A complete series of N-heterocyclic tetrylenes (Si – Pb) with a 1,1'-ferrocenediyl backbone enabled by 1,3,2-diazaborolyl N-substituents†

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A – Experimental Section S2

Crystallographic data S2

Plots of NMR spectra S3

B – Computational Details S15

Frontier orbital discussion S15

Cartesian coordinates for the optimized structures S20

C – References S25

A – Experimental Section

Crystallographic data

Table S1. X-ray crystallographic details.

	1H_2	[**1**Li_2(TMEDA)$_2$]·1.5 C_6H_6	**1**Si·C_6H_6	**1**Ge	**1**Sn	**1**Pb	**1**Si(OH)H
Empirical formula	$C_{62}H_{82}B_2FeN_6$	$C_{83}H_{121}B_2FeLi_2N_{10}$	$C_{68}H_{86}B_2FeN_6Si$	$C_{62}H_{80}B_2FeGeN_6$	$C_{62}H_{80}B_2FeN_6Sn$	$C_{62}H_{80}B_2FeN_6Pb$	$C_{62}H_{82}B_2FeN_6OSi$
Formula weight	988.80	1349.23	1092.98	1059.38	1105.48	1193.98	1032.89
Crystal system	orthorhombic	triclinic	monoclinic	monoclinic	triclinic	triclinic	monoclinic
Space group	*Aea*2	*P*-1	$P2_1/c$	$P2_1/c$	*P*-1	*P*-1	$P2_1/c$
a/Å	8.9740(4)	13.5366(7)	20.8000(8)	20.4144(11)	10.6958(3)	10.7135(5)	12.2033(8)
b/Å	29.2515(17)	16.4231(9)	22.0814(6)	21.9544(8)	14.2662(4)	14.3200(7)	23.7917(17)
c/Å	21.3053(9)	19.0854(10)	14.5347(6)	14.6481(7)	20.2598(6)	20.0251(10)	19.6371(12)
α/°	90	94.408(4)	90	90	109.087(2)	108.398(4)	90
β/°	90	108.594(4)	102.468(3)	104.662(4)	100.421(3)	101.468(4)	92.103(5)
γ/°	90	96.918(4)	90	90	94.724(2)	94.946(4)	90
Volume/Å^3	5592.7(5)	3962.1(4)	6518.3(4)	6351.3(5)	2839.77(15)	2820.1(2)	5697.5(7)
Z	4	2	4	4	2	2	4
ρ_{calcd}/g cm^{-3}	1.174	1.131	1.114	1.108	1.293	1.406	1.204
μ/mm^{-1}	2.485	1.886	2.348	2.704	5.870	3.282	0.332
F(000)	2128.0	1460.0	2344.0	2248.0	1160.0	1224.0	2216.0
Crystal size/mm^3	0.13 × 0.12 × 0.04	0.10 × 0.09 × 0.09	0.28 × 0.19 × 0.03	0.17 × 0.10 × 0.03	0.24 × 0.11 × 0.02	0.17 × 0.11 × 0.04	0.43 × 0.21 × 0.05
Radiation used	Cu K_α (λ = 1.54186 Å)	Cu K_α (λ = 1.54186 Å)	Cu K_α (λ = 1.54186 Å)	Cu K_α (λ = 1.54186 Å)	Cu K_α (λ = 1.54186 Å)	Mo K_α (λ = 0.71073 Å)	Mo K_α (λ = 0.71073 Å)
2*Θ* range for data collection/°	6.042 to 140.918	5.462 to 142.496	5.912 to 142.034	6.02 to 137.986	6.634 to 141.846	2.208 to 51.704	2.69 to 52.77
Index ranges	-7 ≤ h ≤ 10 -33 ≤ k ≤ 35 -25 ≤ l ≤ 12	-14 ≤ h ≤ 16 -16 ≤ k ≤ 20 -19 ≤ l ≤ 23	-25 ≤ h ≤ 24 -25 ≤ k ≤ 13 -17 ≤ l ≤ 16	-24 ≤ h ≤ 24 -26 ≤ k ≤ 19 -17 ≤ l ≤ 11	-7 ≤ h ≤ 12 -16 ≤ k ≤ 17 -24 ≤ l ≤ 21	-12 ≤ h ≤ 13 -17 ≤ k ≤ 17 -24 ≤ l ≤ 24	-15 ≤ h ≤ 14 -27 ≤ k ≤ 29 -24 ≤ l ≤ 24
Refl. collected	10412	34905	27165	23235	22454	19459	25310
Independent refl.	3424 [R_{int} = 0.0902]	14695 [R_{int} = 0.0432]	11825 [R_{int} = 0.0533]	11270 [R_{int} = 0.0870]	10527 [R_{int} = 0.0308]	10646 [R_{int} = 0.0605]	11500 [R_{int} = 0.0687]
Data/restr./param.	3424/1/330	14695/57/974	11825/0/719	11270/0/665	10527/0/665	10646/0/666	11500/0/693
Goodness-of-fit on F^2	1.055	1.021	1.025	1.035	1.035	1.093	1.020
Final *R* indexes [$I > 2\sigma(I)$]	R_1 = 0.0738 wR_2 = 0.1533	R_1 = 0.0549 wR_2 = 0.1093	R_1 = 0.0650 wR_2 = 0.1446	R_1 = 0.0748 wR_2 = 0.1752	R_1 = 0.0407 wR_2 = 0.1039	R_1 = 0.0551 wR_2 = 0.1463	R_1 = 0.0850 wR_2 = 0.2209
Final *R* indexes [all data]	R_1 = 0.1146 wR_2 = 0.1736	R_1 = 0.0930 wR_2 = 0.1273	R_1 = 0.1112 wR_2 = 0.1667	R_1 = 0.1347 wR_2 = 0.2146	R_1 = 0.0491 wR_2 = 0.1098	R_1 = 0.0654 wR_2 = 0.1575	R_1 = 0.1209 wR_2 = 0.2537
Largest diff. peak/hole / e Å^{-3}	0.76/-0.34	0.72/-0.61	0.70/-0.55	0.72/-0.83	1.05/-1.11	1.67/-2.38	1.28/-0.82
Flack parameter	0.362(15)						
CCDC No.	2289080	2289081	2289082	2289083	2289084	2289085	2289086

Plots of NMR spectra

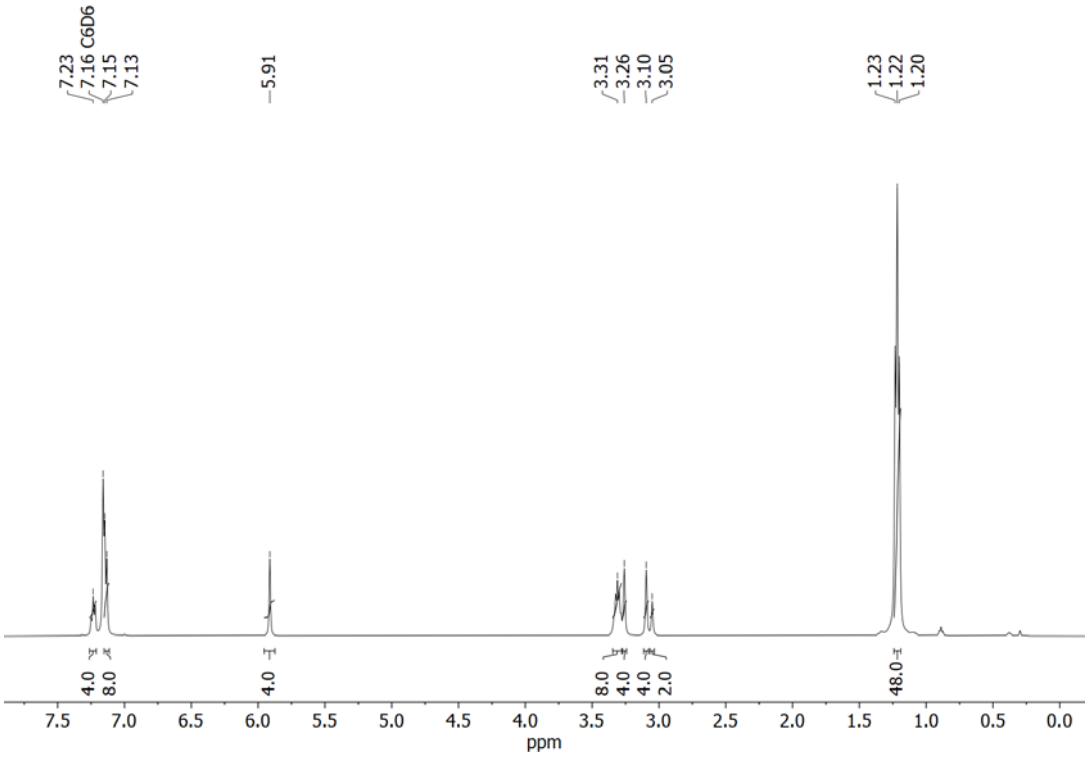


Figure S1: ^{1}H NMR (C_6D_6, 500 MHz) of **1**H_2.

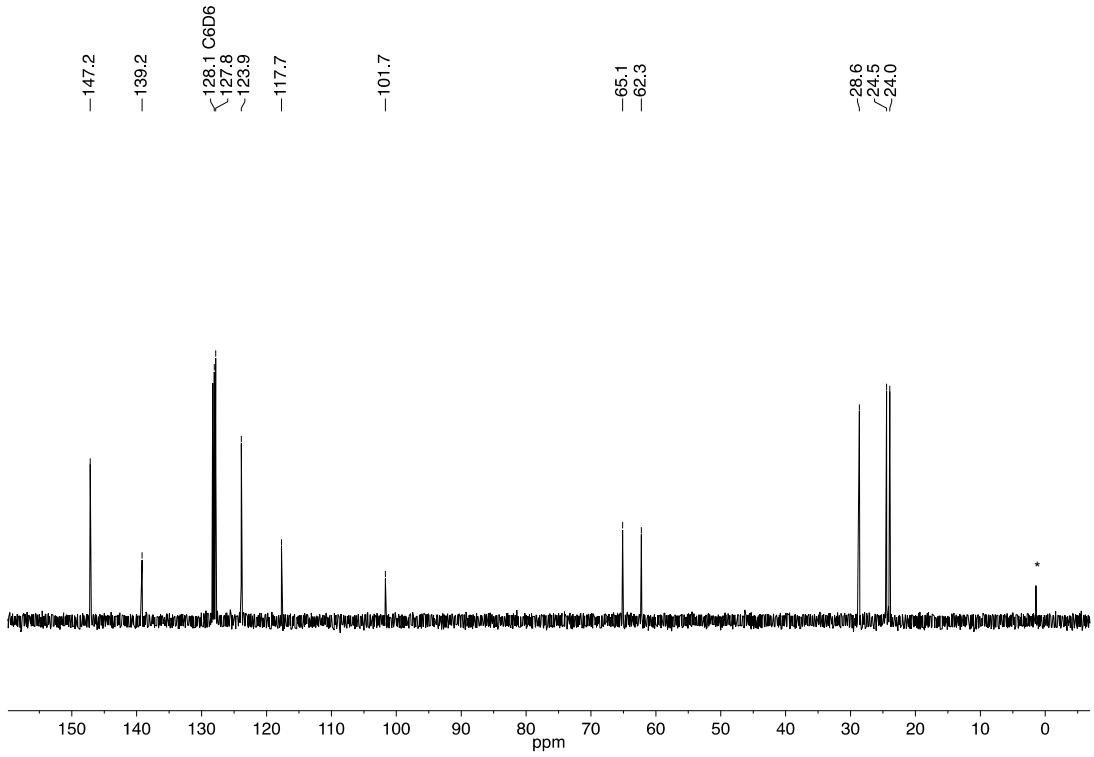


Figure S2: ^{13}C{^{1}H} NMR (C_6D_6, 100 MHz) of **1**H_2. The signal marked (*) belongs to silicon grease.

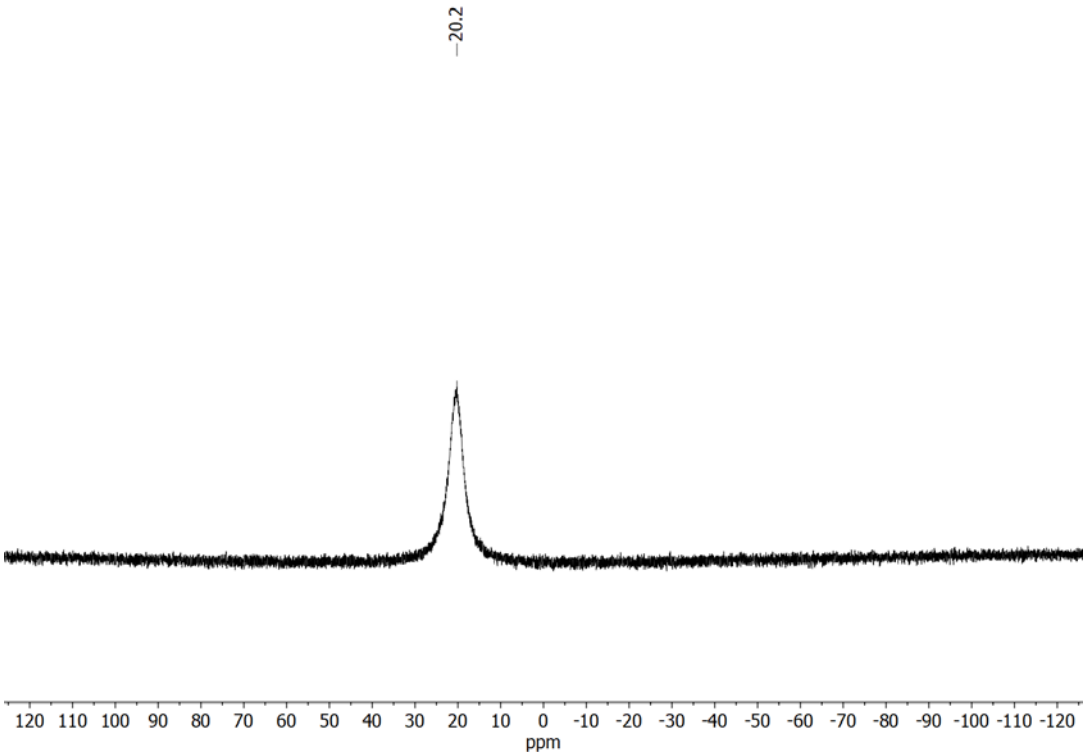


Figure S3: ^{11}B NMR (C_6D_6, 160 MHz) of **1**H_2.

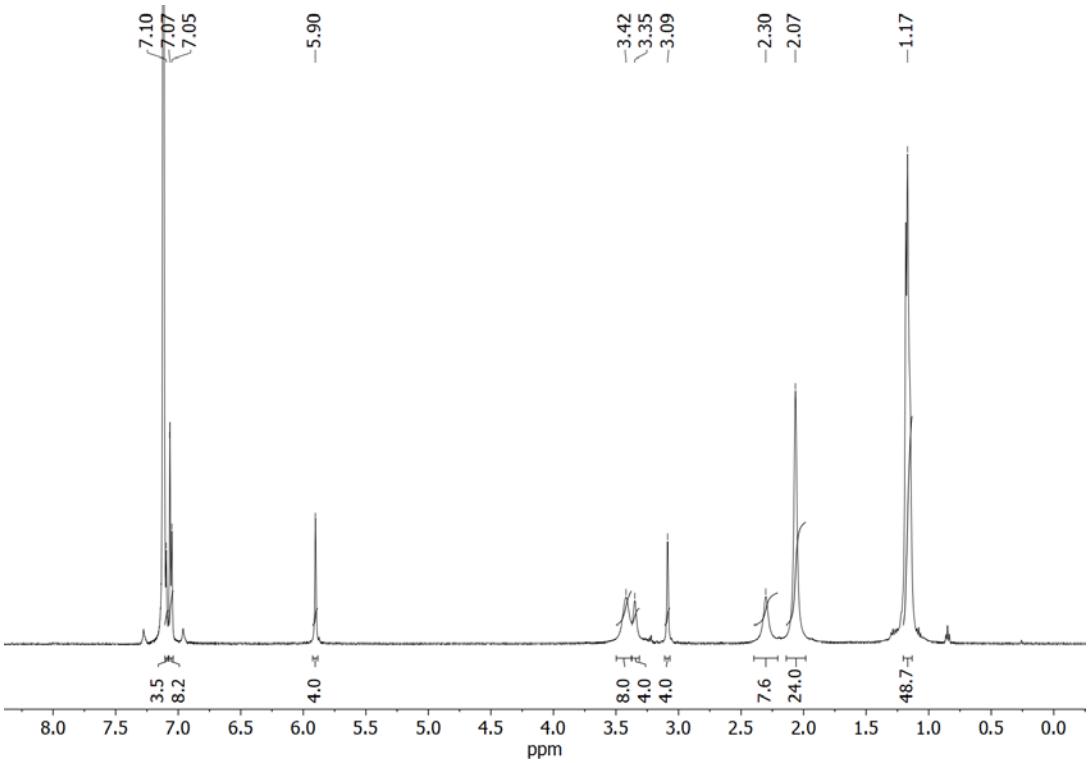


Figure S4: ^{1}H NMR (C_6D_6, 500 MHz) of [**1**Li_2(TMEDA)$_2$].

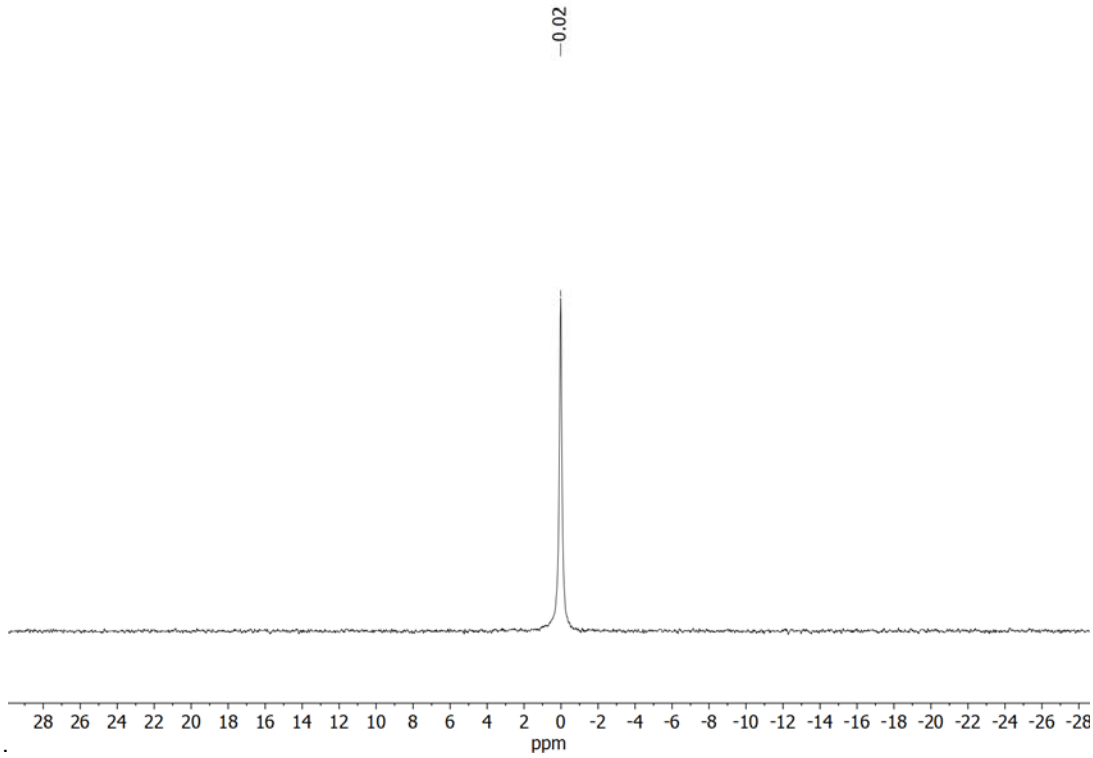


Figure S5: ^{7}Li NMR (C_6D_6, 194 MHz) of [**1**Li_2(TMEDA)$_2$].

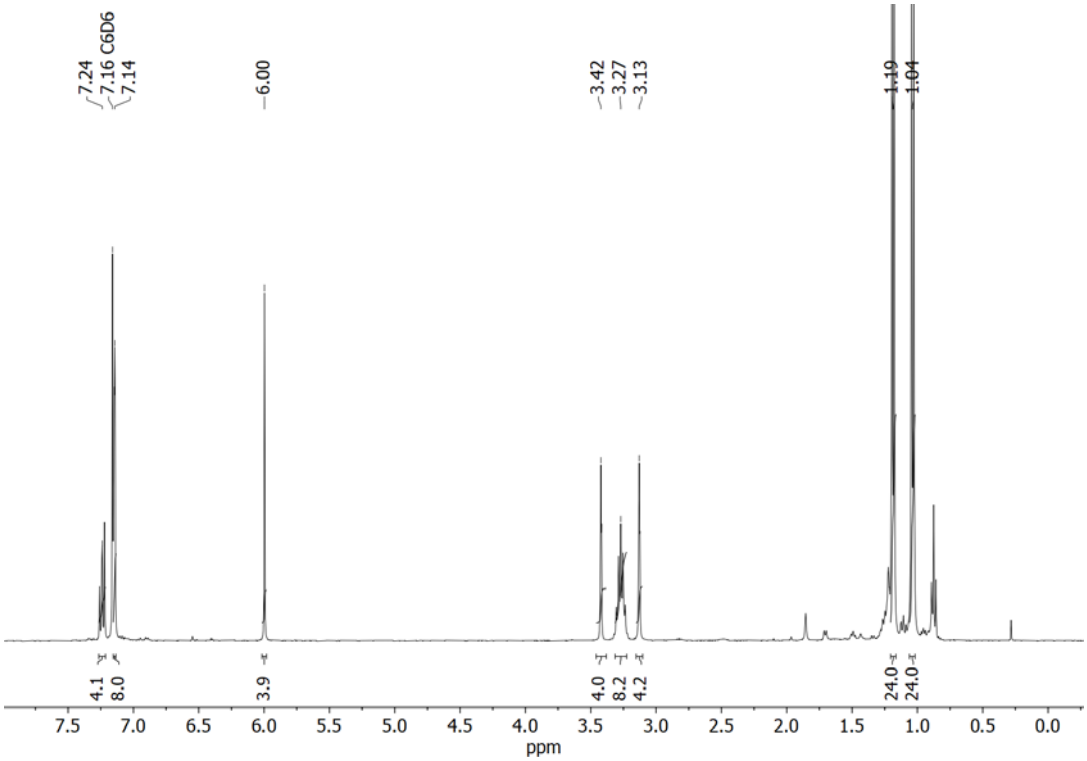


Figure S6: ^{1}H NMR (C_6D_6, 500 MHz) of **1**Si.

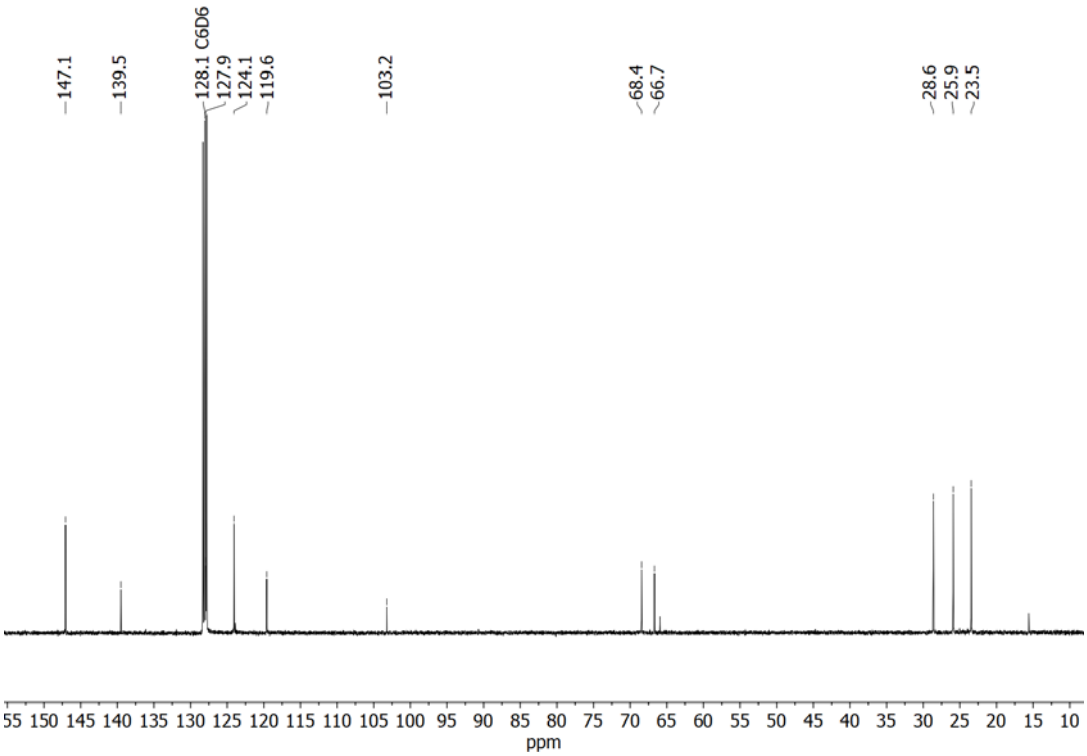


Figure S7: ^{13}C NMR (C_6D_6, 101 MHz) of **1**Si**.**

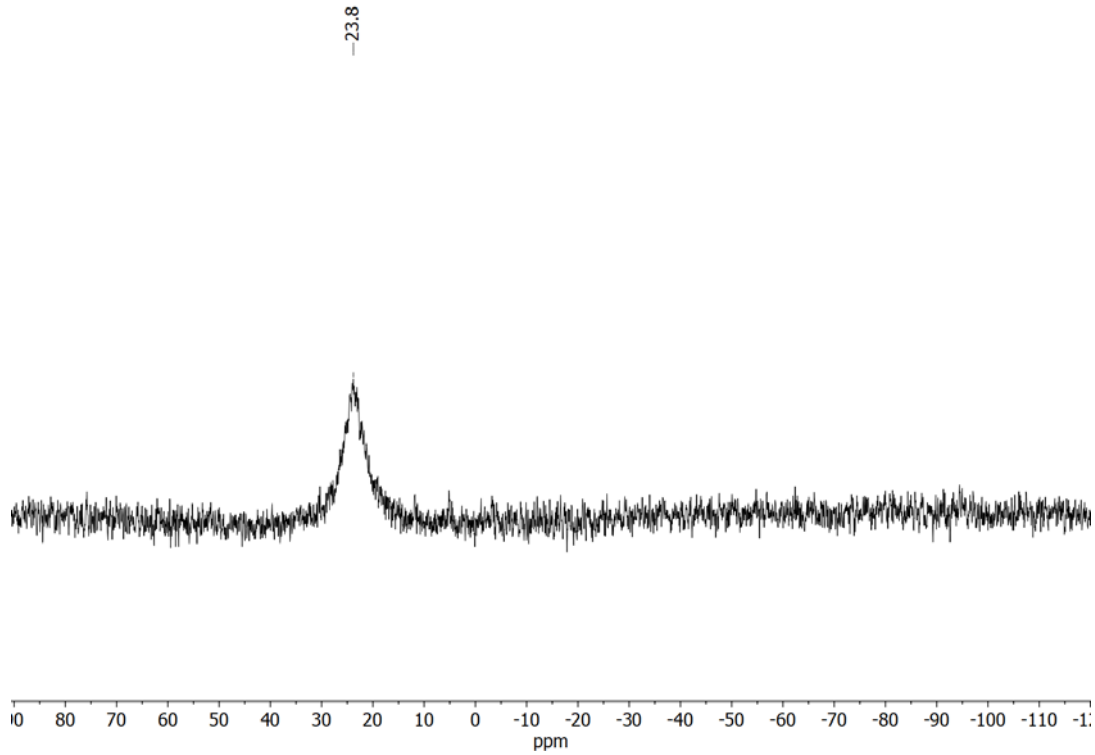


Figure S8: ^{11}B NMR (C_6D_6, 160 MHz) of **1**Si**.**

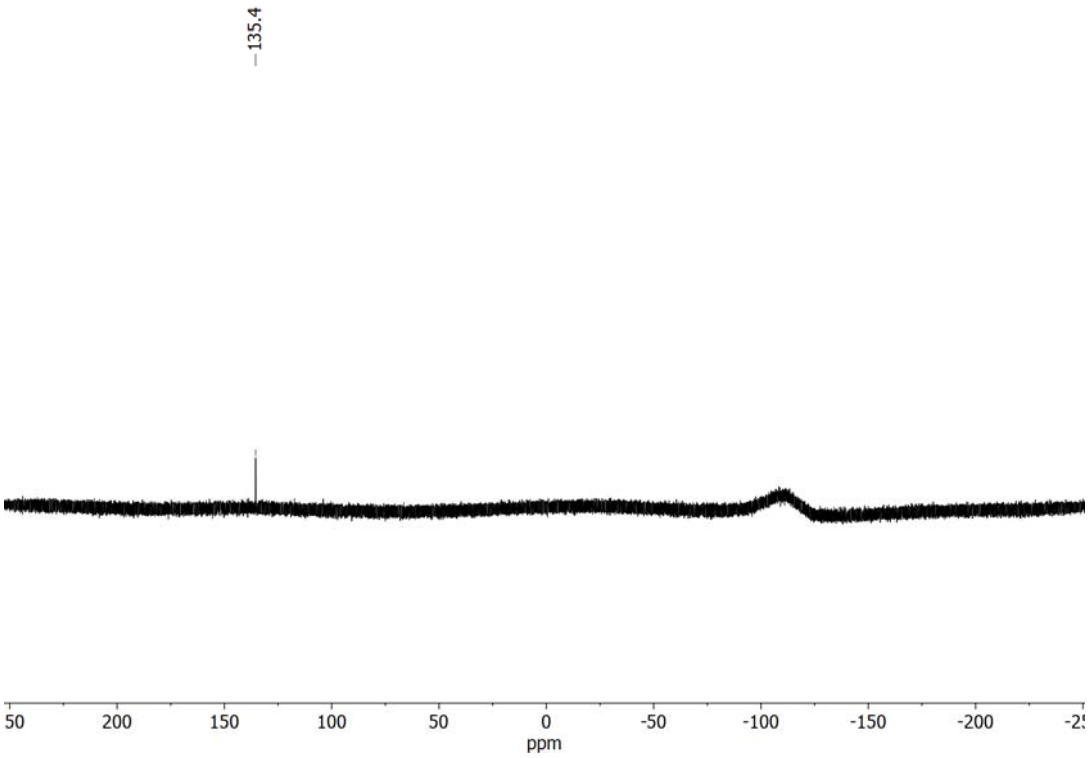


Figure S9: ^{29}Si NMR (C_6D_6, 99 MHz) of **1**Si.

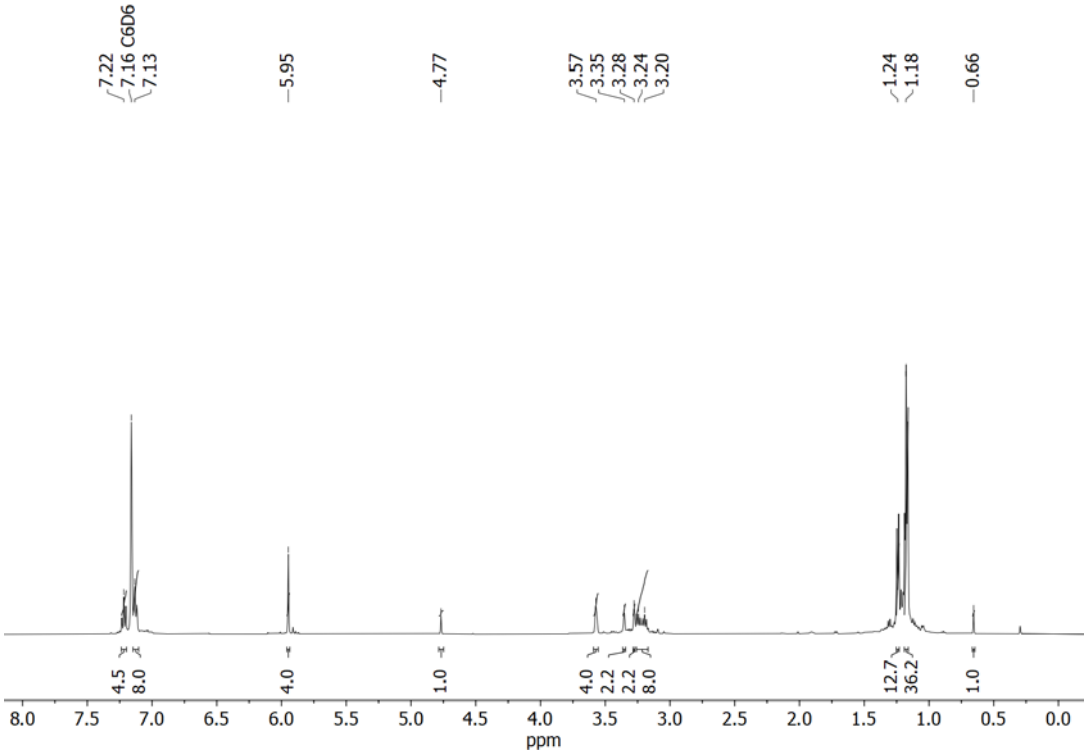


Figure S10: ^{1}H NMR (C_6D_6, 500 MHz) of **1**Si(OH)H.

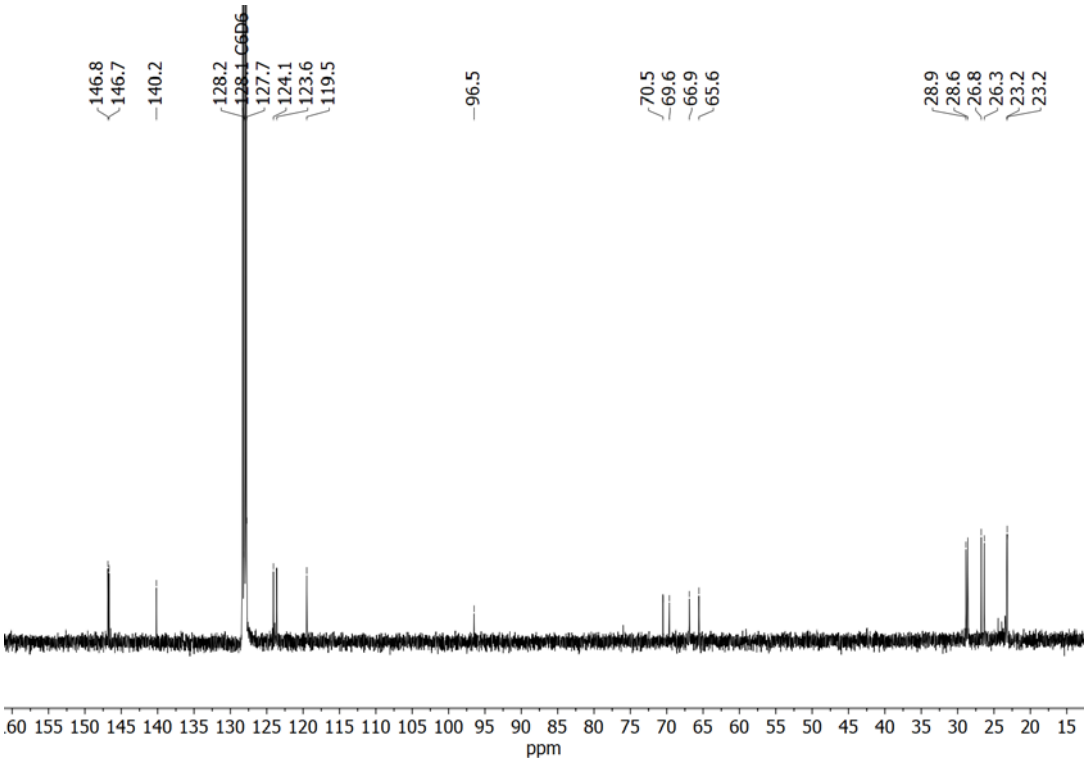


Figure S11: ^{13}C NMR (C_6D_6, 101 MHz) of **1**Si(OH)H.

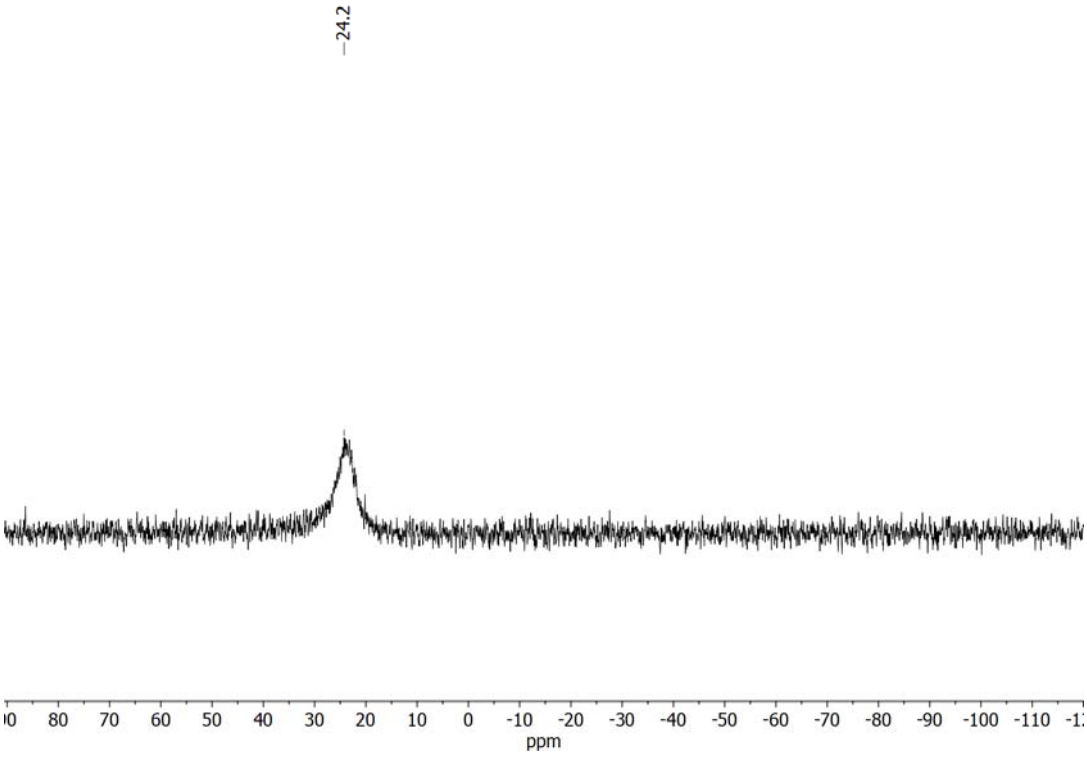


Figure S12: ^{11}B NMR (C_6D_6, 160 MHz) of **1**Si(OH)H.

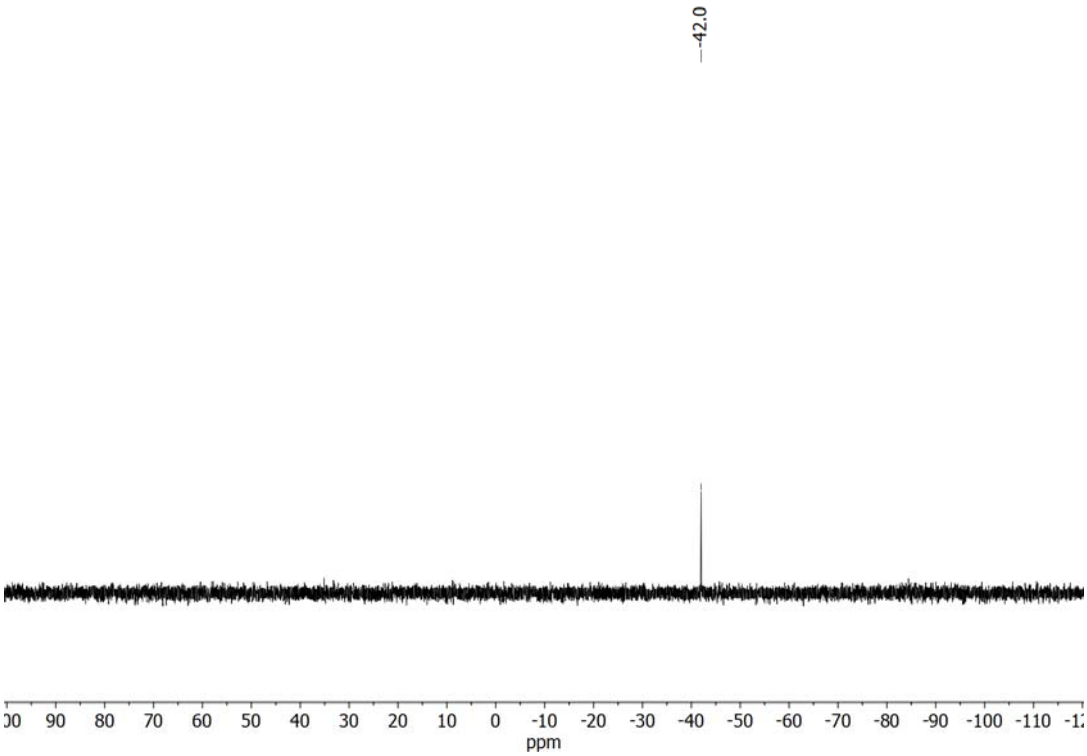


Figure S13: $^{29}Si\{^{1}H\}$ DEPT NMR (C_6D_6, 99 MHz) of **1**Si(OH)H.

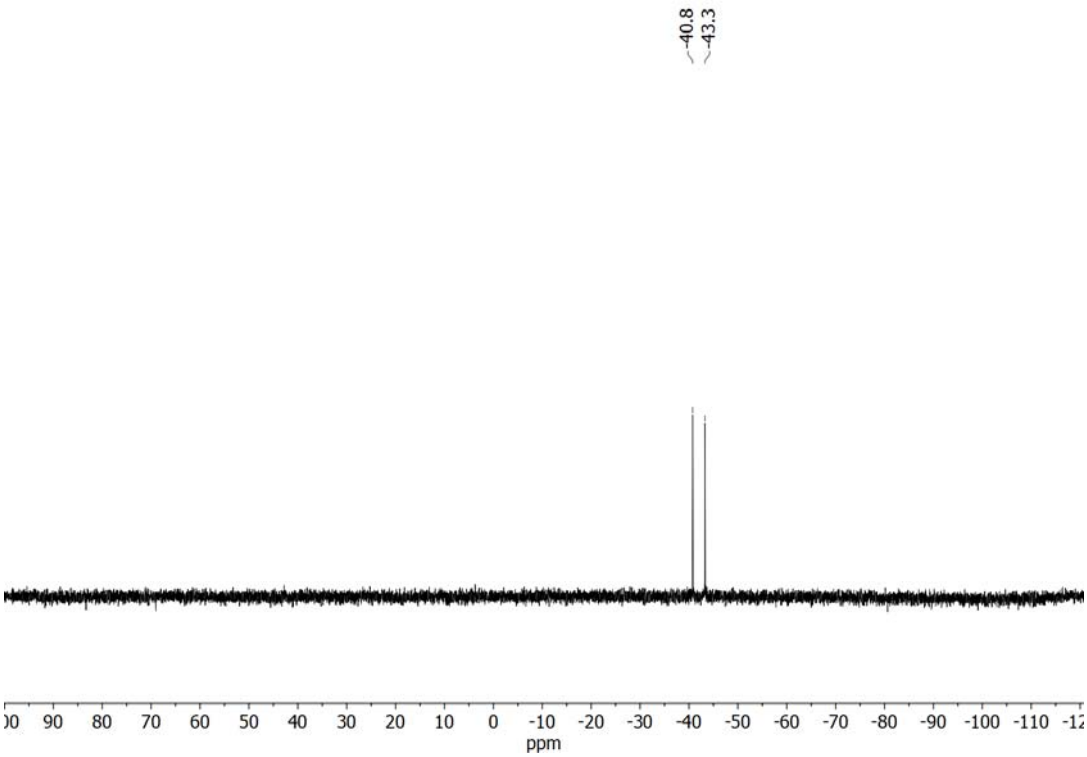


Figure S14: ^{29}Si DEPT NMR (C_6D_6, 99 MHz) of **1**Si(OH)H.

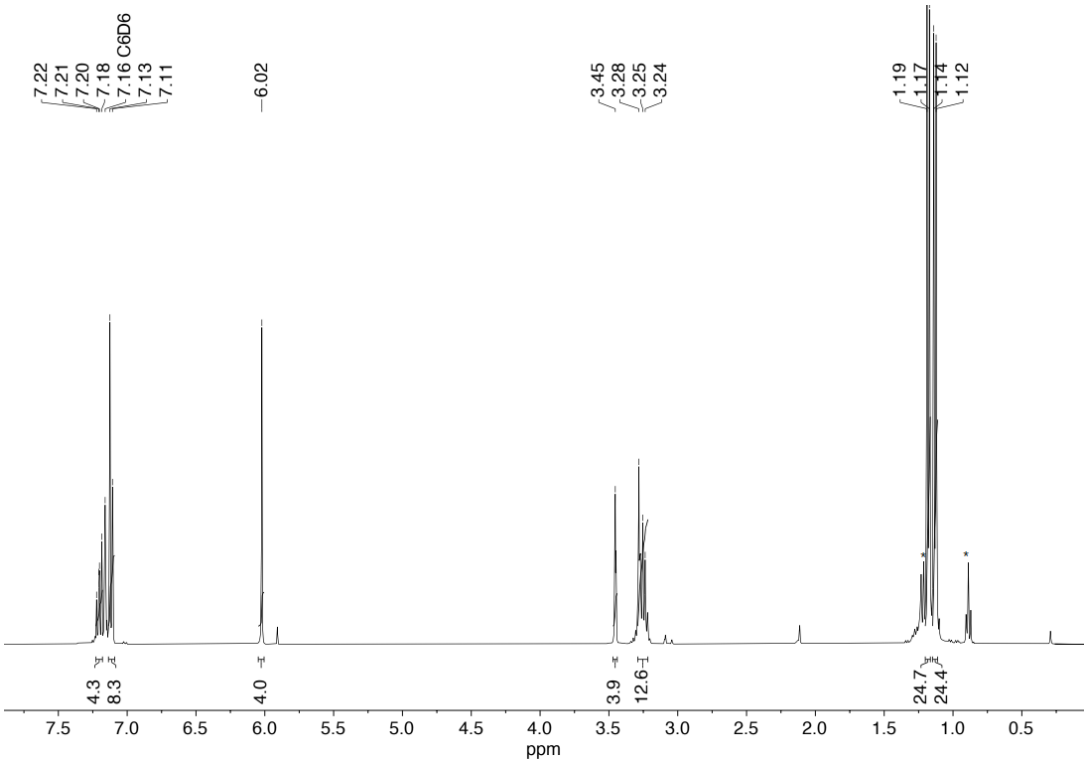


Figure S15: ^{1}H NMR (C_6D_6, 400 MHz) of **1**Ge. The signal marked (*) belongs to trace amounts of *n*-hexane.

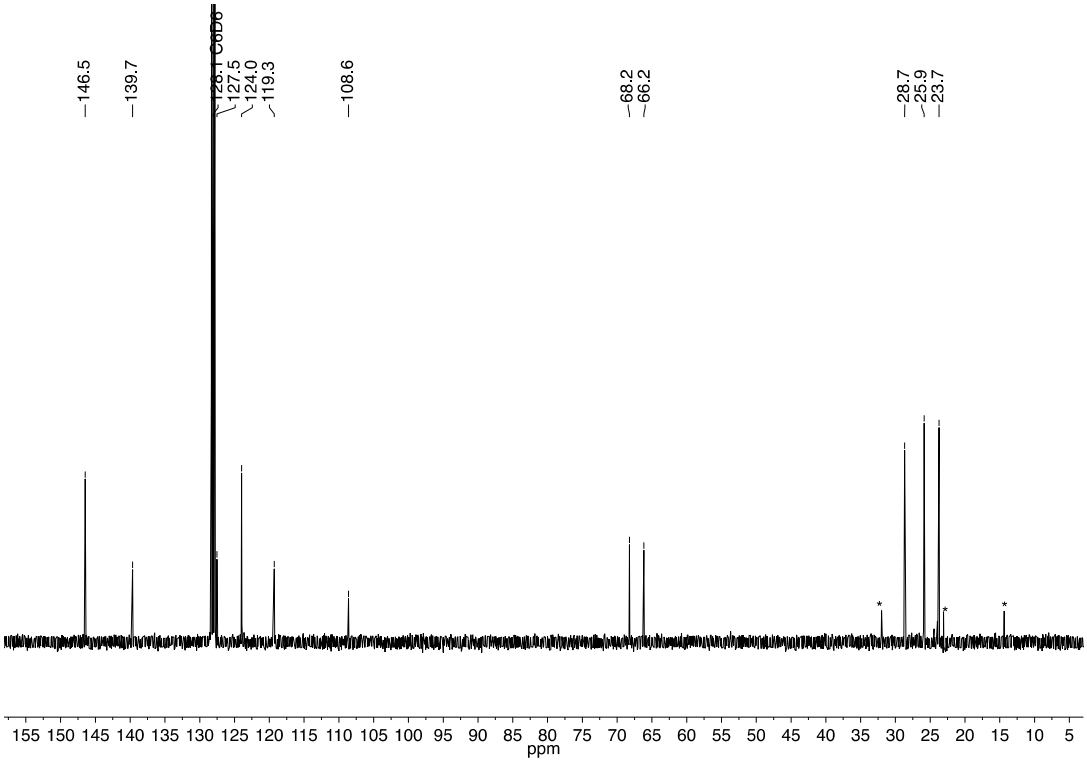


Figure S16: ^{13}C NMR (C_6D_6, 100 MHz) of **1**Ge. The signals marked (*) belong to trace amounts of *n*-hexane.

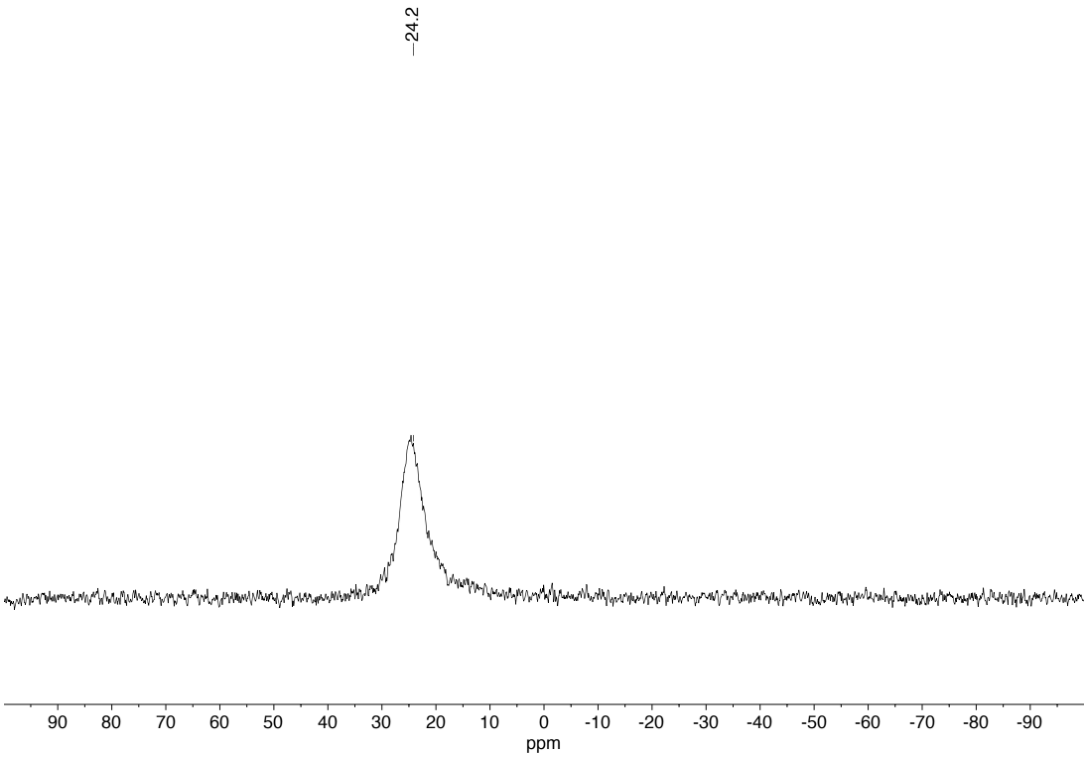


Figure S17: ^{11}B NMR (C_6D_6, 160 MHz) of **1**Ge.

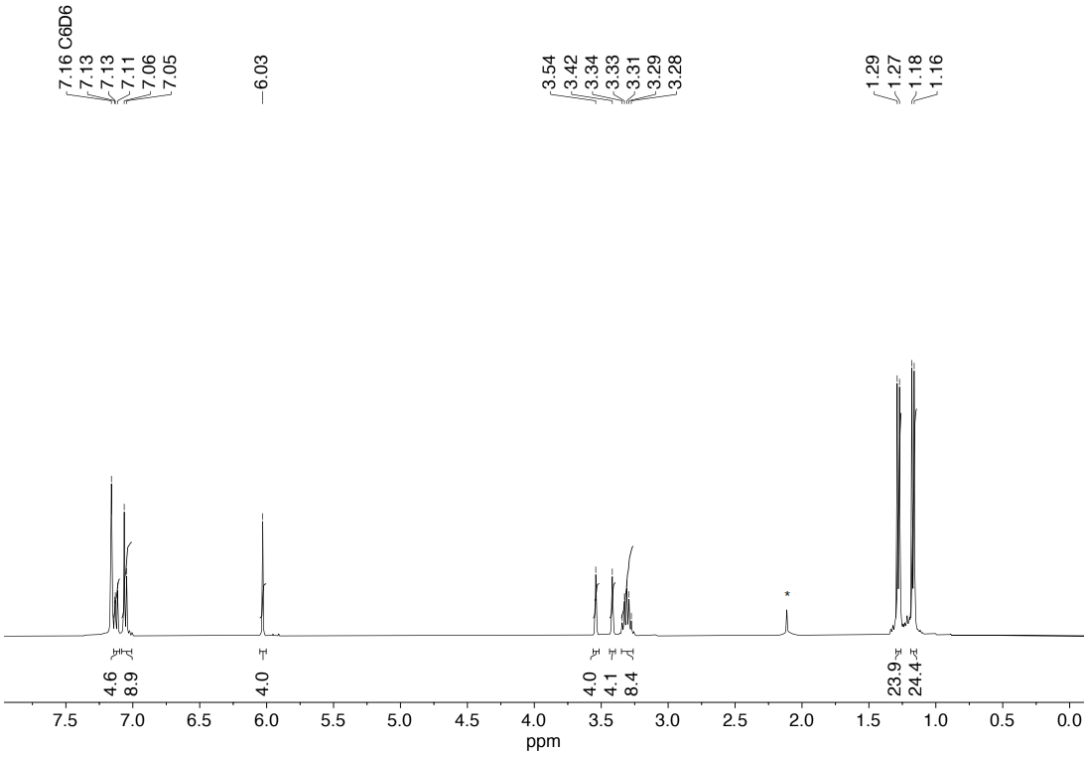


Figure S18: ^{1}H NMR (C_6D_6, 400 MHz) of **1**Sn. The signal marked (*) belongs to trace amounts of toluene.

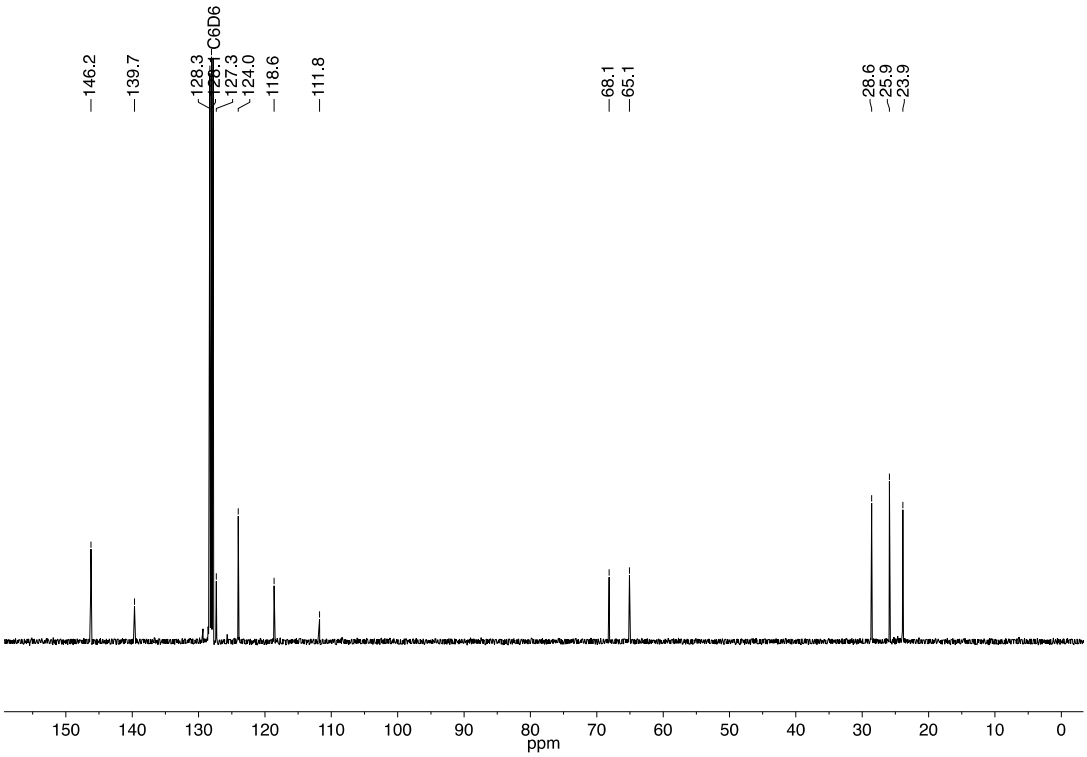


Figure S19: ^{13}C NMR (C_6D_6, 100 MHz) of **1**Sn.

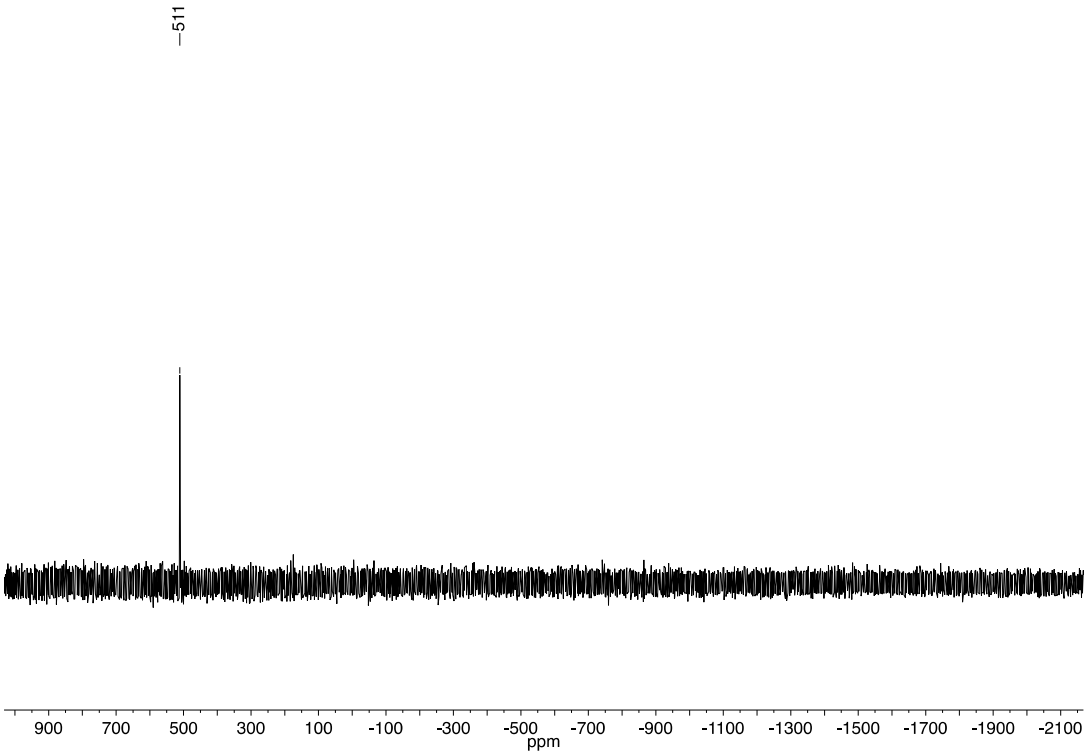


Figure S20: ^{119}Sn NMR (C_6D_6, 186 MHz) of **1**Sn.

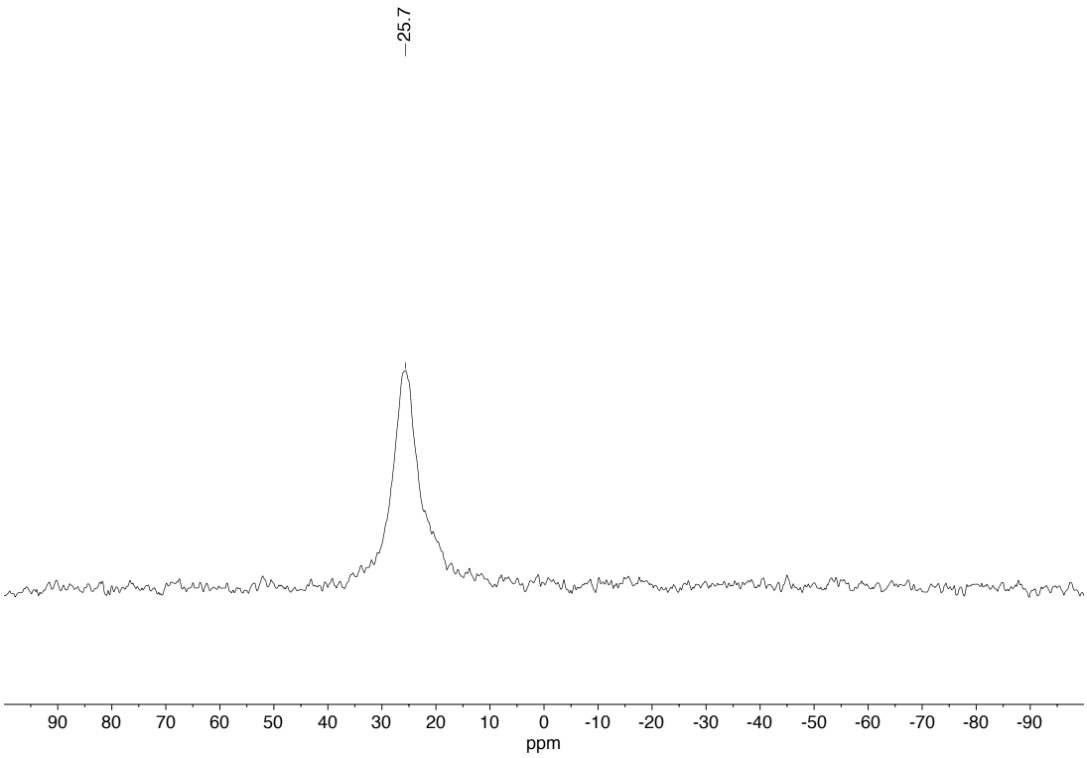


Figure S21: ^{11}B NMR (C_6D_6, 160 MHz) of **1**Sn.

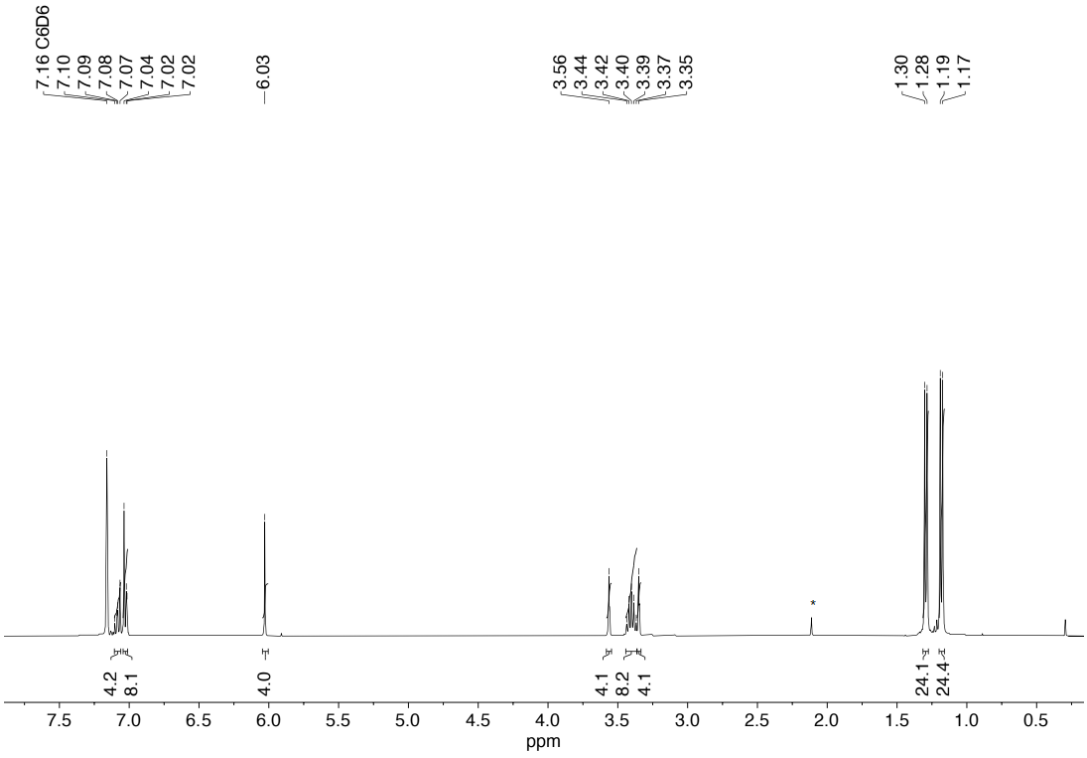


Figure S22: ^{1}H NMR (C_6D_6, 400 MHz) of **1**Pb. The signal marked (*) belongs to trace amounts of toluene.

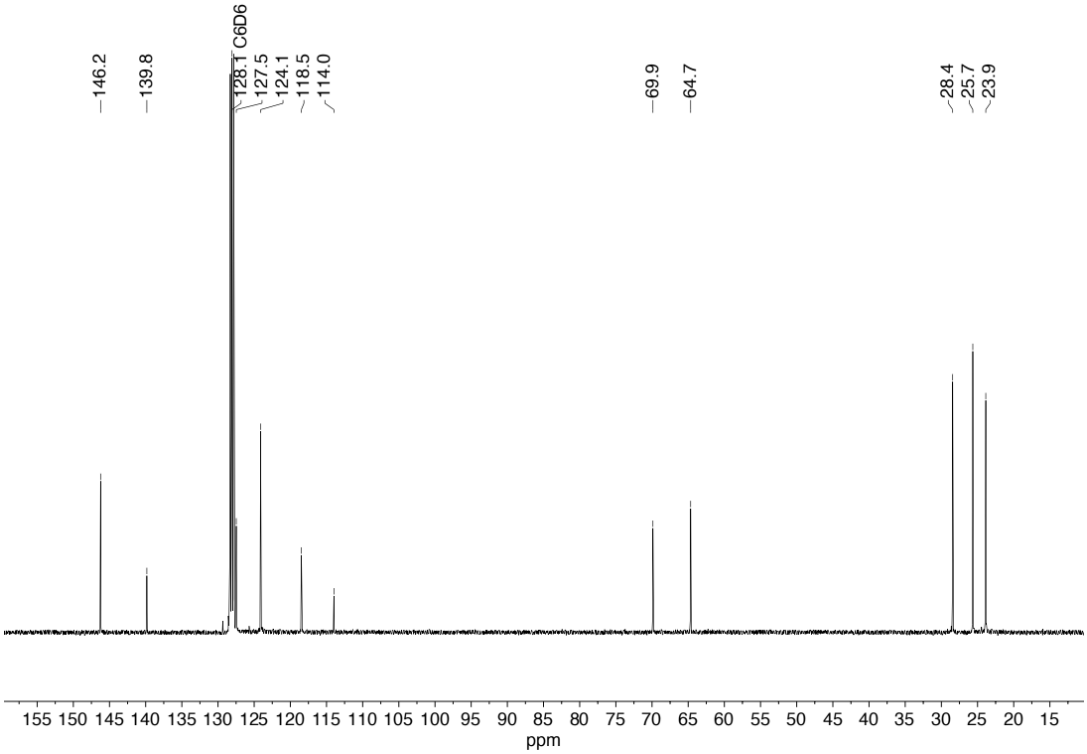


Figure S23: ^{13}C NMR (C_6D_6, 100 MHz) of **1**Pb.

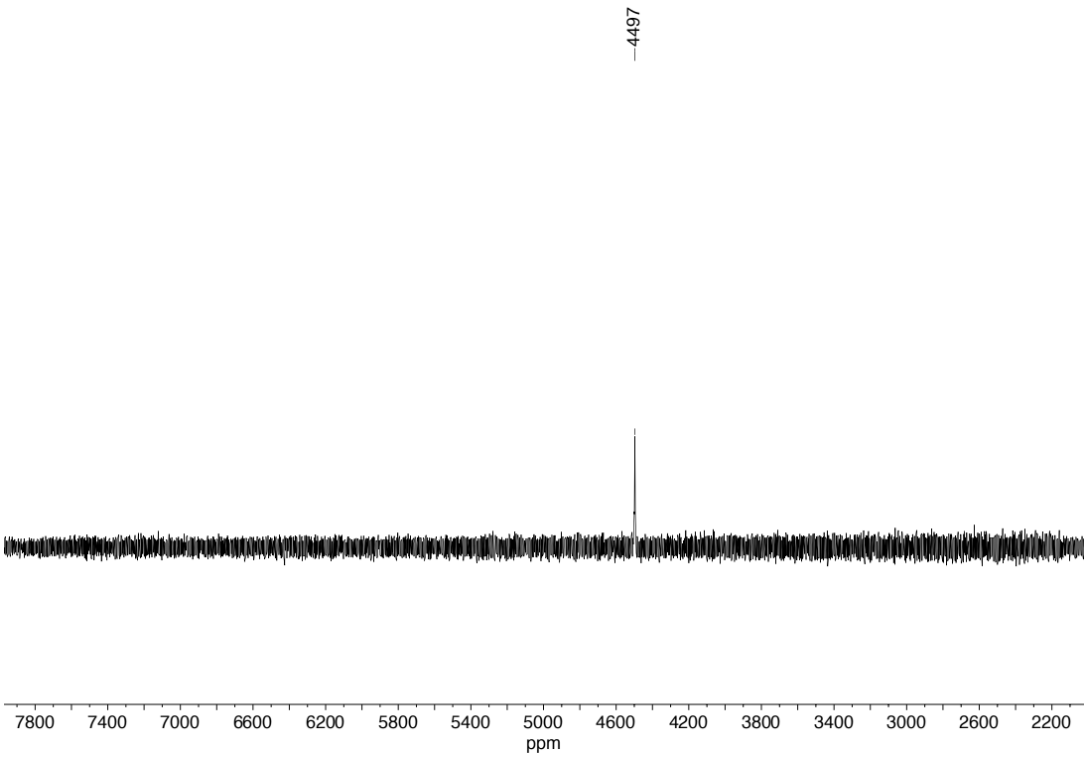


Figure S24: ^{207}Pb NMR (C_6D_6, 105 MHz) of **1**Pb.

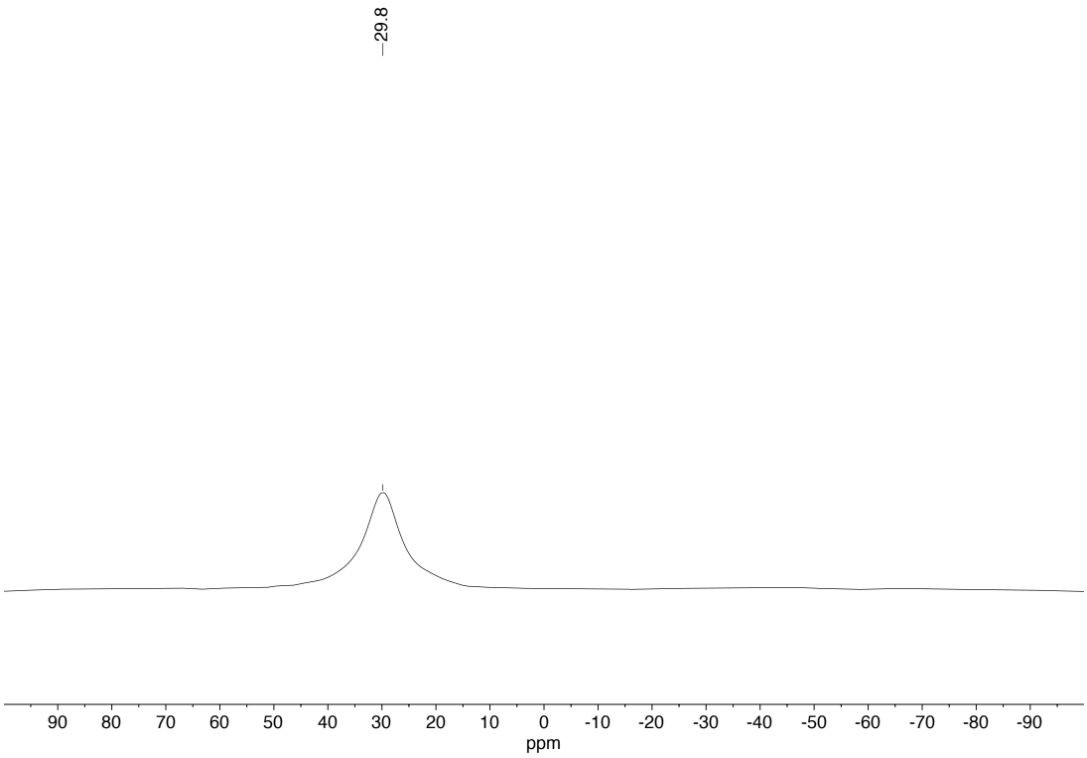


Figure S25: ^{11}B NMR (C_6D_6, 160 MHz) of **1**Pb.

B – Computational Details

The geometries of **1**Si, fc[(NDipp)$_2$Si] and fc[(NBMe$_2$)$_2$Si] were optimised with the ORCA program package (Version 5.0.3)[S1] employing the PBEh-3c[S2] method and checked for imaginary frequencies to confirm the geometries as minima on the energy hypersurface. Single-point calculations with further methods were performed with Gaussian09[S3] employing the functionals B3LYP,[S4] M06-L[S5] and ωB97XD[S6] in combination with the def2-TZVP[S7] basis set with Grimme's dispersion correction (D3) and Becke-Johnson damping.[S8] Pictures were generated with the ChemCraft program.[S9]

Frontier orbital discussion

As previously reported[S10] it is becoming commonplace to tentatively correlate the energy difference $\Delta E_{LP/LUMO}$ of assigned lone pair orbital (LP) and vacant orbital (LUMO) of a silylene with its reactivity, which, however, cannot be particularly reliable due to the method dependence of the energies. We find a higher $\Delta E_{LP/LUMO}$ for **1**Si in comparison to fc[(NDipp)$_2$Si] for each method, as is illustrated in Table S1.[S10] For the optimised model compound fc[(NBMe$_2$)$_2$Si] the orbitals are shown in Table S2.

Table S2. Frontier molecular orbitals of **1**Si obtained from calculations with different methods (PBEh-3c, B3LYP/def2-TZVP, M06-L/def2-TZVP and ωB97XD/def2-TZVP; H atoms not shown, energies in eV, surfaces at 0.05 $a_0^{-3/2}$). Values used to calculate $\Delta E_{LP/LUMO}$ are highlighted in red. For each method $\Delta E_{LP/LUMO}$, E_{LP} and E_{LUMO} of **1**Si are compared with the corresponding values of fc[(NDipp)$_2$Si].[S10]

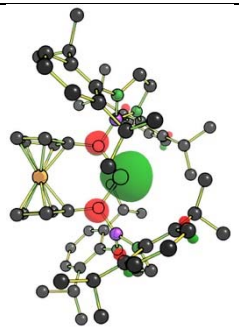
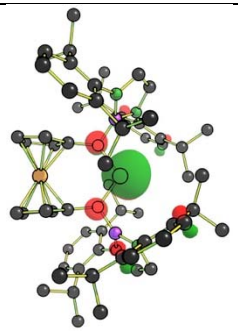
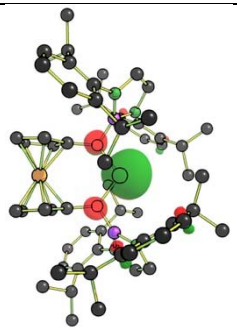
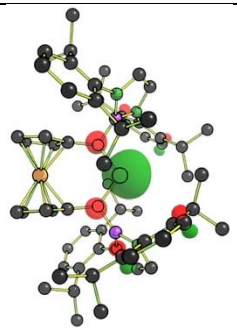
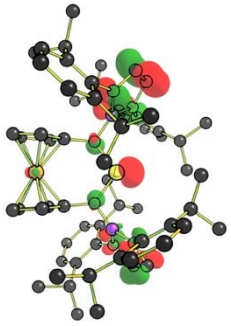
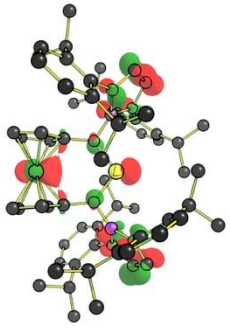
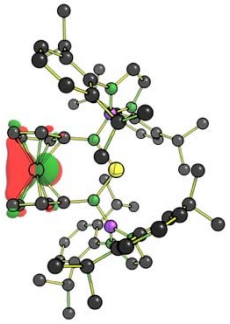
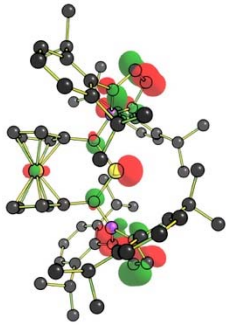
	PBEh-3c		B3LYP		M06-L		ωB97XD	
LUMO		–0.061		–0.854		–1.418		1.013
HOMO		–6.223		–5.360		–4.353		–7.309

Table S2 (continued)

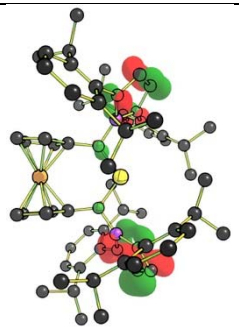
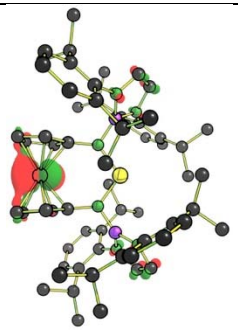
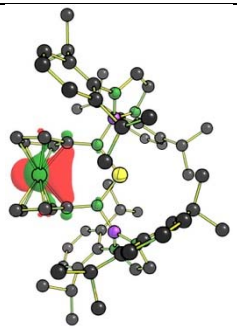
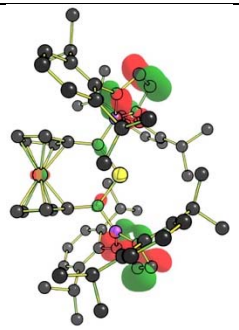
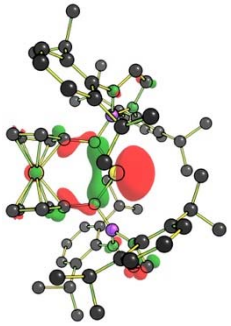
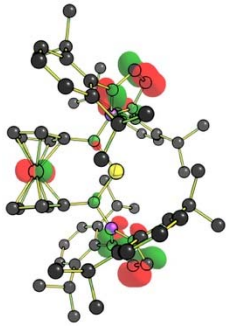
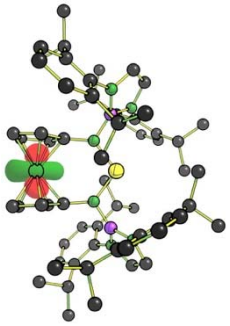
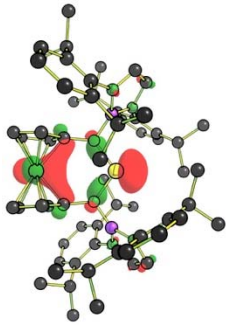
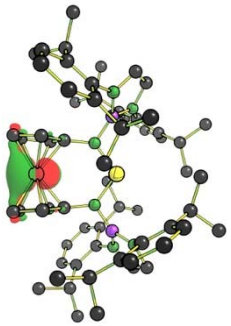
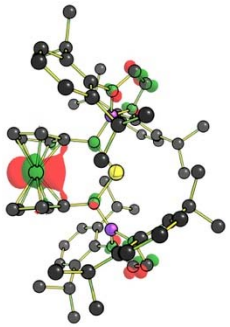
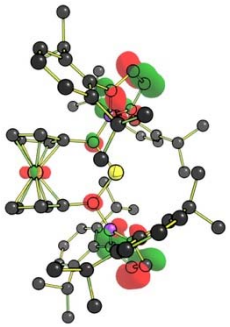
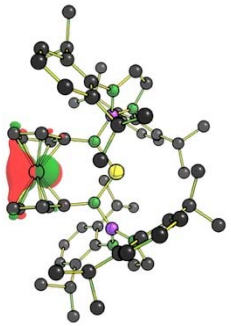
HOMO–1		–6.336		–5.398		–4.393		–7.418
HOMO–2		–6.651		–5.483		–4.633		–7.698
HOMO–3		–6.977		–5.504		–4.691		–7.857

Table S2 (continued)

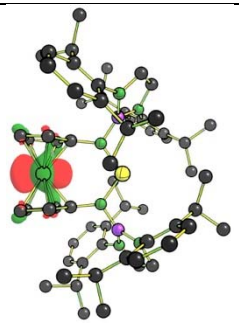
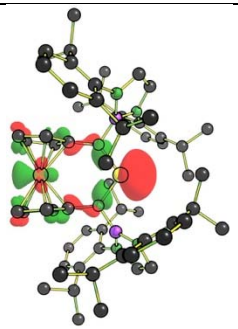
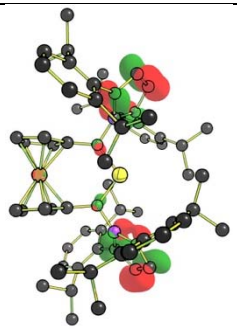
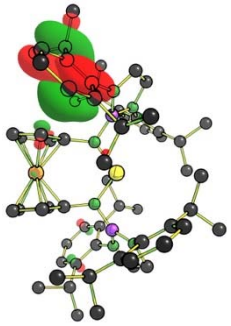
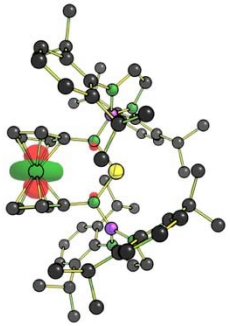
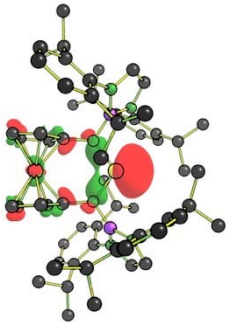
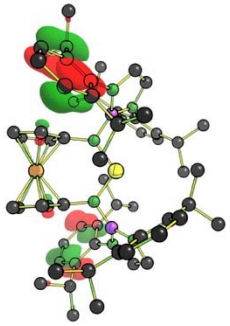
HOMO–4		–7.065		–5.810		–4.733		–8.486
HOMO–5		–7.406		–6.253		–5.236		–8.496
$\Delta E_{LP/LUMO}$		6.59		4.96		3.82		8.71
$\Delta E_{LP/LUMO}$ (fc[(NDipp)$_2$Si])		6.32		4.71		3.74		8.58
$\Delta E_{LP/LUMO}$ (**1**Si) – $\Delta E_{LP/LUMO}$ (fc[(NDipp)$_2$Si])		0.27		0.25		0.08		0.14
E_{LUMO} (**1**Si) – E_{LUMO} (fc[(NDipp)$_2$Si])		0.49		0.46		0.40		0.48
E_{LP} (**1**Si) – E_{LP} (fc[(NDipp)$_2$Si])		0.23		0.21		0.32		0.35

Table S3. Frontier molecular orbitals of fc[$(BMe_2)_2Si$] calculated with PBEh-3c (H atoms not shown, energies in eV, energy surfaces with 0.5 $a_0^{-3/2}$). LUMO and lone pair energies are highlighted in red.

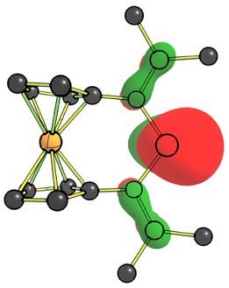
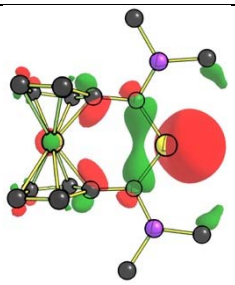
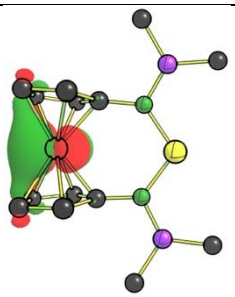
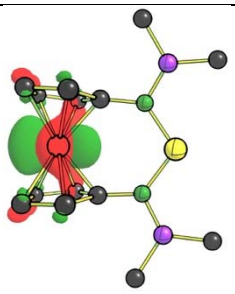
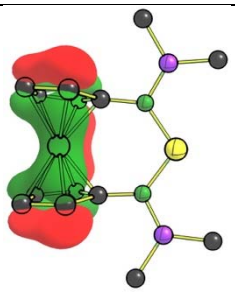
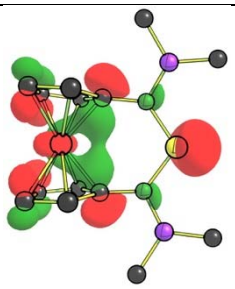
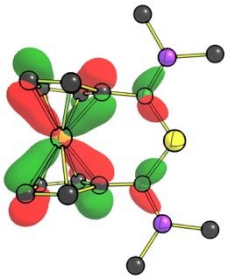
LUMO		–0.696
HOMO		–6.732
HOMO–1		–7.264
HOMO–2		–7.342
HOMO–3		–8.081

Table S3 (continued)

HOMO–4		–8.127
HOMO–5		–8.891
$\Delta E_{LP/LUMO}$		6.036

Cartesian coordinates for the optimized structures

1Si:

Fe	0.002095000	0.001917000	-3.029978000
Si	-0.000105000	0.001751000	0.672462000
N	-1.419526000	0.090573000	-0.342996000
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N	-3.598551000	-1.035470000	0.514154000
N	1.420321000	-0.087324000	-0.341354000
N	3.598326000	1.037033000	0.520680000
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C	-1.608220000	0.938468000	-3.902237000
H	-1.582809000	1.612084000	-4.745971000
C	-1.770738000	-0.469087000	-3.958194000
H	-1.897157000	-1.060627000	-4.852708000
C	-1.738560000	-0.972054000	-2.634867000
H	-1.839156000	-2.008144000	-2.348229000
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C	1.743132000	0.974896000	-2.633389000
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C	1.776499000	0.471003000	-3.956347000
H	1.904594000	1.061868000	-4.851071000
C	1.612625000	-0.936353000	-3.899831000
H	1.587481000	-1.610395000	-4.743232000
C	1.484367000	-1.306575000	-2.538856000
H	1.323592000	-2.303516000	-2.154916000
C	-4.536705000	-0.735858000	1.494193000
H	-5.351068000	-1.404501000	1.721358000
C	-4.234679000	0.448220000	2.051451000
H	-4.749858000	0.975730000	2.837557000
C	-2.725649000	2.318568000	1.701483000
C	-3.171295000	3.316987000	0.816602000
C	-2.922969000	4.644552000	1.144754000

H	-3.257536000	5.433726000	0.484857000
C	-2.262250000	4.982291000	2.312890000
H	-2.091464000	6.022378000	2.558655000
C	-1.808738000	3.988192000	3.157113000
H	-1.286027000	4.266119000	4.063508000
C	-2.017100000	2.642044000	2.865567000
C	-3.956060000	2.989143000	-0.438072000
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C	-5.453648000	2.902064000	-0.133694000
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H	-6.009531000	2.619737000	-1.030391000
H	-5.837098000	3.865067000	0.208933000
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C	-2.264644000	-4.477526000	1.867519000
H	-3.214158000	-4.265999000	2.359483000
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H	-2.335254000	-5.470005000	1.417818000
C	-0.574139000	-3.694882000	0.175513000
H	-0.549828000	-4.684961000	-0.283707000
H	0.227304000	-3.655597000	0.910563000
H	-0.350942000	-2.966834000	-0.604742000
C	4.536353000	0.734353000	1.499928000
H	5.350670000	1.402249000	1.729467000
C	4.234251000	-0.451430000	2.053509000
H	4.749153000	-0.981270000	2.838226000
C	3.784086000	2.131380000	-0.357957000
C	3.012451000	3.288711000	-0.209751000
C	3.234943000	4.344376000	-1.089313000

H	2.653015000	5.253208000	-0.991303000
C	4.183479000	4.252176000	-2.091362000
H	4.343281000	5.083720000	-2.765703000
C	4.924537000	3.091884000	-2.233917000
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C	1.926107000	3.413525000	0.833876000
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H	0.537824000	4.649288000	-0.305439000
H	-0.232213000	3.636952000	0.908328000
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H	3.196911000	4.306841000	2.357811000
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H	5.189579000	-0.012310000	-0.897425000
C	5.431616000	0.196855000	-2.989860000
H	4.393021000	-0.026709000	-3.232865000
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H	7.484804000	1.751322000	-1.860482000
H	7.607585000	0.082215000	-1.308093000
H	7.130194000	1.350387000	-0.182682000
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C	2.016288000	-2.647470000	2.860896000
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C	2.264145000	-4.986357000	2.303626000
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C	3.172373000	-3.317053000	0.811314000
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C	0.036080000	-1.860275000	4.197860000
H	-0.602327000	-1.897657000	3.314359000
H	-0.339079000	-1.058192000	4.834867000
H	-0.090786000	-2.790116000	4.754180000
C	2.370428000	-1.498912000	5.063806000
H	2.352883000	-2.425789000	5.640429000
H	2.021424000	-0.698106000	5.718347000
H	3.408503000	-1.285023000	4.810688000
C	3.958605000	-2.986208000	-0.441615000
H	3.642456000	-2.006423000	-0.806103000
C	5.455910000	-2.901485000	-0.135169000
H	5.670571000	-2.161663000	0.634394000
H	6.013233000	-2.617084000	-1.030313000
H	5.837959000	-3.865877000	0.205110000
C	3.719325000	-3.969783000	-1.585290000
H	4.195338000	-4.936024000	-1.407842000
H	4.139773000	-3.568841000	-2.508177000
H	2.657441000	-4.149100000	-1.756026000
B	-2.638203000	0.027859000	0.464640000
B	2.638180000	-0.026322000	0.467644000

Fc[(NDipp)$_2$Si]:

C	1.524527000	-0.671768000	1.059342000
C	2.015347000	0.051291000	2.183598000

H	2.387200000	1.065143000	2.167301000
C	1.912194000	-0.784536000	3.320762000
H	2.193300000	-0.518696000	4.328621000
C	1.368346000	-2.026490000	2.908581000
H	1.165455000	-2.873762000	3.546378000
C	1.146970000	-1.967027000	1.510618000
H	0.733661000	-2.751673000	0.892380000
C	-1.443147000	0.056309000	1.247314000
C	-1.048386000	1.155353000	2.062660000
H	-0.663981000	2.101005000	1.707719000
C	-1.206355000	0.776829000	3.418044000
H	-0.972131000	1.386342000	4.277923000
C	-1.733125000	-0.537514000	3.448465000
H	-1.969131000	-1.106189000	4.335459000
C	-1.886723000	-0.982863000	2.115446000
H	-2.256839000	-1.949931000	1.809920000
C	2.619766000	0.256722000	-0.859323000
C	3.521828000	-0.688717000	-1.371479000
C	4.701189000	-0.235222000	-1.948998000
H	5.412257000	-0.950196000	-2.344300000
C	4.979526000	1.116896000	-2.041354000
H	5.899032000	1.451344000	-2.503750000
C	4.077892000	2.038761000	-1.544789000
H	4.301804000	3.095237000	-1.628985000
C	2.894313000	1.631526000	-0.937013000
C	3.253999000	-2.175407000	-1.298970000
H	2.214114000	-2.316423000	-1.003359000
C	3.421911000	-2.861111000	-2.654404000
H	4.454039000	-2.834179000	-3.006978000
H	2.797321000	-2.392827000	-3.415204000
H	3.133907000	-3.911028000	-2.583101000
C	4.135888000	-2.829786000	-0.234672000
H	3.899710000	-3.890677000	-0.134090000
H	3.996373000	-2.362645000	0.739973000
H	5.192645000	-2.749177000	-0.496822000
C	1.950496000	2.686660000	-0.395009000
H	1.173783000	2.182503000	0.183872000
C	2.650778000	3.651147000	0.562190000
H	3.402716000	4.260563000	0.059216000
H	3.150525000	3.119708000	1.372571000
H	1.927181000	4.336134000	1.007673000
C	1.264026000	3.448647000	-1.529317000
H	0.718104000	2.773774000	-2.190273000
H	1.989194000	3.989780000	-2.139613000
H	0.553959000	4.176771000	-1.132491000
C	-2.670348000	-0.001638000	-0.801252000
C	-3.252664000	-1.214434000	-1.199530000
C	-4.503606000	-1.182544000	-1.807493000
H	-4.964142000	-2.106951000	-2.134224000
C	-5.173397000	0.009945000	-2.004985000
H	-6.151019000	0.013924000	-2.469077000
C	-4.583636000	1.198724000	-1.616304000
H	-5.109756000	2.130415000	-1.783801000
C	-3.324849000	1.218888000	-1.026443000
C	-2.559556000	-2.550186000	-1.030046000
H	-1.672435000	-2.402376000	-0.411824000
C	-2.087168000	-3.083260000	-2.382838000
H	-1.413953000	-2.378008000	-2.872436000
H	-2.927815000	-3.256668000	-3.057162000
H	-1.556977000	-4.030327000	-2.265252000
C	-3.439824000	-3.573367000	-0.313734000
H	-2.876340000	-4.486560000	-0.115151000

H	-4.310367000	-3.857261000	-0.906895000
H	-3.807679000	-3.190632000	0.639055000
C	-2.712288000	2.551634000	-0.655585000
H	-1.680537000	2.379982000	-0.346743000
C	-2.651876000	3.501401000	-1.850862000
H	-3.644454000	3.787221000	-2.202055000
H	-2.118745000	3.049753000	-2.687596000
H	-2.129694000	4.419605000	-1.576740000
C	-3.449779000	3.188367000	0.521897000
H	-2.960999000	4.115743000	0.826384000
H	-3.473002000	2.520615000	1.382930000
H	-4.481199000	3.429977000	0.258457000
N	1.397589000	-0.179812000	-0.255629000
N	-1.385039000	-0.008810000	-0.163418000
Fe	0.068263000	-0.504515000	2.423359000
Si	-0.025264000	-0.002352000	-1.269896000

fc[(NBMe$_2$)$_2$Si]:

Fe	-0.000023000	-1.564234000	-0.040498000
Si	-0.000172000	2.160685000	-0.114283000
N	-1.443806000	1.130860000	-0.059819000
N	1.443644000	1.131044000	-0.059866000
C	-1.527319000	-0.282580000	-0.045748000
C	-1.617376000	-1.122349000	-1.189398000
H	-1.588001000	-0.788250000	-2.216677000
C	-1.716073000	-2.462559000	-0.740887000
H	-1.779906000	-3.337486000	-1.370726000
C	-1.713106000	-2.453684000	0.676514000
H	-1.773713000	-3.320818000	1.317348000
C	-1.611136000	-1.108098000	1.108255000
H	-1.575551000	-0.762566000	2.131572000
C	1.527161000	-0.282394000	-0.047115000
C	1.615102000	-1.120942000	-1.191797000
H	1.583836000	-0.785801000	-2.218686000
C	1.714761000	-2.461629000	-0.744909000
H	1.777433000	-3.335864000	-1.375826000
C	1.714509000	-2.454253000	0.672502000
H	1.776427000	-3.322077000	1.312273000
C	1.613232000	-1.109138000	1.105860000
H	1.579510000	-0.764643000	2.129580000
B	-2.718813000	1.817546000	-0.003741000
B	2.718444000	1.817690000	-0.001628000
C	-2.882531000	3.389414000	-0.035861000
H	-3.317125000	3.704911000	0.918418000
H	-2.006180000	4.007706000	-0.213300000
H	-3.635405000	3.645542000	-0.786650000
C	-4.049422000	0.969660000	0.122412000
H	-4.939702000	1.598886000	0.118363000
H	-4.155104000	0.238241000	-0.682760000
H	-4.067263000	0.382228000	1.044240000
C	4.048956000	0.970130000	0.127975000
H	4.939244000	1.599325000	0.121013000
H	4.066632000	0.387716000	1.053018000
H	4.154758000	0.234445000	-0.673253000
C	2.882660000	3.389400000	-0.037304000
H	3.328127000	3.707349000	0.911020000
H	3.628072000	3.642029000	-0.796887000
H	2.005421000	4.008227000	-0.208175000

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