Supporting Information

Synthesis and structures of lithium alkoxytris(dimethyl-phenylsilyl)borates

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Contents

1. Experimental Details

Reactions

All experiments were performed under a nitrogen or argon atmosphere unless otherwise noted. Tetrahydrofuran (THF) was distilled from sodium benzophenone ketyl. Toluene was distilled from sodium. THF, hexane and benzene-d_6 used in a glovebox were dried over a potassium mirror, degassed by freeze–pump–thaw cycles, distilled in a vacuum line and stored in the glovebox. Lithium was provided by Shin-Etsu Chemical Co., Ltd. Chlorodimethylphenylsilane was prepared according to the reported procedure.[S1] Trimethyl borate (Kishida) and triisopropyl borate (Tokyo Kasei) were purchased and used without further purification.

Measurements

^{1}H (600 MHz), ^{13}C (151 MHz), ^{7}Li (233 MHz), ^{11}B (193 MHz) and ^{29}Si NMR (119 MHz) spectra were measured with a JEOL JNM-ECA600 spectrometer. Melting points were measured under an argon atmosphere in a sealed tube on a Yanaco MP-J3 micro melting point apparatus and were uncorrected.

Synthesis of lithium tris(dimethylphenylsilyl)methoxyborate (1a). Chlorodimethylphenylsilane (2.51 mL, 15.0 mmol) was added to a mixture of coarsely cut lithium (0.37 g, 53 mmol) in THF (19 mL) at 0 °C, and the mixture was stirred at 0 °C for 4.5 h. After the solvent was removed under reduced pressure, toluene (30 mL) was added to the mixture. The resulting silyllithium solution was added dropwise through a cannula to a solution of trimethyl borate (0.352 mL, 3.16 mmol) in toluene (8 mL) at −78 °C, and the mixture was stirred at −78 °C for 30 min. The supernatant solution of the reaction mixture was transferred, and the solvents were removed under reduced pressure. In a glovebox, the residue was recrystallized by slow vapor diffusion of hexane to a solution of **1a** in THF to give **1a** (0.604 g, 32%) as colorless crystals.

1a. Mp: 108−109 °C. ^{1}H NMR (600 MHz, C_6D_6): δ 0.69 (s, 18H), 1.20−1.22 (m, 8H), 3.04−3.06 (m, 8H), 3.44 (s, 3H), 7.06–7.09 (m, 3H), 7.10−7.13 (m, 6H), 7.57−7.59 (m, 6H). ^{13}C NMR (151 MHz, C_6D_6): δ 3.0, 25.3, 59.4, 68.1, 127.0, 128.3, 134.6, 150.4. ^{7}Li NMR (233 MHz, C_6D_6): δ 0.3. ^{11}B NMR (193 MHz, C_6D_6): δ −7.5 ($\Delta\nu_{1/2}$ = 162 Hz). ^{29}Si NMR (119 MHz, C_6D_6): δ −13.8 ($\Delta\nu_{1/2}$ = 126 Hz). Measurement of a mass spectrum and elemental analysis were not successful due to its high sensitivity to moisture.

Synthesis of lithium tris(dimethylphenylsilyl)isopropoxyborate (1b). Compound **1b** was synthesized with the similar method by using triisopropyl borate (0.69 mL, 2.99 mmol) and dimethylphenylsilyllithium prepared from chlorodimethylphenylsilane (2.51 mL, 15.0 mmol),

lithium (0.31 g, 45 mmol) in THF (19 mL). Compound **1b** (0.712 g, 31%) was obtained as colorless crystals.

1b. Mp: 138−139 °C. ^{1}H NMR (600 MHz, C_6D_6): δ 0.61 (s, 18H), 1.08 (d, 6H, J = 6.1 Hz), 1.26−1.29 (m, 12H), 3.25−3.30 (m, 12H), 4.23 (sept, 1H, J = 6.1 Hz), 7.04–7.07 (m, 3H), 7.11–7.14 (m, 6H), 7.59−7.61 (m, 6H). ^{13}C NMR (151 MHz, C_6D_6): δ 2.6, 25.5, 26.1, 68.2, 74.1, 127.2, 128.3, 134.6, 150.0. ^{7}Li NMR (233 MHz, C_6D_6): δ 0.5. ^{11}B NMR (193 MHz, C_6D_6): δ −7.8 ($\Delta\nu_{1/2}$ = 171 Hz). ^{29}Si NMR (119 MHz, C_6D_6): δ −14.8 ($\Delta\nu_{1/2}$ = 117 Hz). Measurement of a mass spectrum and elemental analysis were not successful due to its high sensitivity to moisture.

Attempt at further silylation of 1a with dimethylphenylsilyllithium. Compound **1a** was synthesized with the similar method by using trimethyl borate (0.360 mL, 3.23 mmol) and dimethylphenylsilyllithium prepared from chlorodimethylphenylsilane (2.00 mL, 11.9 mmol) and lithium (0.24 g, 35 mmol) in THF (15 mL). After the reaction was completed, the supernatant solution of the reaction mixture was transferred, and the solvents were removed under reduced pressure. The residue was dissolved in THF (3.8 mL). To this solution, dimethylphenylsilyllithium prepared from chlorodimethylphenylsilane (0.76 mL, 4.5 mmol) and lithium (0.12 g, 17 mmol) in THF (9.6 mL) was added at –78 ºC. The reaction mixture was warmed to room temperature and then refluxed. The reaction progress was monitored by ^{1}H, ^{7}Li and ^{11}B NMR measurement, but no reaction took place.

Attempt at further silylation of 1b with dimethylphenylsilyllithium. Compound **1b** was synthesized with the similar method by using triisopropyl borate (0.69 mL, 3.0 mmol) and dimethylphenylsilyllithium prepared from chlorodimethylphenylsilane (2.52 mL, 15.0 mmol) and lithium (0.34 g, 49 mmol) in THF (19 mL). After the reaction was completed, the supernatant solution of the reaction mixture was transferred, and the solvents were removed under reduced pressure. The residue was dissolved in toluene (13.8 mL). To this solution, dimethylphenylsilyllithium prepared from chlorodimethylphenylsilane (0.76 mL, 4.5 mmol) and lithium (0.14 g, 20 mmol) in THF (6 mL) was added at –78 ºC. The reaction mixture was warmed to room temperature and then refluxed. The reaction progress was monitored by ^{1}H, ^{7}Li and ^{11}B NMR measurement, but no reaction took place.

2. Spectral Data

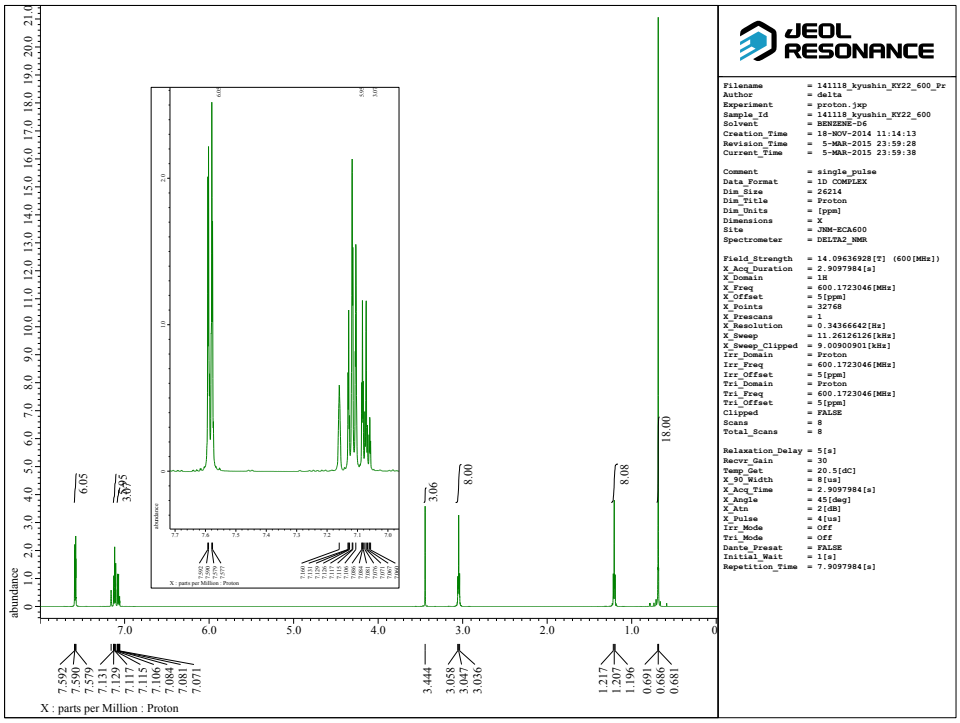


Fig. S1 ^{1}H NMR spectrum of **1a** in C_6D_6 at room temperature.

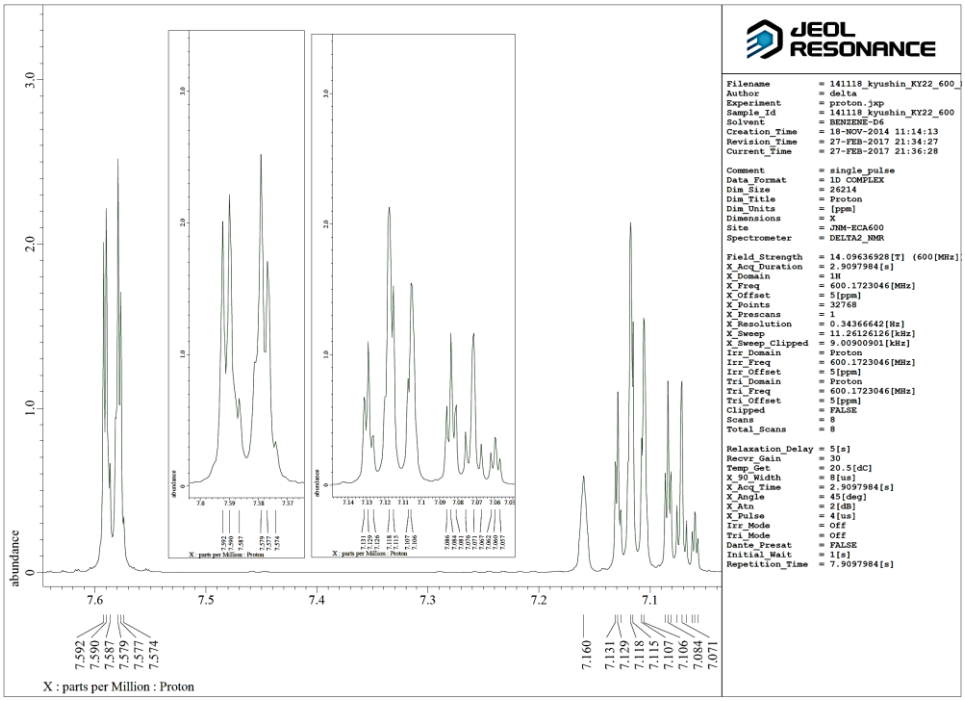


Fig. S2 Expansion of ^{1}H NMR spectrum of **1a** in C_6D_6 at room temperature.

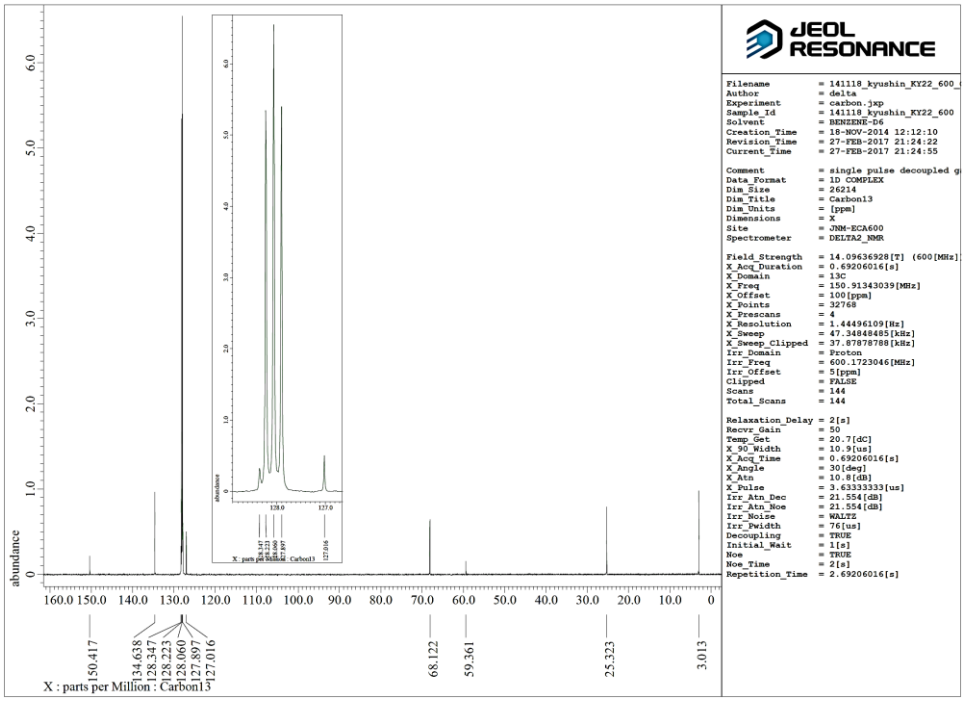


Fig. S3 ^{13}C NMR spectrum of **1a** in C_6D_6 at room temperature.

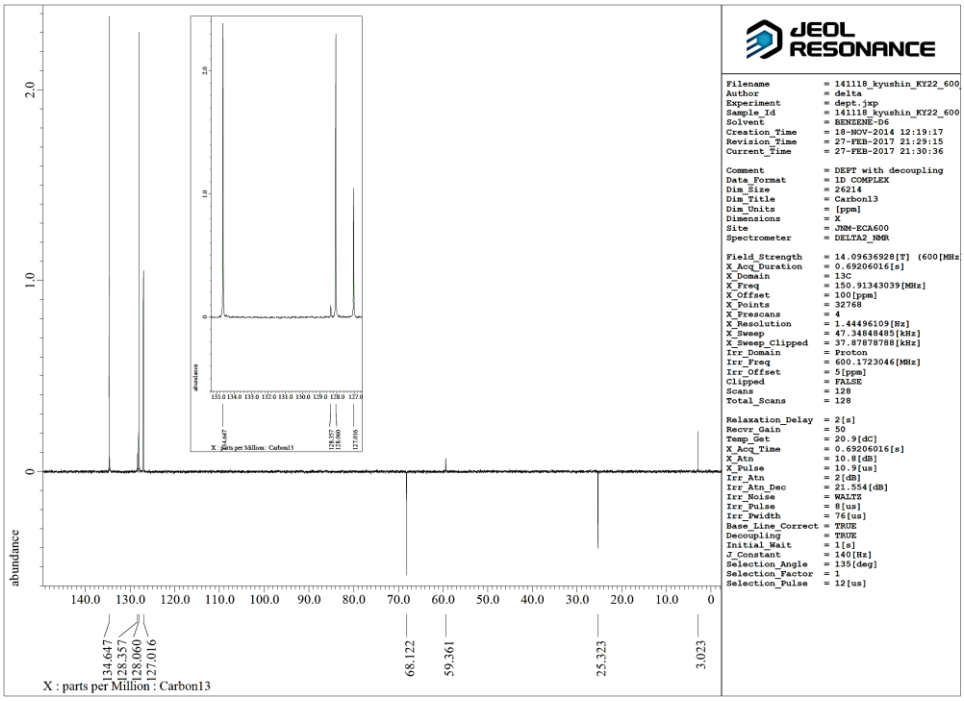


Fig. S4 ^{13}C DEPT NMR spectrum of **1a** in C_6D_6 at room temperature.

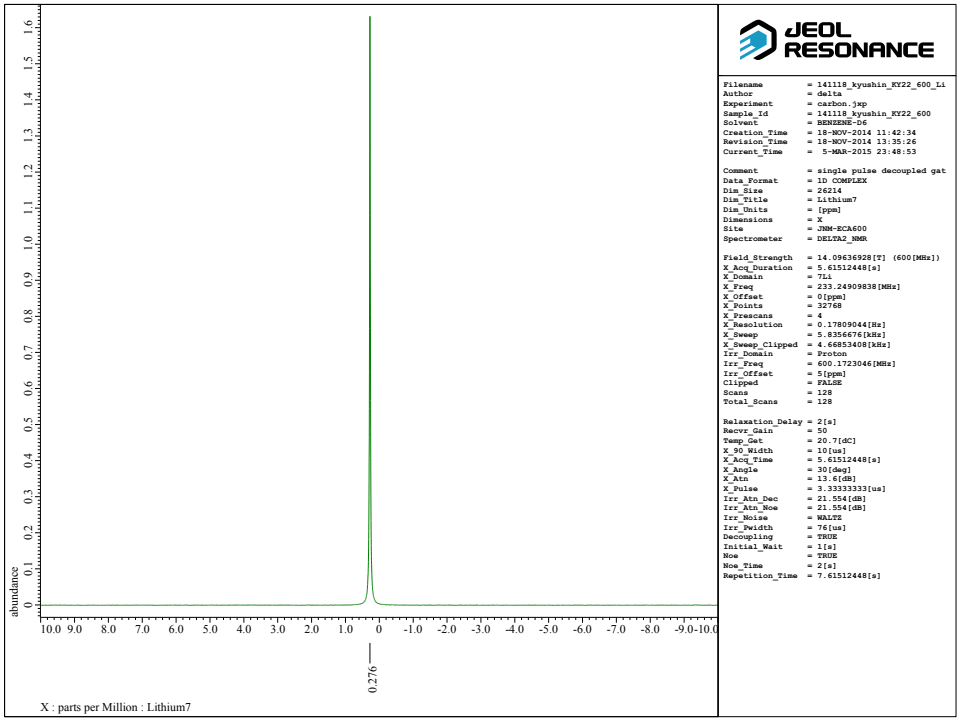


Fig. S5 ^{7}Li NMR spectrum of **1a** in C_6D_6 at room temperature.

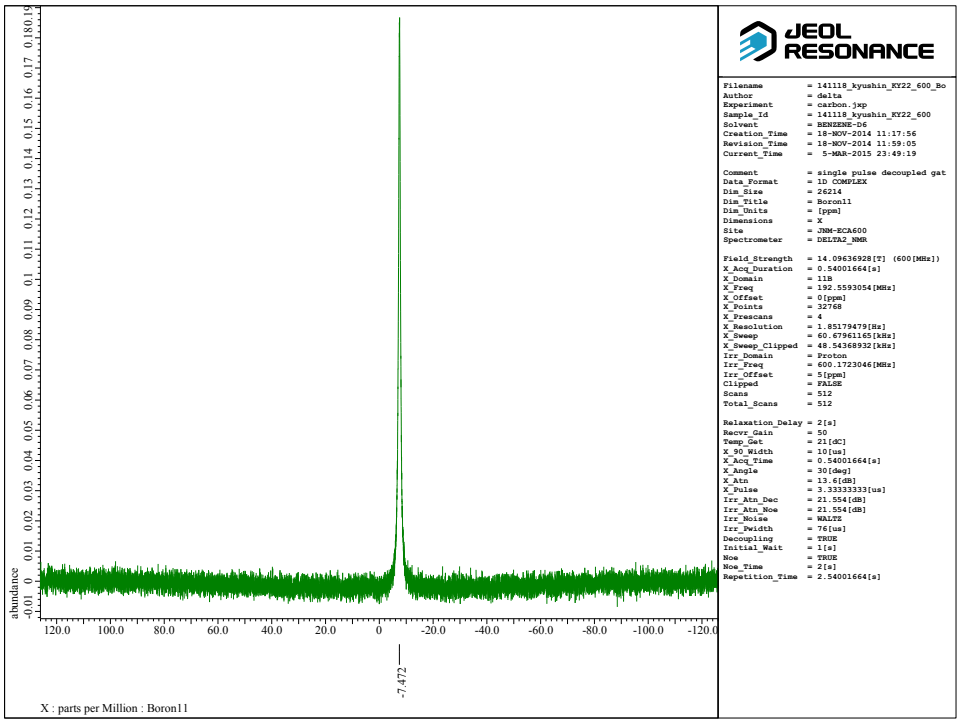


Fig. S6 ^{11}B NMR spectrum of **1a** in C_6D_6 at room temperature.

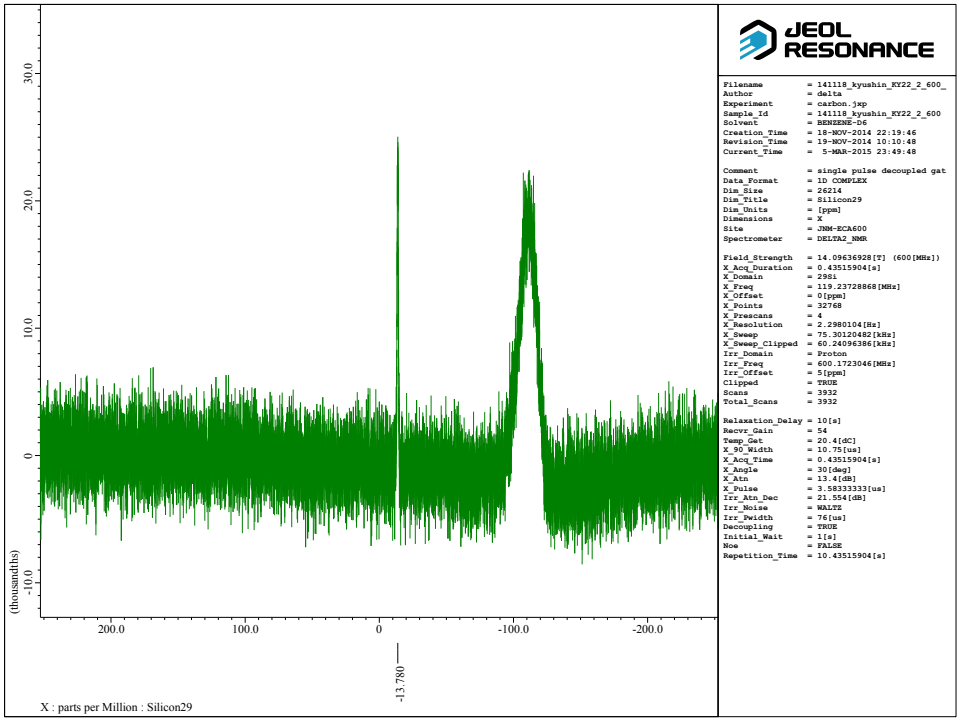


Fig. S7 ^{29}Si NMR spectrum of **1a** in C_6D_6 at room temperature.

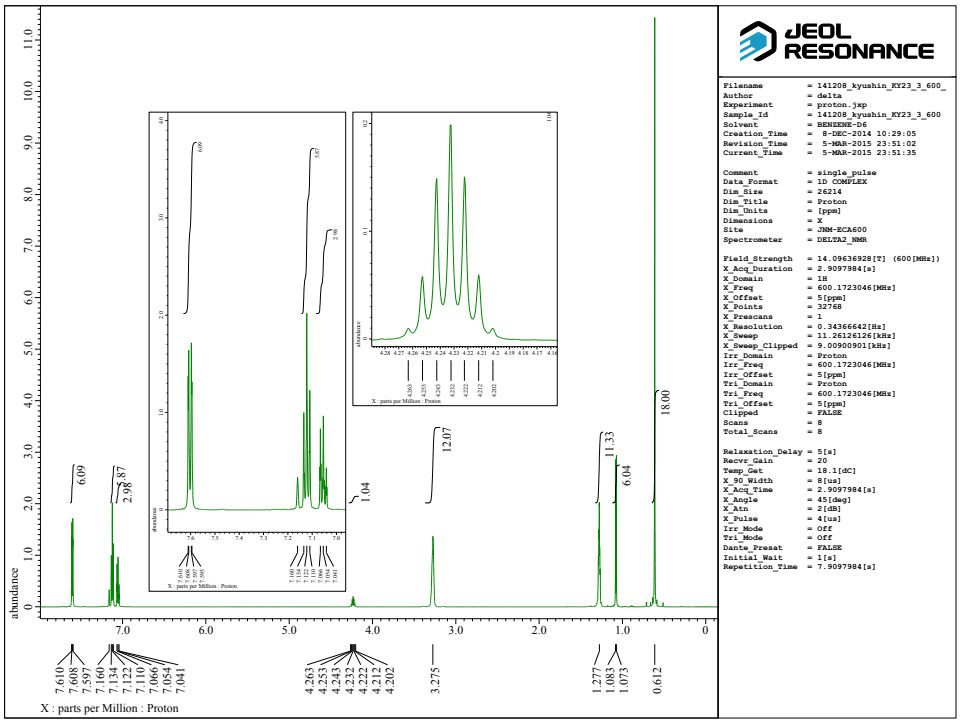


Fig. S8 ^{1}H NMR spectrum of **1b** in C_6D_6 at room temperature.

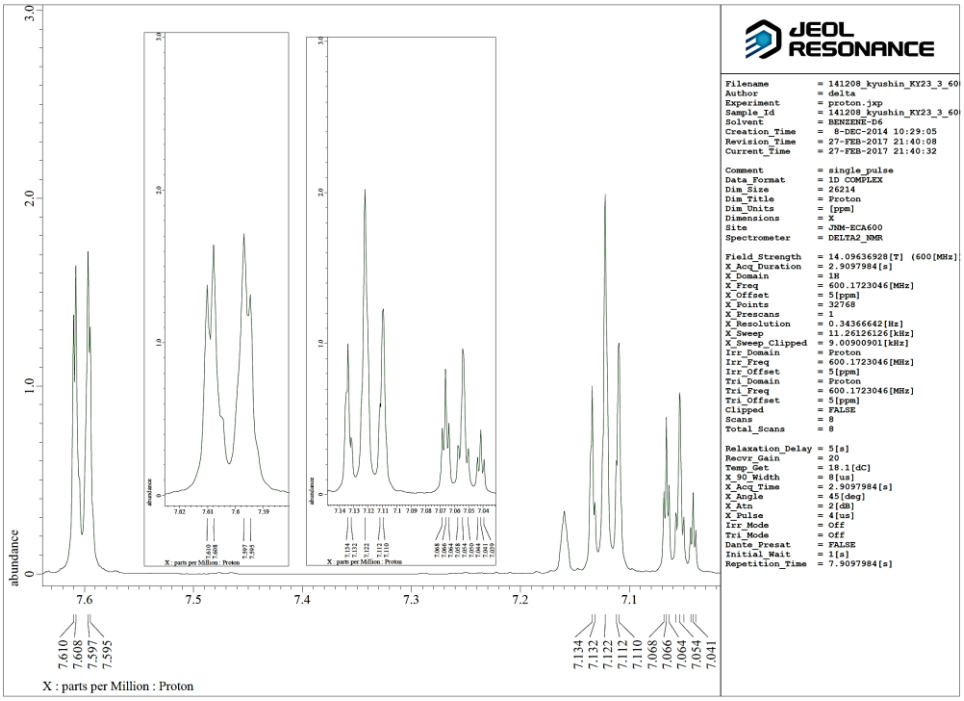


Fig. S9 Expansion of ^{1}H NMR spectrum of **1b** in C_6D_6 at room temperature.

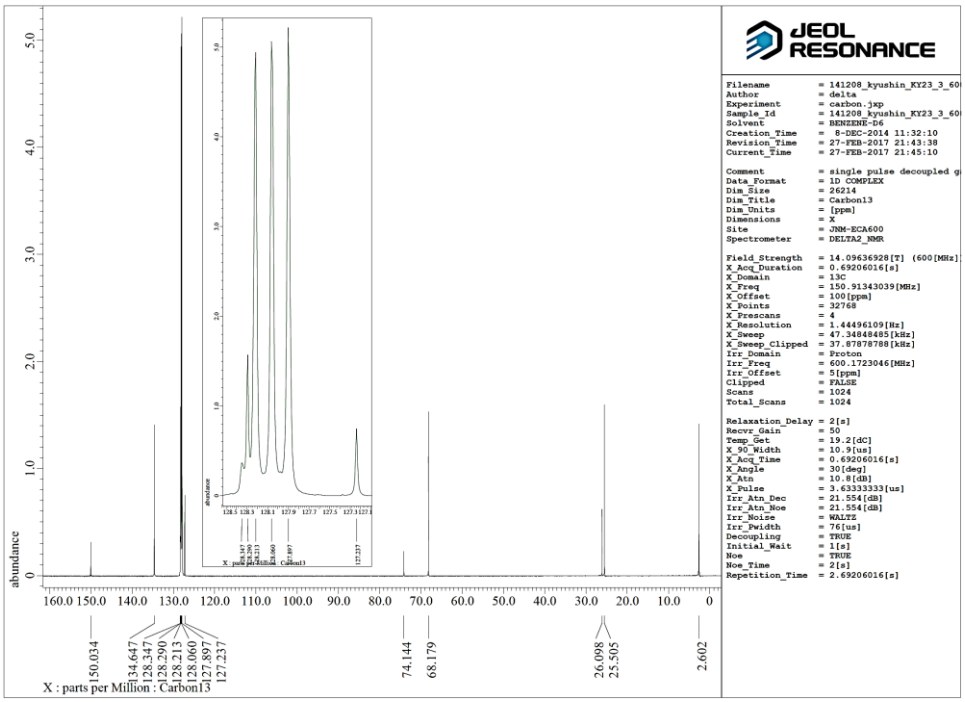


Fig. S10 ^{13}C NMR spectrum of **1b** in C_6D_6 at room temperature.

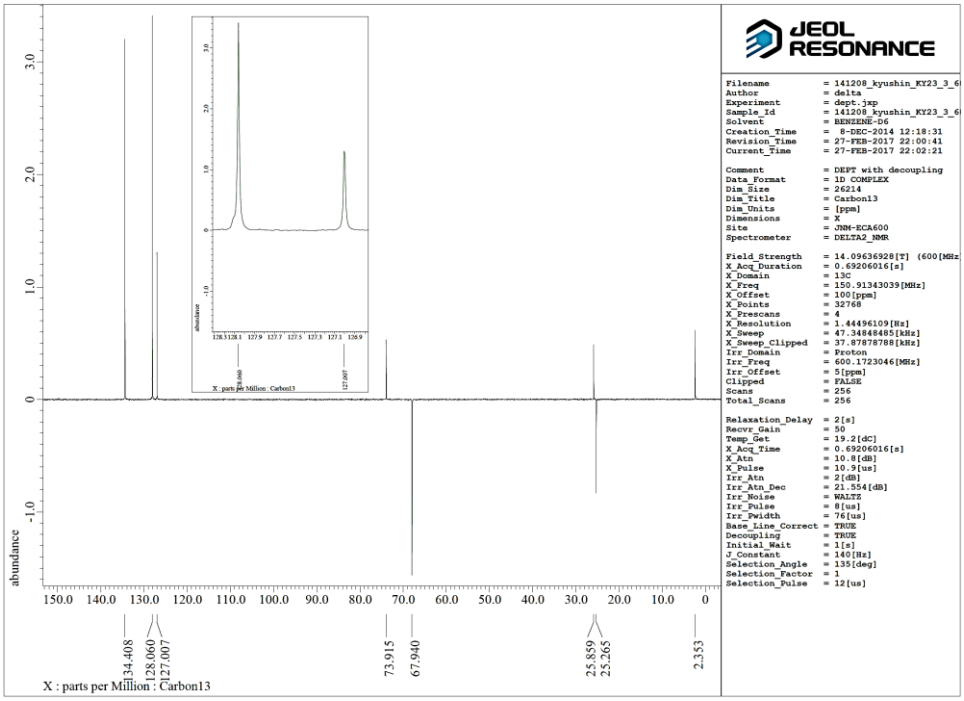


Fig. S11 ^{13}C DEPT NMR spectrum of **1b** in C_6D_6 at room temperature.

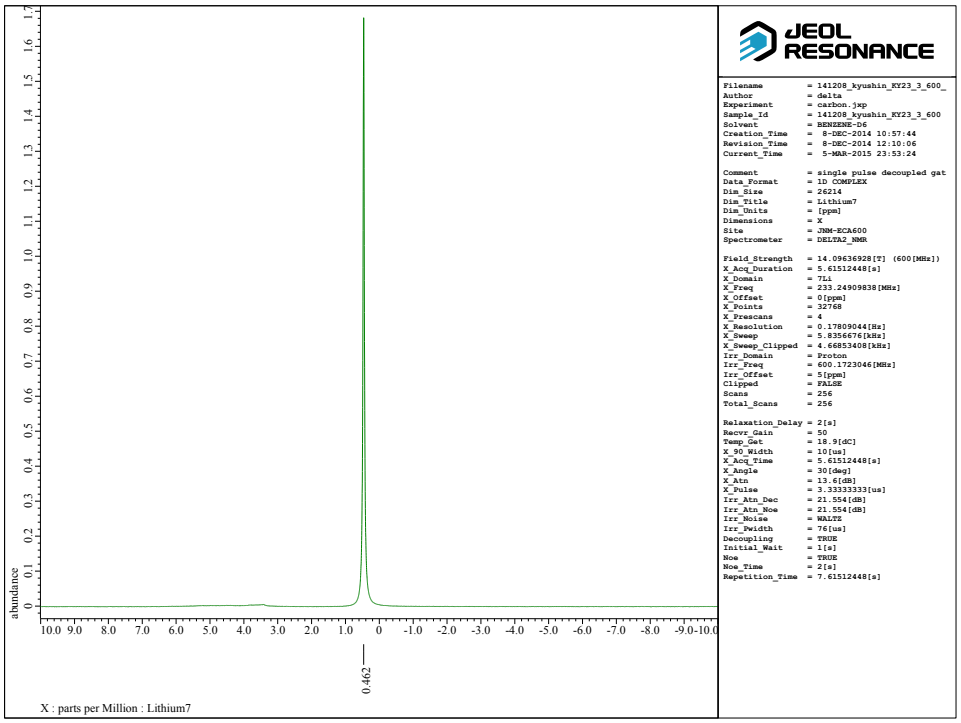


Fig. S12 ^{7}Li NMR spectrum of **1b** in C_6D_6 at room temperature.

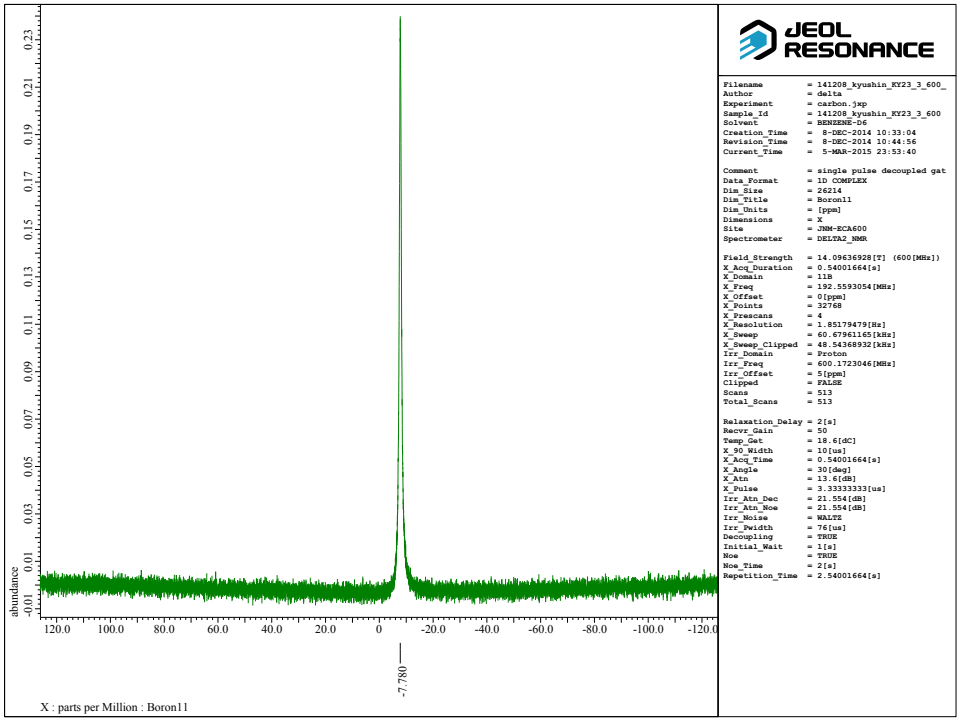


Fig. S13 ^{11}B NMR spectrum of **1b** in C_6D_6 at room temperature.

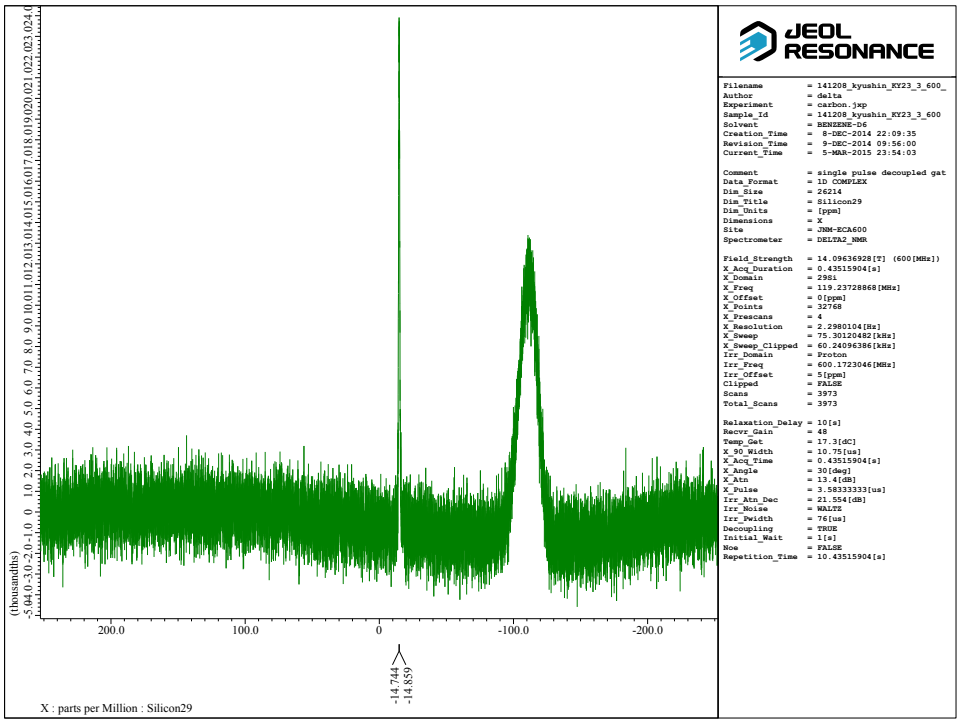


Fig. S14 ^{29}Si NMR spectrum of **1b** in C_6D_6 at room temperature.

3. X-ray Crystallographic Analysis

Colorless crystals of **1a** and **1b** were grown by recrystallization with slow diffusion of hexane vapor into THF solutions at room temperature under an argon atmosphere. Colorless crystals of **1a'** were grown by recrystallization with slow diffusion of hexane vapor into a toluene−TMEDA solution at room temperature under an argon atmosphere. Intensity data were collected on a Rigaku XtaLAB P200 diffractometer using multilayer mirror monochromated Mo Kα radiation. The data were corrected for Lorentz and polarization effects. An empirical absorption correction based on multi-scan was also applied. The structures were solved by a direct method using SIR2004[S2] and refined by the full-matrix least-squares method on F^2 for all reflections using SHELXL-97.[S3,S4] Non-hydrogen atoms were refined anisotropically. All hydrogen atoms were generated by AFIX instructions and were not refined. All calculations were carried out using Yadokari-XG 2009.[S5]

Crystal data for **1a** (123 K): $C_{33}H_{52}BLiO_3Si_3$, fw 598.77, monoclinic, space group $P2_1/c$, colorless crystal, a = 11.216(2), b = 20.479(4), c = 30.789(5) Å, β = 95.103(4)°, V = 7044(2) Å^3, Z = 8, D_{calcd} = 1.129 g cm^{-3}, R_1 = 0.107 (all data), wR_2 = 0.268 (all data), GOF = 1.13.

Crystal data for **1a'** (98 K): $C_{31}H_{52}BLiN_2OSi_3$, fw 570.77, orthorhombic, space group $P2_12_12_1$, colorless crystal, a = 12.5945(17), b = 13.796(2), c = 19.569(3) Å, V = 3400.2(9) Å^3, Z = 4, D_{calcd} = 1.115 g cm^{-3}, R_1 = 0.051 (all data), wR_2 = 0.089 (all data), GOF = 1.05.

Crystal data for **1b** (123 K): $C_{43}H_{72}BLiO_5Si_3$, fw 771.03, monoclinic, space group $P2_1/n$, colorless crystal, a = 16.4003(19), b = 14.5611(18), c = 19.366(2) Å, β = 97.897(3)°, V = 4580.9(9) Å^3, Z = 4, D_{calcd} = 1.118 g cm^{-3}, R_1 = 0.070 (all data), wR_2 = 0.187 (all data), GOF = 1.07.

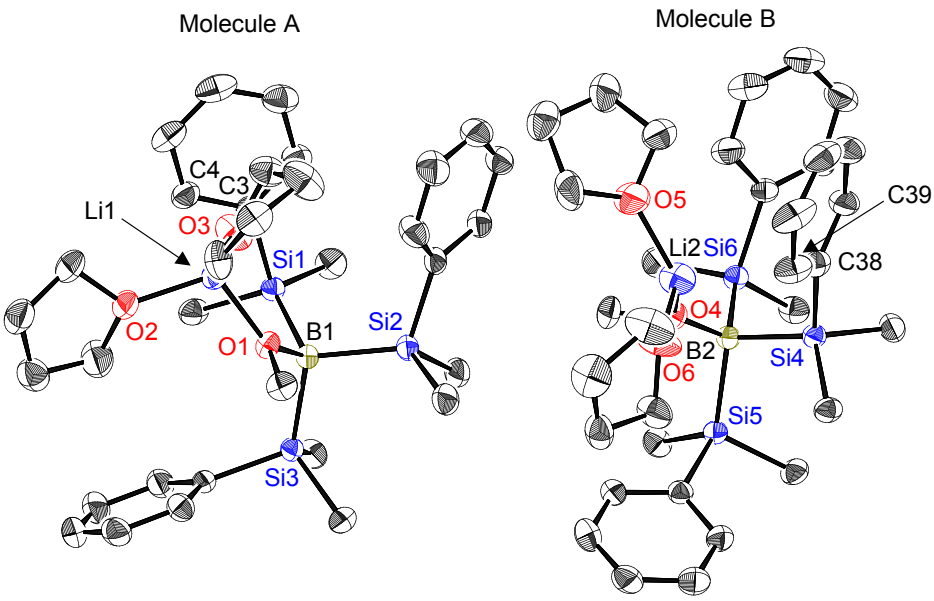


Fig. S15 Molecular structures of **1a**. Selected bond lengths (Å), angles (deg) and atomic distances (Å) of molecule B: Si4−B2 2.043(5), Si5−B2 2.063(5), Si6−B2 2.057(5), B2−O4 1.530(5), Li2−O4 1.852(9), Li2−O5 1.904(10), Li2−O6 1.992(17); Si4−B2−Si5 107.3(2), Si4−B2−Si6 110.1(2), Si5−B2−Si6 106.8(2); Li2···C38 2.867(11), Li2···C39 2.526(12).

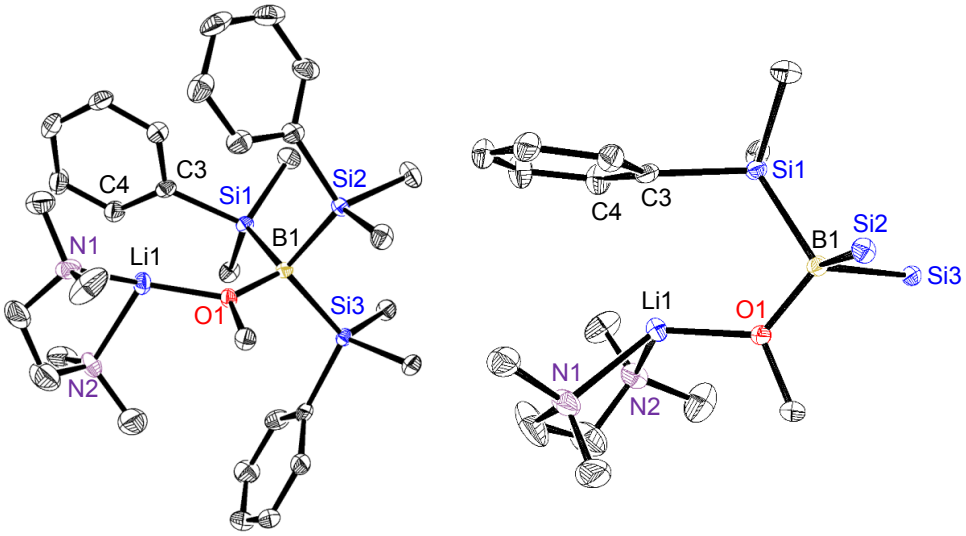
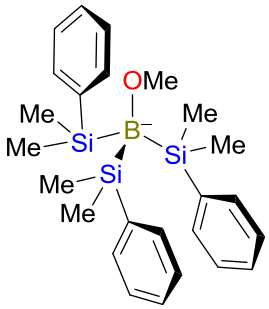


Fig. S16 Molecular structure of **1a'**. Selected bond lengths (Å), angles (deg) and atomic distances (Å): Si1−B1 2.054(2), Si2−B1 2.056(2), Si3−B1 2.071(2), B1−O1 1.535(2), Li1−O1 1.866(4), Li1−N1 2.129(4), Li1−N2 2.124(4); Si1−B1−Si2 109.37(10), Si1−B1−Si3 108.95(10), Si2−B1−Si3 106.13(10); Li1···C3 2.733(4), Li1···C4 2.957(4).

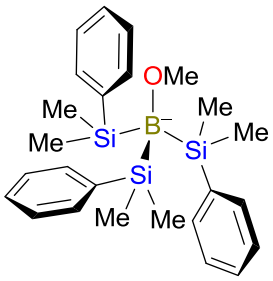
4. Theoretical Calculations

All theoretical calculations were performed using the Gaussian 09[S6] on a Fujitsu PRIMERGY RX300 system of the Research Center for Computational Science, Japan. The structures were optimized at the B3LYP/6-31+G(d) level. It was confirmed by frequency calculations that the optimized structures have no imaginary frequency. The results are summarized in Tables S1–S3.

Table S1 Structural parameters of **1a-X** and **1a-Y**



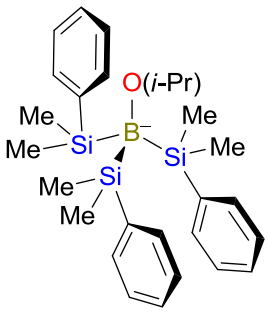
1a-X
parallel geometry
(2.5 kcal mol^{-1})



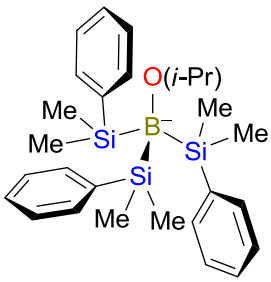
1a-Y
Propeller-like geometry
(0 kcal mol^{-1})

Structural parameter	Calculated		Observed		
	1a-X	**1a-Y**	**1a** (Molecule A)	**1a** (Molecule B)	**1a'**
d(Si−B) / Å	2.076	2.084	2.050(5)	2.043(5)	2.054(2)
	2.088	2.073	2.051(5)	2.063(5)	2.056(2)
	2.084	2.093	2.073(5)	2.057(5)	2.071(2)
d(B−O) / Å	1.506	1.499	1.526(5)	1.530(5)	1.535(2)
angle(Si−B−Si) / º	108.9	109.4	110.6(2)	107.3(2)	109.37(10)
	108.6	109.5	107.3(2)	110.1(2)	108.95(10)
	108.4	109.2	105.9(2)	106.8(2)	106.13(10)

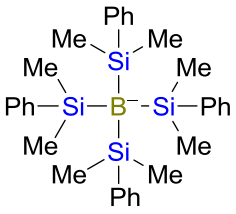
Table S2 Structural parameters of **1b-X**, **1b-Y**, $\mathbf{4}^-$ and $\mathbf{5}^-$



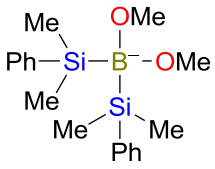
1b-X
Parallel geometry
(9.5 kcal mol^{-1})



1b-Y
Propeller-like geometry
(0 kcal mol^{-1})



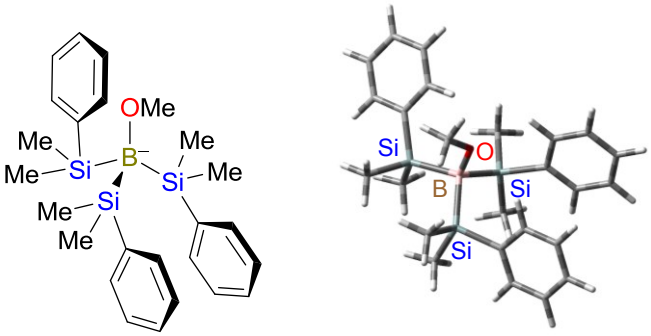
$\mathbf{4}^-$



$\mathbf{5}^-$

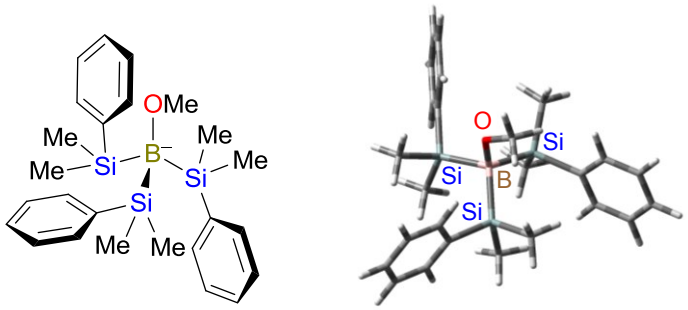
Structural parameter	Calculated		Observed	Calculated	
	1b-X	**1b-Y**	**1b**	**4^-**	**5^-**
d(Si−B) / Å	2.099	2.078	2.046(2)	2.058, 2.066	2.107
	2.094	2.083	2.048(2)	2.068, 2.072	2.108
	2.105	2.093	2.040(2)		
d(B−O) / Å	1.500	1.504	1.521(3)	–	1.484, 1.493
angle(Si−B−Si) / °	109.0	108.8	107.98(10)	105.3, 108.1	111.5
	109.9	109.7	109.41(10)	109.0, 109.2	
	104.8	108.5	108.91(10)	109.6, 115.5	

Table S3 Atomic coordinates of the optimized structures



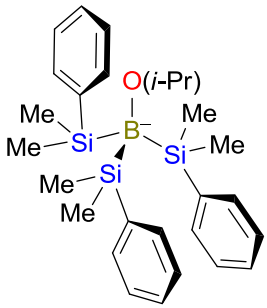
1a-X

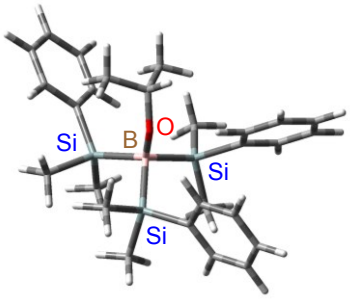
Si	2.34386700	-1.18911000	0.31604200	C	-0.73981600	-3.29556900	-1.71805200
Si	-0.87604500	-2.08412500	-0.22019400	H	0.28951000	-3.64012700	-1.87906600
Si	-0.15584100	0.90761400	1.19765200	H	-1.08567100	-2.82767400	-2.64837000
O	0.45463300	0.28663800	-1.51670200	H	-1.37164200	-4.17957500	-1.54475200
C	3.78199000	0.04110200	-0.08508900	C	-1.31848800	2.81499700	-0.66122100
C	-2.73370700	-1.58290400	-0.31043100	H	-0.41659900	2.63259500	-1.24010500
C	-1.52158700	2.09229100	0.53369700	B	0.45919300	-0.47900300	-0.22005500
C	3.57225100	1.22381600	-0.82087800	C	5.10382600	-0.21997800	0.32934000
H	2.56562900	1.46180600	-1.15521200	H	5.31905900	-1.12101500	0.90287100
C	2.93825600	-2.81801000	-0.53284000	C	-5.07780900	-1.78052300	0.39593900
H	3.96260200	-3.07234500	-0.22340500	H	-5.81766500	-2.22019600	1.06390600
H	2.93432400	-2.73078700	-1.62677700	C	-2.72429900	2.33701300	1.22285100
H	2.29250600	-3.66612000	-0.26886800	H	-2.93702400	1.79658200	2.14280300
C	0.96226200	-0.28583800	-2.69121400	C	5.92321700	1.81157000	-0.70371300
H	2.03815000	-0.52381800	-2.61476400	H	6.74145600	2.48992900	-0.93948300
H	0.83757800	0.43695900	-3.51145500	C	-3.44235200	3.96285200	-0.42483200
H	0.43905100	-1.21334200	-2.97195300	H	-4.17716800	4.67771300	-0.79183600
C	1.18454100	2.15617400	1.78764000	C	-0.84928200	0.17521600	2.83055900
H	0.74814300	2.85907300	2.51195100	H	-0.11119900	-0.48616800	3.30170900
H	1.58476900	2.74531700	0.95361200	H	-1.76252600	-0.41102800	2.67022800
H	2.03519100	1.65730100	2.26886200	H	-1.08200100	0.97149800	3.55189000
C	-0.73505700	-3.26631800	1.28935200	C	-5.47554900	-0.87254000	-0.58887500
H	-0.88624500	-2.76093000	2.25055700	H	-6.52364900	-0.59745900	-0.69365800
H	0.25811300	-3.73256400	1.31714100	C	-2.25807800	3.73581600	-1.13466400
H	-1.46932000	-4.08153800	1.21726600	H	-2.06858500	4.27388000	-2.06272700
C	2.56555400	-1.58384000	2.18606000	C	6.16148400	0.64538600	0.03109600
H	3.55714700	-2.01769900	2.37907200	H	7.16940500	0.41119100	0.37149400
H	1.81801100	-2.30827100	2.53271000	C	-3.67330100	3.25500500	0.75741700
H	2.47122100	-0.68704600	2.81004900	H	-4.59493000	3.41160500	1.31636200
C	4.62264300	2.09679400	-1.12829100	C	-3.16409600	-0.65979900	-1.28632200
H	4.42248300	3.00295600	-1.69812700	H	-2.42713800	-0.18700300	-1.93257300
C	-3.72712700	-2.12591300	0.52725800	C	-4.50938700	-0.31028100	-1.42981300
H	-3.44856000	-2.83714300	1.30273300	H	-4.80170600	0.41492200	-2.18703700



1a-Y

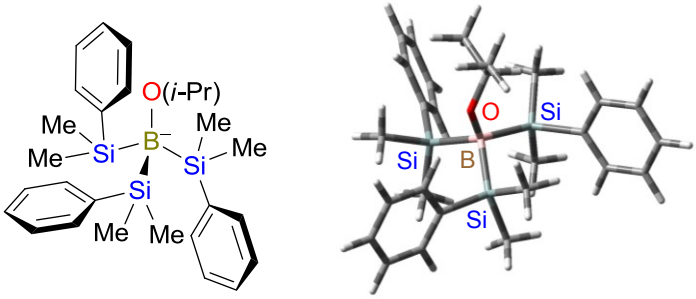
Si	-0.52567300	-1.88427500	-0.26220600	H	0.22854400	-4.27344300	0.06770200
Si	1.87728800	0.53589900	-0.19755600	H	0.02934100	-3.48603200	1.63988000
Si	-1.40175600	1.38867600	-0.43215100	H	1.47267500	-3.15448600	0.66786000
O	-0.30053800	0.28224200	1.85874800	C	-0.44081900	5.05716800	1.43362800
C	-0.89865900	3.22741800	-0.13910400	H	-0.35797400	5.40587500	2.46210000
C	2.61002600	1.96181400	0.85837100	C	-1.78374800	1.26128300	-2.30854000
H	3.64314900	2.18740900	0.55829600	H	-2.28299100	0.30745000	-2.52166200
H	2.61557800	1.71902800	1.92859500	H	-0.88931600	1.31389000	-2.94139800
H	2.01017400	2.87166300	0.74069900	H	-2.46827600	2.06204700	-2.62304700
C	-2.37485300	-2.38676300	-0.04120000	C	-0.78245600	3.72655400	1.17616900
C	3.89509900	-1.14499200	1.11846300	H	-0.94878900	3.05231900	2.01380900
H	3.61138100	-0.61724000	2.02736700	C	-3.11445100	1.28697500	0.42085900
B	-0.06666500	0.03809700	0.39836600	H	-3.77510300	2.09352400	0.07221000
C	3.68418300	-1.54647200	-1.22995400	H	-3.00871100	1.37717200	1.50870500
H	3.23830800	-1.33557200	-2.19990000	H	-3.60405700	0.32743100	0.21712400
C	2.01026600	1.14648600	-2.01432200	C	-5.09855800	-3.12245300	0.36080100
H	1.47408800	2.09650900	-2.13009000	H	-6.13945800	-3.40117900	0.51478700
H	1.58022500	0.43918000	-2.73464000	C	4.67860500	-2.52893500	-1.15913400
H	3.05845600	1.31982600	-2.29649300	H	4.97625900	-3.06338500	-2.06021500
C	-0.64627900	4.13828200	-1.18281600	C	0.38042700	-0.44675900	2.83684800
H	-0.72226300	3.80514000	-2.21639700	H	0.13434200	-1.52271300	2.81407500
C	-2.93894300	-2.47301200	1.24907900	C	-3.23151600	-2.67895700	-1.12036400
H	-2.32541900	-2.23623700	2.11689500	H	-2.84957700	-2.62536700	-2.13824500
C	-0.13950900	-2.17386700	-2.12042100	C	-4.27289300	-2.83556400	1.45357200
H	-0.43958300	-3.18561800	-2.42875500	H	-4.67210700	-2.88631100	2.46550300
H	0.94055100	-2.09043100	-2.29181200	C	-0.19682700	5.93978400	0.37516400
H	-0.63262300	-1.45605700	-2.78659900	H	0.07299300	6.97582600	0.57248000
C	-4.57086300	-3.04064300	-0.93046100	C	5.28921800	-2.82323500	0.06284200
H	-5.20134400	-3.25711300	-1.79191100	H	6.06238800	-3.58683400	0.12468000
C	-0.29949400	5.47290600	-0.93778400	C	4.89295300	-2.12025200	1.20533200
H	-0.10902400	6.14593200	-1.77284200	H	5.36062000	-2.33285300	2.16570400
C	3.25389200	-0.82689100	-0.09664200	H	1.47754800	-0.36520900	2.74009000
C	0.39200900	-3.33353900	0.61540800	H	0.09873400	-0.05477800	3.82566000





1b-X

Si	-2.22393200	-1.12490500	-0.63979900	H	1.83536000	1.12345300	1.46779800
Si	0.91316400	-2.13308700	-0.18411100	B	-0.33977500	-0.46868400	0.03061900
Si	0.35920600	1.07572200	-1.20701100	C	-4.18490500	1.05941700	-0.87757100
O	-0.11616600	-0.23844100	1.49637300	H	-3.53985000	1.44112700	-1.66385100
C	-3.82385200	-0.11957300	-0.19352800	C	5.09827900	-1.56822200	-0.71106900
C	2.78600400	-1.76550100	0.09671700	H	5.80074600	-1.59545100	-1.54293300
C	1.75578600	2.15725300	-0.41680800	C	2.33101100	3.22354100	-1.13902800
C	-4.71668900	-0.55172000	0.80876200	H	1.99179800	3.43304700	-2.15280200
H	-4.50235300	-1.46434100	1.36033500	C	-6.21190500	1.31750300	0.42762900
C	-2.73882800	-2.90381300	-0.10127800	H	-7.12113600	1.86669900	0.66517400
H	-3.76099800	-3.12751800	-0.43833000	C	3.79914000	3.79685600	0.69936800
H	-2.70242600	-3.04990500	0.98580800	H	4.58123800	4.42220900	1.12681600
H	-2.07382300	-3.65247600	-0.54807200	C	1.12746400	0.48790900	-2.87203600
C	-0.77052300	0.59092900	2.43758600	H	0.42073900	-0.12566300	-3.44532300
H	0.02161600	0.90705200	3.14025800	H	2.03772900	-0.10235400	-2.71794100
C	-0.88729800	2.41480100	-1.82934000	H	1.39624100	1.35150700	-3.49714100
H	-0.35251100	3.23287900	-2.33240400	C	5.55546500	-1.30571400	0.58285800
H	-1.48113400	2.85576000	-1.02075300	H	6.61294300	-1.12636600	0.76850600
H	-1.58380800	1.98953000	-2.56386200	C	3.25052900	2.74543700	1.43741300
C	0.87398900	-3.13193500	-1.82773800	H	3.60792600	2.54341500	2.44594100
H	1.07811200	-2.51591800	-2.71169200	C	-5.35287700	1.76836300	-0.57933000
H	-0.10835000	-3.59759100	-1.97742000	H	-5.59069000	2.67486600	-1.13392700
H	1.61871400	-3.94015000	-1.80256100	C	3.33518500	4.03293600	-0.59902400
C	-2.31870100	-1.21173000	-2.56013800	H	3.75589300	4.84555200	-1.19015600
H	-3.26853500	-1.67012900	-2.86928300	C	3.27821800	-1.49713500	1.39097200
H	-1.50336800	-1.81671200	-2.97398200	H	2.58175300	-1.45741500	2.22575200
H	-2.26140600	-0.22329400	-3.03089700	C	4.63569700	-1.27198300	1.63589100
C	-5.88690700	0.14891600	1.12159800	H	4.97630900	-1.06419300	2.64931500
H	-6.54553600	-0.22103200	1.90619000	C	-1.78775200	-0.22014500	3.25739500
C	3.73659000	-1.79522700	-0.94181600	H	-2.16732300	0.37082900	4.10375300
H	3.41343900	-2.00462800	-1.95968200	H	-2.64418000	-0.51777800	2.64397300
C	0.57517800	-3.43715200	1.18609900	H	-1.31148400	-1.12551500	3.65157800
H	-0.39642600	-3.92711800	1.05824600	C	-1.39456200	1.87019200	1.86823400
H	0.57587100	-2.96356700	2.17503600	H	-2.20528200	1.64745700	1.16909100
H	1.35210800	-4.21453400	1.17983900	H	-1.81088000	2.47388900	2.68660000
C	2.24709400	1.94102000	0.88447700	H	-0.64195300	2.47575200	1.35405000



1b-Y

Si	0.74278800	1.76278100	-0.47530400	C	-0.18633700	-5.08422000	1.33062400
Si	-1.95539500	-0.32291700	-0.47741000	H	-0.29848100	-5.40317100	2.36593000
Si	1.18604100	-1.58924300	-0.61418700	C	1.59677900	-1.57757300	-2.49145900
O	0.07151000	-0.39103800	1.65509900	H	2.21534200	-0.70486200	-2.73513400
C	0.46840500	-3.34780600	-0.27798800	H	0.70629700	-1.53631500	-3.13022100
C	-2.83214900	-1.67233800	0.56189300	H	2.17269500	-2.47131500	-2.77166400
H	-3.88920400	-1.77274200	0.27779400	C	0.30906300	-3.80869500	1.04653200
H	-2.78413100	-1.44681400	1.63436100	H	0.56016600	-3.14525500	1.87088100
H	-2.34192000	-2.64217800	0.42016400	C	2.89799000	-1.67002300	0.24896000
C	2.65226700	2.06990800	-0.33809100	H	3.47788000	-2.53068700	-0.11386600
C	-3.86028700	1.47649000	0.83778000	H	2.78366000	-1.77786100	1.33442300
H	-3.69874100	0.85527800	1.71582600	H	3.48345800	-0.76099700	0.06641300
B	0.01261000	-0.06674200	0.18734400	C	1.06168300	-0.22055700	3.81733300
C	-3.46102900	2.00769000	-1.46147700	H	2.00109300	-0.64902300	3.45106500
H	-2.98214800	1.81174500	-2.41883300	H	0.43335900	-1.04046200	4.18930000
C	-2.13944800	-0.89997100	-2.30142100	H	1.28788000	0.45120800	4.65705500
H	-1.70469900	-1.90001100	-2.42196600	C	5.46552800	2.51525300	-0.14390800
H	-1.63664200	-0.23686200	-3.01625200	H	6.53860500	2.68088300	-0.06841900
H	-3.19904900	-0.96187700	-2.58676200	C	-4.34798100	3.08612300	-1.37491000
C	0.09501900	-4.23847300	-1.30307500	H	-4.53324600	3.70635100	-2.25083400
H	0.19560500	-3.93364700	-2.34321000	C	0.33599500	0.52404800	2.68915400
C	3.26148400	2.48481400	0.86386500	H	1.00596300	1.32056200	2.32503700
H	2.64913600	2.64273800	1.74989600	C	3.51339600	1.89608400	-1.44069800
C	0.38494300	2.02735400	-2.34423700	H	3.10125200	1.58610000	-2.39868200
H	0.89875700	2.92848400	-2.70746600	C	4.63837300	2.70509300	0.96750100
H	-0.68886800	2.17821900	-2.50524500	H	5.06581000	3.02290700	1.91742000
H	0.69476400	1.18499200	-2.97318800	C	-0.54656800	-5.94847600	0.29045600
C	4.89347000	2.10995300	-1.35282900	H	-0.93500800	-6.94182500	0.50841900
H	5.52139300	1.95856800	-2.22966600	C	-4.99647700	3.36710500	-0.16868400
C	-0.40585800	-5.51780500	-1.03124600	H	-5.68599500	4.20604600	-0.09463200
H	-0.68601600	-6.17617300	-1.85258300	C	-4.74938900	2.55139500	0.93984300
C	-3.18070300	1.17176900	-0.36059200	H	-5.25086300	2.75114100	1.88582000
C	0.00300000	3.34294400	0.33659300	C	-0.94858300	1.18751300	3.20956100
H	0.35997000	4.24080200	-0.18829400	H	-1.46095500	1.72631400	2.40791100
H	0.27532500	3.45094400	1.39378100	H	-0.72749000	1.90229100	4.01555300
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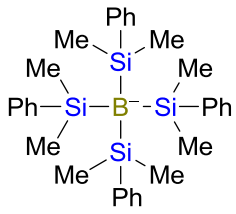

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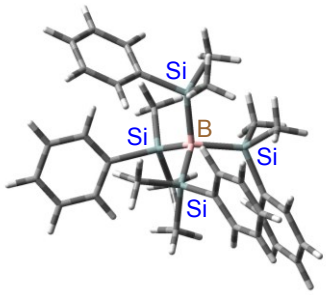
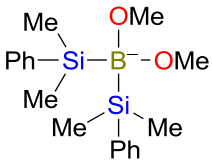


Si	-1.69471300	-0.30579600	1.76344800	C	5.40035300	1.30173700	1.56413000
Si	1.13999700	1.34696700	1.51614000	H	6.17165200	0.97150500	2.25830700
Si	1.02284800	-1.85121800	0.47442300	C	3.55766600	-1.47409700	-0.96170500
C	-3.27735100	-1.15144100	1.02291800	H	3.83424400	-0.82348300	-0.13798400
C	3.00953700	1.51836500	1.02447700	C	-5.68256000	-2.37497500	0.08979500
C	2.28514800	-2.08042100	-0.97660200	H	-6.59878000	-2.84131900	-0.26787500
C	-3.43680300	-2.55167100	0.98400200	C	4.17868100	-2.50383100	-3.06767000
H	-2.62968100	-3.19408000	1.32195400	H	4.90060100	-2.66236000	-3.86686600
C	-2.41796100	1.35091700	2.41975600	C	2.09515100	-2.23244900	2.02404500
H	-3.34980400	1.16443300	2.97136800	H	1.48474500	-2.22044300	2.93566500
H	-2.63852000	2.05799400	1.61107000	H	2.91763400	-1.52280900	2.16426300
H	-1.72386200	1.85038600	3.10519500	H	2.53680600	-3.23431600	1.92724700
C	-0.02945400	-3.45625600	0.34782200	C	5.75696700	1.90846000	0.35707500
H	0.62898700	-4.31429000	0.15297600	H	6.80455200	2.05485700	0.10065400
H	-0.79751700	-3.43160300	-0.43266400	C	2.92776900	-3.12516100	-3.10923500
H	-0.53461300	-3.65140800	1.30131200	H	2.66728700	-3.77497600	-3.94345500
C	1.25684100	1.12394800	3.42521700	C	-5.56101800	-0.98357100	0.12475000
H	1.61917800	0.13503400	3.72843800	H	-6.38588400	-0.35458900	-0.20661500
H	0.27913500	1.27009700	3.89694000	C	4.49004400	-1.67737300	-1.98419500
H	1.93659900	1.87781700	3.84626600	H	5.45903900	-1.18444000	-1.93216700
C	-1.42758600	-1.34289600	3.36320400	C	3.40462700	2.13018300	-0.18204600
H	-2.35375700	-1.35658800	3.95487500	H	2.64923000	2.45906500	-0.89010700
H	-0.63370200	-0.92174300	3.98977300	C	4.74773300	2.32511800	-0.51635700
H	-1.15651800	-2.38432900	3.15301400	H	5.00542800	2.79700200	-1.46300700
C	-4.61058000	-3.15887300	0.52622000	Si	-0.62339000	0.41217400	-1.34724800
H	-4.68635200	-4.24508900	0.51208200	C	-1.35606400	-1.08786600	-2.29138300
C	4.05047800	1.11730500	1.88620300	H	-0.58460300	-1.84932100	-2.44706300
H	3.81145500	0.64925300	2.83799800	H	-2.18714100	-1.56218400	-1.75642400
C	0.58034600	3.18098400	1.35887400	H	-1.71630900	-0.78171400	-3.28338100
H	-0.49875600	3.30633700	1.49532900	C	0.74685800	1.06098200	-2.52657700
H	0.84463800	3.61090200	0.38552400	H	1.03121800	2.09574900	-2.29819700
H	1.09435900	3.78101000	2.12343700	H	1.65292900	0.44633800	-2.48533700
C	2.00582300	-2.91539300	-2.07774400	H	0.37398200	1.05143100	-3.56062100
H	1.04713800	-3.42522900	-2.13840400	C	-1.98600900	1.77561900	-1.58553300
B	-0.02284700	-0.07208900	0.56118500	C	-1.71033600	3.14636800	-1.40649800
C	-4.38007000	-0.39052600	0.58526600	C	-3.28124200	1.45964700	-2.04250900
H	-4.32454300	0.69393500	0.59930300	C	-2.66199100	4.14066100	-1.65387400

H	-0.72606500	3.45558100	-1.06785700	H	-2.40325200	5.18694800	-1.49849000
C	-4.24444800	2.44326900	-2.29641400	H	-5.23351300	2.15183900	-2.64717800
H	-3.55445500	0.42098700	-2.20454300	H	-4.68587900	4.56160000	-2.29556600
C	-3.94046400	3.79271800	-2.10038200				



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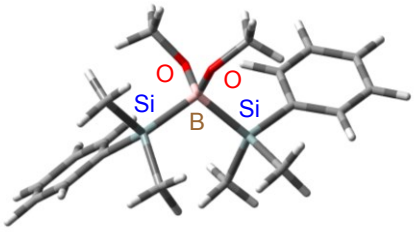

Si	1.92695300	1.21457500	-0.11746100	H	-2.25020200	2.19838000	-2.10688800
Si	-1.26734700	0.13389900	-0.99512200	H	-2.20490500	0.84721700	-3.26149400
O	-0.21707000	0.01721100	1.66504100	C	-3.07907700	-1.27223900	0.79247200
C	-2.98504000	-0.51305200	-0.39453900	H	-2.17700000	-1.44301200	1.37544800
C	3.01063900	-0.38527600	-0.07842600	C	-0.49073400	-1.41150000	-1.83503400
B	-0.06609800	0.96704900	0.52260400	H	-1.14070400	-1.79813000	-2.63346500
C	-4.18823400	-0.27631300	-1.08866700	H	-0.33712400	-2.22003000	-1.10902500
H	-4.17291300	0.31187400	-2.00459000	H	0.48869200	-1.18153900	-2.27487200
C	2.52103800	-1.58727000	0.47043800	C	4.60848800	-2.73890400	0.01873400
H	1.50696300	-1.60812100	0.86375100	H	5.21867800	-3.64003900	0.05434000
C	2.11866700	1.87892000	-1.91331200	C	0.43906900	0.32506400	2.86993000
H	3.17197500	2.07002600	-2.16592500	H	1.53595000	0.22206400	2.78253400
H	1.57319600	2.82601000	-2.02307700	C	4.32963100	-0.40718600	-0.57535900
H	1.72071000	1.17856600	-2.65849400	H	4.75367600	0.49786500	-1.00991900
C	5.12199800	-1.55905800	-0.53088000	C	3.30354800	-2.74745900	0.51962000
H	6.13759700	-1.53793100	-0.92483400	H	2.89116500	-3.66014100	0.94766200
C	-5.41734500	-0.77340200	-0.63796700	C	-5.47865100	-1.53091900	0.53528000
H	-6.32614200	-0.56892300	-1.20334300	H	-6.43138800	-1.92036900	0.89079800
C	2.91698000	2.49080700	0.92978900	H	0.22828800	1.35206000	3.20806500
H	3.90733900	2.70067900	0.49850700	H	0.09499200	-0.37478300	3.64615200
H	3.06596700	2.13979200	1.95897300	O	-0.43936200	2.36006000	0.87140900
H	2.35564700	3.43280200	0.98136800	C	-1.74900600	2.61148300	1.31406100
C	-4.30073100	-1.77665800	1.24978700	H	-1.82427200	3.67187100	1.59787200
H	-4.33554200	-2.35701500	2.17107400	H	-2.49933300	2.41217200	0.52886600
C	-1.65730200	1.33718000	-2.44306500	H	-2.02261800	1.99718700	2.18788400
H	-0.72486100	1.73413300	-2.86298500				

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