Electronic Supplementary Material (ESI) for Dalton Transactions.

Probing the non-innocent nature of an amino-functionalised β-diketiminate ligand in silylene/iminosilane systems

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Supporting Information (27 pages in total)

1. NMR spectra of novel compounds

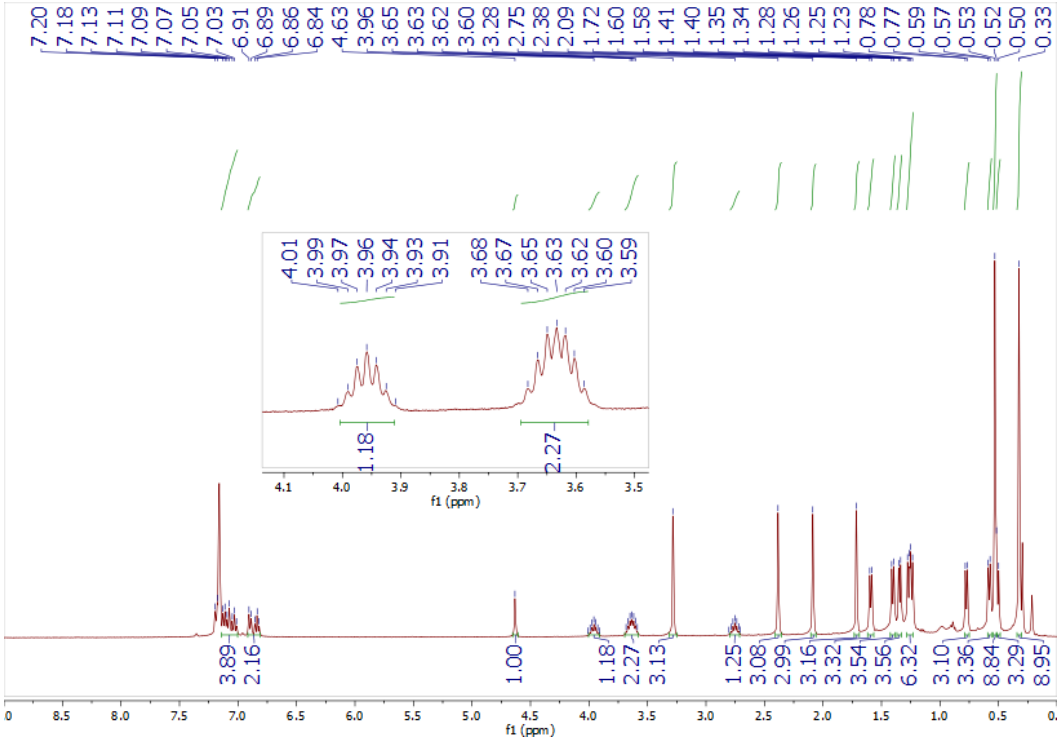

Figure s1: ^{1}H NMR spectrum of (**2-Dipp**)Si(NDipp){N(SiMe$_3$)$_2$}

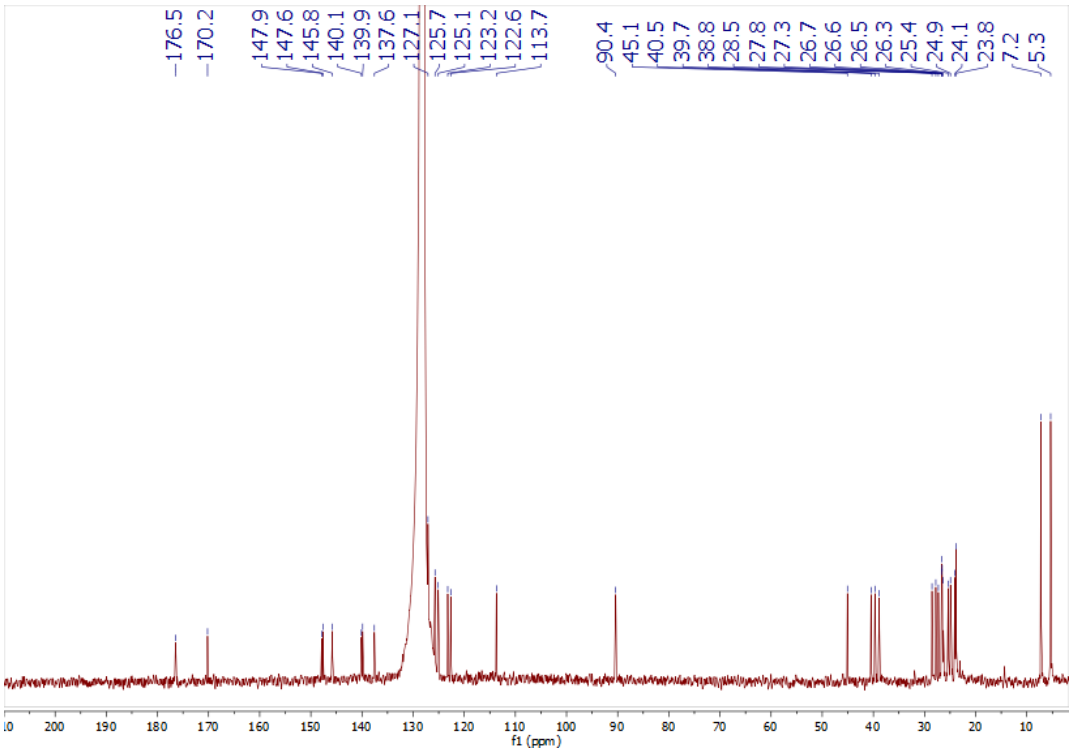

Figure s2: ^{13}C{^{1}H} NMR spectrum of (**2-Dipp**)Si(NDipp){N(SiMe$_3$)$_2$}

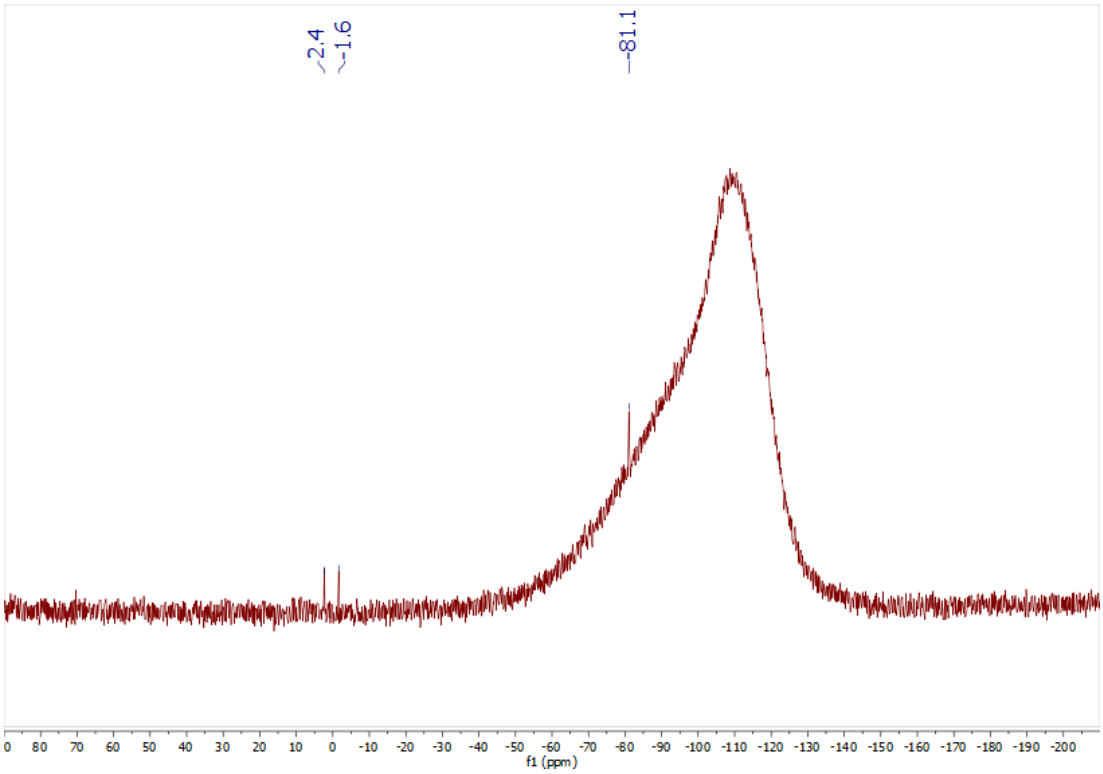

Figure s3: $^{29}Si\{^{1}H\}$ NMR spectrum of (**2-Dipp**)Si(NDipp){$N(SiMe_3)_2$}

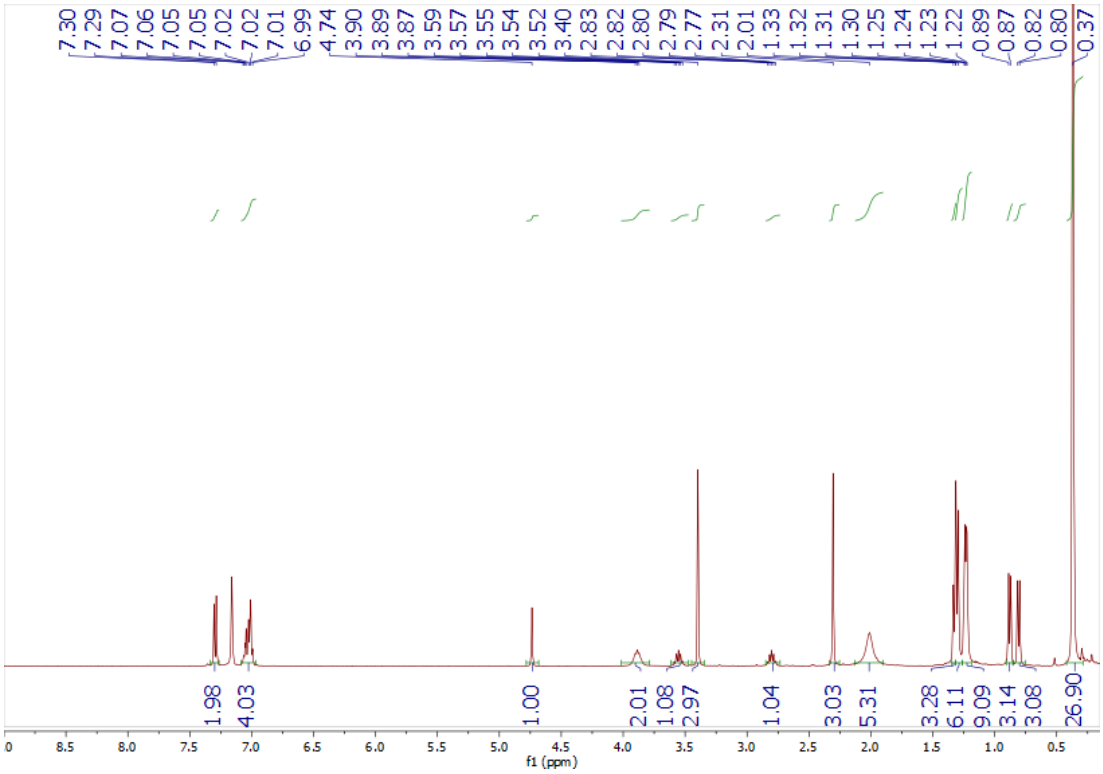

Figure s4: ^{1}H NMR spectrum of (**2-Dipp**)Si(NDipp){Si(SiMe$_3$)$_3$}

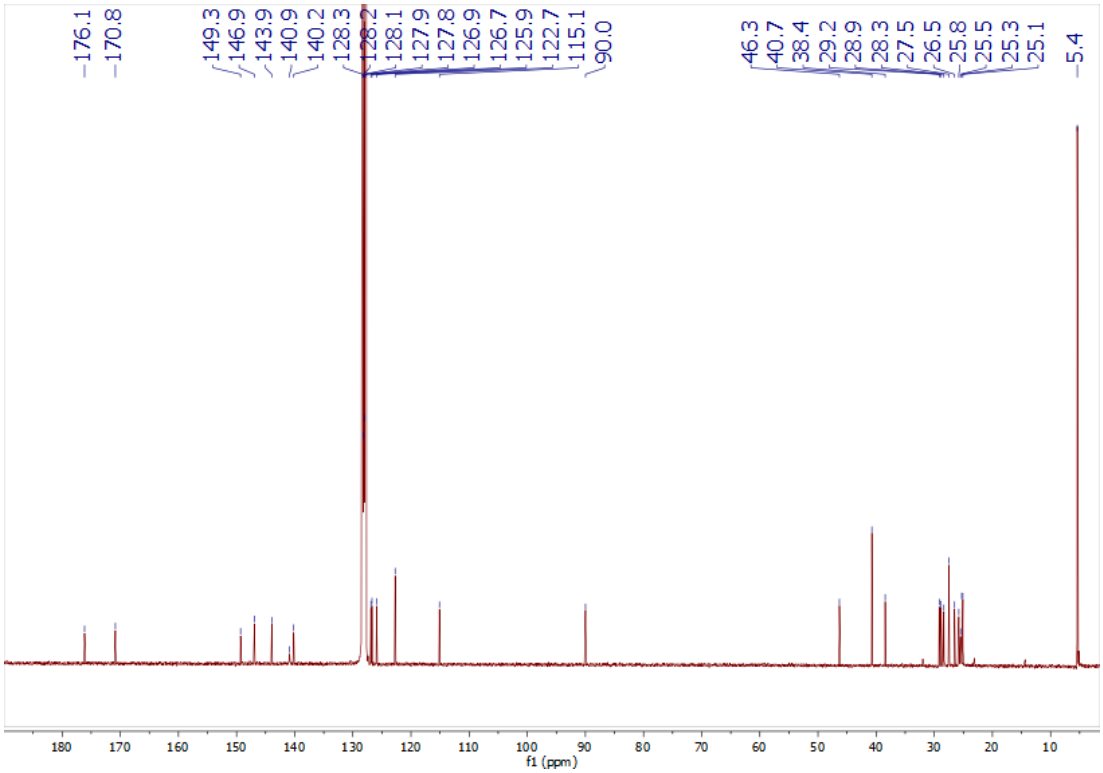

Figure s5: ^{13}C{^{1}H} NMR spectrum of (**2-Dipp**)Si(NDipp){Si(SiMe$_3$)$_3$}

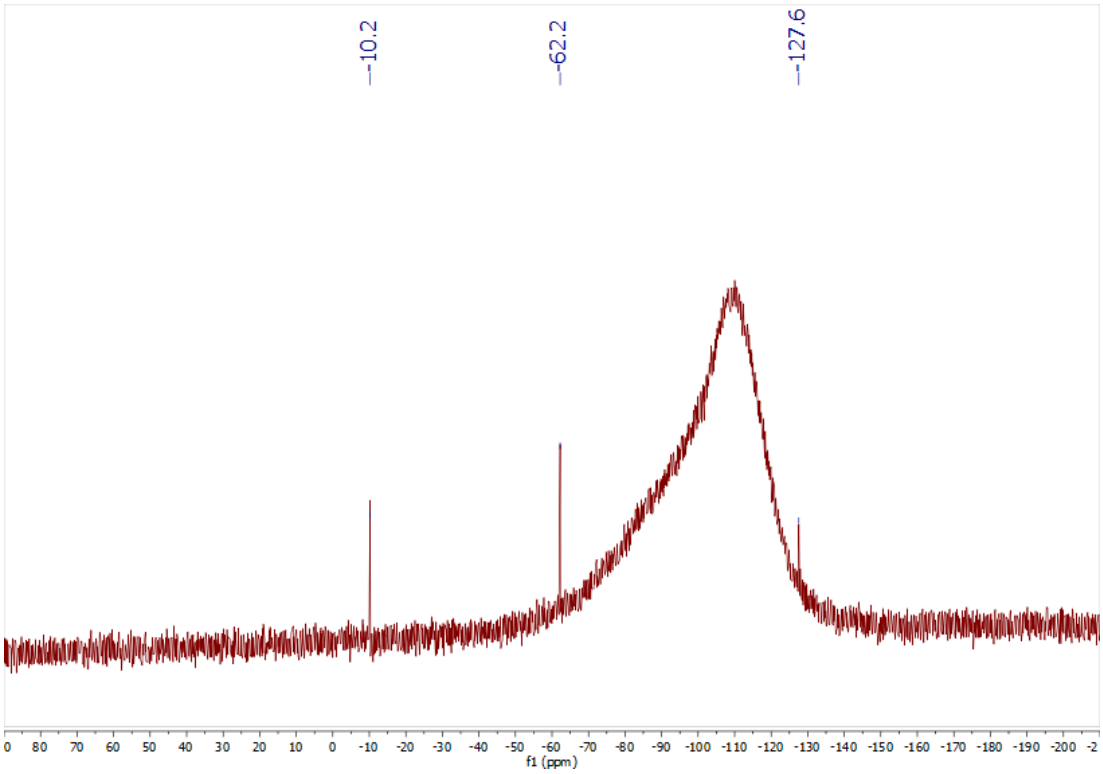

Figure s6: $^{29}Si\{^{1}H\}$ NMR spectrum of (**2-Dipp**)Si(NDipp){Si($SiMe_3$)$_3$}

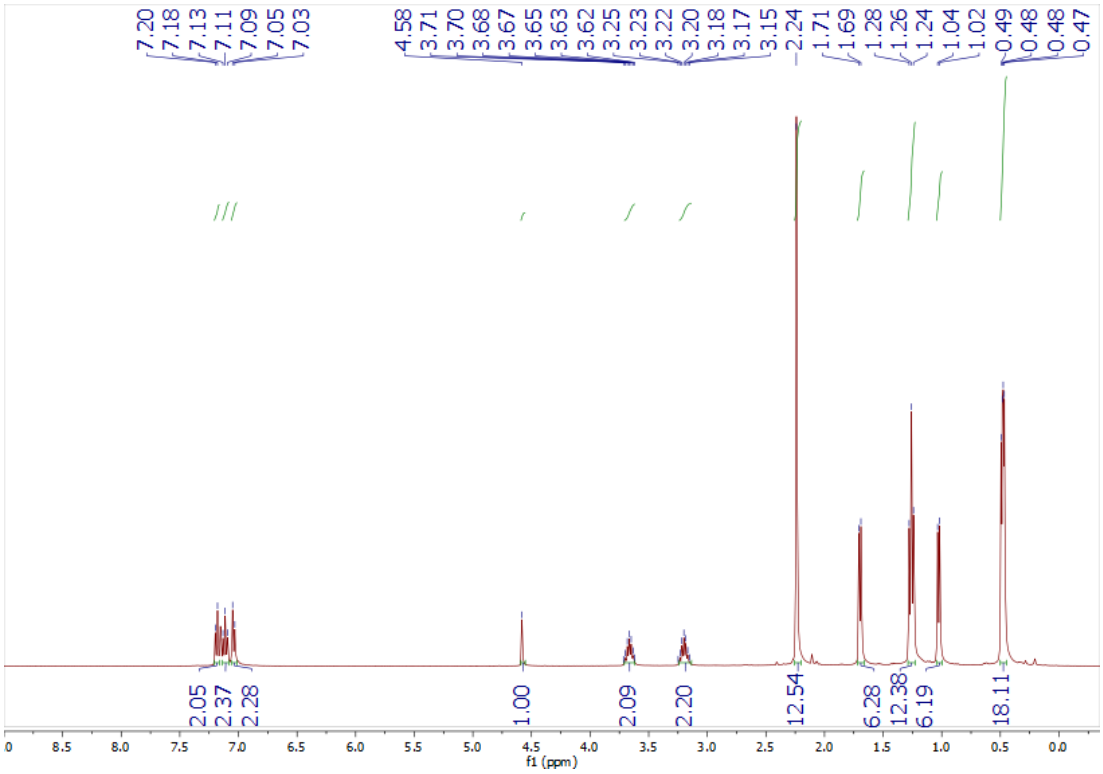

Figure s7: ^{1}H NMR spectrum of (**1-Dipp**)Si{P(SiMe$_3$)$_2$}

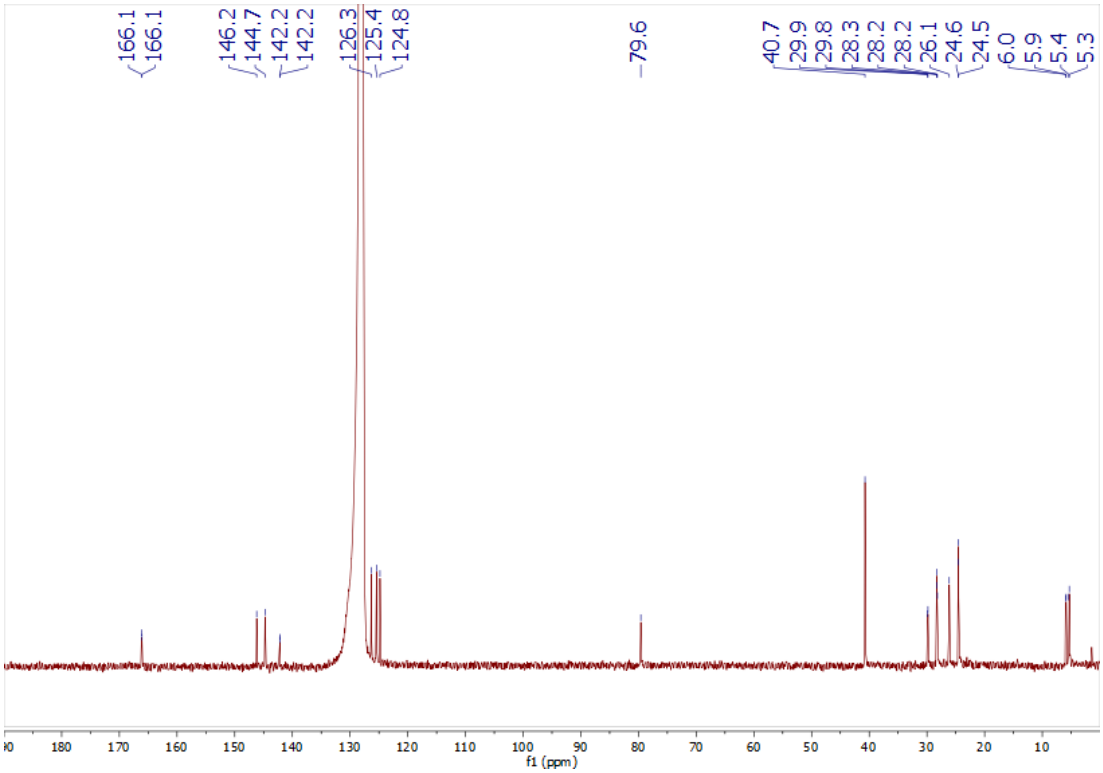

Figure s8: ^{13}C{^{1}H} NMR spectrum of (**1-Dipp**)Si{P(SiMe$_3$)$_2$}

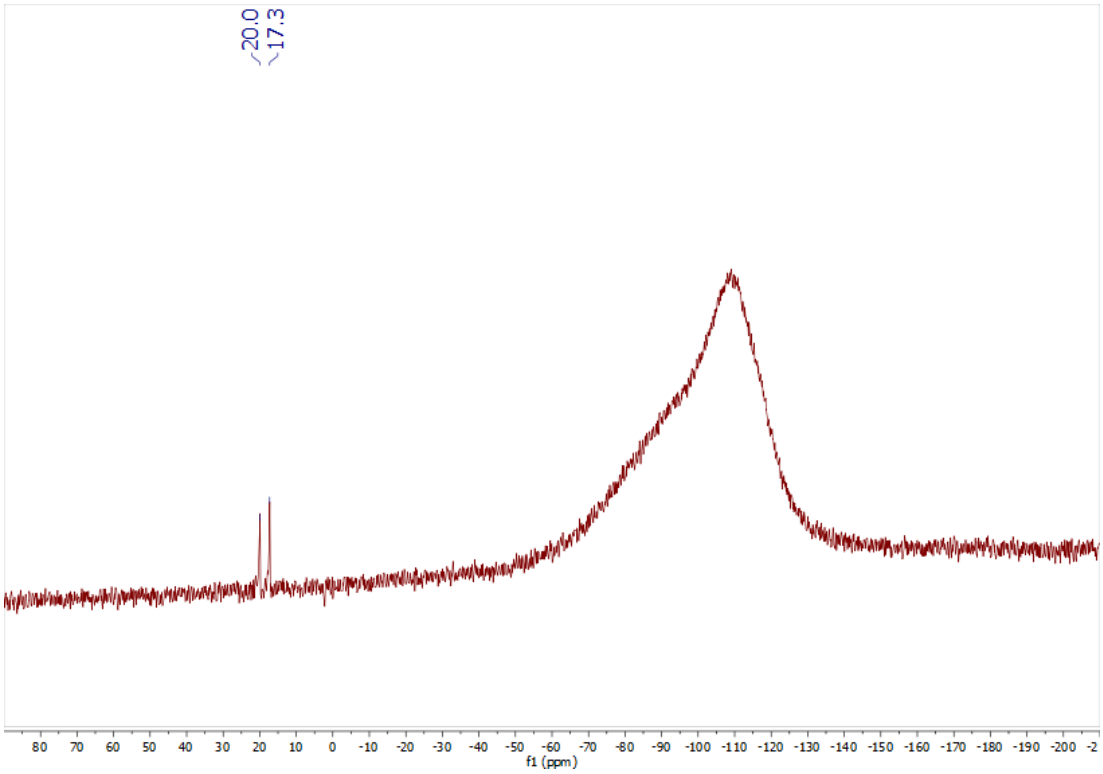

Figure s9: $^{29}Si\{^{1}H\}$ NMR spectrum of (**1-Dipp**)Si{$P(SiMe_3)_2$}

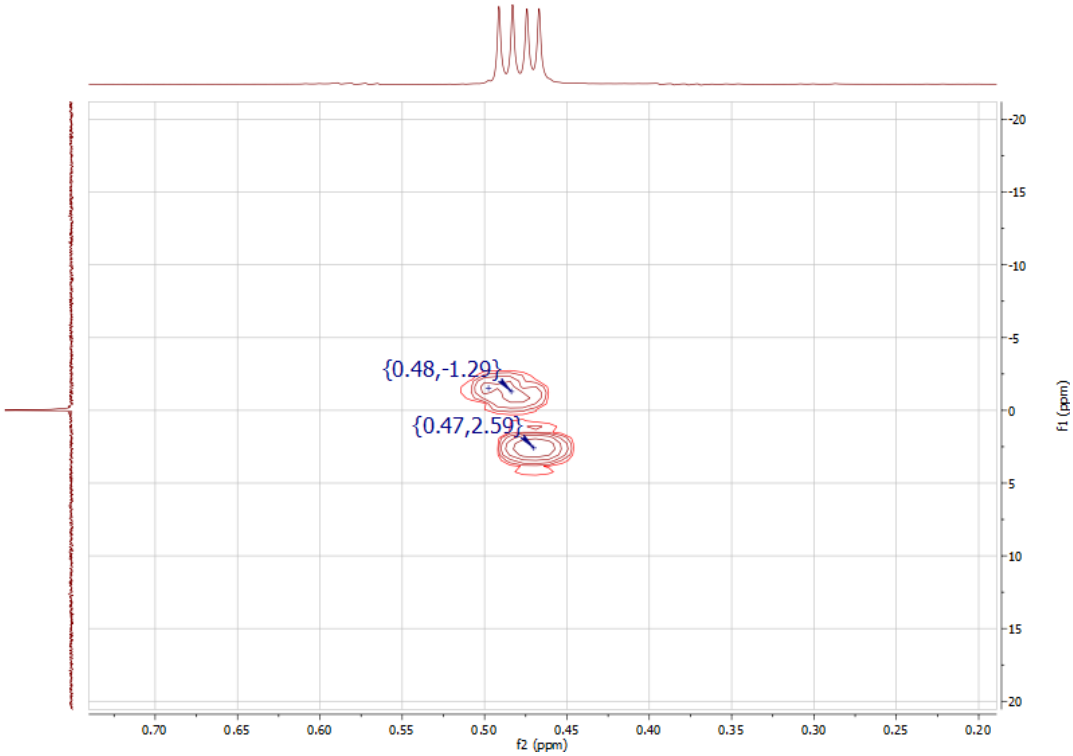

Figure s10: ^{1}H-^{29}Si 2D-NMR spectrum of (**1-Dipp**)Si{$P(SiMe_3)_2$}

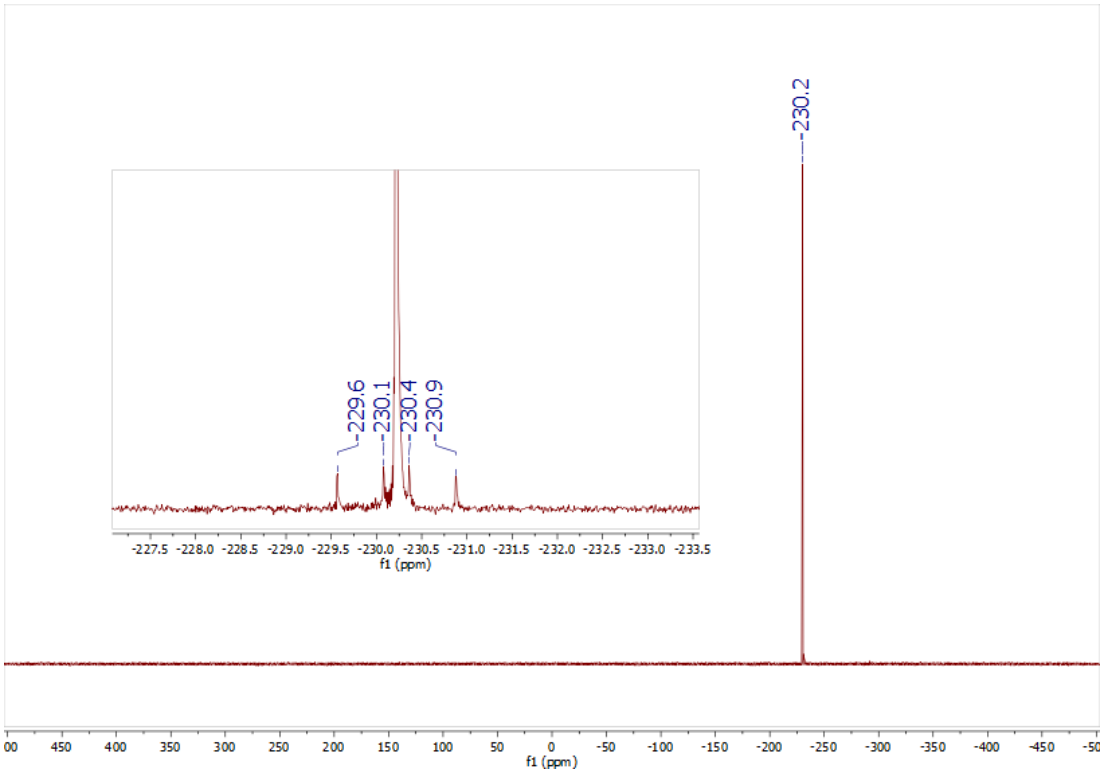

Figure s11: $^{31}P\{^{1}H\}$ NMR spectrum of (**1-Dipp**)Si{$P(SiMe_3)_2$}

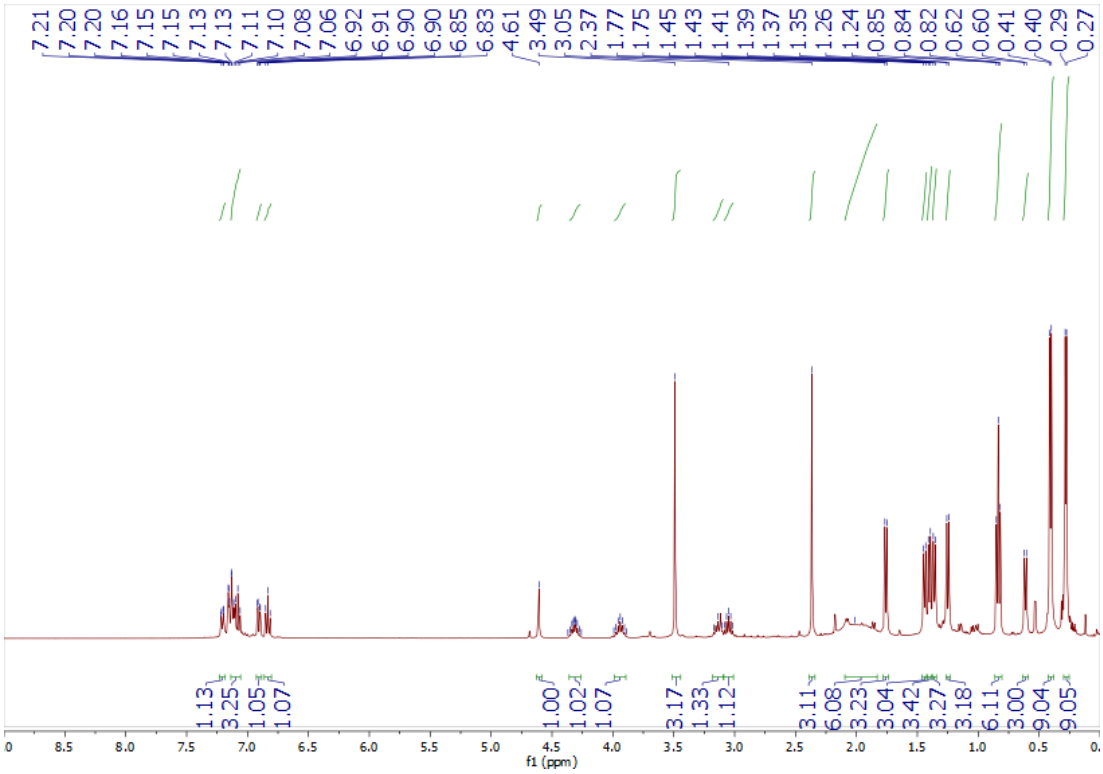

Figure s12: ^{1}H NMR spectrum of (**2-Dipp**)Si(NDipp){P(SiMe$_3$)$_2$}

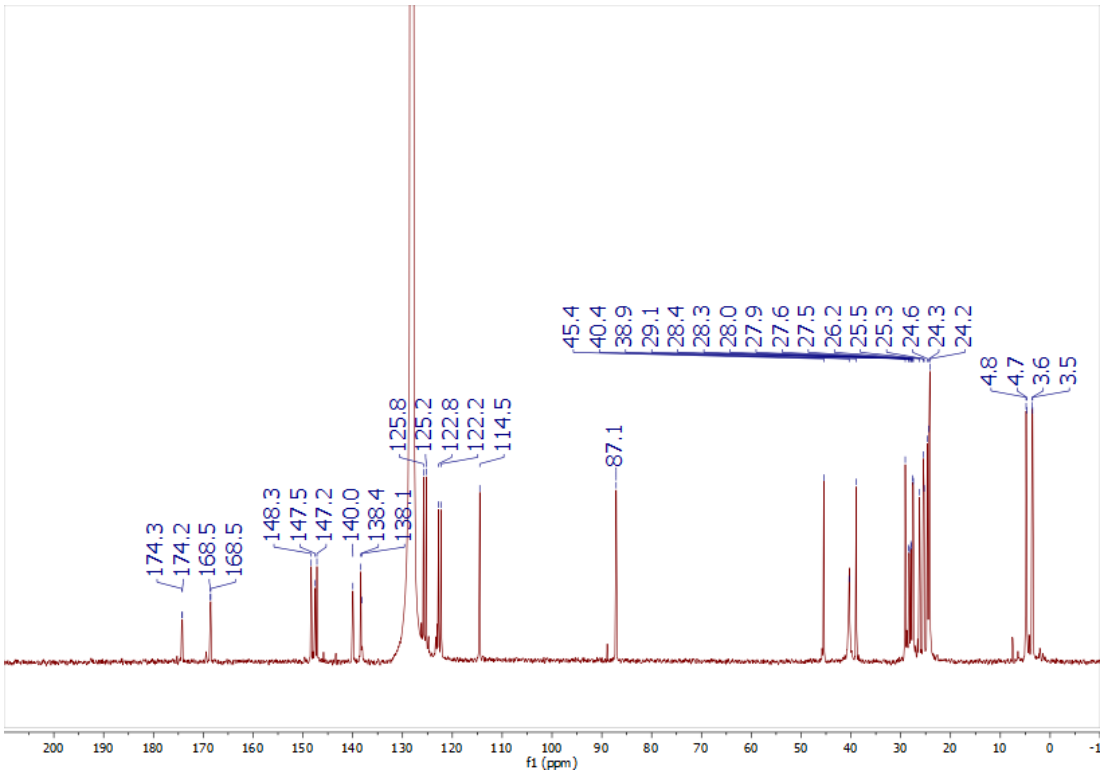

Figure s13: ^{13}C{^{1}H} NMR spectrum of (**2-Dipp**)Si(NDipp){P(SiMe$_3$)$_2$}

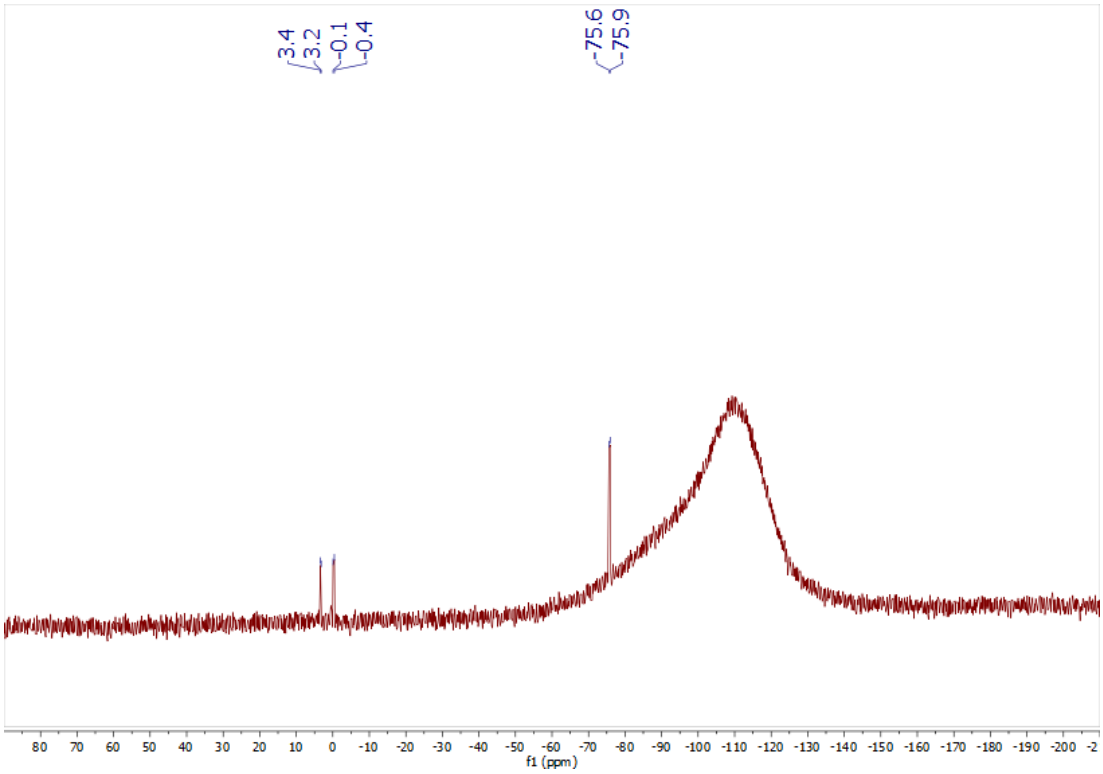

Figure s14: $^{29}Si\{^{1}H\}$ NMR spectrum of (**2-Dipp**)Si(NDipp){$P(SiMe_3)_2$}

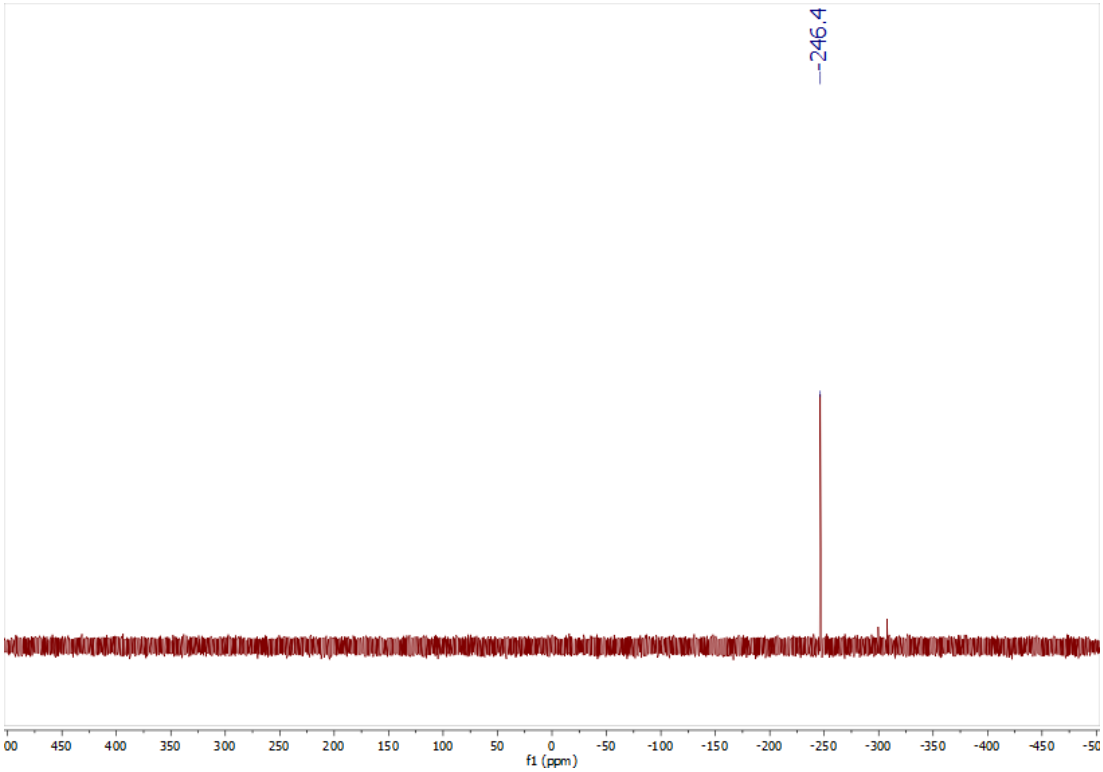

Figure s15: $^{31}P\{^{1}H\}$ NMR spectrum of (**2-Dipp**)Si(NDipp){$P(SiMe_3)_2$}

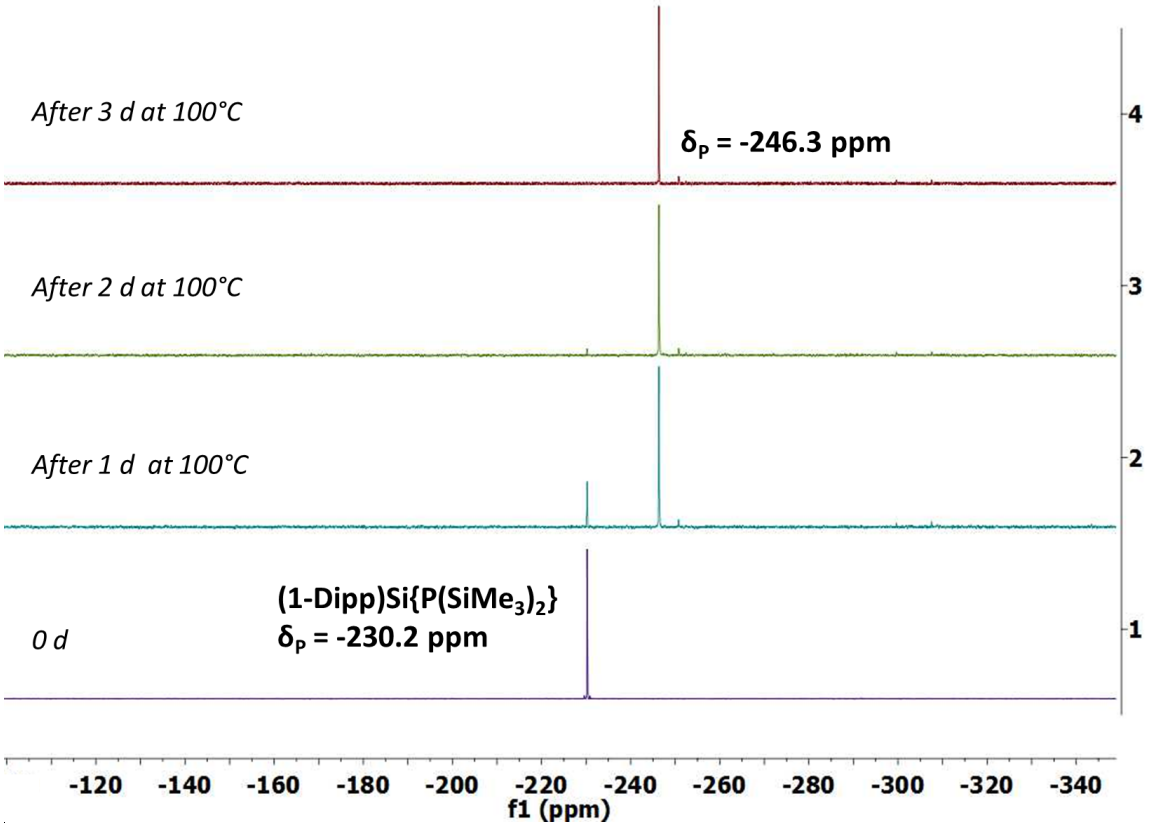

Figure s16: $^{31}P\{^{1}H\}$ NMR spectra of a sample of (**1-Dipp**)Si{$P(SiMe_3)_2$} in C_6D_6 heated to 100°C, over the course of 3 d.

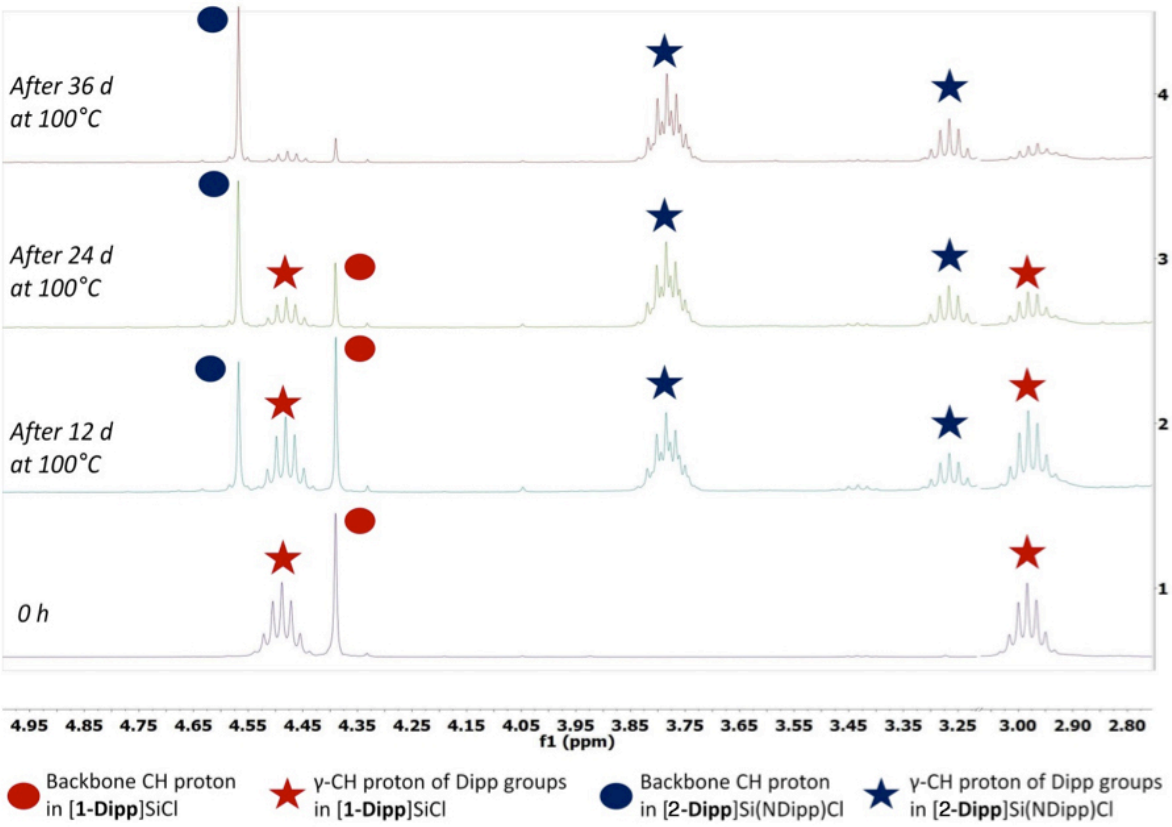

Figure s17: Thermally-induced ring contraction in (**1-Dipp**)SiCl: *in situ* ^{1}H NMR spectra in C_6D_6 (selected region) measured after 0, 12, 24, and 36 d at 100°C.

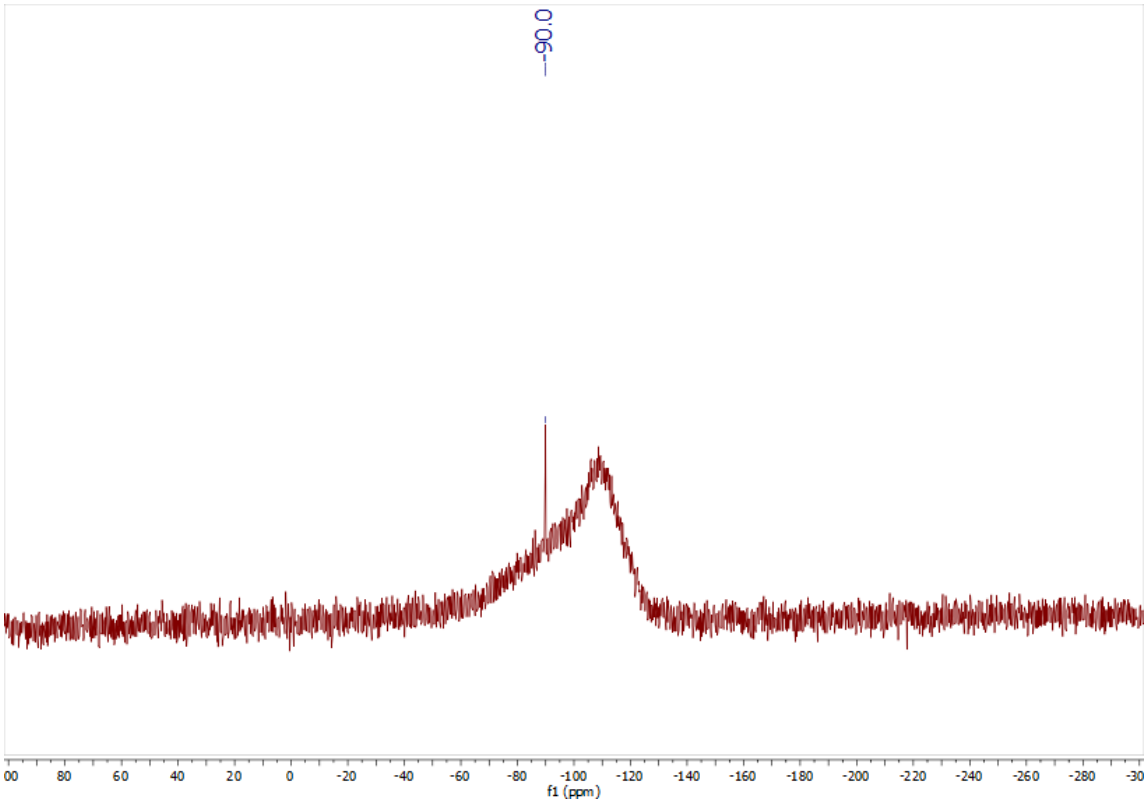

Figure s18: $^{29}Si\{^{1}H\}$ NMR spectrum of (**2-Dipp**)Si(NDipp)Cl

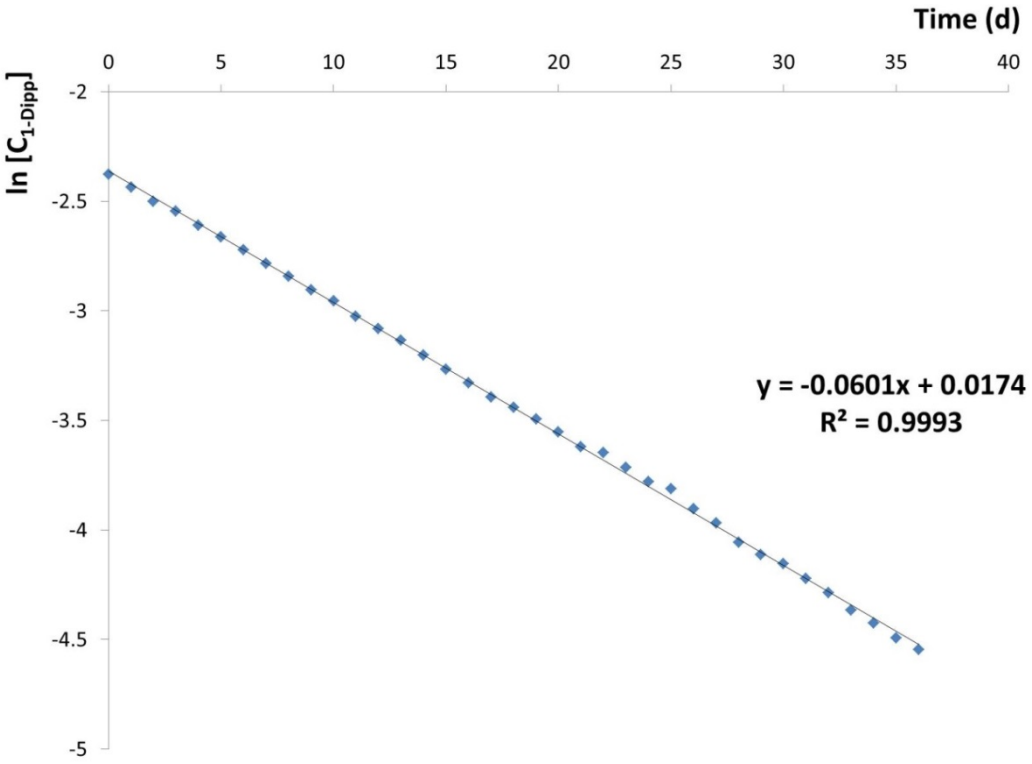

Figure s19: Plot of the natural logarithm of the concentration of (**1-Dipp**)SiCl versus time for the ring contraction to (**2-Dipp**)Si(NDipp)Cl over 36 d at 100°C.

2. Details of crystallographic studies

Compound	**(2-Dipp)Si(NDipp){N(SiMe$_3$)$_2$}**	**(2-Dipp)Si(NDipp){Si(SiMe$_3$)$_3$}**
Empirical formula	$C_{37}H_{65}N_5Si_3$	$C_{40}H_{74}N_4Si_5$
Formula weight	664.21	751.48
Temperature (K)	150(2)	150(2)
Space group	$P2_1/c$	$P2_1/c$
Crystal system	Monoclinic	Monoclinic
a (Å)	10.5277(5)	19.7161(5)
b (Å)	17.6961(8)	10.7126(2)
c (Å)	21.6670(10)	22.3580(5)
α (°)	90	90
β (°)	101.098(5)	98.430(2)
γ (°)	90	90
Volume (Å^3)	3961.1(3)	4671.23(18)
Z	4	4
ρ_{calc} (g.cm^{-3})	1.114	1.069
μ (mm^{-1})	1.327	1.643
F(000)	1456.0	1648.0
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2Θ range for data collection (°)	8.56 to 153.242	7.996 to 148.98
	-11 ≤ h ≤ 13	-24 ≤ h ≤ 22
Index ranges	-21 ≤ k ≤ 22	-13 ≤ k ≤ 13
	-27 ≤ l ≤ 24	-27 ≤ l ≤ 20
Reflections collected	22980	37395
Independent reflections	8201 [R_{int} = 0.053]	9523 [R_{int} = 0.0449]
Data/restraints/parameters	8201/0/406	9523/0/463
Goodness-of-fit on F^2	0.978	1.057
Final R indexes [I>2σ (I)]	R_1 = 0.0450, wR_2 = 0.1025	R_1 = 0.0351, wR_2 = 0.0887
Final R indexes [all data]	R_1 = 0.0669, wR_2 = 0.1144	R_1 = 0.0454, wR_2 = 0.0966
Largest diff. peak/hole (e Å^{-3})	0.46/-0.42	0.37/-0.27

Compound	**(2-Dipp)Si(NDipp)P(SiMe$_3$)$_2$·C$_6$H$_6$**	**(1-Dipp)SiP(SiMe$_3$)$_2$**
Empirical formula	$C_{43}H_{71}N_4PSi_3$	$C_{37}H_{65}N_4PSi_3$
Formula weight	759.27	681.17
Temperature (K)	150(2)	115(2)
Space group	$P2_1/n$	P-1
Crystal system	Monoclinic	Triclinic
a (Å)	11.5822(5)	9.9161(3)
b (Å)	22.3841(9)	10.3439(3)
c (Å)	17.9474(9)	20.8211(9)
α (°)	90	77.111(3)
β (°)	102.035(4)	85.335(3)
γ (°)	90	72.843(3)
Volume (Å^3)	4550.7(4)	1988.92(13)
Z	4	2
ρ_{calc} (g.cm^{-3})	1.108	1.137
μ (mm^{-1})	0.172	1.694
F(000)	1656.0	744.0
Radiation	MoKα (λ = 0.71073)	CuKα (λ = 1.54184)
2Θ range for data collection (°)	2.948 to 57.71	8.714 to 148.982
	-14 ≤ h ≤ 10	-12 ≤ h ≤ 12
Index ranges	-18 ≤ k ≤ 28	-12 ≤ k ≤ 11
	-14 ≤ l ≤ 23	-25 ≤ l ≤ 26
Reflections collected	21049	32411
Independent reflections	10425 [R_{int} = 0.0544]	8110 [R_{int} = 0.0338]
Data/restraints/parameters	10425/0/478	8110/0/424
Goodness-of-fit on F^2	1.030	1.035
Final R indexes [I>=2σ (I)]	R_1 = 0.0601, wR_2 = 0.1077	R_1 = 0.0329, wR_2 = 0.0884
Final R indexes [all data]	R_1 = 0.1166, wR_2 = 0.1321	R_1 = 0.0368, wR_2 = 0.0914
Largest diff. peak/hole (e Å^{-3})	0.50/-0.28	0.41/-0.34

3. Cartesian coordinates of DFT optimized structures

(1-Dipp)SiCl

84

Cl	0.119400	2.620700	1.455100
Si	0.085100	1.266700	-0.311400
N	-1.351400	0.257900	0.300700
C	-1.255400	-0.333900	1.517800
N	-2.374600	-0.517700	2.269800
C	-3.481900	0.413900	2.213000
C	-2.363100	-1.379200	3.425900
C	-0.026200	-0.755500	2.026800
C	1.223400	-0.670500	1.392100
N	1.415400	0.106400	0.309100
C	2.584900	-0.015800	-0.524800
C	2.781400	-1.170600	-1.302100
C	3.931100	-1.264700	-2.081900
C	4.849000	-0.236400	-2.146900
C	4.621500	0.913900	-1.417200
C	3.510100	1.046100	-0.592700
C	3.361900	2.328200	0.199100
C	4.632300	2.706800	0.960400
C	2.937000	3.482900	-0.708100
C	1.791500	-2.313300	-1.379300
C	2.373100	-3.610200	-0.819400
C	1.329500	-2.517800	-2.822100
N	2.253800	-1.380500	1.938700
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H	-1.978900	4.453800	-1.641400
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H	-1.430800	2.931600	-2.355900

(2-Dipp)Si(NDipp)Cl

84

Si	-0.137200	0.752600	-1.012600
N	-1.340600	-0.098900	-0.476200
C	-2.346000	-0.907300	-0.063700
C	-2.277000	-2.318800	-0.226600
C	-1.110300	-2.934100	-0.960500
C	-1.401000	-2.974800	-2.461400
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C	-3.311100	-3.117100	0.240300
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C	-4.509000	-1.207400	1.007000
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C	3.096300	3.424800	1.698100

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H	5.071500	-2.187800	-1.594700
H	5.167300	-0.483300	-1.160800
H	2.799400	-1.942800	-3.656700
H	2.861400	-3.194700	-2.409600
H	1.429700	-2.169000	-2.568400
Cl	0.363300	0.577600	-3.046600

Cl system– transition state

84

Cl	-0.462200	-3.112300	0.372700
Si	-0.102500	-1.111300	0.089000
N	1.420500	-0.414700	0.363500
C	0.936900	-0.342300	1.687600
N	1.610000	-1.030900	2.721600
C	2.794900	-1.778600	2.390400
C	0.781500	-1.684400	3.712400
C	0.016900	0.716100	2.096600
C	-1.127200	0.912200	1.387100
N	-1.436400	-0.039100	0.387500
C	-2.443300	0.201700	-0.611500
C	-2.254300	1.213700	-1.569000
C	-3.255100	1.433400	-2.508200
C	-4.408500	0.670600	-2.524100
C	-4.569500	-0.338000	-1.594300
C	-3.604000	-0.593300	-0.624500
C	-3.845000	-1.729200	0.350100
C	-5.111300	-1.530500	1.183100
C	-3.920300	-3.067700	-0.385000
C	-0.980600	2.025700	-1.659100
C	-1.249900	3.527400	-1.639000
C	-0.182100	1.632800	-2.902300
N	-1.943900	2.026400	1.518800
C	-1.379400	3.167700	2.199500
C	-3.330100	1.812000	1.885300
C	2.578600	0.007100	-0.337500
C	3.209800	-0.909900	-1.204600
C	4.325200	-0.492300	-1.922500
C	4.848400	0.776900	-1.776300
C	4.240200	1.656200	-0.901400
C	3.102100	1.306900	-0.182200
C	2.476900	2.328400	0.740400
C	3.096200	2.266200	2.137100
C	2.543200	3.753800	0.199700
C	2.729000	-2.333600	-1.387800
C	3.867600	-3.351000	-1.360700
C	1.908400	-2.487000	-2.667400
H	3.316400	-2.035500	3.315900
H	2.578800	-2.718100	1.857200
H	3.469800	-1.184900	1.774800
H	0.457200	-2.685900	3.393700
H	-0.106200	-1.083400	3.906300
H	1.338200	-1.786400	4.648000
H	0.198100	1.265800	3.013500
H	-3.120200	2.210300	-3.252600
H	-5.175500	0.855600	-3.267800

H	-5.467500	-0.945500	-1.617300
H	-2.996100	-1.766500	1.035500
H	-5.236500	-2.365400	1.877600
H	-5.081400	-0.611600	1.771000
H	-6.002100	-1.492200	0.550700
H	-3.996000	-3.891100	0.330000
H	-3.039000	-3.237500	-1.004400
H	-4.800000	-3.108200	-1.033300
H	-0.363800	1.791700	-0.789900
H	-0.307900	4.081800	-1.633700
H	-1.820600	3.810500	-0.752700
H	-1.811600	3.847900	-2.520300
H	0.769800	2.169100	-2.933100
H	0.036900	0.562600	-2.910600
H	-0.734800	1.869200	-3.815800
H	-2.015700	4.036900	2.013900
H	-1.314600	3.030500	3.290100
H	-0.380700	3.376400	1.817400
H	-3.435900	1.582400	2.957100
H	-3.758800	0.999700	1.308200
H	-3.903600	2.715900	1.668200
H	4.804100	-1.188800	-2.601100
H	5.725300	1.078900	-2.337700
H	4.647400	2.653600	-0.786500
H	1.421500	2.067700	0.839500
H	2.624700	2.998400	2.799700
H	2.977800	1.280100	2.590300
H	4.165000	2.495100	2.091900
H	1.929500	4.414000	0.818600
H	3.558800	4.157500	0.218700
H	2.176700	3.814100	-0.827500
H	2.079400	-2.572300	-0.544900
H	3.458400	-4.364700	-1.355900
H	4.489600	-3.231000	-0.470900
H	4.516000	-3.269600	-2.236600
H	1.550300	-3.514100	-2.777500
H	2.511500	-2.240200	-3.546000
H	1.038900	-1.824100	-2.665300

(1-Dipp)SiH

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Si	0.065200	1.445700	-0.092100
N	-1.390200	0.334800	0.417800
C	-1.271600	-0.400300	1.549000
N	-2.392400	-0.785700	2.241700
C	-3.571000	0.050100	2.313200
C	-2.341200	-1.844800	3.218400
C	-0.016700	-0.801300	2.039200
C	1.239400	-0.674400	1.396900
N	1.429600	0.198100	0.393400
C	2.621000	0.231900	-0.402100
C	2.918200	-0.808400	-1.309400
C	4.110300	-0.740700	-2.040200
C	4.974200	0.339700	-1.924400
C	4.644700	1.384400	-1.069500
C	3.480900	1.353900	-0.297200
C	3.189700	2.525500	0.628500
C	4.349500	2.829900	1.580300
C	2.812600	3.775800	-0.171700
C	1.978800	-1.971300	-1.571100
C	2.585700	-3.311200	-1.151600
C	1.562100	-1.998100	-3.044100
N	2.258300	-1.474200	1.860600
C	1.968400	-2.706200	2.553000
C	3.623600	-1.019900	2.018200
C	-2.561800	0.294400	-0.398800
C	-3.246400	1.499000	-0.706800
C	-4.367700	1.446100	-1.540300
C	-4.840900	0.245500	-2.051800
C	-4.169500	-0.929500	-1.742200
C	-3.025700	-0.932200	-0.937200
C	-2.317100	-2.259700	-0.726800
C	-3.194700	-3.269600	0.015300
C	-1.842700	-2.841800	-2.059600
C	-2.847100	2.858100	-0.149000
C	-3.980200	3.508700	0.652700
C	-2.371500	3.805400	-1.253400
H	-3.862200	0.177500	3.369500
H	-3.358400	1.042000	1.905700
H	-4.425800	-0.374500	1.759800
H	-3.351800	-2.260900	3.347500
H	-1.990800	-1.500700	4.210900
H	-1.685600	-2.657400	2.878300
H	0.004700	-1.255100	3.025400
H	4.355100	-1.549100	-2.734100
H	5.895500	0.375100	-2.511000
H	5.312200	2.246400	-0.992500
H	2.318100	2.255500	1.245600
H	4.064900	3.630100	2.281300
H	4.642500	1.952800	2.177900
H	5.245100	3.174100	1.039000
H	2.543700	4.601300	0.506500
H	1.952300	3.579000	-0.829200
H	3.653500	4.113900	-0.799300
H	1.069300	-1.806200	-0.973200
H	1.861100	-4.129100	-1.293600
H	2.887000	-3.302000	-0.094300
H	3.477200	-3.553500	-1.752400
H	0.867200	-2.828500	-3.238200
H	1.067700	-1.058300	-3.332900
H	2.431400	-2.136300	-3.705900
H	2.802400	-3.408900	2.395800
H	1.850400	-2.571900	3.646300
H	1.055400	-3.167700	2.155700
H	3.951400	-1.212800	3.054600
H	3.700500	0.054900	1.840900
H	4.319100	-1.529800	1.330100
H	-4.890700	2.374600	-1.783600
H	-5.725300	0.226000	-2.693300
H	-4.529700	-1.875700	-2.154800
H	-1.420700	-2.076200	-0.117200
H	-2.632100	-4.192000	0.232900
H	-3.565900	-2.861800	0.965500
H	-4.071000	-3.555800	-0.588300

H	-1.231800	-3.744300	-1.895300
H	-2.692100	-3.131100	-2.698700
H	-1.239000	-2.113900	-2.618200
H	-2.005900	2.707800	0.548000
H	-3.632600	4.449800	1.107200
H	-4.348000	2.861200	1.463000
H	-4.842000	3.752900	0.011600
H	-2.040100	4.763400	-0.821800
H	-3.182700	4.022800	-1.967400
H	-1.526300	3.368800	-1.804700
H	0.113300	2.138500	1.290200

(2-Dipp)Si(NDipp)H

84

Si	-0.022400	0.569700	-1.006900
N	1.360600	0.122500	0.123000
N	2.999600	1.153300	1.481800
N	-1.524800	0.147900	-0.710100
N	-0.180400	3.464300	-1.246800
C	1.971600	1.219000	0.615600
C	0.448900	2.410400	-0.741500
C	1.998600	-1.154000	0.004400
C	3.162300	-1.283800	-0.777000
C	1.474500	2.480400	0.178900
H	1.814800	3.391800	0.649500
C	-3.680800	-0.888300	-0.709400
C	3.768000	-0.140700	-1.567400
H	3.172700	0.757300	-1.393700
C	-2.686500	-0.098000	-0.063400
C	-2.970200	0.391000	1.241900
C	1.413200	-2.276700	0.615700
C	-4.881200	-1.153500	-0.070000
H	-5.628200	-1.759700	-0.571500
C	3.235900	0.024000	2.357600
H	2.358700	-0.611800	2.405000
H	3.437300	0.405400	3.362200
H	4.087700	-0.579600	2.031500
C	-4.190400	0.097700	1.838700
H	-4.399000	0.480800	2.833000
C	3.761500	-2.536000	-0.867300
H	4.662900	-2.648700	-1.460000
C	-1.977900	1.275200	1.960500
H	-1.002600	1.094100	1.499300
C	-5.150700	-0.667600	1.200800
H	-6.094900	-0.886000	1.686800
C	3.218700	-3.642000	-0.240700
H	3.698800	-4.610100	-0.328500
C	0.124500	-2.207600	1.408900
H	-0.214200	-1.169900	1.415200
C	-3.405600	-1.401400	-2.103000
H	-2.322700	-1.555600	-2.159300
C	3.710100	-0.424900	-3.068300
H	4.314700	-1.296700	-3.331200
H	4.095000	0.429500	-3.631800
H	2.685700	-0.615100	-3.392800
C	5.201900	0.161800	-1.136400
H	5.263300	0.385200	-0.069100
H	5.593100	1.021700	-1.686700
H	5.863700	-0.684900	-1.336100
C	2.046400	-3.507800	0.478400
H	1.606200	-4.380100	0.948400
C	-1.305400	3.331300	-2.147700
H	-1.575000	2.280000	-2.245000
H	-1.063600	3.746300	-3.131400
H	-2.174400	3.863400	-1.750000
C	0.195100	4.807100	-0.868200
H	-0.097300	5.024100	0.165200
H	-0.300500	5.520300	-1.525600
H	1.276000	4.943400	-0.960600
C	3.803700	2.320700	1.768000
H	3.919000	2.937100	0.878100
H	4.795500	1.988400	2.079000
H	3.378300	2.928600	2.575500
C	-3.757000	-0.341400	-3.147400
H	-4.831700	-0.135000	-3.138800
H	-3.482900	-0.672500	-4.154200
H	-3.230600	0.591700	-2.938600
C	-0.970000	-3.036400	0.739300
H	-1.136700	-2.705100	-0.286300
H	-1.912200	-2.925300	1.280000
H	-0.707400	-4.098400	0.723700
C	-2.314900	2.750700	1.745700
H	-2.387200	2.980600	0.680700
H	-1.554700	3.401200	2.192100
H	-3.278800	2.993800	2.202600
C	-4.094700	-2.719000	-2.431600
H	-3.880900	-3.482100	-1.679200
H	-3.751300	-3.091700	-3.400800
H	-5.181200	-2.609300	-2.498000
C	-1.842500	0.973400	3.449000
H	-2.756700	1.210900	3.999700
H	-1.038800	1.572600	3.888300
H	-1.616100	-0.081100	3.622800
C	0.313900	-2.656500	2.857600
H	0.628800	-3.701900	2.914200
H	-0.629800	-2.567100	3.401100
H	1.060400	-2.058800	3.387000
H	0.537900	0.140600	-2.320900

H system – transition state

84

Si	0.120400	-1.271800	0.294800
N	1.446500	-0.146100	0.435000
C	1.160600	0.913400	1.312300
N	2.025200	1.999900	1.342900
C	3.390000	1.751200	1.766900
C	1.505000	3.227500	1.895100
C	0.011900	0.824300	2.036100
C	-0.928000	-0.260400	1.750100
N	-1.387100	-0.481800	0.434800
C	-2.537700	-0.153000	-0.314000
C	-3.070300	1.152600	-0.320400
C	-4.209800	1.405800	-1.075900
C	-4.811600	0.423300	-1.838900

C	-4.277000	-0.849900	-1.834100
C	-3.159500	-1.170400	-1.071000
C	-2.665900	-2.602500	-1.091200
C	-3.790900	-3.615800	-0.889900
C	-1.893100	-2.908100	-2.372900
C	-2.443000	2.281400	0.465300
C	-3.089500	2.424100	1.843600
C	-2.469000	3.617100	-0.272100
N	-1.647700	-0.783600	2.848700
C	-0.825000	-1.273600	3.931900
C	-2.731100	-1.684100	2.549900
C	2.469900	-0.075400	-0.565100
C	3.566100	-0.951800	-0.471100
C	4.547600	-0.896600	-1.455400
C	4.464400	0.003800	-2.500900
C	3.376100	0.853300	-2.585000
C	2.359100	0.825800	-1.637100
C	1.144900	1.706100	-1.836900
C	1.514400	3.178900	-1.984600
C	0.328300	1.225600	-3.036700
C	3.693100	-1.968800	0.644500
C	5.045100	-1.904500	1.351500
C	3.438400	-3.382200	0.120100
H	3.462100	1.652800	2.861400
H	3.777000	0.845900	1.308700
H	4.023800	2.583700	1.453100
H	2.184300	4.044400	1.637900
H	1.415300	3.203300	2.992600
H	0.523600	3.441800	1.472600
H	-0.162400	1.483300	2.878900
H	-4.623100	2.407600	-1.082600
H	-5.690000	0.649100	-2.432600
H	-4.747700	-1.625000	-2.428500
H	-1.979100	-2.727100	-0.250700
H	-3.374300	-4.621700	-0.790200
H	-4.369700	-3.396200	0.010000
H	-4.482800	-3.635400	-1.735500
H	-1.523800	-3.937700	-2.367900
H	-1.035100	-2.241200	-2.488200
H	-2.533800	-2.782500	-3.250400
H	-1.394900	2.018900	0.620900
H	-2.611100	3.227600	2.412000
H	-3.005500	1.504500	2.426300
H	-4.151100	2.669800	1.745100
H	-1.864000	4.351000	0.267500
H	-2.069300	3.526300	-1.284700
H	-3.478000	4.031200	-0.345000
H	-0.361600	-2.243900	3.679000
H	-0.026700	-0.566800	4.151800
H	-1.433800	-1.400500	4.830100
H	-3.284900	-1.884000	3.469500
H	-2.376100	-2.651900	2.153700
H	-3.416400	-1.247400	1.825300
H	5.394700	-1.571400	-1.398900
H	5.242100	0.037100	-3.255700
H	3.303400	1.543700	-3.418300
H	0.509500	1.613200	-0.954800
H	0.611600	3.791100	-2.057800
H	2.094800	3.523700	-1.126900
H	2.104200	3.358100	-2.887500
H	-0.581900	1.821000	-3.145400
H	0.902000	1.311800	-3.963700
H	0.032400	0.180300	-2.921600
H	2.921200	-1.741000	1.384200
H	5.063600	-2.603400	2.191800
H	5.253500	-0.905600	1.740900
H	5.864600	-2.177700	0.681900
H	3.464500	-4.107600	0.937800
H	4.202200	-3.669100	-0.608300
H	2.467000	-3.459300	-0.372800
H	0.334300	-2.640200	0.792500

(1-Dipp)SiP($SiMe_3$)$_2$

110

P	5.299700	11.017600	16.630300
Si	6.720100	11.325700	18.332900
Si	3.243300	11.270300	17.500400
N	6.015500	10.055500	13.679600
Si	5.111500	9.223700	15.132300
N	6.524200	8.078700	15.498000
N	7.970200	10.796400	12.568300
N	8.765000	7.940100	16.209900
C	5.127500	10.762000	12.802000
C	7.343300	10.154700	13.619400
C	6.272500	6.667100	15.555300
C	8.153000	9.620600	14.648000
H	9.181000	9.929900	14.668600
C	7.797100	8.556900	15.475300
C	5.110100	12.173700	12.775500
C	6.893200	5.791100	14.636900
C	6.010100	13.068700	13.606200
H	6.593700	12.440000	14.281000
C	4.216100	10.025600	12.016200
C	4.626900	6.990400	17.522000
H	4.947900	8.032400	17.417500
C	5.368600	6.146800	16.504700
C	4.193600	12.803900	11.938400
H	4.176600	13.887400	11.907200
C	6.636500	4.426700	14.726700
H	7.120200	3.756000	14.024900
C	4.197500	8.511300	11.946400
H	4.965000	8.133400	12.626300
C	3.296000	12.093800	11.166300
H	2.586400	12.613400	10.532300
C	5.130900	4.776200	16.530300
H	4.433800	4.380500	17.260200
C	3.309800	10.714500	11.218000
H	2.605400	10.151100	10.616400
C	7.804400	6.239200	13.510100
H	7.894200	7.324400	13.541300
C	5.764500	3.909800	15.663400
H	5.571900	2.843900	15.709200
C	8.466300	7.154800	17.385700
H	8.621000	6.084300	17.215400

H	7.435900	7.308700	17.686500
H	9.113800	7.479200	18.205400
C	9.364800	11.146700	12.684200
H	9.608300	11.831600	11.870000
H	10.035400	10.278400	12.605000
H	9.561900	11.666500	13.621800
C	5.198300	14.020200	14.482300
H	5.869000	14.606200	15.116700
H	4.525300	13.466100	15.134900
H	4.614200	14.722300	13.881400
C	7.598400	10.497600	11.199400
H	7.740600	11.383300	10.575000
H	6.559000	10.201000	11.122700
H	8.226900	9.688700	10.800100
C	4.928000	6.556800	18.957600
H	4.563600	5.545000	19.152600
H	4.432700	7.226200	19.665300
H	5.996900	6.570000	19.180800
C	2.859400	7.941000	12.409400
H	2.044100	8.254200	11.751300
H	2.636000	8.270300	13.425200
H	2.891600	6.848000	12.402500
C	2.987300	10.468600	19.188600
H	1.941300	10.571000	19.495800
H	3.603500	10.945800	19.954800
H	3.234400	9.405600	19.174800
C	1.966200	10.597100	16.300500
H	2.074200	11.058600	15.315800
H	0.964200	10.828000	16.677300
H	2.049500	9.518100	16.168400
C	6.963900	13.880700	12.729400
H	7.558400	13.244100	12.074400
H	7.647000	14.464300	13.353100
H	6.411900	14.585500	12.101300
C	6.243000	12.895900	19.257800
H	6.180600	13.752100	18.582600
H	7.004800	13.112600	20.014100
H	5.285100	12.799000	19.772700
C	7.214700	5.879600	12.147300
H	7.837900	6.282600	11.343500
H	6.208200	6.281800	12.031300
H	7.158600	4.796800	12.009500
C	4.525600	8.017500	10.536400
H	3.787500	8.370500	9.811800
H	4.518800	6.924800	10.504900
H	5.508500	8.355500	10.199500
C	3.121600	6.935100	17.264800
H	2.891700	7.272800	16.252900
H	2.584300	7.571800	17.971600
H	2.742000	5.916400	17.382300
C	8.461900	11.592500	17.673400
H	8.831000	10.708600	17.151800
H	9.142400	11.815100	18.501500
H	8.488800	12.430300	16.972600
C	10.165400	8.216700	16.000000
H	10.398200	8.260600	14.935000
H	10.747800	7.404300	16.437000
H	10.487200	9.154500	16.470700
C	2.865400	13.104000	17.715600
H	2.843900	13.615000	16.750300
H	3.596200	13.612900	18.346300
H	1.880000	13.221900	18.178800
C	9.207500	5.648100	13.641500
H	9.190000	4.561700	13.521200
H	9.647300	5.864300	14.616100
H	9.868600	6.051600	12.869100
C	6.795000	9.942200	19.608100
H	7.132400	9.003000	19.167200
H	5.815900	9.765200	20.057600
H	7.492700	10.208000	20.409500

(2-Dipp)Si(NDipp)P(SiMe$_3$)$_2$

110

P	2.091300	0.603200	-0.799000
Si	0.245000	0.193900	0.453700
Si	2.385700	2.810200	-1.214500
Si	3.999100	-0.164800	0.109500
N	0.038900	-1.659000	0.427000
N	0.284000	-3.510300	1.900100
N	1.138300	1.012000	3.118800
N	-1.061700	1.025400	0.122100
C	-0.853900	-2.337100	-0.475900
C	-2.075200	1.820600	-0.290200
C	0.768900	0.036300	2.294100
C	-0.404500	-2.767400	-1.739100
C	-2.181000	-2.580700	-0.072200
C	-2.511600	1.850300	-1.646700
C	0.777400	-1.294000	2.644700
H	1.154200	-1.674500	3.582200
C	-2.773400	-2.083700	1.231400
H	-2.020500	-1.490300	1.753200
C	-1.853500	0.992600	-2.702300
H	-0.999100	0.510600	-2.220800
C	0.353000	-2.193600	1.626500
C	-1.283200	-3.476400	-2.551300
H	-0.942500	-3.813900	-3.523700
C	0.997100	-2.524100	-2.261300
H	1.553100	-1.987000	-1.490900
C	-2.763800	2.661500	0.633300
C	-3.009600	-3.311600	-0.918800
H	-4.029500	-3.512500	-0.610500
C	-2.571100	-3.766500	-2.146300
H	-3.235900	-4.329000	-2.792100
C	0.333900	-3.981300	3.268300
H	1.362700	-4.115000	3.623400
H	-0.169700	-4.947800	3.315100
H	-0.190400	-3.298000	3.934000
C	0.356000	-4.558600	0.903900
H	-0.625400	-4.988000	0.682900
H	1.010300	-5.346100	1.286300
H	0.784100	-4.180000	-0.015700
C	-3.964200	-1.162700	0.973400
H	-3.672300	-0.290500	0.387600
H	-4.379700	-0.813400	1.922100

H	-4.763300	-1.684700	0.440400
C	-3.190400	-3.238800	2.142100
H	-4.002600	-3.818900	1.695900
H	-3.550100	-2.855200	3.100600
H	-2.363800	-3.924500	2.338700
C	3.707900	3.650200	-0.167700
H	3.813800	4.684500	-0.511800
H	4.685900	3.173200	-0.255700
H	3.436100	3.680400	0.889200
C	1.229400	2.390200	2.699300
H	0.840200	2.488200	1.688100
H	2.269900	2.729800	2.718700
H	0.639900	3.029900	3.360400
C	1.536600	0.720700	4.476500
H	0.776000	0.114000	4.976100
H	1.651400	1.653900	5.025900
H	2.489100	0.179200	4.512300
C	-3.576200	2.660400	-2.018400
H	-3.894600	2.660300	-3.056900
C	0.976000	-1.638600	-3.505100
H	0.451900	-2.130200	-4.329800
H	1.996600	-1.425500	-3.832400
H	0.487300	-0.685500	-3.306600
C	-1.332900	1.807200	-3.884600
H	-2.150600	2.289600	-4.427700
H	-0.805800	1.162200	-4.594500
H	-0.644500	2.592100	-3.564300
C	0.799800	3.782600	-1.021700
H	0.548700	3.958600	0.025700
H	-0.059800	3.291200	-1.477700
H	0.931900	4.759200	-1.499200
C	-3.821600	3.451100	0.207600
H	-4.333000	4.078900	0.932100
C	-2.359500	2.716400	2.089500
H	-1.515100	2.032200	2.199500
C	4.499800	0.563800	1.770500
H	5.457800	0.137400	2.085900
H	3.758800	0.327200	2.536500
H	4.612400	1.648100	1.724700
C	1.743500	-3.820900	-2.577800
H	1.839900	-4.481100	-1.713000
H	2.752800	-3.591800	-2.930500
H	1.243100	-4.386700	-3.367800
C	3.877100	-2.027200	0.339100
H	3.678600	-2.540000	-0.604000
H	3.090500	-2.292100	1.049000
H	4.826300	-2.403400	0.734400
C	-4.243700	3.462900	-1.110500
H	-5.073300	4.086300	-1.423700
C	2.949600	2.889400	-3.004700
H	3.139800	3.925600	-3.301900
H	2.184800	2.477700	-3.667300
H	3.867600	2.317300	-3.160700
C	5.371700	0.173500	-1.131200
H	5.522900	1.240900	-1.304900
H	5.147300	-0.293200	-2.093200
H	6.316200	-0.240700	-0.764200
C	-2.796600	-0.102400	-3.194700
H	-3.136100	-0.732000	-2.370500
H	-2.302100	-0.744900	-3.929200
H	-3.680400	0.332800	-3.671100
C	-3.470500	2.233500	3.019500
H	-4.353900	2.874400	2.947900
H	-3.138500	2.243400	4.062900
H	-3.778800	1.217400	2.768600
C	-1.908500	4.118200	2.496300
H	-1.095900	4.478000	1.860700
H	-1.569100	4.137100	3.537700
H	-2.728800	4.836000	2.409300

$P(SiMe_3)_2$ system– transition state

110

P	-2.008800	-1.281700	-0.078100
Si	-2.345200	-2.372700	1.872000
Si	-2.357700	-2.737800	-1.774900
N	-0.398100	1.521300	0.093200
Si	-0.097800	-0.208800	-0.076800
N	1.527900	-0.478600	0.404900
N	0.023500	3.489300	1.394100
N	1.362900	-1.007200	2.763800
C	-1.268200	2.225000	-0.802300
C	0.209200	2.111400	1.183400
C	2.809600	-0.737200	-0.162800
C	0.915700	1.299500	2.032900
H	1.267000	1.699000	2.975200
C	1.165700	-0.085500	1.716300
C	-2.566300	2.586700	-0.400700
C	3.866600	0.194400	-0.075000
C	-3.104600	2.348900	0.993700
H	-2.357700	1.773900	1.545400
C	-0.818400	2.504700	-2.108700
C	1.970400	-3.027300	-1.021800
H	1.016700	-2.623400	-0.675700
C	3.041400	-1.978900	-0.795700
C	-3.398600	3.201000	-1.331300
H	-4.402400	3.483300	-1.033600
C	5.132100	-0.173000	-0.522700
H	5.944600	0.539300	-0.431800
C	0.596100	2.209000	-2.572000
H	1.186900	1.956200	-1.687400
C	-2.983100	3.446600	-2.625700
H	-3.655600	3.914200	-3.336400
C	4.321900	-2.282900	-1.245800
H	4.496700	-3.243600	-1.717600
C	-1.700100	3.100300	-3.004500
H	-1.369500	3.307100	-4.016200
C	3.703100	1.598700	0.461700
H	2.636800	1.784500	0.577200
C	5.375900	-1.405100	-1.093700
H	6.370300	-1.670700	-1.433800
C	2.578200	-1.787200	2.805300
H	3.426100	-1.225200	3.230000
H	2.861700	-2.123700	1.813000
H	2.417000	-2.668700	3.433100

C	0.214900	3.933400	2.752100
H	-0.130400	4.967000	2.831100
H	1.269100	3.908000	3.075700
H	-0.373000	3.321200	3.437100
C	-4.400300	1.540300	0.975000
H	-4.735100	1.344800	1.997500
H	-4.261300	0.585000	0.466800
H	-5.203000	2.084700	0.470500
C	0.672300	4.378500	0.451200
H	0.268200	5.386400	0.574200
H	0.473700	4.063800	-0.569400
H	1.762700	4.421800	0.602700
C	2.247200	-4.305800	-0.231700
H	3.203200	-4.750200	-0.521200
H	1.468500	-5.050800	-0.418100
H	2.277400	-4.117800	0.842900
C	0.643100	1.009500	-3.514400
H	0.048600	1.195000	-4.413600
H	0.247700	0.115900	-3.027900
H	1.671600	0.802800	-3.822600
C	-1.737900	-4.484500	-1.467700
H	-1.920700	-5.104900	-2.351100
H	-2.258800	-4.946900	-0.626100
H	-0.669100	-4.506700	-1.252500
C	-1.646100	-2.048000	-3.360600
H	-1.997400	-1.028000	-3.531100
H	-1.978500	-2.666300	-4.200600
H	-0.556400	-2.040000	-3.360100
C	-3.328400	3.671600	1.726900
H	-2.416400	4.268100	1.743300
H	-3.644900	3.487500	2.757600
H	-4.113300	4.258000	1.240600
C	-3.939400	-3.360600	1.722700
H	-4.778000	-2.729500	1.420300
H	-4.177300	-3.784000	2.704300
H	-3.860300	-4.190800	1.018300
C	4.248600	2.646700	-0.506800
H	4.009000	3.651300	-0.147200
H	3.816500	2.532100	-1.503100
H	5.335500	2.591200	-0.606500
C	1.252800	3.415700	-3.242200
H	0.768100	3.663500	-4.189700
H	2.300100	3.194800	-3.463400
H	1.222300	4.307000	-2.612300
C	1.839700	-3.341100	-2.511900
H	1.673700	-2.432600	-3.094700
H	1.009300	-4.026600	-2.697100
H	2.745300	-3.815800	-2.897900
C	-2.614800	-1.049400	3.173100
H	-1.889900	-0.240500	3.070200
H	-2.527000	-1.467000	4.180300
H	-3.613100	-0.619700	3.066100
C	0.920000	-0.633600	4.081700
H	1.649400	-0.002200	4.615800
H	0.769500	-1.536500	4.681600
H	-0.021500	-0.091100	4.030300
C	-4.226600	-2.797500	-1.961100
H	-4.621400	-1.806100	-2.195100
H	-4.725200	-3.155100	-1.058600
H	-4.493200	-3.472400	-2.780800
C	4.349000	1.761300	1.835500
H	5.427200	1.583700	1.784800
H	3.929700	1.060400	2.559700
H	4.194000	2.774700	2.217500
C	-0.950700	-3.524900	2.348800
H	-0.027900	-2.953500	2.474600
H	-0.784900	-4.285100	1.582300
H	-1.183800	-4.034900	3.289300

(1-Dipp)SiSi(SiMe$_3$)$_3$

123

N	0.505600	1.529300	0.078500
Si	0.156800	-0.128700	-0.806900
N	1.331700	-1.058600	0.295300
N	1.131100	2.713800	2.039600
N	1.422000	-1.913700	2.489500
C	0.446700	2.711600	-0.739100
C	0.789600	1.542800	1.382900
C	2.548700	-1.606800	-0.225500
C	0.738300	0.342100	2.141500
H	0.666800	0.439300	3.209500
C	1.136800	-0.895200	1.637200
C	-0.516400	3.715200	-0.492200
C	3.820100	-1.243500	0.289500
C	-1.524700	3.684200	0.638100
H	-1.429300	2.728800	1.152400
C	1.328700	2.841000	-1.834700
C	1.214700	-3.078300	-1.894500
H	0.369100	-2.686800	-1.320200
C	2.492800	-2.496400	-1.323500
C	-0.568800	4.812800	-1.346200
H	-1.304400	5.585900	-1.156000
C	4.965700	-1.755700	-0.312900
H	5.932600	-1.475100	0.089800
C	2.472600	1.890900	-2.131100
H	2.475700	1.105300	-1.371400
C	0.269000	4.933400	-2.435700
H	0.194900	5.790700	-3.095000
C	3.675700	-2.942100	-1.904400
H	3.617400	-3.610400	-2.755800
C	1.203200	3.946000	-2.670500
H	1.872000	4.037500	-3.518700
C	4.069400	-0.319800	1.471200
H	3.120100	0.075600	1.824400
C	4.912800	-2.583600	-1.414000
H	5.821800	-2.950400	-1.876700
C	1.634100	-3.270100	2.041400
H	2.692000	-3.552400	2.078000
H	1.285800	-3.381000	1.020900
H	1.062900	-3.953600	2.673700
C	1.135600	2.732400	3.482800
H	1.225000	3.771800	3.803500
H	1.976200	2.171100	3.916800
H	0.200600	2.345600	3.887800

C	-2.956200	3.792200	0.117600
H	-3.667300	3.703300	0.943300
H	-3.181600	3.017400	-0.611700
H	-3.136700	4.759700	-0.357400
C	2.161000	3.582600	1.498500
H	1.940900	4.622900	1.751300
H	2.223600	3.509300	0.419300
H	3.139100	3.322700	1.925100
C	1.209900	-4.603400	-1.758600
H	1.981000	-5.057500	-2.385800
H	0.246600	-5.010100	-2.073300
H	1.396300	-4.925300	-0.731200
C	2.313600	1.215800	-3.490600
H	2.360400	1.947500	-4.302100
H	1.359000	0.692100	-3.546000
H	3.115000	0.489100	-3.647200
C	-1.288300	4.805700	1.650000
H	-0.275400	4.790400	2.049100
H	-1.986000	4.710700	2.486700
H	-1.456200	5.783800	1.190600
C	4.926300	0.885200	1.089300
H	5.040000	1.553900	1.948000
H	4.478600	1.450400	0.272600
H	5.929800	0.587500	0.775600
C	3.819600	2.615400	-2.070400
H	3.909900	3.350500	-2.874100
H	4.636600	1.898600	-2.186400
H	3.964700	3.145700	-1.126300
C	1.014800	-2.681400	-3.355300
H	0.902100	-1.600600	-3.446400
H	0.122400	-3.158000	-3.768400
H	1.863800	-2.996300	-3.967600
C	1.452700	-1.705000	3.917200
H	2.055000	-0.829500	4.173600
H	1.910200	-2.575300	4.386600
H	0.451200	-1.576300	4.343300
C	4.725400	-1.066500	2.633700
H	5.726000	-1.413700	2.363400
H	4.146100	-1.939900	2.936200
H	4.830400	-0.409300	3.502100
Si	-2.153000	-0.738800	-0.049600
Si	-3.191400	-0.367200	2.082300
Si	-3.483000	0.205800	-1.817200
Si	-2.644700	-3.074100	-0.282200
C	-2.439000	-3.792800	-2.018300
H	-1.583800	-3.384700	-2.555700
H	-2.301300	-4.875600	-1.930900
H	-3.326900	-3.620500	-2.626500
C	-4.445900	-3.431100	0.173700
H	-4.667900	-4.470500	-0.091700
H	-4.638800	-3.314600	1.241700
H	-5.147500	-2.792900	-0.368300
C	-1.610400	-4.194900	0.834000
H	-0.608000	-4.331500	0.427100
H	-1.519500	-3.825000	1.855300
H	-2.083800	-5.182000	0.871400
C	-4.092600	-1.042500	-3.096800
H	-3.270600	-1.536900	-3.616600
H	-4.742900	-1.808600	-2.670400
H	-4.675500	-0.491500	-3.843000
C	-2.487900	1.434600	-2.845800
H	-2.017500	2.234900	-2.274100
H	-1.689200	0.906000	-3.372400
H	-3.143400	1.891800	-3.594900
C	-5.075900	1.024000	-1.210400
H	-5.552200	1.540200	-2.050800
H	-5.774600	0.265000	-0.849600
H	-4.931300	1.749200	-0.409600
C	-5.081300	-0.389800	2.055500
H	-5.443200	-0.417600	3.089400
H	-5.478700	0.513700	1.589800
H	-5.499600	-1.248800	1.530900
C	-2.778200	1.254700	2.956900
H	-1.703400	1.398700	3.070600
H	-3.189700	2.119500	2.434900
H	-3.226300	1.227300	3.956000
C	-2.655600	-1.716700	3.296300
H	-1.569700	-1.832700	3.312900
H	-2.985700	-1.448000	4.305200
H	-3.092100	-2.687000	3.052200

(2-Dipp)Si(NDipp)Si(SiMe$_3$)$_3$

123

Si	-0.241900	-0.166000	0.552700
Si	2.074700	-0.673100	0.022500
Si	3.526500	0.228700	1.701100
Si	2.613500	-3.021500	0.147300
Si	2.885500	-0.259800	-2.202000
N	-0.702100	1.627800	0.117400
N	-1.719200	3.481300	1.189700
N	-0.141200	-0.357300	3.481100
N	-1.301500	-1.327900	0.201700
C	-0.314600	0.406600	2.403200
C	-0.747800	1.712000	2.479700
H	-1.094800	2.171700	3.393400
C	-1.050200	2.309500	1.229500
C	-0.042800	-1.795500	3.395300
H	-0.935800	-2.263700	3.823900
H	0.831300	-2.154900	3.943300
H	0.019600	-2.096900	2.353000
C	-0.327900	0.179000	4.809500
H	0.179700	1.140800	4.905900
H	0.099700	-0.512200	5.535800
H	-1.390600	0.315500	5.044200
C	-1.842400	4.293600	2.379700
H	-2.040800	5.322600	2.076700
H	-0.915100	4.286500	2.950600
H	-2.666200	3.962400	3.023900
C	-2.639400	3.824200	0.123600
H	-3.565700	4.187100	0.576200
H	-2.878400	2.946800	-0.466700
H	-2.242500	4.597300	-0.540200
C	-0.552200	2.291600	-1.144600
C	-1.294600	1.849400	-2.259600

C	-1.081900	2.458100	-3.492600
H	-1.639200	2.103500	-4.352300
C	-0.215700	3.522300	-3.636600
H	-0.075600	3.993000	-4.603000
C	0.455100	3.993000	-2.525400
H	1.119300	4.843300	-2.631500
C	0.324100	3.395400	-1.274900
C	1.122300	4.019700	-0.140900
H	0.984100	3.422100	0.761700
C	2.621000	4.056400	-0.429800
H	2.840200	4.608700	-1.346300
H	3.035600	3.056500	-0.538600
H	3.144900	4.559800	0.387100
C	0.654200	5.448100	0.148300
H	0.888900	6.108200	-0.690800
H	1.166300	5.843500	1.029700
H	-0.419000	5.507900	0.323000
C	-2.391900	0.807400	-2.178500
H	-2.496600	0.497700	-1.138000
C	-3.735900	1.373800	-2.644000
H	-4.007100	2.299900	-2.131200
H	-4.523900	0.640500	-2.456700
H	-3.730100	1.586600	-3.716300
C	-2.065900	-0.441800	-2.987800
H	-2.898600	-1.145600	-2.933700
H	-1.183500	-0.943100	-2.591900
H	-1.890800	-0.199100	-4.040400
C	-2.535000	-1.880600	0.039700
C	-3.741600	-1.308800	0.550100
C	-4.968900	-1.908400	0.295500
H	-5.869400	-1.449800	0.691800
C	-5.081000	-3.077200	-0.434500
H	-6.049900	-3.524500	-0.624500
C	-3.919200	-3.668800	-0.896900
H	-3.983800	-4.602000	-1.448800
C	-2.670200	-3.109700	-0.674100
C	-1.452000	-3.858600	-1.157300
H	-0.602300	-3.204800	-0.945100
C	-1.482200	-4.154700	-2.654800
H	-1.570200	-3.240800	-3.244400
H	-2.325400	-4.800600	-2.915400
H	-0.571100	-4.674400	-2.967500
C	-1.275900	-5.158800	-0.373000
H	-1.270400	-4.976100	0.703800
H	-0.341800	-5.661500	-0.641900
H	-2.097700	-5.850400	-0.581500
C	-3.714500	-0.096200	1.449200
H	-2.762800	0.406000	1.277500
C	-3.748500	-0.523400	2.916300
H	-3.644400	0.338900	3.584000
H	-2.947400	-1.232000	3.134300
H	-4.696600	-1.017600	3.147800
C	-4.823400	0.915200	1.176900
H	-4.674300	1.814700	1.783100
H	-5.809400	0.520400	1.435400
H	-4.851700	1.209200	0.125600
C	3.064900	1.922200	2.387600
H	3.233100	2.723000	1.669500
H	3.699800	2.118300	3.258600
H	2.023100	1.965600	2.711700
C	5.285300	0.377900	1.037500
H	5.330800	1.060800	0.185200
H	5.691600	-0.584100	0.720700
H	5.938700	0.777800	1.819900
C	3.564400	-0.870800	3.238500
H	4.388000	-0.546000	3.883000
H	3.699900	-1.931900	3.030700
H	2.638400	-0.750500	3.805500
C	4.466400	-3.245700	0.459000
H	5.086700	-2.782600	-0.308800
H	4.673800	-4.321400	0.446500
H	4.787600	-2.862600	1.428500
C	2.261400	-3.950000	-1.454200
H	1.205900	-3.927200	-1.723000
H	2.546900	-4.997300	-1.308300
H	2.832500	-3.566900	-2.300400
C	1.764900	-3.997500	1.515300
H	0.679300	-3.993600	1.414200
H	2.026900	-3.634000	2.510200
H	2.100600	-5.037300	1.442900
C	4.541000	-1.131200	-2.466400
H	4.878900	-0.886900	-3.479400
H	4.494200	-2.216700	-2.388000
H	5.302000	-0.770400	-1.770900
C	3.249600	1.512700	-2.708200
H	2.379600	2.164500	-2.639800
H	3.564900	1.485300	-3.757300
H	4.067200	1.952700	-2.133800
C	1.656300	-0.915300	-3.465200
H	0.805000	-0.237500	-3.552100
H	1.274600	-1.908400	-3.226100
H	2.144000	-0.965300	-4.444400

$Si(SiMe_3)_3$ system– transition state

123

Si	0.193300	-0.190700	0.327000
Si	-2.134600	-0.860900	0.027200
Si	-3.067800	-0.368800	2.201300
Si	-2.662200	-3.189900	-0.252600
Si	-3.464100	0.069800	-1.764200
N	0.473400	1.604100	0.195700
N	1.703500	3.333700	1.336000
N	1.212000	-1.217500	2.927800
N	1.702600	-0.998600	0.331500
C	1.233000	-0.318500	1.867500
C	1.728600	1.032200	2.110700
H	2.418700	1.269100	2.907500
C	1.328600	1.994100	1.237700
C	0.509500	-2.455900	2.714400
H	1.081400	-3.165900	2.102800
H	0.293400	-2.925400	3.678300
H	-0.434800	-2.259600	2.206500
C	2.445500	-1.415800	3.664000
H	2.882200	-0.460000	3.950900

H	2.226000	-1.967000	4.581600
H	3.190300	-1.985600	3.089200
C	2.172500	3.766600	2.630800
H	2.212200	4.858900	2.639200
H	1.483900	3.436900	3.409500
H	3.180800	3.393600	2.872100
C	2.485300	3.912900	0.257800
H	3.558200	3.715500	0.388600
H	2.175100	3.517800	-0.705800
H	2.336100	4.996400	0.239400
C	-0.027200	2.513200	-0.778700
C	0.368800	2.329800	-2.124200
C	-0.174900	3.154700	-3.104700
H	0.108500	3.007400	-4.140800
C	-1.030400	4.190900	-2.777200
H	-1.433500	4.834500	-3.551400
C	-1.347200	4.413100	-1.449800
H	-1.999000	5.241500	-1.192800
C	-0.874100	3.587500	-0.432300
C	-1.298000	3.906800	0.988600
H	-0.798200	3.200400	1.650600
C	-2.804700	3.756600	1.184300
H	-3.362200	4.446000	0.544300
H	-3.137200	2.745900	0.950500
H	-3.075400	3.972400	2.221800
C	-0.865400	5.314000	1.400400
H	-1.396400	6.077900	0.825600
H	-1.090600	5.484300	2.457100
H	0.204400	5.457200	1.250400
C	1.447400	1.331300	-2.510200
H	1.982900	1.071700	-1.593200
C	2.462400	1.931200	-3.483400
H	2.880600	2.868900	-3.110000
H	3.285000	1.229000	-3.639600
H	2.019700	2.128800	-4.463100
C	0.898900	0.031900	-3.094000
H	1.714000	-0.675600	-3.264600
H	0.172900	-0.447500	-2.430900
H	0.395600	0.211900	-4.048100
C	2.874400	-1.554700	-0.202100
C	4.127800	-0.878500	-0.220000
C	5.265500	-1.530600	-0.686600
H	6.212100	-1.001500	-0.665500
C	5.230300	-2.816400	-1.185100
H	6.129800	-3.299300	-1.550400
C	4.013100	-3.465000	-1.212800
H	3.961700	-4.471300	-1.615700
C	2.849800	-2.877300	-0.728300
C	1.597800	-3.722700	-0.807500
H	0.789400	-3.153400	-0.342600
C	1.219900	-4.008000	-2.261400
H	1.000900	-3.087400	-2.807400
H	2.036600	-4.512700	-2.784100
H	0.345100	-4.660700	-2.316000
C	1.772800	-5.042300	-0.051800
H	2.041900	-4.876800	0.994200
H	0.856400	-5.637400	-0.080800
H	2.564400	-5.649000	-0.498400
C	4.330800	0.540900	0.261000
H	3.345400	0.975600	0.417900
C	5.071100	0.574000	1.598000
H	5.153800	1.599600	1.972500
H	4.561800	-0.025100	2.353400
H	6.084600	0.176400	1.488500
C	5.079500	1.399200	-0.759100
H	5.134100	2.436700	-0.418300
H	6.108300	1.059700	-0.902000
H	4.588700	1.387700	-1.733300
C	-1.984300	0.781600	3.234800
H	-1.827600	1.749000	2.759500
H	-2.476800	0.952400	4.198000
H	-1.004900	0.336000	3.426300
C	-4.801600	0.380300	2.014500
H	-4.798100	1.323600	1.467100
H	-5.482000	-0.305300	1.503700
H	-5.212500	0.572700	3.010900
C	-3.297100	-1.934600	3.250400
H	-3.772700	-1.634400	4.190300
H	-3.939800	-2.676400	2.775300
H	-2.345900	-2.406400	3.501200
C	-4.502500	-3.443200	0.201600
H	-5.013600	-2.536700	0.525000
H	-5.050900	-3.839900	-0.656300
H	-4.576600	-4.175300	1.010000
C	-2.456900	-3.716200	-2.061100
H	-1.461800	-3.497400	-2.447600
H	-2.626900	-4.794000	-2.149900
H	-3.184300	-3.210900	-2.700000
C	-1.728400	-4.399100	0.861900
H	-0.647700	-4.354100	0.751200
H	-1.974400	-4.225300	1.911200
H	-2.054800	-5.413400	0.608400
C	-5.118000	-0.860400	-1.858100
H	-5.691700	-0.401300	-2.670500
H	-5.017800	-1.922300	-2.081100
H	-5.704600	-0.756700	-0.943300
C	-3.959100	1.883000	-1.612400
H	-3.102800	2.552500	-1.551800
H	-4.525900	2.140700	-2.513700
H	-4.607100	2.061000	-0.752600
C	-2.618500	-0.133700	-3.444100
H	-1.834700	0.613900	-3.570400
H	-2.181300	-1.122200	-3.592700
H	-3.367900	0.027500	-4.225900