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$(PhC(NtBu)_2Al)_2(SiH_2)_4$ Six-Membered Heterocycle: Comparable in Structure to Cyclohexane

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Contents:

S1. Experimental Section

All manipulations were carried out under a dry argon or nitrogen atmosphere using Schlenk line and glovebox techniques. Solvents including THF, diethyl ether, toluene and n-hexane were dried by refluxing with sodium/potassium benzophenone under N_2 prior to use. The NMR (^{1}H, ^{13}C, ^{27}Al, ^{29}Si) spectra were recorded on Bruker Avance 300 MHz and/or Bruker Avance 500 MHz spectrometer. Melting points of compounds were measured in a sealed glass tube using the Büchi-540 instrument. Elemental analysis were performed by the Analytisches Labor des Instituts für Anorganische Chemie der Universität Göttingen. IR spectra of solid samples were measured with a Cary 630 FTIR spectrometer with Dial Path Technology and analyzed by FTIR MicroLab software. Commercial reagents were purchased from Aldrich, Acros or Alfa-Aesar Chemical Co. and used as received. LSiMes[1] (L = PhC(N*t*Bu)$_2$, Mes = 2,4,6-Me$_3$C$_6$H$_2$), LSi-SiL[2] (L = PhC(N*t*Bu)$_2$) were prepared according to the literatures.

LAl(SiH$_2$SiH$_2$)$_2$AlL (**1**): To a solution of LSi-SiL (L=PhC(N*t*Bu)$_2$) (519 mg, 1 mmol) in toluene (40 mL) at -78 ^{o}C, a solution of AlH$_3$·NEtMe$_2$ (0.5 M in toluene, 3 mL, 1.5 mmol) was added dropwise under stirring. The mixture was kept at this temperature for one hour and then allowed to warm to -30 ^{o}C slowly. Then the solution was placed in a fridge at -26 ^{o}C for 2 days. The resulted colorless solution was filterred over a G4 frit. The volume of toluene was reduced to 5 mL and the solution was cooled to −26 °C. After one night, big crystals of L$_2$AlH were found and collected by filtration. The volatiles of the filtrate were removed under vacuum and the residues were extracted with n-hexane. The volume of n-hexane was reduced to 5 mL and the solution was cooled to −26 °C again. After one day, several big colorless crystals of L$_2$AlH were found. The clear solution was transferred to another clean flask which then was placed in the fridge at -26 ^{o}C. After several days, small colorless crystals (**1**) were found. Yield: 18%. Mp: 210 °C. ^{1}H NMR (C$_6$D$_6$, 298K, 300 MHz, ppm): δ 7.10-6.85 (m, 10H, Ph-*H*), 3.63 (s, 8H, Si*H*$_2$), 1.11 (s, 36H, C(C*H*$_3$)$_3$). ^{13}C {^{1}H} NMR (C$_6$D$_6$, 298K, 125 MHz, ppm): δ = 173.5 (Ph*C*(N*t*Bu)$_2$), 135.0, 130.1, 129.1, 128.9, 127.6, 127.1, 52.3 (N*C*Me$_3$), 32.3 (NC*Me*$_3$). ^{29}Si INEPT NMR (C$_6$D$_6$, 298 K, 99 MHz, ppm) δ= -128.9 (br, *Si*H$_2$). IR (solid, FTIR): *v* = 2074 cm^{-1} (Si−H). Anal. Calcd (%) for C$_{30}$H$_{54}$N$_4$Al$_2$Si$_4$ (Mr = 636.31): C, 56.56; H, 8.54; N, 8.79. Found: C, 57.71; H, 8.03; N, 8.15. No signal was found for aluminum atom in the ^{27}Al NMR spectrum.

LSi(AlMe$_3$)-Si(AlMe$_3$)L(**2**) To a solution of LSi-SiL (L=PhC(N*t*Bu)$_2$) (519 mg, 1 mmol) in toluene (40 mL) at -78 ^{o}C, a solution of AlMe$_3$ (1 M in hexane, 2 mL, 2 mmol) was added dropwise under stirring. The mixture was kept at this temperature for one hour and then warmed to room temperature. The solution was stirred overnight. After filtration, the solution was concentrated to afford colorless crystalline solid of **3**. Yield: 82%. Mp: 174°C. ^{1}H NMR (C$_6$D$_6$, 298K, 300 MHz, ppm): δ 7.52 (br), 7.07-6.86 (m, 10H, Ph-*H*), 1.21 (s, 36H, C*Me*$_3$), -0.02 (s, 18H, Al*Me*$_3$). ^{13}C{^{1}H} NMR (C$_6$D$_6$, 298K, 125 MHz, ppm): δ = 162.5 (Ph*C*(N*t*Bu)$_2$), 132.1, 130.7, 129.9, 128.9, 128.5, 128.3, 128.2, 128.0, 127.8, 54.0 (N*C*Me$_3$), 31.3 (NC*Me*$_3$), -5.8 (Al*Me*$_3$). ^{29}Si{^{1}H} NMR (C$_6$D$_6$, 298 K, 99 MHz, ppm) δ= +56.9 ppm(br, *Si*AlMe$_3$). Anal. Calcd (%) for C$_{36}$H$_{64}$N$_4$Al$_2$Si$_2$ (M$_r$ = 662.43): C, 65.21; H, 9.73; N, 8.45. Found: C, 65.62; H, 9.68; N, 8.31. No signal was found for aluminum atom in the ^{27}Al NMR spectrum.

[LAlHSiH$_2$Mes]$_2$ (**3**): To a solution of LSiMes (L = PhC(N*t*Bu)$_2$, Mes = 2,4,6-Me$_3$C$_6$H$_2$) (378 mg, 1 mmol) in toluene (40 mL) at -78 ^{o}C, a solution of AlH$_3$·NEtMe$_2$ (0.5 M in toluene, 2 mL, 1 mmol) was added dropwise under stirring. The mixture was warmed to room temperature slowly and stirred overnight. The resulted colorless solution was filtered over a G4 frit. Then the solvent was removed under vacuum and the remaining was washed with n-hexane (5 mL) to get a white solid. X-ray quality crystals were grown from a solution in toluene at -26 °C. Yield: 76%. Mp: 146 °C. ^{1}H NMR (C$_6$D$_6$, 298K, 300 MHz, ppm): δ 7.15-6.75 (m, 10H, Ph-*H*), 6.88 (s, 10H, C$_6$*H*$_2$) 5.14 (br, 2H, Al*H*), 4.53 (s, 4H, Si*H*$_2$), 2.69 (s, 12H, *o*-C*H*$_3$), 2.17 (s, 6H, *p*-CH$_3$), 0.92 (s, 36H, C(C*H*$_3$)$_3$). ^{13}C{^{1}H}

NMR (C_6D_6, 298K, 125 MHz, ppm): δ = 175.0(Ph*C*(N*t*Bu)$_2$), 144.0, 138.4, 134.9, 130.6, 129.4, 129.0, 128.7, 128.5,128.3, 128.1, 127.9,127.5, 51.8 (N*C*Me$_3$), 31.8 (NC*Me*$_3$), 25.0(*o*-*Me*), 21.2 (*p*-*Me*). ^{29}Si{^{1}H} NMR (C_6D_6, 298 K, 99 MHz, ppm) δ= -91.7 (m, *Si*H$_2$Mes). IR (solid, FTIR): *v* = 2095 cm^{-1} (Si−H), 1645 cm^{-1} (Al−H). Anal. Calcd (%) for $C_{48}H_{74}N_4Al_2Si_2$ (Mr = 816.51): C, 70.54; H, 9.13; N, 6.86. Found: C, 70.22; H, 9.27; N, 6.75. No signal was found for aluminum atom in the ^{27}Al NMR spectrum.

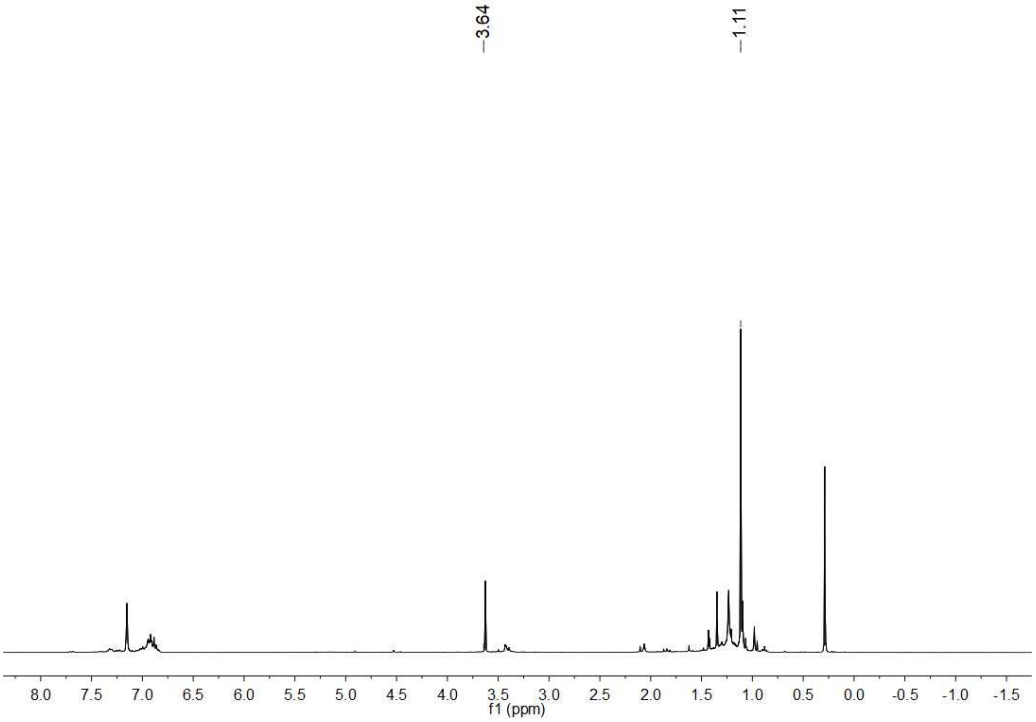

Figure S1.1 ^{1}H NMR spectrum of **1**

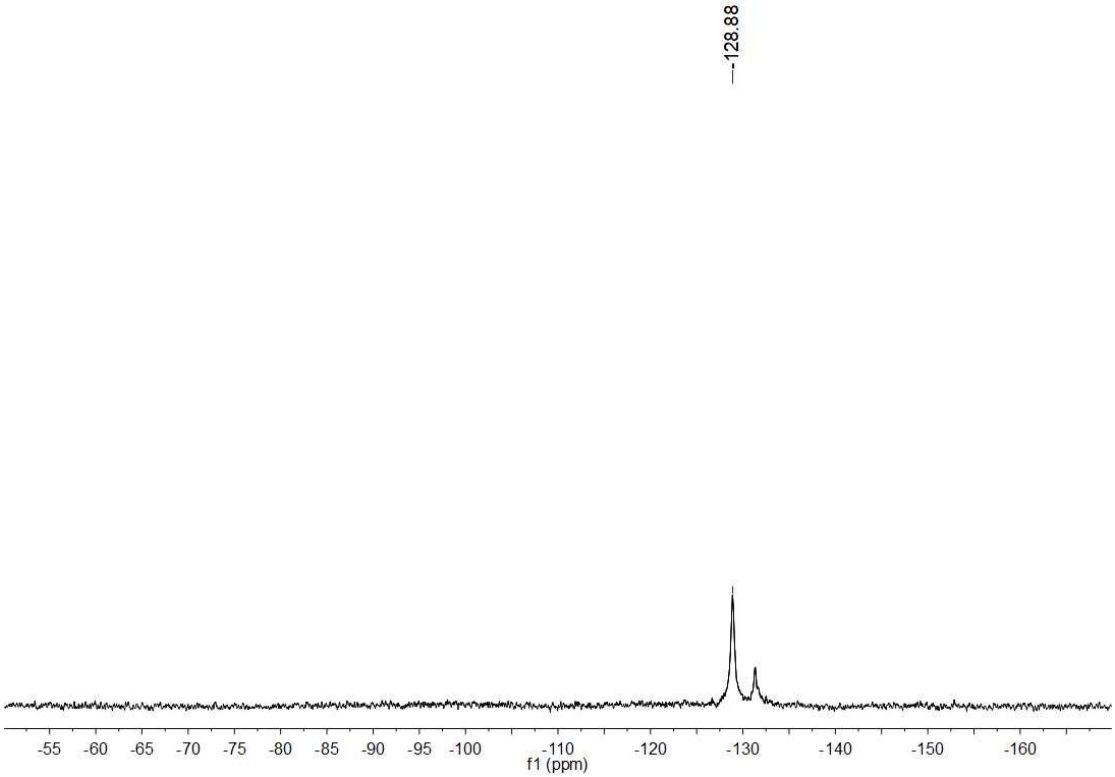

Figure S1.2 ^{29}Si INEPT NMR spectrum of **1**

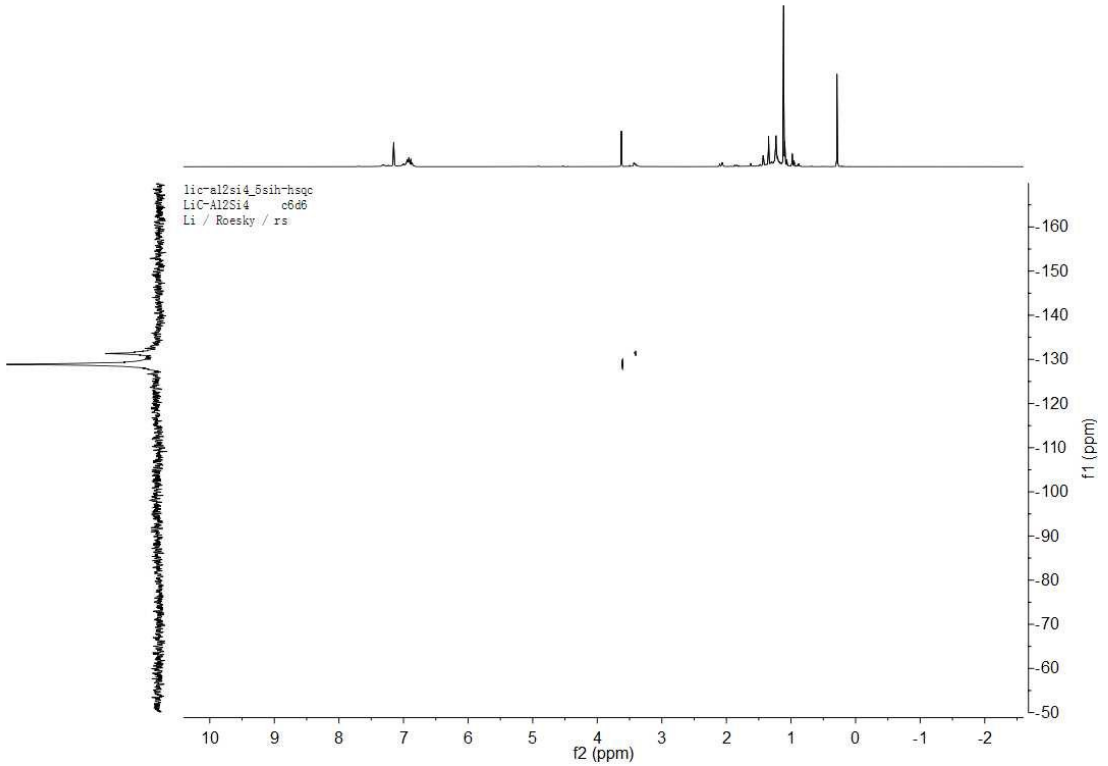

Figure S1.3 Si-H HSQC NMR spectrum of **1**

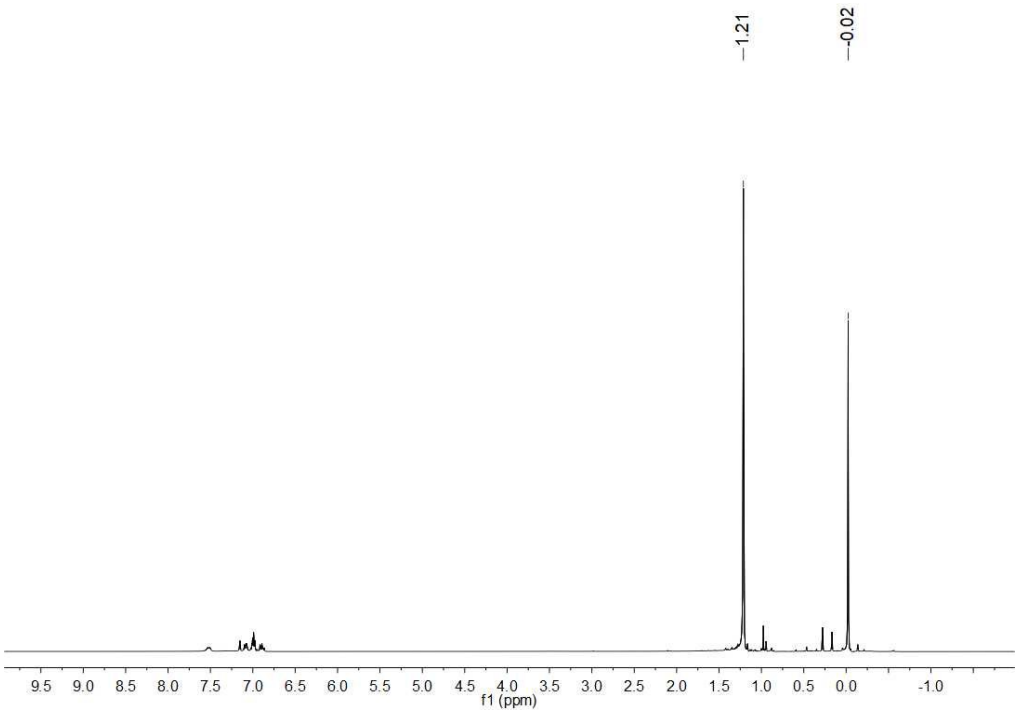

Figure S1.4 1H NMR spectrum of **2**

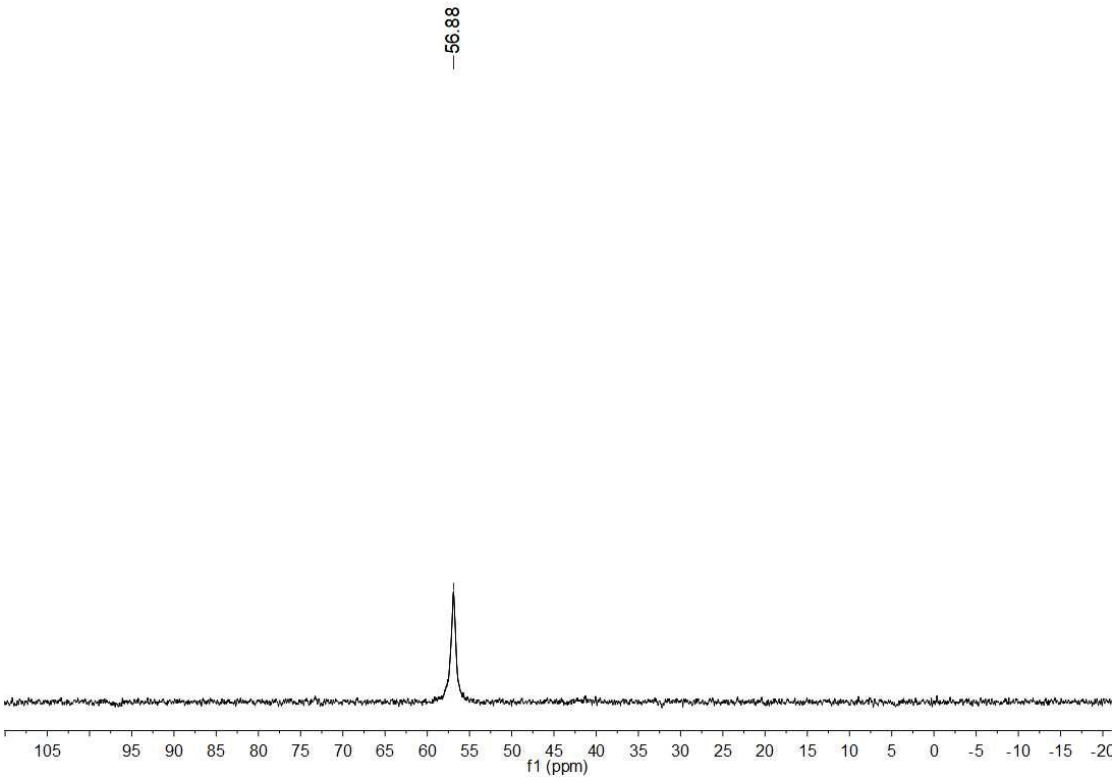

Figure S1.5 ^{29}Si NMR spectrum of **2**

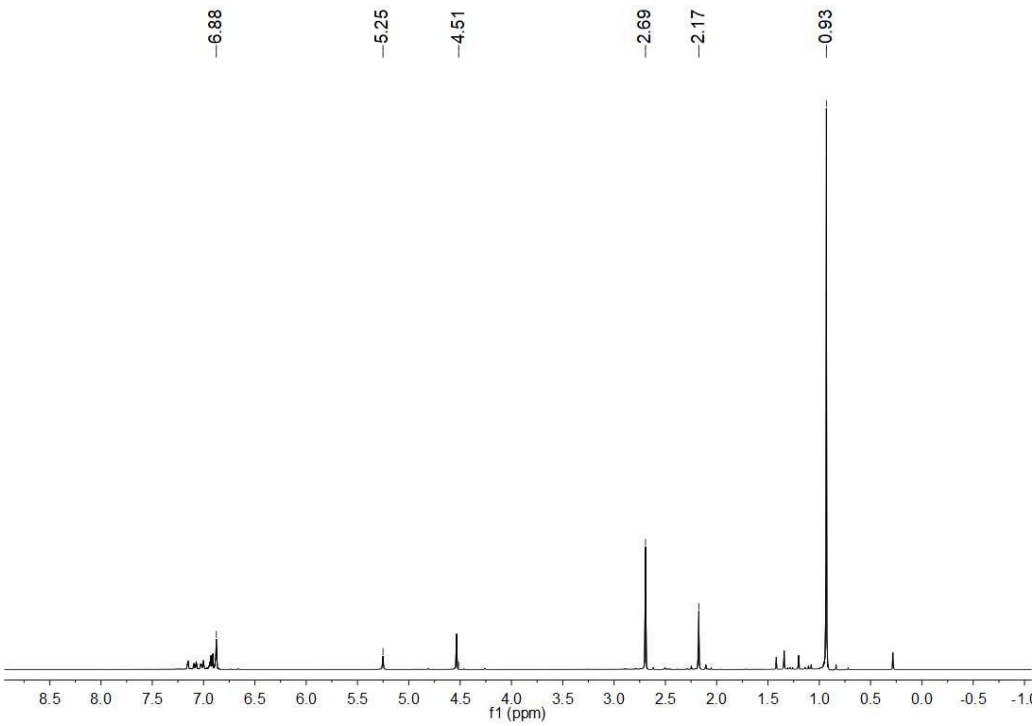

Figure S1.6 1H NMR spectrum of **3**

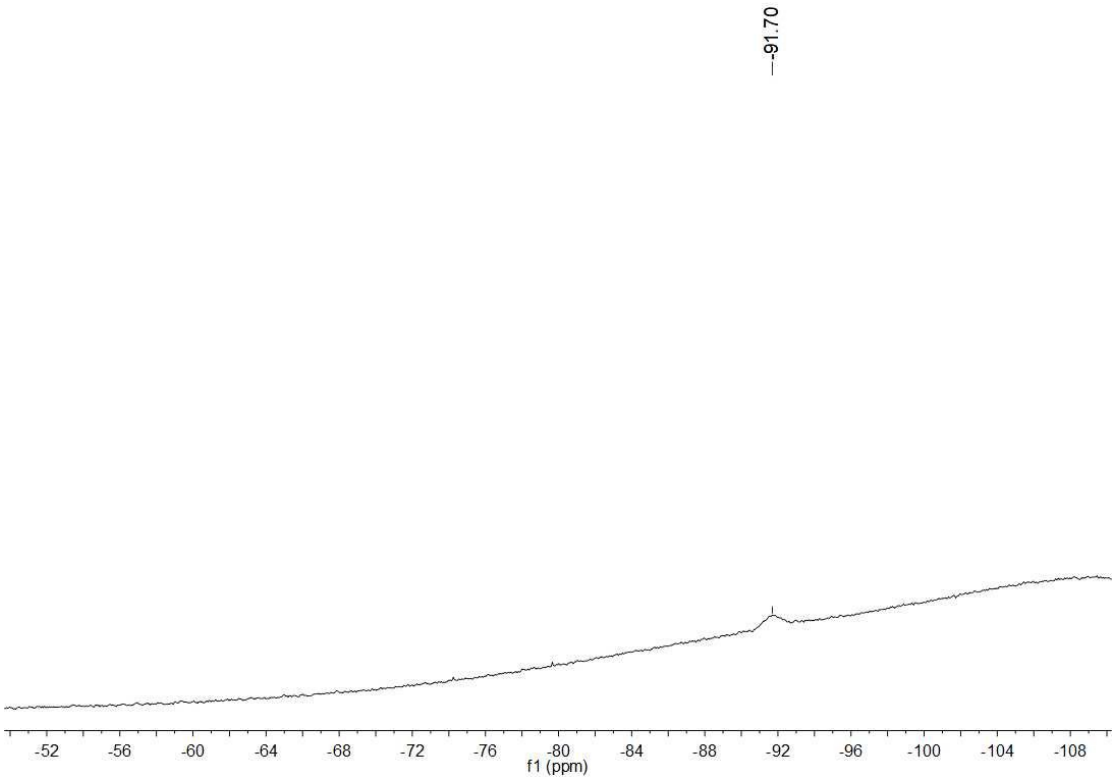

Figure S1.7 ^{29}Si NMR spectrum of **3**

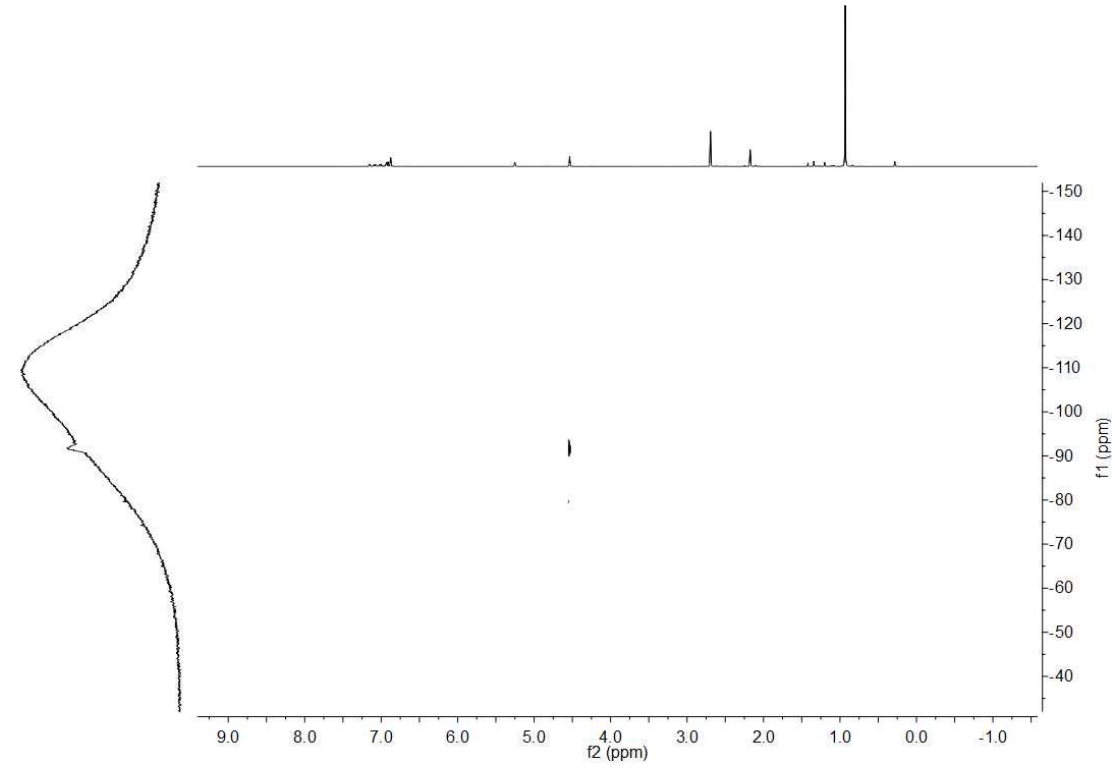

Figure S1.8 Si-H HSQC NMR spectrum of **3**

S2. X-Ray Crystallographic Analysis

The data were collected from shock-cooled crystals at 100(2) K, on a BRUKER D8 three circle diffractometer equipped with an INCOATEC Mo Microsource and Ag Microsource with mirror optics (MoK_α radiation, λ = 0.71073 Å, AgK_α radiation, λ = 0.56086 Å) The data were integrated with SAINT.[3] A multi-scan absorption correction was applied using SADABS.[4] The structures were solved by SHELXT[5] and refined on F^2 using SHELXL[6] in the graphical user interface SHELXLE.[7]

Identification code	1	2	3
CCDC number	1875009	1875010	1875008
Empirical formula	$C_{30}H_{54}Al_2N_4Si_4$	$C_{39.50}H_{68}Al_2N_4Si_2$	$C_{48}H_{74}Al_2N_4Si_2$
Formula weight	637.09	709.11	817.25
Temperature	100(2) K	100(2) K	100(2) K
Wavelength	0.71073 Å	0.71073 Å	0.56086 Å
Crystal system	Monoclinic	monoclinic	triclinic
Space group	$P2_1/c$	$P2_1/c$	P-1
Unit cell dimensions Å/°	a = 13.559(2)	a = 18.949(2)	a = 10.039(2)
	b = 8.253(2)	b = 11.775(2)	b = 10.144(2)
	c = 17.689(3)	c = 20.216(3)	c = 13.835(3)
	□= 90	□= 90	□= 103.40(2)
	□= 103.31(2)	□= 102.27(2)	□= 97.39(2)
	□ = 90	□ = 90	□ = 114.85(3)
Volume Å^3	1926.3(7)	4407.6(11)	1202.2(5)
Z	2	4	1
Density (calculated) Mg/m^3	1.098	1.069	1.129
Absorption coefficient mm^{-1}	0.224	0.150	0.083
F(000)	688	1548	444
Crystal size mm	0.210 x 0.150 x 0.150	0.260 x 0.170 x 0.100	0.195 x 0.150 x 0.144
Theta range for data collection	1.543 to 26.403°.	1.100 to 26.454°.	1.825 to 20.548°.
Reflections collected	32188	86568	46064
Independent reflections	3950	9064	4929
R_{int}	0.0532	0.0665	0.0469
Data / restraints / parameters	3950 / 335 / 258	9064 / 447 / 544	4929 / 181 / 305
Goodness-of-fit on F^2	1.052	1.017	1.041
R1 [I>2sigma(I)]	0.0410	0.0368	0.0370
wR2(all data)	0.1143	0.0922	0.0955
Largest diff. peak and hole	0.425/-0.266 e.Å^{-3}	0.276/-0.211 e.Å^{-3}	0.313/ -0.335 e.Å^{-3}

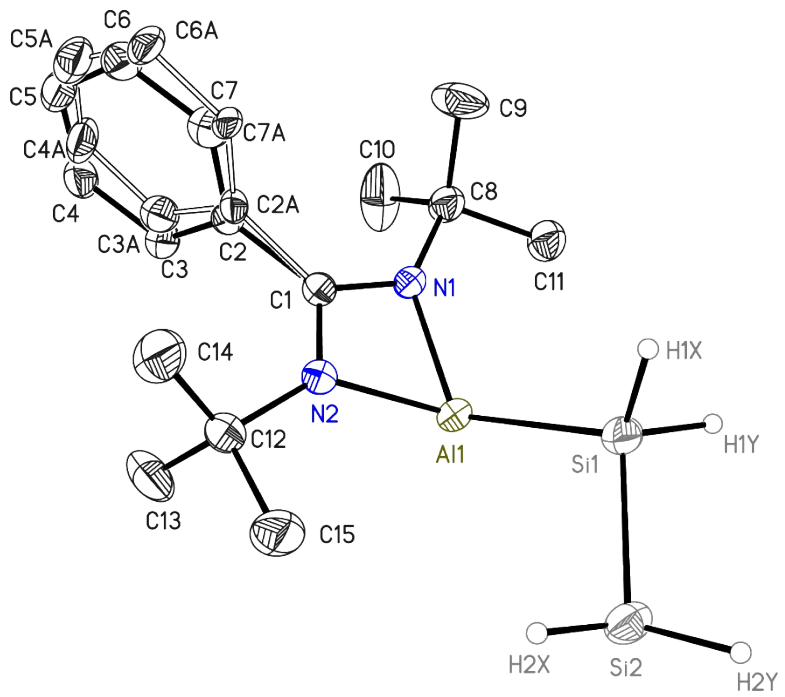

Figure S2.1. The asymmetric unit of **1** with anisotropic displacement parameters at 50% probability level. The hydrogen atoms are omitted for clarity. The disordered phenyl ring was refined on two positions. The occupancy of the main positions refined to 0.680(18). For the refinement distance restraints and restraints for the anisotropic displacement parameters were used.[8]

Table S2.1. Bond lengths [Å] and angles [°] for **1**.

Si(1)-H(1Y)	1.440(17)	C(1)-C(2A)	1.507(10)
Si(1)-H(1X)	1.445(17)	C(2)-C(3)	1.390(6)
Si(1)-Si(2)	2.3413(9)	C(2)-C(7)	1.391(6)
Si(1)-Al(1)	2.4473(9)	C(3)-C(4)	1.380(6)
Si(2)-H(2X)	1.439(18)	C(4)-C(5)	1.379(6)
Si(2)-H(2Y)	1.448(18)	C(5)-C(6)	1.377(6)
Si(2)-Al(1)#1	2.4545(9)	C(6)-C(7)	1.386(6)
Al(1)-N(1)	1.9100(16)	C(2A)-C(7A)	1.388(11)
Al(1)-N(2)	1.9236(17)	C(2A)-C(3A)	1.393(11)
Al(1)-C(1)	2.3451(19)	C(3A)-C(4A)	1.393(11)
C(15)-C(12)	1.530(3)	C(4A)-C(5A)	1.367(11)
N(1)-C(1)	1.340(2)	C(5A)-C(6A)	1.370(10)
N(1)-C(8)	1.472(2)	C(6A)-C(7A)	1.370(10)
N(2)-C(1)	1.336(2)	C(8)-C(10)	1.526(3)
N(2)-C(12)	1.482(2)	C(8)-C(11)	1.526(3)
C(1)-C(2)	1.493(5)	C(8)-C(9)	1.527(3)

C(12)-C(14)	1.526(3)	N(2)-C(1)-C(2A)	124.5(12)
C(12)-C(13)	1.529(3)	N(1)-C(1)-C(2A)	125.6(13)
		N(2)-C(1)-Al(1)	55.11(9)
H(1Y)-Si(1)-H(1X)	101.3(14)	N(1)-C(1)-Al(1)	54.53(9)
H(1Y)-Si(1)-Si(2)	107.7(10)	C(2)-C(1)-Al(1)	171.5(3)
H(1X)-Si(1)-Si(2)	112.8(10)	C(2A)-C(1)-Al(1)	177.7(6)
H(1Y)-Si(1)-Al(1)	110.5(10)	C(3)-C(2)-C(7)	119.4(4)
H(1X)-Si(1)-Al(1)	116.6(10)	C(3)-C(2)-C(1)	120.5(5)
Si(2)-Si(1)-Al(1)	107.57(3)	C(7)-C(2)-C(1)	120.1(5)
H(2X)-Si(2)-H(2Y)	105.6(16)	C(4)-C(3)-C(2)	119.6(4)
H(2X)-Si(2)-Si(1)	105.4(11)	C(5)-C(4)-C(3)	120.6(4)
H(2Y)-Si(2)-Si(1)	111.3(11)	C(6)-C(5)-C(4)	120.4(4)
H(2X)-Si(2)-Al(1)#1	110.5(11)	C(5)-C(6)-C(7)	119.3(4)
H(2Y)-Si(2)-Al(1)#1	110.7(11)	C(6)-C(7)-C(2)	120.6(5)
Si(1)-Si(2)-Al(1)#1	112.90(3)	C(7A)-C(2A)-C(3A)	119.8(9)
N(1)-Al(1)-N(2)	69.47(7)	C(7A)-C(2A)-C(1)	121.1(9)
N(1)-Al(1)-C(1)	34.86(6)	C(3A)-C(2A)-C(1)	119.0(9)
N(2)-Al(1)-C(1)	34.73(7)	C(4A)-C(3A)-C(2A)	120.0(9)
N(1)-Al(1)-Si(1)	120.62(6)	C(5A)-C(4A)-C(3A)	118.3(8)
N(2)-Al(1)-Si(1)	119.55(6)	C(4A)-C(5A)-C(6A)	122.3(8)
C(1)-Al(1)-Si(1)	129.74(5)	C(7A)-C(6A)-C(5A)	119.6(9)
N(1)-Al(1)-Si(2)#1	112.85(6)	C(6A)-C(7A)-C(2A)	119.7(9)
N(2)-Al(1)-Si(2)#1	111.82(6)	N(1)-C(8)-C(10)	111.30(17)
C(1)-Al(1)-Si(2)#1	115.39(5)	N(1)-C(8)-C(11)	105.49(15)
Si(1)-Al(1)-Si(2)#1	114.84(3)	C(10)-C(8)-C(11)	108.24(19)
C(1)-N(1)-C(8)	130.52(16)	N(1)-C(8)-C(9)	110.69(18)
C(1)-N(1)-Al(1)	90.62(12)	C(10)-C(8)-C(9)	111.7(2)
C(8)-N(1)-Al(1)	138.86(12)	C(11)-C(8)-C(9)	109.13(18)
C(1)-N(2)-C(12)	129.16(16)	N(2)-C(12)-C(14)	112.79(17)
C(1)-N(2)-Al(1)	90.16(11)	N(2)-C(12)-C(13)	109.97(18)
C(12)-N(2)-Al(1)	137.79(12)	C(14)-C(12)-C(13)	111.1(2)
N(2)-C(1)-N(1)	109.40(16)	N(2)-C(12)-C(15)	104.87(16)
N(2)-C(1)-C(2)	125.3(6)	C(14)-C(12)-C(15)	108.44(19)
N(1)-C(1)-C(2)	125.1(6)	C(13)-C(12)-C(15)	109.42(19)

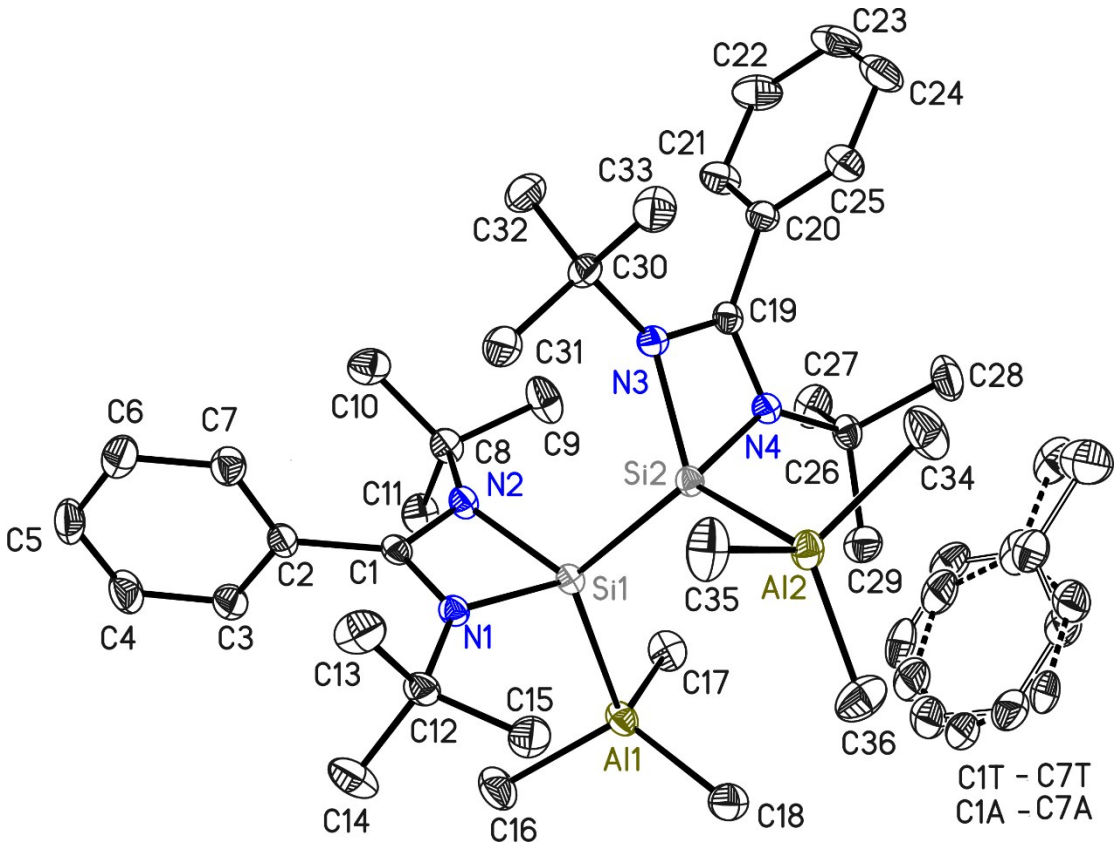

Figure S2.2. The asymmetric unit of **2** with anisotropic displacement parameters at 50% probability level. The hydrogen atoms are omitted for clarity. The disordered toluene on an inversion centre was refined on four positions (two generated by the inversion centre). The occupancy of the main positions refined to 0.381(8). For the disordered group distance restraints and restraints for the anisotropic displacement parameters were used.[8]

Table S2.2. Bond lengths [Å] and angles [°] for **2**.

C(1)-N(1)	1.341(2)	Al(2)-C(36)	1.9855(19)
C(1)-N(2)	1.3450(19)	Al(2)-C(35)	1.9858(19)
C(1)-C(2)	1.484(2)	Al(2)-C(34)	1.9932(19)
C(1)-Si(1)	2.3080(16)	Al(2)-Si(2)	2.5799(8)
Al(1)-C(18)	1.984(2)	N(2)-C(8)	1.483(2)
Al(1)-C(17)	1.9898(18)	Si(2)-N(3)	1.8379(14)
Al(1)-C(16)	1.9921(18)	Si(2)-N(4)	1.8407(13)
Al(1)-Si(1)	2.5921(7)	Si(2)-C(19)	2.3085(16)
N(1)-C(12)	1.4857(19)	C(3)-C(4)	1.387(2)
N(1)-Si(1)	1.8451(13)	N(3)-C(19)	1.344(2)
Si(1)-N(2)	1.8401(14)	N(3)-C(30)	1.484(2)
Si(1)-Si(2)	2.3937(7)	C(4)-C(5)	1.381(3)
C(2)-C(7)	1.389(2)	N(4)-C(19)	1.341(2)
C(2)-C(3)	1.392(2)	N(4)-C(26)	1.4858(19)

C(5)-C(6)	1.385(3)	N(2)-C(1)-C(2)	126.52(14)
C(6)-C(7)	1.388(2)	N(1)-C(1)-Si(1)	53.05(8)
C(8)-C(11)	1.526(2)	N(2)-C(1)-Si(1)	52.84(8)
C(8)-C(9)	1.527(2)	C(2)-C(1)-Si(1)	172.50(12)
C(8)-C(10)	1.528(2)	C(18)-Al(1)-C(17)	112.53(8)
C(12)-C(14)	1.525(2)	C(18)-Al(1)-C(16)	115.05(9)
C(12)-C(15)	1.525(2)	C(17)-Al(1)-C(16)	110.93(9)
C(12)-C(13)	1.526(2)	C(18)-Al(1)-Si(1)	107.15(6)
C(19)-C(20)	1.488(2)	C(17)-Al(1)-Si(1)	106.58(6)
C(20)-C(25)	1.389(2)	C(16)-Al(1)-Si(1)	103.78(6)
C(20)-C(21)	1.394(2)	C(1)-N(1)-C(12)	130.69(13)
C(21)-C(22)	1.388(2)	C(1)-N(1)-Si(1)	91.43(9)
C(22)-C(23)	1.378(3)	C(12)-N(1)-Si(1)	137.19(11)
C(23)-C(24)	1.381(3)	N(2)-Si(1)-N(1)	70.89(6)
C(24)-C(25)	1.391(2)	N(2)-Si(1)-C(1)	35.63(5)
C(26)-C(29)	1.519(2)	N(1)-Si(1)-C(1)	35.51(6)
C(26)-C(27)	1.526(2)	N(2)-Si(1)-Si(2)	112.10(5)
C(26)-C(28)	1.530(2)	N(1)-Si(1)-Si(2)	107.50(5)
C(30)-C(32)	1.524(2)	C(1)-Si(1)-Si(2)	117.75(4)
C(30)-C(31)	1.526(2)	N(2)-Si(1)-Al(1)	115.17(5)
C(30)-C(33)	1.528(2)	N(1)-Si(1)-Al(1)	113.89(5)
C(1T)-C(6T)	1.386(9)	C(1)-Si(1)-Al(1)	117.43(4)
C(1T)-C(2T)	1.398(9)	Si(2)-Si(1)-Al(1)	124.58(2)
C(1T)-C(7T)	1.507(8)	C(7)-C(2)-C(3)	119.72(15)
C(2T)-C(3T)	1.395(9)	C(7)-C(2)-C(1)	120.57(15)
C(3T)-C(4T)	1.374(9)	C(3)-C(2)-C(1)	119.68(15)
C(4T)-C(5T)	1.384(9)	C(36)-Al(2)-C(35)	114.30(9)
C(5T)-C(6T)	1.381(8)	C(36)-Al(2)-C(34)	114.31(9)
C(1A)-C(2A)	1.385(13)	C(35)-Al(2)-C(34)	113.03(9)
C(1A)-C(6A)	1.391(13)	C(36)-Al(2)-Si(2)	106.71(6)
C(1A)-C(7A)	1.499(16)	C(35)-Al(2)-Si(2)	106.32(6)
C(2A)-C(3A)	1.388(13)	C(34)-Al(2)-Si(2)	100.64(6)
C(3A)-C(4A)	1.393(14)	C(1)-N(2)-C(8)	130.41(13)
C(4A)-C(5A)	1.382(14)	C(1)-N(2)-Si(1)	91.53(10)
C(5A)-C(6A)	1.374(13)	C(8)-N(2)-Si(1)	134.47(11)
		N(3)-Si(2)-N(4)	70.89(6)
N(1)-C(1)-N(2)	105.43(13)	N(3)-Si(2)-C(19)	35.58(6)
N(1)-C(1)-C(2)	128.02(14)	N(4)-Si(2)-C(19)	35.50(6)

N(3)-Si(2)-Si(1)	112.43(5)	C(25)-C(20)-C(21)	119.57(15)
N(4)-Si(2)-Si(1)	106.70(5)	C(25)-C(20)-C(19)	120.12(15)
C(19)-Si(2)-Si(1)	117.01(4)	C(21)-C(20)-C(19)	120.15(15)
N(3)-Si(2)-Al(2)	113.93(5)	C(22)-C(21)-C(20)	120.07(17)
N(4)-Si(2)-Al(2)	112.17(5)	C(23)-C(22)-C(21)	120.03(18)
C(19)-Si(2)-Al(2)	115.93(4)	C(22)-C(23)-C(24)	120.32(17)
Si(1)-Si(2)-Al(2)	126.65(2)	C(23)-C(24)-C(25)	120.11(17)
C(4)-C(3)-C(2)	119.89(16)	C(20)-C(25)-C(24)	119.88(17)
C(19)-N(3)-C(30)	131.03(13)	N(4)-C(26)-C(29)	104.79(12)
C(19)-N(3)-Si(2)	91.69(10)	N(4)-C(26)-C(27)	110.79(13)
C(30)-N(3)-Si(2)	135.52(11)	C(29)-C(26)-C(27)	110.08(14)
C(5)-C(4)-C(3)	120.39(17)	N(4)-C(26)-C(28)	112.09(13)
C(19)-N(4)-C(26)	131.48(13)	C(29)-C(26)-C(28)	109.29(15)
C(19)-N(4)-Si(2)	91.65(10)	C(27)-C(26)-C(28)	109.68(14)
C(26)-N(4)-Si(2)	136.31(11)	N(3)-C(30)-C(32)	110.50(14)
C(4)-C(5)-C(6)	119.81(16)	N(3)-C(30)-C(31)	105.45(13)
C(5)-C(6)-C(7)	120.30(17)	C(32)-C(30)-C(31)	109.15(14)
C(6)-C(7)-C(2)	119.88(16)	N(3)-C(30)-C(33)	110.60(13)
N(2)-C(8)-C(11)	109.94(13)	C(32)-C(30)-C(33)	111.14(14)
N(2)-C(8)-C(9)	104.56(13)	C(31)-C(30)-C(33)	109.84(15)
C(11)-C(8)-C(9)	109.39(15)	C(6T)-C(1T)-C(2T)	118.7(7)
N(2)-C(8)-C(10)	112.13(14)	C(6T)-C(1T)-C(7T)	121.7(8)
C(11)-C(8)-C(10)	110.77(14)	C(2T)-C(1T)-C(7T)	119.6(9)
C(9)-C(8)-C(10)	109.87(15)	C(3T)-C(2T)-C(1T)	120.3(8)
N(1)-C(12)-C(14)	111.31(14)	C(4T)-C(3T)-C(2T)	120.4(8)
N(1)-C(12)-C(15)	105.03(12)	C(3T)-C(4T)-C(5T)	119.1(8)
C(14)-C(12)-C(15)	109.81(15)	C(6T)-C(5T)-C(4T)	121.3(8)
N(1)-C(12)-C(13)	110.67(13)	C(5T)-C(6T)-C(1T)	120.2(8)
C(14)-C(12)-C(13)	110.50(15)	C(2A)-C(1A)-C(6A)	119.5(15)
C(15)-C(12)-C(13)	109.36(15)	C(2A)-C(1A)-C(7A)	122.9(17)
N(4)-C(19)-N(3)	105.23(13)	C(6A)-C(1A)-C(7A)	117.7(16)
N(4)-C(19)-C(20)	125.90(14)	C(1A)-C(2A)-C(3A)	119.4(16)
N(3)-C(19)-C(20)	128.84(14)	C(2A)-C(3A)-C(4A)	120.8(16)
N(4)-C(19)-Si(2)	52.85(8)	C(5A)-C(4A)-C(3A)	119.3(15)
N(3)-C(19)-Si(2)	52.73(8)	C(6A)-C(5A)-C(4A)	120.0(16)
C(20)-C(19)-Si(2)	173.29(12)	C(5A)-C(6A)-C(1A)	121.0(16)

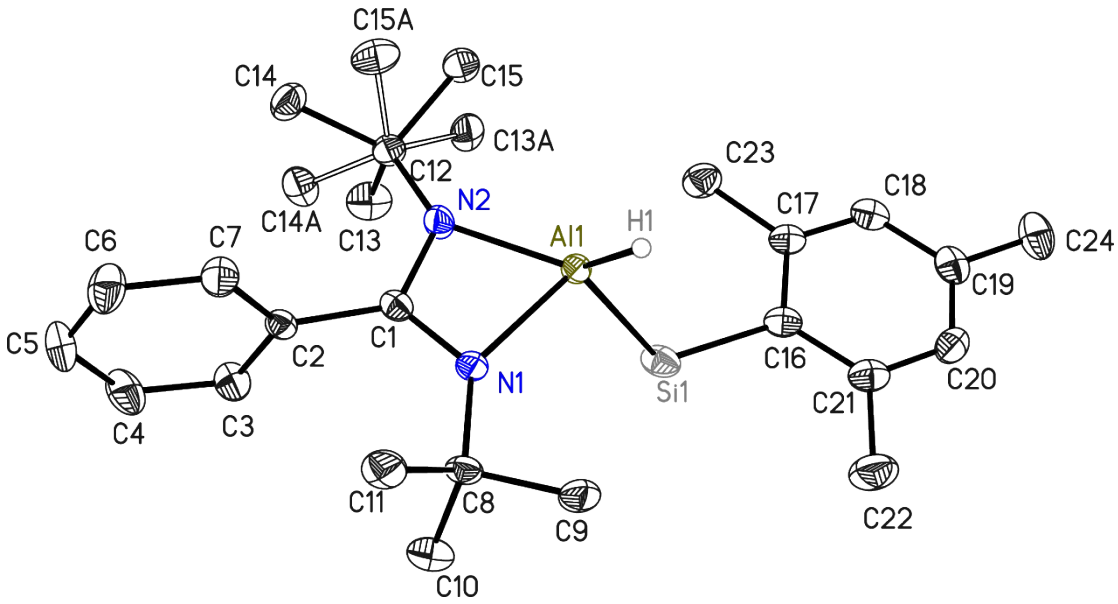

Figure S2.3. The asymmetric unit of **3** with anisotropic displacement parameters at 50% probability level. The hydrogen atoms are omitted for clarity. The disordered t-butyl group was refined on two positions. The occupancy of the main positions refined to 0.804(3). For the refinement distance restraints and restraints for the anisotropic displacement parameters were used.[8]

Table S2.3. Bond lengths [Å] and angles [°] for **3**.

C(3)-C(2)	1.385(2)	Al(1)-C(1)	2.3716(17)
C(3)-C(4)	1.387(2)	Al(1)-Al(1)#1	2.7004(12)
C(4)-C(5)	1.377(3)	C(1)-N(2)	1.347(2)
C(7)-C(6)	1.381(2)	N(2)-C(12)	1.482(2)
C(7)-C(2)	1.392(2)	C(12)-C(15A)	1.453(8)
C(6)-C(5)	1.378(2)	C(12)-C(13)	1.508(3)
C(8)-N(1)	1.475(2)	C(12)-C(15)	1.522(3)
C(8)-C(9)	1.525(2)	C(12)-C(14A)	1.526(7)
C(8)-C(11)	1.527(2)	C(12)-C(14)	1.562(3)
C(8)-C(10)	1.529(2)	C(12)-C(13A)	1.617(7)
C(2)-C(1)	1.490(2)	C(17)-C(18)	1.386(2)
Si(1)-H(2Y)	1.414(16)	C(17)-C(16)	1.411(2)
Si(1)-H(2X)	1.425(16)	C(17)-C(23)	1.505(2)
Si(1)-C(16)	1.9025(18)	C(18)-C(19)	1.385(2)
Si(1)-Al(1)	2.4602(8)	C(19)-C(20)	1.391(3)
N(1)-C(1)	1.327(2)	C(19)-C(24)	1.501(2)
N(1)-Al(1)	1.9543(16)	C(20)-C(21)	1.394(3)
Al(1)-H(1)	1.653(16)	C(21)-C(16)	1.405(2)
Al(1)-H(1)#1	1.796(17)	C(21)-C(22)	1.512(3)
Al(1)-N(2)	1.9220(14)		

C(2)-C(3)-C(4)	119.76(15)	H(1)-Al(1)-Al(1)#1	40.4(6)
C(5)-C(4)-C(3)	120.46(16)	H(1)#1-Al(1)-Al(1)#1	36.6(5)
C(6)-C(7)-C(2)	119.87(15)	N(2)-Al(1)-Al(1)#1	113.57(5)
C(5)-C(6)-C(7)	120.46(16)	N(1)-Al(1)-Al(1)#1	131.70(5)
C(4)-C(5)-C(6)	119.78(16)	C(1)-Al(1)-Al(1)#1	130.92(5)
N(1)-C(8)-C(9)	105.73(12)	Si(1)-Al(1)-Al(1)#1	112.72(3)
N(1)-C(8)-C(11)	112.66(13)	N(1)-C(1)-N(2)	109.58(13)
C(9)-C(8)-C(11)	108.26(13)	N(1)-C(1)-C(2)	126.14(14)
N(1)-C(8)-C(10)	110.38(13)	N(2)-C(1)-C(2)	124.17(14)
C(9)-C(8)-C(10)	109.16(14)	N(1)-C(1)-Al(1)	55.49(8)
C(11)-C(8)-C(10)	110.46(14)	N(2)-C(1)-Al(1)	54.12(8)
C(3)-C(2)-C(7)	119.63(14)	C(2)-C(1)-Al(1)	177.70(11)
C(3)-C(2)-C(1)	122.19(14)	C(1)-N(2)-C(12)	127.50(13)
C(7)-C(2)-C(1)	118.15(13)	C(1)-N(2)-Al(1)	91.29(10)
H(2Y)-Si(1)-H(2X)	102.7(11)	C(12)-N(2)-Al(1)	139.28(10)
H(2Y)-Si(1)-C(16)	107.9(8)	C(15A)-C(12)-N(2)	104.3(4)
H(2X)-Si(1)-C(16)	105.3(8)	N(2)-C(12)-C(13)	109.64(14)
H(2Y)-Si(1)-Al(1)	109.8(8)	N(2)-C(12)-C(15)	107.04(14)
H(2X)-Si(1)-Al(1)	108.4(8)	C(13)-C(12)-C(15)	110.06(16)
C(16)-Si(1)-Al(1)	121.16(5)	C(15A)-C(12)-C(14A)	116.7(5)
C(1)-N(1)-C(8)	129.46(13)	N(2)-C(12)-C(14A)	117.9(3)
C(1)-N(1)-Al(1)	90.49(10)	N(2)-C(12)-C(14)	113.66(14)
C(8)-N(1)-Al(1)	140.05(10)	C(13)-C(12)-C(14)	109.77(16)
H(1)-Al(1)-H(1)#1	77.0(9)	C(15)-C(12)-C(14)	106.57(15)
H(1)-Al(1)-N(2)	123.3(6)	C(15A)-C(12)-C(13A)	109.6(5)
H(1)#1-Al(1)-N(2)	95.5(5)	N(2)-C(12)-C(13A)	105.6(3)
H(1)-Al(1)-N(1)	95.7(6)	C(14A)-C(12)-C(13A)	102.1(5)
H(1)#1-Al(1)-N(1)	155.4(5)	C(18)-C(17)-C(16)	120.55(15)
N(2)-Al(1)-N(1)	68.60(6)	C(18)-C(17)-C(23)	118.62(15)
H(1)-Al(1)-C(1)	113.6(6)	C(16)-C(17)-C(23)	120.82(15)
H(1)#1-Al(1)-C(1)	128.0(5)	C(19)-C(18)-C(17)	122.40(16)
N(2)-Al(1)-C(1)	34.59(6)	C(18)-C(19)-C(20)	117.18(16)
N(1)-Al(1)-C(1)	34.02(5)	C(18)-C(19)-C(24)	120.71(17)
H(1)-Al(1)-Si(1)	118.0(6)	C(20)-C(19)-C(24)	122.11(17)
H(1)#1-Al(1)-Si(1)	98.5(5)	C(19)-C(20)-C(21)	121.90(16)
N(2)-Al(1)-Si(1)	118.66(5)	C(20)-C(21)-C(16)	120.64(16)
N(1)-Al(1)-Si(1)	105.58(5)	C(20)-C(21)-C(22)	117.74(16)
C(1)-Al(1)-Si(1)	116.15(4)	C(16)-C(21)-C(22)	121.59(16)

C(21)-C(16)-C(17)	117.31(15)	C(17)-C(16)-Si(1)	119.54(13)
C(21)-C(16)-Si(1)	123.13(12)		

S3. Computational Details:

All computational calculations were carried out employing a method of density functional theory (DFT) implemented in the Gaussian 09 program package.[9] Geometries of all the intermediates and transition states without any symmetry constraints were optimized with the generalized gradient approximation (GGA) by means of Becke exchange functional[10] in addition with the Perdew correlation functional[11] (BP86). For basis sets Ahlrich's split valence plus polarization (def2-SVP)[12] had been used for the treatment of all the atoms. Harmonic force constants were computed at the optimized geometries to characterize the stationary points as minima or saddle points. All transition states were located from a linear transit scan in which the reaction coordinate was kept fixed at different distances while all other degrees of freedom were optimized. After the linear transit search the transition states were optimized using Berny algorithm implemented in the Gaussian 09 code.[9] IRC (Intrinsic Reaction Coordinate) calculations were carried out to authenticate that the transition state connects the corresponding stationary points. Furthermore, to refine the energies obtained from BP86/def2-SVP calculations, single point calculations were performed using the BP86 functional including the Grimme empirical dispersion correction D3[13] employing a triple-ζ quality split valence plus polarization (def2-TZVP) basis set[14] on the optimized geometries. The effect of solvation by toluene (dielectric constant ε = 2.37) was assessed by a self-consistent reaction field (SCRF) approach, using the SMD continuum solvation model.[15] The tight wave function convergence criteria and an "ultrafine" (99950) grid was used for all solvent single point calculations. In this present calculations, the four tert-butyl (-^{t}Bu) groups and two phenyl (-Ph) groups of LSi-SiL [L = PhC(N^{t}Bu)$_2$] were replaced by methyl (-Me) groups and this model substrate is designated as **I**. All energy values reported in the manuscript are at BP86-D3/def2-TZVP/SMD(Toluene)//BP86/def2-SVP level of theory. Figures were generated using the Chem Draw and CYLview visualization software.[16]

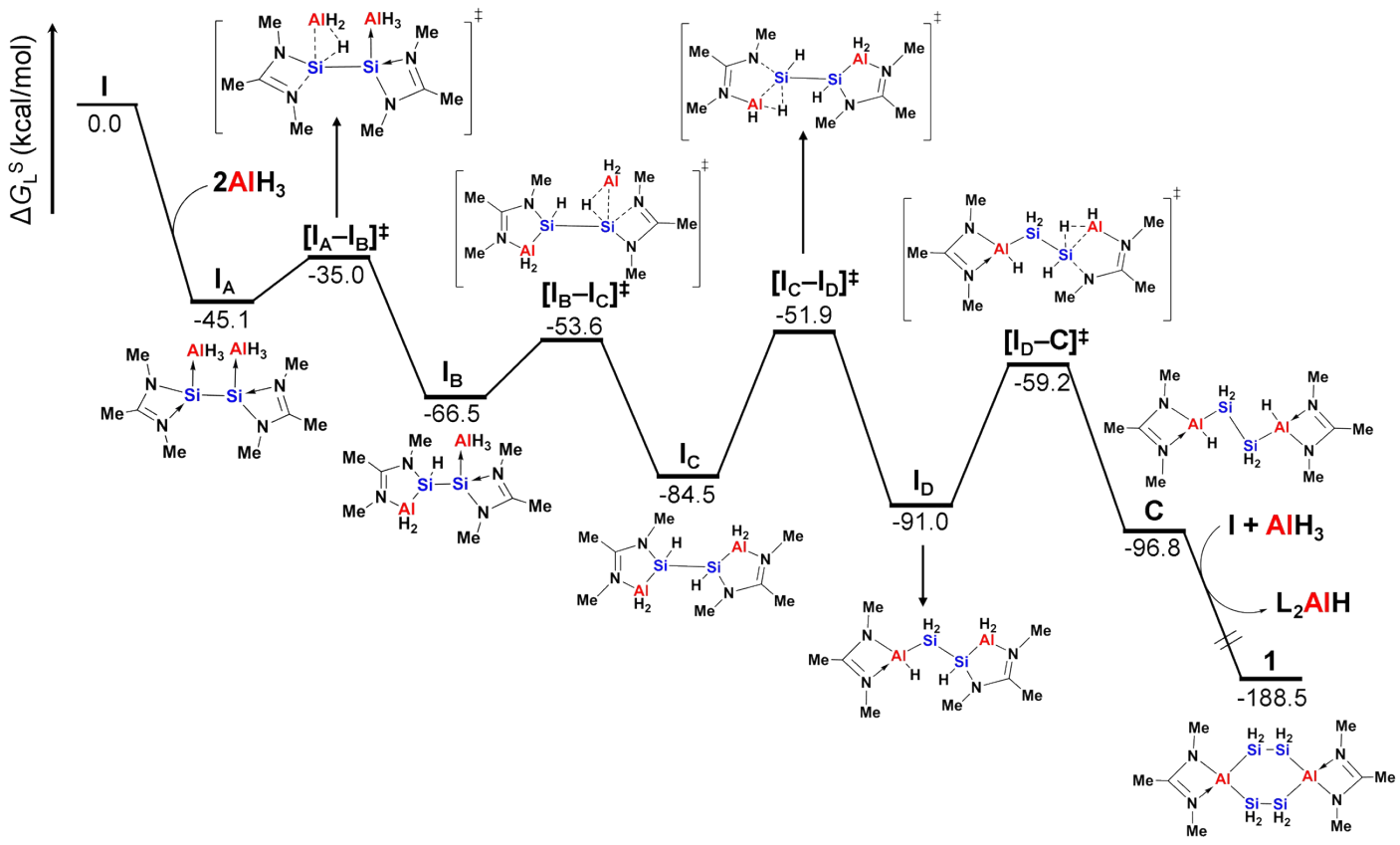

Figure S3.1 Overall free energy profile diagram for the formation of silicon-aluminum heterocycle **1**. All values are in kcal/mol.

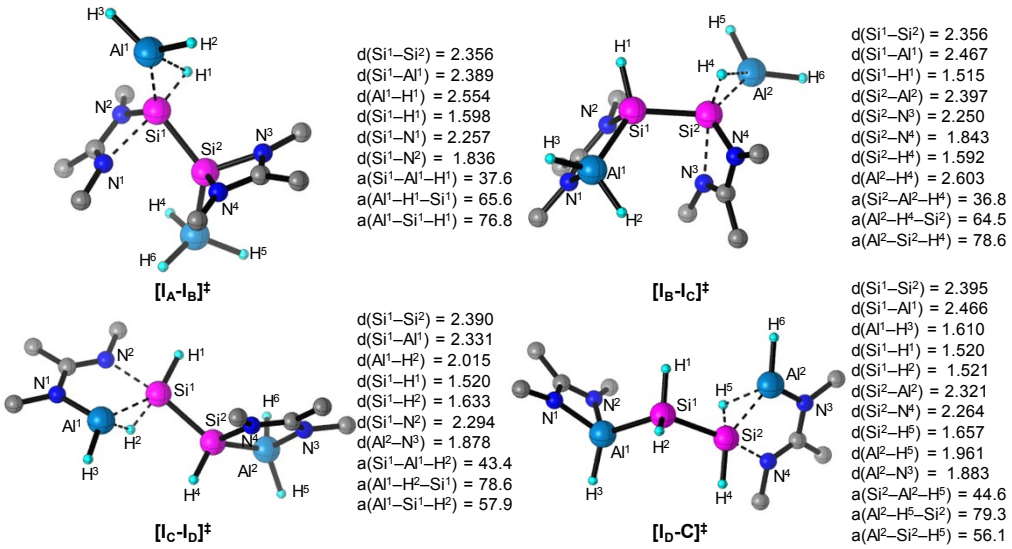

Figure S3.2 Optimized geometries of the selected transition states involved in the reaction mechanism. All hydrogen atoms (except AlH_3) are omitted for clarity. Color code: C: grey; N: blue; Si: pink; Al: light blue; H: sky blue. Distances (d) are in Å and angles (a) are in degree (°).

Table S3.1 Cartesian Coordinates

I				H	3.85531	-2.52430	0.32753
C	-2.80391	0.11776	0.04299	H	2.18836	-3.16987	0.34227
N	-2.27330	-1.09275	-0.20782	C	-2.83349	-2.38443	0.09887
Si	-0.69841	-0.35113	-1.02591	H	-2.88486	-2.57970	1.19525
Si	0.69807	-0.35157	1.02492	H	-3.85590	-2.52419	-0.32256
N	-1.87009	1.01636	-0.33835	H	-2.18914	-3.16995	-0.34586
N	1.86980	1.01644	0.33863	C	-4.18572	0.42735	0.53968
N	2.27333	-1.09252	0.20695	H	-4.84124	0.78733	-0.28585
C	2.80394	0.11821	-0.04277	H	-4.66073	-0.46841	0.98401
C	4.18605	0.42818	-0.53839	H	-4.16250	1.22484	1.31114
H	4.84169	0.78548	0.28822	C	-2.04882	2.44349	-0.43668
H	4.66052	-0.46676	-0.98496	H	-2.82276	2.73862	-1.18475
H	4.16354	1.22771	-1.30774	H	-2.33253	2.90077	0.53940
C	2.04775	2.44368	0.43670	H	-1.09445	2.90966	-0.75475
H	2.82192	2.73932	1.18432				
H	2.33065	2.90104	-0.53958	**AlH_3**			
H	1.09329	2.90932	0.75525	Al	-0.00000	-0.00001	0.00002
C	2.83487	-2.38391	-0.09850	H	0.98794	-1.25818	-0.00008
H	2.89134	-2.57796	-1.19484	H	0.59571	1.48470	-0.00008

H	-1.58364	-0.22641	-0.00008

I_A

C	2.80499	-0.36277	0.12697
N	2.11496	-0.60709	-1.00384
Al	-0.80494	-3.15950	-0.31971
Si	0.56850	-1.05866	-0.03579
Si	-0.56869	1.05906	-0.03562
Al	0.80513	3.15968	-0.31931
N	1.97602	-0.66181	1.14874
N	-1.97614	0.66170	1.14881
N	-2.11505	0.60736	-1.00379
C	-2.80502	0.36260	0.12697
C	-4.18486	-0.19718	0.23871
H	-4.78501	0.02495	-0.66406
H	-4.11393	-1.30254	0.34610
H	-4.70777	0.20204	1.12973
C	-2.24012	0.53207	2.56481
H	-3.15776	1.08388	2.86627
H	-2.35184	-0.53063	2.87533
H	-1.39485	0.97079	3.13031
C	-2.51729	0.35505	-2.37179
H	-2.37981	-0.71362	-2.65148
H	-3.58049	0.63168	-2.53681
H	-1.90197	0.97817	-3.05048
C	2.51738	-0.35476	-2.37179
H	2.37983	0.71390	-2.65150
H	3.58064	-0.63126	-2.53663
H	1.90224	-0.97795	-3.05058
C	4.18503	0.19651	0.23884
H	4.78529	-0.02615	-0.66373
H	4.11454	1.30193	0.34586
H	4.70757	-0.20266	1.13009
C	2.23997	-0.53254	2.56478
H	3.15674	-1.08570	2.86645
H	2.35315	0.53000	2.87528
H	1.39394	-0.96999	3.13013
H	1.99780	2.83237	0.74783
H	1.25068	2.86446	-1.86293
H	-0.08654	4.47539	-0.04310
H	0.08717	-4.47502	-0.04399
H	-1.25086	-2.86418	-1.86321
H	-1.99757	-2.83274	0.74766

$[I_A\text{-}I_B]^{‡}$

C	2.94344	-0.38393	-0.10086
N	2.41765	0.66822	-0.75821
Si	0.74915	-0.19660	-0.92778
Si	-0.79316	0.85768	0.50807
Al	-0.51346	1.58435	2.76694
N	1.93699	-1.25914	0.08493
N	-1.94949	-1.06538	0.26668
N	-2.39348	0.98701	-0.38353
C	-2.79659	-0.31771	-0.41083
C	-4.01209	-0.76541	-1.17216
H	-4.34142	-1.77124	-0.85020
H	-4.85365	-0.05429	-1.05404
H	-3.75910	-0.81949	-2.25352
C	-2.06731	-2.49073	0.46717
H	-3.11947	-2.82423	0.62546
H	-1.65477	-3.06607	-0.39411
H	-1.49482	-2.78524	1.37216
C	-2.99453	2.06407	-1.14658
H	-3.00133	1.85450	-2.23972
H	-4.03895	2.27353	-0.82257
H	-2.40387	2.98589	-0.98195

C	3.10629	1.82554	-1.28126	H	3.63783	2.04568	1.17274
H	3.56901	1.63129	-2.27549	C	4.23278	-1.60126	0.77974
H	2.38405	2.65741	-1.40147	H	5.19664	-1.37426	0.27244
H	3.90304	2.17257	-0.58865	H	4.32098	-1.31387	1.85126
C	4.38176	-0.54885	0.28454	H	4.10400	-2.70190	0.75098
H	4.51957	-1.38238	0.99791	C	1.88733	2.37789	-0.81972
H	5.00419	-0.74967	-0.61384	H	1.78497	2.91356	0.14932
H	4.76497	0.37966	0.75453	H	2.77897	2.77092	-1.35437
C	1.96027	-2.57073	0.68789	H	0.99648	2.63217	-1.42366
H	2.99801	-2.94053	0.82265	C	-3.71574	0.07446	-1.92443
H	1.46141	-2.57280	1.68264	H	-4.04487	-0.88310	-2.38349
H	1.42594	-3.29294	0.03594	H	-4.62198	0.63763	-1.60441
H	0.99423	1.82593	3.27682	H	-3.21513	0.66799	-2.71430
H	-0.41409	2.40290	0.35004	C	-4.00781	-2.04104	0.33018
H	-1.71616	2.19229	3.64446	H	-3.86216	-2.66577	1.23035
Al	0.05394	-1.31918	-3.09758	H	-5.00186	-1.55013	0.39865
H	-1.28040	-0.51434	-3.56397	H	-4.02614	-2.70710	-0.55750
H	1.35148	-1.20879	-4.06319	C	-1.55926	-1.42232	2.27411
H	-0.24487	-2.80748	-2.49260	H	-2.42193	-1.95863	2.72194
				H	-0.73987	-2.15304	2.09162
I_B				H	-1.20400	-0.68053	3.01771
C	-2.92581	-1.01465	0.19182	H	1.06946	-2.99939	0.69002
N	-2.78842	-0.14910	-0.83734	H	0.28993	0.35816	-2.62503
Si	-1.34799	0.71944	0.01231	H	2.36130	-3.12972	-1.73180
Si	0.51959	-0.14279	-1.21128	Al	-1.59530	3.00418	1.08223
Al	1.69979	-2.21641	-0.57998	H	-1.41822	4.00818	-0.18202
N	-1.93537	-0.73806	1.05638	H	-3.04568	2.97073	1.80372
N	3.08372	-0.97735	0.11903	H	-0.29547	2.92566	2.06569
N	1.94661	0.92081	-0.64836				
C	3.00688	0.35009	-0.01620	**$[I_B\text{-}I_C]^{\ddagger}$**			
C	4.08333	1.26876	0.51889	Si	-1.31932	1.09390	-2.12150
H	4.85016	0.72592	1.09581	Al	-2.11443	2.65003	-3.76290
H	4.58974	1.80108	-0.31344	N	-1.83804	1.29212	-0.36406

H	-1.96656	2.26089	-5.31921	H	5.07461	-0.03350	-2.39430
H	-3.07670	3.88779	-3.39559	H	4.39443	-0.23279	-4.03954
C	-0.72240	1.85090	0.18701	H	4.14431	1.29432	-3.15836
C	-3.02755	0.88683	0.35499	H	-0.39902	-1.44064	-3.74068
N	0.18205	2.05318	-0.74725				
C	-0.60701	2.12450	1.66135	**I_C**			
H	-2.80722	0.15233	1.16244	Si	-0.85799	0.35177	-0.68266
H	-3.56545	1.75014	0.81004	Al	-2.58892	2.07540	-0.33116
H	-3.72129	0.40158	-0.35894	N	-3.76857	0.52440	0.08091
C	1.49883	2.59677	-0.54563	N	-2.09451	-1.03040	-0.43118
H	0.23292	2.81052	1.88121	C	-3.37179	-0.74192	-0.06026
H	-1.54129	2.56175	2.06682	C	-4.31363	-1.90335	0.17555
H	-0.41703	1.17123	2.20000	H	-5.31271	-1.57383	0.50535
H	2.25376	1.79736	-0.35670	H	-4.43476	-2.49829	-0.75349
H	1.82288	3.14644	-1.45564	H	-3.90227	-2.59041	0.94319
H	1.55948	3.31467	0.30630	C	-5.13774	0.84483	0.49050
H	-2.67897	0.40267	-2.57670	H	-5.90111	0.48333	-0.23437
Si	0.11897	-0.73242	-2.50528	H	-5.38905	0.44446	1.49782
Al	1.21128	-1.85034	-0.59705	H	-5.24146	1.94684	0.54738
N	1.76087	-0.07883	-3.13437	C	-1.68695	-2.42268	-0.64619
N	2.89036	-1.07885	-1.34374	H	-1.79057	-3.04303	0.27141
H	0.97404	-1.15159	0.84562	H	-2.27116	-2.90888	-1.45854
H	1.38186	-3.45474	-0.59108	H	-0.62054	-2.44645	-0.94082
C	2.91156	-0.34999	-2.46228	H	-2.43249	2.94722	1.02011
C	1.80262	0.69214	-4.37817	H	-0.26399	-0.00432	-2.03278
C	4.12631	-1.39484	-0.62514	H	-3.21181	2.83244	-1.61461
C	4.20477	0.19401	-3.03255	Si	0.88140	-0.14283	0.87908
H	2.19488	1.72270	-4.22752	Al	2.44072	-2.03039	0.57522
H	2.41999	0.19991	-5.16214	N	2.20021	1.09965	0.40380
H	0.77361	0.78604	-4.77385	N	3.68622	-0.63465	-0.10666
H	4.84824	-1.97558	-1.24179	H	3.12854	-2.71159	1.86698
H	4.64405	-0.48887	-0.23709	H	2.08802	-3.01366	-0.65967
H	3.87426	-2.02311	0.25245	C	3.40395	0.66915	-0.06174

C	1.91752	2.53453	0.50449	H	4.90142	2.21482	0.67283
C	4.98077	-1.10927	-0.60035	H	0.44625	0.42839	2.00754
C	4.39885	1.71665	-0.51369	Si	-0.92265	0.83553	-0.75966
H	2.64993	3.06240	1.15390	Al	-2.44349	2.00204	0.56633
H	1.90975	3.03904	-0.48761	N	-4.07935	1.80314	-0.33364
H	0.91577	2.67059	0.95447	N	-2.87633	0.65426	-1.94786
H	5.15903	-0.83902	-1.66501	C	-4.04004	1.10306	-1.51760
H	5.83674	-0.73884	0.00694	C	-5.34623	0.87561	-2.25434
H	4.99742	-2.21601	-0.54291	H	-6.06421	0.32680	-1.60933
H	5.30911	1.27138	-0.94832	H	-5.82649	1.84126	-2.51762
H	3.94334	2.38675	-1.27076	H	-5.20691	0.29420	-3.18142
H	4.70287	2.35746	0.34047	C	-5.35247	2.29277	0.18985
H	0.42088	0.39141	2.22029	H	-5.84730	3.02261	-0.49031
				H	-6.08056	1.47426	0.38997
$[I_C\text{-}I_D]^‡$				H	-5.17293	2.81038	1.15336
Si	0.87377	0.03550	0.59796	C	-2.75349	-0.04279	-3.21456
Al	2.25886	-1.96713	0.19338	H	-3.17426	-1.07421	-3.18319
N	2.35340	1.16754	0.32047	H	-3.22484	0.49985	-4.06459
N	3.73245	-0.66633	-0.14329	H	-1.67167	-0.13983	-3.45055
H	2.71029	-2.88139	1.44819	H	-1.93672	0.07446	0.26987
H	2.00516	-2.74719	-1.20076	H	-0.41692	0.65519	-2.18211
C	3.56591	0.65102	-0.01914	H	-2.58483	2.56956	2.05300
C	2.20170	2.61073	0.50511				
C	5.02908	-1.23274	-0.51609	**I_D**			
C	4.70736	1.62145	-0.24468	Al	2.68018	-1.12262	0.83451
H	2.80046	2.99499	1.36162	N	2.96230	0.81797	0.75700
H	2.48482	3.19172	-0.40066	N	3.98225	-0.65132	-0.55003
H	1.13659	2.82901	0.71309	C	3.81277	0.65733	-0.27138
H	5.37090	-0.90229	-1.52273	Si	0.45828	-1.72282	-0.07950
H	5.83053	-1.00142	0.22132	C	4.47643	1.76557	-1.04435
H	4.93470	-2.33636	-0.55450	H	4.05068	1.81792	-2.06919
H	5.64275	1.11070	-0.52752	H	4.33430	2.75015	-0.56242
H	4.45214	2.34533	-1.04601	H	5.56320	1.57128	-1.15118

C	4.83098	-1.15452	-1.60495	Al	2.67406	-0.68317	0.74396
H	4.54039	-0.77886	-2.61424	N	3.42665	1.09716	0.35248
H	5.90667	-0.90023	-1.45266	N	4.24199	-0.80230	-0.44121
H	4.76166	-2.25977	-1.63645	C	4.36536	0.53776	-0.43093
C	2.49745	2.08638	1.27625	Si	0.47856	-1.06378	-0.31312
H	3.32282	2.82178	1.40970	C	5.41307	1.28380	-1.21591
H	1.71942	2.55692	0.63092	H	5.27324	1.10935	-2.30390
H	2.04289	1.92791	2.27460	H	5.37818	2.37264	-1.02830
H	0.35556	-1.35481	-1.54695	H	6.42654	0.91237	-0.95686
H	0.16220	-3.21117	-0.02434	C	5.08569	-1.68807	-1.20808
H	3.25514	-1.88176	2.12642	H	5.03519	-1.49588	-2.30611
Si	-1.26794	-0.51307	1.00284	H	6.15961	-1.62787	-0.91058
Al	-1.69508	1.86664	0.52881	H	4.76211	-2.73524	-1.04659
N	-2.89619	-1.01848	0.21830	C	3.26605	2.51558	0.57577
N	-3.33708	1.20216	-0.37831	H	4.13007	2.97157	1.11468
H	-2.16125	2.83025	1.73917	H	3.11408	3.09195	-0.36662
H	-0.76135	2.55281	-0.60095	H	2.36855	2.68409	1.20314
C	-3.68101	-0.08797	-0.38761	H	0.45942	-0.48715	-1.72062
C	-3.29989	-2.42530	0.23179	H	0.22852	-2.55353	-0.48248
C	-4.17846	2.21173	-1.02350	H	2.95042	-1.19882	2.24406
C	-4.94743	-0.56938	-1.06410	Si	-1.41238	-0.15258	0.84023
H	-4.27498	-2.57885	0.74496	Al	-2.67028	1.16291	-0.60069
H	-3.37373	-2.85858	-0.79042	N	-3.57692	2.33410	0.56281
H	-2.53583	-3.00812	0.77992	N	-2.51384	1.19991	2.28302
H	-4.27095	2.05715	-2.12198	C	-3.33327	2.16538	1.90309
H	-5.20116	2.26499	-0.58749	C	-4.01301	3.10992	2.87656
H	-3.71271	3.20673	-0.87677	H	-3.75301	4.16333	2.64126
H	-5.48963	0.24634	-1.57033	H	-5.11780	3.02910	2.80028
H	-4.71247	-1.35001	-1.81629	H	-3.72402	2.91242	3.92267
H	-5.63255	-1.03317	-0.32416	C	-4.45918	3.40323	0.10353
H	-1.40329	-1.11414	2.38880	H	-5.49995	3.30013	0.48644
				H	-4.09640	4.41662	0.39028
$[I_D\text{-}C]^{\ddagger}$				H	-4.51216	3.37891	-1.00338

C	-2.26816	0.92783	3.68729
H	-1.61696	1.69348	4.16919
H	-3.19959	0.83492	4.28950
H	-1.73747	-0.04622	3.75957
H	-0.98081	1.37796	0.37195
H	-1.43952	-1.00329	2.10238
H	-2.73215	1.59689	-2.13594

C

Al	3.11870	-1.16387	0.34525
N	3.60395	0.56356	1.15214
N	4.59149	-0.30098	-0.63158
C	4.55086	0.74509	0.21519
Si	-0.91475	-1.10940	0.75721
H	-0.70489	-2.28301	1.69407
H	-0.74476	0.11638	1.63735
Si	0.91372	-1.10710	-0.75891
Al	-3.11922	-1.16332	-0.34811
N	-4.59226	-0.30240	0.62995
N	-3.60338	0.56638	-1.15096
C	-4.55051	0.74601	-0.21389
C	-5.45062	1.94802	-0.09331
H	-6.51525	1.63689	-0.14370
H	-5.30457	2.44109	0.89092
H	-5.26398	2.69057	-0.89057
C	-5.49220	-0.40054	1.75513
H	-5.31810	0.39133	2.52201
H	-6.56547	-0.34162	1.45637
H	-5.34841	-1.37703	2.25822
C	-3.28791	1.49742	-2.21082
H	-4.11154	1.60143	-2.95588
H	-3.04133	2.51736	-1.83467
H	-2.39757	1.13243	-2.75955
C	5.45199	1.94667	0.09793
H	5.30739	2.44190	-0.88541
H	5.26509	2.68768	0.89656
H	6.51635	1.63464	0.14885
C	5.49104	-0.39669	-1.75730
H	5.31590	0.39612	-2.52297
H	6.56437	-0.33729	-1.45892
H	5.34788	-1.37257	-2.26176
C	3.28999	1.49151	2.21515
H	4.11386	1.59181	2.96044
H	3.04486	2.51305	1.84243
H	2.39917	1.12599	2.76276
H	-3.55181	-2.45721	-1.19583
H	0.74370	0.12133	-1.63536
H	0.70390	-2.27787	-1.69934
H	3.55207	-2.45973	1.18959

L_2AlH

N	-1.80290	0.89934	0.38628
N	-1.24861	-1.17068	-0.14578
C	-2.23282	-0.24569	-0.14287
C	-3.62346	-0.52163	-0.66028
H	-4.08363	-1.36469	-0.10282
H	-4.28436	0.36073	-0.57400
H	-3.58324	-0.82690	-1.72720
C	-1.37841	-2.49238	-0.70687
H	-2.11896	-3.13248	-0.16762
H	-1.67804	-2.48471	-1.78286
H	-0.39902	-3.00771	-0.64842
C	-2.63901	2.04549	0.65075
H	-2.99529	2.55318	-0.27842
H	-3.54224	1.80865	1.26314
H	-2.05663	2.79590	1.22315

Al	0.00278	-0.00250	0.81162	Si	0.92299	0.68782	2.08167
N	1.80151	-0.89984	0.36281	H	0.35569	2.09430	2.13842
N	1.24044	1.17046	-0.16203	H	1.71731	0.52688	3.36256
C	2.22641	0.24892	-0.16614	Al	-2.24402	-0.43572	-0.00068
C	2.66937	-2.01617	0.64872	N	-4.13617	-0.95498	-0.00056
C	1.33928	2.49486	-0.72498	N	-3.41929	1.13946	0.00039
C	3.63318	0.49778	-0.65277	C	-4.50130	0.34243	0.00022
H	2.07261	-2.84730	1.07598	C	-5.93423	0.80455	0.00058
H	3.18187	-2.41663	-0.25974	H	-6.46516	0.41106	-0.89168
H	2.06339	3.15378	-0.18742	H	-6.46500	0.41057	0.89273
H	1.63041	2.49441	-1.80293	H	-6.01574	1.90689	0.00091
H	0.34708	2.98484	-0.66229	C	-5.06827	-2.05876	-0.00078
H	4.30427	0.68947	0.21253	H	-5.72872	-2.06657	0.89820
H	4.03215	-0.38916	-1.18490	H	-5.72978	-2.06534	-0.89901
H	3.69007	1.37400	-1.32608	H	-4.50827	-3.01446	-0.00176
H	0.01473	0.00382	2.42326	C	-3.44333	2.58555	0.00118
H	3.46825	-1.77860	1.39324	H	-3.94578	3.01021	-0.89865
				H	-3.94375	3.00918	0.90263
1				H	-2.40266	2.96414	0.00023
Si	0.92340	0.68952	-2.08057	C	5.96332	-0.70447	-0.00045
H	0.35645	2.09619	-2.13632	H	6.17164	-1.33449	-0.89071
H	1.71836	0.52971	-3.36121	H	6.66198	0.15205	-0.00375
Si	-0.94489	-0.77076	-2.07910	H	6.17355	-1.32884	0.89339
H	-0.38323	-2.17947	-2.12383	C	3.61155	-2.55649	-0.00078
H	-1.73465	-0.61399	-3.36324	H	4.14648	-2.94050	-0.90103
Al	2.22764	0.39125	0.00064	H	4.15062	-2.94117	0.89668
N	4.09231	1.01118	0.00028	H	2.60404	-3.01602	0.00134
N	3.48285	-1.11713	0.00006	C	4.94299	2.18011	0.00057
C	4.52352	-0.26381	-0.00009	H	5.59517	2.24167	0.90274
Si	-0.94512	-0.77278	2.07771	H	5.60024	2.23842	-0.89809
H	-0.38332	-2.18149	2.12120	H	4.31005	3.08929	-0.00288
H	-1.73545	-0.61765	3.36171				

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