-1.62006	0.66502
H	6.86684	-2.28706	-1.38839	H	5.27591	0.76301	0.03019	C	0.04556	-2.53996	0.75108
C	-4.11888	-1.81989	1.14049	C	3.34259	0.46326	-0.85131	C	2.72200	-2.60299	1.56044
H	-4.75692	-1.17509	1.75557	C	1.61724	-2.88815	-1.45026	C	0.49744	-3.51579	1.64396
H	-4.57616	-2.81737	1.14205	H	0.72917	-2.86597	-0.80478	C	1.82865	-3.55050	2.05226
H	-3.15174	-1.91951	1.63223	H	2.04085	-3.89427	-1.38728	H	3.76744	-2.62119	1.86451
C	-6.28930	0.55661	-2.69039	H	1.25123	-2.72802	-2.47067	H	-0.21065	-4.25231	2.02079
H	-6.51762	0.20856	-3.70268	C	6.06053	-1.78568	0.60202	H	2.16820	-4.31516	2.74602
H	-7.18102	0.41034	-2.07439	H	6.45928	-2.69374	0.13972	C	-1.38721	-2.49984	0.34675
H	-6.11662	1.63816	-2.76351	H	5.88303	-2.02029	1.65858	C	-1.80135	-3.05294	-0.87714
C	-1.65502	-1.22975	-3.28194	H	6.83715	-1.01709	0.56701	C	-2.31016	-1.80724	1.15056
H	-0.83927	-0.51936	-3.09342	C	3.11991	1.92429	-1.08598	C	-3.12907	-2.88884	-1.28260
H	-1.23052	-2.22926	-3.14367	H	3.91117	2.52825	-0.63350	C	-3.62361	-1.65092	0.70553
H	-1.95986	-1.12250	-4.32650	H	2.15850	2.24396	-0.67258	C	-4.05470	-2.18309	-0.51266
C	-1.45976	3.64419	-0.15388	H	3.07906	2.16827	-2.15422	H	-3.44243	-3.30958	-2.23796
H	-1.84724	4.23315	0.68542	C	-1.02271	4.30369	1.87527	H	-4.32878	-1.09213	1.32247
H	-0.43472	3.32911	0.07658	H	-1.90135	3.65172	1.88031	C	3.26807	-0.63034	0.12440
H	-1.42844	4.29471	-1.03361	H	-1.32354	5.25814	1.42690	C	3.98166	-0.92491	-1.05511
C	-3.72012	2.81301	-0.93292	H	-0.74918	4.49490	2.91767	C	3.47042	0.59724	0.77788
H	-4.40689	1.96508	-0.89732	C	1.92945	4.70351	1.30501	C	4.88288	0.01447	-1.55559
H	-4.15409	3.65034	-0.37893	H	2.14055	4.74467	2.37790	C	4.38023	1.51317	0.24326
H	-3.63576	3.12516	-1.97836	H	1.71935	5.72462	0.96545	C	5.09795	1.24105	-0.92157
C	0.01460	-0.12070	4.08358	H	2.84201	4.37460	0.79725	H	5.42981	-0.21762	-2.46935
H	-0.66900	-0.16244	4.93569	C	0.12679	3.71926	-0.94688	H	4.53083	2.46545	0.75185
H	0.91604	-0.66827	4.37499	H	-0.08147	2.75857	-1.42982	C	2.71353	0.91854	2.03101
H	0.29614	0.92205	3.90662	H	0.99309	4.15859	-1.45342	H	3.01148	0.27190	2.86519
C	-1.05867	-2.17929	3.08232	H	-0.73248	4.37284	-1.13646	H	2.87114	1.95704	2.33782
H	-1.94786	-2.20861	3.72074	C	-0.62152	-1.63689	3.72449	H	1.63606	0.75749	1.89651
H	-1.27832	-2.70182	2.14707	H	-0.00117	-0.84474	4.15657	C	6.06400	2.23779	-1.48811
H	-0.27014	-2.73923	3.59434	H	-0.62077	-2.48309	4.42135	H	5.71725	2.62979	-2.45075
TS-S3 (C_1): $E_{\text{tot}} = -2327.58164030$				H	-1.64562	-1.25548	3.66000	H	6.20255	3.08936	-0.81676
Si	0.82893	1.54187	2.10025	C	-1.12672	-3.52714	1.38314	H	7.04682	1.78958	-1.66719
Si	-0.02071	-0.16981	0.80132	H	-0.75124	-4.00286	0.47167	C	3.75427	-2.22176	-1.77227
H	-1.30033	0.44041	1.37656	H	-2.12567	-3.13353	1.16594	H	2.70500	-2.32448	-2.07884
Si	0.45286	3.58320	0.92209	H	-1.23458	-4.31234	2.14057	H	4.37519	-2.29424	-2.66846
Si	0.01953	-2.17720	2.03548	C	1.75286	-2.88359	2.25385	H	3.97157	-3.08449	-1.13291
C	-0.13152	-0.07630	-1.08804	H	2.10993	-3.39537	1.35533	C	-1.87343	-1.21699	2.45715
C	-1.36292	0.09578	-1.76394	H	1.75687	-3.61045	3.07437	H	-2.62922	-0.53644	2.86200
C	-1.36685	0.40016	-3.12978	H	2.48084	-2.10122	2.49491	H	-1.68595	-1.99066	3.21141
H	-2.32172	0.53651	-3.63490	TS-S4 (C_1): $E_{\text{tot}} = -2327.57877478$				H	-0.92893	-0.66900	2.34945
C	-0.17613	0.50052	-3.84310	Si	0.49399	-0.27919	-1.09566	C	-0.82216	-3.76181	-1.76381
H	-0.19259	0.74700	-4.90138	H	-1.07577	-0.32932	-1.17409	H	-0.10684	-3.05475	-2.20554
C	1.03285	0.23556	-3.20539	Si	-0.66890	1.36712	-0.12047	H	-0.22682	-4.49655	-1.21173
H	1.96373	0.24196	-3.76994	Si	-1.16903	2.56860	1.87379	H	-1.32831	-4.27381	-2.58611
C	1.06801	-0.06447	-1.84033	Si	-2.00837	2.31654	-1.81923	C	-5.47240	-2.01139	-0.96786
C	-2.66343	-0.16607	-1.07887	C	-0.38561	4.26924	1.60770	H	-6.12641	-2.78218	-0.54342
C	-3.41504	0.86847	-0.49275	H	0.70678	4.20301	1.57198	H	-5.87796	-1.04262	-0.65963
C	-4.61386	0.56472	0.15124	H	-0.64583	4.92751	2.44504	H	-5.55695	-2.08085	-2.05620
H	-5.18093	1.37275	0.61306	H	-0.71930	4.75590	0.68697				
C	-5.09936	-0.74366	0.22460	C	-0.54878	1.95235	3.54193				
C	-4.35353	-1.75174	-0.38510	H	-0.99514	1.00468	3.85138				
H	-4.71778	-2.77863	-0.35200	H	-0.81681	2.70256	4.29593				
C	-3.14840	-1.48624	-1.04317	H	0.53771	1.83763	3.57106				
C	-2.91040	2.27505	-0.53730	C	-3.04728	2.73869	1.96771				
H	-1.93366	2.34936	-0.04473	H	-3.45915	3.25328	1.09358				
H	-3.59355	2.96795	-0.03855	H	-3.33329	3.31365	2.85584				
H	-2.75499	2.62495	-1.56441	H	-3.53881	1.76223	2.03353				
C	-6.38675	-1.04703	0.92991	C	-3.71320	1.51654	-1.67242				
H	-7.22881	-0.51362	0.47562	H	-3.64527	0.43951	-1.86156				
H	-6.35113	-0.74070	1.98087	H	-4.40393	1.94644	-2.40727				