Electronic Supplementary Material (ESI) for Dalton Transactions.

Synthetic, structural and reaction chemistry of N-heterocyclic germylene and stannylene compounds featuring N-boryl substituents

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Supporting Information (44 pages)

1. Additional synthetic data

Deprotonation of (L^1)H_2 with ^{n}BuLi/TMEDA (*In Situ*) – Generation of $Li_2(L^1)\cdot(C_6H_5Me)$(TMEDA): To a stirred mixture of (L^1)H_2 (0.20 g, 0.24 mmol) and TMEDA (36 µL, 0.24 mmol) in toluene (2 mL) at -50 °C was added dropwise ^{n}BuLi (0.60 mL of a 1.6 M solution in hexane, 0.96 mmol). The resulting pale orange reaction mixture was warmed to room temperature and stirred for 30 min. The ^{1}H NMR spectrum of the reaction mixture indicates full conversion to $Li_2(L^1)\cdot(C_6H_5Me)$(TMEDA). ^{1}H NMR (C_6D_6, 400 MHz, 298 K): δ_H 6.99-7.18 (overlapping m, *p*-H and *m*-H of Dipp and $C_6D_5\underline{H}$), 6.71 (2H, m, *o*-H of coordinated toluene), 6.25 (2H, m, *m*-H of coordinated toluene), 5.93 (1H, m, *p*-H of coordinated toluene), 5.87 (4H, s, $N(CH)_2N$ of boryl ligand), 3.54-3.60 (8H, br m, $C\underline{H}Me_2$), 2.82-2.85 (4H, br m, NCH_2), 1.76 (3H, s, CH_3 of coordinated toluene), 1.71 (12H, s, CH_3 of coordinated TMEDA), 1.56 (4H, s, CH_2 of coordinated TMEDA), 1.17-1.35 (48H, overlapping m, $CH\underline{Me}_2$). $^{13}C\{^1H\}$ NMR (C_6D_6, 101 MHz, 298 K): δ_C 155.3 (*i*-C of coordinated toluene), 147.2 (*o*-C of Dipp), 143.0 (*i*-C of Dipp), 130.2 (*o*-C of coordinated toluene), 126.7 (*p*-C of Dipp), 124.0 (*m*-C of Dipp), 118.0 ($N(CH)_2N$ of boryl ligand), 115.5 (*m*-C of coordinated toluene), 107.2 (*p*-C of coordinated toluene), 56.2 (CH_2 of coordinated TMEDA), 54.5 (NCH_2), 45.3 (CH_3 of coordinated TMEDA), 38.8 (CH_3 of coordinated toluene), 28.5 ($C\underline{H}Me_2$), 25.6 ($CH\underline{Me}_2$), 23.9 ($CH\underline{Me}_2$). ^{11}B NMR (C_6D_6, 128 MHz, 298 K): δ_B 29 (br s, boryl ligand). ^{7}Li NMR (C_6D_6, 156 MHz, 298 K): δ_{Li} 1.1.

Deprotonation of (L^2)H_2 with ^{n}BuLi/TMEDA (*In Situ*) – Generation of $Li_2(L^2)\cdot(C_6H_5Me)$(TMEDA): $Li_2(L^2)\cdot(C_6H_5Me)$(TMEDA) was prepared by a similar method to $Li_2(L^1)\cdot(C_6H_5Me)$(TMEDA) from (L^2)H_2 (0.20 g, 0.24 mmol), TMEDA (36 µL, 0.24 mmol) and ^{n}BuLi (0.59 mL of a 1.6 M solution in hexane, 0.95 mmol). ^{1}H NMR (C_6D_6, 400 MHz, 298 K): δ_H 7.00-7.20 (overlapping m, *p*-H and *m*-H of Dipp and $C_6D_5\underline{H}$), 6.86 (2H, m, *o*-H coordinated toluene), 6.45 (2H, m, *m*-H of coordinated toluene), 6.03 (1H, m, *p*-H of coordinated toluene), 5.87 (4H, s, $N(CH)_2N$ of boryl ligand), 3.48 (8H, sept, $^3J_{HH}$ = 6.9 Hz, $C\underline{H}Me_2$), 2.78 (4H, m, NCH_2), 2.08 (3H, s, CH_3 of coordinated toluene), 1.75 (12H, s, CH_3 of coordinated TMEDA), 1.61 (4H, s, CH_2 of coordinated TMEDA), 1.22 (24H, d, $^3J_{HH}$ = 6.9 Hz, $CH\underline{Me}_2$), 1.13 (24H, d, $^3J_{HH}$ = 6.9 Hz, $CH\underline{Me}_2$), 0.96 (2H, m, $C\underline{H}_2(CH_2N)_2$). $^{13}C\{^1H\}$ NMR (C_6D_6, 101 MHz, 298 K): δ_C 147.4 (*i*-C of coordinated toluene), 146.8 (*o*-C of Dipp), 142.8 (*i*-C of Dipp), 130.2 (*o*-C of coordinated toluene), 125.7 (*p*-C of Dipp), 124.2 (*m*-C of Dipp), 117.3

($N(CH)_2N$ of boryl ligand), 115.6 (*m*-C of coordinated toluene), 106.6 (*p*-C of coordinated toluene), 56.4 (CH_2 of coordinated TMEDA), 47.5 (NCH_2), 45.3 (CH_3 of coordinated TMEDA), 40.0 ($\underline{C}H_2(CH_2N)_2$), 36.8 ($CH_3$ of coordinated toluene), 28.7 ($\underline{C}HMe_2$), 24.7 ($CH\underline{Me_2}$), 23.8 ($CH\underline{Me_2}$). ^{11}B NMR (C_6D_6, 128 MHz, 298 K): δ_B 26 (br s, boryl ligand). ^{7}Li NMR (156 MHz, C_6D_6, 298 K): δ_{Li} 1.0.

Deprotonation of (L^1)H_2 with Benzyl Potassium (*In situ*) – Generation of $K_2(L^1)$: To a mixture of ($\mathbf{L^1}$)H_2 (48 mg, 0.058 mmol) and benzyl potassium (15 mg, 0.12 mmol) in a J. Young's NMR tube was added C_6D_6 (0.5 mL) and the resulting red solution sonicated for 3 h. The ^1H NMR spectrum of the reaction mixture indicates full conversion to $K_2(\mathbf{L^1})$. ^1H NMR (C_6D_6, 400 MHz, 298 K): δ_H 6.99-7.15 (12H, overlapping m, *m*-H and *p*-H of Dipp), 5.98 (4H, s, $N(CH)_2N$ of boryl ligand), 3.61 (8H, sept, $^3J_{HH}$ = 6.9 Hz, $C\underline{H}Me_2$), 2.66 (4H, s, NCH_2), 1.24 (24H, d, $^3J_{HH}$ = 6.9 Hz, $CH\underline{Me_2}$), 1.09 (24H, d, $^3J_{HH}$ = 6.9 Hz, $CH\underline{Me_2}$).

Deprotonation of (L^2)H_2 with Benzyl Potassium (*In situ*) – Generation of $K_2(L^2)$: $K_2(\mathbf{L^2})$ was prepared by a similar method to $K_2(\mathbf{L^1})$ from ($\mathbf{L^2}$)H_2 (50 mg, 0.059 mmol) and benzyl potassium (15 mg, 0.12 mmol). ^1H NMR (C_6D_6, 400 MHz, 298 K): δ_H 7.00-7.15 (12H, overlapping m, *m*-H and *p*-H of Dipp), 5.90 (4H, s, $N(CH)_2N$ of boryl ligand), 3.61 (8H, sept, $^3J_{HH}$ = 6.9 Hz, $C\underline{H}Me_2$), 2.87 (4H, m, NCH_2), 1.26 (24H, d, $^3J_{HH}$ = 6.9 Hz, $CH\underline{Me_2}$), 1.14 (24H, d, $^3J_{HH}$ = 6.9 Hz, $CH\underline{Me_2}$), 0.94 (2H, m, $C\underline{H_2}(CH_2N)_2$).

(L^4)H: To a stirred solution of $Br\{B(NDippCH)_2\}$ (2.5 g, 5.4 mmol) in benzene (50 mL) was added dropwise *tert*-butylamine (1.1 g, 15 mmol) and the resulting mixture heated to 80˚C for 16 h. After cooling, the mixture was filtered and the residue extracted once more with benzene. The volatiles were removed *in vacuo*, yielding a viscous brown oil. Yield: 2.1 g, 84%. ^1H NMR (C_6D_6, 400 MHz, 298 K): δ_H 7.17-7.27 (m, 6H, Ar), 6.01 (s, 2H, $N(CH)_2N$), 3.49 (sept, *J* = 6.9 Hz, 4H, $C\underline{H}Me_2$), 1.88 (s, 1H, NH), 1.35 (d, *J* = 6.9 Hz, 12H $CH\underline{Me_2}$), 1.25 (d, *J* = 6.9 Hz, 12H, $CH\underline{Me_2}$), 0.82 (s, 9H, $NC(CH_3)_3$). ^{13}C NMR (C_6D_6, 101 MHz, 298 K): δ_C 147.5 (*o*-C), 140.0 (*i*-C), 127.7 (*p*-C), 124.0 (*m*-C), 118.1 ($N(CH)_2N$), 48.7 ($N\underline{C}(CH_3)_3$), 33.3 ($\underline{C}HMe_2$), 28.6 ($NC(\underline{C}H_3)_3$), 25.5 ($CH\underline{Me_2}$), 23.5 ($CH\underline{Me_2}$). ^{11}B NMR (C_6D_6, 128 MHz, 298 K): δ_B 22. MS (ESI): m/*z* (assignment, %) 460.4 $[M]H^+$, 100%).

(L^4)H: To a stirred solution of Br{B(NDippCH)$_2$} (2.5 g, 5.4 mmol) in benzene (50 mL) was added dropwise *tert*-butylamine (1.1 g, 15 mmol) and the resulting mixture heated to 80˚C for 16 h. After cooling, the mixture was filtered and the residue extracted once more with benzene. The volatiles were removed *in vacuo*, yielding a viscous brown oil. Yield: 2.1 g, 84%. ^{1}H NMR (C_6D_6, 400 MHz, 298 K): δ_H 7.17-7.27 (m, 6H, Ar), 6.01 (s, 2H, N(CH)$_2$N), 3.49 (sept, *J* = 6.9 Hz, 4H, C<u>H</u>Me$_2$), 1.88 (s, 1H, NH), 1.35 (d, *J* = 6.9 Hz, 12H CH<u>Me$_2$</u>), 1.25 (d, *J* = 6.9 Hz, 12H, CH<u>Me$_2$</u>), 0.82 (s, 9H, NC(CH$_3$)$_3$). ^{13}C NMR (C_6D_6, 101 MHz, 298 K): δ_C 147.5 (*o*-C), 140.0 (*i*-C), 127.7 (*p*-C), 124.0 (*m*-C), 118.1 (N(CH)$_2$N), 48.7 (N<u>C</u>(CH$_3$)$_3$), 33.3 (<u>C</u>HMe$_2$), 28.6 (NC(<u>C</u>H$_3$)$_3$), 25.5 (CH<u>Me$_2$</u>), 23.5 (CH<u>Me$_2$</u>). ^{11}B NMR (C_6D_6, 128 MHz, 298 K): δ_B 22. MS (ESI): m/*z* (assignment, %) 460.4 [M]H$^+$, 100%).

(L^4)$_2$Sn: To a suspension of LiN^tBu{B(NDippCH)$_2$} (280 mg, 0.56 mmol) (generated in situ from equimolar amounts of (**L^4**)H and phenyl lithium) in benzene (10 mL) and THF (1 mL) was added $SnBr_2$ (35 mg, 0.125 mmol), and the reaction mixture sonicated for 30 min. This resulted in the formation of a red-brown suspension with a white precipitate. The precipitate was removed by filtration and volatiles removed *in vacuo*. The residue was washed with a small amount of cold hexane and dried. This solid consisted of a mixture of yellow and red crystals. Extraction with hexane (2 x 5 mL) allowed the separation of the more soluble red product. Single crystals suitable for X-ray crystallography were grown from a concentrated solution in hexane at 4 °C. ^{1}H NMR (C_6D_6, 400 MHz, 298 K): δ_H 7.25-7.00 (m, 12H, Ar), 5.91 (s, 4H, NCH), 3.47 (sept, *J* = 6.8 Hz, 8H, C<u>H</u>Me$_2$), 1.32 (s, 18H, NC(CH$_3$)$_3$), 1.30 (d, *J* = 6.8 Hz, 24H, CH<u>Me$_2$</u>), 1.17 (d, *J* = 6.8 Hz, 24H, CH<u>Me$_2$</u>). ^{13}C NMR (C_6D_6, 101 MHz, 298 K): δ_C 146.7 (Dipp *o*-CH), 143.0 (*i*-C), 127.7 (*p*-CH), 124.4 (*m*-CH), 120.1 (NCH), 56.9 (N<u>C</u>(CH$_3$)$_3$), 35.4 (NC(<u>C</u>H$_3$)$_3$), 28.7 (<u>C</u>HMe$_2$), 26.5 (CH<u>Me$_2$</u>), 23.2 (CH<u>Me$_2$</u>). ^{11}B NMR (C_6D_6, 128 MHz, 298 K): δ_B 25. ^{119}Sn NMR (C_6D_6, 187 MHz, 298 K): δ_{Sn} 644.

2. Representative ^{1}H NMR spectra for new compounds

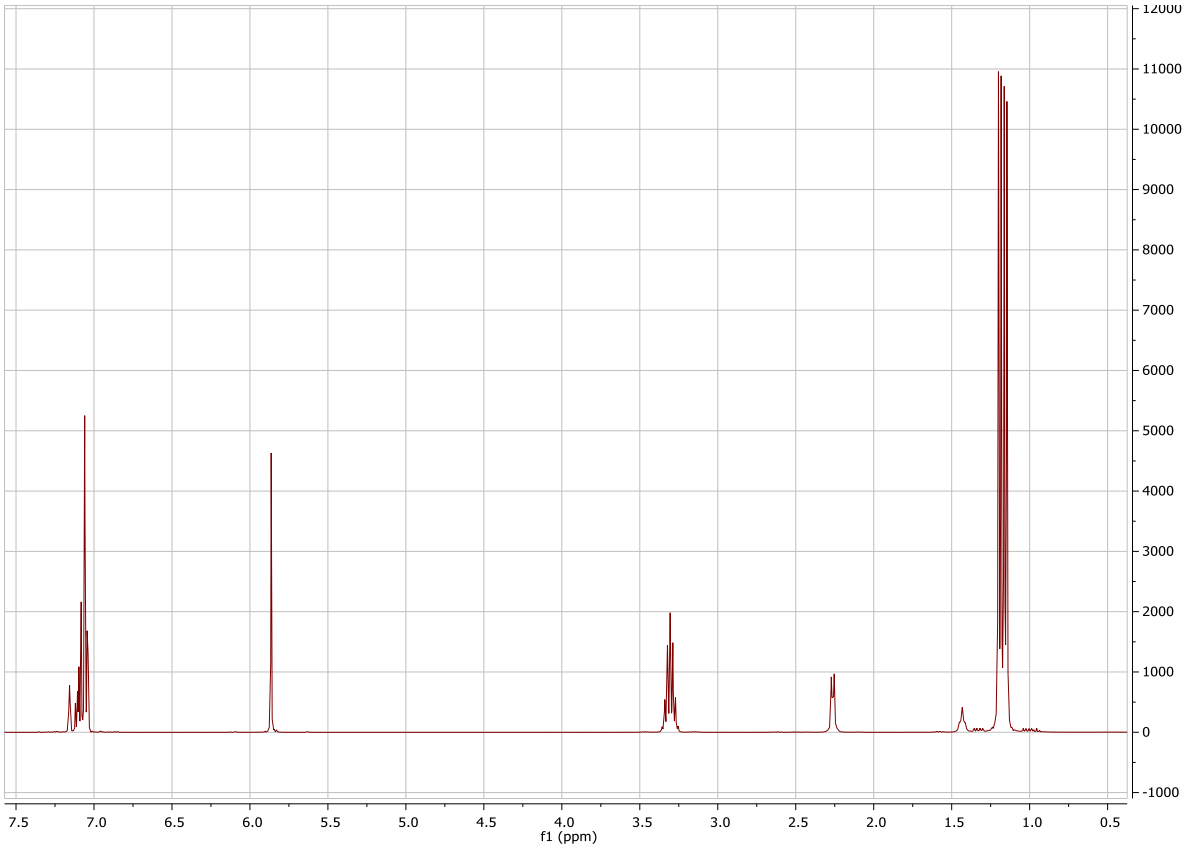

Figure s1: ^{1}H NMR spectrum of (**L^{1}**)H_2 in C_6D_6.

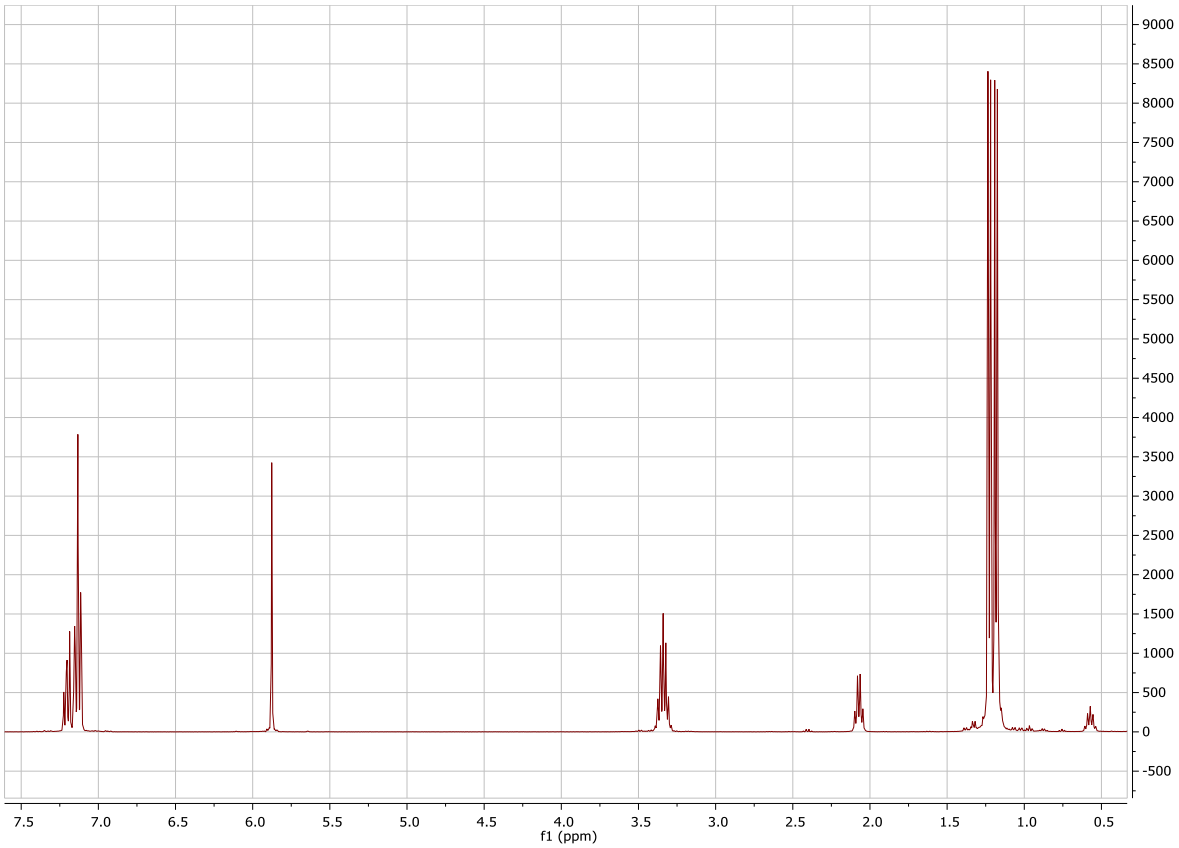

Figure s2: ^{1}H NMR spectrum of (**L^{2}**)H_2 in C_6D_6.

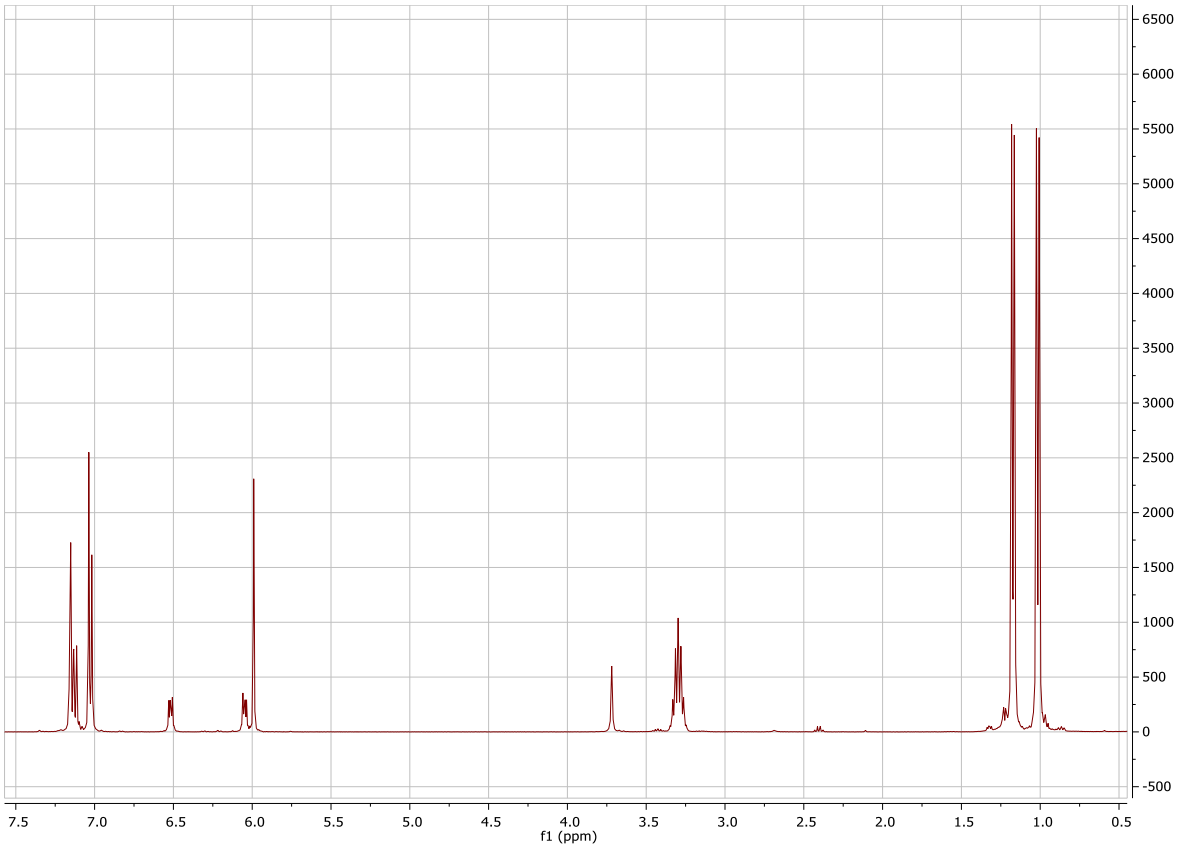

Figure s3: ^{1}H NMR spectrum of (**L^{3}**)H_2 in C_6D_6.

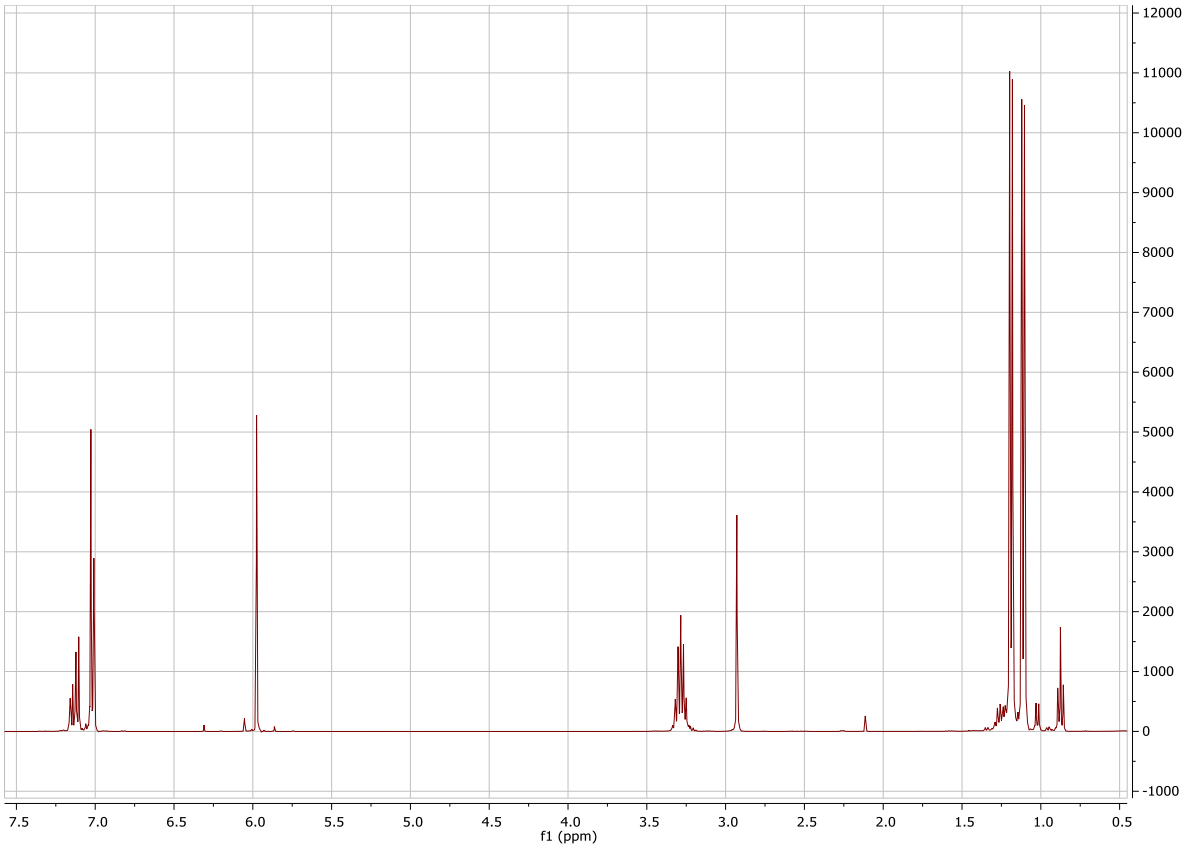

Figure s4: ^{1}H NMR spectrum of (**L^{1}**)Ge in C_6D_6.

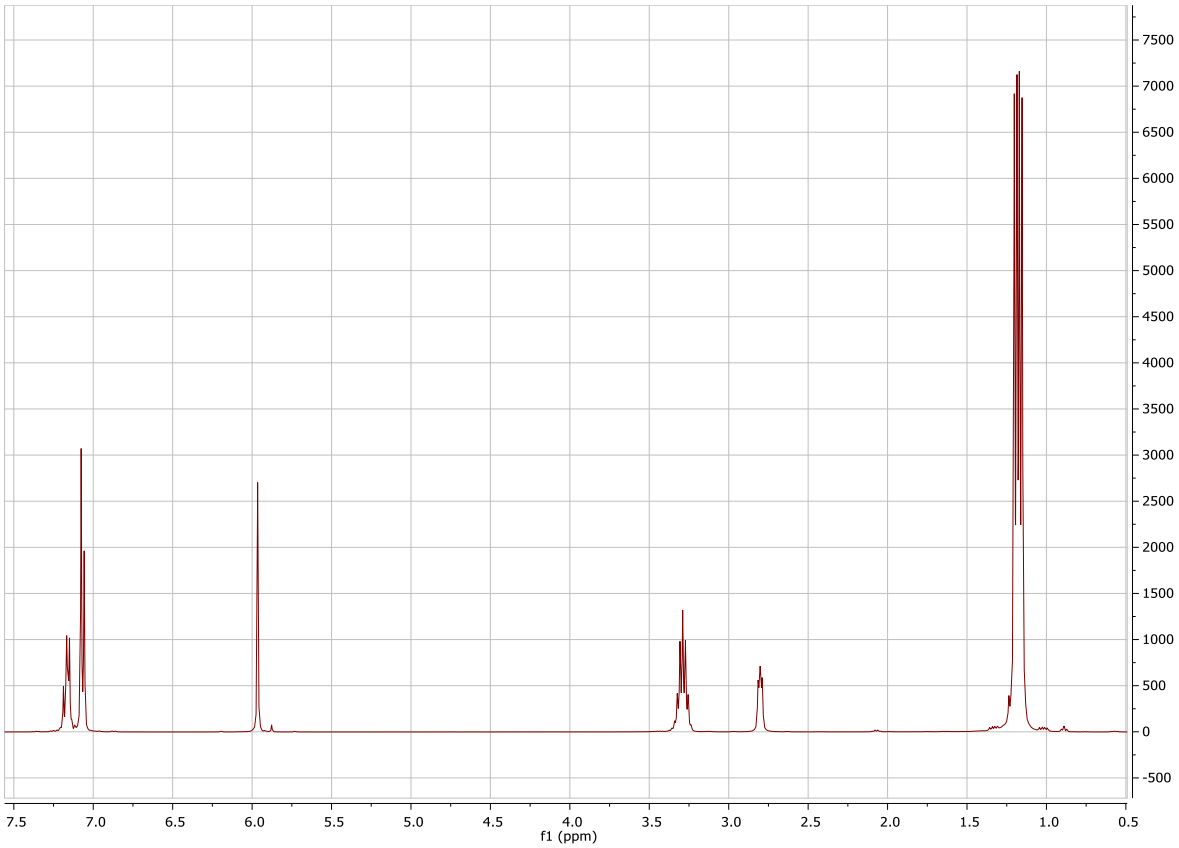

Figure s5: ^{1}H NMR spectrum of (**L^{2}**)Ge in C_6D_6.

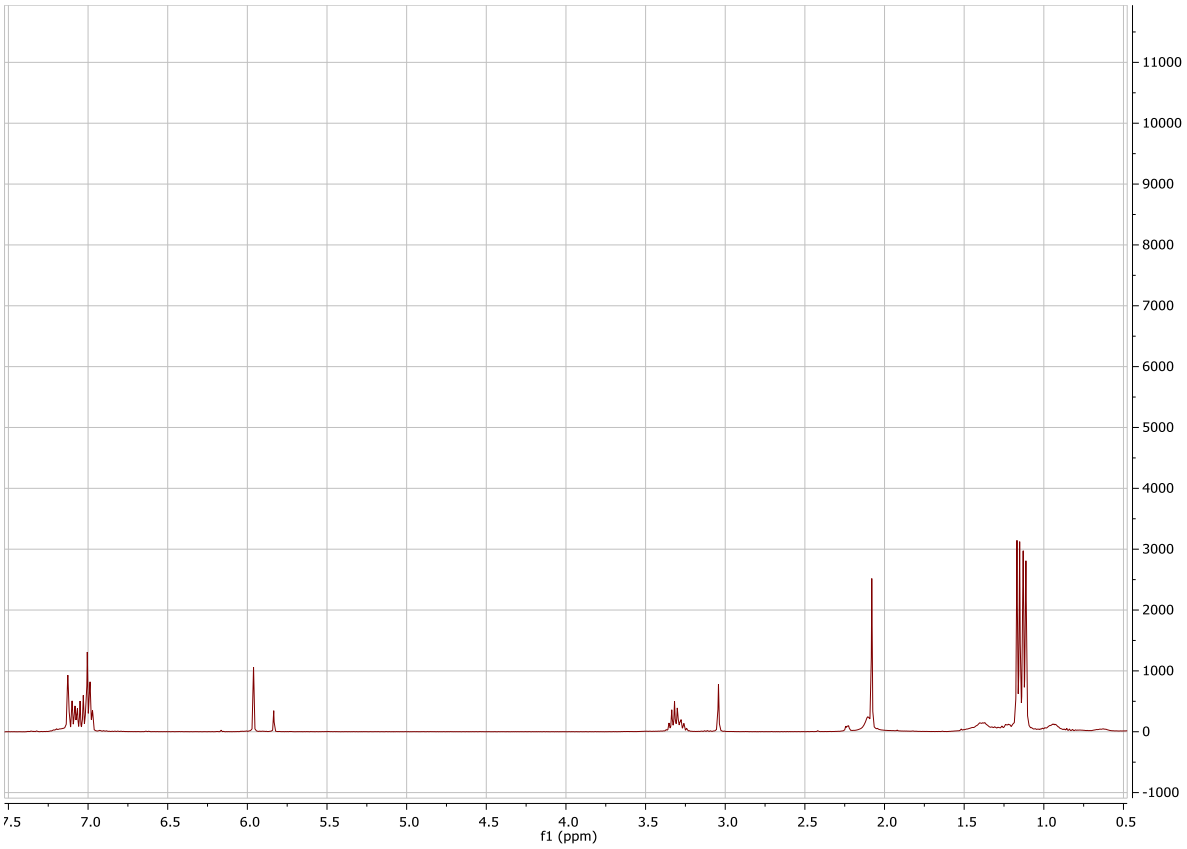

Figure s6: ^{1}H NMR spectrum of (**L**^{1})Sn in C_7D_8 (contaminated with ca. 10% (**L**^{1})H_2).

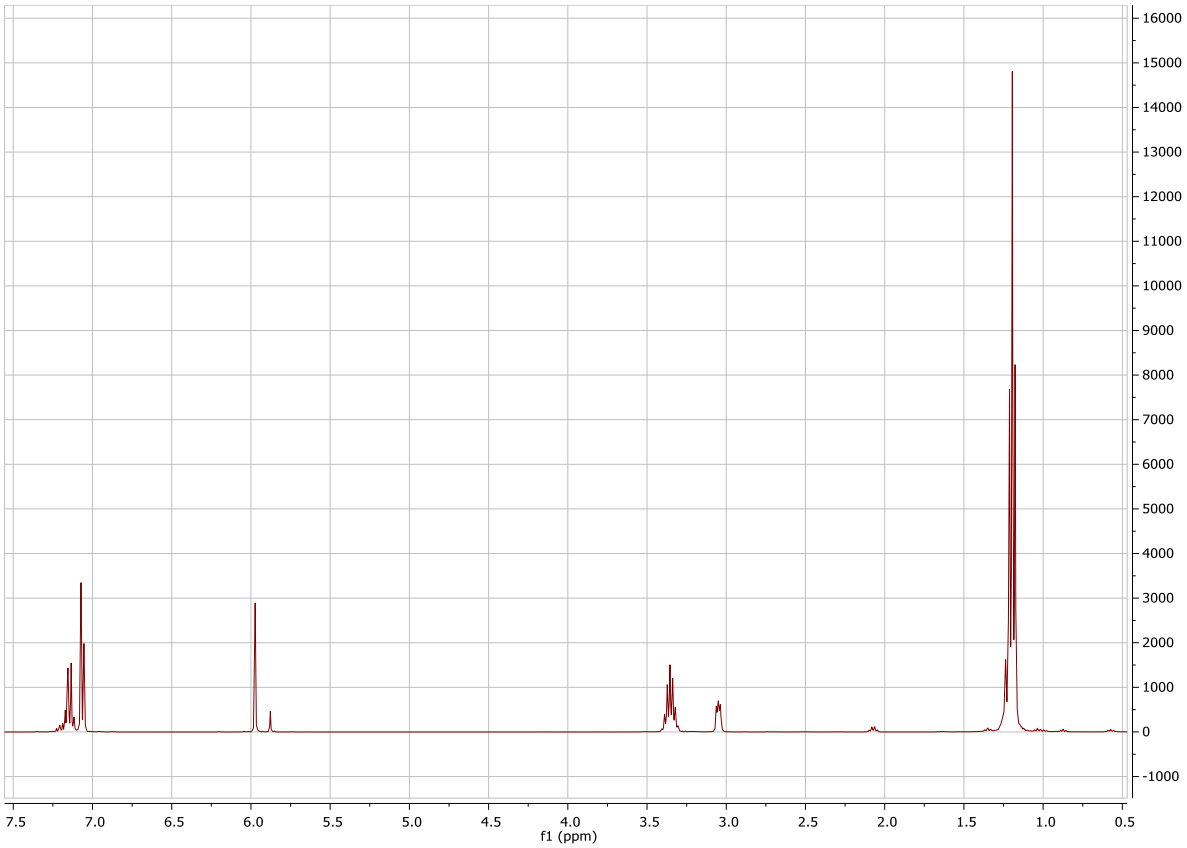

Figure s7: ^{1}H NMR spectrum of (**L^{2}**)Sn in C_6D_6.

3. Crystallographic data for new compounds

($\mathbf{L^1}$)H_2: *a* = 14.2417(2) Å, *b* = 22.3662(4) Å, *c* = 16.4812(3) Å, α = γ = 90°, β = 97.5685(8)°, V = 5204.06(15) Å^3, Monoclinic, *P*2$_1$, *Z* = 4, R_1 for 8834 [data intensity *I* > 2σ(*I*)] unique data = 0.061, wR_2 (all 12110 unique data) = 0.156. CCDC: 1921772.

($\mathbf{L^2}$)H_2: *a* = 19.0773(2) Å, *b* = 13.7845(1) Å, *c* = 20.3735(2) Å, α = γ = 90°, β = 99.780(1)°, V = 5279.78(9) Å^3, Monoclinic, *P*2$_1$/c, *Z* = 4, R_1 for 9261 [data intensity *I* > 2σ(*I*)] unique data = 0.046, wR_2 (all 10581 unique data) = 0.129. CCDC: 1921773.

($\mathbf{L^3}$)H_2: *a* = 10.9110(1) Å, *b* = 12.8255(1) Å, *c* = 38.0195(1) Å, α = γ = 90°, β = 90.504(1)°, V = 5320.21(9) Å^3, Monoclinic, *P*2$_1$/c, *Z* = 4, R_1 for 9667 [data intensity *I* > 2σ(*I*)] unique data = 0.044, wR_2 (all 10581 unique data) = 0.129. CCDC: 1921774.

($\mathbf{L^1}$)Ge: *a* = 12.9973(1) Å, *b* = 20.9096(1) Å, *c* = 21.1512(2) Å, α = γ = 90°, β = 103.4323(7)°, V = 5590.98(8) Å^3, Monoclinic, *P*2$_1$/c, *Z* = 2, R_1 for 10696 [data intensity *I* > 2σ(*I*)] unique data = 0.031, wR_2 (all 11074 unique data) = 0.1169. CCDC: 1921775.

($\mathbf{L^2}$)Ge: *a* = 10.6441(2) Å, *b* = 13.4667(4) Å, *c* = 19.8671(5) Å, α = 70.951(2)°, β = 78.3208(19)°, γ = 89.024(2)°, V = 2632.39(12) Å^3, Triclinic, *P*-1, *Z* = 2, R_1 for 9784 [data intensity *I* > 2σ(*I*)] unique data = 0.035, wR_2 (all 10869 unique data) = 0.097. CCDC: 1921776.

($\mathbf{L^1}$)Sn: *a* = 10.444(1) Å, *b* = 19.182(1) Å, *c* = 27.692(1) Å, α = 93.576(2)°, β = 96.319(3)°, γ = 90.149(2)°, V = 5503.4(3) Å^3, Triclinic, *P*-1, *Z* = 2, R_1 for 14921 [data intensity *I* > 2σ(*I*)] unique data = 0.117, wR_2 (all 20167 unique data) = 0.346. CCDC: 1921777.

($\mathbf{L^2}$)Sn: *a* = 10.5800(2) Å, *b* = 13.7902(2) Å, *c* = 36.8584(4) Å, α = γ = 90°, β = 91.0379(12)°, V = 5376.77(14) Å^3, Monoclinic, *P*2$_1$/c, *Z* = 4, R_1 for 10216 [data intensity *I* > 2σ(*I*)] unique data = 0.101, wR_2 (all 11187 unique data) = 0.322. CCDC: 1921778.

($\mathbf{L^2}$)Ge(OCH_2NMe_2)(OH): *a* = 13.4539(2) Å, *b* = 18.6681(2) Å, *c* = 23.0034(3) Å, α = β = γ = 90°, V = 5777.61(13) Å^3, Orthorhombic, *P*2$_1$2$_1$2$_1$, *Z* = 4, R_1 for 11469 [data intensity *I* > 2σ(*I*)] unique data = 0.027, wR_2 (all 12052 unique data) = 0.071. CCDC: 1921779.

($\mathbf{L^2}$)Ge(C_5H_4NO)(OH): *a* = *b* = 42.2093(12) Å, *c* = 13.8670(5) Å, α = β = γ = 90°, V = 24705.8(17) Å^3, Tetragonal, *I*4$_1$/*a*, *Z* = 16, R_1 for 9904 [data intensity $I > 2\sigma(I)$] unique data = 0.052, wR_2 (all 12758 unique data) = 0.153. CCDC: 1921780.

($\mathbf{L^4}$)$_2$Sn: *a* = 26.1530(3) Å, *b* = 12.3864(1) Å, *c* = 17.6976(2) Å, α = γ = 90°, β = 95.1853(5)°, V = 5709.53(10) Å^3, Monoclinic, *C*2/*c*, *Z* = 3, R_1 for 5980 [data intensity $I > 2\sigma(I)$] unique data = 0.030, wR_2 (all 6511 unique data) = 0.073.

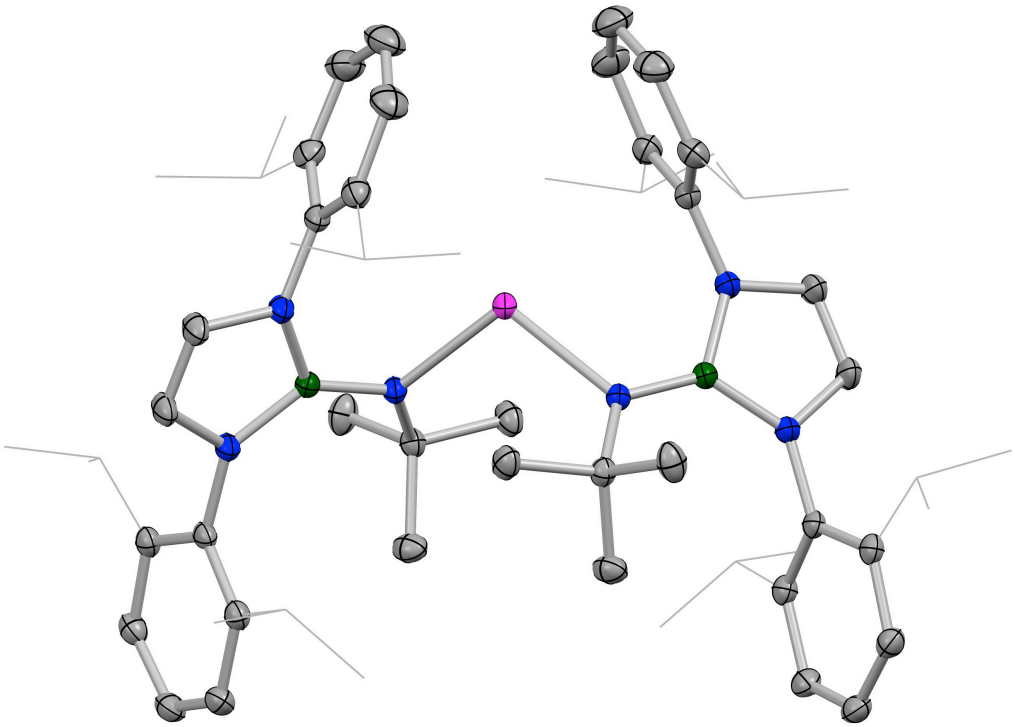

Figure s8: Molecular structure of ($\mathbf{L^4}$)$_2$Sn in the solid state, as determined by X-ray crystallography. Most hydrogen atoms omitted and Dipp and ^{t}Bu groups shown in wireframe format for clarity. Thermal ellipsoids set at the 50% probability level. Colour coding: green – boron; grey - carbon; blue – nitrogen, pink – tin.

4. Xyz files for DFT calculated structures

($\mathbf{L^1}$)Si
139

Si	0.74532954	4.93722387	10.68544675
N	0.15706138	3.28078654	10.92353094
C	-0.15389583	2.61284449	9.63503077
C	0.74856620	3.24090392	8.57830143
N	0.90923658	4.67319166	8.93661705
B	1.31285029	5.63374576	7.92475244
N	1.80830524	5.38078466	6.57000833
C	2.05246911	6.62206898	5.94883593
C	1.74786908	7.62791971	6.80624209
N	1.29349728	7.09083647	8.02345641
C	0.85269878	7.97209706	9.06982337
C	-0.51895670	8.31078990	9.15798464
C	-0.91743995	9.20759081	10.15998967
C	0.00904563	9.76618283	11.03863188
C	1.35794868	9.43203085	10.92970628
C	1.80732154	8.53382462	9.95188066
C	3.29209560	8.20510605	9.84857948
C	3.88016252	7.73768399	11.19141164
C	4.08731528	9.40132949	9.28855138
C	-1.55363139	7.75772165	8.18531447
C	-2.10695072	8.86869147	7.27145229
C	-2.69373582	7.02244571	8.91104499
C	2.10799832	4.16954199	5.85449829
C	1.14936313	3.63813469	4.95695367
C	1.47474383	2.46987350	4.25225319
C	2.70971033	1.84540337	4.42075005
C	3.64864640	2.39025679	5.29505275
C	3.37416345	3.55870725	6.02153184
C	4.44745315	4.16131910	6.92128379
C	5.56141035	4.81359036	6.07748494
C	5.03823585	3.13955303	7.90785234
C	-0.19835277	4.31321687	4.72337043
C	-1.38294623	3.34624206	4.90221608
C	-0.24736348	4.97897403	3.33348075
B	-0.17984853	2.63404670	12.17905567
N	0.31863555	2.96521023	13.51068574
C	1.29498256	3.92383408	13.95036678

C	0.86198411	5.13863849	14.53500319
C	-0.61569990	5.48321897	14.68094873
C	-1.05595717	5.43105679	16.15736921
C	-0.95779588	6.84680112	14.05476876
C	1.83506504	6.03273878	15.00285856
C	3.19422457	5.74311813	14.89511837
C	3.60384917	4.54115974	14.32066555
C	2.67119349	3.60695815	13.84718727
C	3.15776704	2.28015431	13.27676489
C	3.79983771	1.40818029	14.37370535
C	4.12185937	2.47728615	12.09395615
C	-0.25645059	2.07670931	14.43632621
C	-1.07634199	1.21093736	13.78919009
N	-1.07168700	1.49722179	12.40942975
C	-1.91455096	0.73578635	11.52741720
C	-3.19758267	1.23110401	11.19155532
C	-4.00775937	0.45804978	10.34638507
C	-3.57391450	-0.77236891	9.85583370
C	-2.31490094	-1.25467730	10.21030324
C	-1.46435909	-0.51931398	11.04870252
C	-0.10513574	-1.09174952	11.43791421
C	-0.26306827	-2.28205891	12.40510459
C	0.73656612	-1.49801291	10.21430641
C	-3.72987042	2.54272130	11.75774046
C	-4.25750605	3.48775548	10.66457984
C	-4.81327294	2.27744907	12.82253350
H	-1.21532990	2.76388277	9.37329022
H	0.01487072	1.52931190	9.69518217
H	1.73213188	2.74022190	8.56594829
H	0.31210755	3.12423963	7.57776067
H	2.43389036	6.67997218	4.93518393
H	1.81015441	8.69961889	6.65090361
H	2.07760215	9.87605714	11.62012623
H	3.39103088	7.37690002	9.13244000
H	4.92487776	7.42036569	11.05785188
H	3.31172214	6.89379768	11.60507102
H	3.87543109	8.54479306	11.93894510
H	4.01497600	10.27089253	9.95921778
H	3.71441179	9.70637418	8.30113240
H	5.15154476	9.14225182	9.18541197
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H	-2.63207057	9.63945159	7.85543795
H	-2.82099631	8.45141844	6.54597174
H	-1.30076442	9.36220518	6.71147805

H	-2.30355592	6.21722912	9.54864371
H	-3.38805413	6.57793961	8.18306221
H	-3.27468785	7.70469443	9.54924734
H	0.74861528	2.04244646	3.55787584
H	2.94335341	0.93551855	3.86437518
H	4.61845868	1.90239979	5.41119146
H	3.97003991	4.95733211	7.50980595
H	4.67012393	4.31665045	14.24930598
H	5.57807845	2.33423837	7.38822341
H	4.25609200	2.67608374	8.52463391
H	5.75341430	3.63252155	8.58181087
H	-0.29727426	5.10919202	5.47504810
H	-1.37442484	2.87165305	5.89326846
H	-1.37254761	2.54539711	4.14840208
H	-2.33427682	3.88719108	4.79422820
H	0.56059794	5.71316723	3.21301749
H	-1.20523357	5.50005827	3.18879715
H	-0.14484021	4.23056713	2.53327608
H	-1.18297957	4.71386361	14.13820886
H	-0.86757830	4.44315031	16.59994336
H	-2.13148552	5.64453336	16.24638645
H	-0.51346621	6.17694286	16.75775238
H	-0.63916248	6.89478893	13.00476463
H	-0.46952081	7.67304741	14.59260148
H	-2.04289287	7.02226180	14.09730609
H	2.27572384	1.74301376	12.90126736
H	4.10866933	0.43574064	13.96217461
H	3.09648162	1.22258943	15.19707544
H	4.69235094	1.89363330	14.79631567
H	5.04724709	2.98435981	12.40490343
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H	4.40529020	1.50535532	11.66419267
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H	0.43922219	-0.30069178	11.97295483
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H	-0.81500510	-1.99274607	13.30954543
H	1.73250772	-1.83736185	10.53406823
H	0.87249496	-0.65921551	9.51750058
H	0.27107431	-2.32331428	9.65581203

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H	-5.13087754	3.06529401	10.14610407
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H	-0.32071925	10.46635291	11.80865035
H	1.52178914	6.97510262	15.45646765
H	3.93626962	6.45445308	15.26288756
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H	6.07314237	4.06537949	5.45347467

(**L**^{2})Si
142

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N	1.46545954	1.87996496	21.82200994
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N	1.86010878	-0.47336177	23.15337635
B	1.79002342	-1.48040142	24.19861328
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C	1.72999226	-3.65104319	22.83307368
C	2.81914984	-4.20699343	22.12996074
C	2.55637930	-4.87370732	20.92502519
C	1.25481950	-4.98209354	20.43355136
C	0.18861982	-4.44225681	21.15328664
C	0.40148222	-3.77692905	22.36830537
C	-0.77894148	-3.24861707	23.17199224
C	-1.66208137	-4.40546424	23.67281446
C	-1.59799168	-2.21146422	22.39555484
C	4.23251482	-4.12614046	22.68643080
C	4.58762597	1.82729336	25.72646303
C	4.50495891	-0.35668971	27.01075560
C	1.85049984	-3.51859063	25.30805717
C	1.64954790	-2.55591125	26.24713464
N	1.61148842	-1.29644053	25.62338487
C	1.32132576	-0.09202921	26.33667923
C	2.35518061	0.85383951	26.53241394
C	2.04102936	2.02825949	27.22556088

C	0.74883870	2.25973270	27.70243228
C	-0.25663569	1.31946070	27.48822415
C	0.00579620	0.12902349	26.79590958
C	-1.11238586	-0.87118599	26.53032815
C	-1.66245380	-1.45586835	27.84255484
C	-2.23216782	-0.26060077	25.67186832
C	3.76367168	0.56850126	26.02555568
C	4.62481298	-5.46414908	23.34227479
C	5.26888899	-3.70506037	21.63202702
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C	-3.05384391	0.35678802	20.88768660
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C	-3.54830999	1.64249838	22.87392837
C	-2.50646760	2.53326072	22.58809274
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C	-3.34827241	4.75290629	23.43376833
C	-1.96219243	3.27229286	24.96277586
C	-1.16391173	0.97826544	19.30842900
C	-0.28489154	-0.27606863	19.46447217
C	-2.03161651	0.89420683	18.04079588
C	2.57002286	4.88488675	21.35490260
C	3.62658740	4.95315586	20.42067897
C	4.86038714	5.45663340	20.85470989
C	5.04084652	5.87177155	22.17519522
C	3.98067752	5.80966406	23.07932304
C	2.72367730	5.32770388	22.68739241
C	1.56258493	5.31847031	23.67231967
C	1.81780628	4.37779353	24.85672825
C	1.22414021	6.74285070	24.14677813
C	3.41474889	4.52140005	18.97692275
C	3.16601104	5.75228861	18.08413269
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H	2.42367269	1.19854180	20.05876497
H	4.45511740	0.34915669	21.07631254
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H	2.43829924	-1.17299952	21.21897771
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H	5.54399414	1.54367238	25.26447138
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H	4.06304940	2.50136890	25.03637522
H	5.50948206	-0.60052545	26.63387111
H	3.95719011	-1.29703753	27.15710044
H	4.61483272	0.13483773	27.98911924
H	1.92614339	-4.59325451	25.43267672
H	1.54537359	-2.65455518	27.32230020
H	2.81080871	2.78273695	27.38629210
H	0.52475208	3.18658524	28.23359489
H	-1.26870921	1.52050218	27.84449056
H	-0.68357894	-1.70351710	25.95669094
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H	-2.43404757	-2.21153642	27.63441692
H	-2.11759572	-0.67288219	28.46746014
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H	-2.98258668	-1.02660364	25.42624550
H	3.65691675	0.02241348	25.07644960
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H	3.91686300	-5.73578048	24.13723085
H	5.63062342	-5.40269253	23.78332999
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H	5.39944111	-4.47698142	20.85953234
H	0.44341327	6.19486717	20.20522480
H	-1.91991908	4.82853322	20.36164870
H	-3.26790559	-0.49841678	20.24454412
H	-4.62968315	-0.12812924	22.27820589
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H	-1.29957946	4.19223155	23.15450342
H	-3.11256967	5.62539968	24.06070795
H	-4.30026375	4.32814362	23.78628128

H	-3.49727202	5.10122930	22.40222627
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H	-2.85839433	2.82532884	25.41694025
H	-1.67965092	4.14215805	25.57408184
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H	0.36213597	-0.40731473	18.58472294
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H	0.35442912	-0.19705109	20.35385902
H	-2.65437570	1.79221297	17.92683645
H	-2.70052390	0.02115223	18.06666812
H	-1.39668538	0.79846492	17.14785979
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H	6.01191981	6.25129687	22.49879394
H	4.12828033	6.14695778	24.10729291
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H	2.69518073	4.68963608	25.44264590
H	1.98595924	3.34834888	24.51375425
H	0.95074215	4.35385436	25.53062766
H	2.05401472	7.18485699	24.71817009
H	0.33894252	6.72468806	24.79918424
H	1.01039810	7.40233837	23.29423857
H	2.50078683	3.90916988	18.95908170
H	4.04219848	6.41808924	18.08899457
H	2.30151636	6.32915628	18.43972069
H	2.97192667	5.44770986	17.04514337
H	5.49893989	4.24357375	18.33803421
H	4.31649648	3.29281210	17.42430990
H	4.76788795	2.80074530	19.07452402

($\mathbf{L^3}$)$_2$Si

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C	11.44710700	8.73499936	1.27647766
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C	7.92565863	3.30043383	2.23748491
C	8.92147583	2.34759373	2.41118499
C	9.94412404	2.59254179	3.32532939

C	10.02054194	3.79727411	4.03824815
C	11.05640737	3.95262106	5.14871371
C	12.14223514	2.87073536	5.14964925
C	10.38301721	3.96575219	6.53825754
C	6.74336211	5.45370827	2.73400753
C	6.34964561	5.67171206	1.26001270
C	5.52305466	4.89709179	3.50014046
C	8.11130046	6.38578604	5.33992829
C	8.30940710	7.60147851	5.88348676
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C	10.32347811	11.86334648	7.42702696
C	10.19365942	11.83516958	6.04221991
C	9.92201762	10.64502119	5.35279100
C	9.62754670	10.71097608	3.86262275
C	8.10442424	10.78616262	3.62791067
C	10.33080034	11.86293616	3.13082745
C	9.82160819	8.22320530	8.41447127
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H	12.17701503	6.07099842	1.07632405
H	10.62641970	5.36152607	1.58458247
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H	8.69146255	6.83098251	2.04104998
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H	12.54173076	8.66374315	1.33198106
H	11.15229533	9.67003364	1.76701850
H	7.09298388	3.08566412	1.56615043
H	8.88514027	1.40429747	1.86477173
H	10.68930340	1.81947014	3.50530483
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H	12.91131986	3.11930894	5.89331714
H	12.64383218	2.77539907	4.17959020
H	11.72810387	1.88730474	5.42184073
H	11.14458002	4.09294526	7.32198354
H	9.64938770	4.77528330	6.64007679
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H	6.98601103	6.43250537	3.16642357
H	5.54878351	6.42322693	1.19400052
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H	4.67424197	5.59402284	3.42608584
H	5.73686511	4.73365310	4.56493720
H	5.20710380	3.93102886	3.07787421
H	7.30534520	5.69055209	5.53291366
H	7.67847775	8.12965921	6.58363673
H	10.26354107	10.70039005	9.22664217
H	10.52213710	12.80189464	7.94622825
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H	9.99663515	9.77595652	3.42923264
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H	7.69442094	11.70941242	4.06662748
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H	10.16201647	11.77198033	2.04806570
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C	16.24212607	2.23962355	5.66754641
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C	15.87123597	3.96607431	3.98412637
C	15.53229760	4.32227821	2.53716923
C	14.34585322	3.55024992	1.94649114
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C	17.39882129	5.35683180	8.51395577
C	19.27858729	5.23297903	6.84909809
C	17.71642165	6.77507788	3.94974846
C	17.54450254	8.01343213	3.42704354

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C	15.06250197	10.56165981	0.73651511
C	14.83548193	11.77549996	1.37963433
C	15.12286700	11.90062684	2.73766496
C	15.60295137	10.81395567	3.48538665
C	16.05321036	11.02350884	4.92865921
C	17.56825398	11.31504081	4.98920810
C	15.28592767	12.13114973	5.66742891
C	15.90236561	8.17749010	0.65774462
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C	17.24069085	8.38805575	-0.08401231
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H	17.62754281	4.73007972	2.00287350
H	17.09148620	3.06992243	1.64103707
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H	17.91599879	6.13986545	9.08810979
H	16.31993509	5.46567912	8.68552615
H	17.70983944	4.38803370	8.93218050
H	19.84974598	5.95085162	7.45779010
H	19.59570851	5.34742041	5.80417860
H	19.55364048	4.21726282	7.17263953
H	18.62082540	6.18104807	3.99213052
H	18.27671522	8.64918646	2.94484325
H	14.87789565	10.48125066	-0.33584405
H	14.45712069	12.63146126	0.81895880
H	14.98263069	12.86558329	3.22498141

H	15.88776766	10.07796662	5.46120982
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H	17.80738416	12.23812445	4.43830908
H	18.15485681	10.49425639	4.55640397
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H	14.19788773	12.00368452	5.59202017
H	15.54055670	13.12795180	5.27709553
H	16.04271636	7.36661094	1.38452457
H	15.16845372	6.80966640	-0.85904923
H	14.62445062	8.47667176	-1.10865138
H	13.88878195	7.48042960	0.17586414
H	17.54797840	7.45858840	-0.58733272
H	17.14278530	9.17325862	-0.85016324
H	18.04654395	8.68681481	0.59996385

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139

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N	0.93639713	4.72960597	8.93142537
B	1.34875866	5.65001528	7.89889133
N	1.79419507	5.37317243	6.52866939
C	2.06345582	6.60117592	5.89221505
C	1.82567724	7.62355687	6.75214346
N	1.39093343	7.11012825	7.98608981
C	1.03690266	7.99666014	9.05750498
C	-0.31609998	8.38253523	9.22079415
C	-0.63186703	9.27018341	10.25985291
C	0.35599794	9.77315834	11.10477570
C	1.68477867	9.39335480	10.92322315
C	2.05283481	8.50245128	9.90527945
C	3.51747965	8.12208968	9.72125188
C	4.15759711	7.60846291	11.02294246
C	4.32667769	9.30011938	9.14293735
C	-1.41356367	7.89359361	8.28308658
C	-1.92412501	9.04026635	7.38806325
C	-2.57582066	7.22837535	9.04062260
C	2.01845317	4.14779335	5.81097183
C	1.00284142	3.64486615	4.96109304
C	1.25370347	2.45942865	4.25453405
C	2.47139220	1.79140441	4.37419907

C	3.46699540	2.30800198	5.20187206
C	3.26708959	3.49079363	5.92916954
C	4.39767320	4.05579390	6.78180707
C	5.51334741	4.64062782	5.89240568
C	4.97062302	3.02115135	7.76594360
C	-0.33105596	4.36296891	4.78487990
C	-1.53310355	3.45079102	5.09127430
C	-0.45192624	4.96630537	3.37143878
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N	0.22932318	2.96131270	13.55540985
C	1.13350883	3.97955783	14.00813396
C	0.61403793	5.16443208	14.58512527
C	-0.88527310	5.40153306	14.72619827
C	-1.32482100	5.31457869	16.20113168
C	-1.32415390	6.73886032	14.10316798
C	1.51915049	6.12892073	15.04978007
C	2.89574430	5.93746443	14.94476239
C	3.39195686	4.76444565	14.37837759
C	2.53005676	3.76276899	13.90823253
C	3.11031346	2.46895047	13.34912406
C	3.78621694	1.64202846	14.46081561
C	4.08151226	2.72146537	12.18288742
C	-0.30861347	2.02995350	14.46054613
C	-1.07289914	1.13145265	13.78902071
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C	-1.84788082	0.64571712	11.50456698
C	-3.14706208	1.07902251	11.14576745
C	-3.89361234	0.28197336	10.26511841
C	-3.38311191	-0.91368595	9.76247314
C	-2.10962573	-1.33664462	10.14060518
C	-1.32045635	-0.57435832	11.01412724
C	0.06017305	-1.07851896	11.42159651
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C	0.95873338	-1.37595157	10.20695864
C	-3.76211200	2.34908849	11.72293246
C	-4.29090813	3.29813229	10.63349473
C	-4.87205978	2.00580766	12.73686655
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H	-0.08265356	1.60512020	9.69559931
H	1.76802183	2.77923371	8.73430235
H	0.42111877	3.11016172	7.63052238
H	2.41117828	6.63998339	4.86548180
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H	4.21992234	8.39971190	11.78467420
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H	-0.96568033	7.13471148	7.62661787
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H	3.97769454	4.88250553	7.37177932
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H	-2.47170374	4.01837429	5.01154120
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H	-1.06565086	4.34196321	16.64144890
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H	-1.00823273	6.81524689	13.05377959
H	-0.89786270	7.59707994	14.64349850
H	-2.41910513	6.83519768	14.14338141
H	2.27033223	1.87695035	12.96020830
H	4.16261108	0.68994782	14.05822657
H	3.08122367	1.41457599	15.27216435
H	4.63878121	2.18389215	14.89728582
H	4.96573433	3.29087526	12.50542697
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H	-0.09344243	2.08274666	15.52242934

H	-1.63769453	0.29093736	14.17783608
H	-4.89677044	0.60029864	9.97412721
H	-3.98091428	-1.51983150	9.07893710
H	-1.71936528	-2.27830354	9.74897449
H	0.53836909	-0.27937140	12.00527248
H	0.94924658	-2.64638008	12.65705676
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H	-0.64505606	-2.10312026	13.22980845
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H	0.55610531	-2.19622145	9.59467348
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H	-5.28360740	2.92302390	13.18352517
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H	3.58404850	6.70238313	15.30942752
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142

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C	3.37611118	0.61096045	21.84241022
C	2.66117172	-0.69279504	22.18820990
N	1.67108700	-0.52460424	23.27358211
B	1.53633496	-1.62841443	24.21026576
N	1.80002817	-3.05334336	23.96795347
C	2.18186111	-3.78551367	22.78986435
C	3.51425632	-4.24763962	22.66209408
C	3.85401695	-4.99386500	21.52314477
C	2.91188129	-5.27280580	20.53659436
C	1.60155363	-4.81487047	20.67894884
C	1.20655405	-4.07456127	21.80229393
C	-0.24749819	-3.64659723	21.97808128

C	-1.01588082	-4.67657321	22.83362625
C	-0.98465195	-3.40692603	20.65235270
C	4.57731595	-3.96942426	23.72083334
C	4.24091712	1.29646331	26.59860811
C	3.94890320	-1.01286328	27.57927529
C	1.57912457	-3.75679153	25.16734477
C	1.19382105	-2.89353269	26.13871516
N	1.15473637	-1.58512800	25.62304032
C	0.84638299	-0.49130288	26.50229062
C	1.89812784	0.32714903	26.98845574
C	1.57132742	1.36458379	27.87240776
C	0.25588799	1.57306320	28.28922426
C	-0.75975825	0.74156866	27.82445261
C	-0.49066918	-0.30034081	26.92418097
C	-1.62722097	-1.20062891	26.45091727
C	-2.18302779	-2.05154215	27.60998282
C	-2.75519906	-0.40433434	25.77251058
C	3.35267349	0.04415688	26.62491031
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C	5.82027690	-3.27526879	23.13247962
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C	-0.88470697	4.96274073	21.04834310
N	-0.73888661	3.64941236	21.52838227
C	-1.91235995	2.86472441	21.79333206
C	-2.34113517	1.91507712	20.83454056
C	-3.50268065	1.17695354	21.10663464
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($\mathbf{L^3}$)$_2$Ge

159

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139

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159

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