Supporting Information for

Synthesis and Functionalization of the Six-Vertex Anionic Amido-Substituted Silicon Cluster $[Si_6\{N(SiMe_3)Ph\}_5]^-$

Westfälische Wilhelms-Universität Münster, Institut für Anorganische und Analytische Chemie, Corrensstraße 28-30, 48149 Münster,
Email: lips@uni-muenster.de

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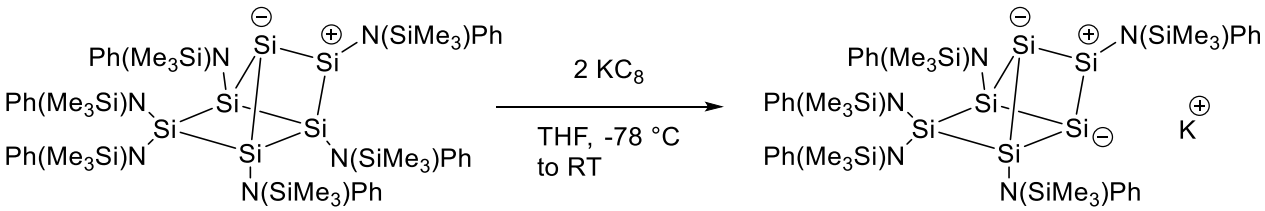
1. General experimental procedures

All reactions were performed with the use of modified Schlenk techniques with additional manipulations using a MBraun Glovebox. All solvents were dried over sodium benzophenone or CaH_2, distilled and stored over 4 Å molecular sieves prior to use. Silicon tetrabromide, silicon tetrachloride and methyliodide were purchased from Aldrich and used without further purification. [2.2.2]cryptant was purchased from Merck and was dried in vacuum for 16 h prior to use. The starting material $Si_6\{N(SiMe_3)Ph\}_6$ was prepared according to a literature procedure.[S1]

All NMR data were obtained on Bruker Avance I and III spectrometer and were referenced to the deuterated solvent (C_6D_6, THF-d_8, PhMe-d_8) according to an IUPAC recommendation. Additionally, the ^1H and ^{13}C NMR spectra were referenced internally to residual solvent resonances at 300 K. ^1H, ^{13}C and ^{29}Si NMR spectra were referenced to tetramethylsilane (TMS; δ = 0 ppm). ^{15}N NMR spectra were referenced to ammonia (NH_3; δ = 0 ppm). Further explanation of the ^{29}Si NMR experiments: ^{29}Si DEPT 19.5 = ^{29}Si NMR measurement with Distortionless Enhancement Polarization Transfer method, pulse angle 19.5°, coupling to 9 protons as polarization source with coupling $^2J_{Si-H}$ = 7 Hz; $^{29}Si\{^1H\}IG$ = Inverse gated decoupled ^{29}Si proton decoupled NMR measurement; $^{29}Si\{/\}$ = ^{29}Si proton coupled NMR measurement. ^{13}C DEPT 135 = Distortionless Enhancement of Polarization Transfer using a 135 degree decoupler pulse. All ^{13}C NMR spectra were recorded proton decoupled. IR spectra were recorded using nujol oil and CsI plates on a Shimadzu IR PRESTIGE 21. UV-visible spectra were recorded as dilute THF or *n*-hexane solutions in 1 mL quartz cuvettes using an Agilent Cary 100 spectrometer. Mass spectrometry was performed with a Varian MAT 212 Micromass Quattro LC-Z device. CHN elemental analysis was done with a Vario EL III CHN Instrument. Melting points were measured in glass capillaries sealed under argon gas by using a Stuart Melting Point Apparatus SMP3 and are uncorrected.

2.1 Synthesis of K[Si$_6${N(SiMe$_3$)Ph}$_5$] (2)



Si$_6${N(SiMe$_3$)Ph}$_6$ (0.200 g, 0.17 mmol, 1.0 equiv.) was dissolved in THF (10 mL) and slowly added to a suspension of KC_8 (0.047 g, 0.35 mmol, 2.0 equiv.) in THF (10 mL) at −78 °C. The reaction mixture was warmed to room temperature over 12 h to obtain an orange solution. Volatile components were removed in vacuo to obtain an orange solid. The crude orange product was extracted in benzene 6 mL to obtain K[Si$_6${N(SiMe$_3$)Ph}$_5$] (**2**) (0.107 g, 0.10 mmol, 61%) as a pale yellow solid that was isolated by filtration. Single crystals of **2** were obtained from a saturated THF/*n*-hexane solution at room temperature.

^{1}H-NMR (THF-d$_8$, 300 K, 400 MHz): δ(ppm) = 7.23 - 7.16 (4H, m); 7.07 - 6.88 (13H, m); 6.83 - 6.74 (8H, m); 0.43 (9H, s); 0.06 (18H, s); −0.01 (18H, s).

^{13}C-NMR (THF-d$_8$, 300 K, 100 MHz): δ(ppm) = 153.9; 150.0; 147.5; 132.6; 131.4; 131.2; 128.5; 128.4; 128.1; 123.0; 122.5; 122.0; 3.9; 3.7; 3.3.

^{15}N,^{1}H-HMBC-NMR (THF-d$_8$, 300 K, 41 MHz): δ(ppm) = 144; 89; 40.

^{29}Si(DEPT 19.5)-NMR (THF-d$_8$, 300 K, 80 MHz): δ(ppm) = 4.7; 3.8; 0.9.

^{29}Si{^{1}H}IG-NMR (THF-d$_8$, 300 K, 80 MHz): δ(ppm) = 164.0; 68.5; 44.4; −44.9.

IR (KBr pellet, $\tilde{\nu}$/cm^{-1} (intensity)) = 523(m), 608(vw), 660(vw), 700(m), 754(w), 837(vs), 874(vs), 937(vs), 1028(vw), 1071(vw), 116 (vw), 1209(s),1246(s), 1404(vw), 1443(vw), 1481(vs), 1587(m), 2891(vw), 2951(w), 3053(vw).

ESI-MS: m/z = 988.31 [Si$_6${N(SiMe$_3$)Ph}$_5$]$^-$, 1038.31 ([Si$_6${N(SiMe$_3$)Ph}$_5$(OH)$_2$O]$^-$.

UV-Vis: (THF, c = 3.0·10^{-4} mol/L, ε/L·mol^{-1}·cm^{-1}): λ = 243 nm (2747), 293 nm (854).

Melting point: Decomposition at 215 °C.

Elemental Analysis for $C_{45}H_{70}KN_5Si_{11}$:	H	C	N
calculated:	6.86	52.52	6.81
found:	6.80	50.95	6.33

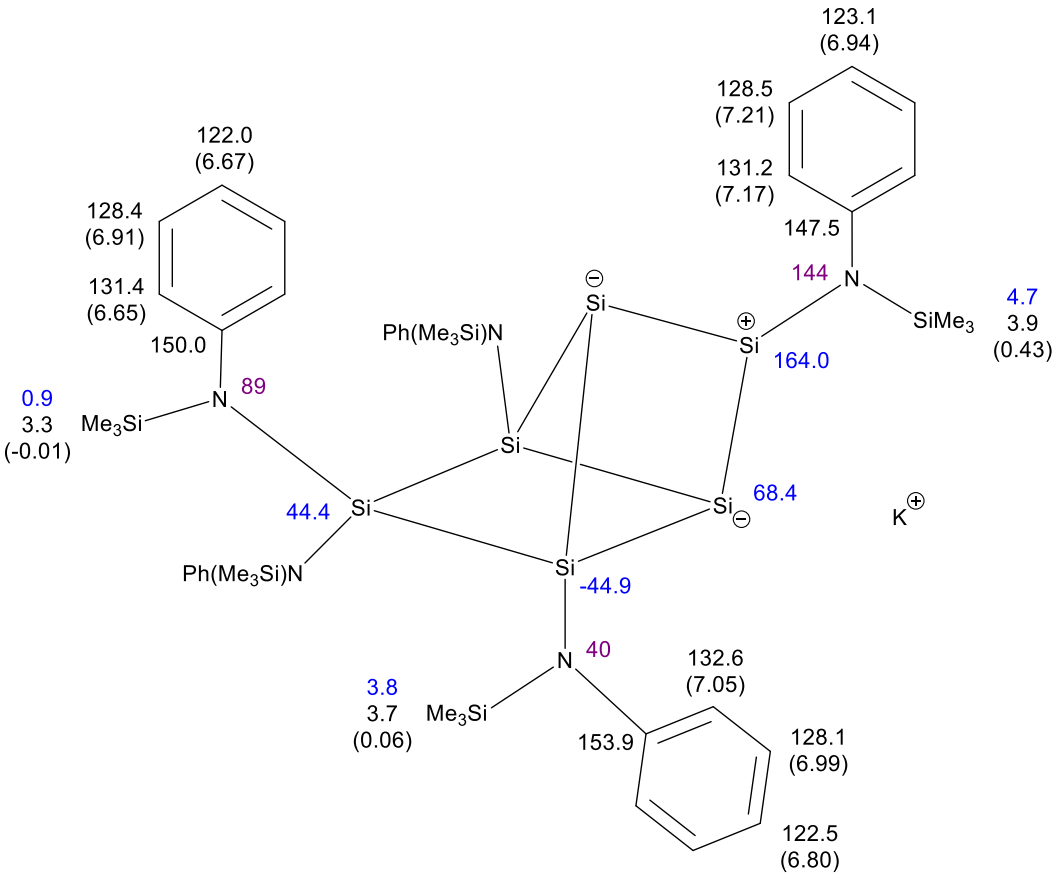


Figure S1. Assignment of chemical shifts to K[Si_6{$N(SiMe_3)Ph$}$_5$], ^{1}H (in brackets), ^{13}C (black), ^{15}N (violet), ^{29}Si (blue).

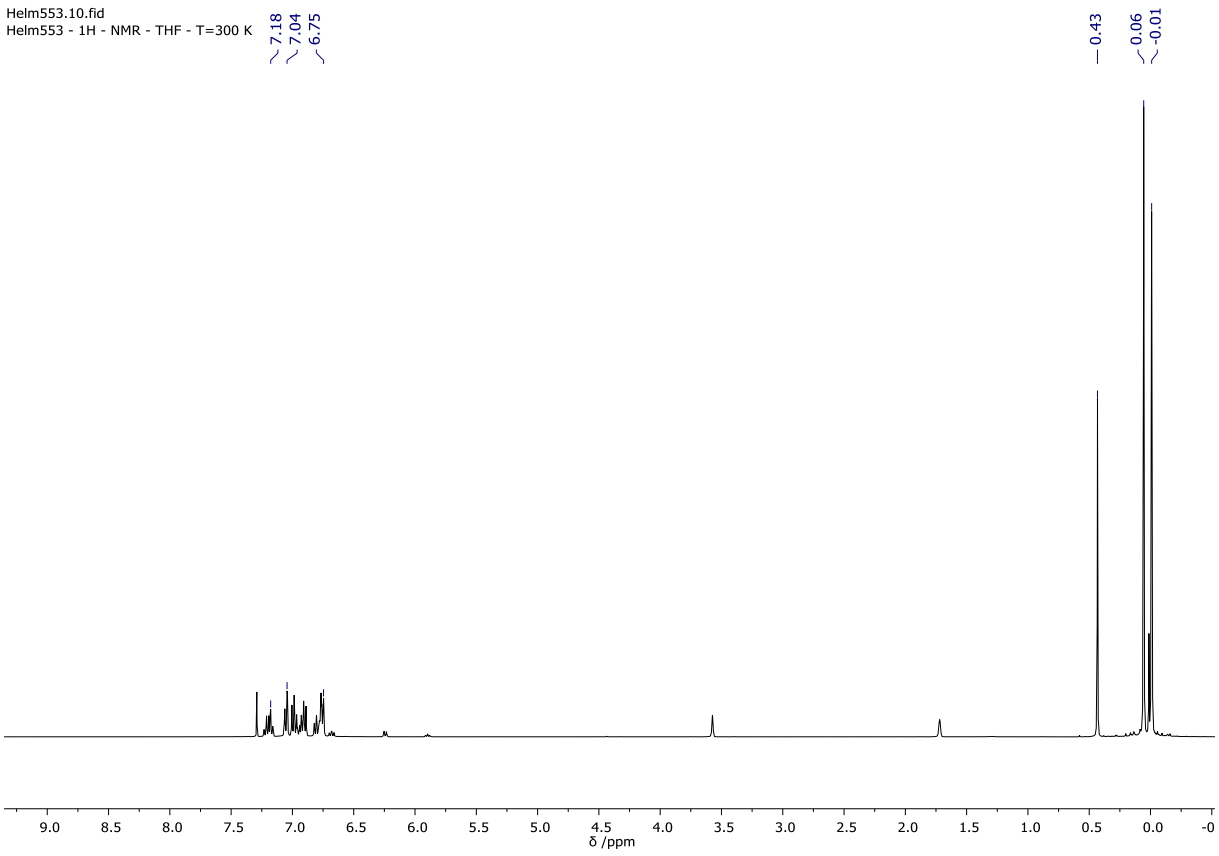


Figure S2. ^{1}H-NMR spectrum (THF-d_8, 300 K, 400 MHz) of K[Si_6{$N(SiMe_3)Ph$}$_5$].

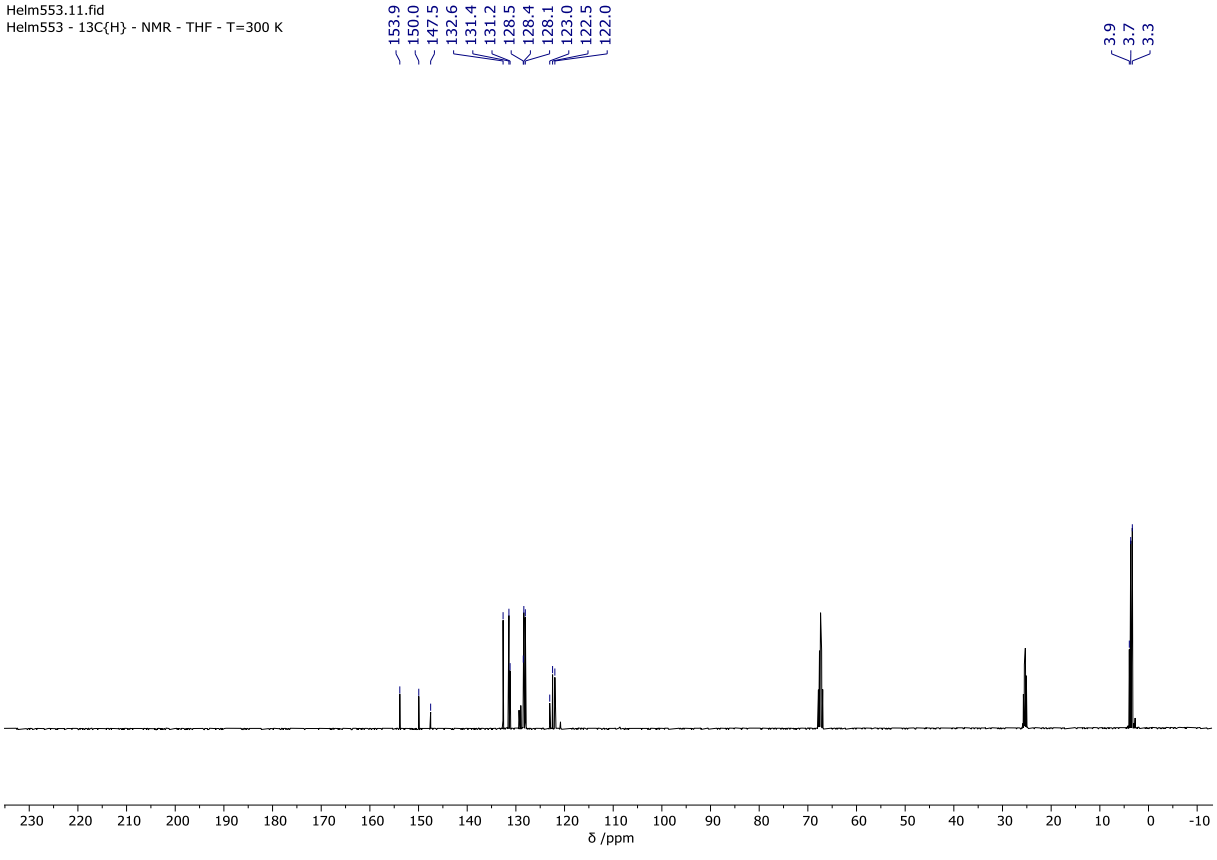


Figure S3. ^{13}C{^{1}H}-NMR spectrum (THF-d_8, 300 K, 100 MHz) of K[Si_6{$N(SiMe_3)Ph$}$_5$].

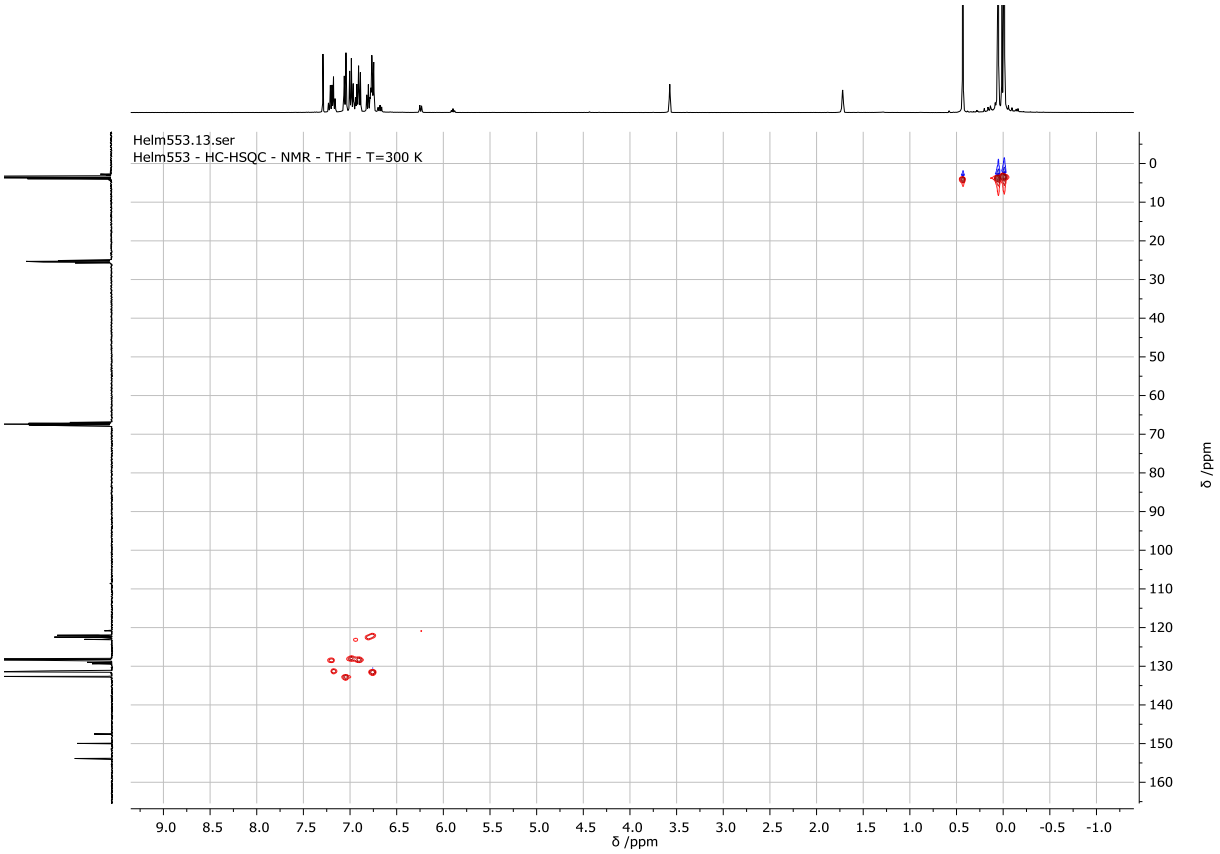


Figure S4. H,C-HSQC-NMR spectrum (THF-d_8, 300 K) of K[Si_6{$N(SiMe_3)Ph$}$_5$].

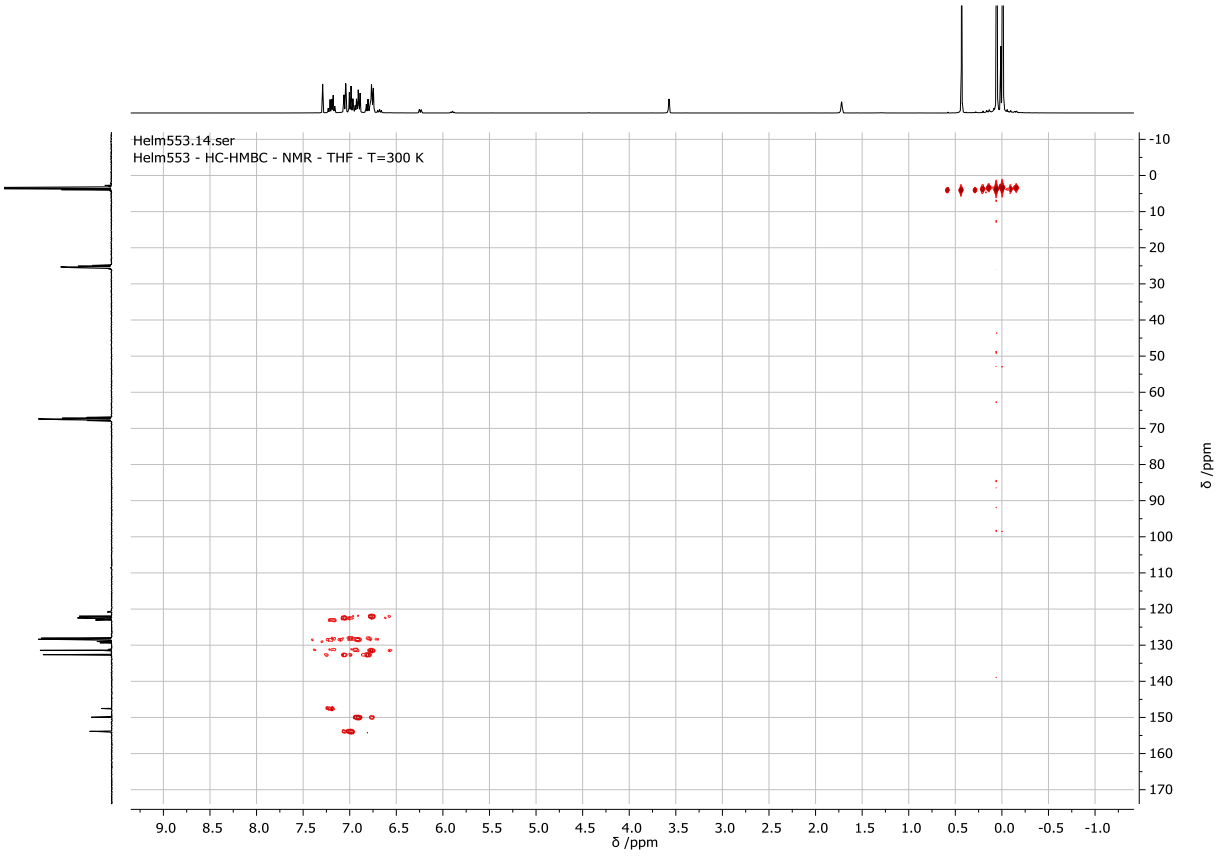


Figure S5. H,C-HMBC-NMR spectrum (THF-d_8, 300 K) of K[Si_6{$N(SiMe_3)Ph$}$_5$].

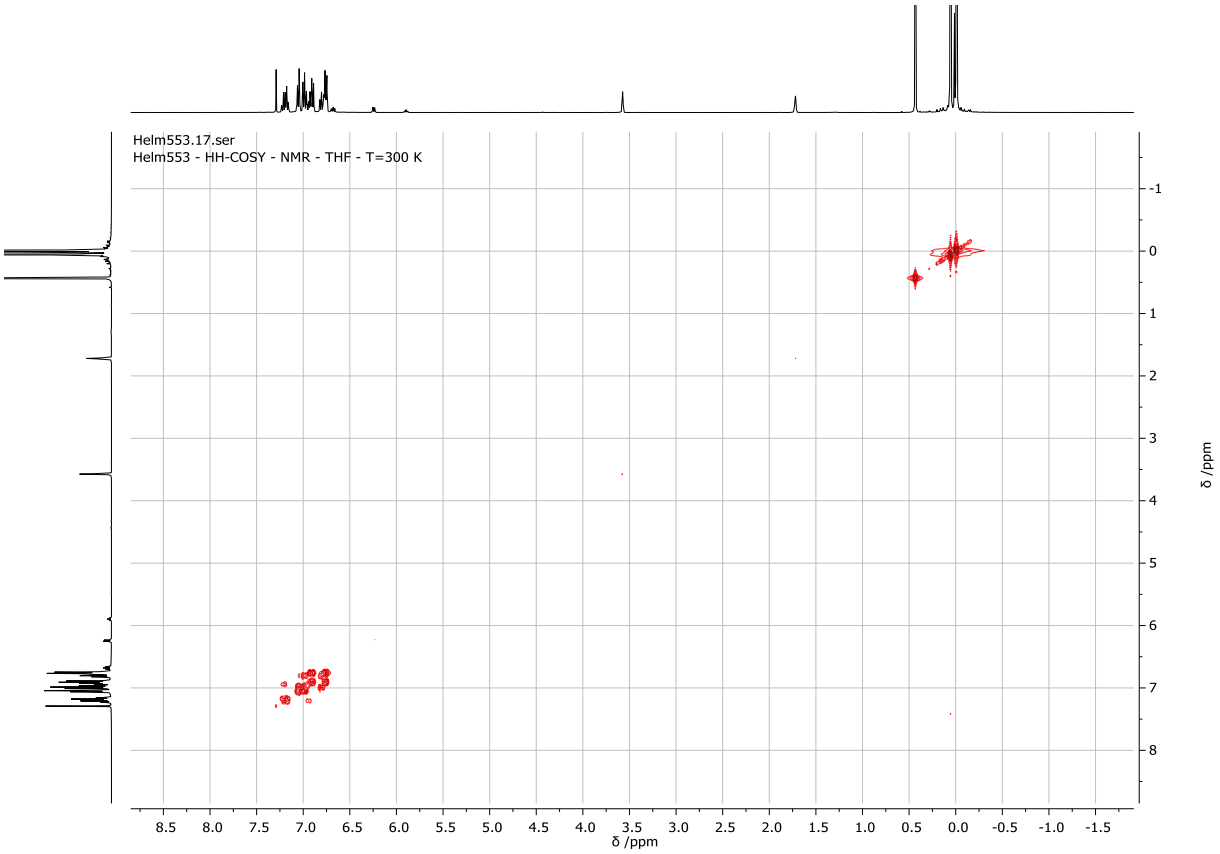


Figure S6. H,H-COSY-NMR spectrum (THF-d_8, 300 K) of K[Si_6{$N(SiMe_3)Ph$}$_5$].

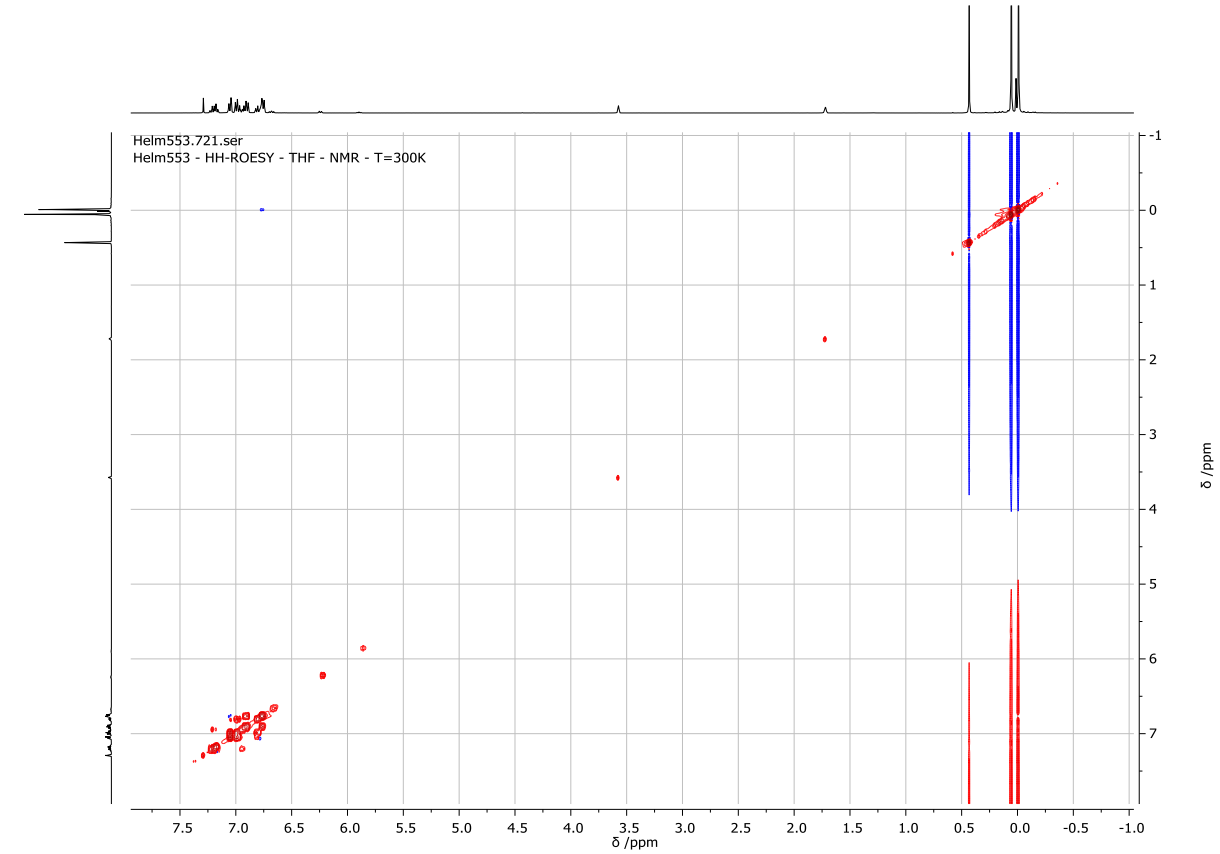


Figure S7. H,H-ROESY-NMR spectrum (THF-d_8, 300 K) of K[Si_6{$N(SiMe_3)Ph$}$_5$].

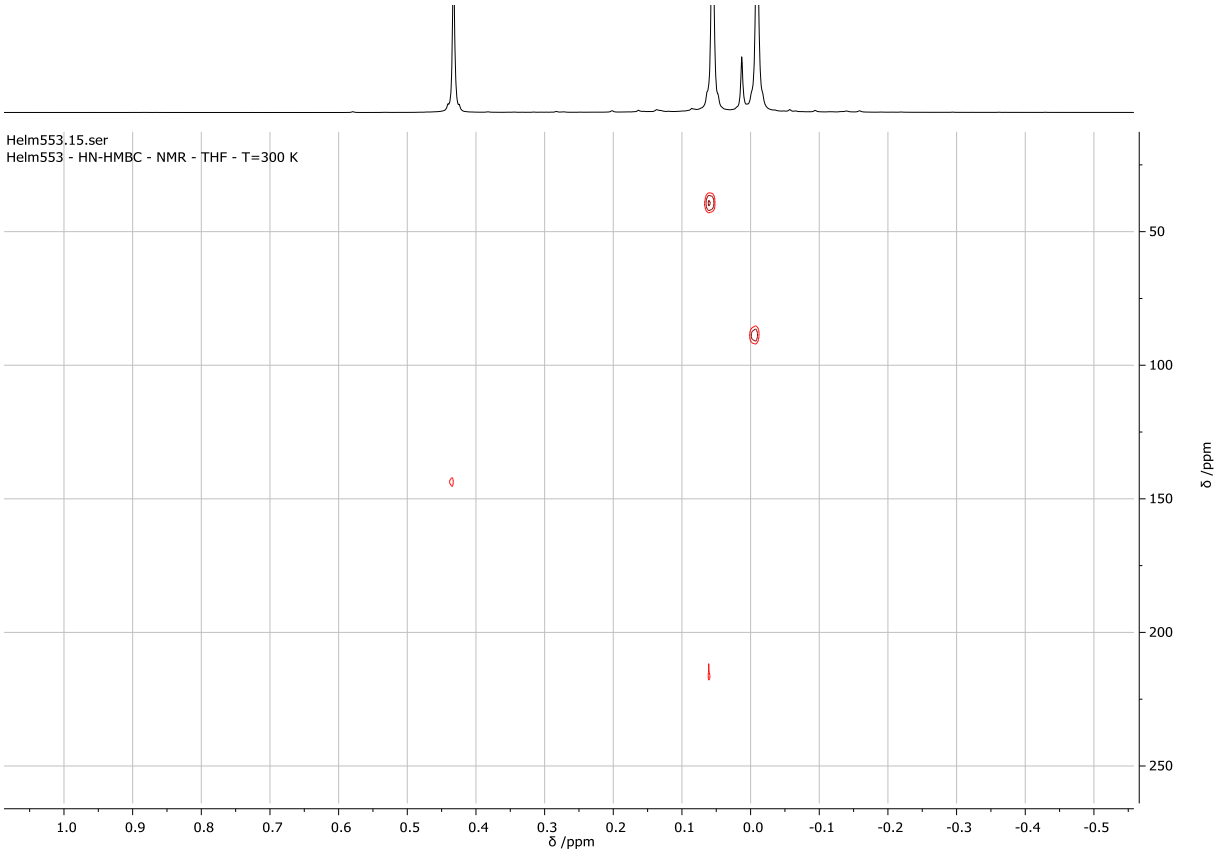


Figure S8. H,N-HMBC-NMR spectrum (THF-d_8, 300 K) of K[Si_6{$N(SiMe_3)Ph$}$_5$].

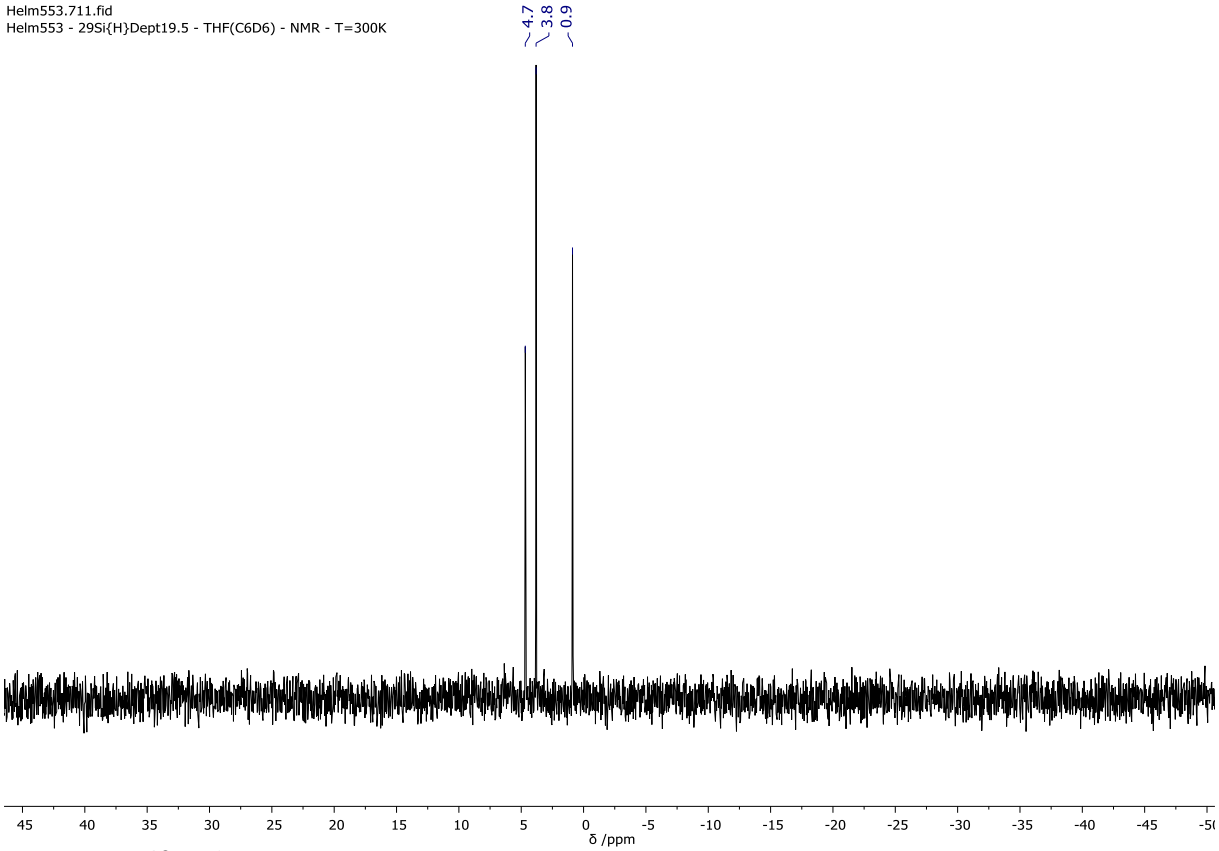


Figure S9. $^{29}Si\{^1H\}$DEPT19.5-NMR spectrum (THF-d_8, 300 K, 80 MHz) of K[Si_6{$N(SiMe_3)Ph$}$_5$].

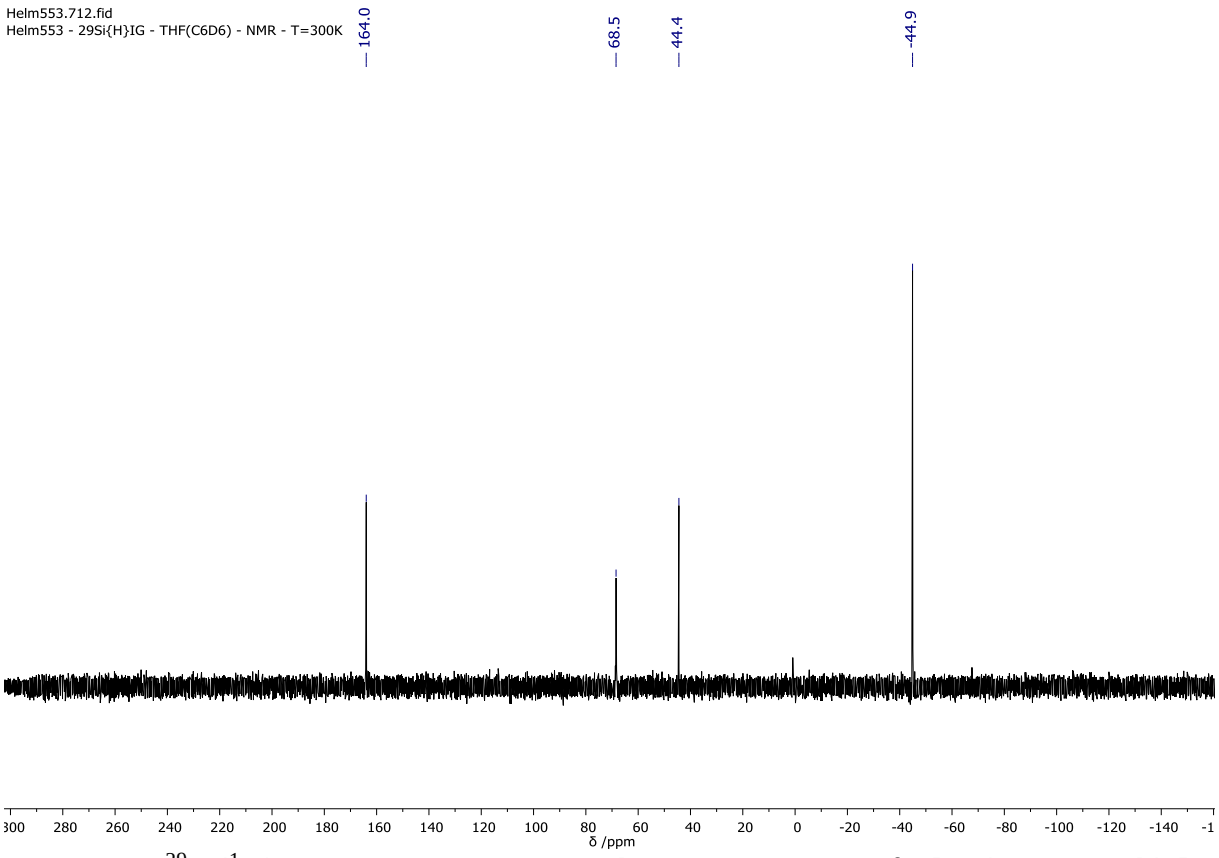


Figure S10. $^{29}Si\{^{1}H\}$IG-NMR spectrum (THF-d_8, 300 K, 80 MHz) of $K[Si_6\{N(SiMe_3)Ph\}_5]$.

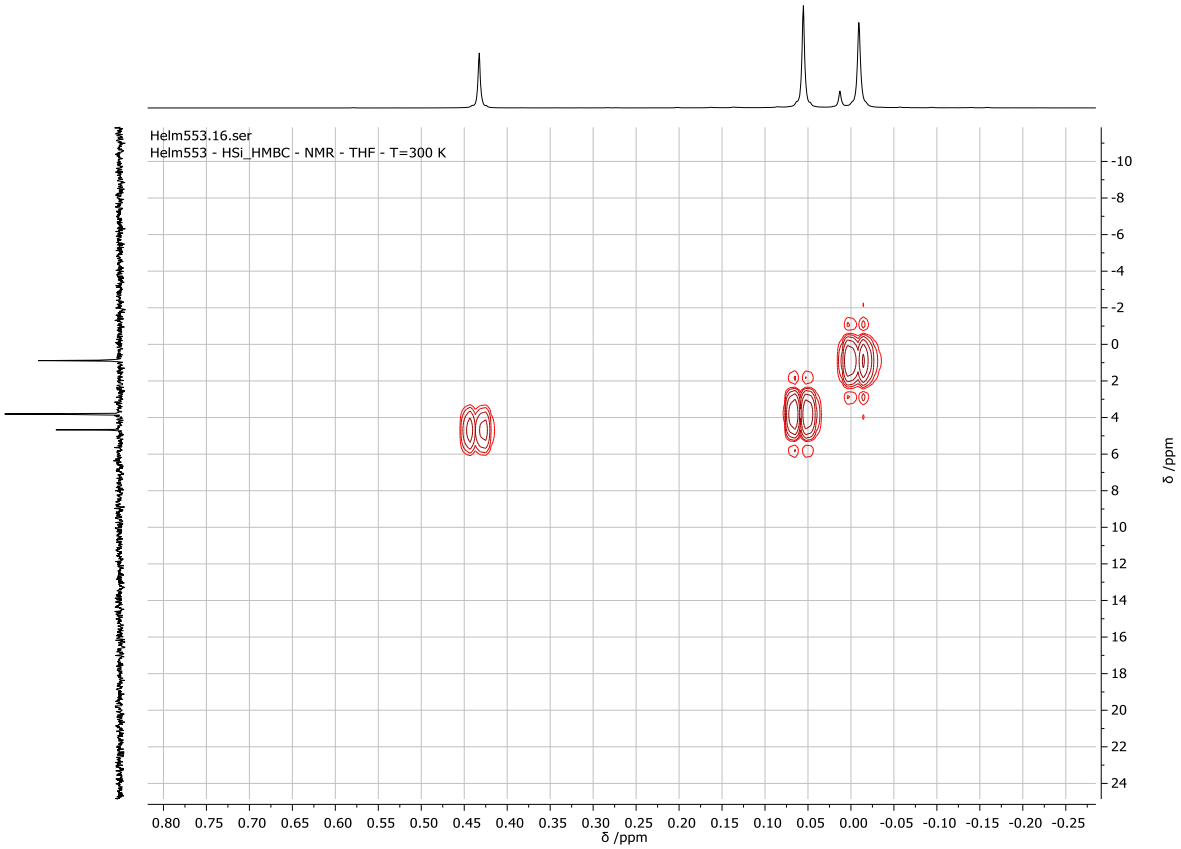


Figure S11. H,Si-HMBC-NMR spectrum (THF-d_8, 300 K) of $K[Si_6\{N(SiMe_3)Ph\}_5]$.

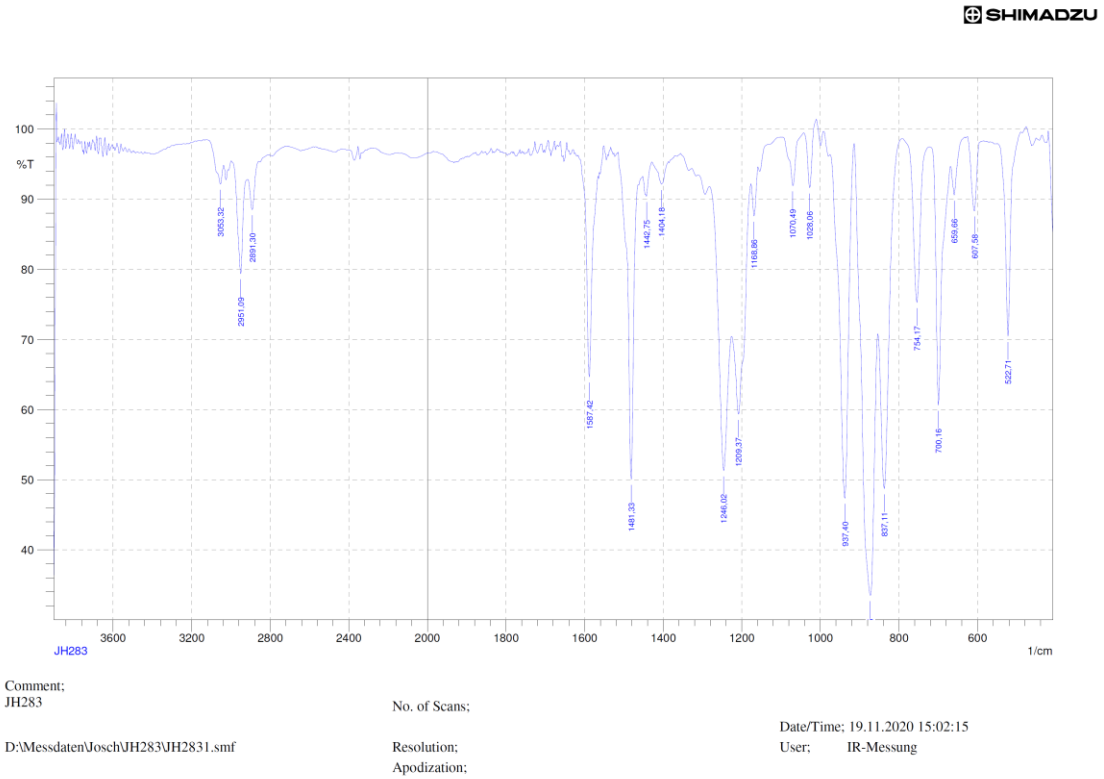


Figure S12. IR spectrum of K[Si_6{$N(SiMe_3)Ph$}$_5$].

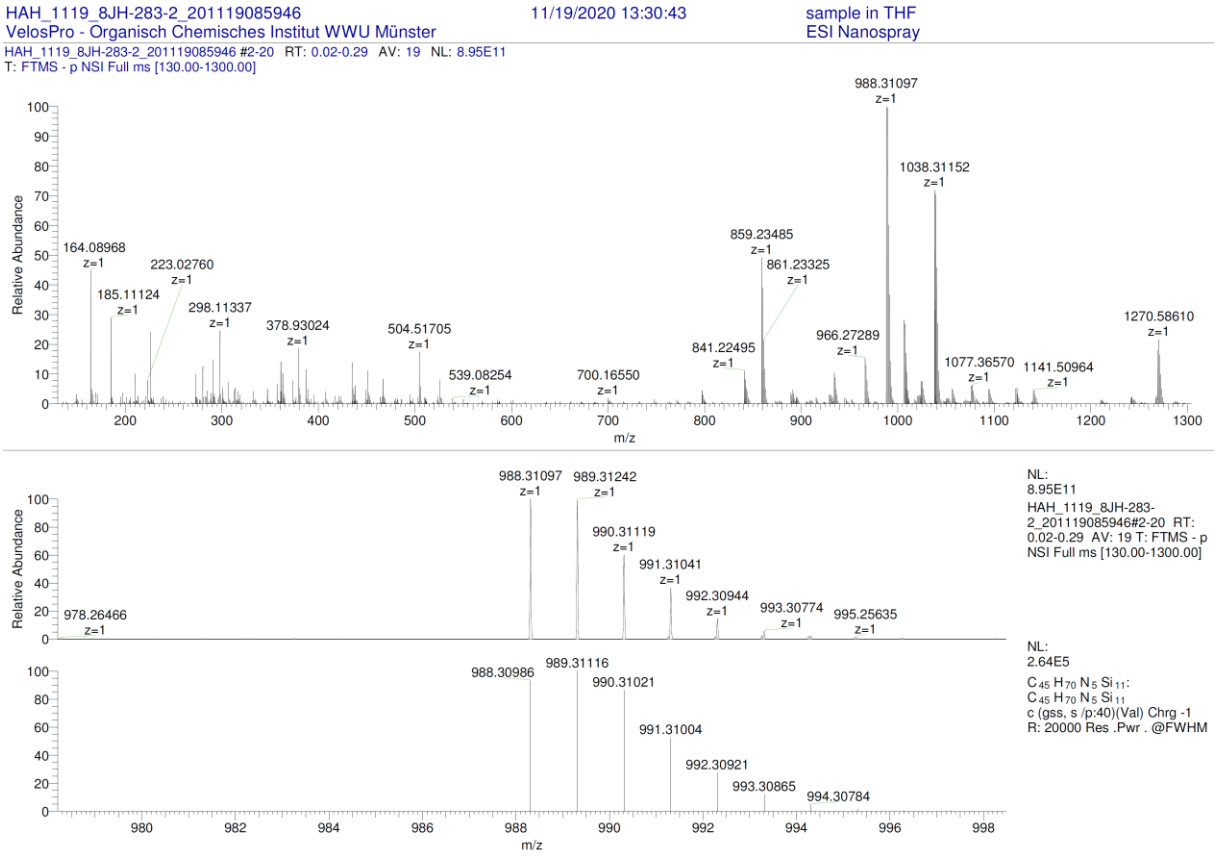


Figure S13. ESI-MS spectrum of K[Si_6{$N(SiMe_3)Ph$}$_5$].

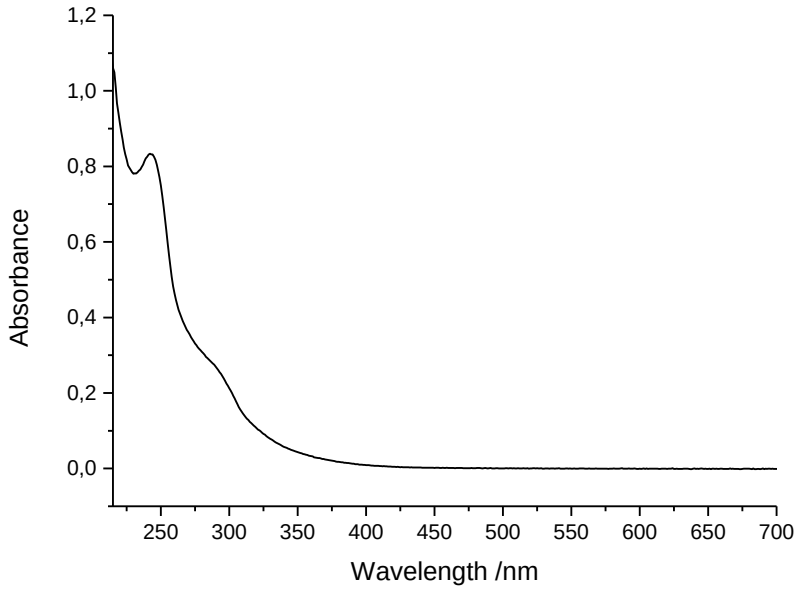
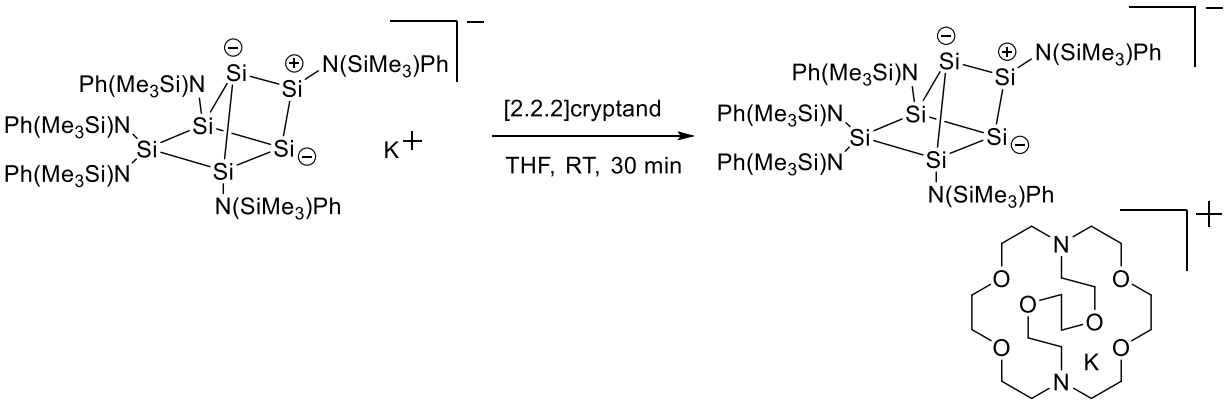


Figure S14. UV-Vis spectrum (THF, c = $3.03 \cdot 10^{-4}$ mol/L) of $K[Si_6\{N(SiMe_3)Ph\}_5]$.

2.2 Synthesis of [K[2.2.2]cryptand] [Si_6{$N(SiMe_3)Ph$}$_5$] (3)



K[Si_6{$N(SiMe_3)Ph$}$_5$] (0.141 g, 0.14 mmol, 1.0 equiv.) and [2.2.2]cryptand (0.052 g, 0.14 mmol, 1.0 equiv.) were dissolved in THF (3 mL) at room temperature. The reaction mixture was stirred for 30 min at room temperature. All volatile components were removed in vacuo, whereupon [K[2.2.2]cryptand][Si_6{$N(SiMe_3)Ph$}$_5$] was obtained as an orange powder in quantitative yield. Single crystals of [K[2.2.2]cryptand][Si_6{$N(SiMe_3)Ph$}$_5$] were obtained by storage of a saturated THF/*n*-hexane solution at −32 °C for 16 h.

^{1}H-NMR (THF-d_8, 300 K, 400 MHz): δ(ppm) = 7.22 - 7.15 (4H, m); 7.08 - 7.06 (4H, m); 7.00 - 6.96 (4H, m); 6.94 - 6.87 (5H, m); 6.81 - 6.77 (2H, m); 6.76 - 6.72 (4H, m); 0.43 (9H, s); 0.05 (18H, s); −0.02 (18H, s).

^{13}C-NMR (THF-d_8, 300 K, 100 MHz): δ(ppm) = 153.7; 150.0; 147.4; 132.7; 131.6; 131.2; 128.5; 128.3; 128.0; 123.0; 122.4; 121.9; 71.4; 68.5; 54.8; 4.0; 3.8; 3.3.

^{15}N,^{1}H-HMBC-NMR (THF-d_8, 300 K, 41 MHz): δ(ppm) = 144; 89; 40.

^{29}Si(DEPT 19.5)-NMR (THF-d_8, 300 K, 80 MHz): δ(ppm) = 4.3; 3.5; 0.7.

^{29}Si{^{1}H}IG-NMR (THF-d_8, 300 K, 80 MHz): δ(ppm) = 164.3; 70.2; 44.3; −45.0.

IR (KBr pellet, $\tilde{\nu}$/cm^{-1} (intensity)) = 463(vw), 521(w), 569(vw), 608(vw), 660(vw), 694(w), 752(m), 841(s), 866(s), 930(m), 949(m), 997(vw), 1076(vs), 1103(vs), 1130(m), 1204(w), 1250(m), 1296(m), 1356(m), 1447(w), 1481(m), 1497(m), 1560(w), 1591(m), 1601(m), 2816(w), 2886(m), 2957(m), 3046(vw), 3381(vw).

UV-Vis: (THF, c =1.42·10^{-5} mol/L, ε/L·mol^{-1}·cm^{-1}): λ = 245 nm (38932), 294 nm (13528),

Melting point: Decomposition at 200 °C.

Elemental Analysis for $C_{63}H_{106}KN_7O_6Si_{11}$:	H	C	N
calculated:	7.40	52.38	6.79
found:	7.57	52.41	6.43

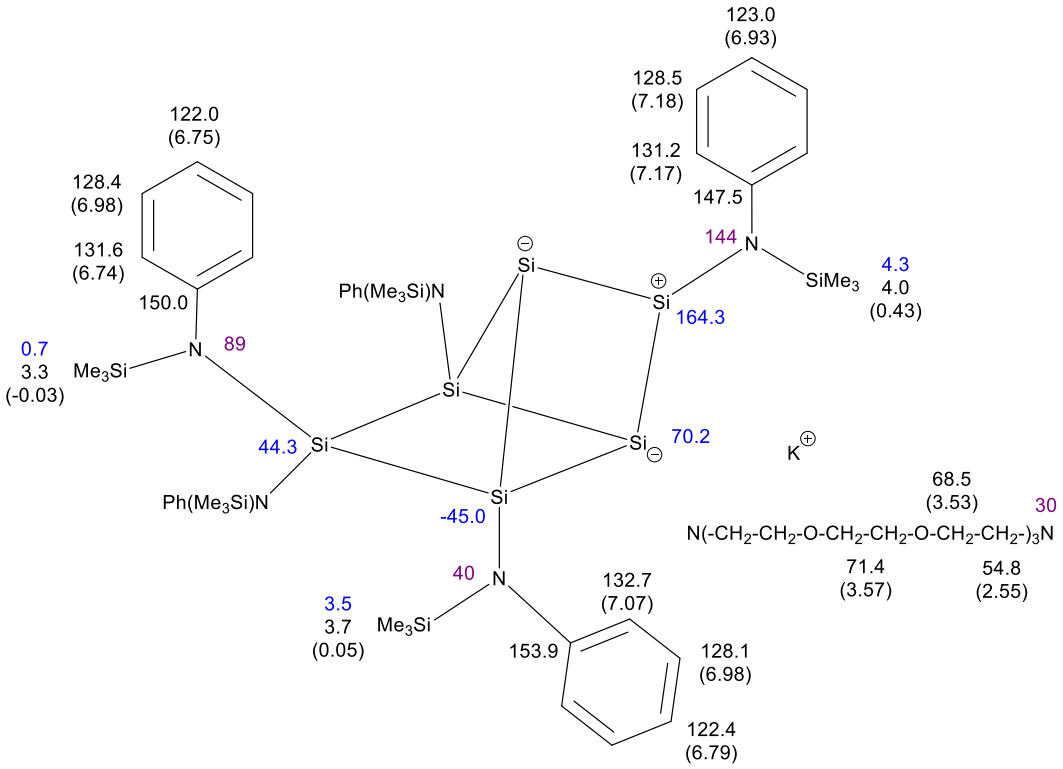


Figure S15. Assignment of chemical shifts to [K[2.2.2]cryptand][Si_6{$N(SiMe_3)Ph$}$_5$], ^{1}H (in brackets), ^{13}C (black), ^{15}N (violet), ^{29}Si (blue).

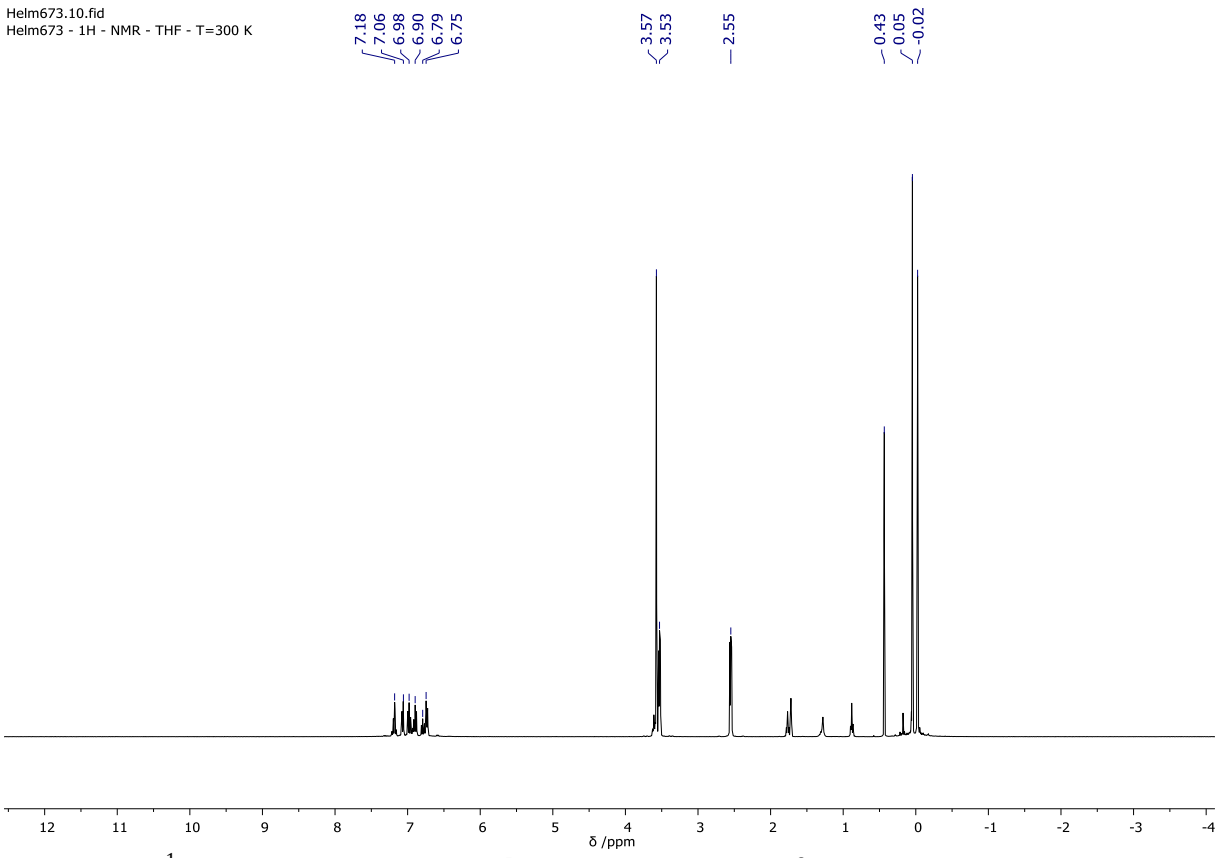


Figure S16. ^{1}H-NMR spectrum (THF-d_8, 300 K, 400 MHz) of **3**.

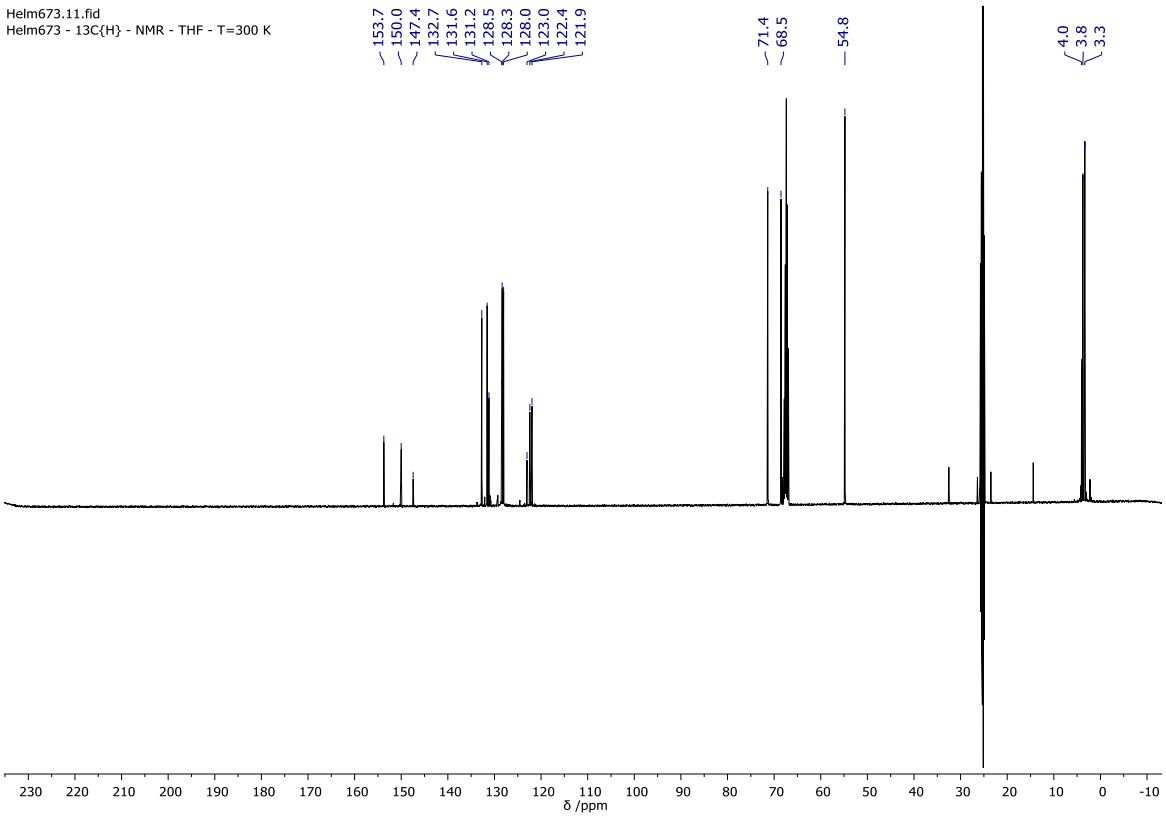


Figure S17. ^{13}C{^{1}H}-NMR spectrum (THF-d_8, 300 K, 100 MHz) of **3**.

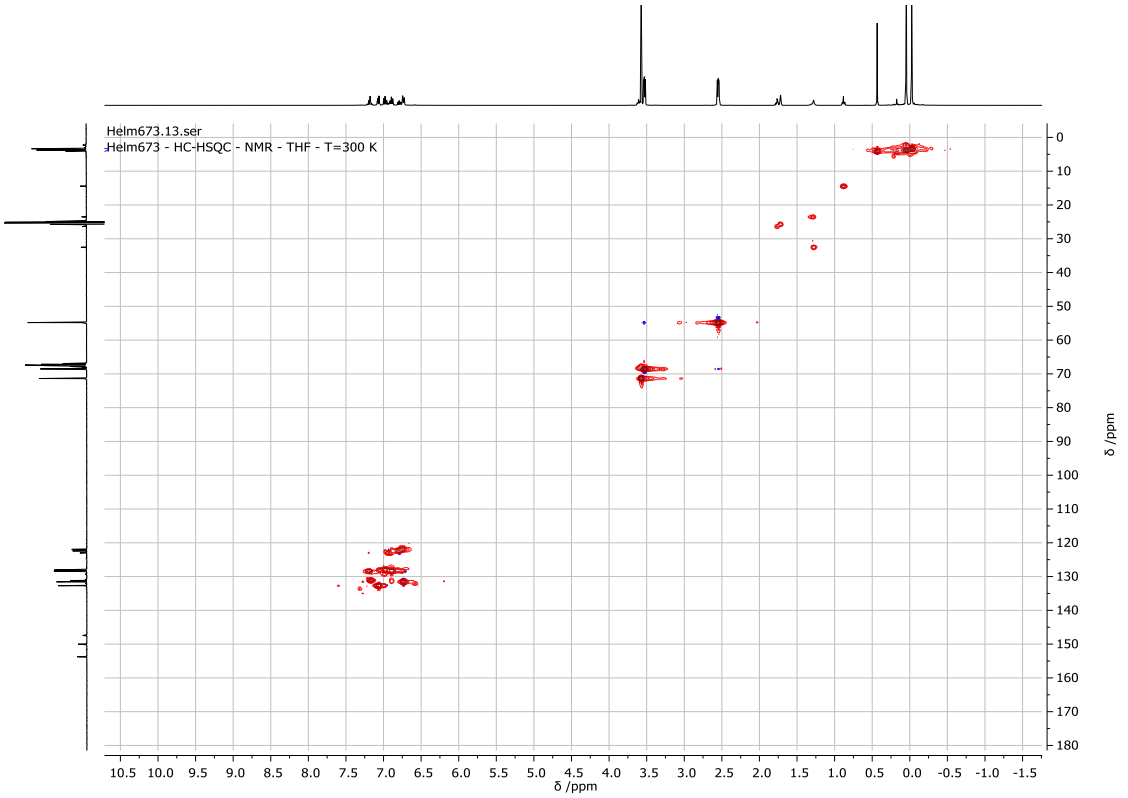


Figure S18. H,C-HSQC-NMR spectrum (THF-d_8, 300 K) of **3**.

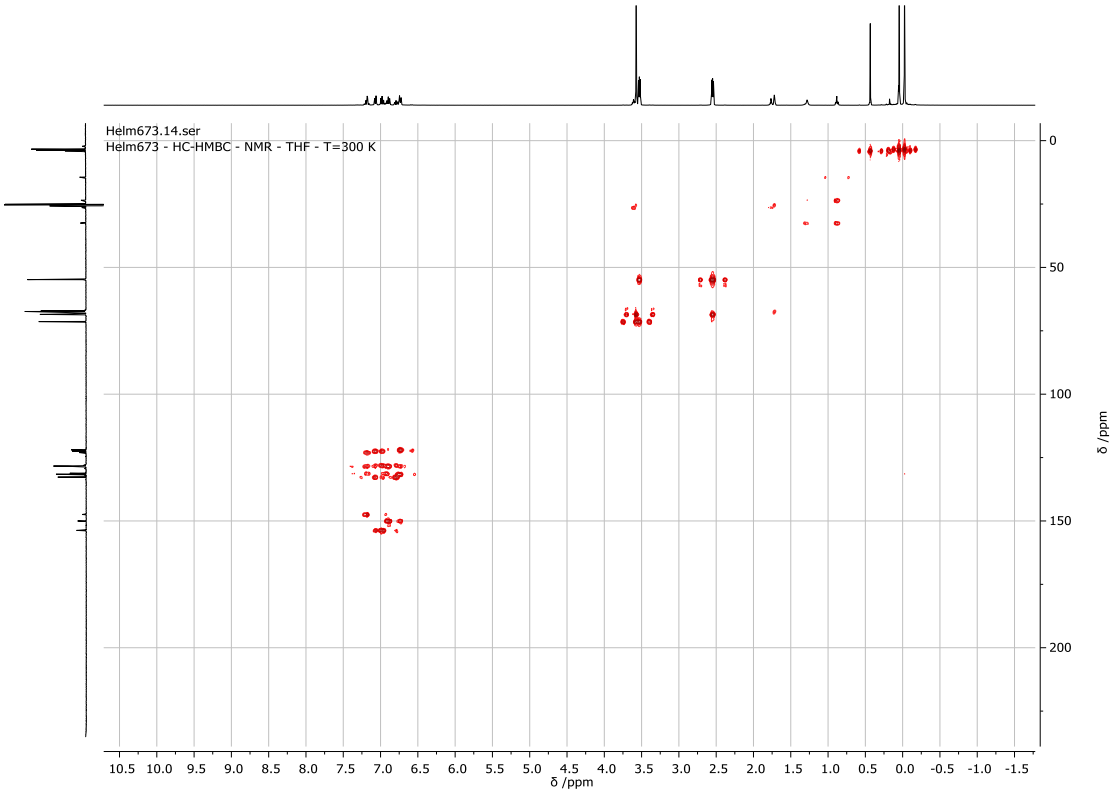


Figure S19. H,C-HMBC-NMR spectrum (THF-d_8, 300 K) of **3**.

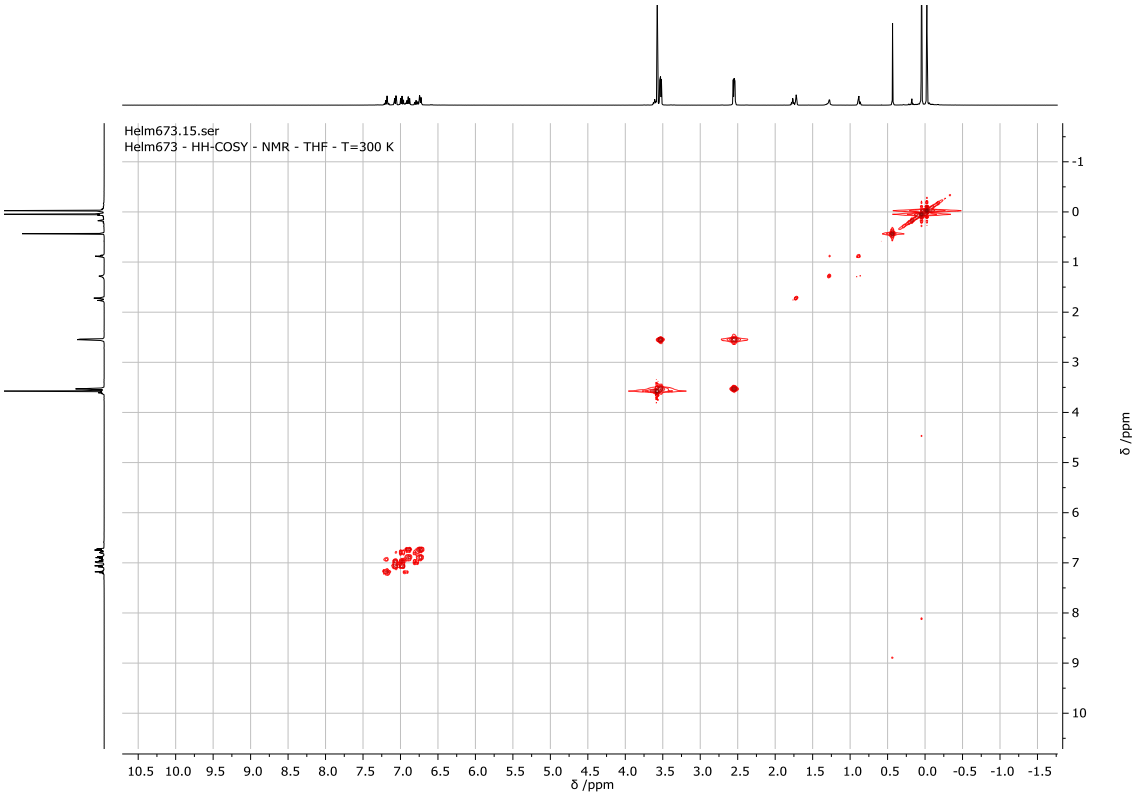


Figure S20. H,H-COSY-NMR spectrum (THF-d_8, 300 K) of **3**.

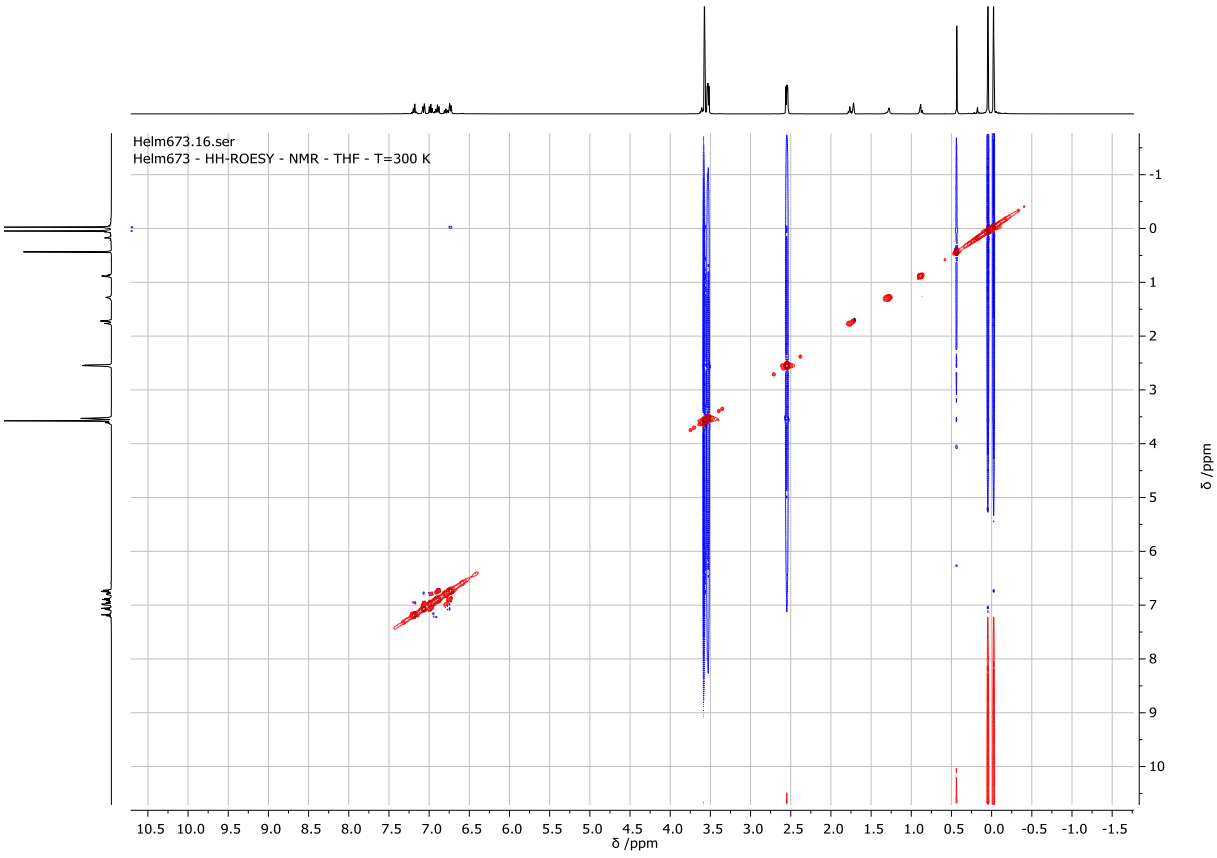


Figure S21. H,H-ROESY-NMR spectrum (THF-d_8, 300 K) of **3**.

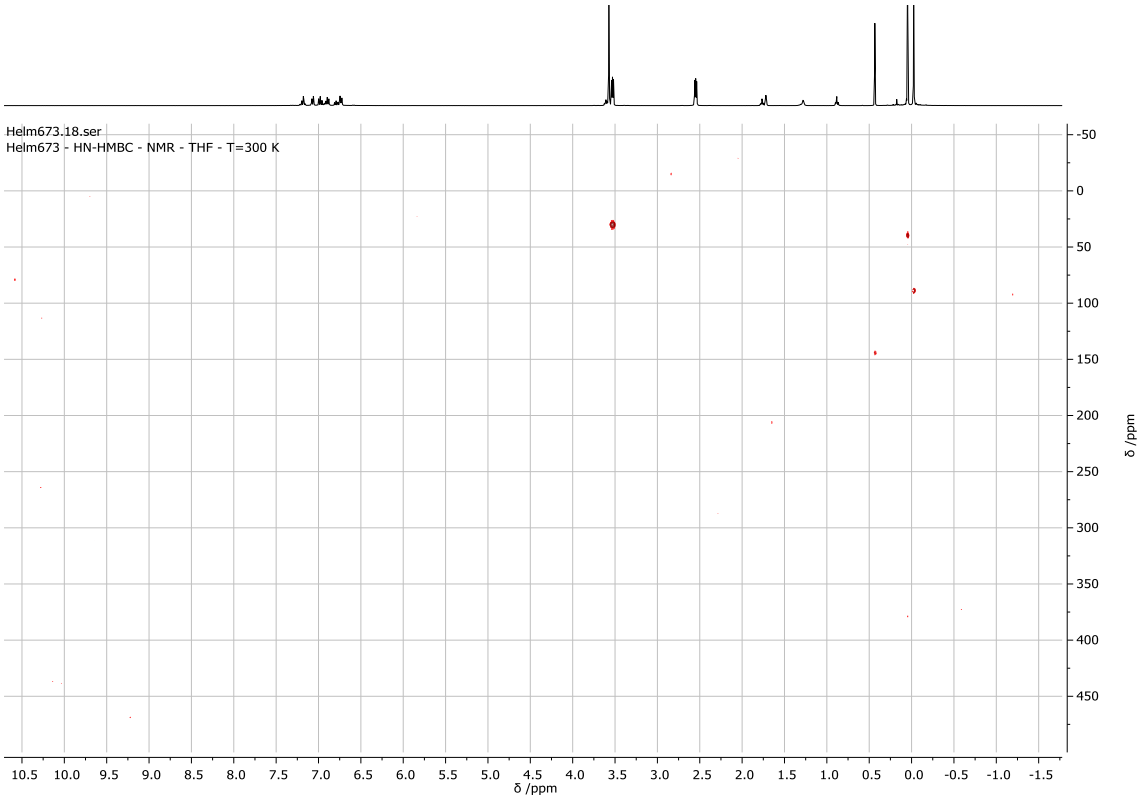


Figure S22. H,N-HMBC-NMR spectrum (THF-d_8, 300 K) of **3**.

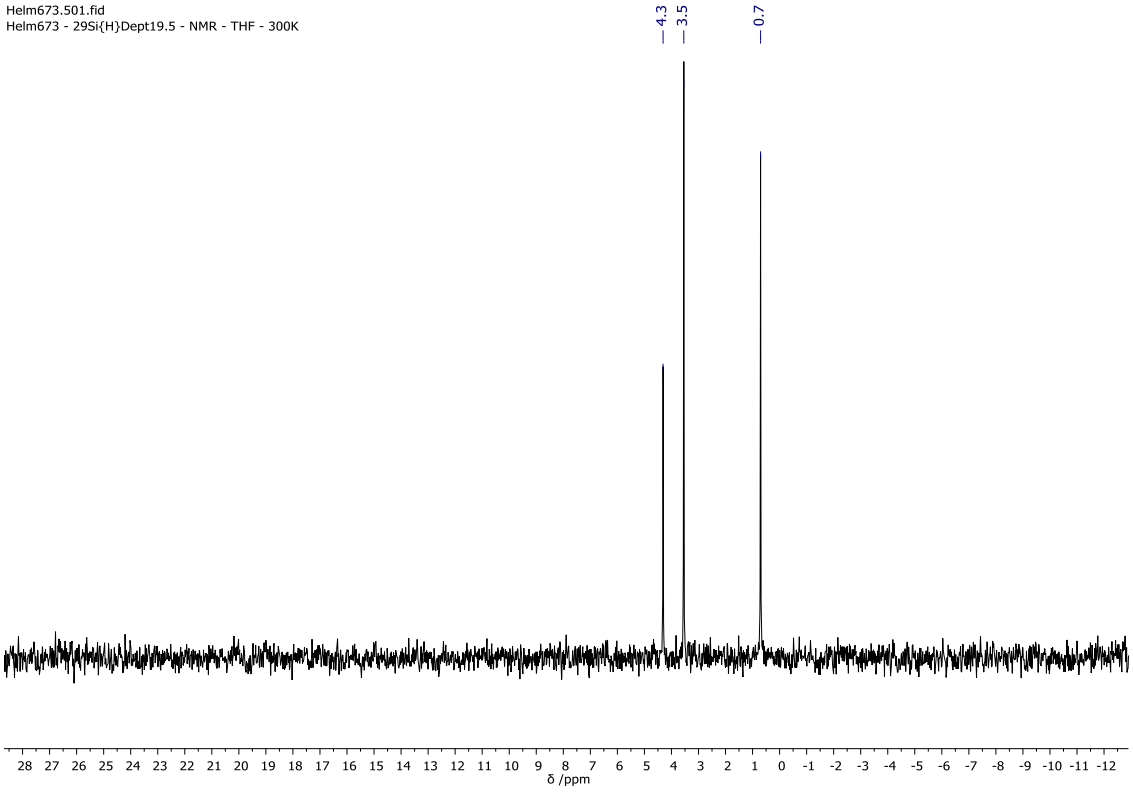


Figure S23. $^{29}Si\{^1H\}$DEPT19.5-NMR spectrum (THF-d_8, 300 K, 80 MHz) of **3**.

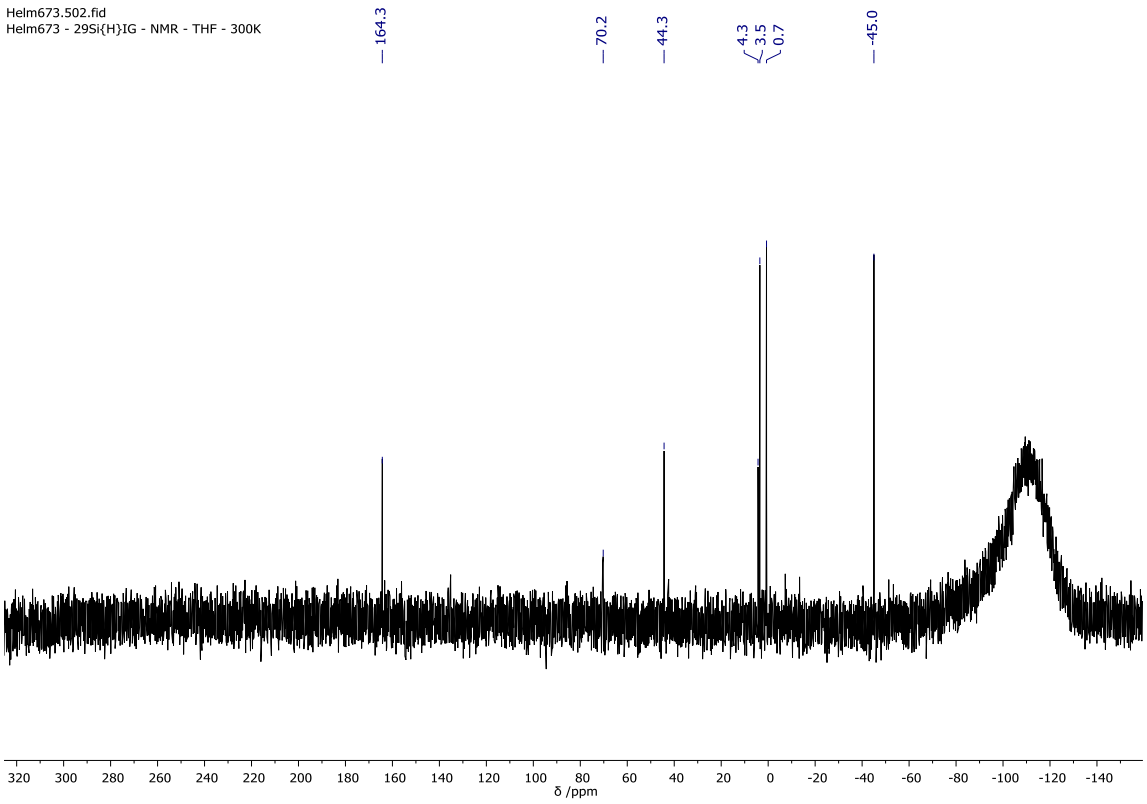


Figure S24. $^{29}Si\{^{1}H\}$IG-NMR spectrum (THF-d_8, 300 K, 80 MHz) of **3**.

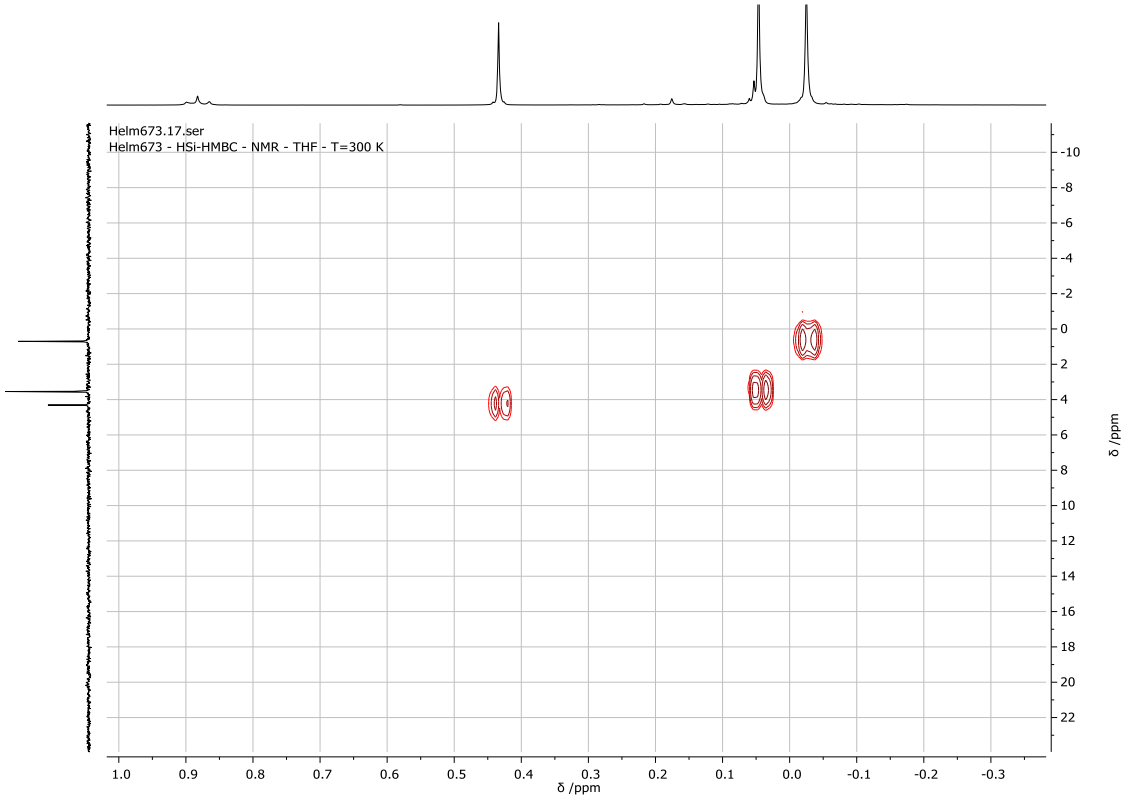


Figure S25. H,Si-HMBC-NMR spectrum (THF-d_8, 300 K, 80 MHz) of **3**.

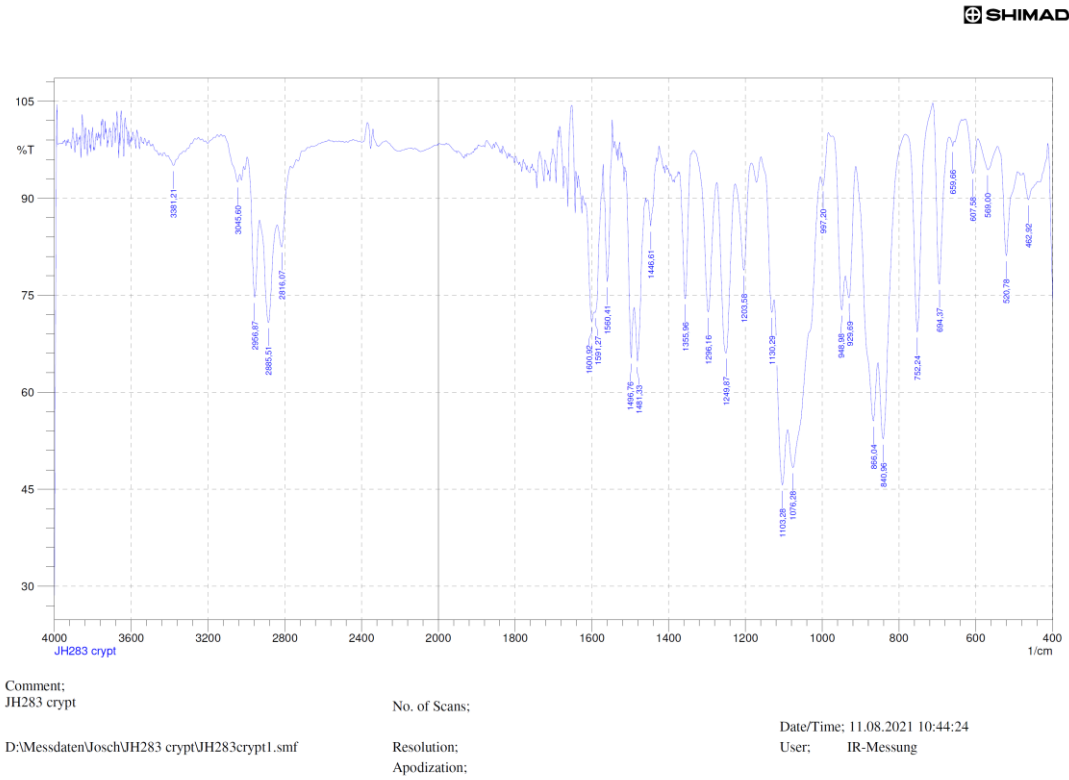


Figure S26. IR spectrum of **3**.

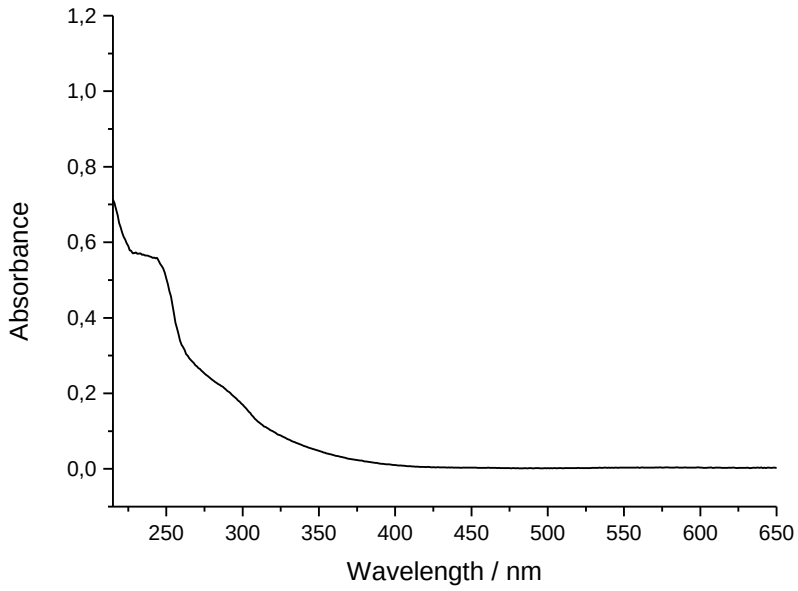


Figure S27. UV-Vis spectrum (THF, c = $1.42 \cdot 10^{-5}$ mol/L) of **3**.

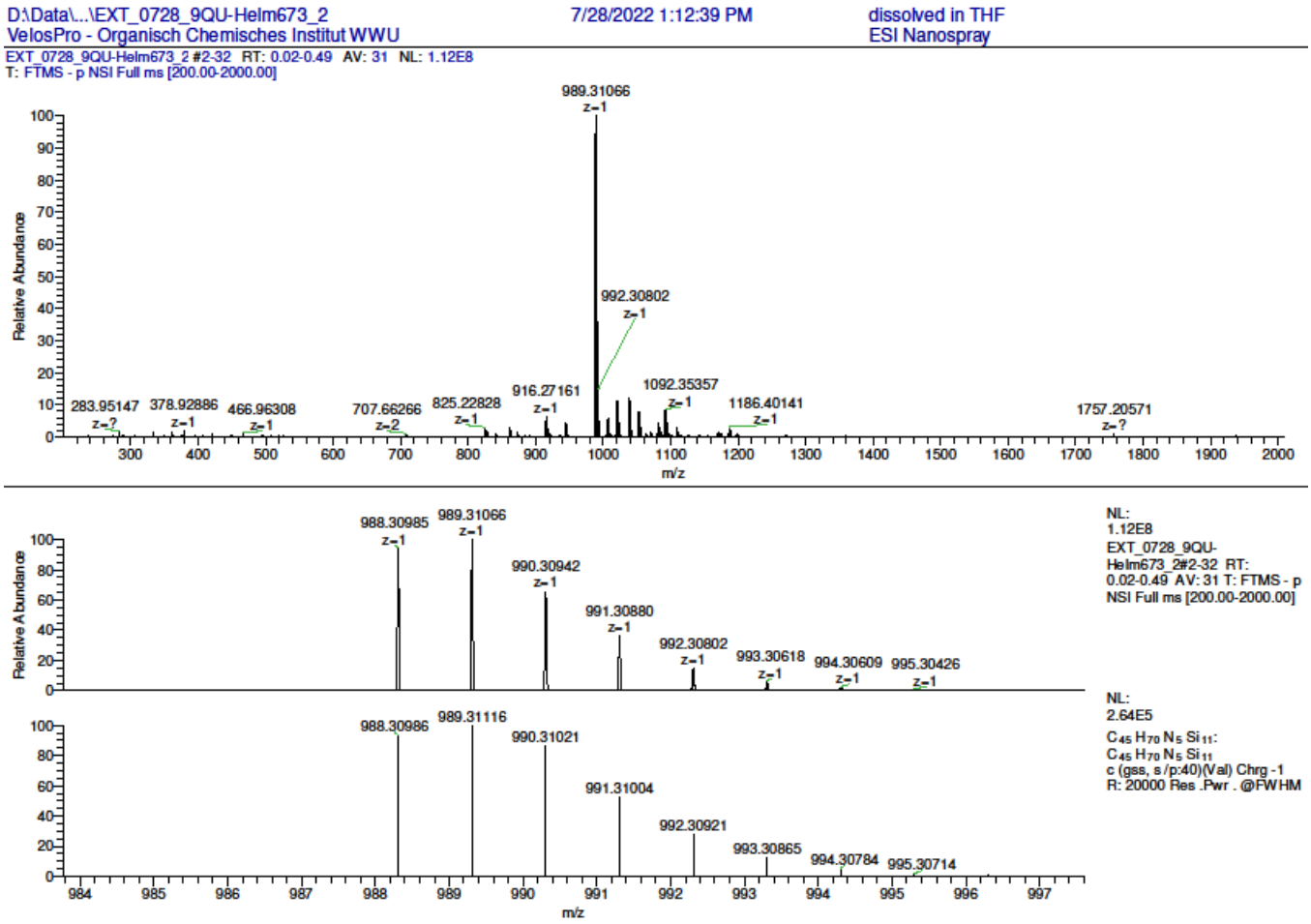
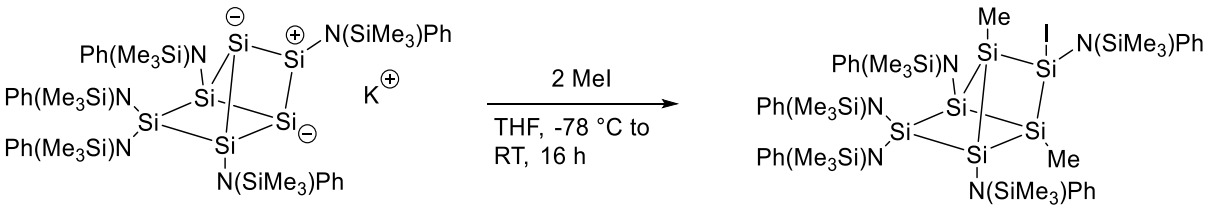


Figure S28. ESI-MS spectrum of **3**.

2.3 Synthesis of $[Si_6\{N(SiMe_3)Ph\}_6Me_2I]$ (4)



$K[Si_6\{N(SiMe_3)Ph\}_5]$ (0.092 g, 0.09 mmol, 1.0 equiv.) was dissolved in THF (10 mL) and MeI (0.1 M in *n*-hexane, 1.8 mL, 0.18 mmol, 2.0 equiv.) was added at −78 °C. The reaction mixture was allowed to warm to room temperature and was stirred for 16 h. Volatile components were removed in vacuo and the orange residue was extracted with benzene (2 mL). Storage of the benzene solution at room temperature resulted in $[Si_6\{N(SiMe_3)Ph\}_5Me_2I]$ (**4**) (0.037 g, 0.03 mmol, 36 %) as pale yellow crystals.

^{1}H-NMR (C_6D_6, 300 K, 400 MHz): δ(ppm) = 7.52 - 7.50 (2H, m); 7.42 - 7.40 (2H, m); 7.13 - 7.11 (6H, m); 7.09 - 7.08 (2H, m); 6.98 - 6.91 (7H, m); 6.89 - 6.82 (4H, br.); 6.80 - 6.76 (2H, m); 0.40 (9H, s); 0.23 (18H, br.); 0.22 (3H, s); 0.21 (9H, s); 0.05 (9H, s); −0.04 (6H, br.).

^{13}C-NMR (C_6D_6, 300K, 100 MHz): δ(ppm) = 151.0; 150.5; 148.4; 148.3; 131.8; 130.8; 129.7; 129.7; 129.4; 129.3; 129.3; 129.2; 129.2; 129.2; 124.8; 124.7; 124.3; 123.5; 123.5; 3.6; 3.3; 2.6; 1.4; 1.4; −6.8.

^{15}N,^{1}H-HMBC-NMR (C_6D_6, 300 K, 41 MHz): δ(ppm) = 81; 27; 27.

^{29}Si(DEPT 19.5)-NMR (C_6D_6, 300 K, 80 MHz): δ(ppm) = 9.5; 8.3; 7.4.

^{29}Si{^{1}H}IG-NMR (C_6D_6, 300 K, 80 MHz): δ(ppm) = 21.8; 9.5; 8.3; 7.4; 5.3; −7.4; −28.3; −49.9; −77.6.

IR (KBr pellet, $\tilde{\nu}$/cm^{-1} (intensity)) = 424(vw), 455(w), 471(w), 488(w), 521(s), 610(w), 677(m), 700(vs), 720(vw), 752(m), 787(vw), 837(vs), 889(vs), 918(s), 955(vs), 1028(w), 1074(w), 1169(w), 1206(vs), 1227(s), 1250(vs), 1404(w), 1447(w), 1481(vs), 1589(s), 1942(vw), 2897(w), 2953(m), 3026(w), 3051(w).

ESI-MS: m/z = 1168.43 $[Si_6\{N(SiMe_3)Ph\}_5Me]^+$, 1186.44 $[Si_6\{N(SiMe_3)Ph\}_6Me+H_3O]^+$.

UV-Vis: (*n*-hexane, c = 5.02·10^{-5} mol/L, ε/L·mol^{-1}·cm^{-1}): λ = 295 nm (12059); 372 (480).

Melting point: 245 °C.

Elemental Analysis for $C_{47}H_{76}IN_5Si_{11}$ + Benzene:	H	C	N
calculated:	6.75	51.96	5.72
found:	6.37	47.98	5.50

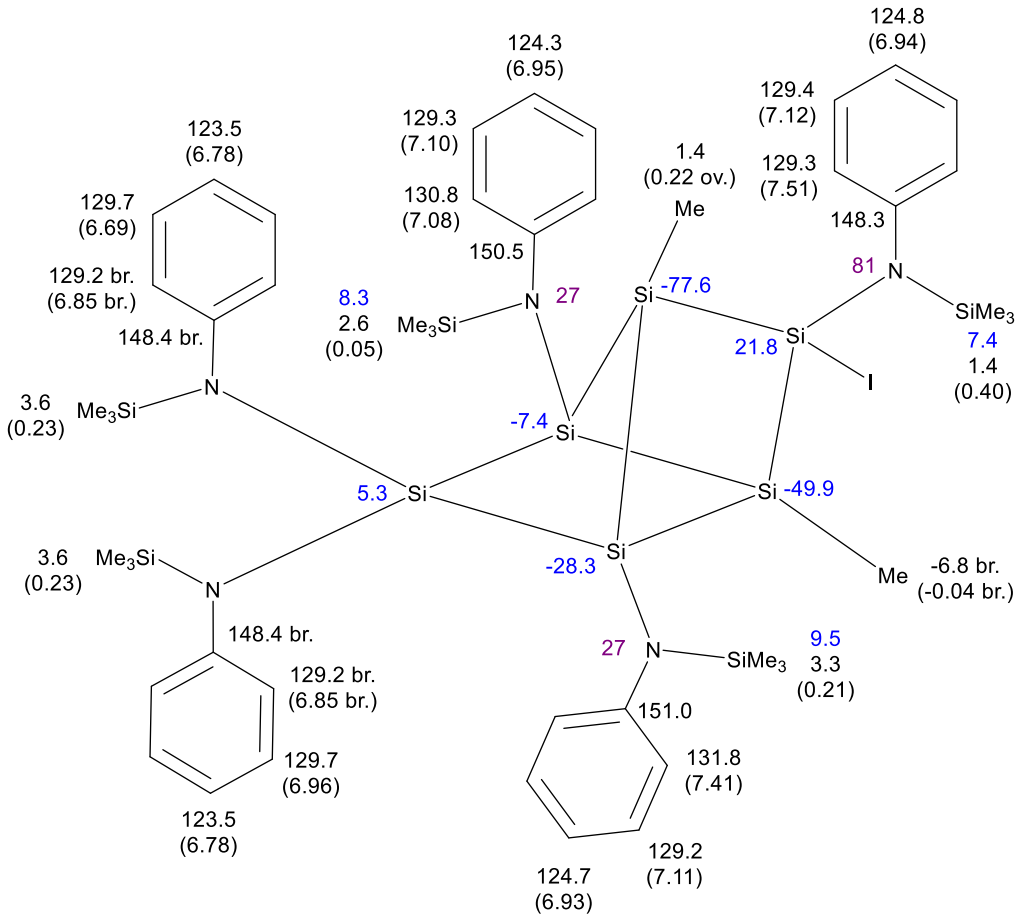


Figure S29. Assignment of chemical shifts to **4**, ^{1}H (in brackets), ^{13}C (black), ^{15}N (violet), ^{29}Si (blue).

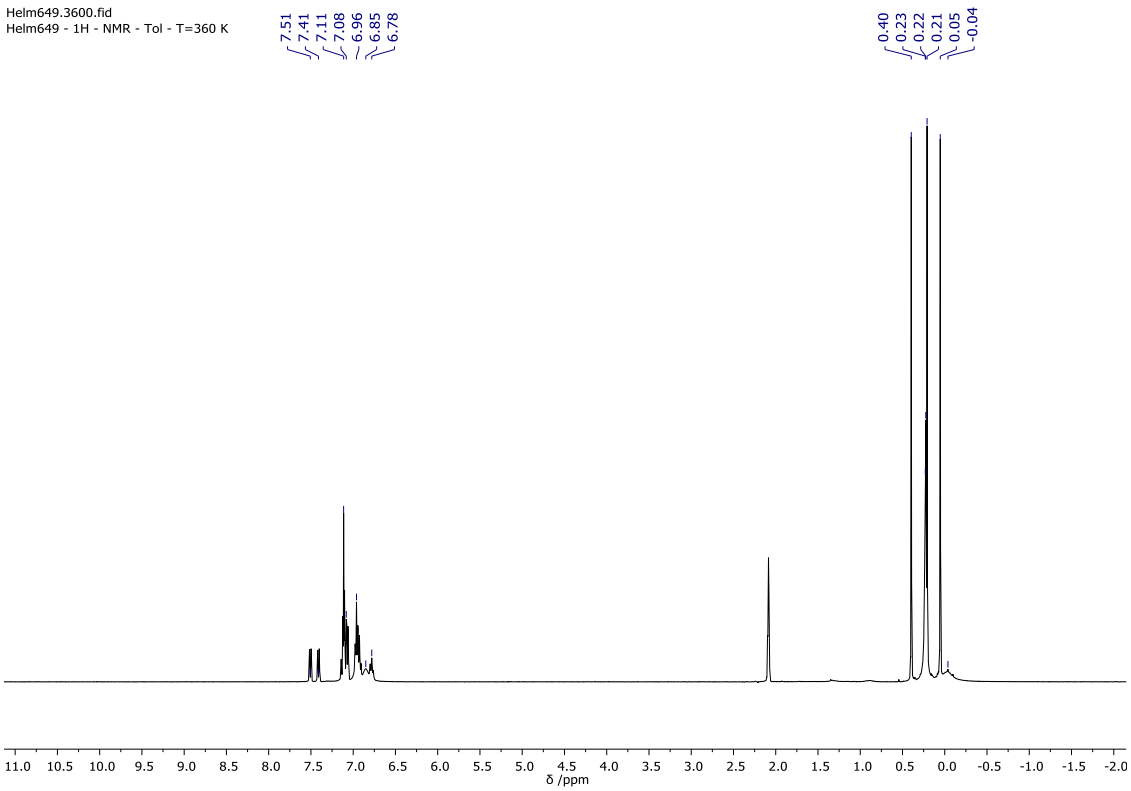


Figure S30. ^{1}H-NMR spectrum (toluene-d_8, 360 K, 400 MHz) of **4**.

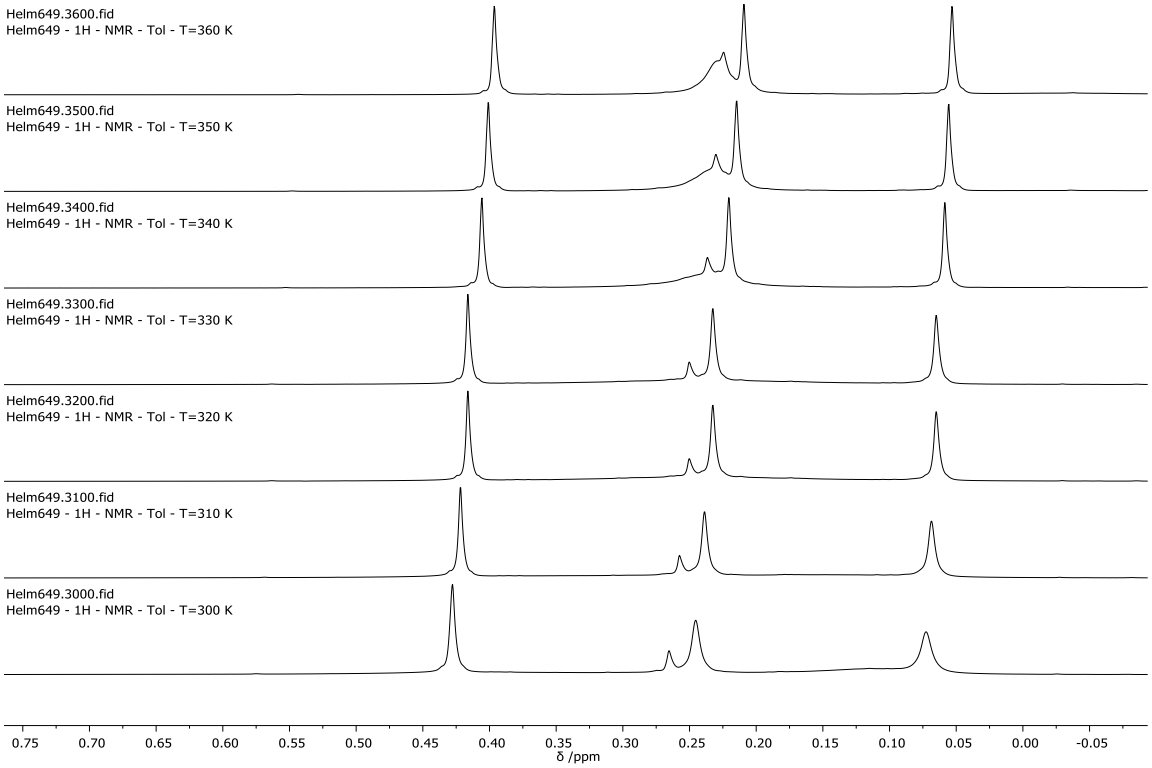


Figure S31. Temperature-dependent ^{1}H-NMR spectra (toluene-d_8, 400 MHz) of **4**.

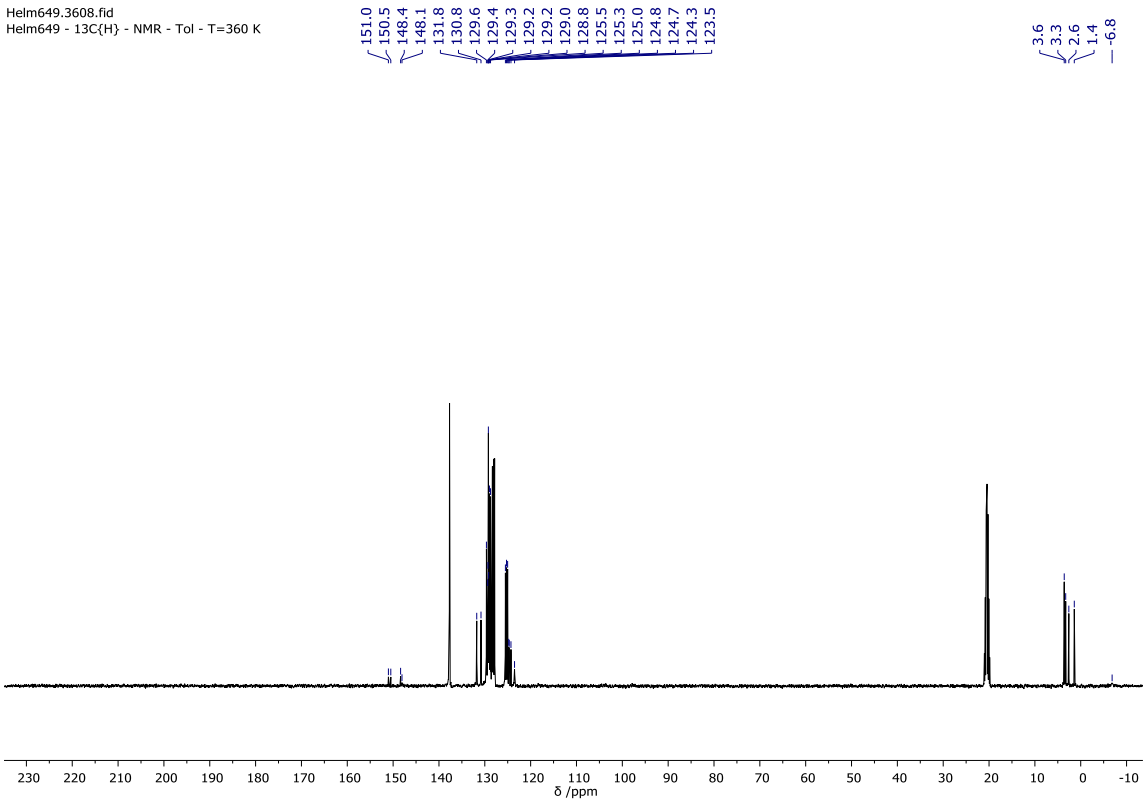


Figure S32. $^{13}C\{^{1}H\}$-NMR spectrum (toluene-d_8, 360 K, 400 MHz) of **4**.

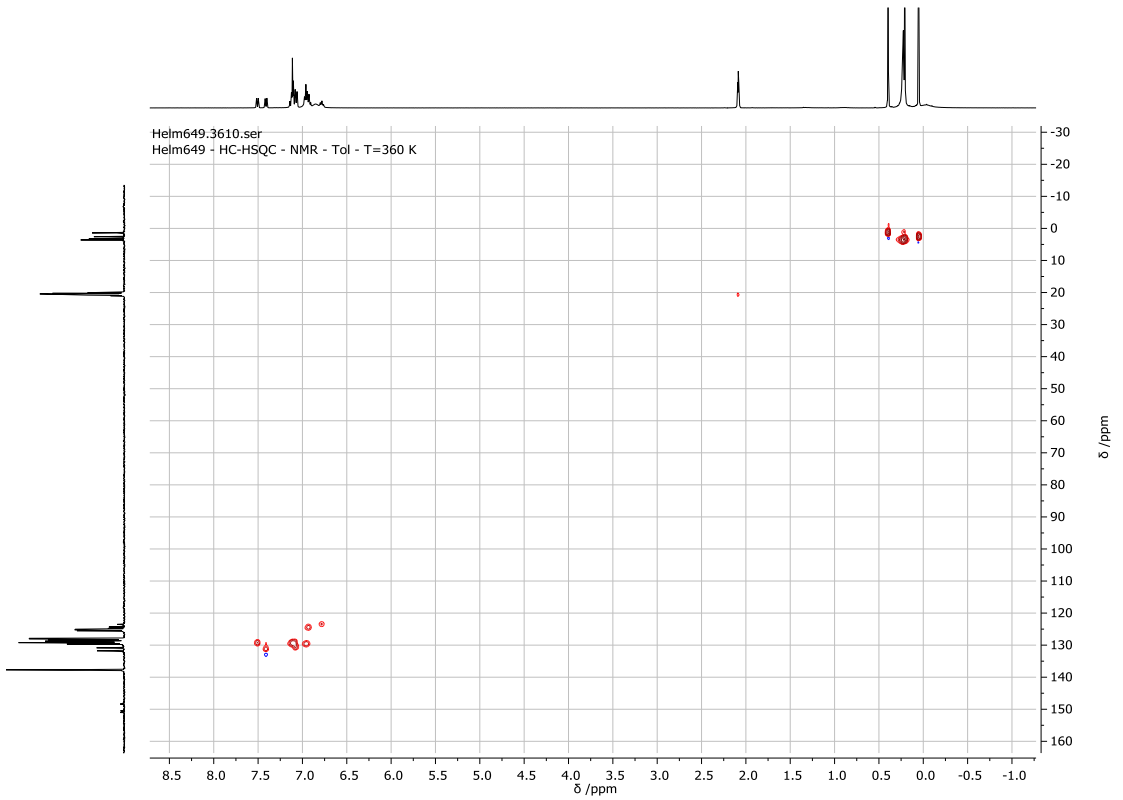


Figure S33. H,C-HSQC-NMR spectrum (toluene-d_8, 360 K, 400 MHz) of **4**.

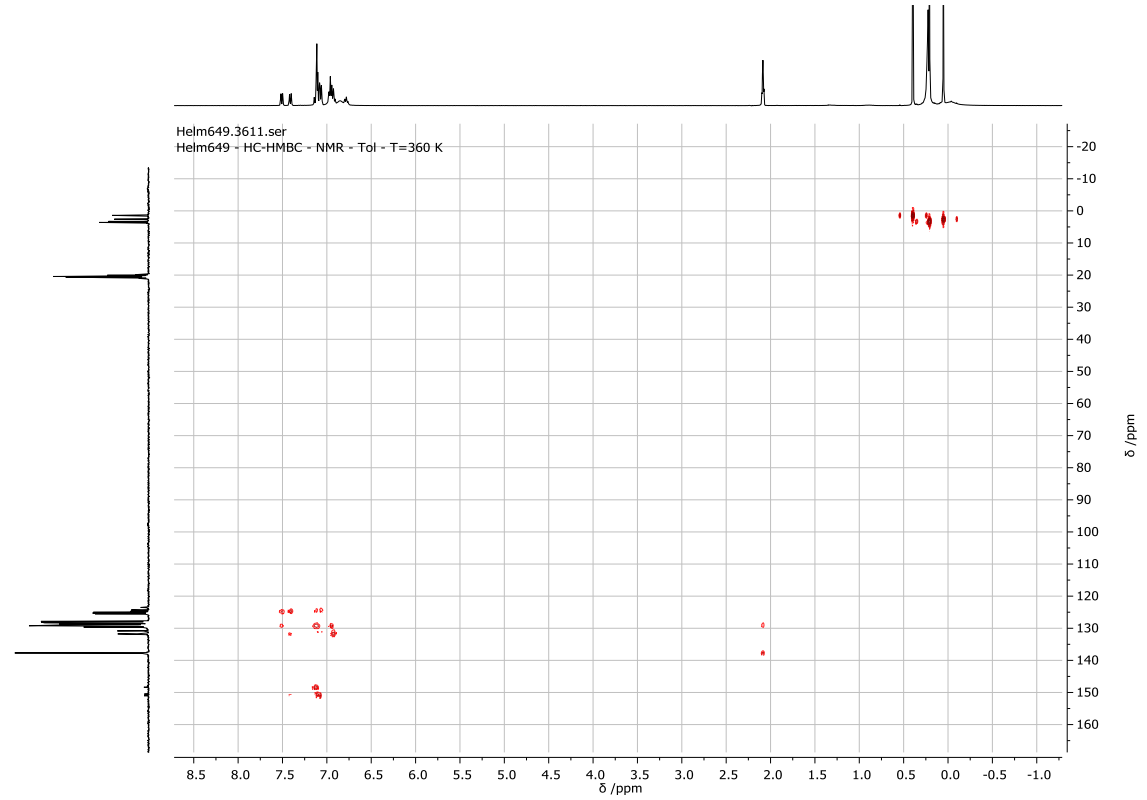


Figure S34. H,C-HMBC-NMR spectrum (toluene-d_8, 360 K, 400 MHz) of **4**.

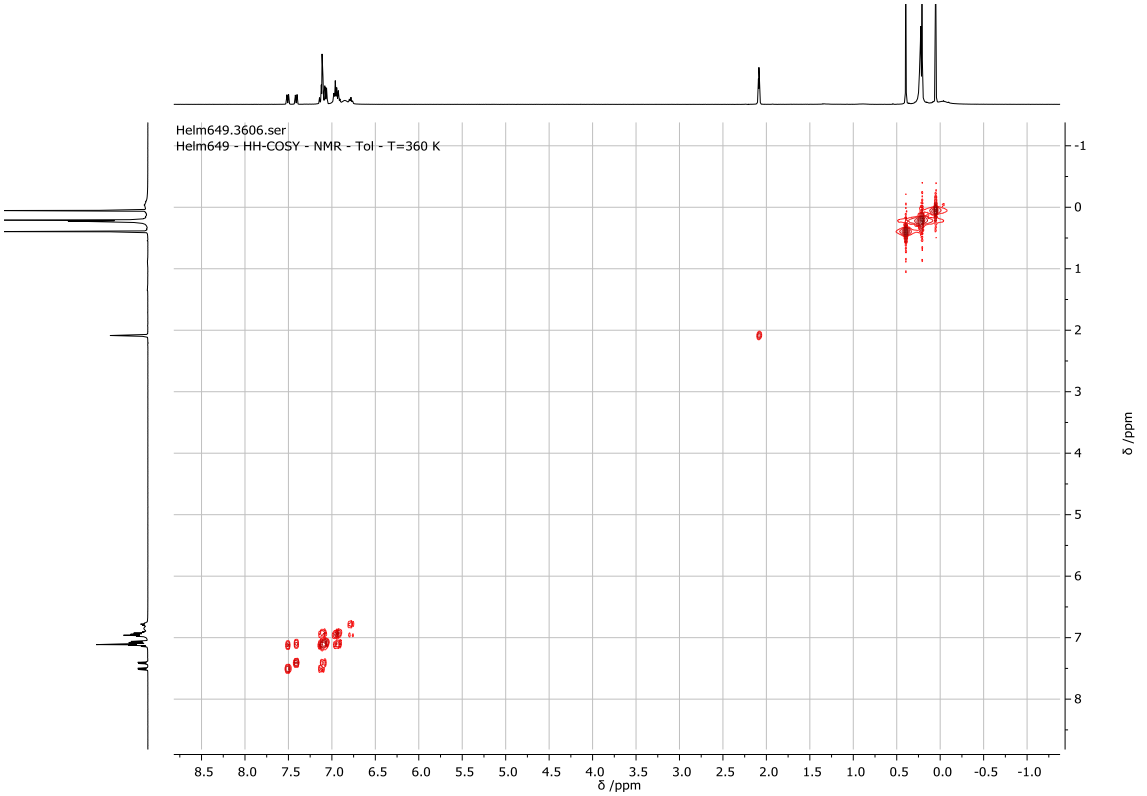


Figure S35. H,H-COSY-NMR spectrum (toluene-d_8, 360 K, 400 MHz) of **4**.

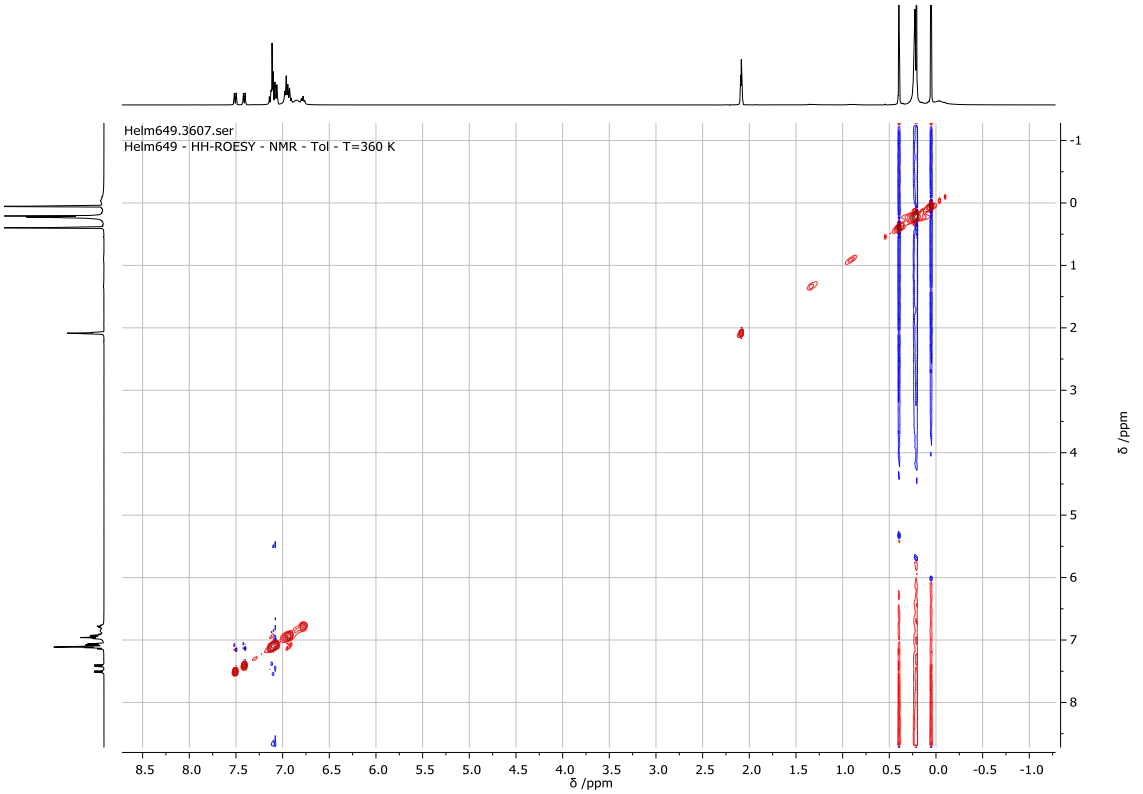


Figure S36. H,H-ROESY-NMR spectrum (toluene-d_8, 360 K, 400 MHz) of **4**.

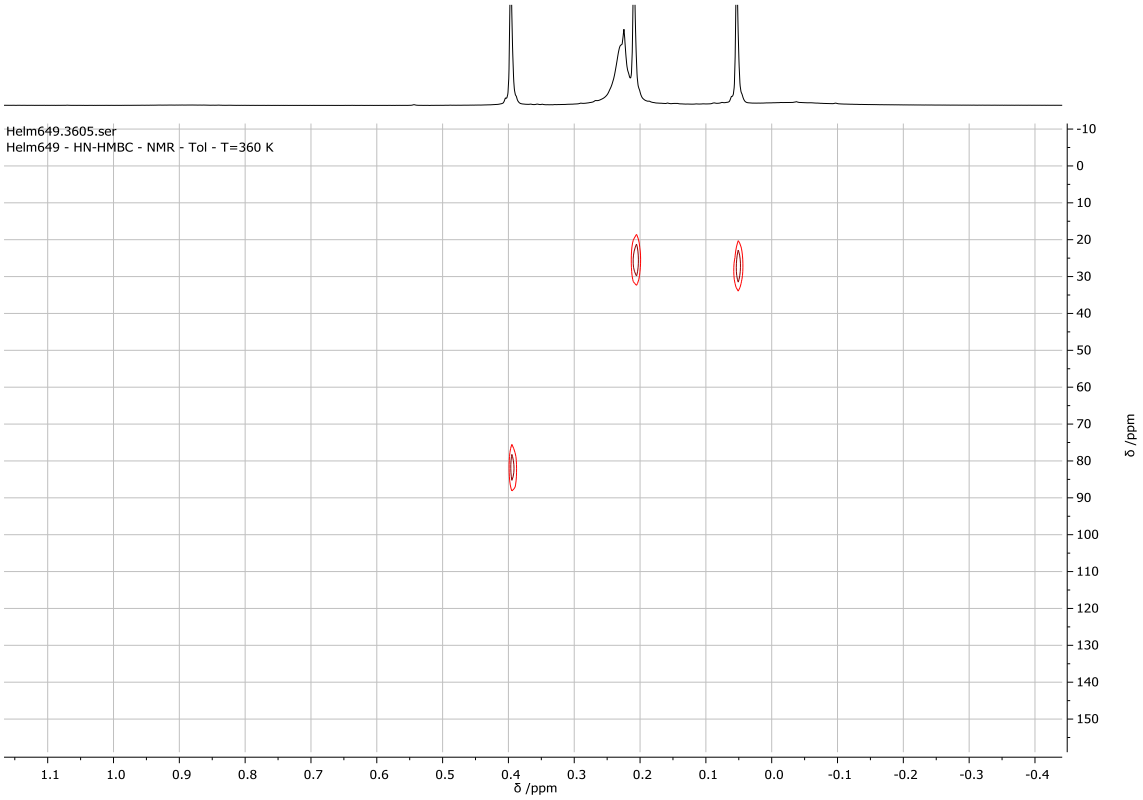


Figure S37. H,N-HSQC-NMR spectrum (toluene-d_8, 360 K, 400 MHz) of **4**.

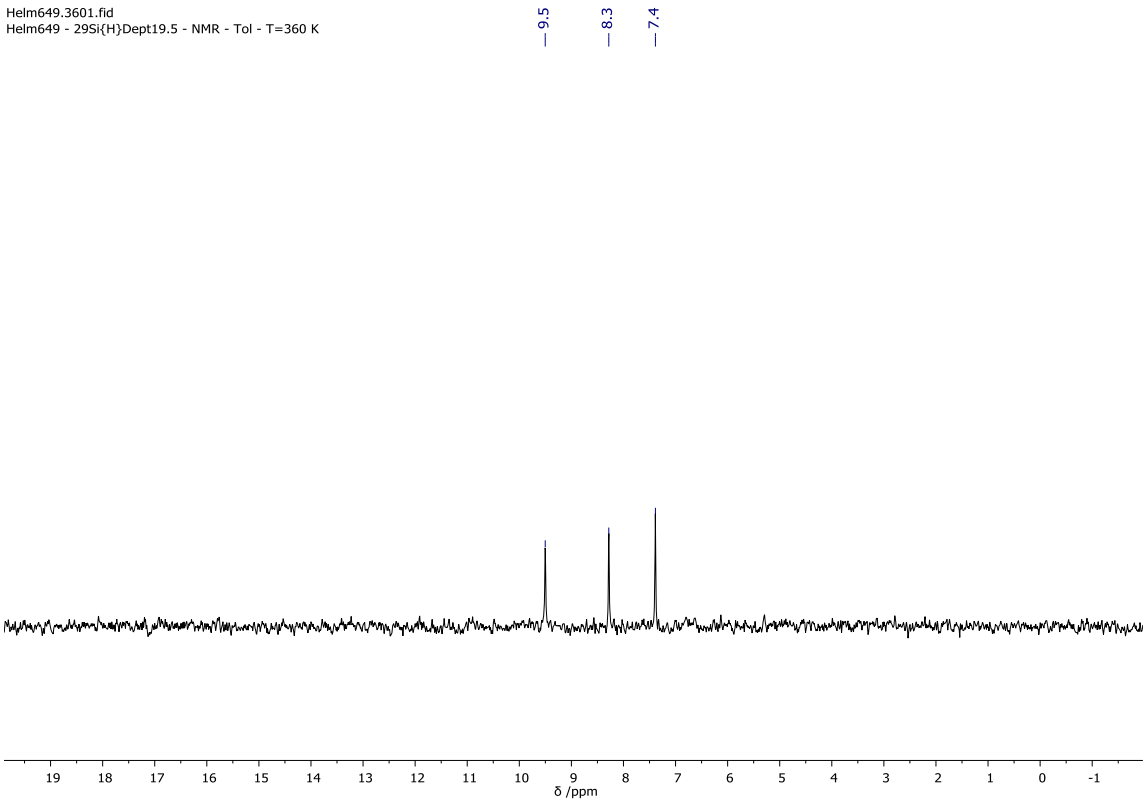


Figure S38. $^{29}Si\{^{1}H\}$DEPT19.5-NMR spectrum (toluene-d_8, 360 K, 80 MHz) of **4**.

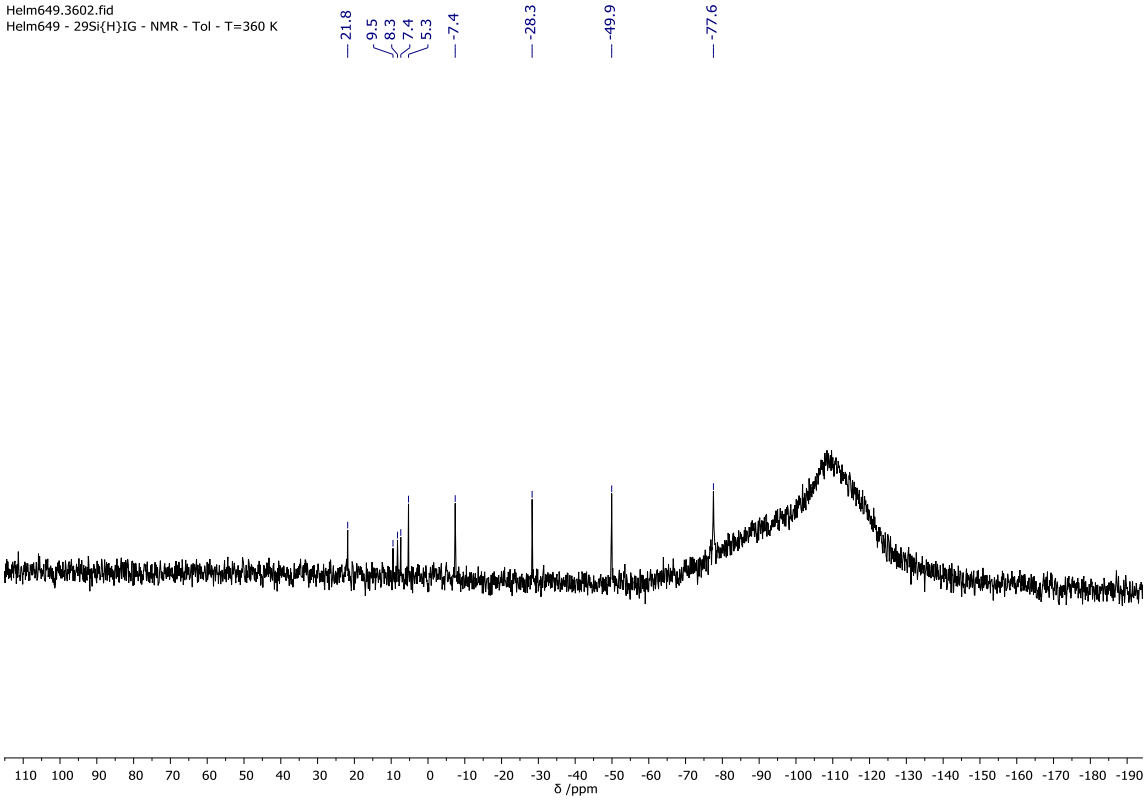


Figure S39. $^{29}Si\{^{1}H\}$IG-NMR spectrum (toluene-d_8, 360 K, 80 MHz) of **4**.

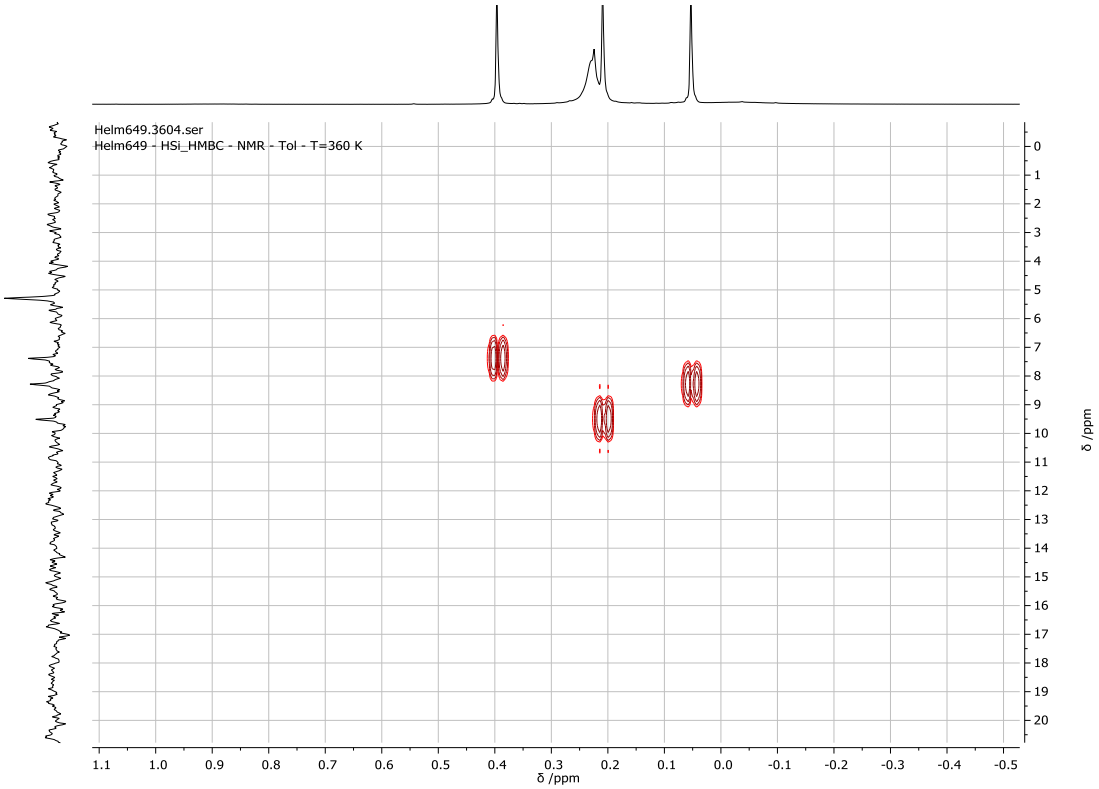


Figure S40. H,Si-HMBC-NMR spectrum (toluene-d_8, 360 K) of **4**.

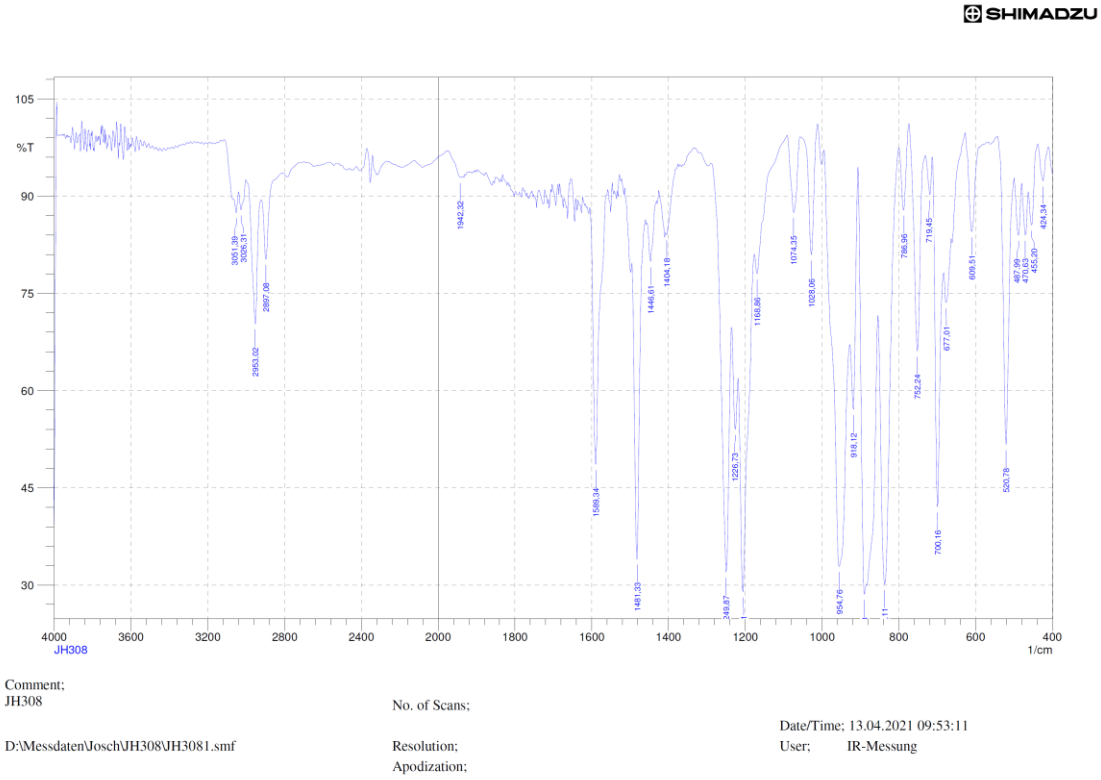


Figure S41. IR spectrum of **4**.

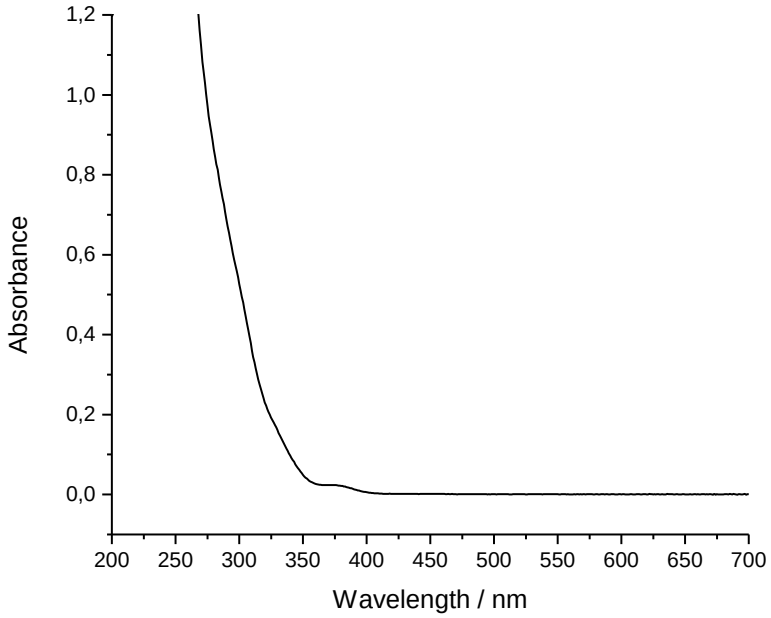


Figure S42. UV-Vis spectrum (*n*-hexane, c = $5.02 \cdot 10^{-5}$ mol/L) of **4**.

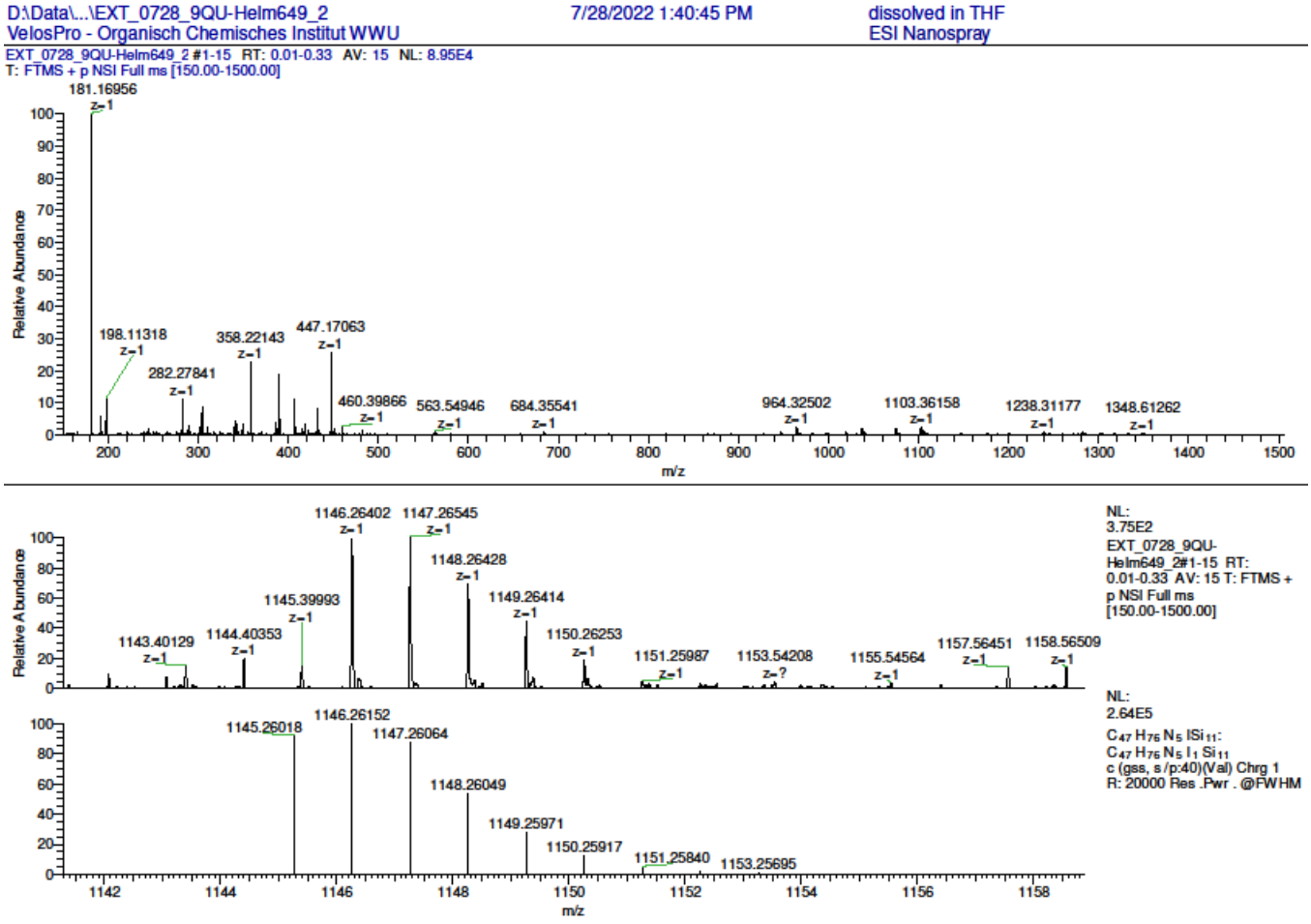
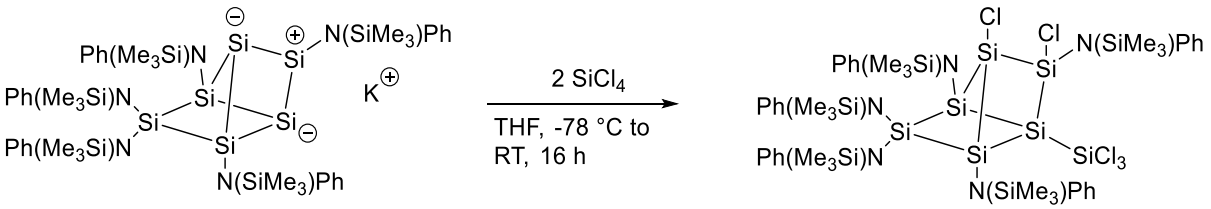


Figure S43. ESI-MS spectrum of **4**.

2.4 Synthesis of $[Si_6\{N(SiMe_3)Ph\}_5Cl_2SiCl_3]$ (5)



$K[Si_6\{N(SiMe_3)Ph\}_5]$ (0.148 g, 0.14 mmol, 1.0 equiv.) was dissolved in THF (10 mL) and $SiCl_4$ (0.1 M in *n*-hexane, 2.8 mL, 0.28 mmol, 2.0 equiv.) was added at −78 °C. The reaction mixture was allowed to warm to room temperature and was stirred for 16 h. All volatile components were removed in vacuo and the yellow residue was extracted with benzene (5 mL). Storage of the benzene solution at room temperature resulted in $[Si_6\{N(SiMe_3)Ph\}_5Cl_2SiCl_3]$ (**5**) (0.037 g, 0.03 mmol, 22 %) as pale yellow crystals.

^{1}H-NMR (C_6D_6, 300 K, 400 MHz): δ(ppm) = 7.49 - 7.46 (2H, m); 7.31 - 7.28 (2H, m); 7.25 - 7.20 (8H, m); 7.12 - 7.10 (3H, m); 7.08 - 7.03 (2H, m); 7.01 - 6.69 (3H, m); 6.95 - 6.91 (1H, m); 6.88 - 6.84 (1H, m); 6.65 - 6.62 (2H, m); 0.49 (9H, s); 0.34 (9H, s); 0.31 (9H, s); 0.15 (9H, s); 0.02 (9H, s).

^{13}C-NMR (C_6D_6, 300 K, 100 MHz): δ(ppm) = 148.9; 147.7; 146.5; 146.5; 146.5; 131.6; 131.6; 130.9; 130.2; 130.1; 129.8; 129.7; 129.6; 129.5; 129.4; 125.8; 125.6; 125.1; 125.0; 125.0; 3.3; 3.1; 2.7; 2.6; 1.3.

^{15}N,^{1}H-HMBC-NMR (C_6D_6, 300 K, 41 MHz): δ(ppm) = 87; 84; 82; 27; 26.

^{29}Si(DEPT 19.5)-NMR (C_6D_6, 300 K, 80 MHz): δ(ppm) = 12.3; 11.2; 9.3; 6.0; 5.4.

^{29}Si{^{1}H}IG-NMR (C_6D_6, 300 K, 80 MHz): δ(ppm) = 33.3; 16.7; 13.8; 12.3; 11.2; 9.3; 6.0; 5.4; −35.3; −39.1; −52.5; −121.7.

IR (KBr pellet, $\tilde{\nu}$/cm^{-1} (intensity)) = 451(vw), 476(w), 517(m), 559(m), 588(w), 611(w), 679(m), 700(m), 754(w), 839(vs), 872(vs), 897(m), 959(vs), 1028(w), 1071(vw), 1169(w), 1196(s), 1251(s), 1404(vw), 1481(s), 1589(w), 1655(w), 1682(vw), 2376(vw), 2895(w), 2955(w), 3030(vw), 3059(vw).

ESI-MS: m/z = 1029.08 $[Si_6\{N(SiMe_3)Ph\}_4Cl_2SiCl_3]^+$.

UV-Vis: (*n*-hexane, c = 1.24·10^{-5} mol/L, ε/L·mol^{-1}·cm^{-1}): λ = 236 nm (68750); 302 (12416).

Melting point: 250 °C, decomposition forming a red solid, melting at 270 °C.

Elemental Analysis for $C_{45}H_{70}Cl_5N_5Si_{12}$:	H	C	N
calculated:	5.90	45.22	5.86
found:	5.96	45.30	5.09

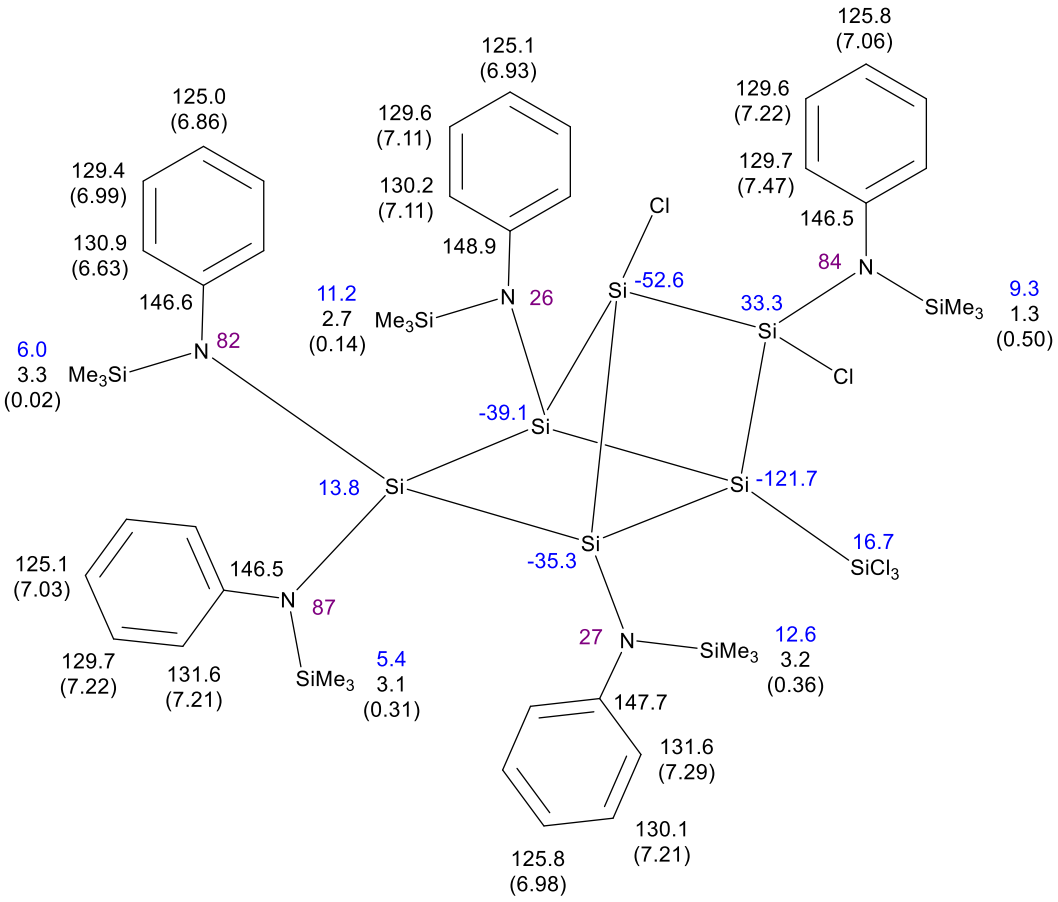


Figure S44. Assignment of chemical shifts to **5**, ^{1}H (in brackets), ^{13}C (black), ^{15}N (violet), ^{29}Si (blue).

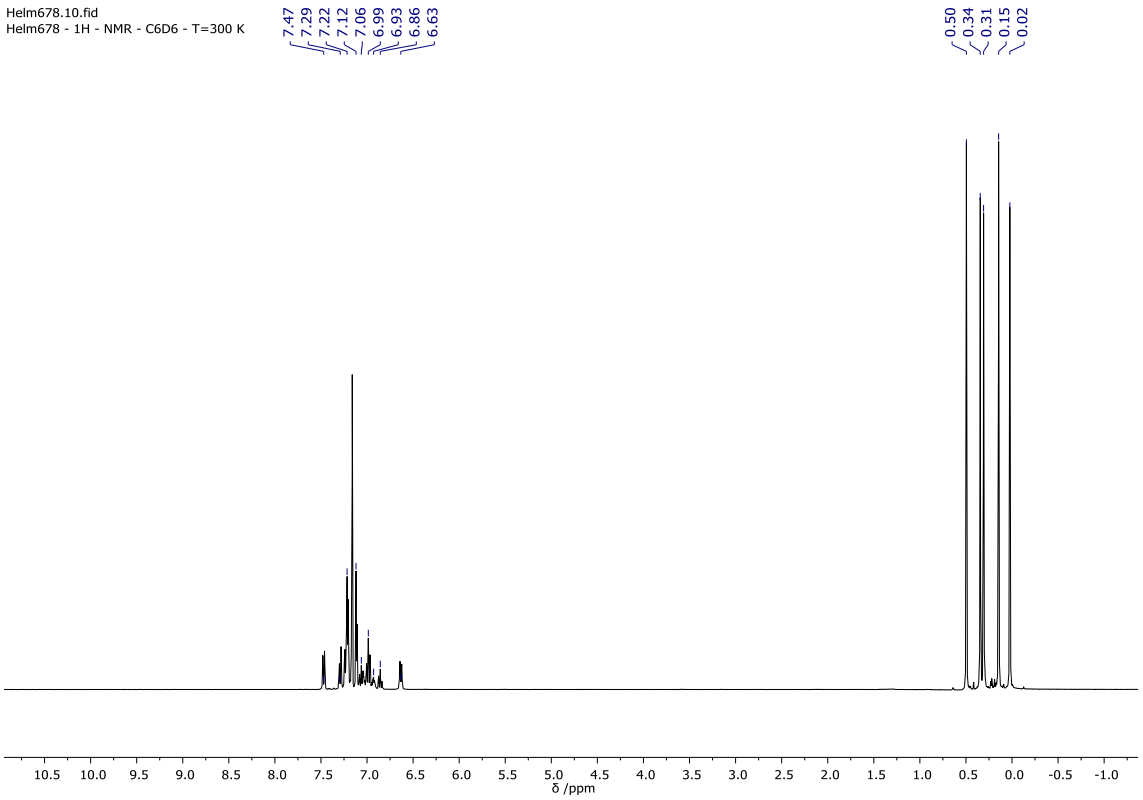


Figure S45. ^{1}H-NMR spectrum (C_6D_6, 300 K, 400 MHz) of **5**.

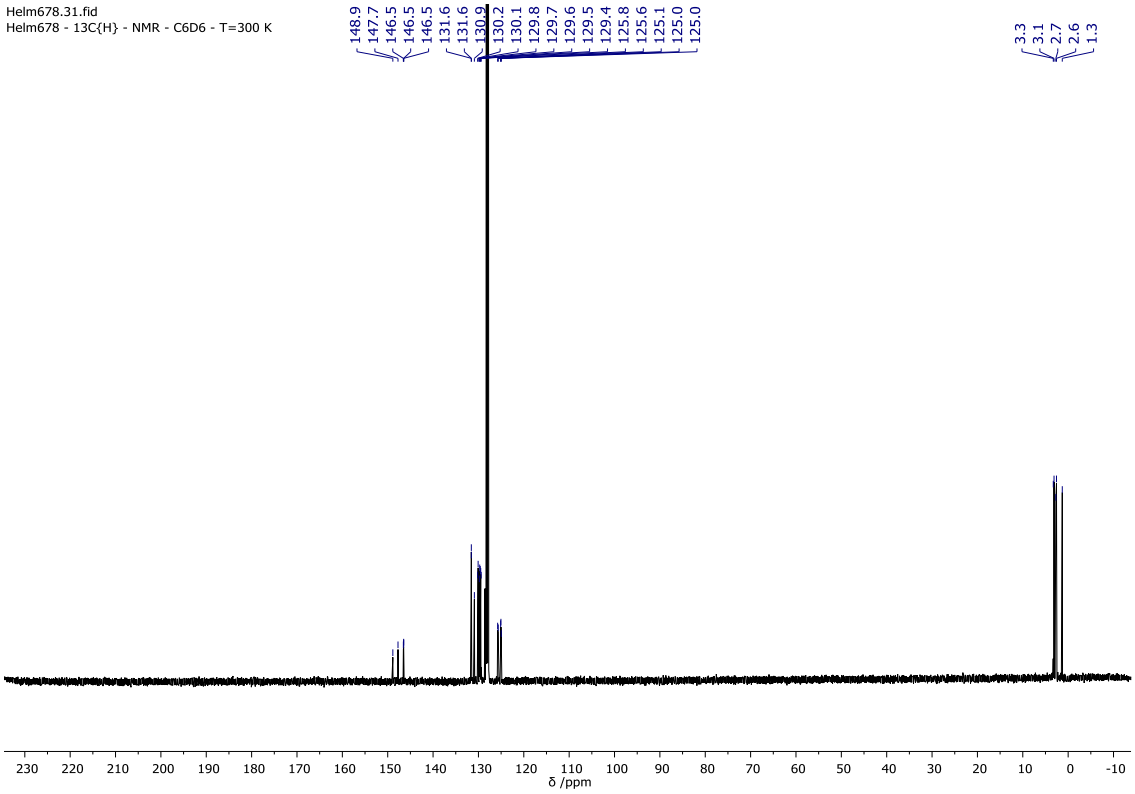


Figure S46. ^{13}C{^{1}H}-NMR spectrum (C_6D_6, 300 K, 100 MHz) of **5**.

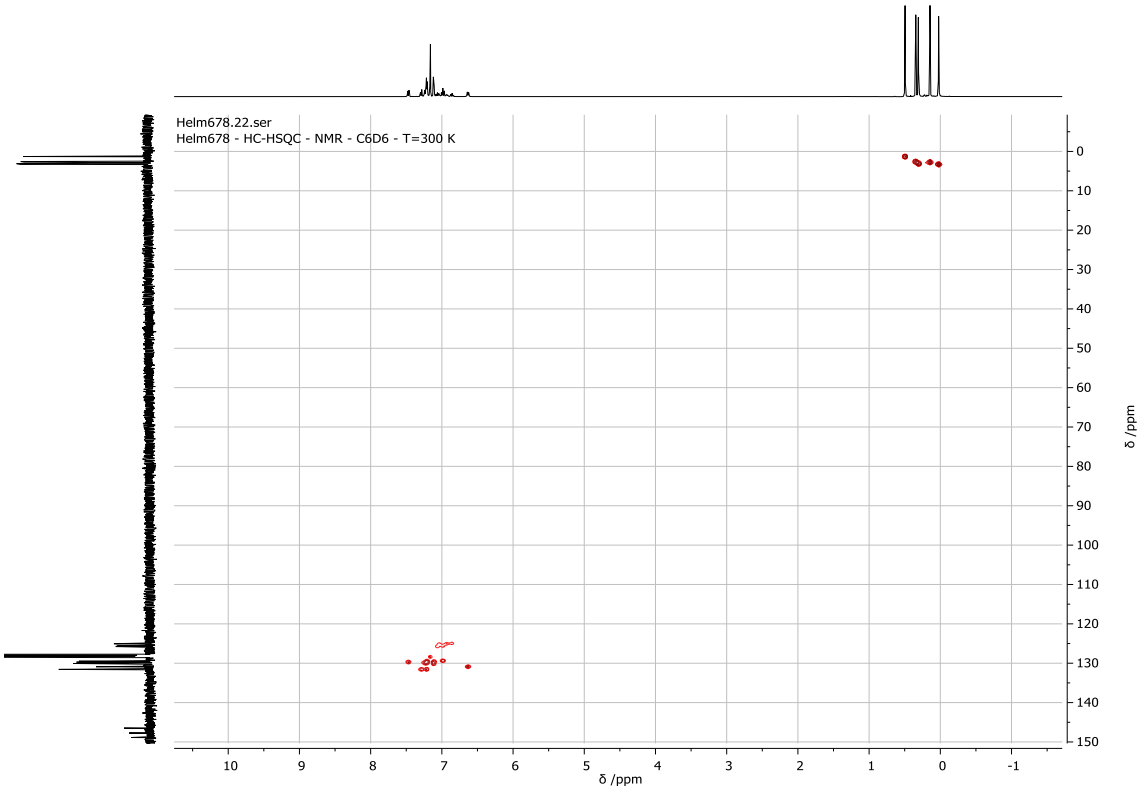


Figure S47. H,C-HSQC-NMR spectrum (C_6D_6, 300 K) of **5**.

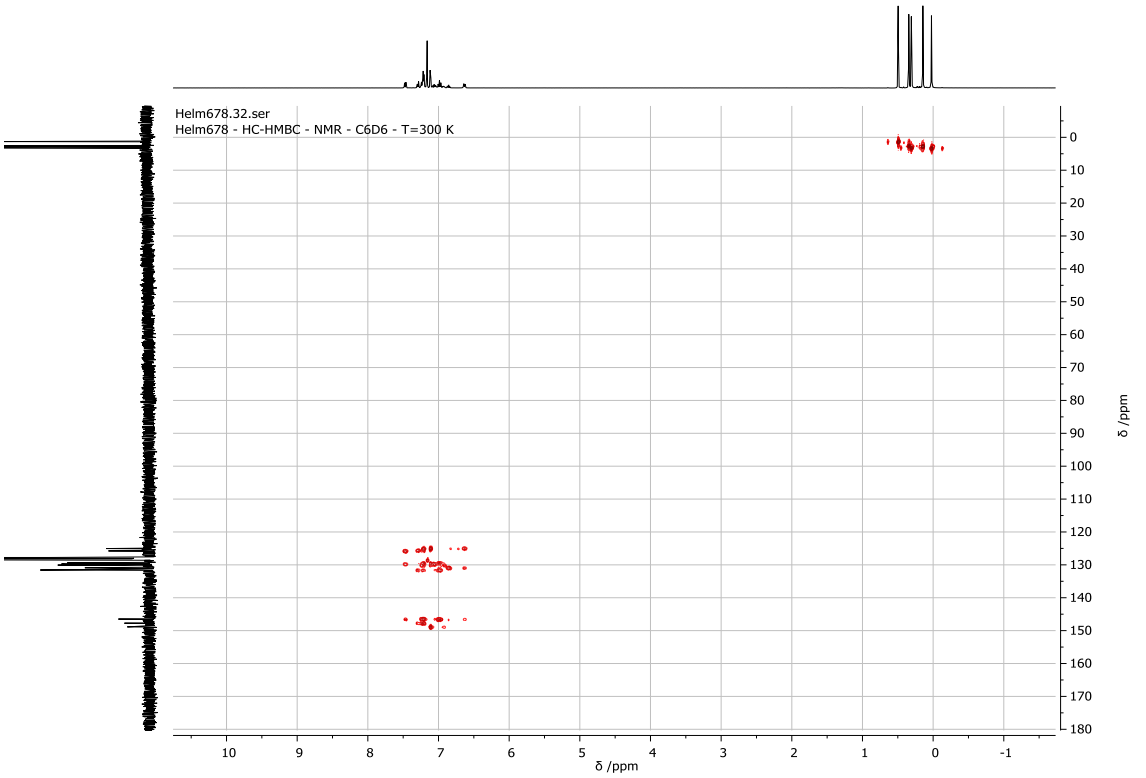


Figure S48. H,C-HMBC-NMR spectrum (C_6D_6, 300 K) of **5**.

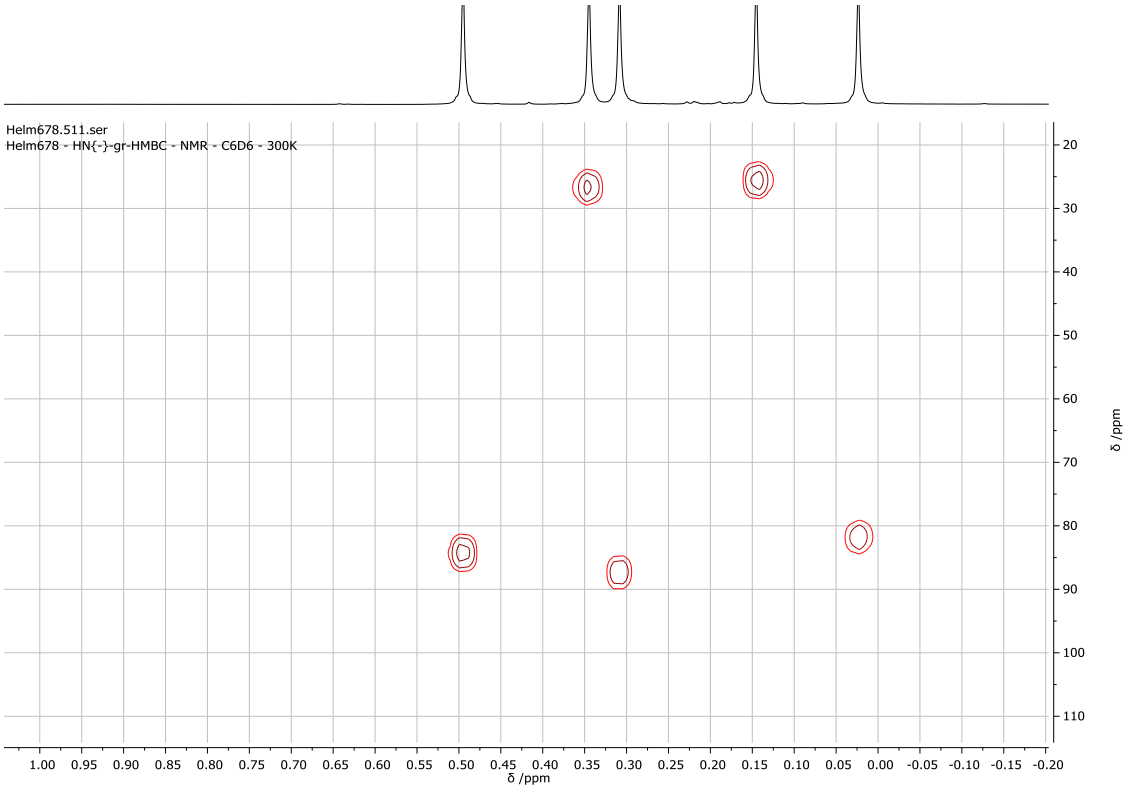


Figure S49. H,N-HMBC-NMR spectrum (C_6D_6, 300 K) of **5**.

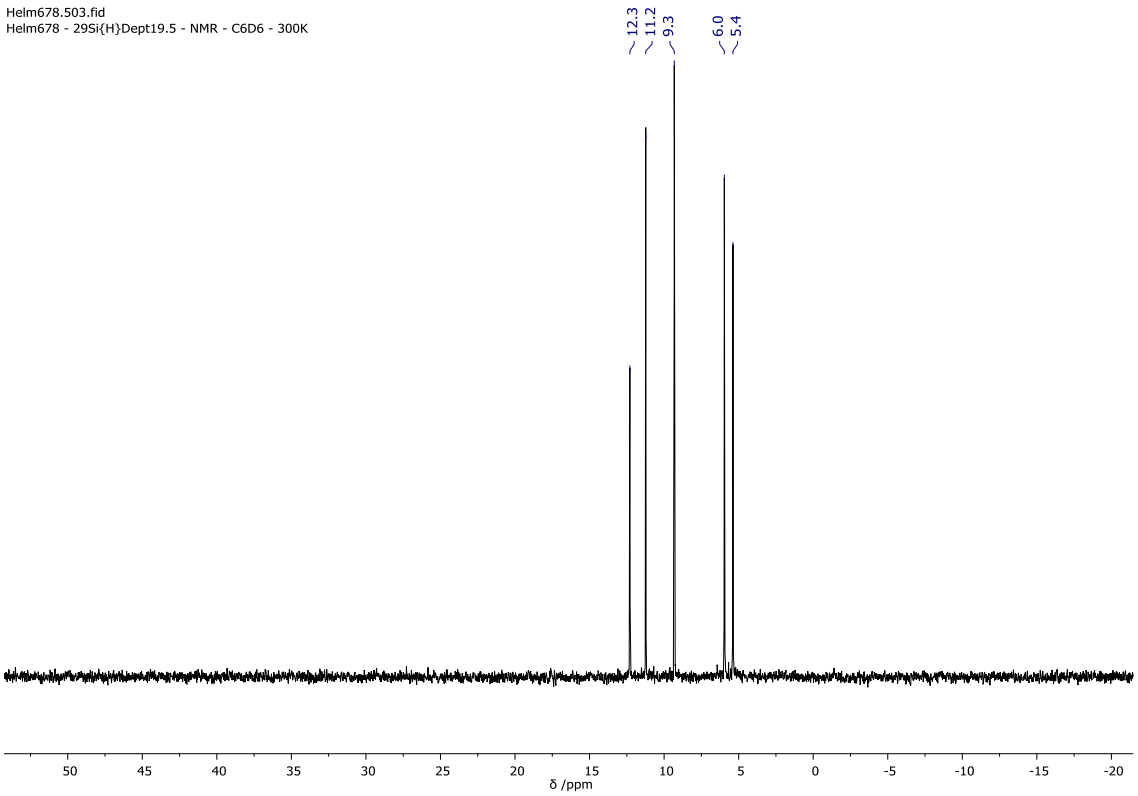


Figure S50. $^{29}Si\{^1H\}$DEPT19.5-NMR spectrum (C_6D_6, 300 K, 80 MHz) of **5**.

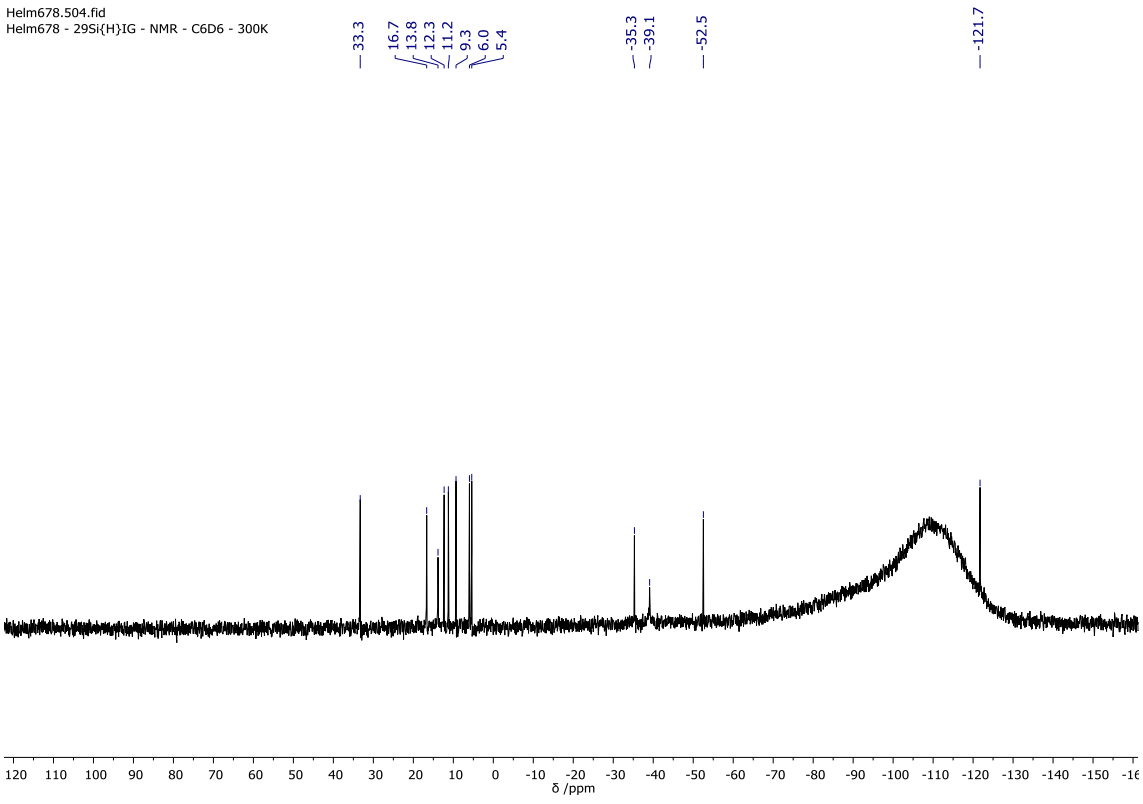


Figure S51. $^{29}Si\{^{1}H\}$IG-NMR spectrum (C_6D_6, 300 K, 80 MHz) of **5**.

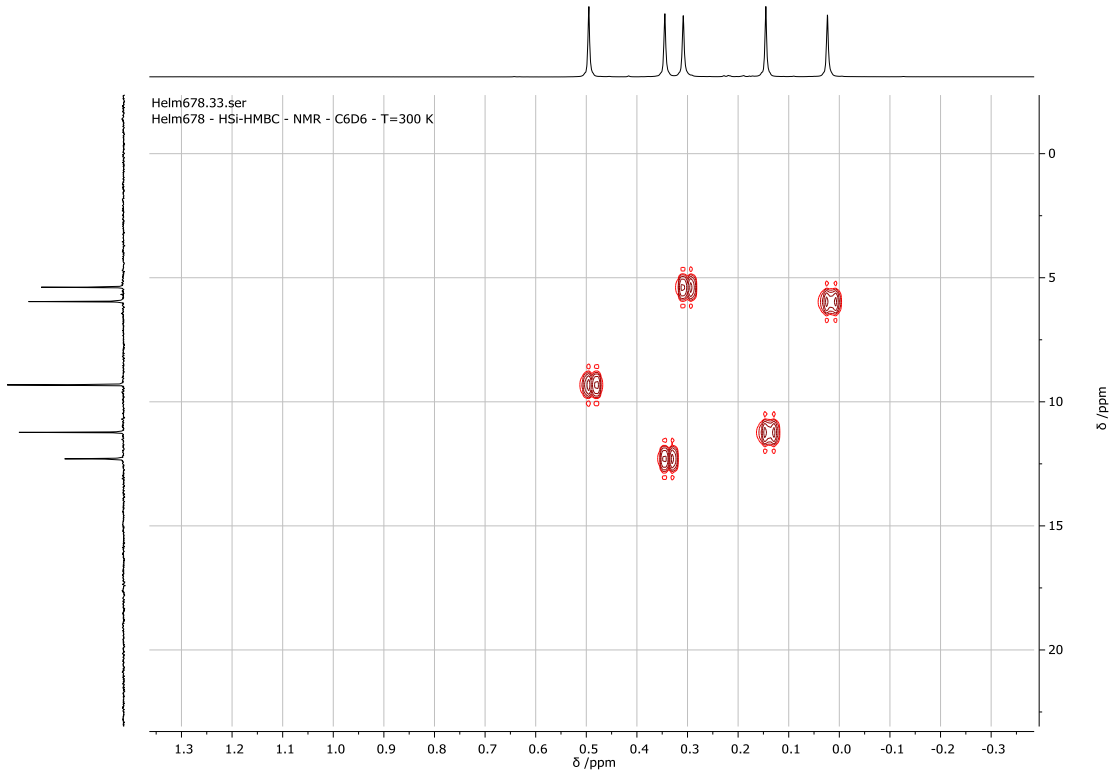


Figure S52. H,Si-HMBC-NMR spectrum (C_6D_6, 300 K) of **5**.

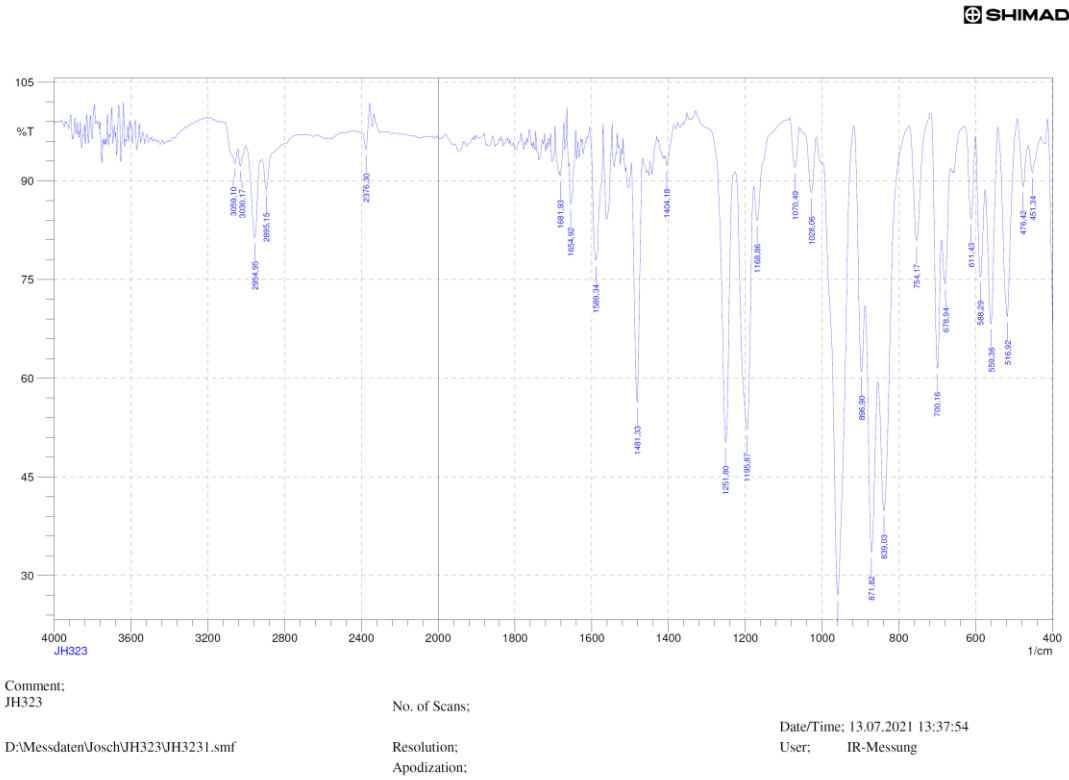


Figure S53. IR spectrum of **5**.

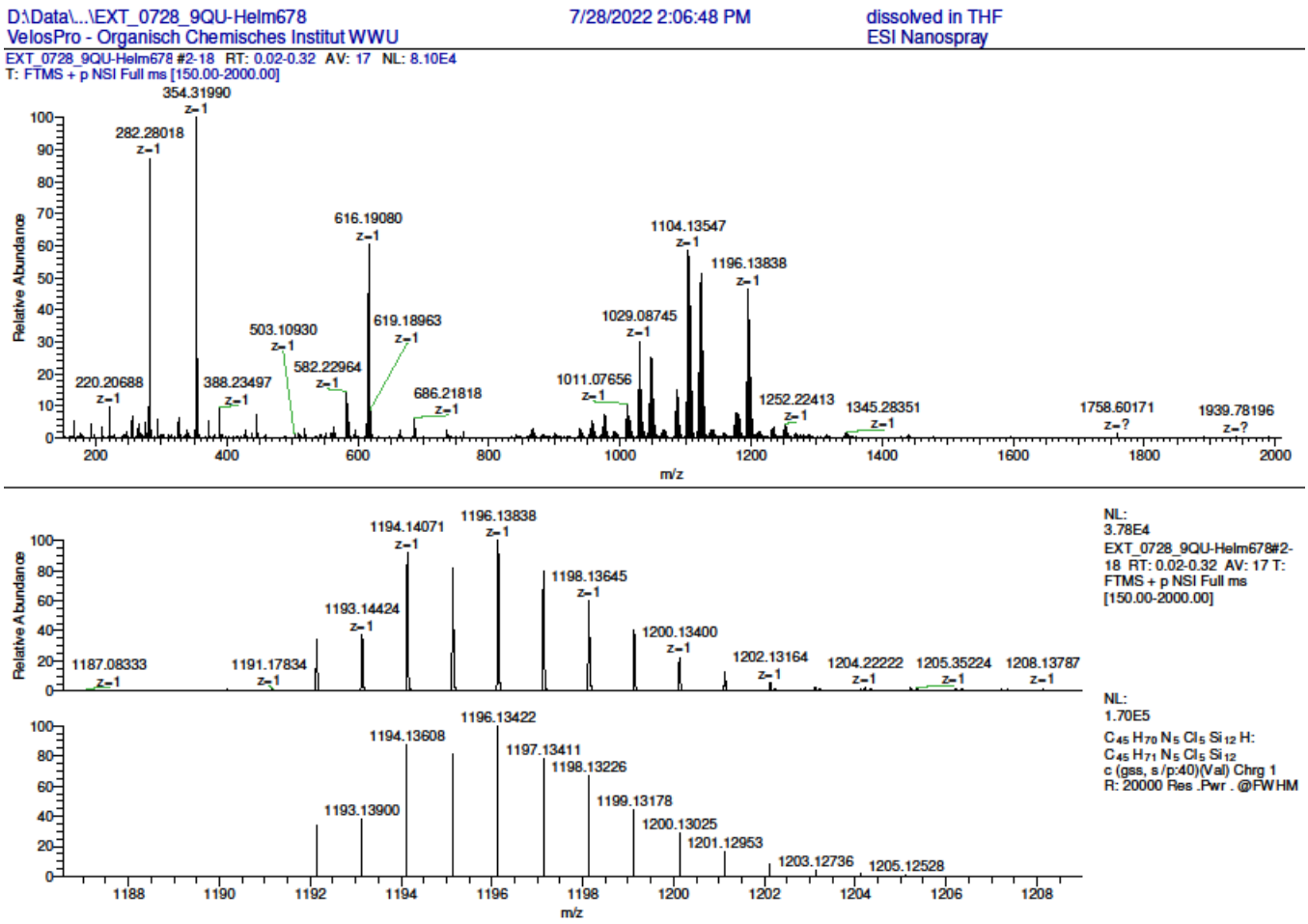


Figure S54. ESI-MS spectrum of **5**.

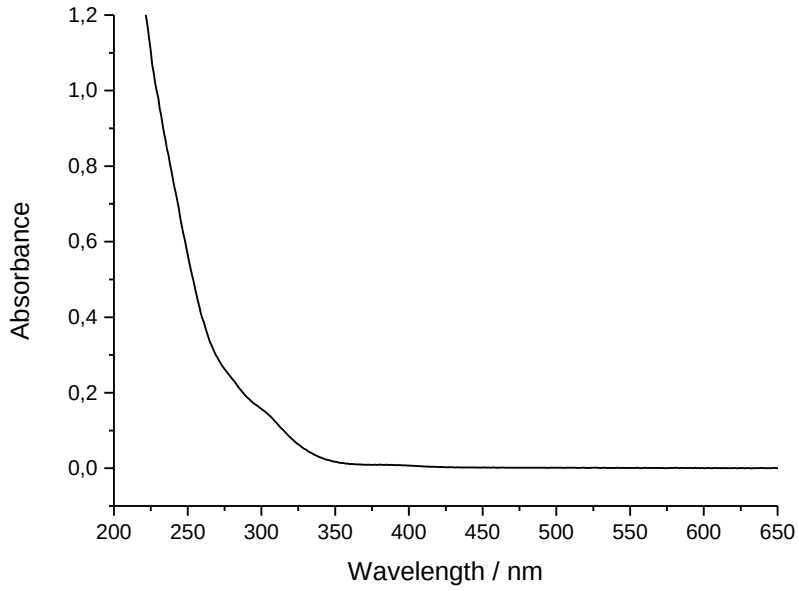
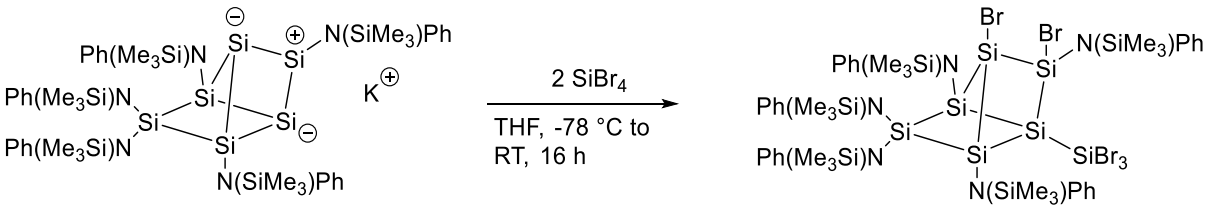


Figure S55. UV-Vis spectrum (*n*-hexane, c = $1.24 \cdot 10^{-5}$ mol/L) of **5**.

2.5 Synthesis of $[Si_6\{N(SiMe_3)Ph\}_5Br_2SiBr_3]$ (6)



$K[Si_6\{N(SiMe_3)Ph\}_5]$ (0.164 g, 0.16 mmol, 1.0 equiv.) was dissolved in THF (10 mL) and $SiBr_4$ (0.1 M in *n*-hexane, 3.2 mL, 0.32 mmol, 2.0 equiv.) was added at −78 °C. The reaction mixture was allowed to warm to room temperature and was stirred for 16 h. All volatile components were removed in vacuo and the yellow residue was extracted with benzene (5 mL). Storage at room temperature obtained $[Si_6\{N(SiMe_3)Ph\}_5Br_2SiBr_3]$ (**6**) (0.025 g, 0.02 mmol, 11 %) as yellow crystals.

^{1}H-NMR (C_6D_6, 300 K, 400 MHz): δ(ppm) = 7.53 -7.51 (2H, m); 7.37 - 7.35 (2H, m); 7.28 - 7.18 (8H, m); 7.14 - 6.97 (9H, m); 6.94 - 6.89 (2H, m); 6.82 - 6.97 (2H, m); 0.52 (9H, s); 0.36 (9H, s); 0.27 (9H, s); 0.18 (9H, s); 0.05 (9H, s).

^{13}C-NMR (C_6D_6, 300 K, 100 MHz): δ(ppm) = 148.8; 147.5; 146.8; 146.5; 146.4; 131.8; 131.5; 131.4; 130.4; 130.1; 129.9; 129.9; 129.7; 129.5; 129.4; 126.1; 125.7; 125.2; 125.2; 125.1; 3.8; 3.3; 3.3; 3.2; 1.5.

^{15}N,^{1}H-HMBC-NMR (C_6D_6, 300 K, 41 MHz): δ(ppm) = 86; 83; 83; 26; 26.

^{29}Si(DEPT 19.5)-NMR (C_6D_6, 300 K, 80 MHz): δ(ppm) = 12.8; 11.7; 10.1; 6.1; 5.5.

^{29}Si{^{1}H}IG-NMR (C_6D_6, 300 K, 80 MHz): δ(ppm) = 18.5; 12.8; 11.8; 11.7; 10.1; 6.1; 5.5; −19.1; −30.9; −39.7; −69.1; −107.9.

IR (KBr pellet, $\tilde{\nu}$/cm^{-1} (intensity)) = 442(m), 469(vw), 498(vw), 525(m), 556(vw), 610(vw), 662(vw), 696(s), 752(w), 837(vs), 868(vs), 897(m), 957(vs), 1026(vw), 1071(vw), 1167(vw), 1196(vs), 1250(s), 1408(vw), 1445(vw), 1481(s), 1557(w), 1586(w), 1668(vw), 1939(vw), 2895(vw), 2955(w), 3055(vw).

ESI-MS: m/z = 1250.78 $[Si_6\{N(SiMe_3)Ph\}_5Br_2SiBr_3]^+$.

UV-Vis: (*n*-hexane, c = 1.41·10^{-5} mol/L, ε/L·mol^{-1}·cm^{-1}): λ = 231 nm (44282); 313 (5106).

Melting point: 260 °C, decomposition forming a red solid, melting at 290 °C.

Elemental Analysis for $C_{45}H_{70}Br_5N_5Si_{12}$ + Benzene**:**	H	C	N
calculated:	5.12	40.95	4.68
found:	4.76	41.08	4.88

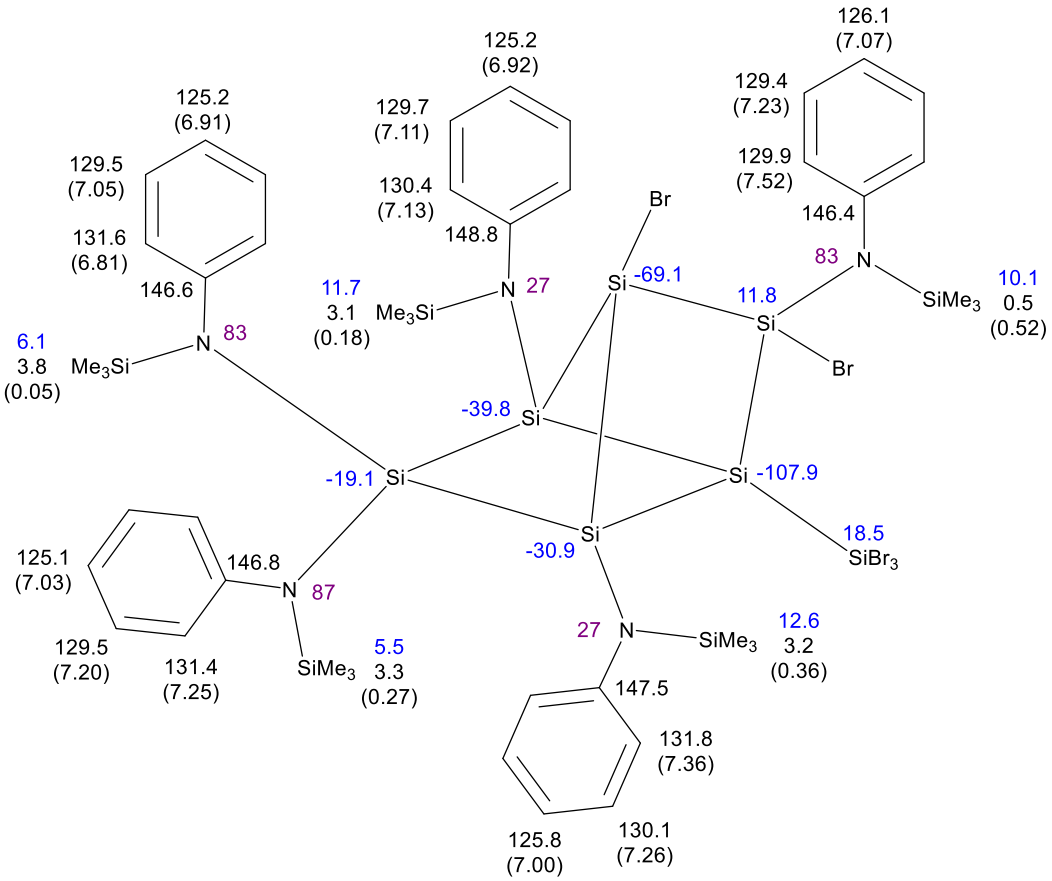


Figure S56. Assignment of chemical shifts to **6**, ^{1}H (in brackets), ^{13}C (black), ^{15}N (violet), ^{29}Si (blue).

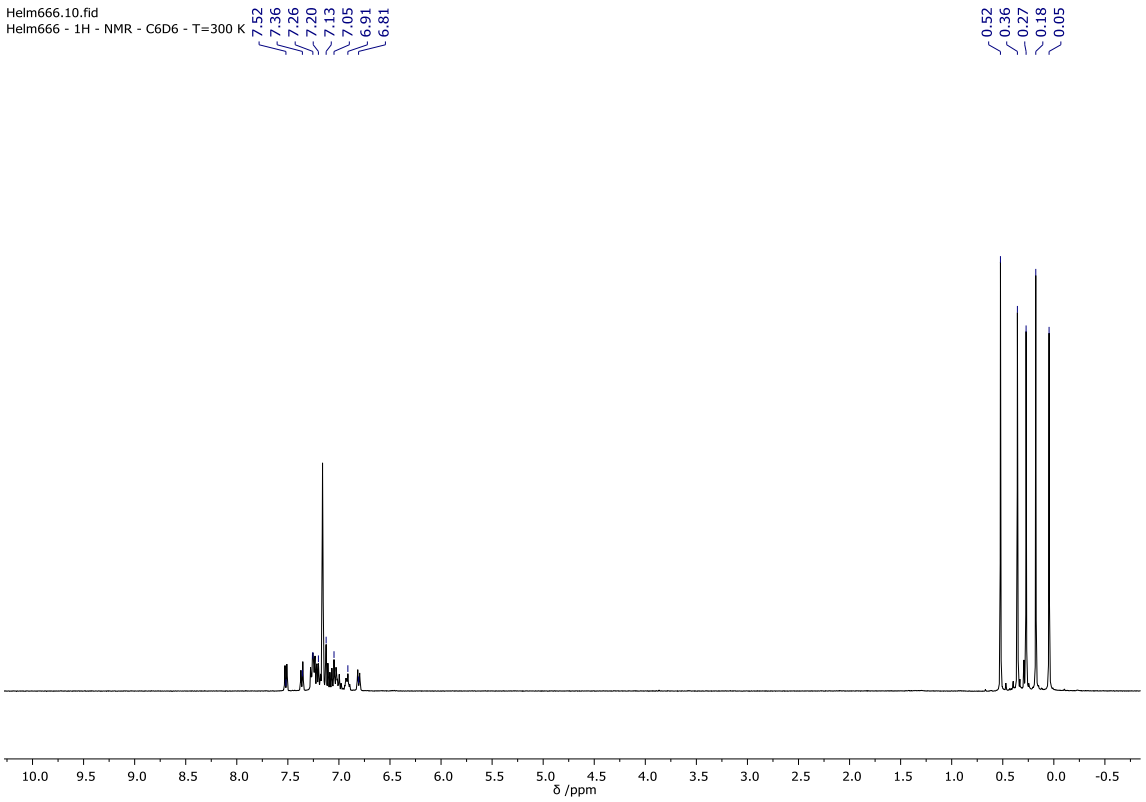


Figure S57. ^{1}H-NMR spectrum (C_6D_6, 300 K, 400 MHz) of **6**.

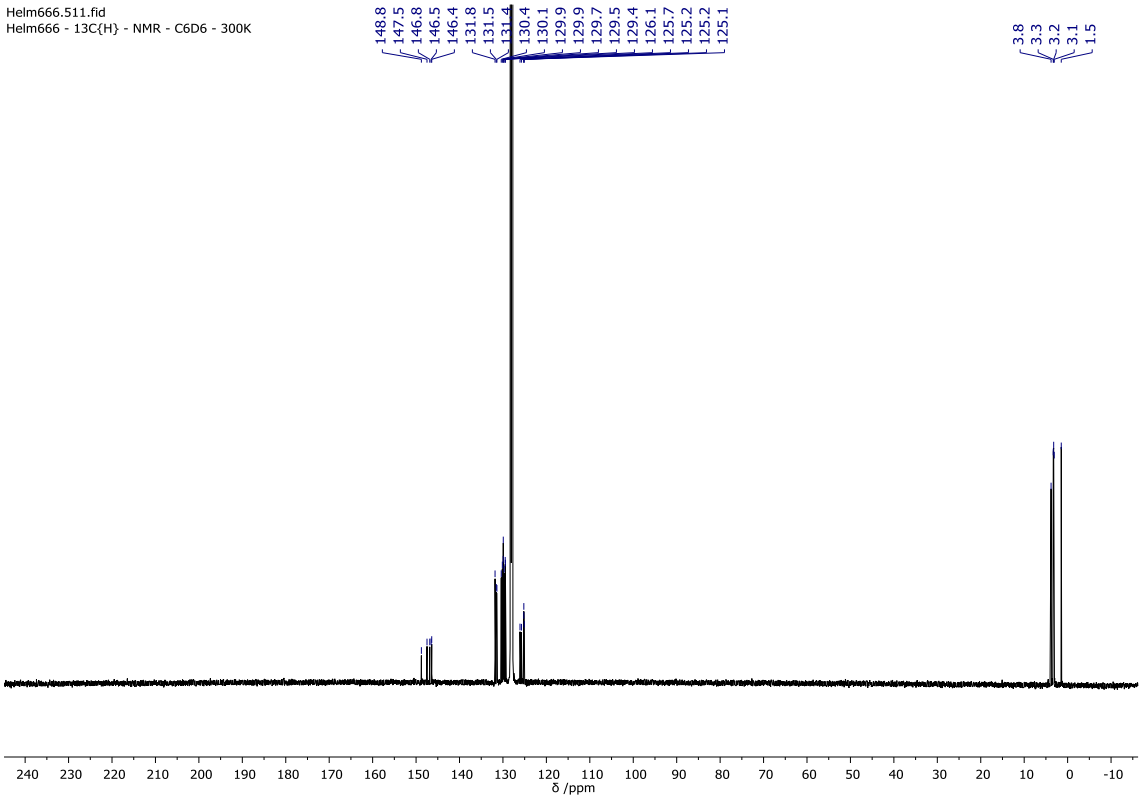


Figure S58. ^{13}C{^{1}H}-NMR spectrum (C_6D_6, 300 K, 100 MHz) of **6**.

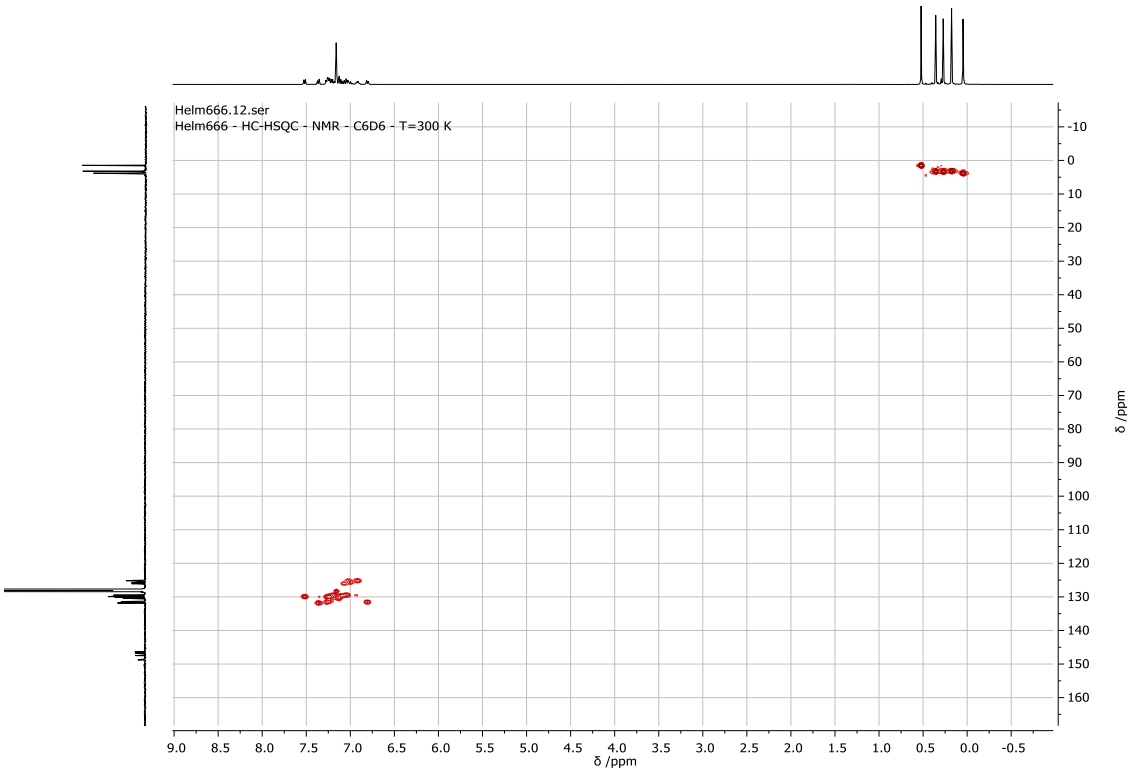


Figure S59. H,C-HSQC-NMR spectrum (C_6D_6, 300 K) of **6**.

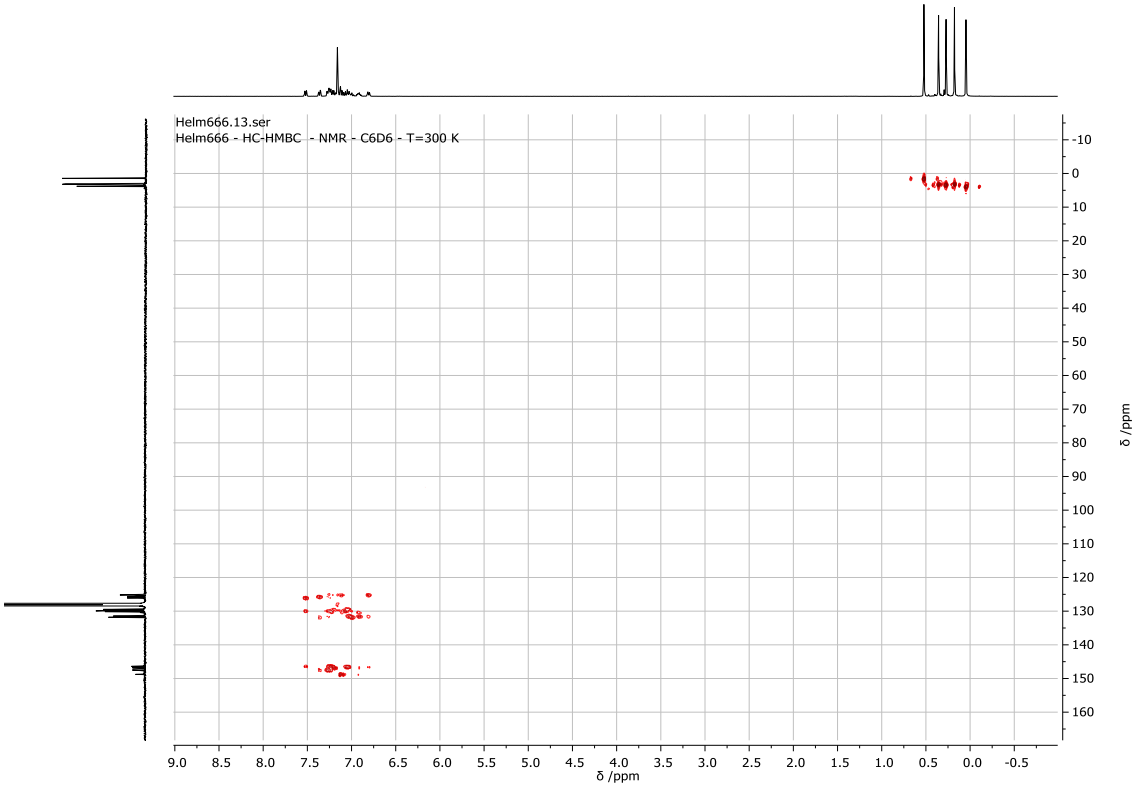


Figure S60. H,C-HMBC-NMR spectrum (C_6D_6, 300 K) of **6**.

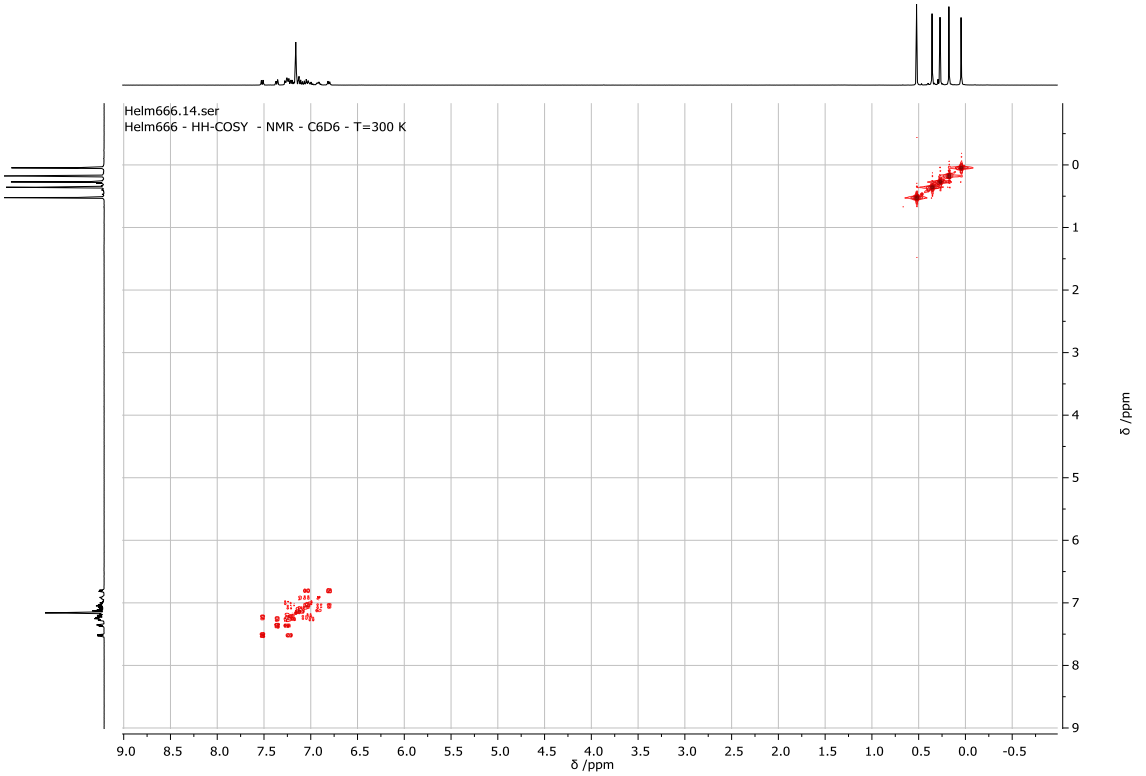


Figure S61. H,H-COSY-NMR spectrum (C_6D_6, 300 K) of **6**.

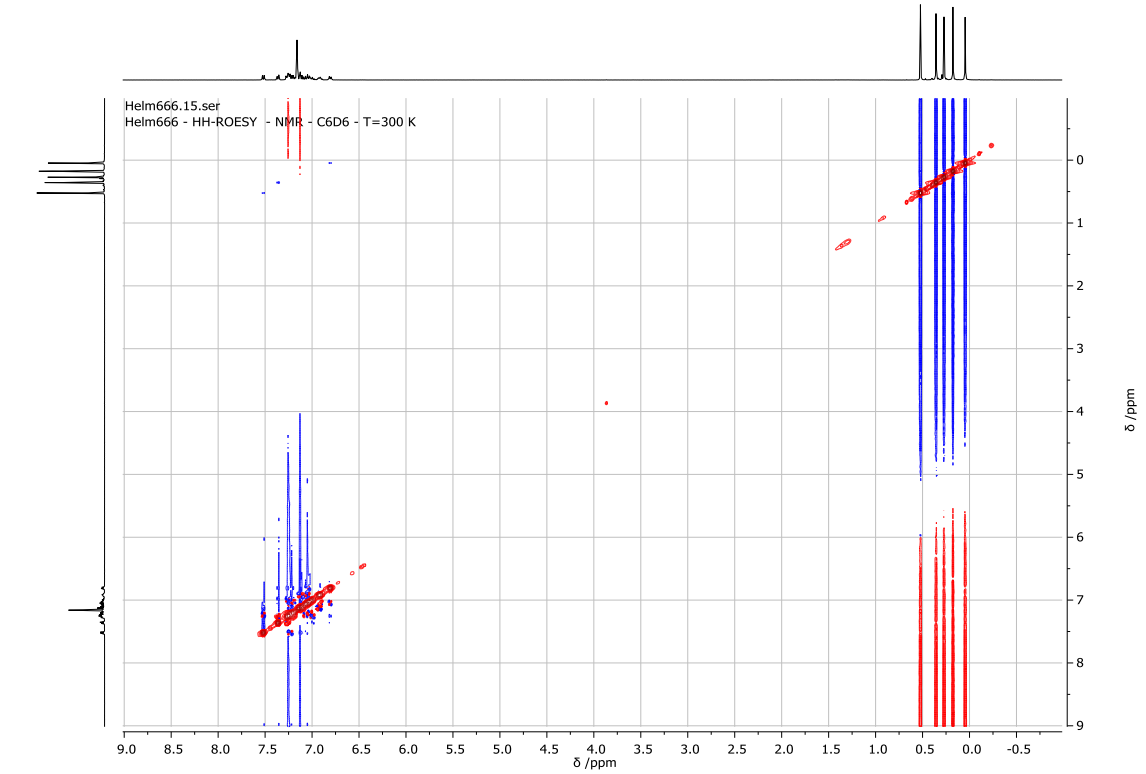


Figure S62. H,H-ROESY-NMR spectrum (C_6D_6, 300 K) of **6**.

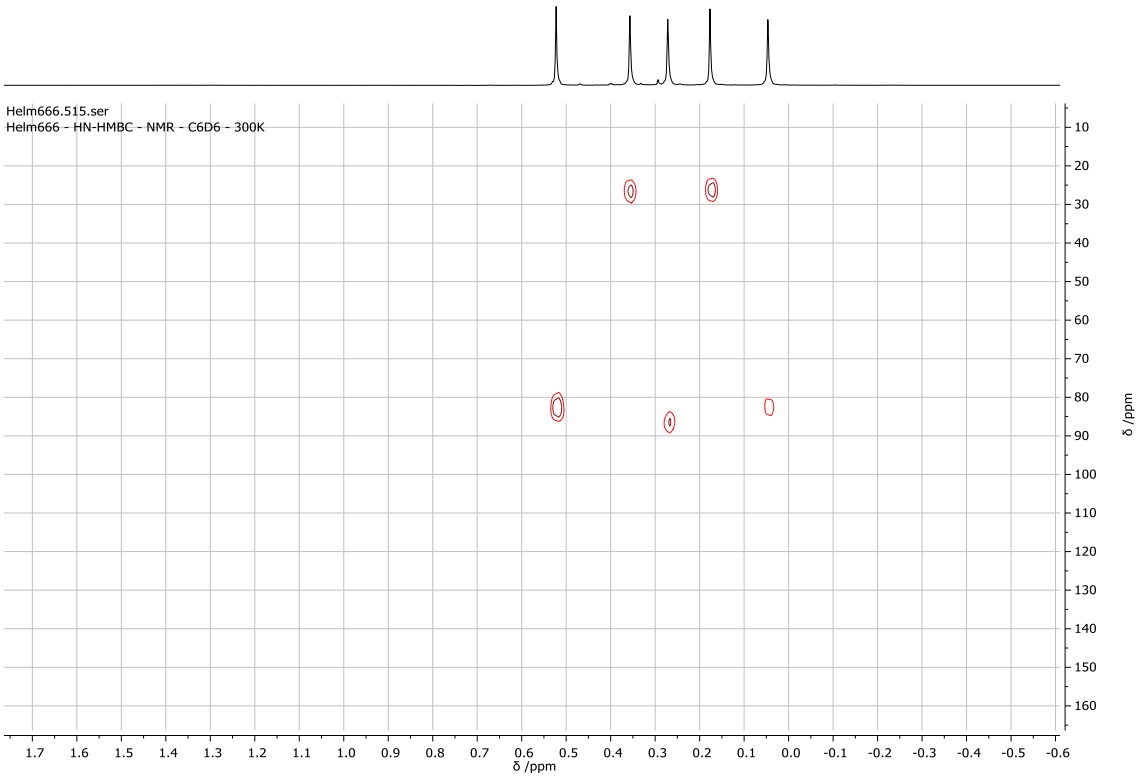


Figure S63. H,N-HMBC-NMR spectrum (C_6D_6, 300 K) of **6**.

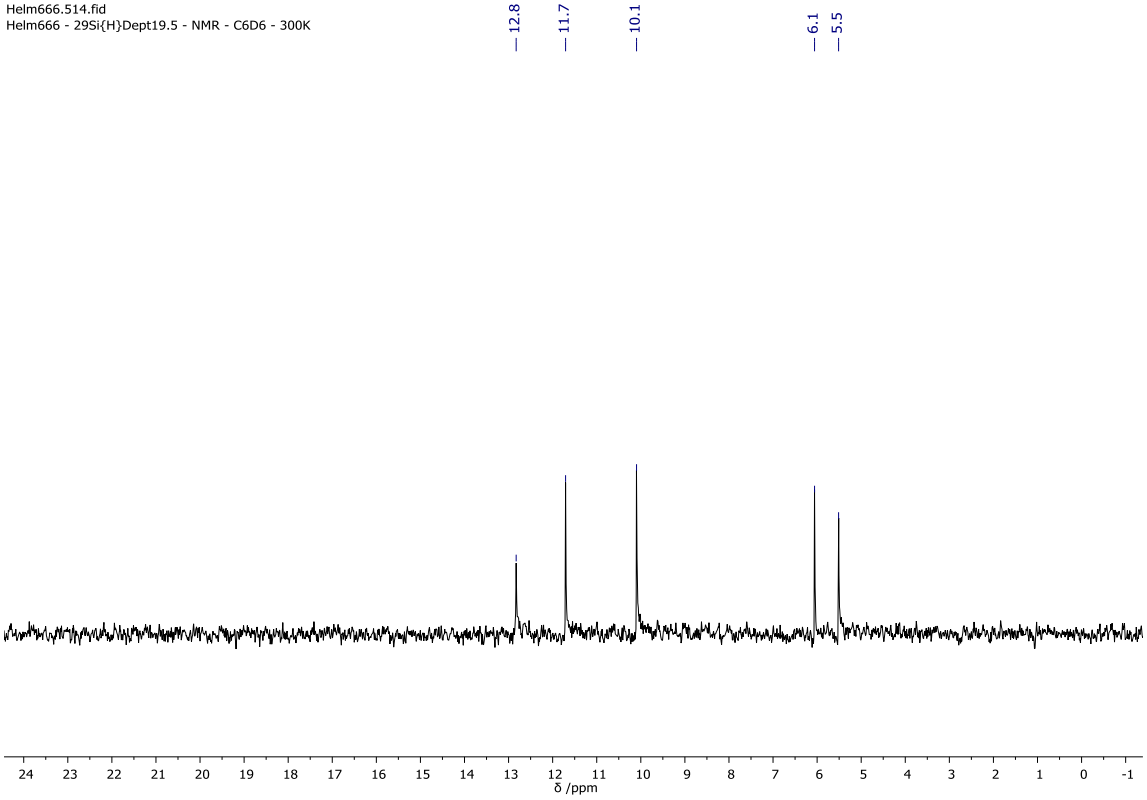


Figure S64. $^{29}Si\{^1H\}$DEPT19.5-NMR spectrum (C_6D_6, 300 K, 80 MHz) of **6**.

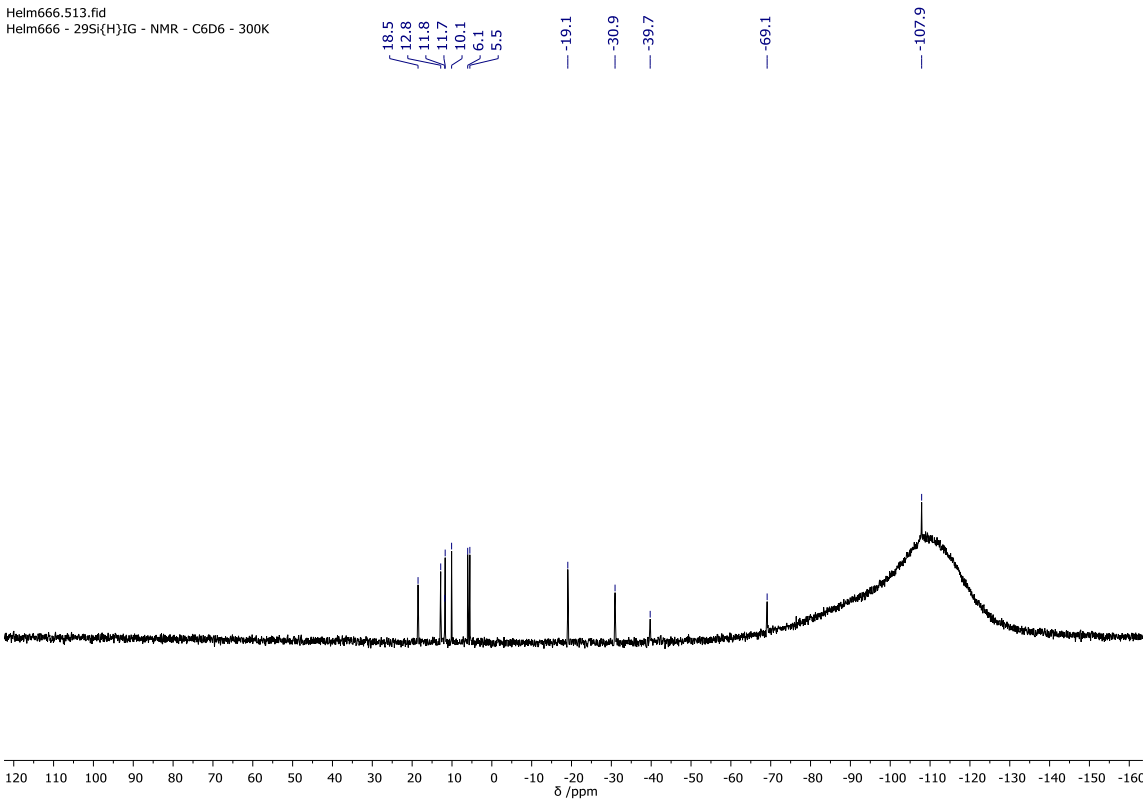


Figure S65. $^{29}Si\{^{1}H\}$IG-NMR spectrum (C_6D_6, 300 K, 80 MHz) of **6**.

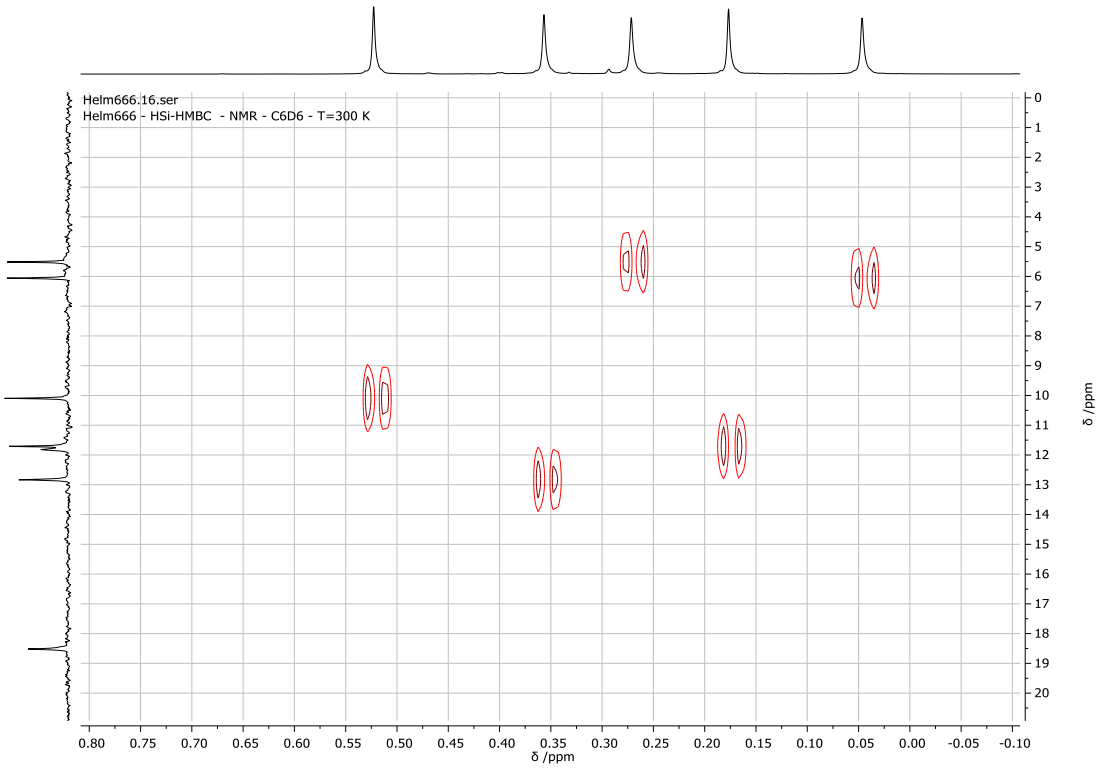


Figure S66. H,Si-HMBC-NMR spectrum (C_6D_6, 300 K) of **6**.

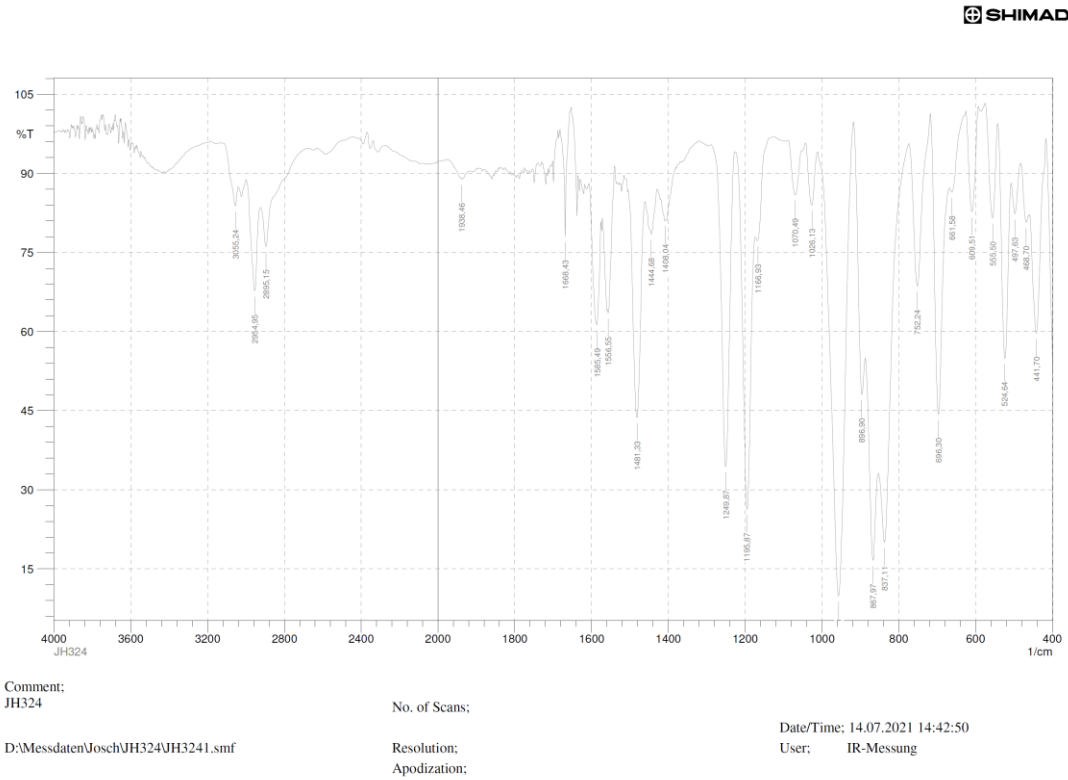


Figure S67. IR spectrum of **6**.

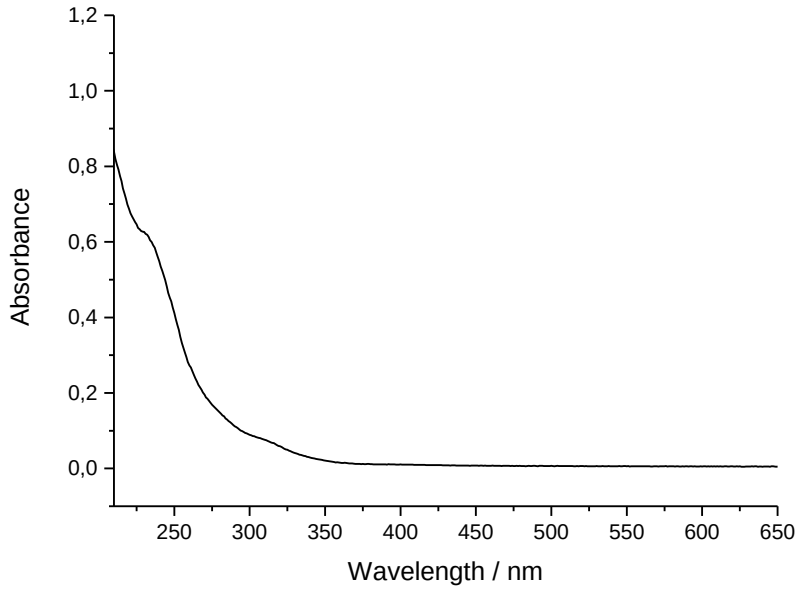


Figure S68. UV-Vis spectrum (*n*-hexane, c = $1.41 \cdot 10^{-5}$ mol/L) of **6**.

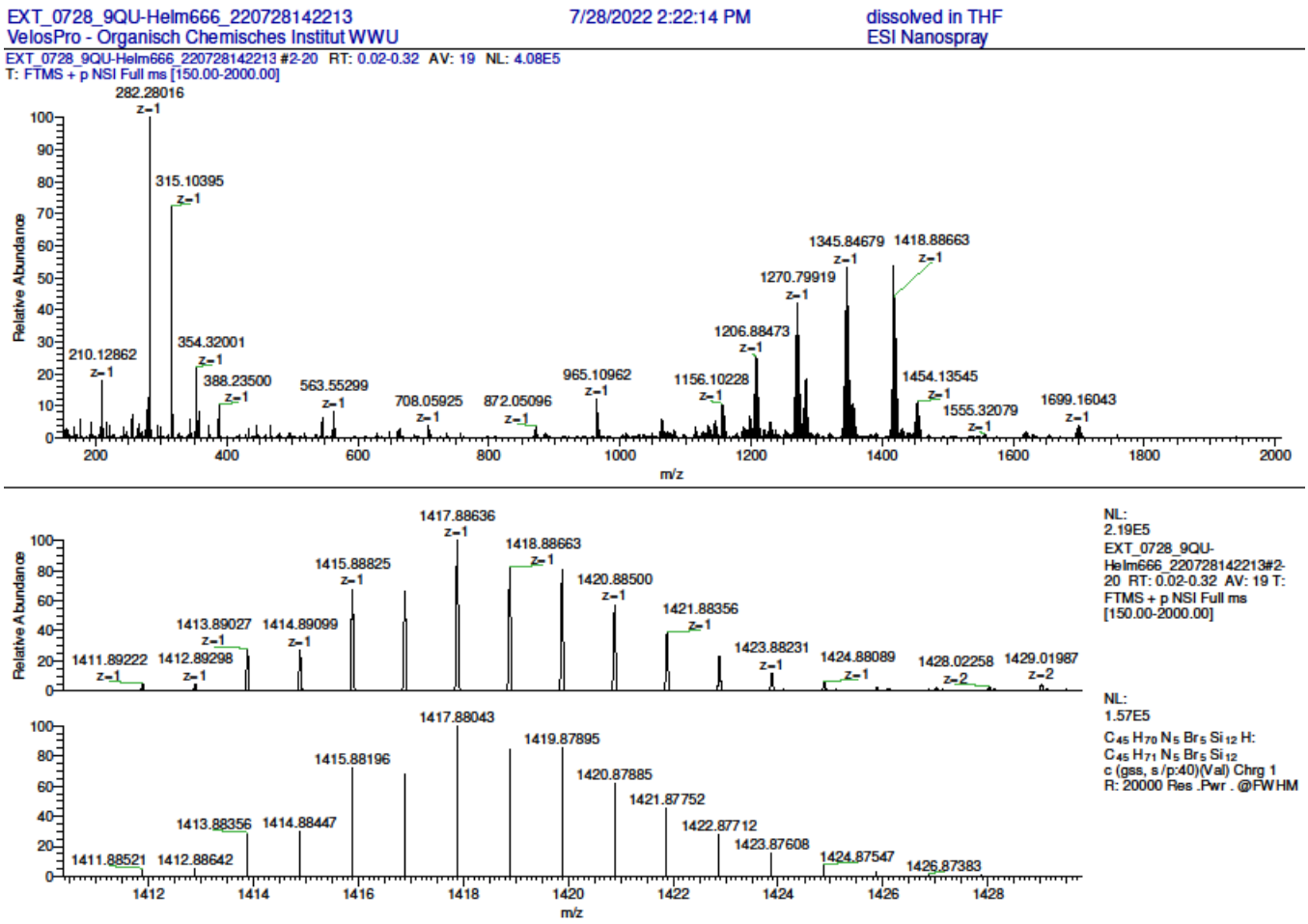


Figure S69. ESI-MS spectrum of **6**.

3. Details of the single crystal X-ray diffraction analysis

Crystals of **2**, **3**(·solvent), **4**(·0.5C_6D_6), **5**(·C_6D_6) and **6** were removed from a Schlenk tube under an argon atmosphere and covered with a layer of hydrocarbon oil. A suitable crystal was selected, attached to a glass fiber and quickly placed in a low temperature Argon stream. The data were collected at 100 K on a Bruker Venture with Mo K_α radiation ($\lambda = 0.71073$ Å), expect **2** which was collected with Cu K_α radiation ($\lambda = 1.54178$ Å) with the same instrument and temperature. The crystal structures were solved by direct methods using SHELX version 6.1 program package.[S2] Non-hydrogen atoms were refined anisotropically. Absorption corrections were applied using SADABS program (*SADABS*, an empirical absorption correction program, part of the SAINTPlus NT version 5.0 package; Bruker AXS: Madison, WI 1998). Data collected were corrected for Lorentz and polarization effects with Saint[S2] and absorption using Blessing's method and merged as incorporated with the program.[S3,S4] The SHELXTL[S5] program package was now implemented to determine the space group based upon intensity statistics. The structure was determined by direct methods with a majority of the non-hydrogen atoms from the molecule of interest being located directly using the program XT.[S6] Refinement of the structure was achieved using the program XL.[S7] Difference-Fourier least-squares refinement cycles were required to locate the remaining non-hydrogen atoms.

3.1. Refinement details

For **2**, **3**(·solvent), **4**(·0.5C_6D_6), **5**(·C_6D_6) and **6** the refinements were performed in the following manner. Compound **2** has one disordered K atom and one disordered phenyl groups next to a symmetry element. The later was refined using PART instructions resulting in 50% occupancy for each part. Compound **3**(·solvent) has one disordered THF molecule per asymmetric unit that was refined with the PLATON SQUEEZE routine.[S8] Compound **4**(·0.5C_6D_6) was refined without using constraints or restraints and two reflexes were omitted. Compound **5**(·C_6D_6) was refined without using constraints or restraints and six reflexes were omitted. Compound **6** was refined without using constraints or restraints and one reflex was omitted.

Table S1. Crystal data and structure refinement for **2**, **3**(·solvent) and **4**(·0.5C_6H_6).

Compound	**2**	**3**(·solvent)	**4**(·0.5C_6H_6)
CCDC number	**2154218**	**2154219**	**2154220**
Empirical formula	$C_{45}H_{70}KN_5Si_{11}$	$C_{63}H_{106}KN_7O_6Si_{11}$	$C_{50}H_{79}IN_5Si_{11}$
Formula weight /g·mol^{-1}	1029.15	1405.63	1186.07
Crystal color, shape	yellow plate	orange block	pale yellow plate
Crystal size /mm^3	0.204 × 0.358 × 0.404	0.321 × 0.367 × 0.457	0.189 × 0.302 × 0.414
Crystal system	monoclinic	triclinic	triclinic
Space group	$P2_1/n$	P-1	P-1
a /Å b /Å c /Å	15.5664(5) 18.7250(6) 19.2084(6)	13.6587(4) 15.9267(5) 21.2413(6)	12.5574(5) 13.3175(5) 20.6076(8)
α /° β /° γ /°	90 100.860(2) 90	78.5250(10) 73.5770(10) 72.8440(10)	91.468(2) 106.579(2) 110.641(2)
V /Å^3	5498.6(3)	4201.3(2)	3060.2(2)
Z	4	2	2
T /K	100(2)	100(2)	100(2)
Completeness to θ 25.24° /%	99.9	98.3	99.6
ρ_{calc} /g·cm^{-3}	1.243	1.111	1.287
μ(Mo) or μ(Cu)/mm^{-1}	0.372	0.266	0.775
2Θ range /°	3.06-54.65	4.18-54.23	2.08-54.81
Reflections measured	61109	53115	42882
Independent reflections	12327	18288	13688
R(int)	0.0508	0.0299	0.0354
Ind. reflections ($I > 2\sigma(I)$)	9063	16658	12545
Parameters	599	808	621
Restraints	0	0	0
R_1 ($I > 2\sigma(I)$)	0.0567	0.0423	0.0353
wR_2 (all data)	0.1621	0.1187	0.0969
GooF (all data)	1.060	1.091	1.045
Max. peak/hole /e$^-$·Å^{-3}	0.753 /-0.302	1.085 /-0.435	1.690 /-0.567
Absorption correction type	Multi-scan	Multi-scan	Multi-scan
Min. /Max. transmission	0.4639 /0.7455	0.5630 /0.7455	0.6102 /0.7455

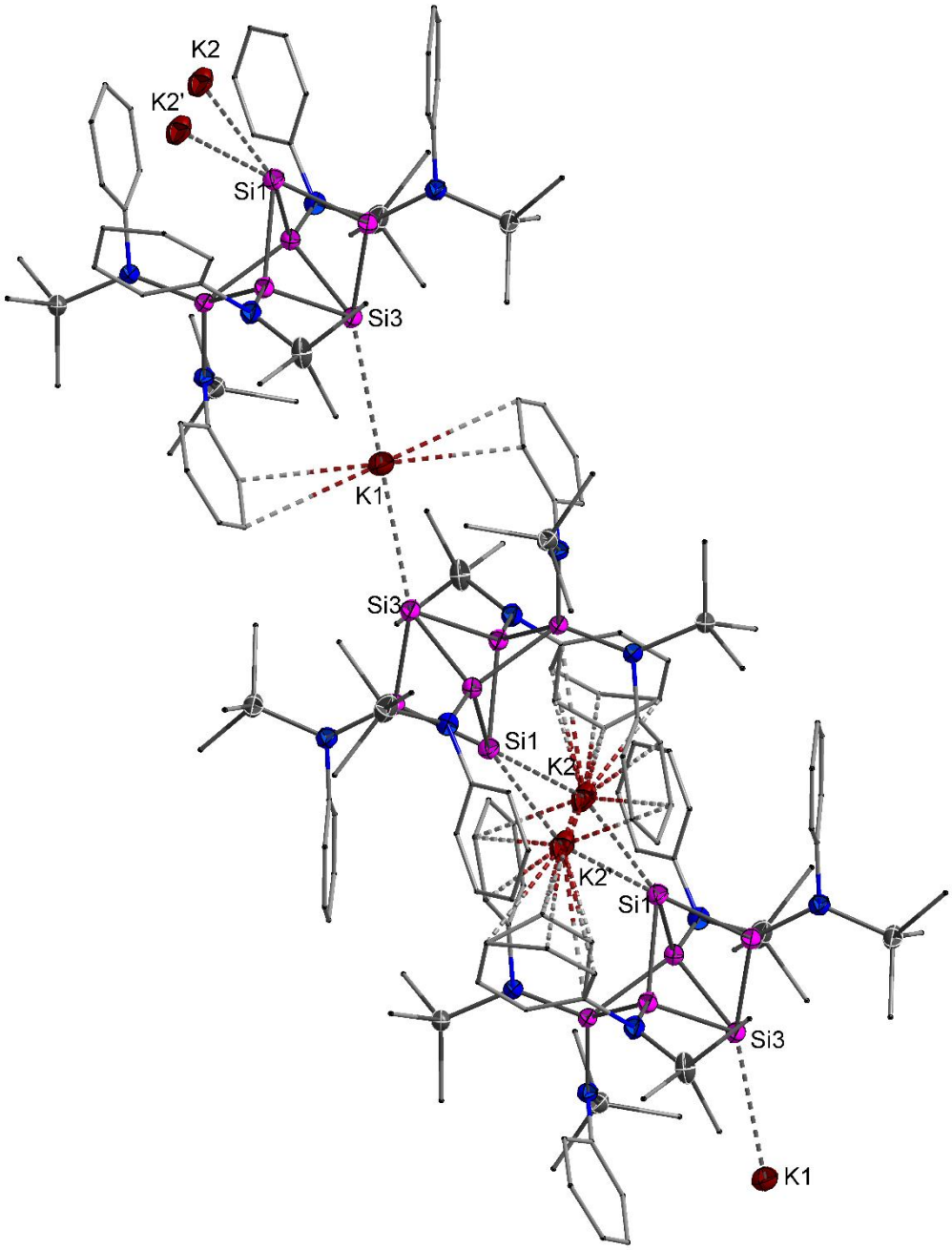


Figure S70. Molecular structure of **2**.

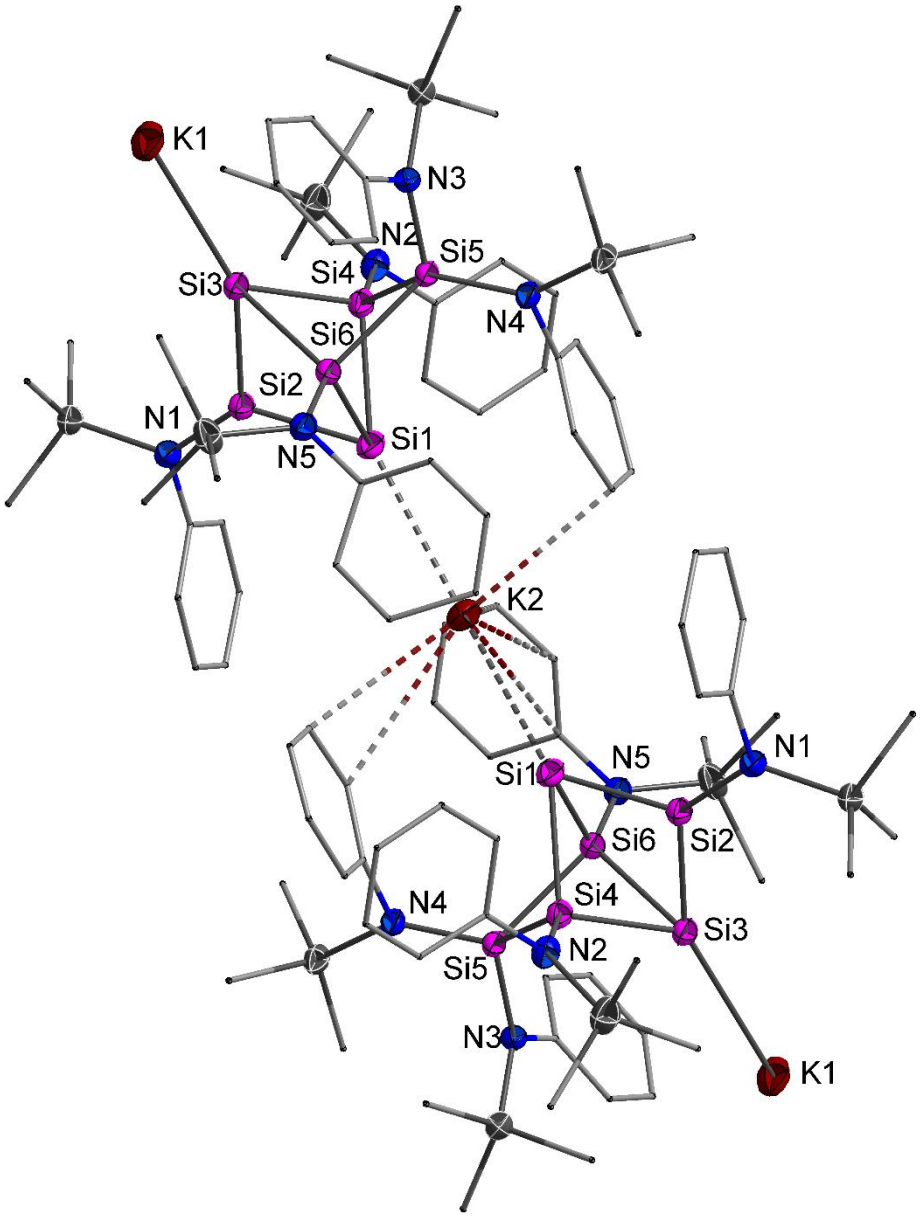


Figure S71. Molecular structure of **2**.

Selected distances /Å:

Si1−Si2 2.2782(11), Si1−Si6 2.4168(11), Si1−Si4 2.4169(11), Si2−Si3 2.2897(10), Si2−Si4 2.6631(11), Si2−Si6 2.6969(11), Si3−Si6 2.4048(11), Si3−Si4 2.4365(11), Si4−Si5 2.3898(11), Si4−Si6 2.6443(12), Si5−Si6 2.3514(11), Si2−N1 1.741(2), Si4−N2 1.756(3), Si5−N3 1.781(2), Si5−N4 1.755(2), Si6−N5 1.760(3), Si7−N1 1.764(2), Si8−N2 1.748(3), Si9−N3 1.761(2), Si10−N4 1.754(2), Si11−N5 1.739(3), Si7−C7 1.862(3), Si7−C8 1.858(4), Si7−C9 1.850(3), Si8−C16 1.851(3), Si8−C17 1.854(4), Si8−C18 1.855(4),

Si9−C25 1.861(3), Si9−C26 1.866(3), Si9−C27 1.851(3), Si10−C34 1.831(3), Si10−C35 1.857(4), Si10−C36 1.867(4), Si11−C43 1.862(4), Si11−C44 1.863(4), Si11−C45 1.857(4), K1····Si3 3.3172(7), K1····C20 3.159(3), K1····C21 3.378(3), K2····Si1 3.4206(16), K2‘····Si1 3.2833(15), K2····C30 3.316(4), K2····C37 3.407(3), K2····C40 3.108(5), K2····C41 3.214(9), K2····C42 3.299(9).

Selected angles /°:

Si2-Si1-Si6 70.05(3), Si2-Si1-Si4 69.04(3), Si6-Si1-Si4 66.33(3), Si1-Si2-Si3 104.08(4), Si1-Si2-Si4 57.94(3), Si3-Si2-Si4 58.36(3), Si1-Si2-Si6 57.39(3), Si3-Si2-Si6 56.96(3), Si4-Si2-Si6 59.12(3), Si2-Si3-Si6 70.08(3), Si2-Si3-Si4 68.51(3), Si6-Si3-Si4 66.21(3), Si5-Si4-Si1 92.71(4), Si5-Si4-Si3 87.42(4), Si1-Si4-Si3 95.82(4), Si5-Si4-Si6 55.41(3), Si1-Si4-Si6 56.83(3), Si3-Si4-Si6 56.32(3), Si5-Si4-Si2 116.38(4), Si1-Si4-Si2 53.02(3), Si3-Si4-Si2 53.13(3), Si6-Si4-Si2 61.08(3), Si6-Si5-Si4 67.79(3), Si5-Si6-Si3 89.04(4), Si5-Si6-Si1 93.68(4), Si3-Si6-Si1 96.66(4), Si5-Si6-Si4 56.79(3), Si3-Si6-Si4 57.47(3), Si1-Si6-Si4 56.84(3), Si5-Si6-Si2 116.49(4), Si3-Si6-Si2 52.96(3), Si1-Si6-Si2 52.56(3), Si4-Si6-Si2 59.80(3), N1-Si2-Si1 127.00(8), N1-Si2-Si3 128.66(8), N1-Si2-Si4 144.78(9), N1-Si2-Si6 156.08(9), N2-Si4-Si5 131.39(9), N2-Si4-Si1 119.07(9), N2-Si4-Si3 121.20(9), N2-Si4-Si6 173.18(9), N2-Si4-Si2 112.16(9), N4-Si5-N3 107.64(11), N4-Si5-Si6 121.66(8), N3-Si5-Si6 116.58(8), N4-Si5-Si4 121.49(8), N3-Si5-Si4 117.55(8), N5-Si6-Si5 128.63(9), N5-Si6-Si3 123.05(9), N5-Si6-Si1 117.57(8), N5-Si6-Si4 173.67(8), N5-Si6-Si2 114.88(8), N1-Si7-C9 109.26(13), N1-Si7-C8 109.72(14), C9-Si7-C8 107.54(18), N1-Si7-C7 109.83(13), C9-Si7-C7 108.98(16), C8-Si7-C7 111.45(18), N2-Si8-C16 114.69(15), N2-Si8-C17 107.86(16), C16-Si8-C17 106.42(18), N2-Si8-C18 111.23(17), C16-Si8-C18 106.6(2), C17-Si8-C18 109.9(3), N3-Si9-C27 107.18(12), N3-Si9-C25 112.24(14), C27-Si9-C25 107.21(15), N3-Si9-C26 112.31(14), C27-Si9-C26 110.51(15), C25-Si9-C26 107.29(15), N4-Si10-C34 114.45(13), N4-Si10-C35 111.59(15), C34-Si10-C35 106.89(17), N4-Si10-C36 108.11(14), C34-Si10-C36 109.58(18), C35-Si10-C36 105.9(2), N5-Si11-C45 110.13(14), N5-Si11-C43 108.00(16), C45-Si11-C43 109.5(2), N5-Si11-C44 111.92(17), C45-Si11-C44 107.79(18), C43-Si11-C44 109.46(18), C1-N1-Si2 116.98(18), C1-N1-Si7 115.95(18), Si2-N1-Si7 126.86(13), C10-N2-Si8 110.34(19), C10-N2-Si4 117.7(2), Si8-N2-Si4 130.54(14), C19-N3-Si9 120.57(17), C19-N3-Si5 117.85(18), Si9-N3-Si5 120.32(13), C28-N4-Si10 109.83(16), C28-N4-Si5 114.30(17), Si10-N4-Si5 135.86(13),

C37-N5-Si11 117.5(2), C37-N5-Si6 115.1(2), Si11-N5-Si6 125.28(14).

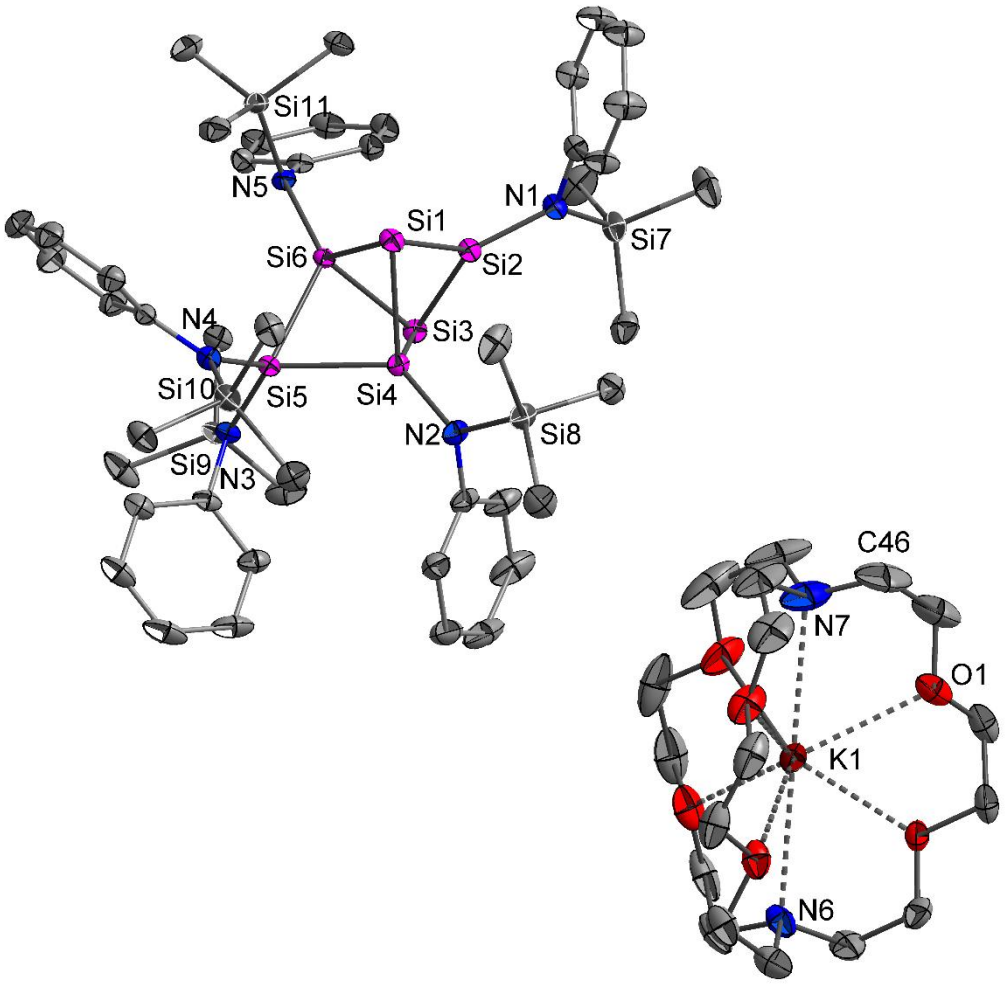


Figure S72. Molecular structure of **3**.

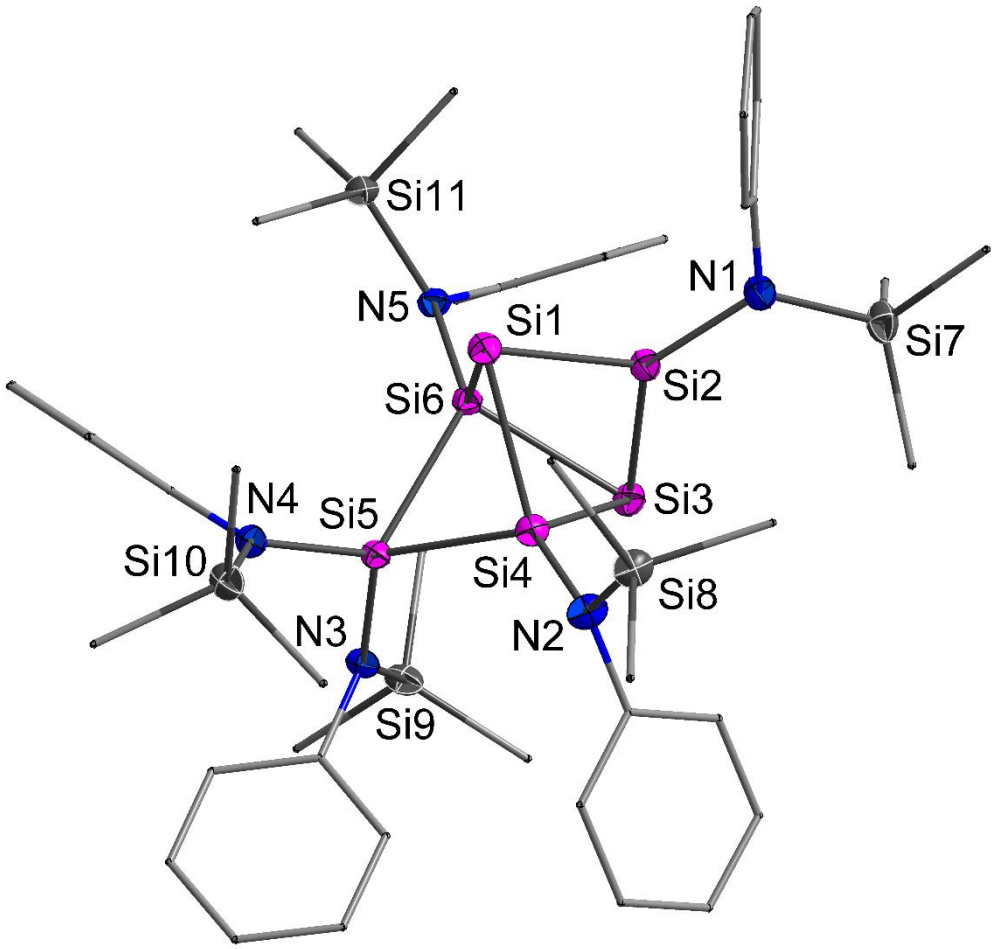


Figure S73. Molecular structure of **3**.

Selected distances /Å:

Si1−Si2 2.2936(6), Si1−Si4 2.4303(6), Si1−Si6 2.4359(6), Si2−Si3 2.2936(6), Si2−Si4 2.6092(6), Si2−Si6 2.6574(6), Si3−Si6 2.4189(6), Si3−Si4 2.4530(6), Si4−Si5 2.3625(6), Si4−Si6 2.6331(6), Si5−Si6 2.3638(6), Si2−N1 1.7541(14), Si4−N2 1.7719(14), Si5−N3 1.7690(13), Si5−N4 1.7892(13), Si6−N5 1.7698(13), Si7−N1 1.7590(14), Si7−C7 1.860(2), Si7−C9 1.863(2), Si7−C8 1.865(2), Si8−N2 1.7452(14), Si8−C18 1.862(2), Si8−C17 1.863(2), Si8−C16 1.865(2), Si9−N3 1.7404(13), Si9−C26 1.8566(17), Si9−C27 1.866(2), Si9−C25 1.874(2), Si10−N4 1.7629(14), Si10−C35 1.8601(19), Si10−C36 1.8734(18), Si10−C34 1.8752(19), Si11−N5 1.7584(14), Si11−C43 1.8546(18), Si11−C45 1.8700(18), Si11−C44 1.873(2), K1····O4 2.7891(15), K1····O5 2.8013(17), K1····O6 2.8111(15), K1····O2 2.8267(13),

K1····O1 2.8382(16), K1····O3 2.8757(16), K1····N7 2.999(2), K1····N6 3.0354(17).

Selected angles /°:

Si2-Si1-Si4 66.983(19), Si2-Si1-Si6 68.294(18), Si4-Si1-Si6 65.516(18),
Si1-Si2-Si3 106.36(2), Si1-Si2-Si4 59.014(17), Si3-Si2-Si4 59.631(17),
Si1-Si2-Si6 58.394(17), Si3-Si2-Si6 57.936(17), Si4-Si2-Si6 59.987(16),
Si2-Si3-Si6 68.593(19), Si2-Si3-Si4 66.594(18), Si6-Si3-Si4 65.427(18),
Si5-Si4-Si1 90.71(2), Si5-Si4-Si3 89.90(2), Si1-Si4-Si3 97.52(2),
Si5-Si4-Si2 117.08(2), Si1-Si4-Si2 54.003(16), Si3-Si4-Si2 53.775(16),
Si5-Si4-Si6 56.167(16), Si1-Si4-Si6 57.344(17), Si3-Si4-Si6 56.661(16),
Si2-Si4-Si6 60.914(16), Si4-Si5-Si6 67.713(18), Si5-Si6-Si3 90.71(2),
Si5-Si6-Si1 90.54(2), Si3-Si6-Si1 98.29(2), Si5-Si6-Si4 56.120(16),
Si3-Si6-Si4 57.912(17), Si1-Si6-Si4 57.140(17), Si5-Si6-Si2 115.22(2),
Si3-Si6-Si2 53.471(16), Si1-Si6-Si2 53.312(16), Si4-Si6-Si2 59.099(16).
N1-Si2-Si1 127.81(5), N1-Si2-Si3 125.82(5), N1-Si2-Si4 147.37(5),
N1-Si2-Si6 152.62(5), N2-Si4-Si5 128.95(5), N2-Si4-Si1 121.53(5),
N2-Si4-Si3 119.68(5), N2-Si4-Si2 113.94(5), N2-Si4-Si6 174.66(5),
N3-Si5-N4 105.38(6), N3-Si5-Si4 120.37(5), N4-Si5-Si4 119.97(5),
N3-Si5-Si6 121.74(5), N4-Si5-Si6 118.81(5), N5-Si6-Si5 130.36(5),
N5-Si6-Si3 120.87(5), N5-Si6-Si1 117.95(5), N5-Si6-Si4 173.16(5),
N5-Si6-Si2 114.38(5).

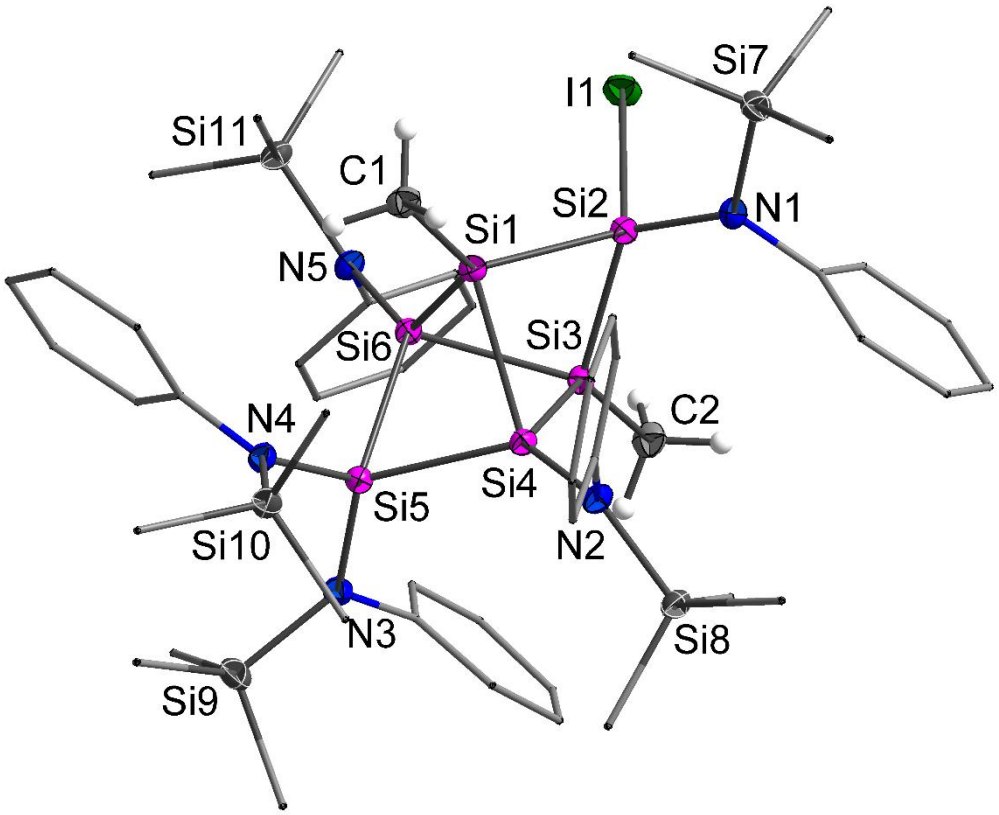


Figure S74. Molecular structure of **4**.

Selected distances /Å:

I1−Si2 2.5352(6), Si1−C1 1.866(2), Si3−C2 1.859(2),
Si1−Si2 2.3137(8), Si1−Si6 2.3335(8), Si1−Si4 2.3982(7), Si2−Si3 2.3096(8),
Si3−Si4 2.3380(8), Si3−Si6 2.3720(8), Si4−Si5 2.3778(7), Si5−Si6 2.3653(7),
Si2−N1 1.7323(18), Si4−N2 1.7525(18), Si5−N3 1.7394(18), Si5−N4 1.7537(18),
Si6−N5 1.7361(17), Si7−N1 1.7592(18), Si7−C9 1.858(2), Si7−C10 1.859(2),
Si7−C11 1.852(2), Si8−N2 1.7593(18), Si8−C18 1.859(2), Si8−C19 1.855(2),
Si8−C20 1.862(2), Si9−N3 1.7600(18), Si9−C27 1.846(3), Si9−C28 1.860(3),
Si9−C29 1.873(3), Si10−N4 1.7629(18), Si10−C36 1.863(2), Si10−C37 1.857(2),
Si10−C38 1.861(2), Si11−N5 1.7472(18), Si11−C45 1.858(2), Si11−C46 1.850(2),
Si11−C47 1.851(2).

Selected angles /°:

C1-Si1-Si2 130.77(7), C1-Si1-Si6 128.22(8), C1-Si1-Si4 126.81(7), C2-Si3-Si2 125.99(8), C2-Si3-Si4 132.62(8), C2-Si3-Si6 127.53(8), Si3-Si2-I1 108.54(3), Si1-Si2-I1 117.13(3), Si2-Si1-Si6 90.47(3), Si2-Si1-Si4 87.81(3), Si6-Si1-Si4 75.19(2), Si3-Si2-Si1 78.55(3), Si2-Si3-Si4 89.36(3), Si2-Si3-Si6 89.61(3), Si4-Si3-Si6 75.60(2), Si3-Si4-Si5 93.92(3), Si3-Si4-Si1 76.33(2), Si5-Si4-Si1 87.28(3), Si6-Si5-Si4 74.99(2), Si1-Si6-Si5 89.09(3), Si1-Si6-Si3 76.92(3), Si5-Si6-Si3 93.37(3), N1-Si2-I1 106.02(6), N1-Si2-Si3 124.28(7), N1-Si2-Si1 120.68(7), N2-Si4-Si3 125.89(6), N2-Si4-Si5 132.23(6), N2-Si4-Si1 123.75(6), N3-Si5-N4 111.13(9), N3-Si5-Si6 120.18(7), N4-Si5-Si6 112.46(6), N3-Si5-Si4 120.00(6), N4-Si5-Si4 113.80(6), N5-Si6-Si1 127.80(6), N5-Si6-Si5 130.68(7), N5-Si6-Si3 123.11(7).

Table S2. Crystal data and structure refinement for **5**(·C_6H_6), **6**.

Compound	**5**(·C_6H_6)	**6**
CCDC number	**2154221**	**2154222**
Empirical formula	$C_{51}H_{76}Cl_5N_5Si_{12}$	$C_{45}H_{70}Br_5N_5Si_{12}$
Formula weight /g·mol^{-1}	1273.49	1417.69
Crystal color, shape	colourless, block	yellow, rod
Crystal size /mm^3	0.639×0.403×0.298	0.627×0.353×0.270
Crystal system	triclinic	monoclinic
Space group	*P*-1	$P2_1/n$
a /Å *b* /Å *c* /Å	13.0493(5) 13.4471(6) 20.7283(9)	20.6155(6) 13.5318(4) 23.7454(7)
α /° *β* /° *γ* /°	71.982(2) 84.352(2) 72.0140(10)	90 111.4260(10) 90
V /Å^3	3289.9(2)	6166.3(3)
Z	2	4
T /K	100(2)	101(2)
Completeness to *θ* 25.24° /%	98.3	99.9
ρ_{calc} /g·cm^{-3}	1.286	1.527
μ(Mo) or *μ*(Cu)/mm^{-1}	0.477	3.527
2*Θ* range /°	3.93-54.27	3.76-54.27
Reflections measured	43541	83454
Independent reflections	14291	13624
R(int)	0.0236	0.0262
Ind. reflections ($I > 2\sigma(I)$)	13411	12669
Parameters	673	619
Restraints	0	0
R_1 ($I > 2\sigma(I)$)	0.0269	0.0232
wR_2 (all data)	0.0765	0.0558
GooF (all data)	1.077	1.096
Max. peak/hole /e$^-$·Å^{-3}	0.487 /-0.406	0.645 /-0.331
Absorption correction type	multi-scan	multi-scan
Min. /Max. transmission	0.6723 / 0.7455	0.4598 / 0.7455

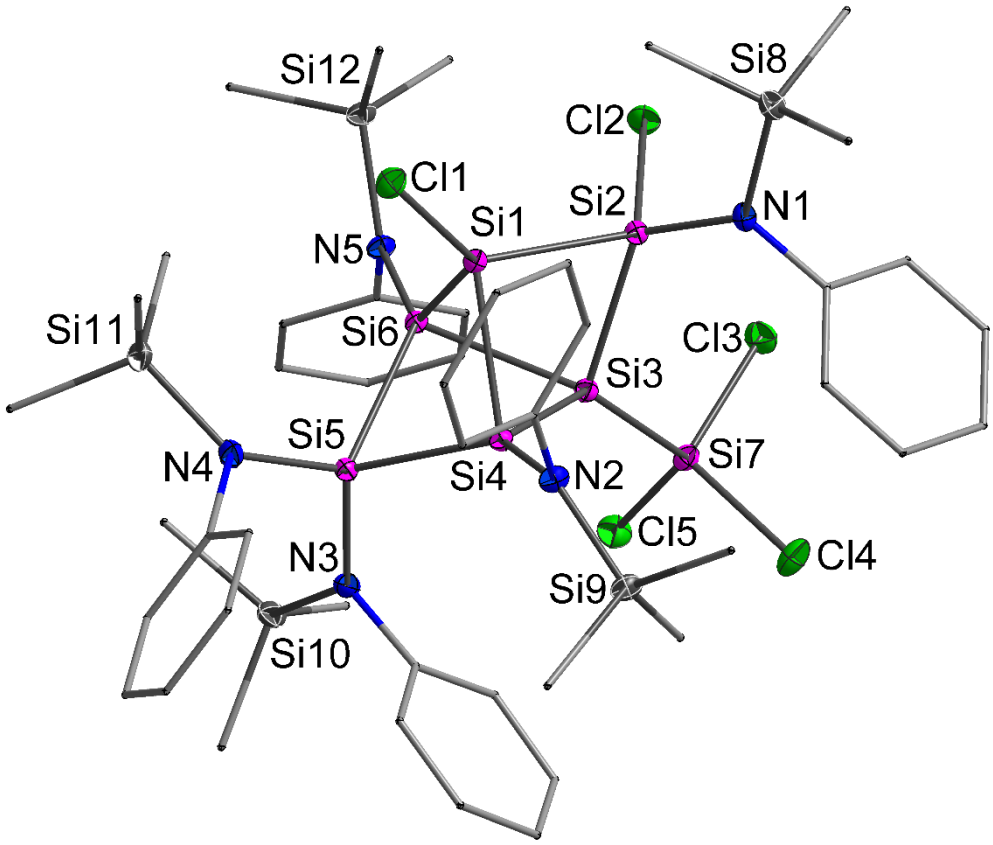


Figure S75. Molecular structure of **5**.

Selected distances /Å:

Si1−Si2 2.3215(5), Si1−Si6 2.3275(5), Si1−Si4 2.3771(5), Si1−Si3 2.8330(5), Si2−Si3 2.3402(5), Si3−Si7 2.3106(5), Si3−Si4 2.3471(5), Si3−Si6 2.4261(5), Si4−Si5 2.3969(5), Si5−Si6 2.3951(5), Cl1−Si1 2.0669(5), Cl2−Si2 2.0967(5), Cl3−Si7 2.0422(5), Cl4−Si7 2.0389(5), Cl5−Si7 2.0351(5), Si2−N1 1.7203(11), Si4−N2 1.7419(11), Si5−N3 1.7393(11), Si5−N4 1.7424(11), Si6−N5 1.7285(11), Si8−N1 1.7613(12), Si8−C7 1.8618(16), Si8−C8 1.8587(17), Si8−C9 1.8705(17), Si9−N2 1.7590(11), Si9−C16 1.8505(14), Si9−C17 1.8707(15), Si9−C18 1.8726(15), Si10−N3 1.7667(11),Si10−C25 1.8665(15), Si10−C26 1.8677(15), Si10−C27 1.8629(15), Si11−N4 1.7607(12), Si11−C34 1.8663(17), Si11−C35 1.8636(15), Si11−C36 1.8552(15), Si12−N5 1.7724(11), Si12−C43 1.8679(14), Si12−C44 1.8654(14), Si12−C45 1.8598(14).

Selected angles /°:

Si2-Si1-Si6 91.770(17), Si2-Si1-Si4 93.617(17), Si6-Si1-Si4 77.888(15),
Si2-Si1-Si3 52.876(13), Si6-Si1-Si3 55.037(13), Si4-Si1-Si3 52.669(13),
Si1-Si2-Si3 74.850(16), Si7-Si3-Si2 116.670(18), Si7-Si3-Si4 140.76(2),
Si2-Si3-Si4 93.917(17), Si7-Si3-Si6 124.813(19), Si2-Si3-Si6 88.878(16),
Si4-Si3-Si6 76.550(15), Si7-Si3-Si1 165.552(18), Si2-Si3-Si1 52.274(13),
Si4-Si3-Si1 53.639(13), Si6-Si3-Si1 51.833(12), Si3-Si4-Si1 73.692(15),
Si3-Si4-Si5 91.786(16), Si1-Si4-Si5 89.797(16), Si6-Si5-Si4 76.218(15),
Si1-Si6-Si5 91.035(16), Si5-Si6-Si3 89.912(16), Si1-Si6-Si3 73.130(15),
Cl1-Si1-Si2 131.56(2), Cl1-Si1-Si6 126.49(2), Cl1-Si1-Si4 120.104(19),
Cl1-Si1-Si3 172.77(2), Cl5-Si7-Cl4 105.06(2), Cl5-Si7-Cl3 106.41(2),
Cl4-Si7-Cl3 107.46(2), Cl5-Si7-Si3 117.64(2), Cl4-Si7-Si3 113.47(2),
Cl3-Si7-Si3 106.233(19), Cl2-Si2-Si1 114.724(19), Cl2-Si2-Si3 112.028(19),
N1-Si2-Cl2 105.59(4), N1-Si2-Si1 124.47(4), N1-Si2-Si3 123.00(4),
N2-Si4-Si3 127.76(4), N2-Si4-Si1 115.72(4), N2-Si4-Si5 136.55(4),
N3-Si5-N4 110.04(5), N3-Si5-Si6 119.26(4), N4-Si5-Si6 116.71(4),
N3-Si5-Si4 112.79(4), N4-Si5-Si4 118.42(4), N5-Si6-Si1 125.14(4),
N5-Si6-Si5 134.57(4), N5-Si6-Si3 123.80(4).

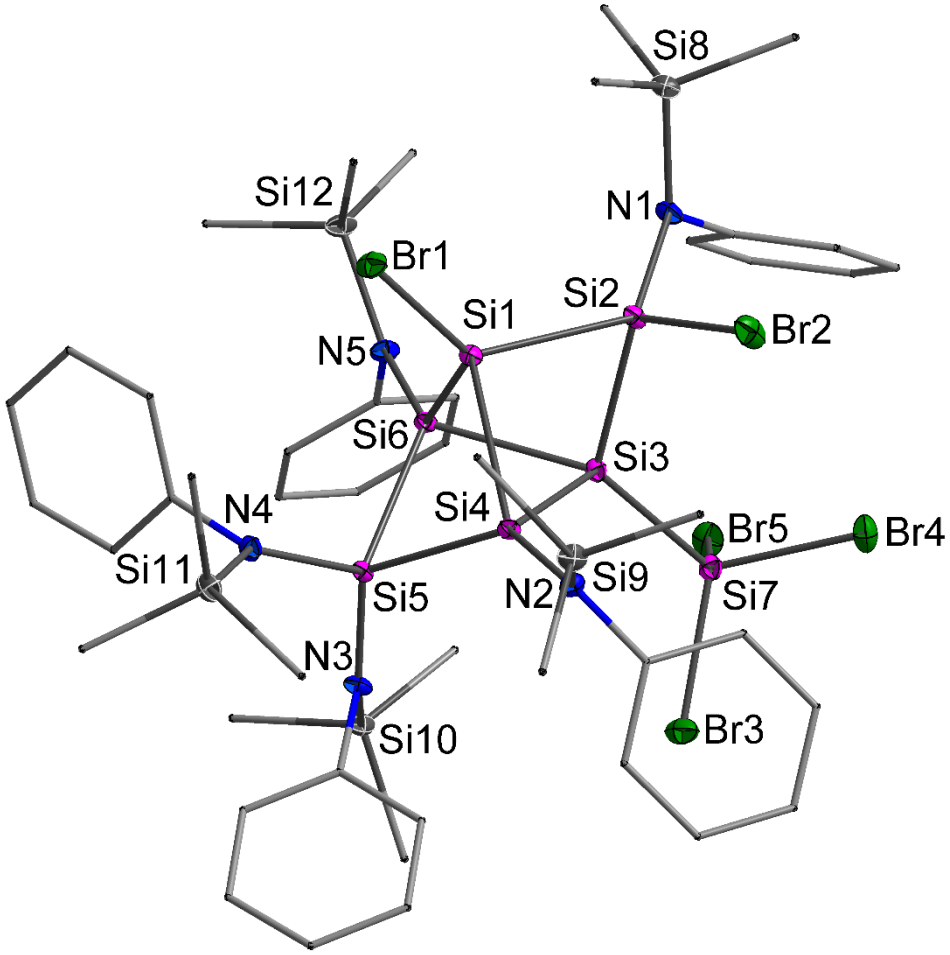


Figure S76. Molecular structure of **6**.

Selected distances /Å:

Si1−Si2 2.3327(7), Si1−Si4 2.3635(6), Si1−Si6 2.3833(6), Si1−Si3 2.8335(7), Si2−Si3 2.3364(7), Si3−Si7 2.3125(7), Si3−Si6 2.3766(7), Si3−Si4 2.3907(6), Si4−Si5 2.3958(6), Si5−Si6 2.3888(6), Br1−Si1 2.2466(5), Br2−Si2 2.2579(5), Br3−Si7 2.2192(5), Br4−Si7 2.2043(5), Br5−Si7 2.2095(5), Si2−N1 1.7190(15), Si4−N2 1.7345(15), Si5−N3 1.7393(15), Si5−N4 1.7441(15), Si6−N5 1.7326(15), Si8−N1 1.7617(15), Si8−C7 1.865(2), Si8−C8 1.858(2), Si8−C9 1.860(2), Si9−N2 1.7641(15), Si9−C16 1.859(2), Si9−C17 1.864(2), Si9−C18 1.857(2), Si10−N3 1.7649(15), Si10−C25 1.8674(19), Si10−C26 1.8636(19), Si10−C27 1.8557(19), Si11−N4 1.7599(15), Si11−C34 1.864(2), Si11−C35 1.861(2), Si11−C36 1.866(2), Si12−N5 1.7638(15), Si12−C43 1.859(2), Si12−C44 1.845(2), Si12−C45 1.865(2).

Selected angles /°:

Si2-Si1-Si4 92.36(2), Si2-Si1-Si6 92.92(2), Si4-Si1-Si6 77.04(2), Si2-Si1-Si3 52.695(17), Si4-Si1-Si3 53.859(17), Si6-Si1-Si3 53.358(17), Si1-Si2-Si3 74.73(2), Si7-Si3-Si2 124.37(3), Si7-Si3-Si6 133.41(3), Si2-Si3-Si6 93.00(2), Si7-Si3-Si4 123.08(3), Si2-Si3-Si4 91.58(2), Si6-Si3-Si4 76.65(2), Si7-Si3-Si1 172.59(3), Si2-Si3-Si1 52.578(18), Si6-Si3-Si1 53.577(17), Si4-Si3-Si1 52.975(17), Si1-Si4-Si5 90.25(2), Si3-Si4-Si5 91.48(2), Si6-Si5-Si4 76.32(2), Si3-Si6-Si1 73.07(2), Si3-Si6-Si5 92.00(2), Si1-Si6-Si5 89.94(2), Si1-Si4-Si3 73.17(2), Br1-Si1-Si2 127.46(2), Br1-Si1-Si4 126.04(2), Br1-Si1-Si6 126.55(2), Br1-Si1-Si3 179.85(3), Br2-Si2-Si1 113.04(2), Br2-Si2-Si3 113.48(2), Br4-Si7-Br5 106.31(2), Br4-Si7-Br3 108.37(2), Br5-Si7-Br3 107.72(2), Br4-Si7-Si3 110.02(2), Br5-Si7-Si3 113.21(2), Br3-Si7-Si3 110.99(2), N1-Si2-Br2 106.43(5), N1-Si2-Si1 125.48(6), N1-Si2-Si3 121.18(6), N2-Si4-Si1 125.86(5), N2-Si4-Si3 122.08(6), N2-Si4-Si5 134.79(6), N3-Si5-N4 111.24(7), N3-Si5-Si6 120.89(5), N4-Si5-Si6 111.71(5), N3-Si5-Si4 119.81(5), N4-Si5-Si4 112.76(5), N5-Si6-Si3 124.97(6), N5-Si6-Si1 125.01(5), N5-Si6-Si5 133.23(6).

4. DFT-calculations

4.1 Methods

All structures were optimized without geometry constraints with density functional theory, using the resolution of the identity approximation[S9] and an atom-pairwise dispersion correction (D3).[S10] A flexible triple zeta basis set (def2-TZVP)[S11] was used in all calculations. Geometry optimizations were performed with the TPSS[S12] functional. For the calculation of zero point vibrational energies and free enthalpy contributions (G_{298}) a rotor approximation was applied for vibrational modes with wave numbers below 100 cm^{-1}.[S13] All geometry optimizations and vibrational frequency calculations were performed with the TURBOMOLE 7.3 program.[S14] Single point calculations were performed with the ORCA program (version 3.0.3).[S15] Intrinsic atomic orbitals were generated with the IBO program.[S16]

4.2 Electronic situation of the anion in 3

The solid state structure of the anion in **3** was taken as a starting point for the vacuum geometry optimization with TPSS-D3/def2-TZVP. The minimum structure was similar to the molecular structure found in the crystal structure.

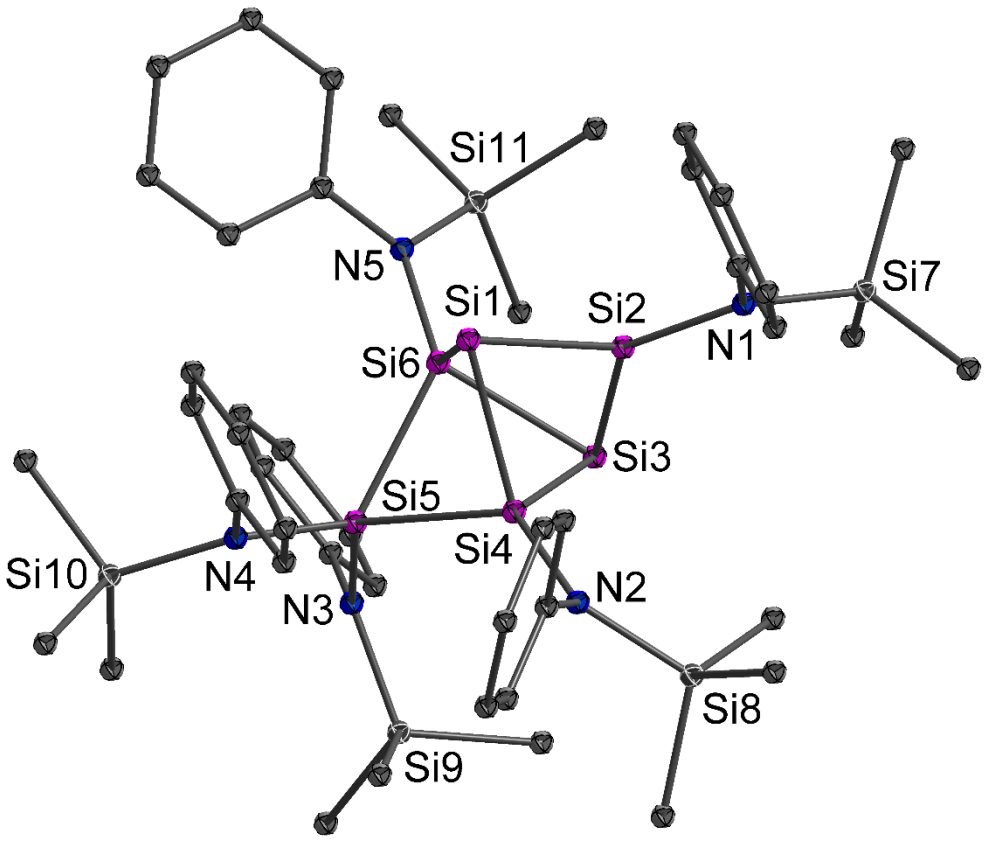


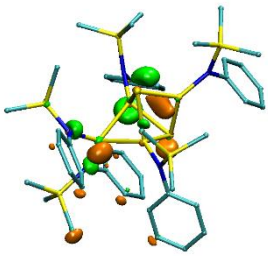
Figure S77. Gas phase (vacuum) structure of the anion in **3** optimized with DFT (TPSS-D3/def2-TZVP). Bond distances and angles are given in Table S3.

Table S3. Structural parameters of the anion in **3** after optimization with DFT (TPSS(D3-BJ)). Bond lengths are given in [Å], angles and dihedral angles in [°]. The numbering is taken from Figure S74.

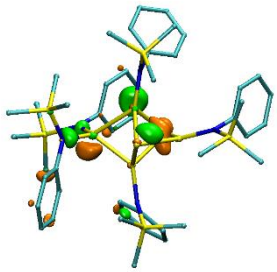
Parameter	TPSS-D3/def2-TZVP	X-ray
Si1-Si2	2.2977	2.2936(6)
Si2-Si3	2.3016	2.2936(6)
Si3-Si4	2.4400	2.4530(6)
Si4-Si5	2.3810	2.3625(6)
Si5-Si6	2.3231	2.3638(6)
Si6-Si3	2.4113	2.4189(6)
Si6-Si1	2.4130	2.4359(6)
Si1-Si4	2.4302	2.4303(6)
Si4···Si6	2.6253	2.6331
Si2···Si4	2.5458	2.6092
Si2···Si6	2.6706	2.6574
Si1···Si5	3.4459	3.4103
Si3···Si5	3.2976	3.4028
Si2-N1	1.7715	1.7541(14)
Si4-N2	1.7800	1.7719(14)
Si5-N3	1.7867	1.7690(13)
Si5-N4	1.7687	1.7892(13)
Si6-N5	1.7834	1.7698(13)
Si1-Si2-Si3	106.166	106.36(2)
Si6-Si3-Si4	65.521	65.427(18)
Si3-Si4-Si5	86.306	89.90(2)
Si4-Si5-Si6	67.834	67.713(18)
Si5-Si6-Si3	88.279	90.71(2)
Si4-Si1-Si6	65.646	65.516(18)
Si3-Si4-Si6-Si5	111.415	116.009

4.3 Electronic Structure of the anion in 3

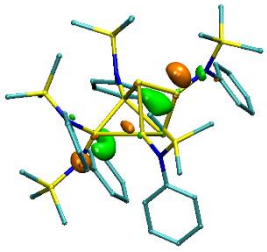
Figure S78. Kohn Sham molecular orbitals of the anion in **3**.



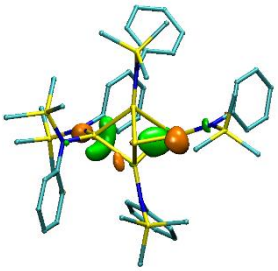
LUMO+18 (+0.847 eV, side view)



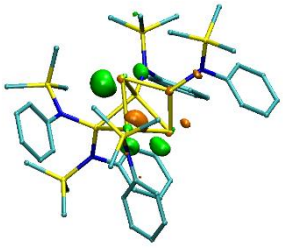
LUMO+18 (+0.847 eV, top view)



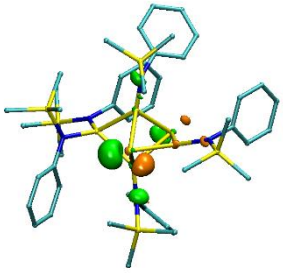
LUMO+14 (+0.457 eV, side view)



LUMO+14 (+0.457 eV, top view)

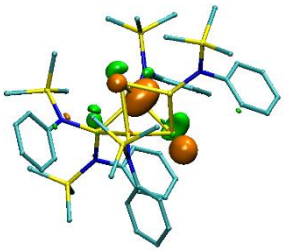


LUMO+13 (+0.390 eV, side view)

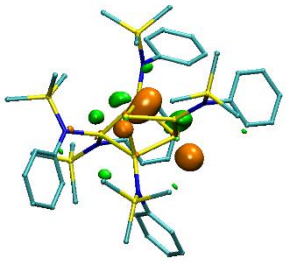


LUMO+13 (+0.390 eV, top view)

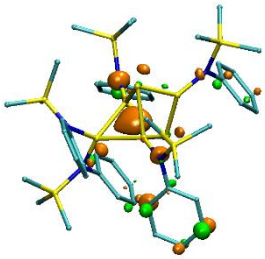
Figure S78 (continued). Kohn Sham molecular orbitals of the anion in **3**.



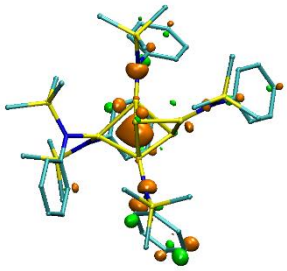
LUMO+12 (+0.195 eV, side view)



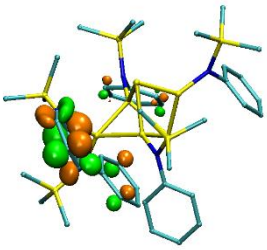
LUMO+12 (+0.195 eV, top view)



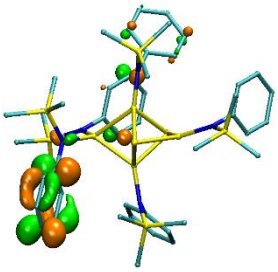
LUMO+11 (-0.343 eV, side view)



LUMO+11 (-0.343 eV, top view)

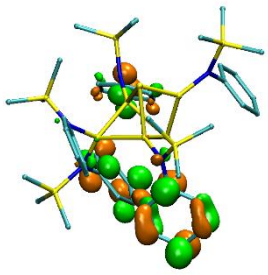


LUMO+10 (-0.509 eV, side view)

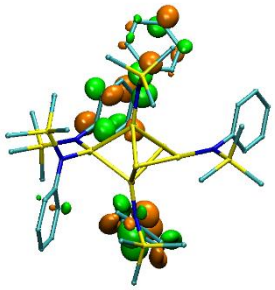


LUMO+10 (-0.509 eV, top view)

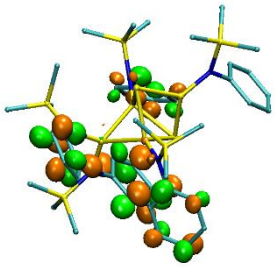
Figure S78 (continued). Kohn Sham molecular orbitals of the anion in **3**.



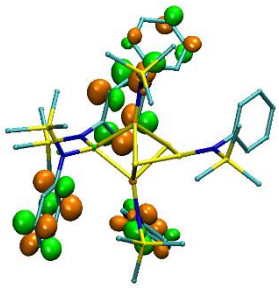
LUMO+9 (-0.579 eV, side view)



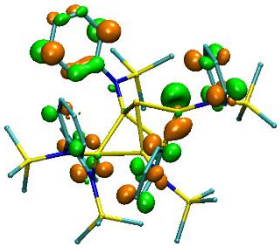
LUMO+9 (-0.579 eV, top view)



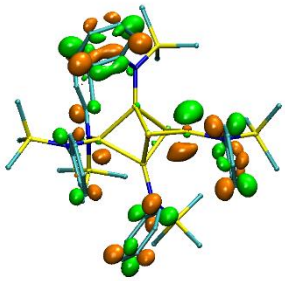
LUMO+8 (-0.658 eV, side view)



LUMO+8 (-0.658 eV, top view)

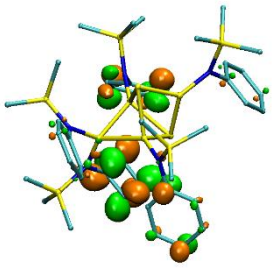


LUMO+7 (-0.676 eV, side view)

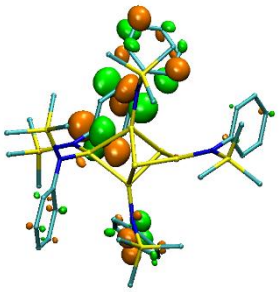


LUMO+7 (-0.676 eV, top view)

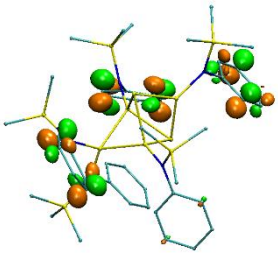
Figure S78 (continued). Kohn Sham molecular orbitals of the anion in **3**.



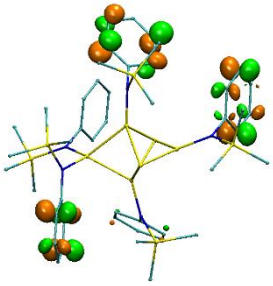
LUMO+6 (-0.692 eV, side view)



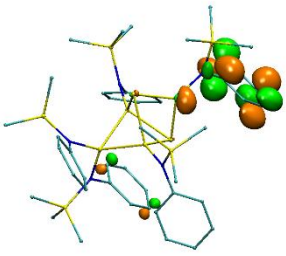
LUMO+6 (-0.692 eV, top view)



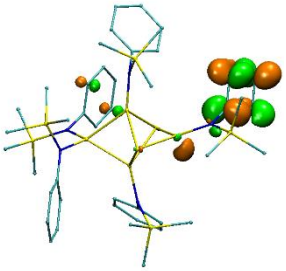
LUMO+5 (-0.816 eV, side view)



LUMO+5 (-0.816 eV, top view)

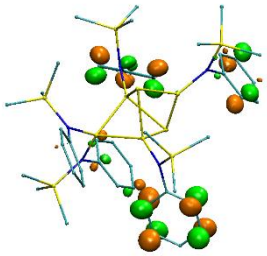


LUMO+4 (-0.863 eV, side view)

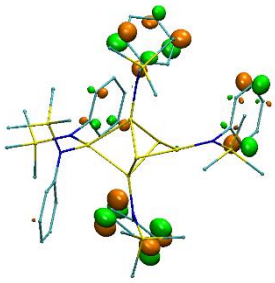


LUMO+4 (-0.863 eV, top view)

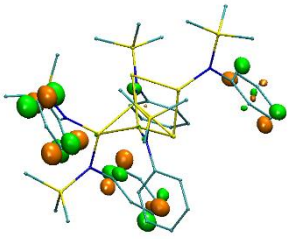
Figure S78 (continued). Kohn Sham molecular orbitals of the anion in **3**.



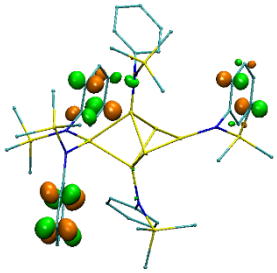
LUMO+3 (-0.877 eV, side view)



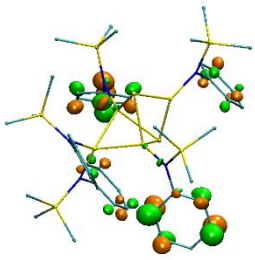
LUMO+3 (-0.877 eV, top view)



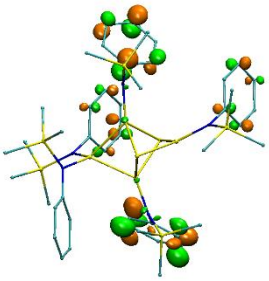
LUMO+2 (-0.930 eV, side view)



LUMO+2 (-0.930 eV, top view)

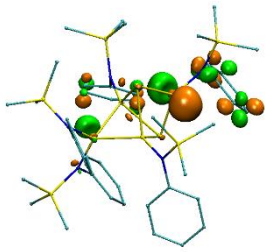


LUMO+1 (-0.978 eV, side view)

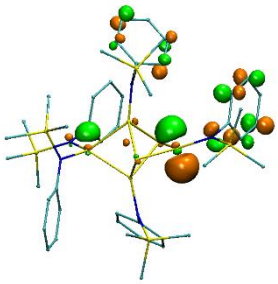


LUMO+1 (-0.978 eV, top view)

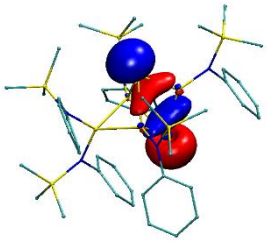
Figure S78 (continued). Kohn Sham molecular orbitals of the anion in **3**.



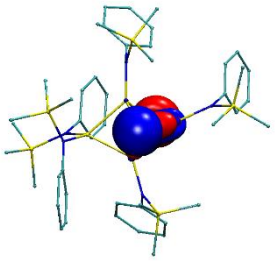
LUMO (-1.155 eV, side view)



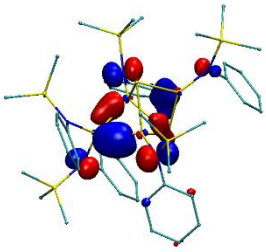
LUMO (-1.155 eV, top view)



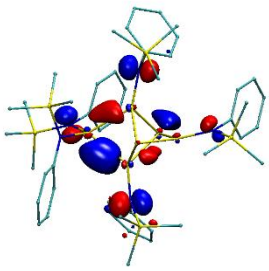
HOMO (-3.531 eV, side view)



HOMO (-3.531 eV, top view)

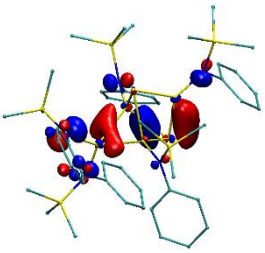


HOMO-1 (-3.977 eV, side view)

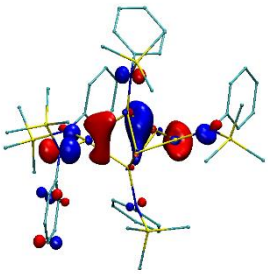


HOMO-1 (-3.977 eV, top view)

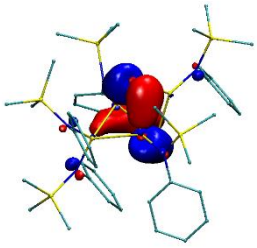
Figure S78 (continued). Kohn Sham molecular orbitals of the anion in **3**.



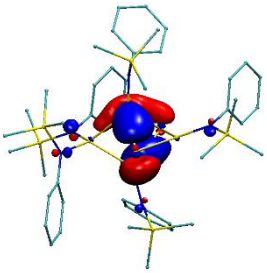
HOMO-2 (-4.266 eV, side view)



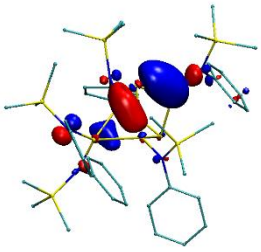
HOMO-2 (-4.266 eV, top view)



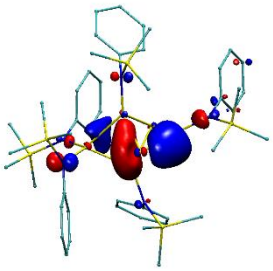
HOMO-3 (-4.418 eV, side view)



HOMO-3 (-4.418 eV, top view)

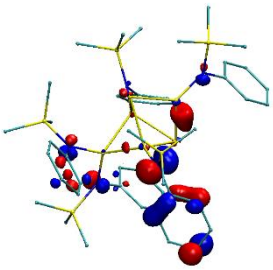


HOMO-4 (-4.734 eV, side view)

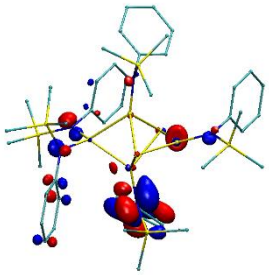


HOMO-4 (-4.734 eV, top view)

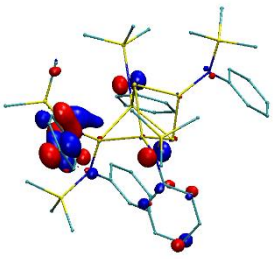
Figure S78 (continued). Kohn Sham molecular orbitals of the anion in **3**.



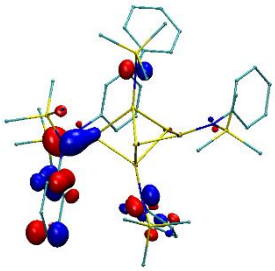
HOMO-5 (-4.960 eV, side view)



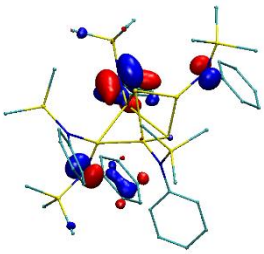
HOMO-5 (-4.960 eV, top view)



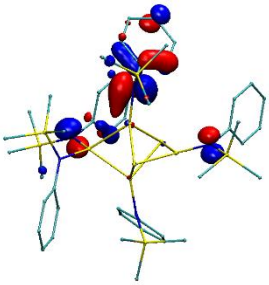
HOMO-6 (-5.075 eV, side view)



HOMO-6 (-5.075 eV, top view)



HOMO-7 (-5.410 eV, side view)



HOMO-7 (-5.410 eV, top view)

Figure S78. Kohn-Sham (frontier) molecular orbitals of the anion in **3** (TPSS-D3/def2-TZVP, 0.04 a.u.).

4.4 Intrinsic bond orbitals of the anion in 3

IBO 236 AB -0.365279 SI 5 0.970 SI 4 0.948 SI 2 0.032 (other: 0.050)

IBO 237 AB -0.355419 SI 2 1.096 SI 3 0.819 SI 5 0.026 (other: 0.059)

IBO 238 AB -0.352912 SI 2 1.091 SI 1 0.823 SI 5 0.028 (other: 0.058)

IBO 239 AB -0.352328 SI 6 0.968 SI 5 0.913 SI 2 0.059 SI 4 0.027 (other: 0.033)

IBO 240 AB -0.338089 SI 6 0.935 SI 1 0.773 SI 2 0.193 SI 5 0.030 SI 4 0.029 (other: 0.041)

IBO 241 AB -0.336673 SI 6 0.950 SI 3 0.768 SI 2 0.186 SI 4 0.032 SI 5 0.025 (other: 0.040)

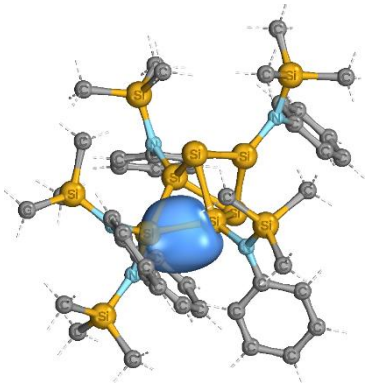
IBO 242 AB -0.334669 SI 4 0.969 SI 1 0.816 SI 2 0.103 SI 5 0.036 SI 6 0.033 (other: 0.043)

IBO 243 AB -0.329309 SI 4 0.956 SI 3 0.826 SI 2 0.110 SI 6 0.041 SI 5 0.028 (other: 0.039)

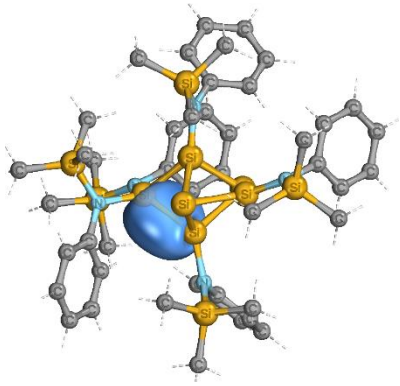
IBO 244 AB -0.289914 SI 3 1.941 SI 1 0.026 (other: 0.033)

IBO 245 AB -0.277143 SI 1 1.921 SI 3 0.023 (other: 0.056)

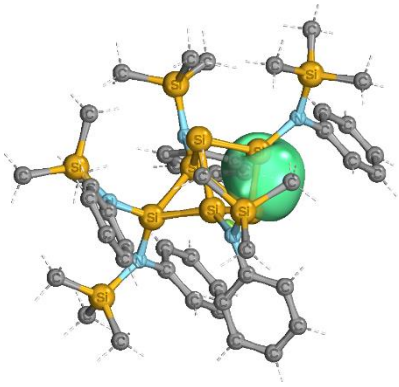
Figure S79. Intrinsic bond orbitals of the anion in **3**.



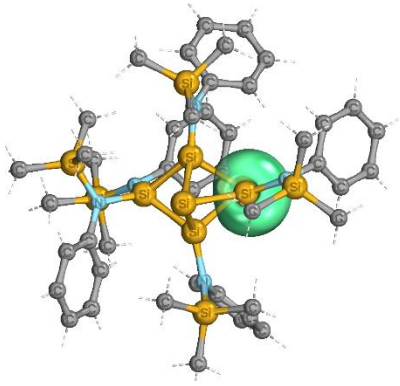
IBO 236 (side)



IBO 236 (top)

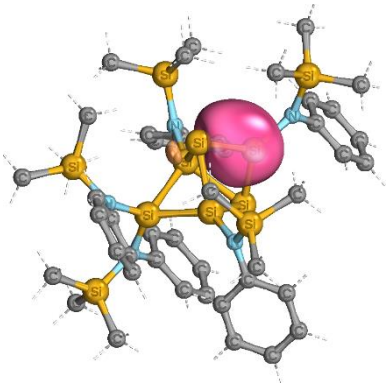


IBO 237 (side)

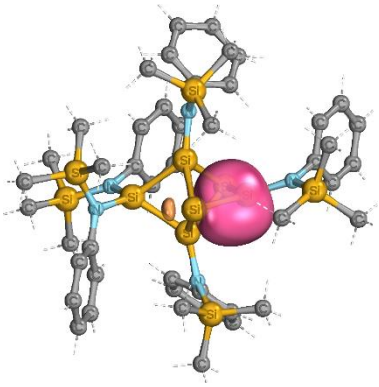


IBO 237 (top)

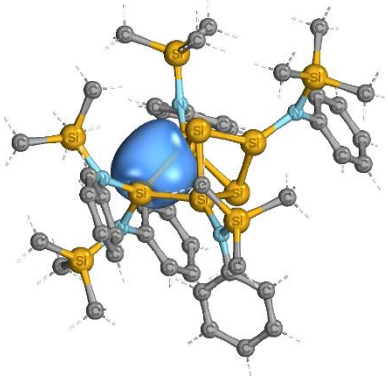
Figure S79 (continued). Intrinsic bond orbitals of the anion in **3**.



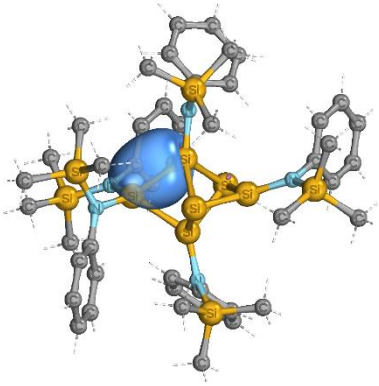
IBO 238 (side)



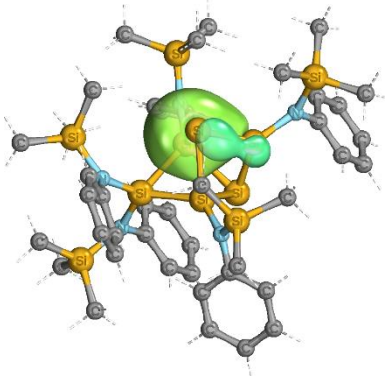
IBO 238 (top)



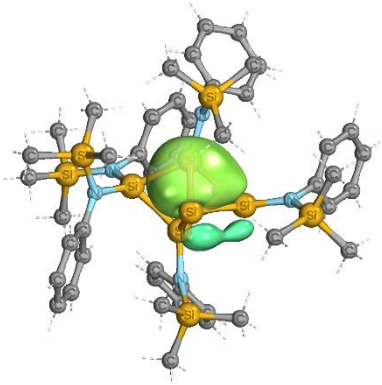
IBO 239 (side)



IBO 239 (top)

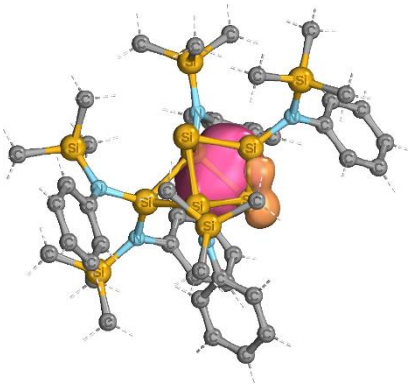


IBO 240 (side)

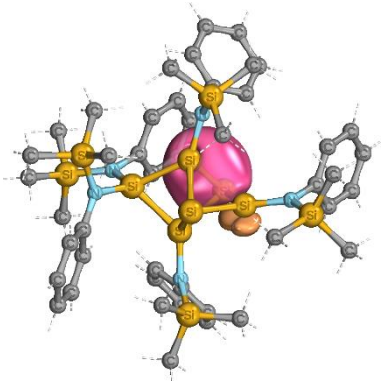


IBO 240 (top)

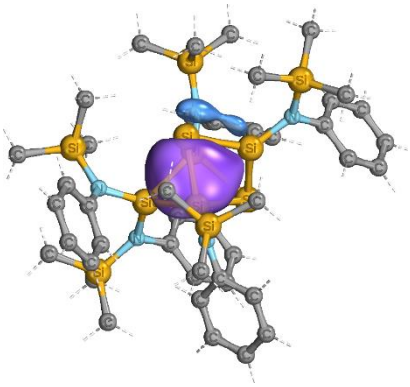
Figure S79 (continued). Intrinsic bond orbitals of the anion in **3**.



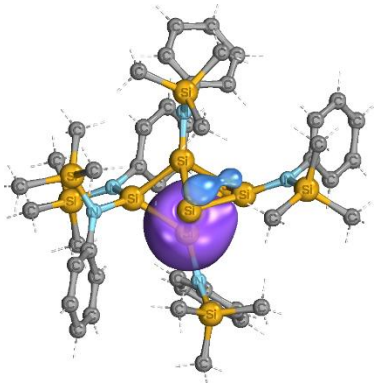
IBO 241 (side)



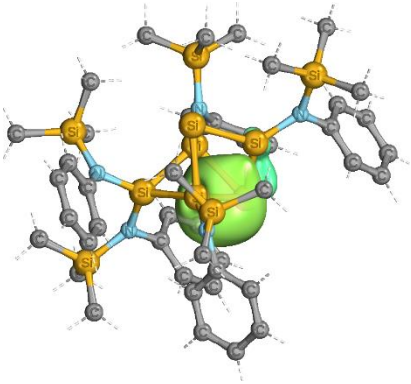
IBO 241 (top)



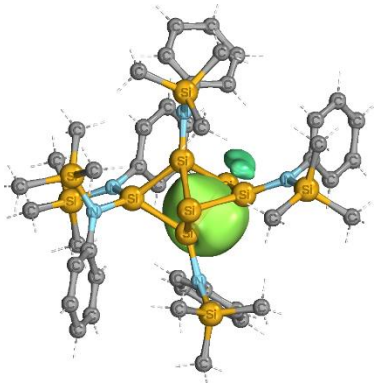
IBO 242 (side)



IBO 242 (top)

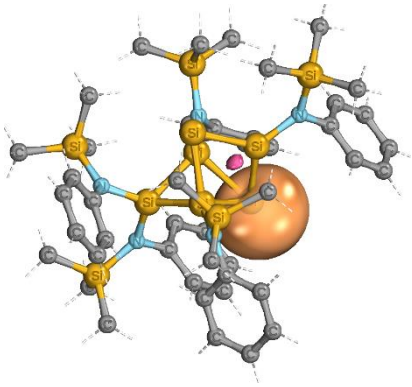


IBO 243 (side)

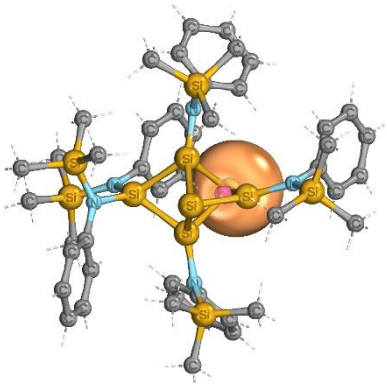


IBO 243 (top)

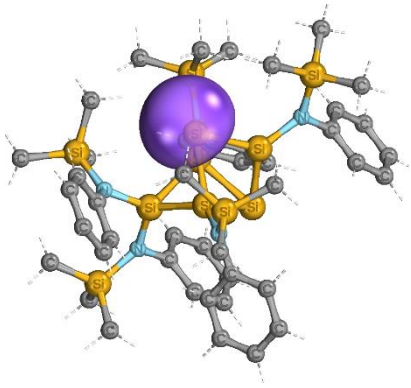
Figure S79 (continued). Intrinsic bond orbitals of the anion in **3**.



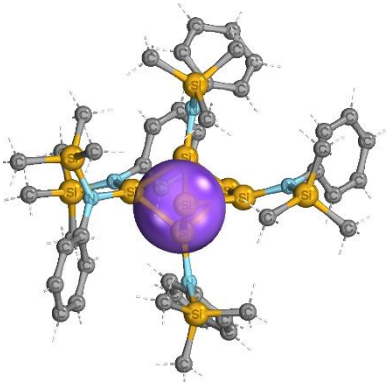
IBO 244 (side)



IBO 244 (top)



IBO 245 (side)



IBO 245 (top)

Figure S79. Intrinsic bond orbitals of the anion in **3**.

4.5 Calculated partial charges and bond orders of the anion in 3

Wiberg bond orders[S17] and Mayer bond orders[S18] were calculated for the anion in **3**.

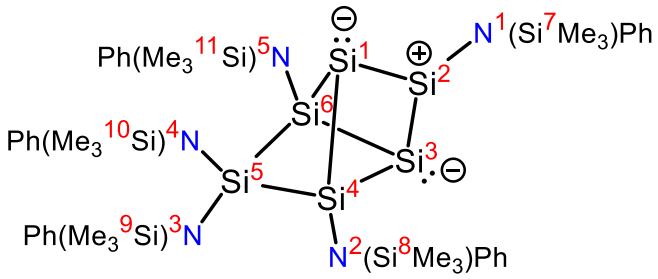


Table S4. Wiberg Bond Orders (B.O.) of the anion in **3** in two population analysis schemes (Wiberg and Mayer).

	Wiberg B.O.	**Mayer B.O.**		**Wiberg B.O.**	**Mayer B.O.**
Si1-Si2	1.0017	0.9926	*Si2-N1*	0.5493	0.9220
Si2-Si3	1.0130	1.0085	*Si4-N2*	0.5589	0.9312
Si3-Si4	0.7629	0.7840	*Si5-N3*	0.5104	1.0881
Si4-Si5	0.8715	0.8695	*Si5-N4*	0.4925	1.0024
Si5-Si6	0.8263	0.8239	*Si6-N5*	0.5532	0.9228
Si6-Si3	0.0767	0.7908			
Si6-Si1	0.0865	0.7363			
Si1-Si4	0.7743	0.8076			
Si4···Si6	0.2470	0.2297			
Si1···Si5	0.0767	-			
Si2···Si4	0.2924	0.2979			
Si2···Si6	0.4156	0.3969			

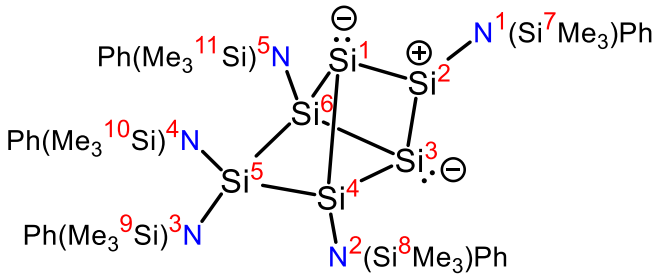


Table S5. Partial atomic charges from natural population analysis[S19] and from Mayer population analysis.[S18]

	Q (NPA)	**Q (Mayer)**
Si1	-0.35607	-0.3868
Si2	0.66665	0.0860
Si3	-0.34638	-0.2451
Si4	0.42884	0.1778
Si5	1.24732	-0.0996
Si6	0.45876	0.1739
N1	-1.29738	-0.2323
N2	-1.25207	-0.1760
N3	-1.34502	-0.0420
N4	-1.27886	0.0367
N5	-1.30534	-0.2235

4.6 Calculated ^{29}Si NMR chemical shifts of the anion in 3

Isotropic chemical shieldings of the anion in **3** were calculated with TPSS/def2-TZVP using the structure optimized with TPSS-D3/def2-TZVP. Isotropic shieldings of $Si(CH_3)_4$ were taken as reference for the chemical shifts.

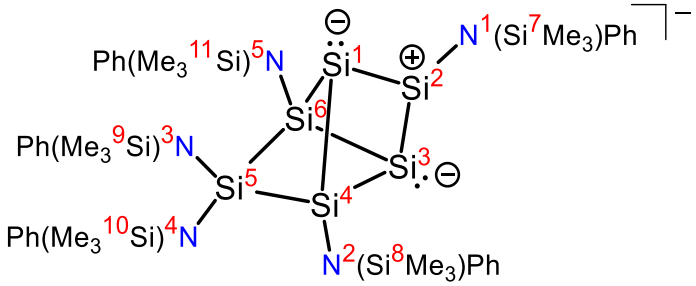


Table S6. ^{29}Si-NMR-chemical shifts[a] of the silicon atoms of the anion in **3**.

Atom	σ_{iso} /ppm	δ /ppm
$SiMe_4$	333.79	0
Si1	292.76	40.4
Si2	195.72	137.4
Si3	273.88	59.2
Si4	389.98	−56.9
Si5	297.68	35.4
Si6	394.12	−61.0
Si7	328.87	4.2
Si8	324.54	8.6
Si9	334.12	−1.0
Si10	332.47	0.6
Si11	329.77	3.3

[a] TPSS//TPSS-D3/def2-TZVP

4.7 Calculated ^{29}Si NMR chemical shifts of 4

Isotropic chemical shieldings of **4** were calculated with TPSS/def2-TZVP using the structure optimized with TPSS-D3/def2-TZVP. Isotropic shieldings of $Si(CH_3)_4$ were taken as reference for the chemical shifts.

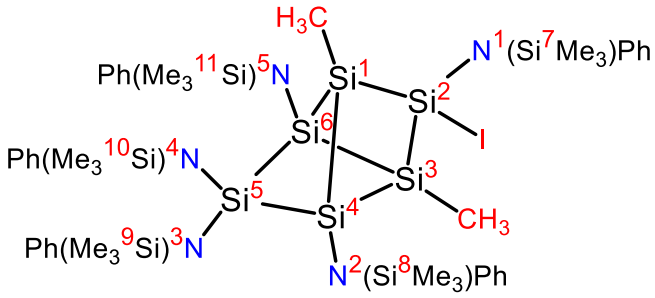


Table S7. ^{29}Si-NMR-chemical shifts[a] of the silicon atoms of **4**.

Atom	σ_{iso} /ppm	δ /ppm
$SiMe_4$	333.79	0
Si1	414.25	−80.5
Si2	313.21	20.6
Si3	407.77	−74.0
Si4	374.00	−40.2
Si5	327.83	6.0
Si6	387.87	−54.1
Si7	325.98	7.8
Si8	323.64	10.2
Si9	330.78	3.0
Si10	329.33	4.5
Si11	322.34	11.5

[a] TPSS//TPSS-D3/def2-TZVP

4.8 Calculated ^{29}Si NMR chemical shifts of 5

Isotropic chemical shieldings of **5** were calculated with TPSS/def2-TZVP using the structure optimized with TPSS-D3/def2-TZVP. Isotropic shieldings of $Si(CH_3)_4$ were taken as reference for the chemical shifts.

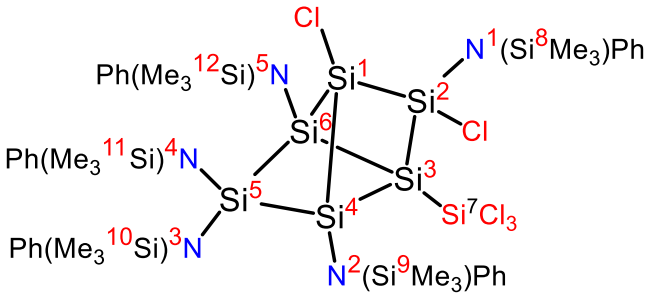


Table S8. ^{29}Si-NMR-chemical shifts[a] of the silicon atoms of **5**.

Atom	σ_{iso} /ppm	δ /ppm
$SiMe_4$	333.79	0
Si1	381.12	−47.3
Si2	299.65	34.1
Si3	472.00	−138.2
Si4	372.47	−38.7
Si5	336.41	−2.6
Si6	378.62	−44.8
Si7	303.40	30.4
Si8	325.15	8.6
Si9	322.81	11.0
Si10	328.32	5.5
Si11	330.58	3.2
Si12	320.36	13.4

[a] TPSS//TPSS-D3/def2-TZVP

4.9 Calculated ^{29}Si NMR chemical shifts of 6

Isotropic chemical shieldings of **6** were calculated with TPSS/def2-TZVP using the structure optimized with TPSS-D3/def2-TZVP. Isotropic shieldings of $Si(CH_3)_4$ were taken as reference for the chemical shifts.

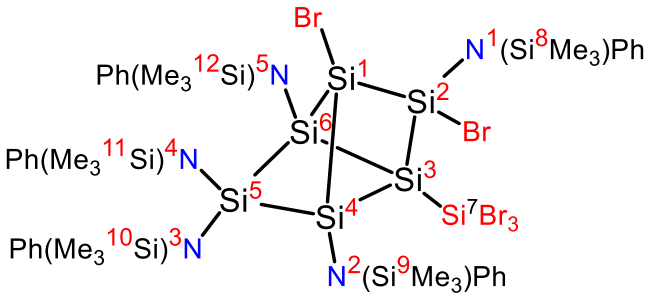


Table S9. ^{29}Si-NMR-chemical shifts[a] of the silicon atoms of **6**.

Atom	σ_{iso} /ppm	δ /ppm
$SiMe_4$	333.79	0
Si1	378.47	−44.7
Si2	295.18	38.6
Si3	444.13	−110.3
Si4	375.42	−41.6
Si5	338.12	−4.3
Si6	375.77	−42.0
Si7	275.19	58.6
Si8	324.94	8.9
Si9	320.03	13.8
Si10	328.50	5.3
Si11	328.86	4.9
Si12	321.37	12.4

[a] TPSS//TPSS-D3/def2-TZVP

4.10 DFT-optimized structure 7

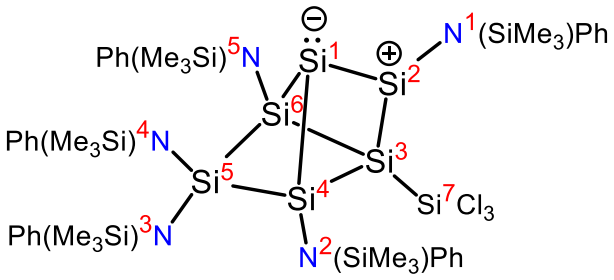


Table S10. Partial atomic charges from natural population analysis[S19] and from Mayer population analysis.[S18]

	Q (NPA)
Si1	-0.24
Si2	0.91
Si3	-0.43
Si4	0.65
Si5	1.37
Si6	0.55
Si7	1.06
N1	-1.30
N2	-1.31
N3	-1.34
N4	-1.32
N5	-1.29

Calculated ^{29}Si NMR chemical shifts of 7

Isotropic chemical shieldings of **7** were calculated with TPSS/def2-TZVP using the structure optimized with TPSS-D3/def2-TZVP. Isotropic shieldings of $Si(CH_3)_4$ were taken as reference for the chemical shifts.

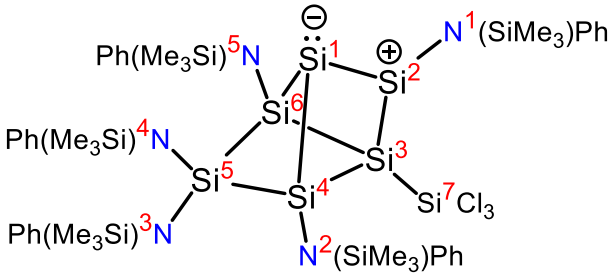
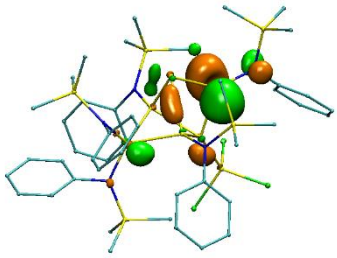


Table S11. ^{29}Si-NMR-chemical shifts[a] of the silicon atoms of **7**.

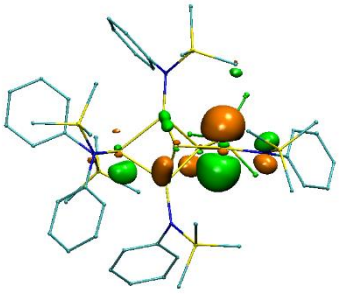
Atom	σ_{iso} /ppm	δ /ppm
$SiMe_4$	333.79	0
Si1	473.02	-139.23
Si2	184.93	148.87
Si3	416.08	-82.29
Si4	375.70	-41.91
Si5	296.59	37.20
Si6	393.62	-59.83
Si7	337.84	-4.05

[a] TPSS//TPSS-D3/def2-TZVP

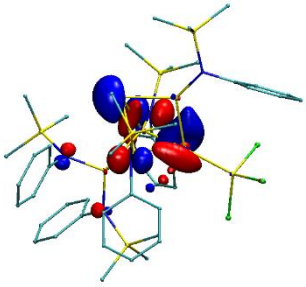
Figure S80. Kohn-Sham (frontier) molecular orbitals of **7** (TPSS-D3/def2-TZVP, 0.04 a.u.).



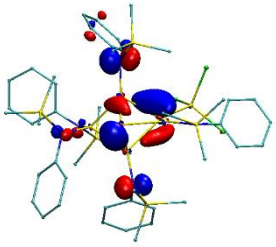
LUMO (-2.138 eV, side view)



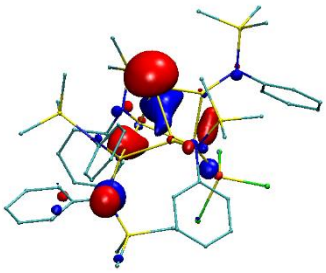
LUMO (-2.138 eV, top view)



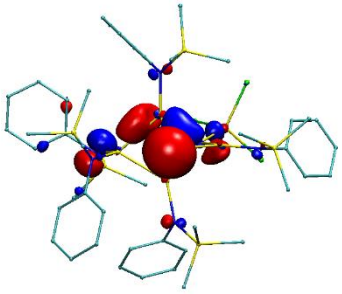
HOMO (-4.747 eV, side view)



HOMO (-4.747 eV, top view)



HOMO−1 (-5.031 eV, side view)



HOMO−1 (-5.031 eV, top view)

4.11 DFT-optimized isomers D_{iso} and 3_{iso}

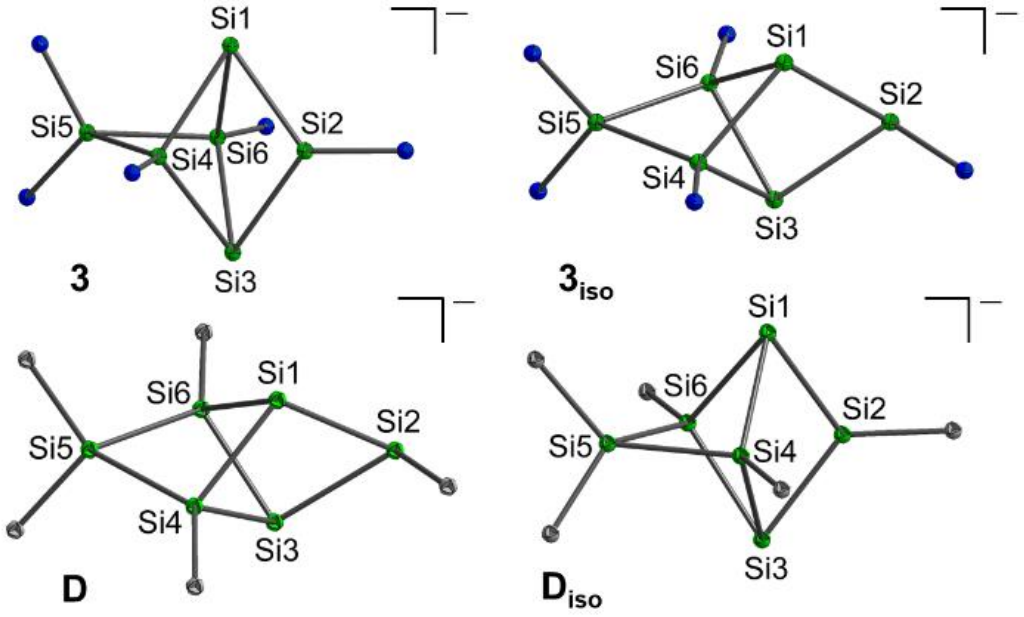


Figure S81. Schematic representation of the molecular structures **3**, **3_{iso}**, **D** and **D_{iso}**.

Table S12. NMR chemical shifts vs. TMS (PW6B95/def2-TZVP//TPSS-D3/def2-TZVP)

D (Si$_6$Trip$_5$); d(Si1-Si5)=2.585 Å

	σ [ppm]	δ [ppm]
si1	530.31	-200.8
si2	204.87	124.6
si3	383.99	-54.5
si4	-70.70	400.2
si5	563.61	-234.1
si8	332.51	-3.0

D_iso (Si$_6$Trip$_5$); d(Si1-Si5)=3.6786 Å ΔG^{solv}_{298} = +5.96 kcal/mol

	σ [ppm]	δ [ppm]
si1	214.60	114.9
si2	442.61	-113.1
si3	466.56	-137.0
si4	39.56	290.0
si5	194.83	134.7
si8	271.77	57.7

Table S13. NMR chemical shifts vs. TMS (PW6B95/def2-TZVP//TPSS-D3/def2-TZVP)

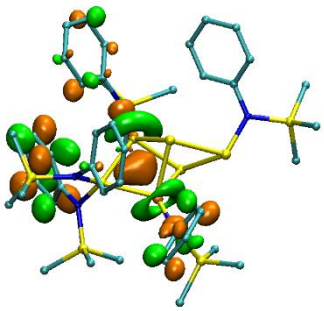
3_opt; d(Si1-Si3) = 3.731 Å

	σ [ppm]	δ [ppm]
si1	234.64	94.9
si2	163.05	166.5
si3	216.63	112.9
si4	395.08	-65.6
si5	383.63	-54.1
si6	292.36	37.1
si7	327.50	2.0
si8	326.22	3.3
si9	321.65	7.9
si10	332.99	-3.5
si11	330.42	-0.9

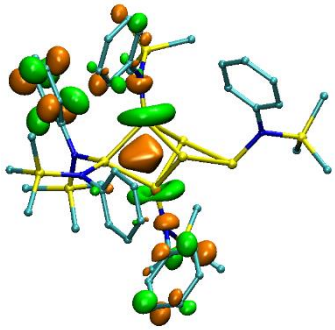
3_iso; d(Si1-Si3) = 2.738 Å ΔG^{solv}_{298} = +7.92 kcal/mol

	σ [ppm]	δ [ppm]
si1	554.37	-224.9
si2	-141.59	471.1
si3	594.74	-265.2
si4	142.11	187.4
si5	339.67	-10.2
si6	316.73	12.8
si7	332.19	-2.7
si8	324.30	5.2
si9	321.03	8.5
si10	330.54	-1.0
si11	327.27	2.2

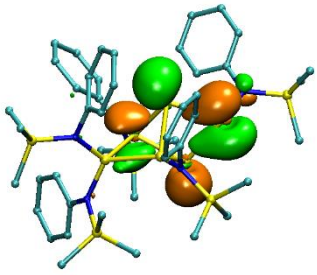
Figure S82. Kohn-Sham (frontier) molecular orbitals of **3$_{iso}$** (TPSS-D3/def2-TZVP, 0.04 a.u.).



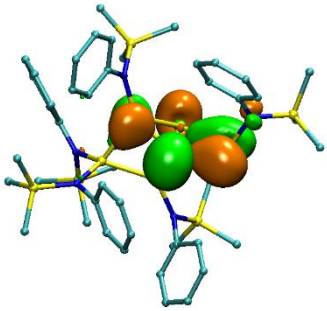
LUMO+1 (+1.018 eV, side view)



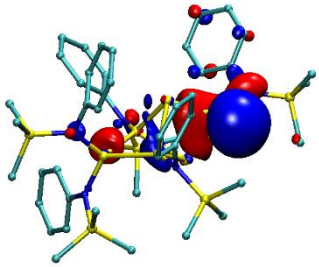
LUMO+1 (+1.018 eV, top view)



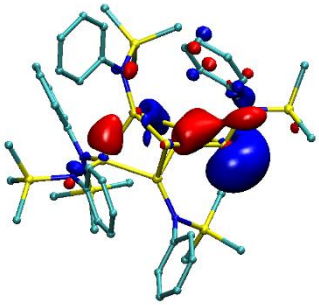
LUMO (+0.510 eV, side view)



LUMO (+0.510 eV, top view)

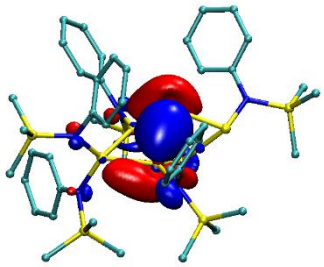


HOMO (-1.252 eV, side view)

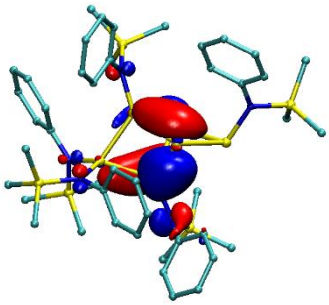


HOMO (-1.252 eV, top view)

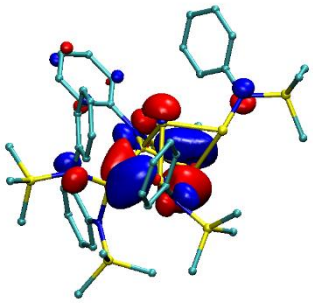
Figure S82 (continued). Kohn-Sham (frontier) molecular orbitals of **3$_{iso}$** (TPSS-D3/def2-TZVP, 0.04 a.u.).



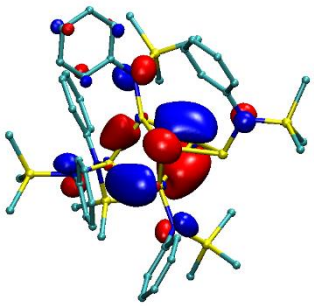
HOMO−1 (-1.794 eV, side view)



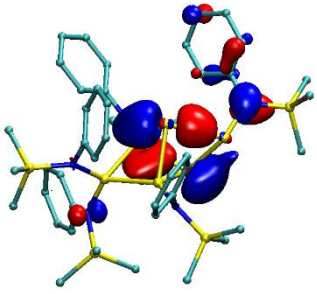
HOMO−1 (-1.794 eV, top view)



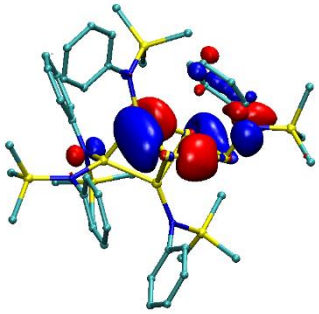
HOMO−2 (-2.054 eV, side view)



HOMO−2 (-2.054 eV, top view)

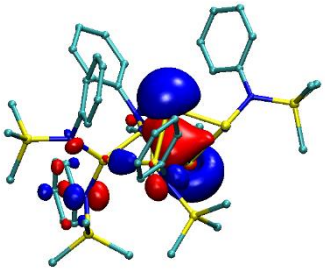


HOMO−3 (-2.341 eV, side view)

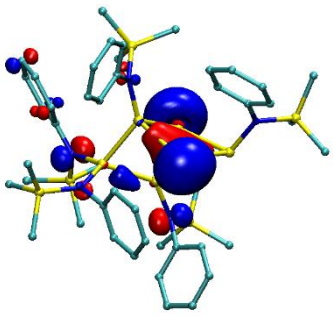


HOMO−3 (-2.341 eV, top view)

Figure S82 (continued). Kohn-Sham (frontier) molecular orbitals of **3$_{iso}$** (TPSS-D3/def2-TZVP, 0.04 a.u.).



HOMO−4 (-2.520 eV, side view)



HOMO−4 (-2.520 eV, top view)

4.12 Calculated isomers 3' and 3_{iso}' and their chemical shielding tensors and orbital imaginary virtual contribution coefficients

Starting from the optimized structures of **3** and $\mathbf{3_{iso}}$ (vide infra) we have replaced all substituents by NH_2 groups, to obtain **3'** and $\mathbf{3_{iso}}$**'** and re-optimized all structural parameters except the Si1····Si3 distance which was fixed to 3.727 Å in **3'** and to 2.738 Å in $\mathbf{3_{iso}}$**'** using Turbomole Version 7.3[S14] at the TPSS(D3/BJ)/def2-TZVP[S12,S10,S11] level of theory and using the RI approximation.[S9]

At the zero gradient geometries we have calculated the chemical shielding tensors using Turbomoles mpshift module.[S20] The following shielding tensors were for the Si1 atom for $\mathbf{3_{iso}}$**'** and **3'**.

3_{iso}'

ATOM si 1 ISOTROPIC: 637.7625485 ANISOTROPIC: 196.6225421

diamagnetic part of magnetic shielding:
Trace = 874.76808881
Tensor :

874.55717265	-3.81120978	0.92604284
-3.74228249	874.69602160	-1.55165903
0.36462755	-0.55548488	875.05107219

paramagnetic undisturbed density part of magnetic shielding:
Trace = 6.73388987
Tensor :

4.22289941	1.40970872	-0.36131673
-4.25280988	9.22982680	-0.49541229
0.99386491	-2.02194054	6.74894340

paramagnetic disturbed density part of magnetic shielding:
Trace = -243.73943022
Tensor :

-257.49341820	23.70545159	-73.46955991
29.47325147	-217.62501193	116.83578527
-20.99714584	84.48605643	-256.09986054

total magnetic shielding:
Trace = 637.76254846
Tensor :

621.28665386	21.30395053	-72.90483380
21.47815910	666.30083647	114.78871395
-19.63865338	81.90863100	625.70015505

3‘

ATOM si 1 ISOTROPIC: 275.0499521 ANISOTROPIC: 553.2410786

diamagnetic part of magnetic shielding:
Trace = 875.14599478
Tensor :

873.71194100	-0.05273061	-0.82347129
0.10958159	871.37685571	-0.56303878
-0.11646651	-0.53807325	880.34918764

paramagnetic undisturbed density part of magnetic shielding:
Trace = 6.25585837
Tensor :

6.41767874	1.54789250	0.89017181
1.87733974	8.52763721	0.77486046
2.11989579	0.31869336	3.82225915

paramagnetic disturbed density part of magnetic shielding:
Trace = -606.35190104
Tensor :

-856.42407359	-4.25042732	89.82745335
6.51729309	-699.83081098	-17.80674706
59.30264671	-12.86688553	-262.80081854

total magnetic shielding:
Trace = 275.04995211
Tensor :

23.70554615	-2.75526544	89.89415387
8.50421442	180.07368193	-17.59492537
61.30607599	-13.08626542	621.37062826

Orbital imaginary virtual contribution coefficients (F_{im}, with virtual orbital *i* and occupied orbital *m*) to the (paramagnetic) wave function response, as described by G. Monaco, R. Zanasi as well as Steiner and Fowler[S21,S22] have been computed using SYSMOIC a program package for the calculation of origin-independent electron current density and derived magnetic properties in molecular systems.[S23] module MO808XL. Thereby, the square norms of the largest matrix elements $|F_{im}|^2 > 15$ in the two conformers have been computed to

		3iso'			**3'**
m	***i***	$\|F_{im}\|^2$	***m***	***i***	$\|F_{im}\|^2$
65	74	17.9327	65	75	15.5270
65	72	18.7265	65	68	54.4939
65	68	23.5785	65	69	60.3172
65	69	26.1357	65	67	97.3227
65	66	155.1367	65	66	107.6409

Visual analysis of F_{im} matrix elements

For the visual analysis of the most significant matrix elements F_{im} we have only included the orbitals HOMO (65), LUMO (66) and LUMO+1 (67) of **3'** and HOMO (65) and LUMO (66) of **3$_{iso}$'**. The molecular orbitals were visualized using VMD.[S24]

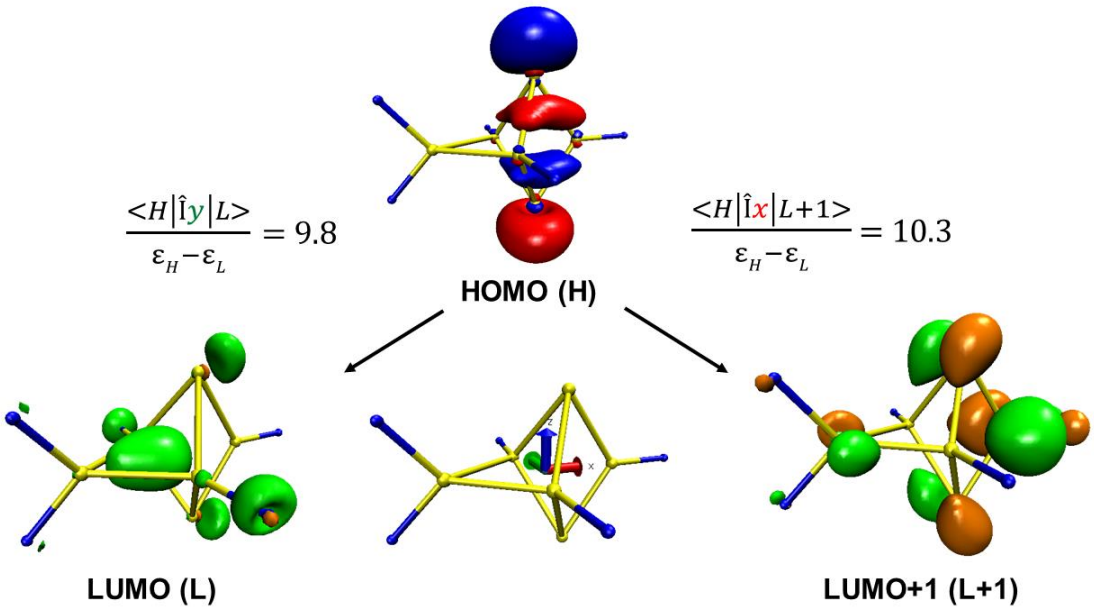


Figure S83. Most significant (> 7, a.u.) paramagnetic response matrix element components (Fi,m)α = <m|ˆlα|i> / ϵi−ϵm in **3′** with long Si1···Si3 distance. The angular momentum axes ˆlα are color coded in red (α = x) green (α = y) and blue (α = z), respectively.

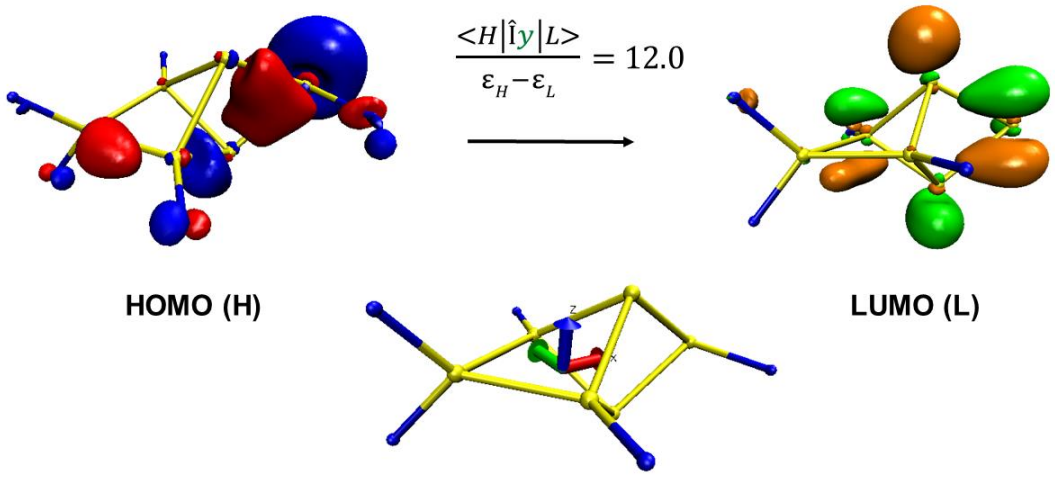


Figure S84. Most significant (> 7, a.u.) paramagnetic response matrix element component (Fi,m)α = <m|ˆlα|i> / ϵi−ϵm in **3$_{iso}$′** with short Si1···Si3 distance. The angular momentum axes ˆlα are color coded in red (α = x) green (α = y) and blue (α = z).

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6. Cartesian Coordinates and Electronic Energies of all Structures

Anion in 3

E(TPSS-D3/def2-TZVP) = -5217.475420433- + 1.0340058 Hartree
Lowest Freq. = 7.31 cm^-1
131
Energy =

Si	6.0922930	10.5827496	6.5120694
Si	4.9753753	10.4131357	4.5112300
Si	6.5957130	10.2602813	2.8837439
Si	7.3361256	9.2402622	4.9393803
Si	7.0770531	11.8398443	4.6801515
Si	9.1490918	10.6926949	4.9252541
Si	2.2304462	10.5149673	2.9047505
Si	6.6303208	6.4073203	3.8766660
Si	6.1489938	14.4281288	3.0582101
Si	11.8619397	10.6533159	6.6990116
Si	10.5813809	11.9955664	2.5554823
N	3.2539042	10.7823201	4.3152883
N	7.2351180	7.4717306	5.1460923
N	6.6985838	13.5700651	4.5021966
N	10.1700653	11.0012902	6.3361435
N	10.2172341	10.5459260	3.5005810
C	2.6002447	11.2417317	5.5072122
C	2.3024622	10.3499681	6.5478001
H	2.5499978	9.3000455	6.4223798
C	1.7082342	10.8073653	7.7241556
H	1.4861387	10.1041706	8.5229616
C	1.4034418	12.1624905	7.8802945
H	0.9438617	12.5183711	8.7982957
C	1.7023046	13.0569956	6.8496774
H	1.4831661	14.1153526	6.9648586
C	2.2977945	12.6003439	5.6732866
H	2.5528010	13.2949011	4.8793776
C	3.2451440	9.8051983	1.4965123
H	4.0414801	10.4859762	1.1791065
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H	2.1717834	12.8822177	2.0954765
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C	8.5411362	7.4211306	7.2140004
H	9.2196125	8.1448191	6.7705372
C	8.7636528	6.9444221	8.5034313
H	9.6310956	7.2901242	9.0605115
C	7.8892919	6.0192647	9.0809861
H	8.0656886	5.6450762	10.0855325
C	6.7786487	5.5922048	8.3481354
H	6.0755271	4.8872900	8.7855333
C	6.5493979	6.0756173	7.0599756
H	5.6640662	5.7590552	6.5169017
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H	8.3448173	4.6568775	4.2912649
H	6.9799691	4.0148328	3.3590971
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H	7.1625752	6.0686008	1.5042588
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C	7.4212556	15.4726674	5.8934491
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H	6.0136059	16.7738029	8.7117318
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H	4.5342373	14.7951235	8.3833534
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H	4.8905330	13.2830767	6.4479203
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H	5.1380269	16.3947120	4.2586501
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H	7.8940616	16.2196370	2.9355971
H	7.1502734	15.9320997	1.3524531
H	8.3734924	14.8098335	1.9771027
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H	9.3880229	9.6211802	8.5229100
C	8.4646815	11.1840894	9.6782835
H	8.2252672	10.5255692	10.5097673
C	8.0878360	12.5271062	9.7140417
H	7.5579008	12.9256991	10.5754080
C	8.3835973	13.3527865	8.6270143
H	8.0767759	14.3933835	8.6301692
C	9.0614997	12.8436593	7.5227371
H	9.2977021	13.4812907	6.6772005
C	12.9525636	10.6524329	5.1759943
H	12.6696201	9.8934581	4.4424085
H	13.9823507	10.4513378	5.5008464
H	12.9411719	11.6288238	4.6838388
C	12.0909462	8.9935039	7.5707728
H	11.5828817	8.9664305	8.5407320
H	13.1604334	8.8206964	7.7508419
H	11.7179012	8.1563010	6.9697452
C	12.4808677	12.0069668	7.8544766
H	12.3605885	12.9958237	7.3953108
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H	11.9386661	12.0110596	8.8061845
C	10.4962502	9.2428394	3.0488661
C	10.6794653	8.9309103	1.6877562
H	10.5675676	9.7076237	0.9386166
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H	10.4765495	8.3984941	5.0312715

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C     9.3703406   12.2599659    1.1397935
H     9.4661555   11.4915351    0.3643968
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H     8.3404245   12.2235081    1.5106439
C    12.3127081   11.9288397    1.8113615
H    13.0957268   11.8984376    2.5745545
H    12.4638311   12.8337490    1.2078481
H    12.4503315   11.0650759    1.1527446
C    10.4706808   13.4523384    3.7390144
H     9.4457438   13.6114692    4.0932410
H    10.7909158   14.3649264    3.2198557
H    11.1143392   13.3103690    4.6134171
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4

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E(TPSS-D3/def2-TZVP) = - 5594.941838802 Hartree
140
Energy =
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Si   -8.1766578    5.3029300   14.4463904
Si   -9.3154838    4.1793335   16.1219479
Si  -11.2551112    4.4391812   14.8346368
Si  -11.7650998    2.1334250   14.8188597
Si   -9.3992606    2.2390599   14.7755171
Si   -7.7355456    8.0301511   13.0313808
Si  -13.0869228    6.4808115   16.2625410
Si  -13.8250085    0.1467661   16.3639375
Si  -13.8097347    2.4397331   12.5167071
Si   -7.3130223    0.2101606   13.5617142
N    -8.3164666    7.0507107   14.3909123
N   -12.3055084    5.8558960   14.7961133
N   -12.5661262    1.3828319   16.1852568
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H   -10.3672851    4.6816512   10.9343097
H   -10.3565226    2.9077938   11.0865886
H    -8.8321755    3.7868072   10.8445272
C    -8.5323916    7.7086486   15.6456265
C    -7.6849657    7.4720623   16.7381079
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C    -8.9806266    8.9928489   18.1048988
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H   -10.2846576    8.7453564   14.9668774
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H    -9.8986565    9.2329047   12.5754995
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H    -5.6455788    9.3201075   12.6091534
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H	-5.3028224	7.8414898	13.5341161
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H	-7.3520297	7.4827638	10.6545227
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C	-12.5969783	6.4677919	13.5403304
C	-11.5594877	6.8408186	12.6731417
H	-10.5331433	6.6886488	12.9967211
C	-11.8404009	7.4151982	11.4354701
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C	-14.1960424	7.3117611	11.9167430
H	-15.2291009	7.4896898	11.6301738
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H	-14.7333704	6.4211785	13.8019475
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H	-13.7208188	8.7583174	16.9756488
H	-14.2677015	8.4850624	15.3138783
C	-11.9234979	6.2336623	17.7071578
H	-11.7610233	5.1749222	17.9301497
H	-12.3569667	6.6961865	18.6036011
H	-10.9519871	6.7014637	17.5238380
C	-14.7020577	5.5915469	16.6581629
H	-15.4795289	5.7701636	15.9073403
H	-15.0896096	5.9381769	17.6251146
H	-14.5564172	4.5081880	16.7264178
C	-11.9528369	1.6822140	17.4603921
C	-12.5507182	2.5780805	18.3547741
H	-13.4476591	3.1061653	18.0511891
C	-12.0190423	2.7587346	19.6331401
H	-12.5021833	3.4460555	20.3219962
C	-10.8727724	2.0647038	20.0233154
H	-10.4607688	2.2073127	21.0179837
C	-10.2438362	1.2067696	19.1191236
H	-9.3342264	0.6826511	19.3949726
C	-10.7810585	1.0188377	17.8476790
H	-10.3141459	0.3297871	17.1522554
C	-14.6087969	-0.3786091	14.7475000
H	-15.1904992	0.4190456	14.2804834
H	-15.3043068	-1.1956928	14.9820325
H	-13.8859194	-0.7552107	14.0199932
C	-15.1955836	0.7944372	17.4825413
H	-14.8434681	0.9900189	18.5004060
H	-16.0009185	0.0512513	17.5462732
H	-15.6306863	1.7216721	17.0908376
C	-13.0604844	-1.3734627	17.1712912
H	-12.2686582	-1.8021629	16.5454460
H	-13.8238224	-2.1482643	17.3164699
H	-12.6266494	-1.1430118	18.1497831
C	-11.8991852	0.4322027	12.6866410
C	-11.3606104	-0.6084493	13.4664921
H	-11.3719483	-0.5188248	14.5500569
C	-10.8513712	-1.7579000	12.8697861
H	-10.4708213	-2.5576596	13.4983282
C	-10.8455584	-1.8987008	11.4815945
H	-10.4473893	-2.7969772	11.0204500
C	-11.3546800	-0.8635768	10.6972681
H	-11.3440196	-0.9444907	9.6137814
C	-11.8699795	0.2878114	11.2883854
H	-12.2467874	1.0898789	10.6612308
C	-14.9282568	1.2227945	11.6017525

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H   -14.7114675    1.2099476   10.5283923
H   -15.9749562    1.5305921   11.7203307
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C   -14.7532813    3.3054404   13.8884771
H   -15.1245505    2.6145492   14.6508671
H   -15.6149505    3.8315354   13.4589828
H   -14.1296227    4.0535733   14.3870801
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H   -12.5877741    4.4793912   11.7355335
H   -14.1288912    4.2776641   10.9040120
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C    -7.6125772    0.7502313   16.2021185
C    -7.8228954   -0.4791549   16.8406958
H    -8.4375763   -1.2281755   16.3511855
C    -7.2547071   -0.7342111   18.0894829
H    -7.4279653   -1.6925084   18.5717601
C    -6.4778109    0.2378678   18.7210044
H    -6.0378700    0.0396476   19.6940872
C    -6.2662231    1.4649283   18.0888426
H    -5.6507950    2.2242300   18.5639513
C    -6.8236163    1.7177573   16.8368902
H    -6.6337765    2.6564111   16.3229440
C    -7.3446227   -1.6627484   13.7553618
H    -6.7400060   -1.9830391   14.6108206
H    -6.9176514   -2.1273951   12.8571002
H    -8.3572459   -2.0535460   13.8819210
C    -5.5079773    0.7245353   13.5902088
H    -5.3946958    1.8018972   13.4338123
H    -4.9495123    0.2013952   12.8033722
H    -5.0415247    0.4749129   14.5503152
C    -8.1173287    0.7360071   11.9566578
H    -9.2037082    0.6028445   11.9644123
H    -7.7165396    0.1330936   11.1324768
H    -7.8979259    1.7854995   11.7373030


5
E(TPSS-D3/def2-TZVP) = - 7808.391815583 Hartree
137
Energy =
Cl   10.9116817   10.7063028   17.9371798
Cl   13.8195288   10.3798040    9.9842600
Cl    8.9425854   11.8708843   13.4160170
Cl   11.1692396   12.2871345   10.3109409
Cl   14.2121753   13.5236530   10.8422028
Si   11.5362904   11.0099671   15.9699911
Si   10.7622981   12.4448768   14.3191787
Si   12.6551768   11.4554641   13.3930737
Si   13.8130297   11.4527238   15.4257239
Si   14.2545829    9.1336949   15.2181110
Si   12.0314062    9.3515871   14.4208280
Si   13.0159906   11.8823169   11.1481361
Si    9.5207927   14.9960917   15.5080672
Si   16.0074558   13.6724192   15.8248772
Si   15.5792017    7.1686599   13.2394408
Si   13.4941004    7.3325915   17.7885983
Si    9.2214921    7.8920643   14.2150376
N    10.7367842   14.1605985   14.5249071
N    14.5684013   12.7539615   16.3127967
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N    14.5417082    8.2401921   16.6964286
N    10.8970280    8.2429729   13.7133319
C    11.5052302   14.9725430   13.6136796
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H	11.3298801	16.4285923	10.5438001
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H	13.5359027	17.3136361	11.2696271
C	13.4863807	16.2908639	13.1671847
H	14.4597937	16.6552718	13.4830497
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H	13.1483701	15.1476715	14.9730239
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H	9.6621237	13.3187128	17.3727704
C	10.3471006	16.4591571	16.3458198
H	11.1907050	16.1574191	16.9747143
H	9.6264992	16.9931093	16.9777092
H	10.7244862	17.1688875	15.6009302
C	8.1152731	15.6183625	14.4285401
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H	7.3426274	16.1032370	15.0385188
H	7.6477560	14.7912509	13.8831211
C	13.9870678	13.1060277	17.5821560
C	12.7189368	13.6960595	17.6434601
H	12.1750061	13.8695099	16.7181276
C	12.1685883	14.0591936	18.8707211
H	11.1818852	14.5115594	18.9027775
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H	12.4451193	14.1311374	21.0089670
C	14.1460088	13.2725140	19.9983079
H	14.7088449	13.1013927	20.9118094
C	14.6972570	12.9011354	18.7717175
H	15.6835068	12.4516954	18.7287844
C	16.1108187	13.5270350	13.9701151
H	16.1711683	12.4846781	13.6409398
H	17.0017809	14.0374169	13.5866873
H	15.2313804	13.9759492	13.4992383
C	15.7730980	15.4561603	16.3755612
H	14.8867059	15.9287308	15.9424824
H	16.6477579	16.0480850	16.0767803
H	15.6858839	15.5235352	17.4656664
C	17.5686006	13.0455568	16.6672848
H	17.5993428	13.3470926	17.7207072
H	18.4546377	13.4695206	16.1780807
H	17.6472200	11.9569798	16.6185980
C	16.5051525	9.6782650	13.6525784
C	16.5453975	10.1656947	12.3392171
H	15.7460011	9.9032745	11.6583545
C	17.5974144	10.9731246	11.9091695
H	17.6033411	11.3415911	10.8871932
C	18.6225815	11.3174385	12.7898997
H	19.4447917	11.9444668	12.4577672
C	18.5730268	10.8600340	14.1070937
H	19.3614969	11.1257034	14.8053627
C	17.5244826	10.0488043	14.5399475
H	17.5086671	9.6678905	15.5550298
C	14.4828517	5.9802608	14.1973024
H	14.9049535	5.7260784	15.1724611
H	14.3560041	5.0553835	13.6217960
H	13.4840968	6.3972041	14.3664676
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H    15.6877188    7.7781504   10.8158889
C    15.8755192    8.4343642   17.2130331
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C    18.1681677    7.6888806   17.4694609
H    18.9400360    6.9498995   17.2735361
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H    16.6368188    6.5964567   16.4096156
C    13.3491965    8.2406063   19.4265803
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C    14.2484840    5.6424512   18.1362740
H    14.3081644    5.0220184   17.2354417
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H    11.3170733    8.4918633    9.1302123
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H    10.9008804    9.4978614   11.3601996
C     8.7071033    8.9393797   15.6784718
H     9.2820637    8.7348939   16.5849986
H     7.6569618    8.7042187   15.8984934
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H     9.2164010    5.4174496   13.8189291
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6

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137
Energy =
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Br   11.7762851    7.1451127    2.2749711
Br   12.1961223    6.3086544    5.7042302
Si    6.3789251    9.0196036    4.5257932
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Si	7.4589772	7.5810015	3.0611709
Si	9.1242536	8.3349464	4.5116062
Si	8.2056298	10.5218917	4.4728842
Si	8.1593687	10.6331296	6.8406656
Si	7.6768083	8.3484275	6.3859786
Si	11.3858957	7.8882879	4.3444838
Si	5.7081496	5.1978093	2.1754670
Si	7.5389356	12.6675801	2.2361867
Si	10.7636782	10.3796835	8.7546256
Si	6.0053837	12.9801732	7.1890919
Si	5.9985763	5.8128049	7.4134061
N	7.1889414	5.8815803	2.8816218
N	8.6198386	11.6299006	3.1951914
N	9.6136655	11.1624034	7.6590126
N	6.7362266	11.4050397	7.5174818
N	7.3514160	6.9672347	7.3940824
C	8.3327439	5.0239062	3.0481979
C	8.8636349	4.8087748	4.3249414
H	8.4135676	5.3190322	5.1707671
C	9.9387776	3.9400201	4.5025344
H	10.3319725	3.7704676	5.4997030
C	10.5104079	3.2921978	3.4085978
H	11.3504831	2.6190955	3.5498362
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H	6.0729530	2.9796632	3.2408537
H	4.3842893	3.1745981	2.7461822
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C	4.3851804	6.5237961	2.2463430
H	4.1447362	6.8444736	3.2636932
H	3.4652048	6.1218296	1.8024722
H	4.6623711	7.4124592	1.6683756
C	5.9294305	4.6878632	0.3775282
H	6.3812370	5.4953030	-0.2093669
H	4.9468605	4.4666497	-0.0593351
H	6.5462619	3.7901399	0.2666940
C	9.9828352	11.6596598	2.7096430
C	10.4760410	10.6239781	1.9089129
H	9.8374343	9.7733841	1.6933119
C	11.7569758	10.7055798	1.3667299
H	12.1245489	9.8952143	0.7455494
C	12.5639204	11.8142410	1.6233935
H	13.5636808	11.8716319	1.2033770
C	12.0787782	12.8453335	2.4270763
H	12.6989917	13.7126063	2.6371732
C	10.7930456	12.7713807	2.9640204
H	10.4009140	13.5756090	3.5752161
C	7.7733133	12.2861692	0.4140048
H	8.8108334	12.4504060	0.1030317
H	7.1366014	12.9478314	-0.1873314
H	7.5086909	11.2511025	0.1797818
C	7.9616607	14.4890536	2.4693522
H	8.0355269	14.7816293	3.5202625
H	7.1798798	15.1029611	2.0028507
H	8.9080042	14.7364986	1.9761517
C	5.7778962	12.3111291	2.7548068
H	5.4677363	11.3129019	2.4307759
H	5.1025960	13.0377746	2.2861435
H	5.6263853	12.3736215	3.8364304
C	9.8349121	12.5817107	7.5191958

C	10.4569906	13.0769706	6.3678947
H	10.7458297	12.3779375	5.5895768
C	10.7241082	14.4387557	6.2431713
H	11.2188240	14.8114058	5.3505401
C	10.3724230	15.3234751	7.2645125
H	10.5825935	16.3842893	7.1656496
C	9.7510061	14.8347986	8.4144560
H	9.4705504	15.5152628	9.2136816
C	9.4807040	13.4722601	8.5397380
H	8.9982467	13.0849521	9.4307456
C	10.1422397	10.3939979	10.5326928
H	10.0291385	11.4180563	10.9081449
H	10.8599871	9.8799901	11.1849205
H	9.1800631	9.8844703	10.6297277
C	12.3640591	11.3644928	8.6960167
H	12.7494021	11.4300890	7.6725837
H	13.1212174	10.8542409	9.3055083
H	12.2527867	12.3830063	9.0816487
C	11.0954684	8.6407324	8.1638283
H	10.3130490	8.2787814	7.4894918
H	11.1690110	7.9248033	8.9870328
H	12.0360067	8.6177717	7.6063822
C	6.1221726	10.6873119	8.6055132
C	5.0221878	9.8526980	8.3673806
H	4.6614893	9.7429610	7.3493166
C	4.3906247	9.2008486	9.4252078
H	3.5281683	8.5706034	9.2273336
C	4.8609588	9.3539972	10.7308503
H	4.3704436	8.8406171	11.5525643
C	5.9662086	10.1716126	10.9723442
H	6.3412256	10.2977426	11.9843992
C	6.5888238	10.8389948	9.9175738
H	7.4358669	11.4909780	10.0979563
C	7.0544942	13.8778871	5.9247782
H	7.8827982	14.4138309	6.3966944
H	6.4397003	14.6062043	5.3831484
H	7.4875762	13.1973436	5.1842219
C	4.2445230	12.7743462	6.5648901
H	4.1952157	12.2322234	5.6165337
H	3.7887931	13.7620278	6.4167512
H	3.6270731	12.2320139	7.2900195
C	5.8834381	13.9842695	8.7770641
H	5.2664166	13.4756267	9.5261247
H	5.4114468	14.9517061	8.5617416
H	6.8639569	14.1832028	9.2188398
C	8.2979034	6.6815805	8.4520815
C	8.1832713	7.3270050	9.6874271
H	7.4154354	8.0833661	9.8175364
C	9.0307294	6.9775594	10.7378198
H	8.9306294	7.4781045	11.6965346
C	9.9993638	5.9876852	10.5633071
H	10.6554792	5.7152241	11.3848023
C	10.1279293	5.3577347	9.3246274
H	10.8915267	4.5999713	9.1735480
C	9.2830992	5.7051169	8.2717270
H	9.3834225	5.2298350	7.3025013
C	5.3201071	5.7099840	9.1621932
H	6.0400159	5.2330110	9.8359894
H	4.4069379	5.1008442	9.1661968
H	5.0778217	6.6937551	9.5718099
C	4.6940194	6.3772192	6.2035956
H	4.2729217	7.3531043	6.4587427
H	3.8727791	5.6498894	6.1856646

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H     5.1004038    6.4398357    5.1885036
C     6.5514429    4.0714518    6.9664537
H     6.8815175    3.9689195    5.9298246
H     5.7020020    3.3909419    7.1131344
H     7.3601863    3.7254477    7.6190592
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7

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Lowest Freq. = 13.40 cm^-1
135
Energy =
Si    3.0909232    5.3693740    8.7259950
Si    4.5235278    3.7238124    9.4486920
Si    6.3508364    5.0310834    9.6160659
Si    5.2221825    5.7709928    7.6424526
Si    5.0351121    8.0101377    8.3985254
Si    4.6108654    6.5253222   10.1962691
Si    2.8561879    1.0935799    9.5496211
Si    4.7548768    3.7476457    5.2651336
Si    2.1201615    9.3478112    8.4298113
Si    8.0250307    9.1713538    8.0882282
Si    3.1207926    5.8133905   12.8278467
N     4.3910901    2.0114648    9.6127778
N     5.5280852    5.1304035    6.0517519
N     3.5695668    8.6628958    7.6955380
N     6.2711820    9.2510405    8.3388126
N     4.2025731    6.8415559   11.8770992
C     5.5637251    1.2492426    9.9750456
C     6.1408173    1.4131399   11.2380381
H     5.7017468    2.1235655   11.9297886
C     7.2589888    0.6651017   11.6016907
H     7.7043824    0.8130965   12.5805864
C     7.8080029   -0.2575031   10.7120778
H     8.6808430   -0.8376562   10.9957991
C     7.2353587   -0.4210787    9.4507240
H     7.6617620   -1.1286866    8.7451845
C     6.1200688    0.3291480    9.0793118
H     5.6855667    0.2123677    8.0930507
C     2.8550533   -0.0532424   11.0342414
H     1.9259863   -0.6353393   11.0668728
H     3.6936305   -0.7567517   11.0025218
H     2.9305556    0.5152784   11.9683363
C     1.4122561    2.2838104    9.6553508
H     0.4880634    1.6967567    9.7408873
H     1.4764777    2.9337480   10.5344880
H     1.3201065    2.9271127    8.7748702
C     2.7430366    0.1037115    7.9572458
H     1.7724237   -0.4053311    7.9016982
H     2.8304769    0.7533972    7.0800091
H     3.5216120   -0.6635407    7.8940226
C     6.6680358    5.6773594    5.3593809
C     7.8713378    4.9649486    5.2862784
H     7.9551868    4.0115239    5.7986578
C     8.9566705    5.4918302    4.5863670
H     9.8876880    4.9338237    4.5398909
C     8.8550359    6.7382084    3.9664502
H     9.7032487    7.1510433    3.4283288
C     7.6594483    7.4542252    4.0499074
H     7.5705174    8.4259263    3.5722993
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H     5.6345267    7.4739374    4.8025424
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C	5.5755032	2.1457879	5.8112988
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H	5.5708212	2.0777304	6.9048480
C	4.9556461	3.9879987	3.4134055
H	4.4293021	3.1930708	2.8706695
H	4.5390552	4.9505540	3.0965302
H	6.0070561	3.9652540	3.1091382
C	2.9270206	3.6330594	5.6768597
H	2.4888392	2.8321254	5.0660058
H	2.7429568	3.3899751	6.7277432
H	2.3889153	4.5585983	5.4527970
C	3.5599434	8.6345516	6.2524663
C	2.9709529	7.5565891	5.5779741
H	2.5399594	6.7540646	6.1689473
C	2.9463350	7.5210259	4.1850305
H	2.4860871	6.6783592	3.6765534
C	3.5156742	8.5591102	3.4448553
H	3.5033376	8.5275890	2.3593221
C	4.1056589	9.6349756	4.1104469
H	4.5511488	10.4478940	3.5431517
C	4.1260854	9.6750234	5.5052531
H	4.5705661	10.5105209	6.0325613
C	0.6018807	8.4618548	7.7611914
H	-0.3047679	8.8510442	8.2420499
H	0.4888219	8.5971187	6.6800728
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H	1.0901890	11.6141301	8.4030068
H	2.8620436	11.7259483	8.4038614
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C	2.1905847	9.1257775	10.2852494
H	1.3317740	9.6388419	10.7375450
H	2.1376693	8.0706202	10.5668734
H	3.0975733	9.5514333	10.7220402
C	5.8311816	10.5432477	8.8074411
C	5.8568565	11.6662298	7.9686309
H	6.1939650	11.5553358	6.9443330
C	5.4601553	12.9152176	8.4446449
H	5.4861424	13.7740255	7.7795002
C	5.0173078	13.0615284	9.7602101
H	4.6997995	14.0335029	10.1260215
C	4.9905339	11.9481850	10.6001911
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H	5.4292700	9.8470398	10.7996487
C	8.5610425	7.4193390	7.7424347
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H	8.1319476	6.6985635	8.4437543
H	8.2886258	7.1106133	6.7320210
C	8.8577670	9.8395229	9.6338169
H	9.9494209	9.7994721	9.5331328
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H	8.5766588	9.2519668	10.5133460
C	8.5435675	10.2259408	6.6137068
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H     3.6492345    3.5529320   11.8609364
H     4.8312644    4.0211122   13.0960144
C     1.3787859    5.8342636   12.1284503
H     0.7525774    5.0977102   12.6479076
H     0.9115287    6.8178303   12.2484770
H     1.3689180    5.5876209   11.0598891
C     3.1135129    6.3970147   14.6142696
H     2.5846817    5.6498898   15.2199695
H     4.1291962    6.4936176   15.0130489
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Si    8.3755541    4.6154772   10.6980158
Cl    9.4408098    3.0898151    9.8120266
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Cartesian coordinates in units of Å

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196
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Si    3.5272948    1.6741637   -0.7090243
Si    1.9619536    1.0264948    1.0595744
C     3.1485307    3.4084714   -1.5103806
C     2.8127967   -2.6727610    0.1543031
Si   -0.6504993   -1.1957673    0.5318336
C    -1.6643480   -1.2745277    2.1610413
C    -1.4084215   -2.5612498   -0.5953282
C    -1.2457032    2.6160415    0.1793470
C     2.7149802   -3.5566676   -0.9525292
C     3.7199539   -2.9941182    1.1949412
C     3.4646330   -4.7352825   -0.9705130
C     1.8636363   -3.2210697   -2.1670967
C     4.3204899   -5.0808787    0.0754240
H     3.3671736   -5.4055877   -1.8214033
C     4.4453445   -4.1891345    1.1389093
C     5.0828669   -6.3932877    0.0679690
H     5.1278844   -4.4395754    1.9482181
C     3.9734906   -2.0260107    2.3386162
C     2.7383449   -2.5098216   -3.2162277
C     1.1446766   -4.4259694   -2.7863604
H     1.0945080   -2.5109529   -1.8405946
H     3.1930883   -1.6086449   -2.7937160
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H     3.5390417   -3.1783974   -3.5567160
H     1.8486352   -5.1271977   -3.2515415
H     0.4582563   -4.0809113   -3.5663345
H     0.5576068   -4.9655676   -2.0385655
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H	4.6718292	-8.5377351	0.1799454
H	5.4319764	-6.5035298	-2.0835349
H	6.5832668	-7.4460016	-1.1188550
H	6.7149156	-5.6727891	-1.1906486
C	4.4025685	-2.6989680	3.6496017
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C	-4.6236890	6.3084576	1.3767514
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H	-3.7245157	-1.2681659	-3.8100957
H	-3.3301392	0.4239221	-3.4821195
H	-4.0771155	-0.5730118	-2.2209935
C	-2.3224455	-6.1153217	-4.1950709
C	-4.6077520	-5.6065127	-3.2242655
H	-3.0563522	-6.7543267	-2.2797329
H	-4.7256925	-4.7160787	-3.8521190
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C	0.2255271	-5.3510213	1.1805058
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H	-2.7017999	-3.8559701	2.3591105
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H	-0.1916367	-6.2887032	0.7947963
H	0.6401521	-5.5528514	2.1751736

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C	-1.1311778	-1.5141806	3.4501709
C	-3.0643699	-1.0578160	2.0530786
C	-3.8782488	-1.1224332	3.1858324
C	-3.7473324	-0.7712318	0.7214815
C	-3.3562728	-1.3652348	4.4560136
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C	-1.9801463	-1.5454386	4.5630636
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C	0.3532128	-1.7363667	3.6958937
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H	-4.1045674	-2.8693496	0.2467755
H	-5.1440041	-1.7436798	-0.6454609
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H	-5.2949876	0.5768055	1.4870590
H	-4.9740445	0.7373675	-0.2484087
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H	-4.2743742	0.7317419	6.0133216
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H	0.2177840	-2.9205636	5.5335595
H	1.7127450	-3.1527073	4.6193048
H	0.2033538	-3.8888192	4.0508152
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Diso

196

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Si	1.1869041	1.6369384	1.2239541
C	3.3302760	2.9919537	-1.4609312
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Si	-1.0346927	-0.8553584	0.4504958
C	-1.7451122	-1.1187864	2.2335844
C	-1.7334874	-2.3626994	-0.5352809
C	-2.2469120	2.6594934	0.0677601
C	2.5141118	-2.5132036	-1.6056443
C	3.7292634	-1.6268378	0.3101667
C	3.5593804	-3.4165818	-1.8187372
C	1.3487284	-2.5635534	-2.5871791
C	4.6897318	-3.4504047	-1.0041441
H	3.4823341	-4.1143745	-2.6502356
C	4.7488553	-2.5512853	0.0572320
C	5.8194832	-4.4309006	-1.2601408

H	5.6205694	-2.5741357	0.7083653
C	3.9022727	-0.6796552	1.4878923
C	1.7605004	-1.9229798	-3.9218960
C	0.8088208	-3.9804405	-2.8357440
H	0.5294162	-1.9665034	-2.1697318
H	2.0158995	-0.8706924	-3.7803807
H	0.9374105	-1.9712516	-4.6439360
H	2.6268953	-2.4468361	-4.3458022
H	1.5382929	-4.6041548	-3.3673826
H	-0.0930741	-3.9202291	-3.4539085
H	0.5404424	-4.4811484	-1.9040755
C	6.4897051	-4.1678821	-2.6208827
C	5.3368822	-5.8889475	-1.1606213
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H	4.5823121	-6.0999338	-1.9267961
H	4.8838434	-6.0836272	-0.1831762
H	6.1710009	-6.5868255	-1.3048567
H	5.7735549	-4.3132387	-3.4376897
H	7.3311714	-4.8533705	-2.7809979
H	6.8605101	-3.1396988	-2.6803260
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H	4.7255157	1.2912930	1.9095011
H	4.1817486	1.0918585	0.2412040
H	4.1313144	-2.2979431	2.9457693
H	4.4841092	-0.6731862	3.5752045
H	5.6525355	-1.4882077	2.5320822
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C	-2.7117999	2.9634306	1.3767864
C	-4.1236804	3.9508689	-0.8121517
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C	-1.9320952	2.5598325	2.6201746
C	-1.2893778	4.0926479	-2.6661058
C	-3.4788459	3.2107922	-3.5544761
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H	-1.6762634	5.1172583	-2.5982017
H	-0.8251685	3.9507085	-3.6487938
H	-0.5134783	3.9643152	-1.9054102
H	-4.3350804	2.5508927	-3.3797507
H	-3.0319822	2.9447569	-4.5189202
H	-3.8534124	4.2386016	-3.6389345
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C	-5.7007060	6.2377778	1.5095887
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H	-3.5124751	1.3759045	3.5581800

H	-0.3243862	3.9628781	2.1666379
H	-0.3546635	3.4305955	3.8548596
H	-1.5647212	4.6042503	3.2706381
C	4.3629761	2.3814011	-2.2072828
C	3.5210069	4.3110956	-0.9868357
C	5.5656166	3.0650580	-2.4111652
C	4.1508787	1.0212496	-2.8543041
C	5.7750319	4.3519624	-1.9120886
H	6.3666052	2.5884276	-2.9746340
C	4.7328668	4.9670443	-1.2130215
C	7.0999222	5.0602482	-2.1328285
H	4.8679052	5.9793052	-0.8338593
C	2.4104056	5.0367947	-0.2384993
C	5.3520038	0.0730491	-2.7397389
C	3.7504893	1.2273589	-4.3279627
H	3.3057547	0.5376649	-2.3444917
H	2.8056990	1.7760102	-4.3947145
H	3.6285227	0.2656481	-4.8375121
H	4.5246507	1.8010836	-4.8523290
H	6.2091373	0.4349256	-3.3211611
H	5.0780400	-0.9150502	-3.1229446
H	5.6644009	-0.0456202	-1.6992394
C	6.9250958	6.3522386	-2.9509145
C	7.8095772	5.3520450	-0.7983053
H	7.7378570	4.3785213	-2.7118121
H	6.2941724	7.0689279	-2.4129941
H	6.4478677	6.1426780	-3.9136022
H	7.8951085	6.8292991	-3.1383142
H	7.9613721	4.4300300	-0.2281793
H	8.7859369	5.8221789	-0.9697646
H	7.2093634	6.0314419	-0.1824506
C	2.0203143	6.3546618	-0.9272189
C	2.7702449	5.2500957	1.2398162
H	1.5218906	4.3869558	-0.2572842
H	1.1700315	6.8152591	-0.4109230
H	1.7374113	6.1796305	-1.9703921
H	2.8508536	7.0706831	-0.9165374
H	2.9297744	4.2854916	1.7319477
H	3.6846662	5.8485164	1.3356063
H	1.9600710	5.7717250	1.7631037
C	-2.5222929	-2.2743343	-1.7122279
C	-1.4562763	-3.6581766	-0.0274659
C	-3.0462992	-3.4329098	-2.2929965
C	-2.8307155	-0.9589860	-2.4151015
C	-2.8120656	-4.7028213	-1.7679029
H	-3.6577738	-3.3344388	-3.1882423
C	-2.0022627	-4.7912557	-0.6398185
C	-3.3928135	-5.9470314	-2.4137043
H	-1.7871551	-5.7756769	-0.2255664
C	-0.5831927	-3.8893584	1.1988053
C	-2.2878323	-0.9734757	-3.8548861
C	-4.3340434	-0.6331895	-2.4404891
H	-2.3120164	-0.1594172	-1.8705183
H	-1.2204212	-1.2032315	-3.8674796
H	-2.4180336	0.0101725	-4.3186013
H	-2.8211376	-1.7160270	-4.4626868
H	-4.8958863	-1.4245514	-2.9514197
H	-4.5037337	0.3038071	-2.9811858
H	-4.7442191	-0.5209406	-1.4352451
C	-2.8242139	-6.1595302	-3.8284572
C	-4.9307843	-5.9040740	-2.4418730
H	-3.0895666	-6.8035569	-1.7960324
H	-5.2834107	-5.0648860	-3.0521133

H	-5.3358117	-5.7768931	-1.4328221
H	-5.3389330	-6.8282254	-2.8693213
H	-1.7317513	-6.2223961	-3.8038425
H	-3.2181955	-7.0817085	-4.2733767
H	-3.0963376	-5.3234403	-4.4826331
C	-1.4115359	-4.4841395	2.3511509
C	0.6444989	-4.7646172	0.8930144
H	-0.1995275	-2.9164935	1.5251776
H	-2.2535797	-3.8337073	2.6019041
H	-0.7953228	-4.6079616	3.2483193
H	-1.8049196	-5.4684280	2.0696410
H	0.3487804	-5.7427479	0.4959203
H	1.2202965	-4.9364652	1.8103423
H	1.3044994	-4.2804738	0.1689814
C	-1.0008123	-1.2436072	3.4325654
C	-3.1623969	-1.1910657	2.3370304
C	-3.7757791	-1.4337683	3.5680223
C	-4.0854914	-1.0265600	1.1369111
C	-3.0405189	-1.5866948	4.7421330
H	-4.8618725	-1.4970011	3.6062873
C	-1.6578485	-1.4750914	4.6476455
C	-3.7183344	-1.8391716	6.0756161
H	-1.0657137	-1.5725872	5.5566805
C	0.5145659	-1.1275540	3.4972103
C	-5.1003566	0.1124343	1.3312887
C	-4.8037724	-2.3487644	0.8153515
H	-3.4688560	-0.7525716	0.2732950
H	-4.0857501	-3.1526633	0.6350419
H	-5.4305711	-2.2425421	-0.0768121
H	-5.4493476	-2.6411497	1.6525985
H	-5.7516490	-0.0769289	2.1927494
H	-5.7396992	0.2021108	0.4448985
H	-4.5971077	1.0700340	1.4804546
C	-4.5147433	-3.1558997	6.0634305
C	-4.6194406	-0.6572226	6.4770587
H	-2.9246866	-1.9305597	6.8298572
H	-4.0475735	0.2754358	6.5093431
H	-5.4300613	-0.5264735	5.7511722
H	-5.0701924	-0.8268134	7.4627410
H	-3.8677611	-4.0003623	5.8049274
H	-4.9663187	-3.3483917	7.0445226
H	-5.3210157	-3.1128918	5.3223923
C	0.9315005	0.0522376	4.3931618
C	1.1804004	-2.4176603	4.0071311
H	0.8780887	-0.9201775	2.4827999
H	0.7880694	-2.6951116	4.9925589
H	2.2599092	-2.2696962	4.1049399
H	1.0125476	-3.2563873	3.3283254
H	0.4653607	0.9813919	4.0580631
H	2.0165095	0.1959205	4.3497304
H	0.6478039	-0.1356741	5.4367035

3opt
131
Energy =
Si -1.2483979 -0.3368232   1.6603357
Si -2.3218134 -0.4328008 -0.3840070
Si -0.6990581 -0.5498682 -2.0239728
Si   0.0328871 -1.5964117   0.0364939
Si -0.2909471   0.9910891 -0.1586226
Si   1.8071035 -0.1093416   0.0429361
Si -5.0497956 -0.3567234 -1.9746386
Si -0.5892787 -4.4161646 -1.1109772
Si -1.2385729   3.6073396 -1.7076954
Si   4.5269164 -0.0427062   1.8026941
Si   3.2033807   1.2425397 -2.3308372
N   -4.0090473   0.1224153 -0.6444611
N   -0.0115914 -3.3754341   0.1856022
N   -0.6826605   2.7289620 -0.2834035
N   2.8378362   0.2680602   1.4320339
N   2.8865595 -0.2119547 -1.3864270
C   -4.5922207   0.8445830   0.4425054
C   -4.7371775   0.2555309   1.7089853
H   -4.4359924 -0.7778685   1.8427691
C   -5.2349731   0.9957019   2.7808265
H   -5.3209668   0.5261816   3.7573083
C   -5.6103252   2.3289343   2.6090875
H   -5.9916304   2.9047640   3.4481429
C   -5.4754891   2.9203622   1.3516690
H   -5.7426807   3.9641492   1.2070309
C   -4.9641313   2.1884754   0.2819912
H   -4.8198289   2.6572029 -0.6853151
C   -4.0503967 -1.1793214 -3.3311973
H   -3.2767884 -0.5148153 -3.7294694
H   -4.7294353 -1.4542645 -4.1505319
H   -3.5469573 -2.0882057 -2.9885352
C   -5.9753567   1.1115419 -2.7202611
H   -6.6387833   1.5904591 -1.9918563
H   -6.5938663   0.7675939 -3.5603027
H   -5.2848645   1.8712634 -3.1038525
C   -6.3371581 -1.5657758 -1.3090280
H   -5.8528605 -2.4773807 -0.9390087
H   -7.0614192 -1.8551583 -2.0813929
H   -6.8937392 -1.1222318 -0.4744621
C   0.2142723 -3.8982818   1.4812512
C   1.3458869 -3.5071997   2.2164822
H   2.0269114 -2.7884906   1.7707450
C   1.5920189 -4.0187435   3.4873111
H   2.4806444 -3.7000441   4.0267164
C   0.7138560 -4.9391080   4.0636281
H   0.9056444 -5.3386372   5.0556345
C   -0.4221486 -5.3252982   3.3505943
H   -1.1303413 -6.0233245   3.7912743
C   -0.6750707 -4.8063539   2.0823579
H   -1.5815893 -5.0847209   1.5536139
C   0.0812911 -6.1588403 -0.8207991
H   1.1775555 -6.1357690 -0.8000956
H   -0.2238119 -6.8095072 -1.6509130
H   -0.2611741 -6.6163174   0.1119617
C   -2.4775354 -4.4504432 -1.1674220
H   -2.9167692 -4.9484430 -0.2950209
H   -2.8450942 -4.9590370 -2.0681000
H   -2.8533256 -3.4199334 -1.1834720
C   0.0540241 -3.8633575 -2.7814065
H   -0.4616639 -2.9786761 -3.1685894

H	-0.0876454	-4.6857558	-3.4973002
H	1.1223267	-3.6315871	-2.7398634
C	-0.7859027	3.4933562	0.9264191
C	0.0283932	4.6183913	1.1243571
H	0.7986340	4.8429951	0.3920082
C	-0.1553555	5.4451638	2.2334863
H	0.4788572	6.3191576	2.3629738
C	-1.1405335	5.1465075	3.1760066
H	-1.2843988	5.7886113	4.0412935
C	-1.9292637	4.0064539	3.0029211
H	-2.6976441	3.7551669	3.7290284
C	-1.7569425	3.1874601	1.8903238
H	-2.3863378	2.3157812	1.7473125
C	-2.0715537	2.4816070	-2.9546661
H	-1.3800346	1.7894875	-3.4455988
H	-2.5456878	3.1029631	-3.7275526
H	-2.8457147	1.8766462	-2.4711607
C	-2.5071672	4.8879630	-1.1449881
H	-3.2806595	4.4296707	-0.5200361
H	-2.9937081	5.3365935	-2.0210577
H	-2.0495771	5.6931148	-0.5608858
C	0.1472465	4.5500174	-2.5779017
H	0.6063358	5.2935022	-1.9161836
H	-0.2534673	5.0834090	-3.4507243
H	0.9347920	3.8786761	-2.9295529
C	2.1037286	0.7225827	2.5944417
C	1.6522816	-0.1754180	3.5668149
H	1.7985781	-1.2377778	3.4167895
C	0.9784636	0.2872619	4.6967839
H	0.6134766	-0.4276597	5.4290961
C	0.7407147	1.6501458	4.8618548
H	0.1979380	2.0108938	5.7315040
C	1.1737131	2.5488644	3.8857834
H	0.9663290	3.6087473	3.9865406
C	1.8493422	2.0884221	2.7591971
H	2.1815562	2.7800786	1.9919550
C	5.6307029	-0.0869622	0.2877066
H	5.3619662	-0.8681959	-0.4272338
H	6.6606164	-0.2711646	0.6230298
H	5.6176307	0.8741248	-0.2336310
C	4.7563280	-1.6662227	2.7427674
H	4.1784180	-1.6696844	3.6734427
H	5.8135279	-1.8063584	3.0052729
H	4.4469678	-2.5334337	2.1484891
C	5.1487456	1.3451723	2.9195734
H	5.0350371	2.3221973	2.4348224
H	6.2140329	1.2008097	3.1434345
H	4.6031561	1.3818814	3.8681296
C	3.1996082	-1.5043918	-1.8470281
C	3.3709815	-1.8088283	-3.2107664
H	3.2087288	-1.0369928	-3.9551296
C	3.7065133	-3.0968452	-3.6225652
H	3.8235672	-3.2976339	-4.6847986
C	3.8557455	-4.1309351	-2.6964110
H	4.0967209	-5.1376919	-3.0250381
C	3.6669571	-3.8500972	-1.3416389
H	3.7633742	-4.6363806	-0.5974454
C	3.3573049	-2.5597450	-0.9264689
H	3.2369652	-2.3499133	0.1322962
C	2.0092799	1.4745150	-3.7676361
H	2.1485641	0.7197086	-4.5494246
H	2.1545266	2.4599090	-4.2296692
H	0.9716713	1.3889755	-3.4271808

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C     4.9477378    1.2223427   -3.0591819
H     5.7209240    1.3374012   -2.2937523
H     5.0482247    2.0552648   -3.7678012
H     5.1573911    0.2956920   -3.6033936
C     3.0549831    2.6984281   -1.1492216
H     2.0344707    2.8132436   -0.7669093
H     3.3229756    3.6262164   -1.6712216
H     3.7244819    2.5807288   -0.2907448
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3iso

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131
Energy =
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Si   -3.2529219    1.0497831   -0.5337015
Si   -1.3556954   -0.2284033   -1.6484984
Si   -0.1585468   -1.2718399    0.0766191
Si   -0.0239211    1.4446817   -0.6507749
Si    1.7627748    0.0925447   -0.0115655
Si   -6.1575399    0.4725179   -1.0073270
Si   -0.5693219   -4.0603915   -1.1022105
Si   -0.5751358    3.7699231   -2.7066679
Si    4.2347193    0.1593938    2.0922090
Si    3.5320574    0.8201270   -2.3496409
N    -4.6934221    0.0266073   -0.1370425
N    -0.2698672   -3.0334285    0.3184858
N    -0.1255829    3.1525407   -1.1114294
N     2.6309988    0.5298784    1.4721973
N     2.9930950   -0.4092624   -1.2026019
C    -4.7383050   -0.9394188    0.8958326
C    -3.7636865   -1.9458167    0.9893693
H    -2.9880646   -1.9871958    0.2327195
C    -3.7894336   -2.8696365    2.0300485
H    -3.0122919   -3.6249219    2.0881966
C    -4.7913737   -2.8221368    3.0022953
H    -4.8012988   -3.5408283    3.8174553
C    -5.7670407   -1.8275603    2.9204070
H    -6.5474495   -1.7632619    3.6757674
C    -5.7377753   -0.8942432    1.8853944
H    -6.4788535   -0.0999550    1.8501479
C    -5.7233138    0.8931723   -2.7929443
H    -5.1425268    1.8185376   -2.8595570
H    -6.6413841    1.0154004   -3.3853747
H    -5.1257328    0.0944036   -3.2471637
C    -7.0289139    1.9681352   -0.2500788
H    -7.3934801    1.7646038    0.7636287
H    -7.8866442    2.2825282   -0.8595744
H    -6.3272330    2.8087322   -0.1907547
C    -7.3329393   -1.0041242   -1.0398904
H    -6.8279718   -1.8820721   -1.4602913
H    -8.2012503   -0.7779320   -1.6725764
H    -7.6983418   -1.2791464   -0.0457445
C    -0.0534687   -3.5665307    1.6037516
C     0.7900452   -2.9107834    2.5188869
H     1.2776040   -1.9893290    2.2075728
C     1.0074828   -3.4197291    3.7951773
H     1.6698204   -2.8874844    4.4728324
C     0.3922036   -4.6052983    4.2024665
H     0.5606615   -5.0020967    5.1994639
C    -0.4535171   -5.2634078    3.3079953
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H	-0.9591794	-6.1781128	3.6085211
C	-0.6806331	-4.7514072	2.0330031
H	-1.3699557	-5.2590881	1.3664974
C	0.1293417	-5.7946616	-0.7974232
H	1.0339576	-5.7622100	-0.1825021
H	0.4049048	-6.2239176	-1.7693181
H	-0.5791607	-6.4790110	-0.3204466
C	-2.4062694	-4.1899079	-1.4885249
H	-2.9907147	-4.5483483	-0.6337784
H	-2.5655866	-4.8835081	-2.3252136
H	-2.8082303	-3.2130414	-1.7804168
C	0.3243052	-3.4104857	-2.6181612
H	-0.0189728	-2.4188682	-2.9237968
H	0.1366537	-4.1093826	-3.4457826
H	1.4047588	-3.3679782	-2.4545183
C	-0.1761440	4.1682552	-0.0976336
C	0.8242487	5.1475680	-0.0227386
H	1.6847328	5.0708414	-0.6803157
C	0.7121927	6.2103164	0.8764588
H	1.4944284	6.9647462	0.9163123
C	-0.3946432	6.3027928	1.7206568
H	-0.4845729	7.1315156	2.4182882
C	-1.3787505	5.3111186	1.6704273
H	-2.2419787	5.3663448	2.3288849
C	-1.2715559	4.2526874	0.7730178
H	-2.0427065	3.4896791	0.7075383
C	-1.2682193	2.4652132	-3.8600274
H	-0.5766677	1.6497418	-4.0853054
H	-1.5258708	2.9645359	-4.8055521
H	-2.1783491	2.0254324	-3.4393380
C	-1.9135361	5.0738513	-2.4706628
H	-2.7774407	4.6253524	-1.9657030
H	-2.2461860	5.4551509	-3.4450634
H	-1.5729173	5.9239174	-1.8701660
C	0.9113467	4.5792256	-3.5515478
H	1.2874190	5.4353227	-2.9800866
H	0.6306883	4.9425871	-4.5492129
H	1.7343245	3.8670537	-3.6738973
C	1.8419369	1.2911744	2.4157490
C	1.1113327	0.6667830	3.4326726
H	1.1021109	-0.4143522	3.4975762
C	0.3714309	1.4263208	4.3396661
H	-0.2074946	0.9231225	5.1094239
C	0.3549725	2.8167241	4.2415002
H	-0.2324929	3.4084129	4.9384061
C	1.0810529	3.4445847	3.2284656
H	1.0590928	4.5240868	3.1259652
C	1.8138776	2.6866494	2.3199944
H	2.3677015	3.1675426	1.5205244
C	5.5024498	-0.2162141	0.7593957
H	5.2808863	-1.1223975	0.1909908
H	6.4728920	-0.3570966	1.2551161
H	5.6062454	0.6166850	0.0575688
C	4.1886744	-1.2887281	3.3018716
H	3.5077305	-1.0780282	4.1343705
H	5.1861558	-1.4679235	3.7246528
H	3.8586545	-2.2163962	2.8224700
C	4.8668126	1.6613035	3.0447646
H	4.9159825	2.5494082	2.4036257
H	5.8790736	1.4606361	3.4204430
H	4.2291017	1.9067586	3.9000481
C	3.3133201	-1.7707663	-1.3274648
C	3.8096973	-2.3252345	-2.5230184

H	3.9207372	-1.6972082	-3.4006485
C	4.1237457	-3.6801766	-2.6111482
H	4.4941427	-4.0752776	-3.5540542
C	3.9383946	-4.5320719	-1.5214431
H	4.1672065	-5.5907029	-1.6002704
C	3.4417369	-3.9970431	-0.3305404
H	3.2828272	-4.6328778	0.5363923
C	3.1461966	-2.6430306	-0.2333506
H	2.7725818	-2.2440327	0.7049533
C	2.3927897	0.8518762	-3.8430808
H	2.4255510	-0.0971823	-4.3910188
H	2.6438986	1.6581234	-4.5432656
H	1.3617169	0.9953019	-3.5009028
C	5.3143075	0.4996142	-2.9124485
H	5.8645977	-0.1194802	-2.1972693
H	5.8437638	1.4564942	-3.0056119
H	5.3609209	0.0027631	-3.8877600
C	3.4949048	2.4837200	-1.4728205
H	2.4747113	2.8084576	-1.2444246
H	3.9515747	3.2430270	-2.1216893
H	4.0614530	2.4526324	-0.5357379

Cartesian coordinates in units of Å

3'

Si	0.000000	0.000000	0.000000
Si	0.000000	0.000000	3.727252
Si	1.353138	0.000000	1.863529
Si	-0.912893	-1.300723	1.837220
Si	-0.899282	1.311574	1.890427
Si	-2.861873	0.014710	1.861957
N	-4.004559	-0.223869	3.184445
H	-4.703295	0.508697	3.295567
H	-3.567671	-0.406782	4.084705
N	-3.997225	0.270595	0.536421
H	-4.706226	-0.451702	0.422846
H	-3.555232	0.447747	-0.362515
N	-0.798355	-3.080270	1.770839
H	-0.725823	-3.521752	2.685295
H	-0.021745	-3.410232	1.202060
N	-0.769294	3.089868	1.956117
H	-0.694313	3.530426	1.041490
H	0.010319	3.413767	2.524190
N	3.102293	0.015813	1.863153
H	3.662278	0.031597	2.709109
H	3.661605	0.014192	1.016627

3iso'

Si	0.000000	0.000000	0.000000
Si	2.095110	0.000000	1.277269
Si	0.000000	0.000000	2.607072
Si	-1.660730	-1.032453	1.321446
Si	-0.948176	1.720245	1.297760
Si	-3.099320	0.832376	1.262140
N	-4.298861	0.872937	2.556046
H	-4.758119	1.771145	2.696354
H	-3.966254	0.524605	3.451428
N	-4.112225	1.346205	-0.085389
H	-4.961455	0.807182	-0.240463
H	-3.623018	1.476606	-0.966323
N	-0.388433	3.406221	1.210937

H	-0.071792	3.770023	2.107292
H	0.375397	3.522989	0.548239
N	-2.153196	-2.733007	1.463496
H	-2.664906	-3.092203	0.660016
H	-1.385446	-3.371123	1.660968
N	2.645764	-1.683687	1.205933
H	2.054178	-2.504135	1.279498
H	3.613572	-1.898981	1.413162