A Bromo(boryloxy) Silylene and its Heavier Analogues

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1 Experimental Details

1.1 General Information

All reactions were performed under an inert gas atmosphere using nitrogen and standard Schlenk line and glove box techniques. Toluene, benzene, *n*-hexane, diethyl ether and THF were dried with a MBraun Solvent Purification System and degassed prior to use. Acetonitrile was used in a technical grade as received. Deuterated benzene (C_6D_6) was dried over elemental sodium, distilled and stored over a sodium mirror. Commercially available but air sensitive compounds (BBr_3, $SiBr_4$, $SiCl_4$, $SiHCl_3$) were filled in J.-Young tap flasks and stored under inert conditions or stored in a glovebox. [$GeCl_2$(1,4-dioxane)], Triethylamine and di*iso*propylethylamine were used as received. BzK[S1], [{(MesNacnac)Mg}$_2$] (Nacnac = [HC(MeCNMes)$_2$]$^-$, Mes = mesityl),[S2] (HCNDipp)$_2$BBr[S3] (Dipp = di*iso*propylphenyl) and [CH_2N{(HCNDipp)$_2$B}H]$_2$[S4] were synthesized according to literature protocols.
For NMR experiments one of the two devices BrukerAvance Neo 400 (^{1}H 400.1 MHz, ^{7}Li 155.5 MHz, ^{11}B 128.4 MHz, ^{13}C 100.6 MHz, ^{29}Si 79.5 MHz) or BrukerAvance III (^{1}H 400.1 MHz, ^{13}C

100.6 MHz) was used for characterization of all new compounds. An Agilent Cary 630 attenuated total reflectance (ATR) spectrometer was used for IR measurements. Melting points were determined in glue sealed capillaries with a Mettler Toledo MP50 device. Microanalysis were performed by the Science Centre, London Metropolitan University.

1.2 Synthesis of New Compounds

1.2.1 Synthesis of {B}*Br

To a stirred solution of $[CH_2N\{(HCNDipp)_2B\}H]_2$ (5.30 g, 6.0 mmol) and NEt_3 (1.69 mL, 12.2 mmol) in toluene (30 mL) at –80 °C was added BBr_3 (0.63 mL, 6.6 mmol) with a syringe. The cooling bath was removed and the mixture was warmed up to room temperature before a preheated oil bath (70 °C) was used to heat the reaction mixture for 15 h. The reaction mixture was cooled to ambient temperature and filtered through a filter canula into another flask. The residue was extracted with toluene (2 × 15 mL). All solutions were combined and dried under vacuum to get a reddish-brown solid. The crude product was washed with ice cooled *n*-hexane (3 × 15 mL) yielding 3.597 g (65 %) of product as a colourless to off-white solid. The combined *n*-hexane solutions were stored at –30 °C to get a second crop of the product (503 mg, 9 %) as colorless crystals. Yield: 4.100 g (74 %). $C_{54}H_{76}B_3BrN_6$ (921.58): calcd. C 70.38, H 8.31, N 9.12; found C 70.37, H 8.29, N 9.16. m. p. 277 °C. ^{1}H NMR (400 MHz, C_6D_6) δ = 7.24 – 7.19 (m, 4H, *p*-aryl CH), 7.13 – 7.09 (m, 8H, *m*-aryl CH), 6.09 (s, 4H, C_2H_2), 3.25 (sept., $J_{H,H}$=6.8 Hz, 8H, C<u>H</u>CH$_3$), 2.97 (s, 4H, C_2H_4), 1.13, 1.09 ppm (2 d, J = 6.8 Hz, 2 × 24H, CHC<u>H</u>$_3$). ^{13}C NMR (151 MHz, C_6D_6) δ = 146.2 (C_{ipso}–C), 139.0 (C_{ipso}–N), 127.4 (*p*-aryl CH), 123.8 (*m*-aryl CH), 118.7 (C_2H_2), 49.3 (C_2H_4), 28.6(<u>C</u>H(CH$_3$)$_2$), 26.2, 23.3 ppm (2 × CH(<u>C</u>H$_3$)$_2$). ^{11}B NMR (128 MHz, C_6D_6) δ = 27.8, 22.9 ppm.

1.2.2 Synthesis of {B}*OH

To an ice cooled and thoroughly stirred solution of {B}*Br (2.64 g, 3.0 mmol) and triethylamine (0.5 mL, 3.6 mmol) in toluene (40 mL) water (0.16 mL, 9 mmol) was added with a pipette. The mixture was stirred for three hours at room temperature within the formation of a colourless solid was observed. 500 mg of $MgSO_4$ were added and the mixture was stirred for additional 30 minutes before all insoluble material was filtered off and subsequently washed with toluene (2 × 20 mL). All solutions were combined and dried under vacuum to get the crude product as an off-white powder in sufficient purity (>95 % by NMR) for further reactions. Yield: 2.21 g (86 %). To get the compound analytically pure, the material could be either washed with acetonitrile or recrystallized from hot *n*-hexane. Crystalline material, suitable for X-ray diffraction experiments was received from *n*-hexane at –30 °C.
$C_{54}H_{77}B_3N_6O$ (858.68): calcd. C 75.53, H 9.04, N 9.79; found C 75.84, H 8.95, N 9.36. m. p. 267 °C.^{1}H NMR (400 MHz, C_6D_6) δ = 7.16 – 7.08 (m, 4H, *p*-aryl CH), 7.06 – 7.00 (m, 8H, *m*-aryl CH), 5.91 (s, 4H, $C_2H_2$3.29 (sept, $J_{H,H}$=6.9 Hz, 8H, C<u>H</u>(CH$_3$)$_2$), 2.83 (s, 4H, C_2H_4), 1.96 (s, 1H, BOH), 1.18, 1.14 ppm (2 d, J = 6.9 Hz, 2 × 24H, CH(<u>C</u>H$_3$)$_2$).^{13}C NMR (101 MHz, C_6D_6) δ = 146.5 (C_{ipso}–C), 140.1 (C_{ipso}–N), 127.6 (*p*-aryl CH), 123.7 (*m*-aryl CH), 118.5 (C_2H_2), 46.9 (C_2H_4), 28.6 (<u>C</u>H(CH$_3$)$_2$), 25.2, 23.5 ppm (2 × CH(<u>C</u>H$_3$)$_2$).^{11}B NMR (128 MHz, C_6D_6) δ = 26.9, 22.3 ppm.

1.2.3 Synthesis of {B}*OK

Toluene (20 ml) was added to a flask filled with {B}*OH (859 mg, 1.0 mmol) and BzK (132 mg, 1.0 mmol). The orange suspension was briefly sonicated after which the suspension turned into a clear and nearly colourless solution in less than 5 minutes. The quantitatively formed product could be used directly at this stage or isolated as an amorphous powder by removing

all volatile components in *vacuo*. The addition of 1 mL of benzene and storage at room temperature overnight lead to the formation of the crystalline benzene solvate, which could be filtered off and dried under vacuum. Yield 802 mg (82 %).
$C_{54}H_{76}B_3KN_6 \cdot C_6H_6$ (927.76): calcd. C 73.92, H 8.48, N 8.62; found C 73.09, H 8.14, N 8.69. m. p. 269 °C. ^{1}H NMR (400 MHz, C_6D_6) δ = 6.94 – 6.82 (m, 12H, aryl CH), 5.85 (s, 4H, C_2H_2), 3.64 (sept, $J_{H,H}$=6.9 Hz, 8H, C<u>H</u>$(CH_3)_2$), 2.83 (s, 4H, C_2H_4), 1.13, 1.09 ppm (m, 48H, CH($\underline{C}H_3)_2$). ^{13}C NMR (101 MHz, C_6D_6) δ = 147.3 (C_{ipso}–C), 144.9 (C_{ipso}–N), 125.4 (*p*-aryl CH), 122.5 (*m*-aryl CH), 118.7 (C_2H_2), 47.1 (C_2H_4), 28.5 (<u>C</u>H$(CH_3)_2$), 24.5, 23.6 ppm (2 × CH($\underline{C}H_3)_2$). ^{11}B NMR (128 MHz, C_6D_6) δ = 23.1 ppm.

1.2.4 Synthesis of {B}*OSiCl$_3$

A freshly prepared solution of {B}*OK (0.5 mmol; see description above) in toluene (10 mL) was cooled to –80 °C and a solution of $SiCl_4$ (68 µL, 0.6 mmol) in toluene (5 mL) was added. The cooling bath was removed, the solution was allowed to warm up to room temperature and stirred for additional 3 h before all volatile components were removed under vacuum. The product was extracted with *n*-hexane (2 × 10 mL). The amount of solvent of the combined extracts was reduced to ca. 5 mL and the solution was stored at –30 °C overnight. The colourless crystalline product was filtered off, washed with a minimal amount of *n*-hexane (ca. 0.8 mL) and dried under vacuum. Yield 365 mg (79 %).
$C_{54}H_{76}B_3Cl_3N_6Si$ (992.11): calcd. C 65.38, H 7.72, N 8.47; found C 65.31, H 7.96, N 7.67. m.p. 227 °C (dec.). ^{1}H NMR (600 MHz, C_6D_6) δ = 7.20 – 7.14 (m, 4H, *p*-aryl CH), 7.09 – 7.06 (m, 8H, *m*-aryl CH), 6.00 (s, 4H, C_2H_2), 3.30 (sept, $J_{H,H}$=6.8 Hz, 8H, C<u>H</u>$(CH_3)_2$), 3.04 (s, 4H, C_2H_4), 1.16 – 1.07 ppm (m, 48H, CH($\underline{C}H_3)_2$). ^{13}C NMR (151 MHz, C_6D_6) δ = 145.8 (C_{ipso}–C), 139.6 (C_{ipso}–N), 127.5 (*p*-aryl CH), 124.1 (*m*-aryl CH), 119.3 (C_2H_2), 48.7 (C_2H_4), 28.5 (<u>C</u>H$(CH_3)_2$), 26.1, 23.5 ppm (2 × CH($\underline{C}H_3)_2$). ^{11}B NMR (128 MHz, C_6D_6) δ = 23.1 ppm. ^{29}Si NMR (80 MHz, C_6D_6) δ = –48.3 ppm.

1.2.5 Synthesis of {B}*OSiHCl$_2$

A freshly prepared solution of {B}*OK (0.5 mmol; see description 1.2.3) in toluene (10 mL) was cooled to –80 °C and a solution of $HSiCl_3$ (60 µl, 0.6 mmol) in toluene (5 mL) was added slowly. The cooling bath was removed, the solution was allowed to warm up to room temperature and stirred for additional 3 h before all volatile components were removed under vacuum. The product was extracted with *n*-hexane (2 × 10 mL). The amount of solvent of the combined extracts was reduced to ca. 5 mL and the solution was stored at –30 °C overnight. The colourless crystalline product was filtered off, washed with a minimal amount of *n*-hexane (ca. 0.8 mL) and dried under vacuum. Yield: 355 mg (74 %). $C_{54}H_{77}B_3Cl_2N_6Si$ (957.67): calcd. C 67.73, H 8.10, N 8.78; found C 67.23, H 8.31, N 8.21. m. p. 232 °C (dec.). ^{1}H NMR (400 MHz, C_6D_6) δ = 7.15 – 7.10 (m, 4H, *p*-aryl CH), 7.10 – 6.98 (m, 8H, *m*-aryl CH), 6.01 (s, 4H, C_2H_2), 5.19 (s, $^1J_{SiH}$= 84.2 Hz, 1H, SiH), 3.33 (sept, $J_{H,H}$=6.9 Hz, 8H, C<u>H</u>$(CH_3)_2$), 2.95 (s, 4H, C_2H_4), 1.26 – 1.06 ppm (m, 48H, CH($\underline{C}H_3)_2$). ^{13}C NMR (101 MHz, C_6D_6) δ = 145.9 (C_{ipso}–C), 139.8 (C_{ipso}–N), 127.5 (*p*-aryl CH), 123.9 (*m*-aryl CH), 119.2 (C_2H_2), 47.2 (C_2H_4), 28.4 (<u>C</u>H$(CH_3)_2$), 26.3, 23.4 ppm (2 × CH($\underline{C}H_3)_2$). ^{11}B NMR (128 MHz, C_6D_6) δ = 23.2 ppm. ^{29}Si NMR (79 MHz, C_6D_6) δ = –38.7 ppm.

1.2.6 Synthesis of {B}*OSiBr$_3$

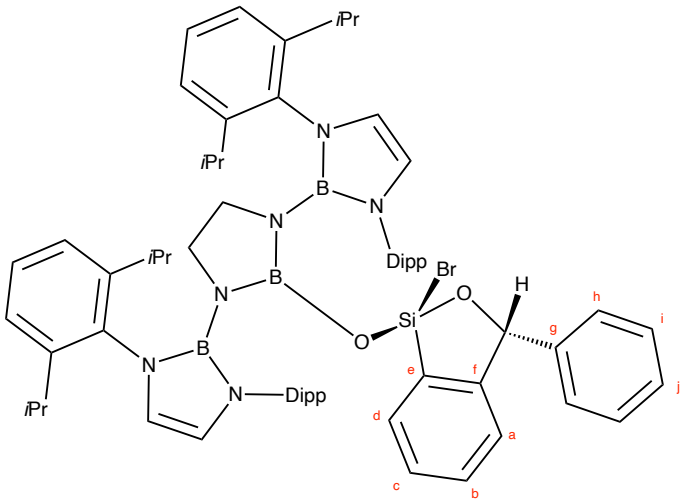
To a solution of {B}*OK (854 mg, 1.0 mmol) in toluene (25 mL) at –80 °C a solution of $SiBr_4$ (1.05 mmol) in toluene (5 mL) was added slowly. After warming to room temperature and additional stirring for three hours, all volatile components were removed under vacuum. The product was extracted with *n*-hexane (3 × 15 mL) and the amount of solvent of the

combined solutions was reduced to a volume of ca. 10 mL before the product was crystallized at –30 °C. The slightly yellow crystals were filtered off, washed with *n*-hexane (ca. 2 mL) and dried under vacuum. First crop: 852 mg. The mother liquor and the washing were combined, reduced to a volume of ca. 5 mL and stored at –30 °C to isolate a second crop of crystalline material (183 mg). Yield: 1.035 g (92 %).
$C_{54}H_{76}B_3Br3N_6OSi$ (1125.47): calcd. C 57.63, H 6.81, N 7.47; found C 56.69, H 7.33, N 6.69. M. P. 223 °C (dec.). ^{1}H NMR (400 MHz, C_6D_6) δ = 7.21 – 7.17 (m, 4H, *p*-aryl CH), 7.12 – 7.06 (m, 8H, *m*-aryl CH), 6.01 (s, 4H, C_2H_2), 3.32 (sept, $J_{H,H}$ = 6.9 Hz, 8H, C<u>H</u>$(CH_3)_2$), 3.05 (s, 4H, C_2H_4), 1.15, 1.13 ppm (2 d, *J* = 6.9 Hz, 2 × 24H, CH(<u>C</u>$H_3)_2$). ^{13}C NMR (151 MHz, C_6D_6) δ = 145.8 (C_{ipso}–C), 139.7 (C_{ipso}–N), 127.4 (*p*-aryl CH), 124.2 (*m*-aryl CH), 119.4 (C_2H_2), 49.1 (C_2H_4), 28.5 (<u>C</u>H$(CH_3)_2$), 26.2, 23.8 ppm (2 × CH(<u>C</u>$H_3)_2$). ^{11}B NMR (128 MHz, C_6D_6) δ = 22.5 ppm. ^{29}Si NMR (80 MHz, C_6D_6) δ = –89.0 ppm.

1.2.7 Synthesis of {B}*OSiBr

A solution of {B}*$OSiBr_3$ (675 mg, 0.6 mmol) in toluene (5 mL) was added to a suspension of [MesNacNacMg(I)]$_2$ (430 mg, 0.66 mmol) in toluene (5 mL) at –40 °C and the mixture was stirred for 15 h without further cooling. All volatile components were removed under vacuum and the product was extracted with *n*-hexane (10 mL). Removing of the solvent under vacuum lead first to a yellow viscous oil which finally solidified under the formation of a foamlike solid. Yield 532 mg (83 %).
$C_{54}H_{76}B_3BrN_6OSi$ (965.66): calcd. C 67.17, H 7.93, N 8.70; found C 66.72, H 8.09, N 8.57. ^{1}H NMR (400 MHz, C_6D_6) δ = 7.12 – 7.02 (m, 12H, aryl CH), 5.95 (s, 4H, C_2H_2), 3.42 (sept, $J_{H,H}$ = 6.8 Hz, 8H, C<u>H</u>$(CH_3)_2$), 2.95 (s, 4H, C_2H_4), 1.32, 1.14 ppm (2 d, *J* = 6.8 Hz, 2 × 24H, CH(<u>C</u>$H_3)_2$). ^{13}C NMR (101 MHz, C_6D_6) δ = 146.0 (C_{ipso}–C), 141.4 (C_{ipso}–N), 127.5 (*p*-aryl CH), 124.5 (*m*-aryl CH), 119.0 (C_2H_2), 47.7 (C_2H_4), 28.7 (<u>C</u>H$(CH_3)_2$), 25.8, 23.4 ppm (2 × CH(<u>C</u>$H_3)_2$). ^{11}B NMR (128 MHz, C_6D_6) δ = 22.0 ppm. ^{29}Si NMR (79 MHz, C_6D_6) δ = 82.8ppm

1.2.8 Synthesis of 1



To a stirred solution of {B}*OSiBr (145 mg, 0.15 mmol) in *n*-hexane (15 mL) benzophenone (27 mg, 0.15 mmol) was added as a solid. The mixture was stirred for 5 h before the amount of solvent was reduced to ca. 1 mL. Storage of the solution at 5 °C afforded colourless crystalline material which was filtered off and washed with a minimal amount of *n*-hexane (ca. 0.5 mL) and dried under vacuum. Yield: 149 mg (87 %).$C_{67}H_{86}B_3BrN_6O_2Si$ (1147.88): calcd. C 70.11, H 7.55, N 7.32; found C 69.30, H 7.76, N 7.30. ^{1}H NMR (400 MHz, C_6D_6) δ = 7.39 (d, *J* = 7.4 Hz, 2H, C_dH) 7.25 – 7.18 (m, 4H, *p*-aryl CH), 7.16 – 7.07 (m, 10H, aryl CH), 7.05 – 6.96

(m, 4H, aryl CH), 6.86 (d, J = 7.8 Hz, 2H, C_aH), 6.03 (s, 4H, C_2H_2), 5.85 (s, 1H, OCH), 3.51 – 3.30 (m, 8H, C<u>H</u>$(CH_3)_2$), 3.17 – 2.98 (m, 4H, C_2H_4), 1.28 (d, J = 6.8 Hz, 12H, CH(<u>C</u>$H_3)_2$), 1.09 – 1.00 (m, 24H, CH(<u>C</u>$H_3)_2$), 0.85 ppm (d, J = 7.0 Hz, 12H, CH(<u>C</u>$H_3)_2$). ^{13}C NMR (MHz, C_6D_6) δ = 153.8 (C_e–Si), 146.0 (Dipp C_{ipso}–C), 140.9 (C_g), 140.3 (C_{ipso}–N), 134.2 (C_d), 131.4 (C_b), 128.9 (C_h), 128.8 (C_c), 127.3 (Dipp *p*-CH), 127.1 (C_j), 126.8 (C_f), 124.4 (C_i), 123.8 (Dipp *m*-CH), 123.7 (C_a), 119.5 (C_2H_2), 78.8 (OCH), 48.0 (m, C_2H_4), 28.6, 28.2 (2 × <u>C</u>H(,$CH_3)_2$), 26.5, 26.2, 24.4, 23.1 ppm (4 × CH(<u>C</u>$H_3)_2$). ^{11}B NMR (128 MHz, C_6D_6) δ = 23.8 ppm. ^{29}Si NMR (79 MHz, C_6D_6) δ = –39.4 ppm.

1.2.9 Synthesis of {B}*OGeCl

A solution of {B}*OK (269 mg, 0.3 mmol) in toluene (5 mL) was added dropwise to a solution of [$GeCl_2$(1,4-dioxane)] (70 mg, 0.3 mmol) in toluene (3 mL) at –40 °C. The mixture was stirred for 10 h at room temperature before all volatile components were removed under vacuum. The product was extracted with *n*-hexane (2 × 10 mL) and insoluble components were filtered off. The solution was dried under vacuum to get the crude product as an off-white to yellow amorphous powder. Yield 235 mg (81 %). The product could be recrystallized from *n*-hexane at –40 °C. Single crystals suitable for X-ray diffraction experiments were obtained from a concentrated benzene solution at room temperature. $C_{54}H_{76}B_3BrClGeN_6O$ (965.75): calcd. C 67.16, H 7.93, N 8.70; found C 66.80, H 8.10, N 8.36. ^{1}H NMR (400 MHz, C_6D_6) δ = 7.04 (br, 12H, aryl CH), 5.94 (s, 4H, C_2H_2), 3.46 (sept, $J_{H,H}$ = 6.9 Hz, 8H, C<u>H</u>$(CH_3)_2$), 2.92 (s, 4H, C_2H_4), 1.33, 1.15 ppm (2 d, J = 6.9 Hz, 2 × 24H, CH(<u>C</u>$H_3)_2$). ^{13}C NMR (MHz, C_6D_6) δ = 146.4 (C_{ipso}–C), 142.1 (C_{ipso}–N), 127.3 (*p*-aryl CH), 124.5 (*m*-aryl CH), 118.9 (C_2H_2), 47.5 (C_2H_4), 28.7 (<u>C</u>H$(CH_3)_2$), 25.7, 23.2 ppm (2 × CH(<u>C</u>$H_3)_2$). ^{11}B NMR (128 MHz, C_6D_6) δ = 27.3, 22.4 ppm.

1.2.10 Synthesis of {B}*OSnCl

A solution of {B}*OK (269 mg, 0.3 mmol) in toluene (5 mL) was added dropwise to a solution of $SnCl_2$ (57 mg, 0.3 mmol) in THF (3 mL) at –40 °C. The mixture was stirred for 10 h at room temperature before all volatile components were removed under vacuum. The product was extracted with *n*-hexane (2 × 10 mL) and insoluble components were filtered off. The volume of the solution was reduced to ca. 3 mL and the product was crystallized at –30 °C. Yield 209 mg (69%). ^{1}H NMR (400 MHz, C_6D_6) δ = 7.06 – 6.96 (m, 12H, aryl CH), 5.94 (s, 4H, C_2H_2), 3.52 (sept, $J_{H,H}$ = 6.9 Hz, 8H, C<u>H</u>$(CH_3)_2$), 2.90 (s, 4H, C_2H_4), 1.36, 1.16 ppm (2 d, J = 6.9 Hz, 2 × 24H, CH(<u>C</u>$H_3)_2$). ^{13}C NMR (MHz, C_6D_6) δ = 146.8 (C_{ipso}–C), 142.8 (C_{ipso}–N), 127.0 (*p*-aryl CH), 124.5 (*m*-aryl CH), 118.8 (C_2H_2), 47.3 (C_2H_4), 28.7 (<u>C</u>H$(CH_3)_2$), 25.6, 23.3 ppm (2 × CH(<u>C</u>$H_3)_2$). ^{11}B NMR (128 MHz, C_6D_6) δ = 27.6, 21.6 ppm. ^{119}Sn NMR (186 MHz, C_6D_6) δ = 180.8 ppm.

1.3 Plots of NMR Spectra

1.3.1 NMR Spectra of {B}*Br

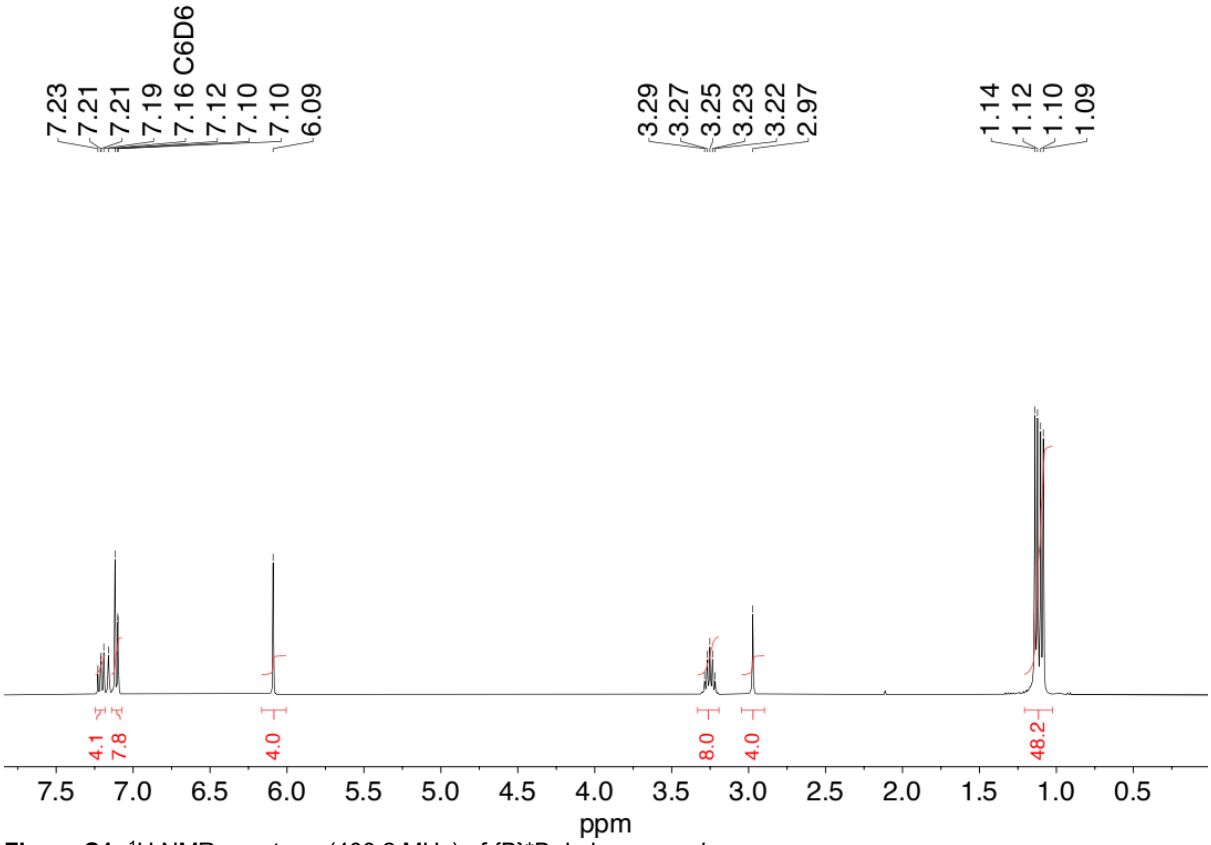


Figure S1: ^{1}H NMR spectrum (400.2 MHz) of {B}*Br in benzene-d_6

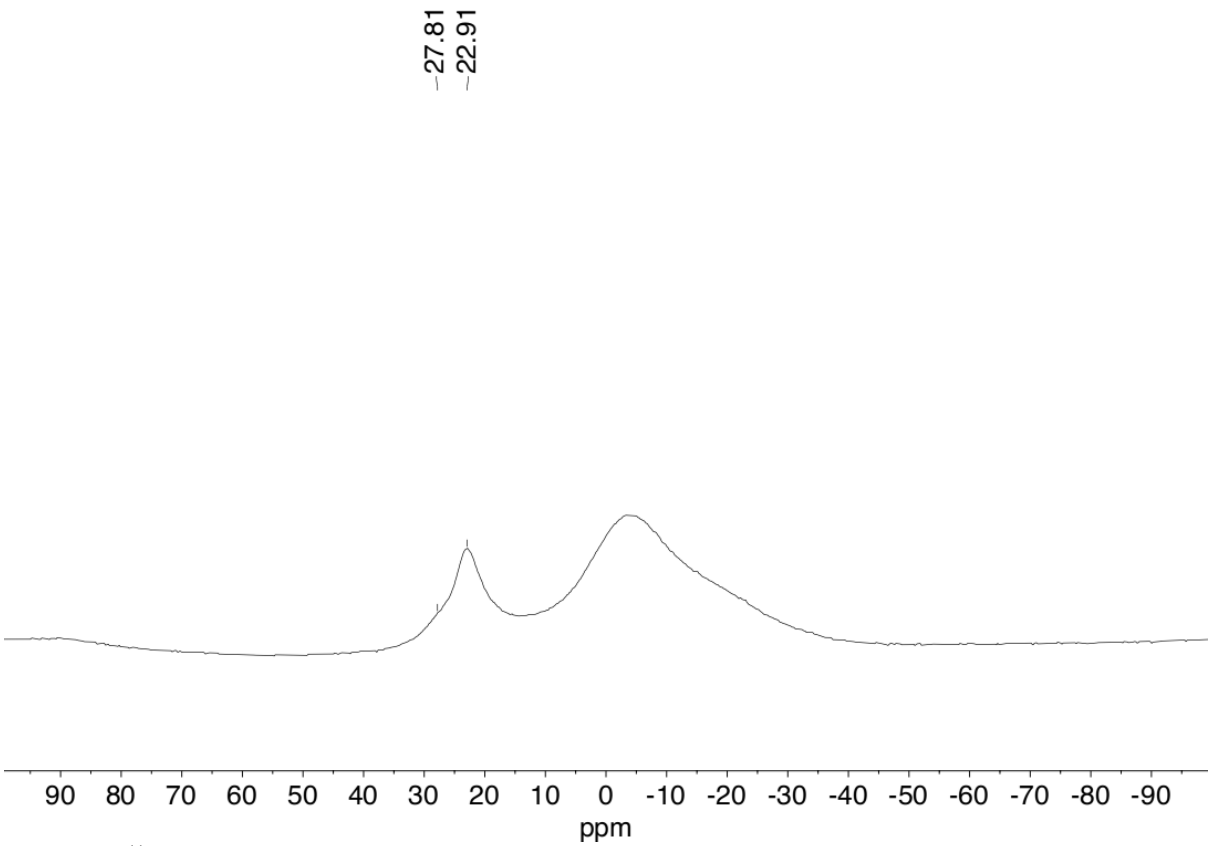


Figure S2: ^{11}B NMR spectrum (128.4 MHz) of {B}*Br in benzene-d_6

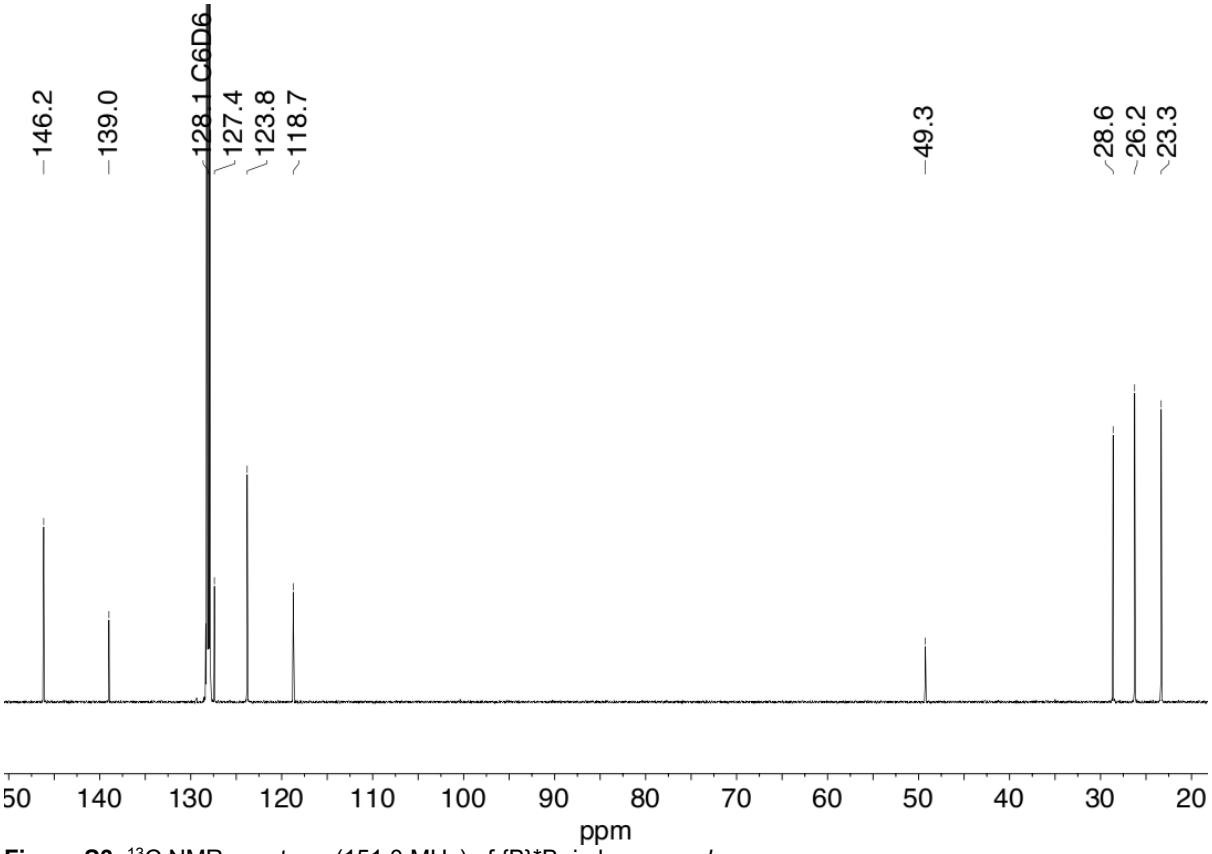


Figure S3: ^{13}C NMR spectrum (151.0 MHz) of {B}*Br in benzene-d_6

1.3.2 NMR Spectra of {B}*OH

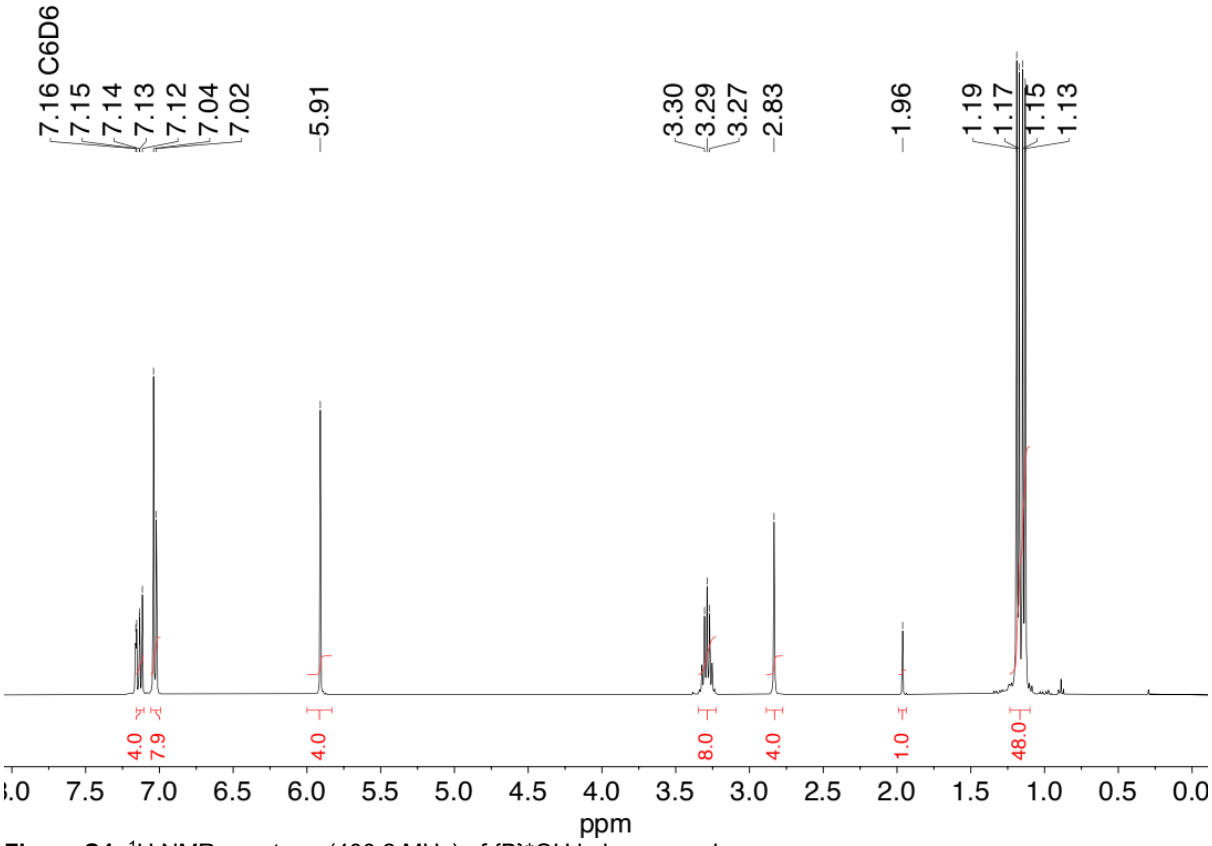


Figure S4: ^{1}H NMR spectrum (400.2 MHz) of {B}*OH in benzene-d_6.

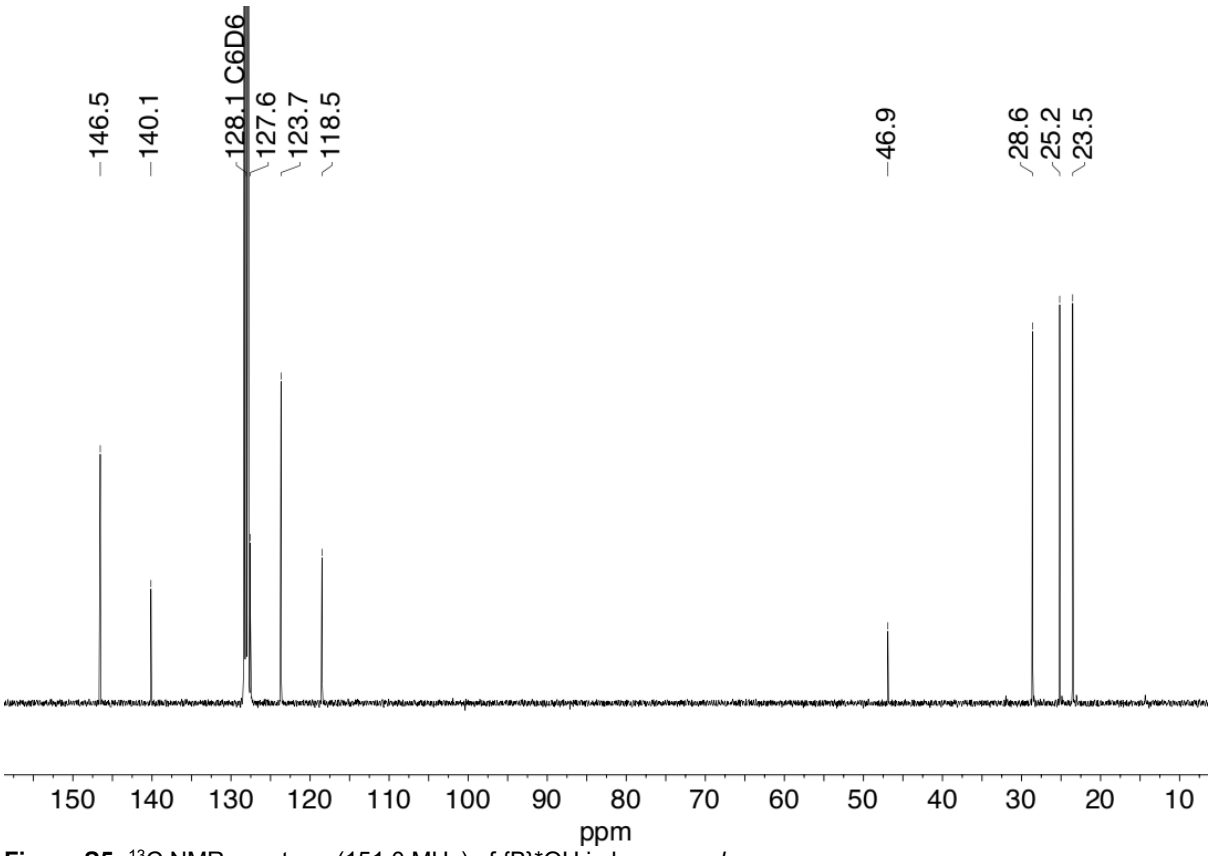


Figure S5: ^{13}C NMR spectrum (151.0 MHz) of {B}*OH in benzene-d_6.

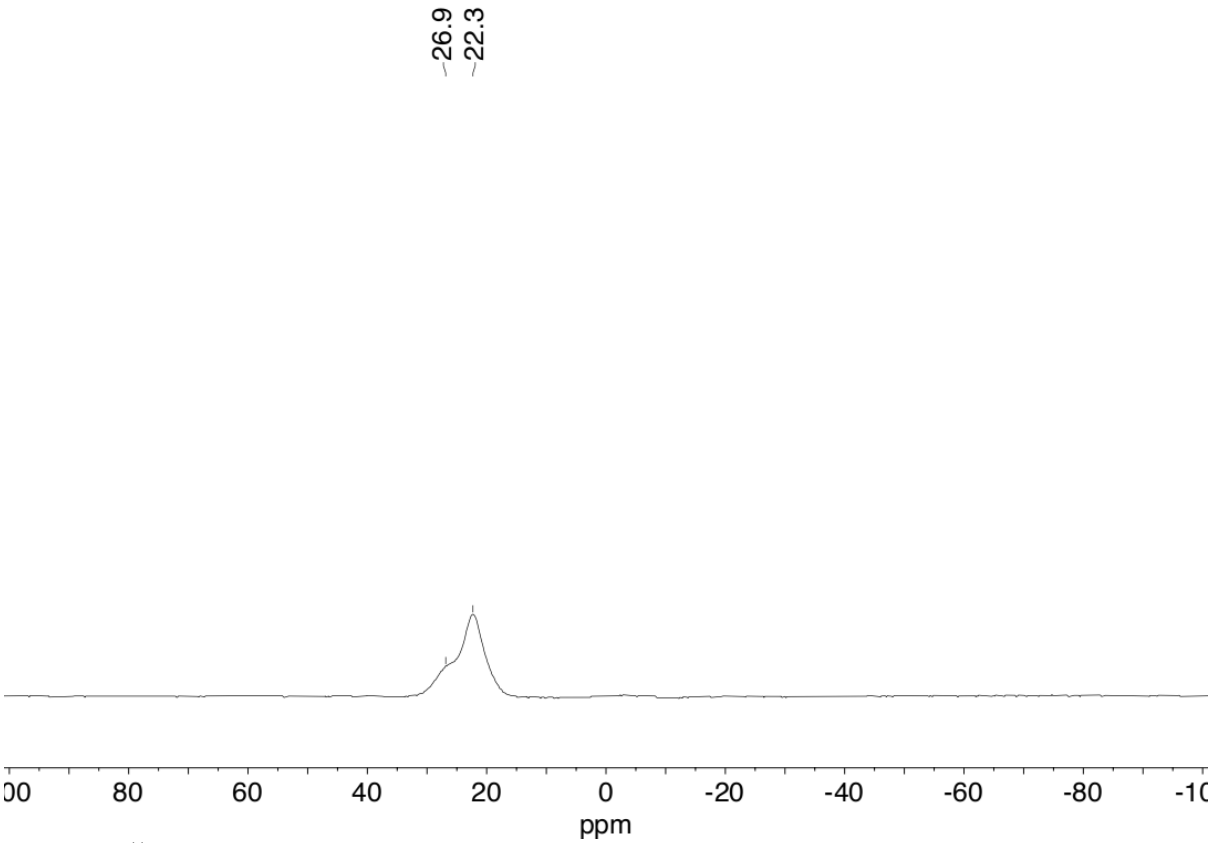


Figure S6: ^{11}B NMR spectrum (128.4 MHz) of {B}*OH in benzene-d_6.

1.3.3 NMR Spectra of {B}*OK

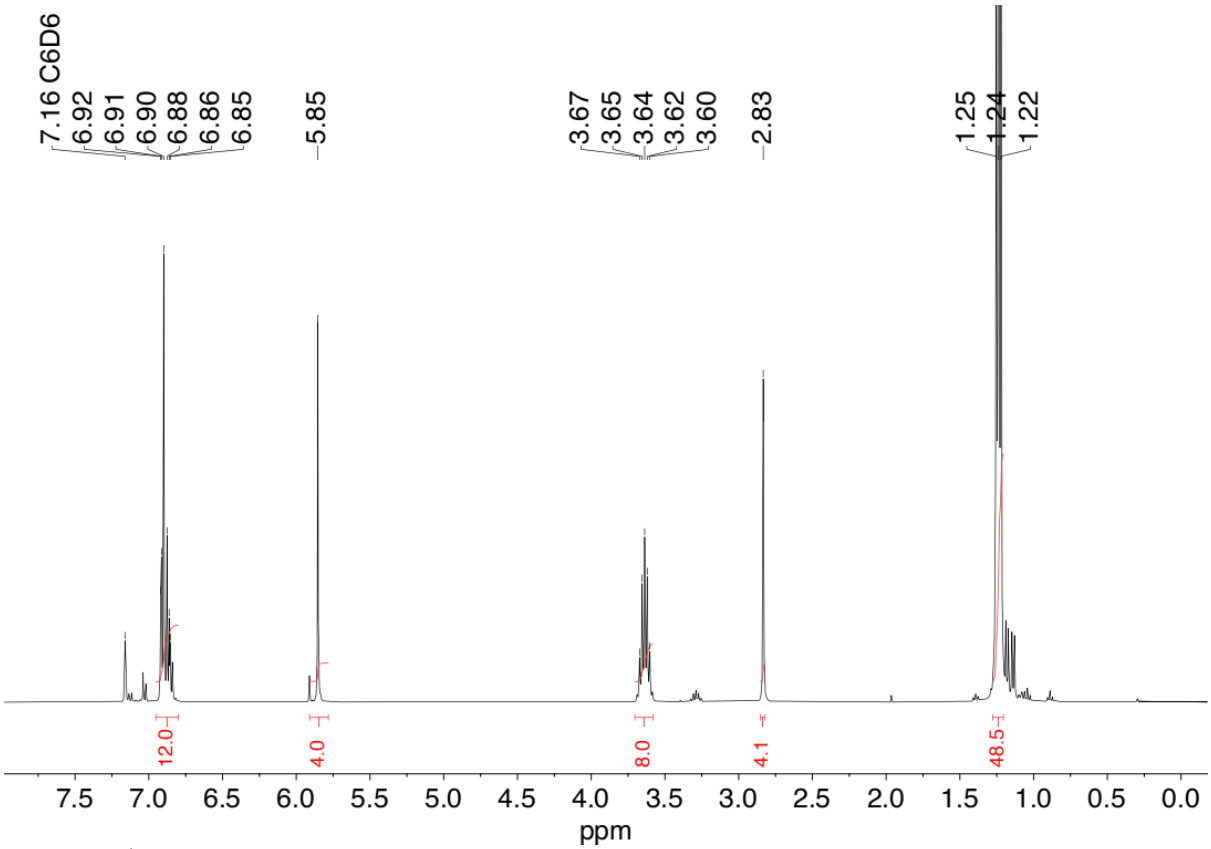


Figure S7: ^{1}H NMR spectrum (400.1 MHz) of {B}*OK in benzene-d_6.

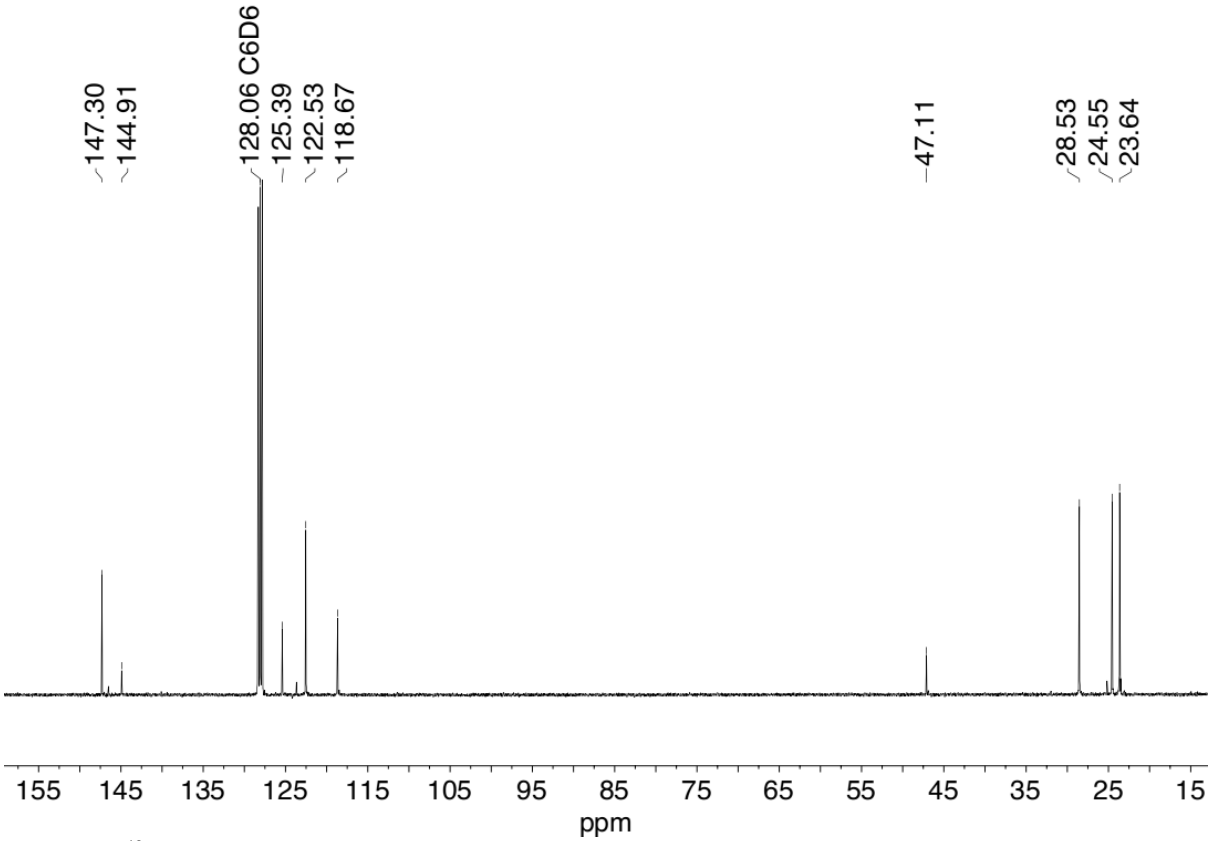


Figure S8: ^{13}C NMR spectrum (100.6 MHz) of {B}*OK in benzene-d_6.

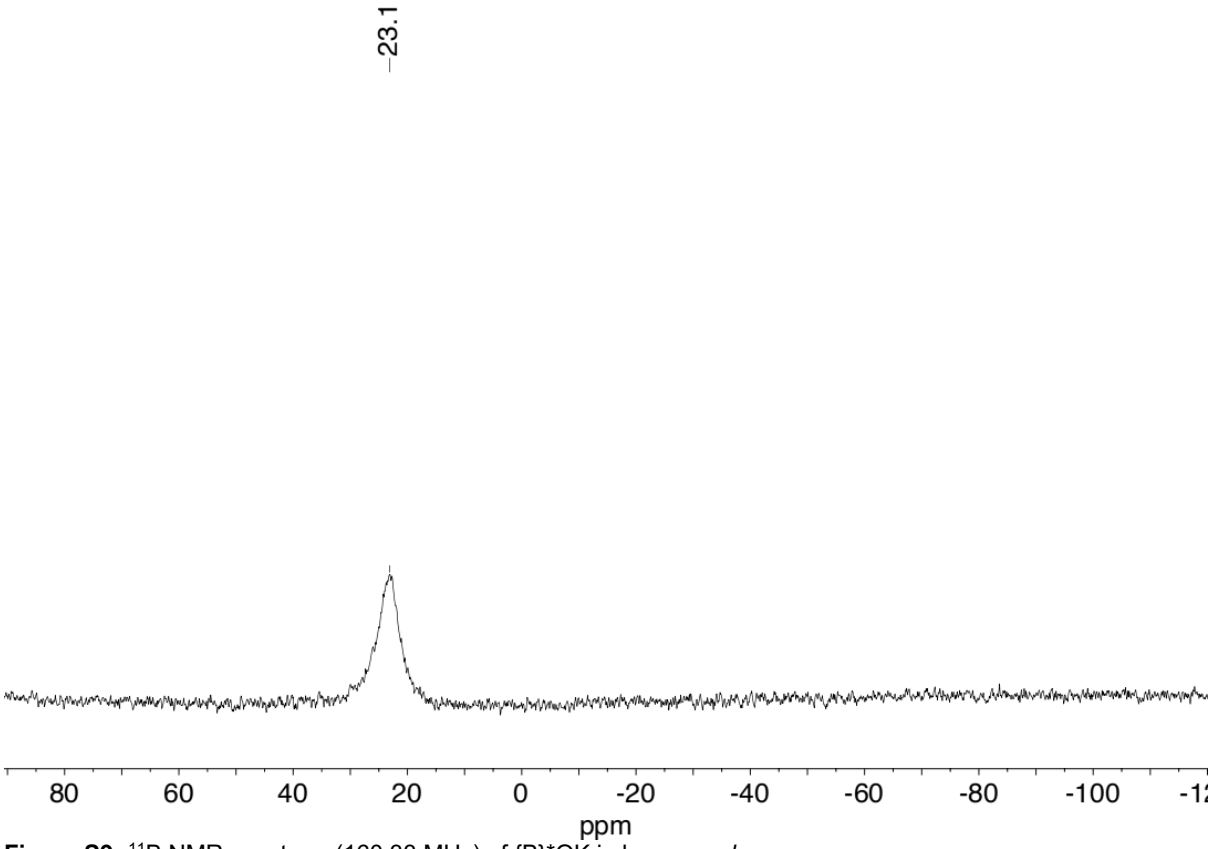


Figure S9: ^{11}B NMR spectrum (160.33 MHz) of {B}*OK in benzene-d_6.

1.3.4 NMR Spectra of {B}*OSiCl$_3$

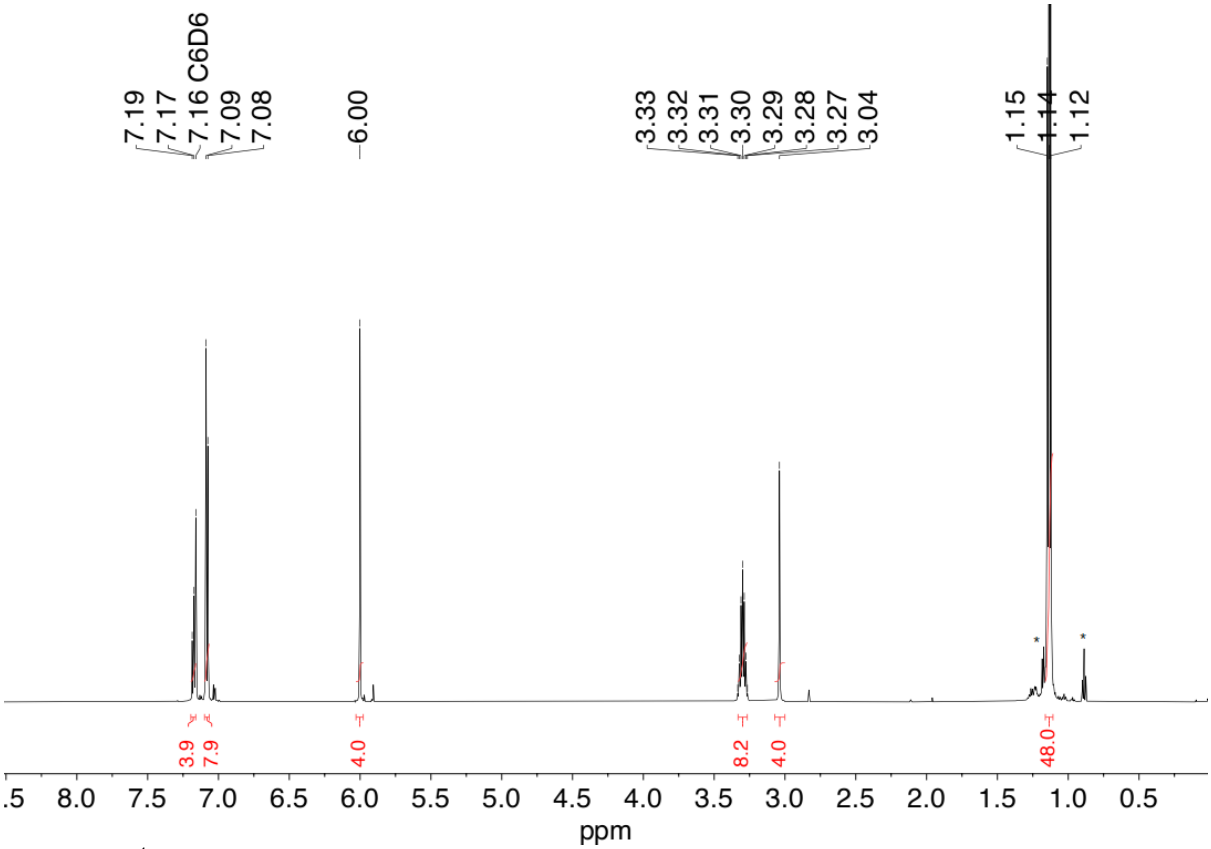


Figure S10: ^{1}H NMR spectrum (400.1 MHz) of {B}*SiCl$_3$ in benzene-d_6. Marked (*) signals are due to trace amounts of *n*-hexane.

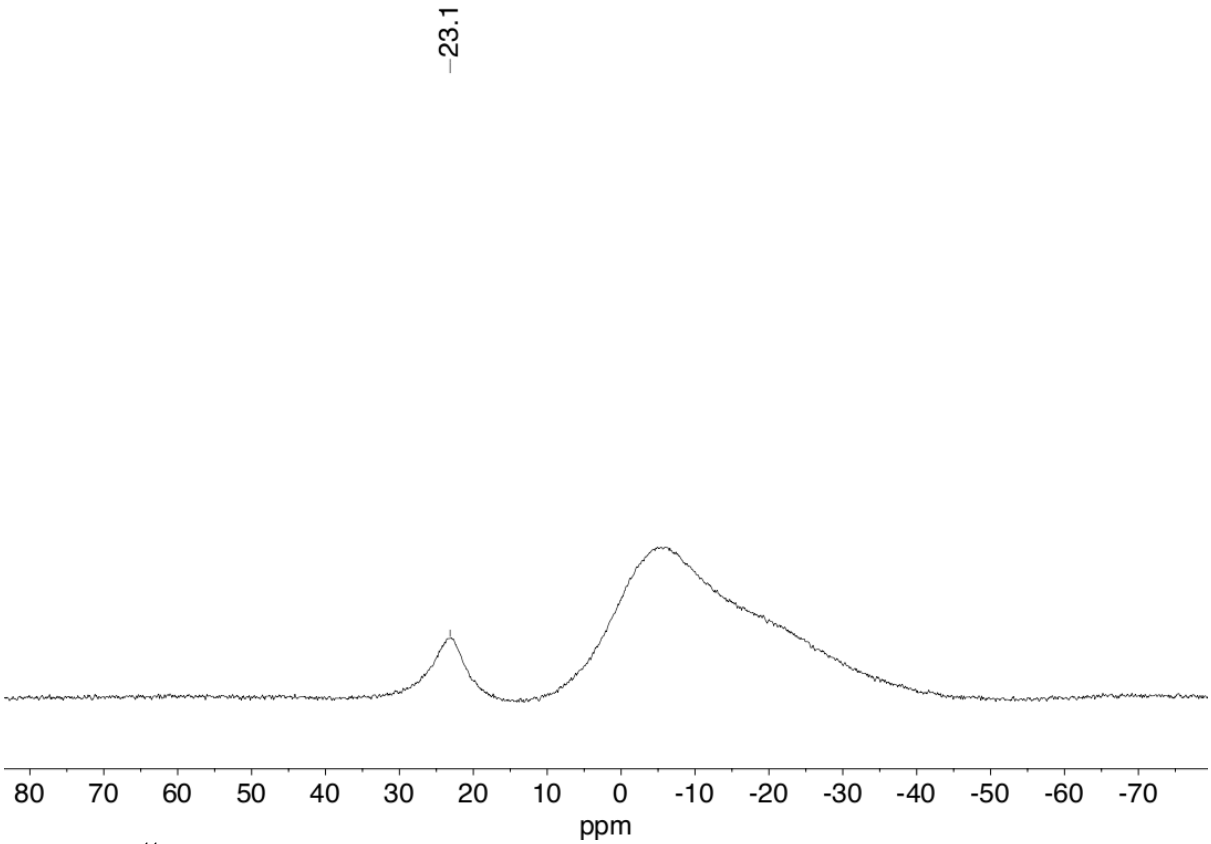


Figure S11: ^{11}B NMR spectrum (128.4 MHz) of {B}*SiCl$_3$ in benzene-d_6.

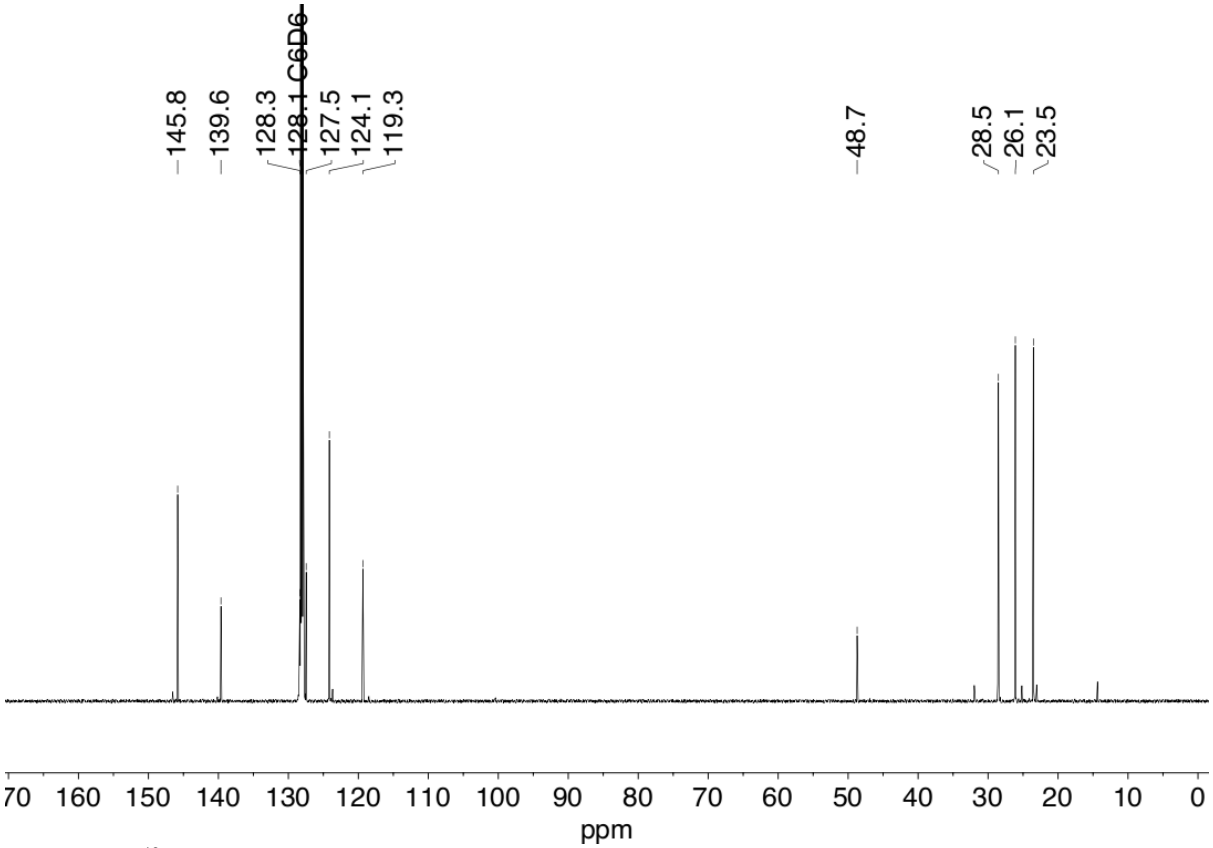


Figure S12: ^{13}C NMR spectrum (100.6 MHz) of {B}*$SiCl_3$ in benzene-d_6.

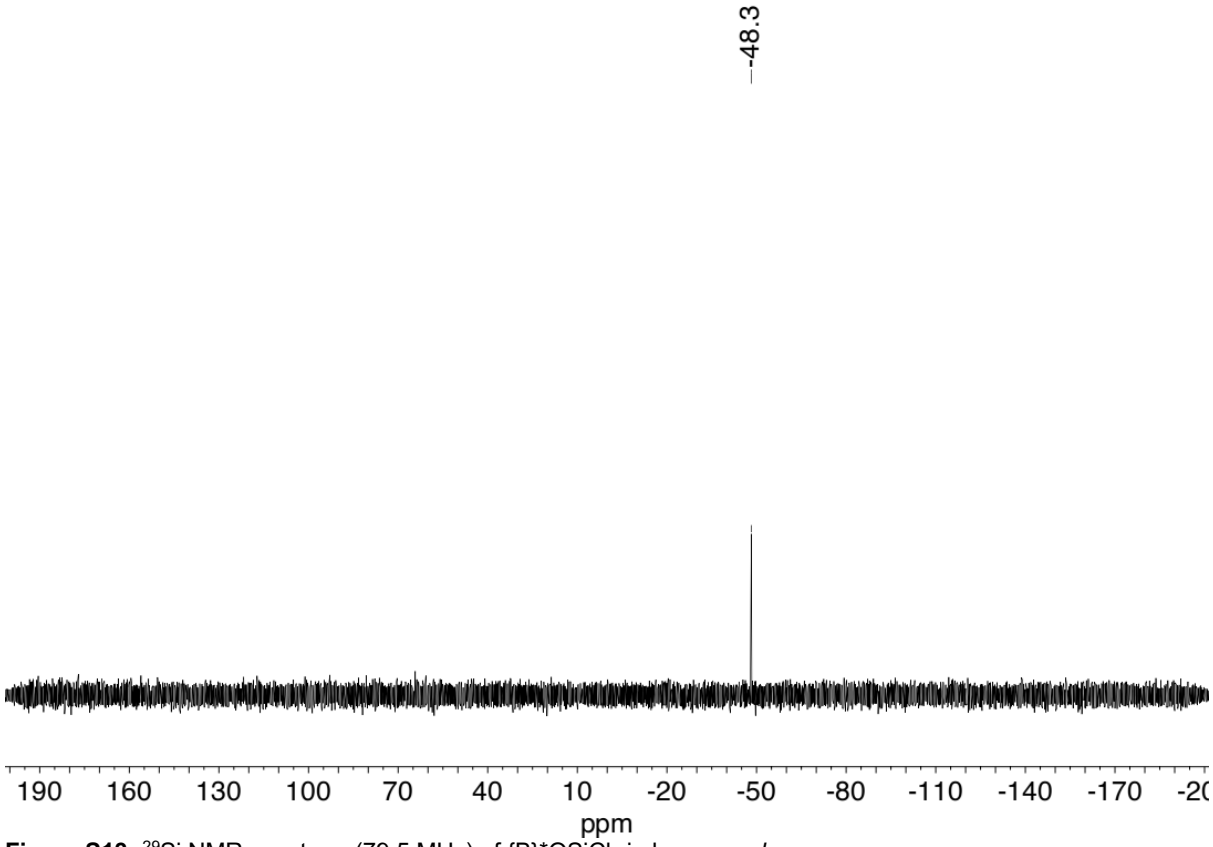


Figure S13: ^{29}Si NMR spectrum (79.5 MHz) of {B}*$OSiCl_3$ in benzene-d_6.

1.3.5 NMR Spectra of {B}*OSiHCl$_2$

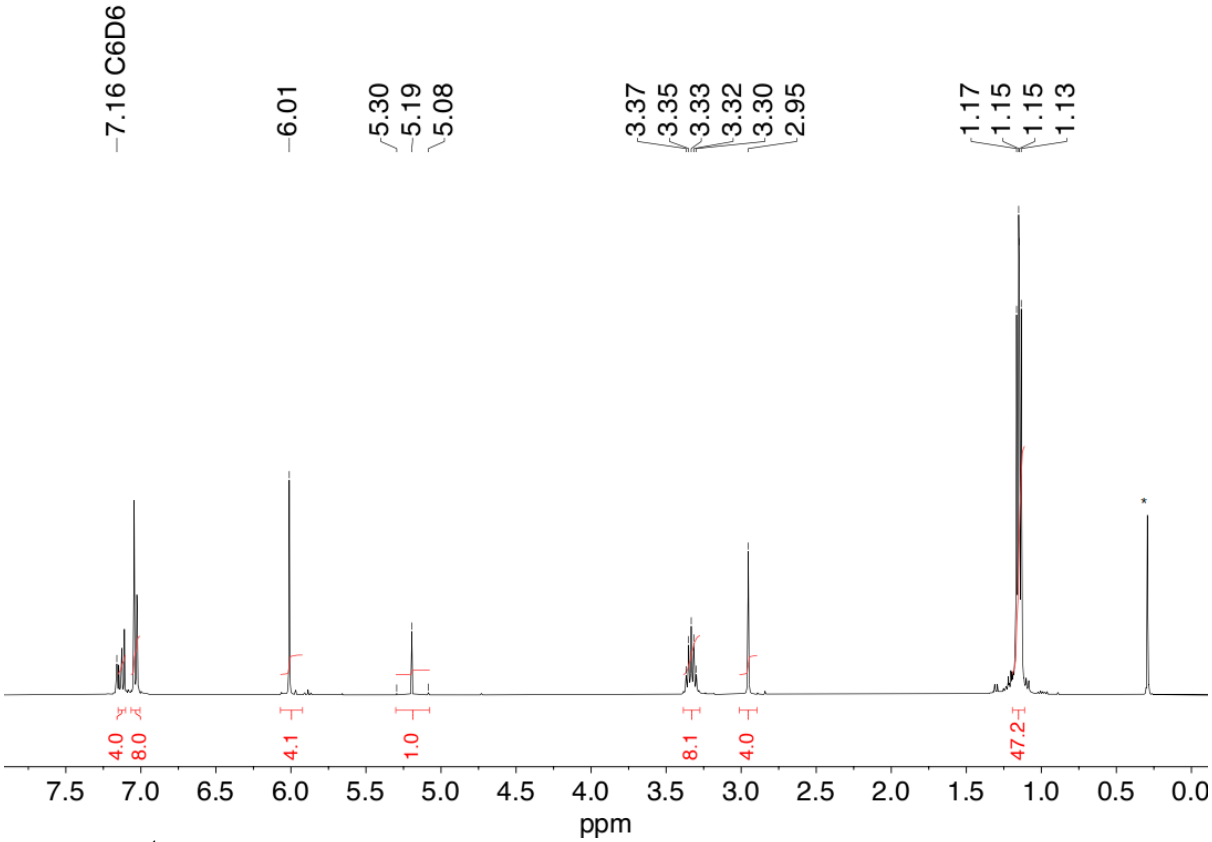


Figure S14: ^{1}H NMR spectrum (400.1 MHz) of {B}*OSiHCl$_2$ in benzene-d_6. Marked (*) signal is due to trace amounts of silicon grease.

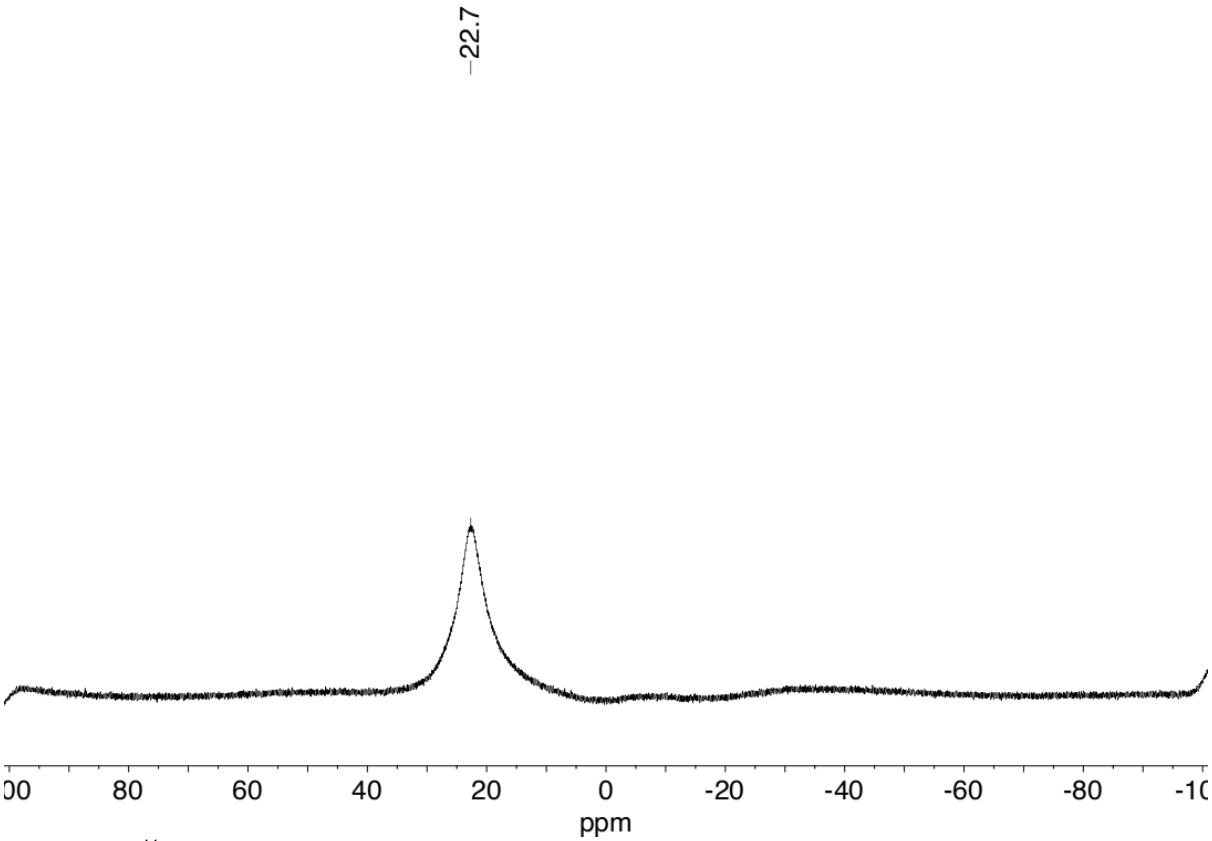


Figure S15: ^{11}B NMR spectrum (128.4 MHz) of {B}*OSiHCl$_2$ in benzene-d_6.

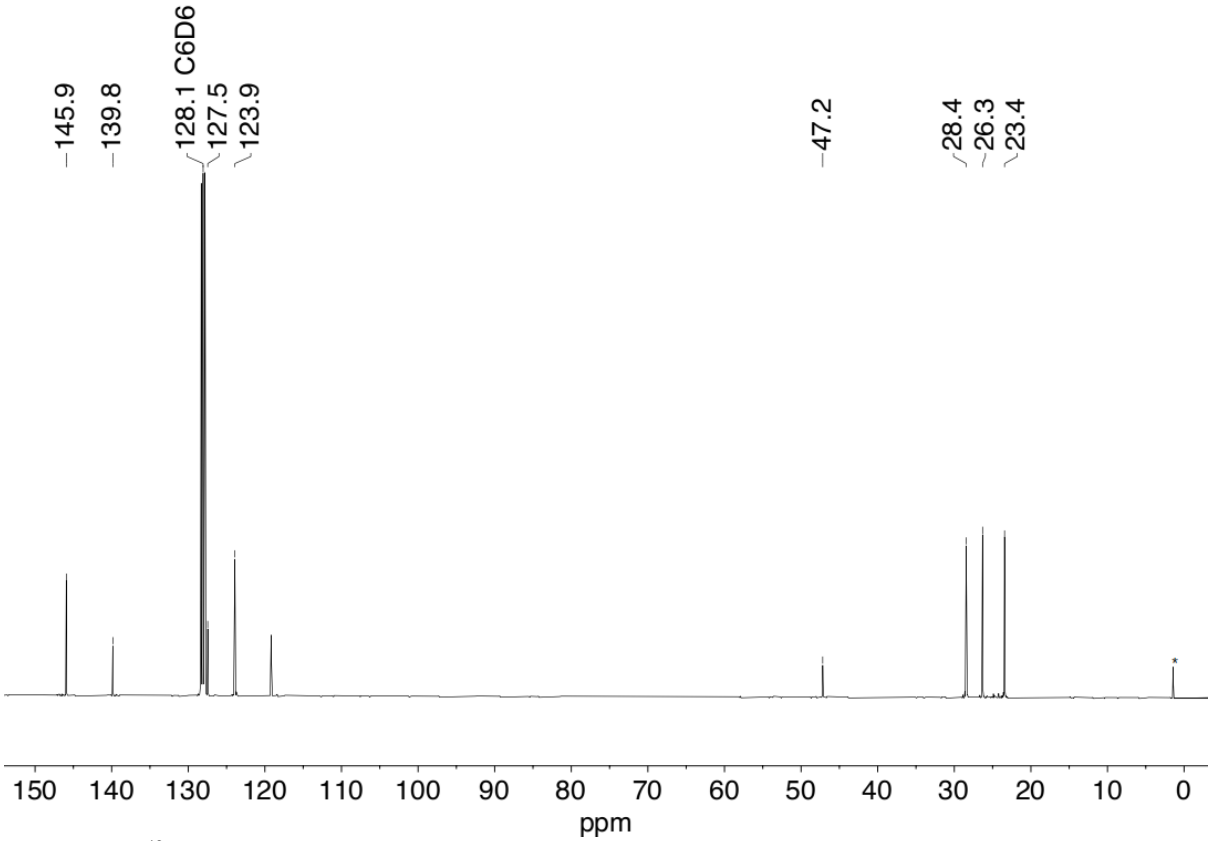


Figure S16: ^{13}C NMR spectrum (100.6 MHz) of {B}*OSiHCl$_2$ in benzene-d_6. Marked (*) signal is due to silicon grease.

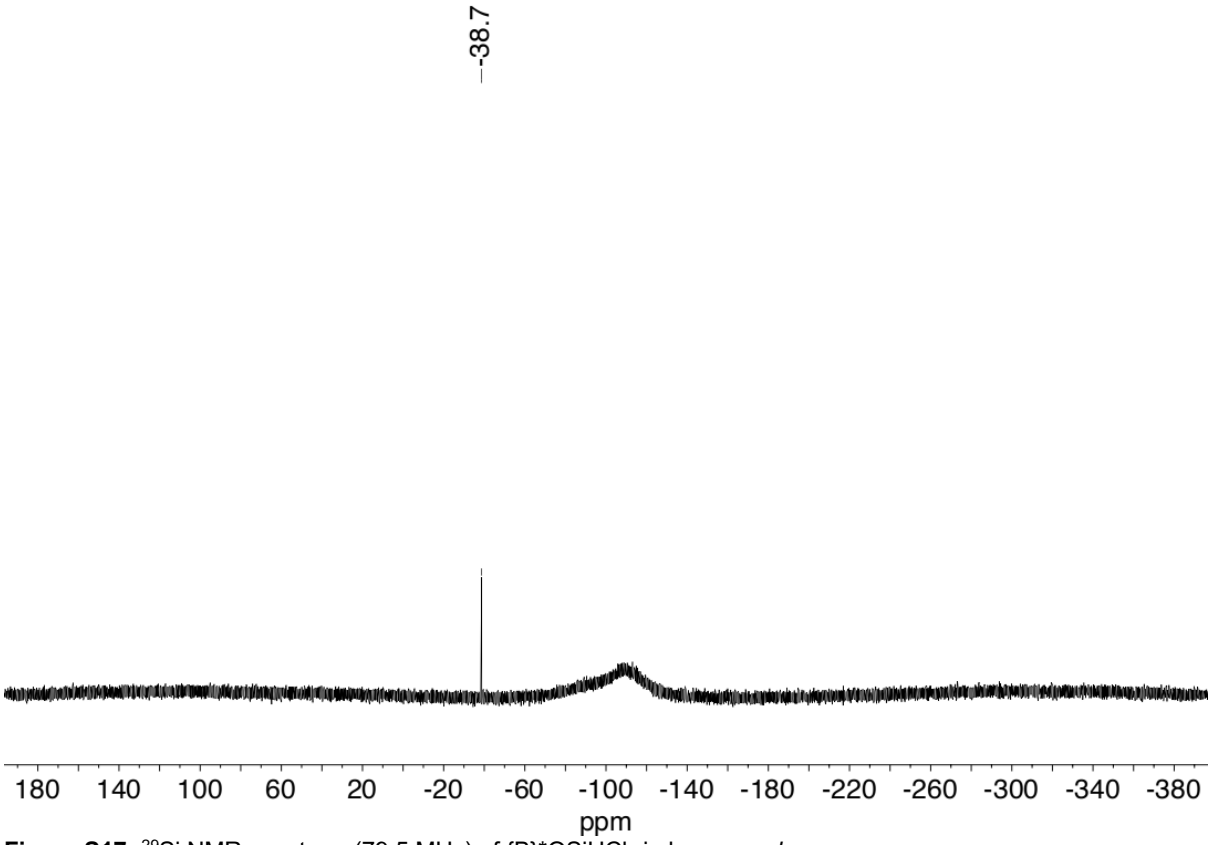


Figure S17: ^{29}Si NMR spectrum (79.5 MHz) of {B}*OSiHCl$_2$ in benzene-d_6.

1.3.6 NMR Spectra of {B}*OSiBr$_3$

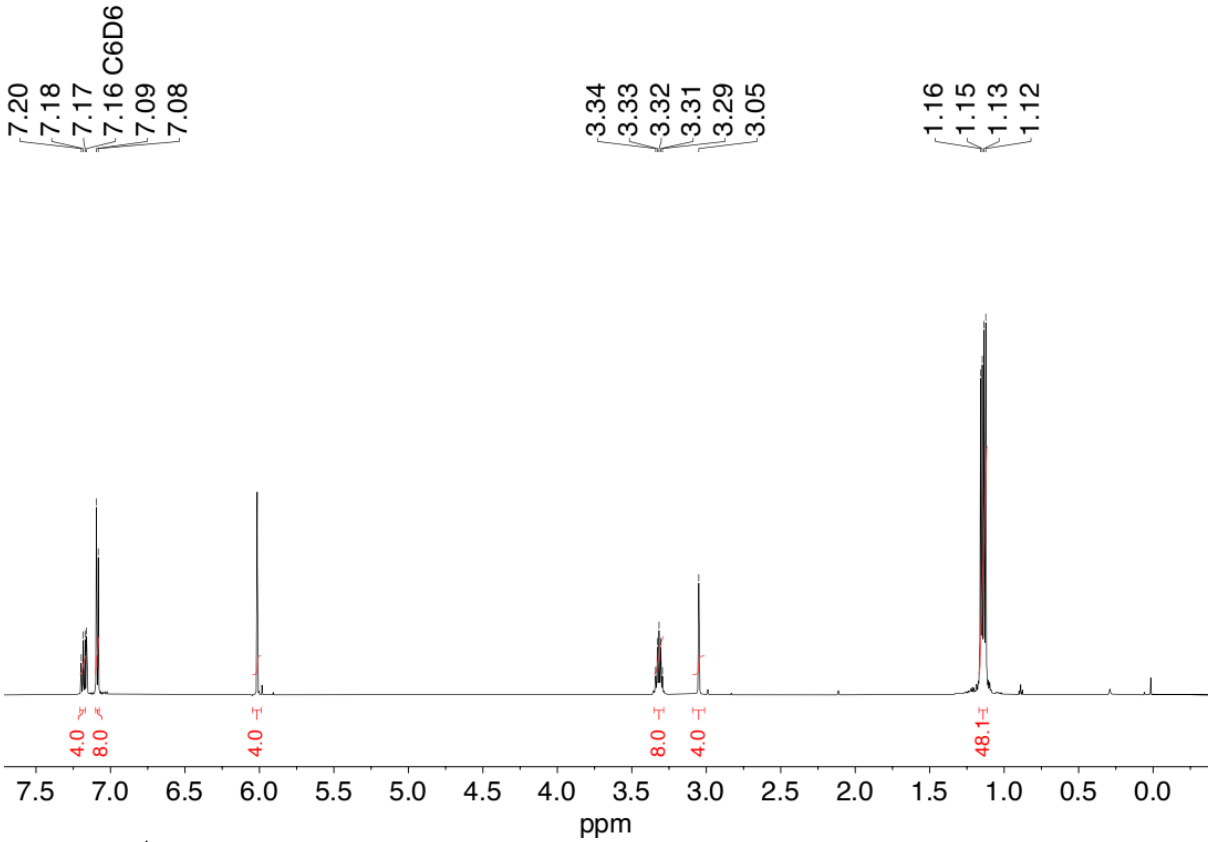


Figure S18: ^{1}H NMR spectrum (400.2 MHz) of {B}*OSiBr$_3$ in benzene-d_6

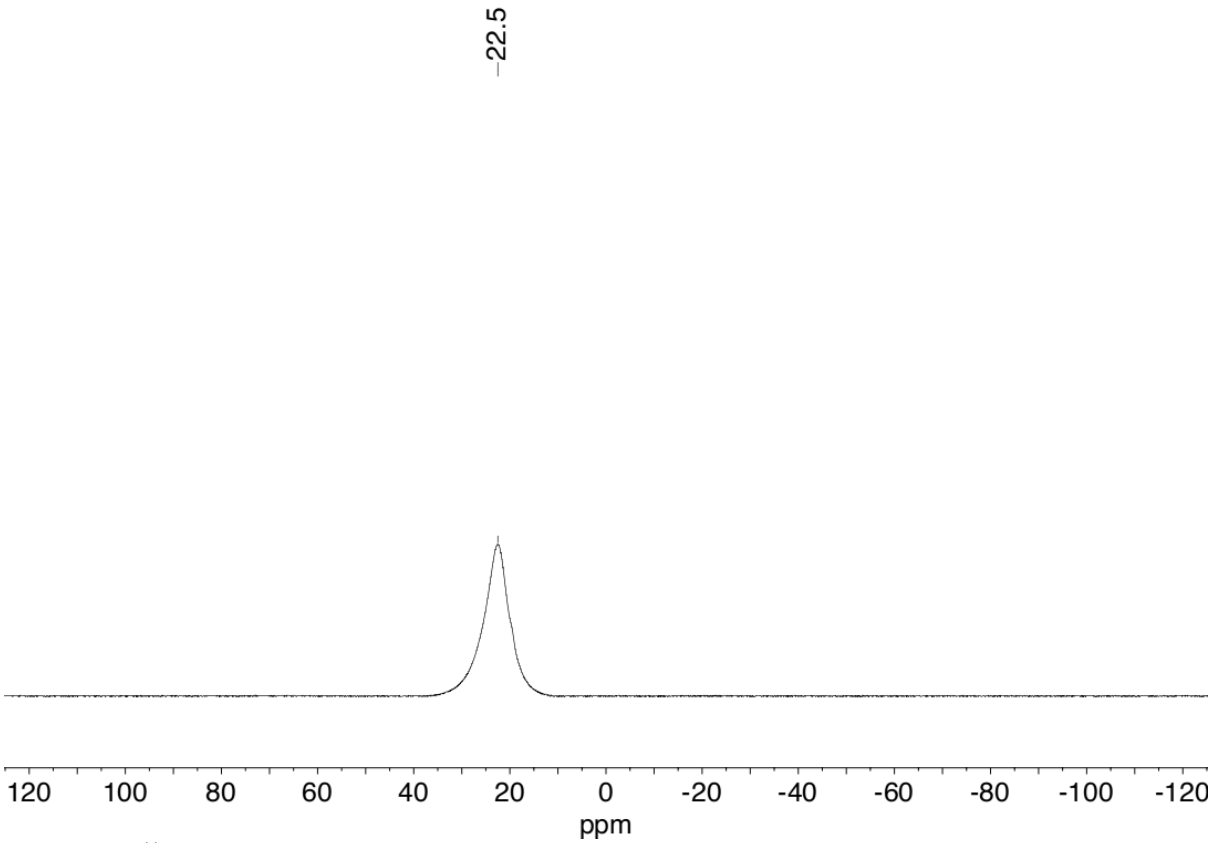


Figure S19: ^{11}B NMR spectrum (128.4 MHz) of {B}*OSiBr$_3$ in benzene-d_6.

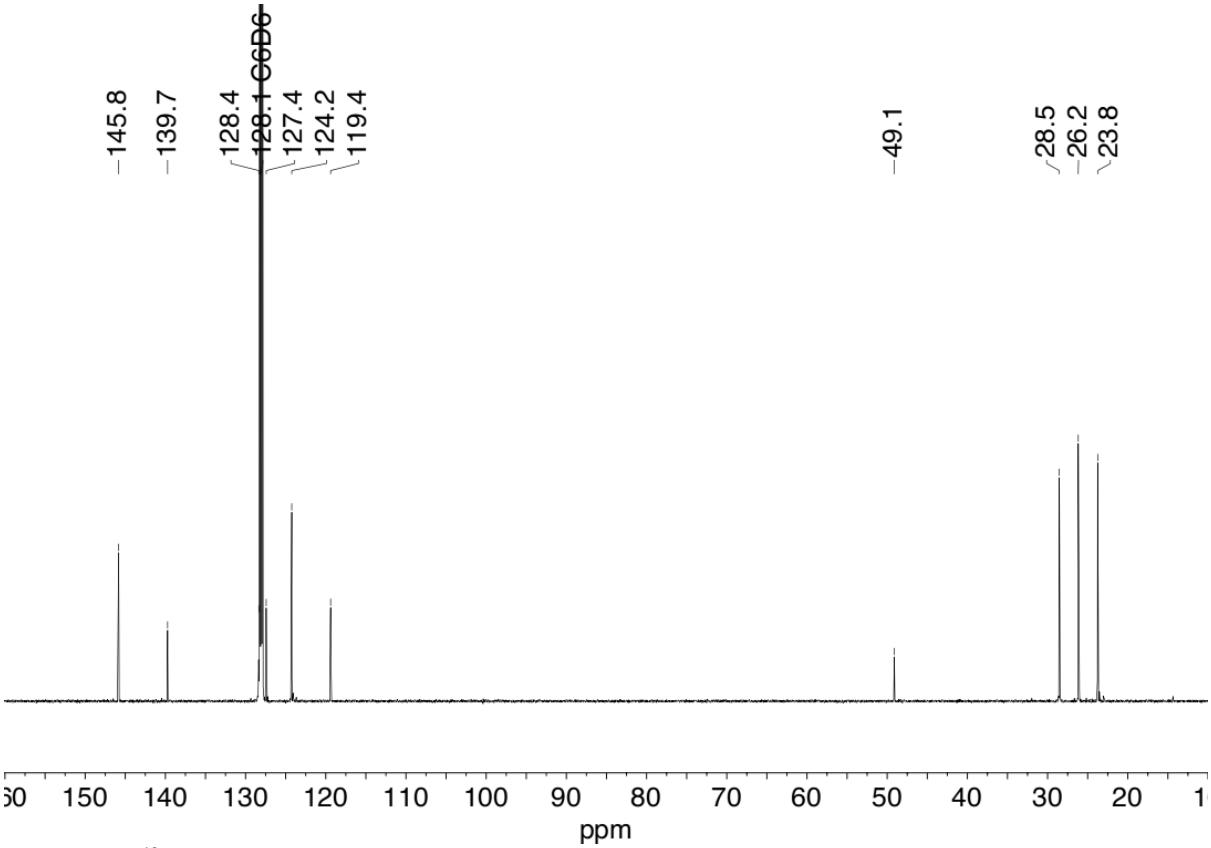


Figure S20: ^{13}C NMR spectrum (151.0 MHz) of {B}*Br in benzene-d_6

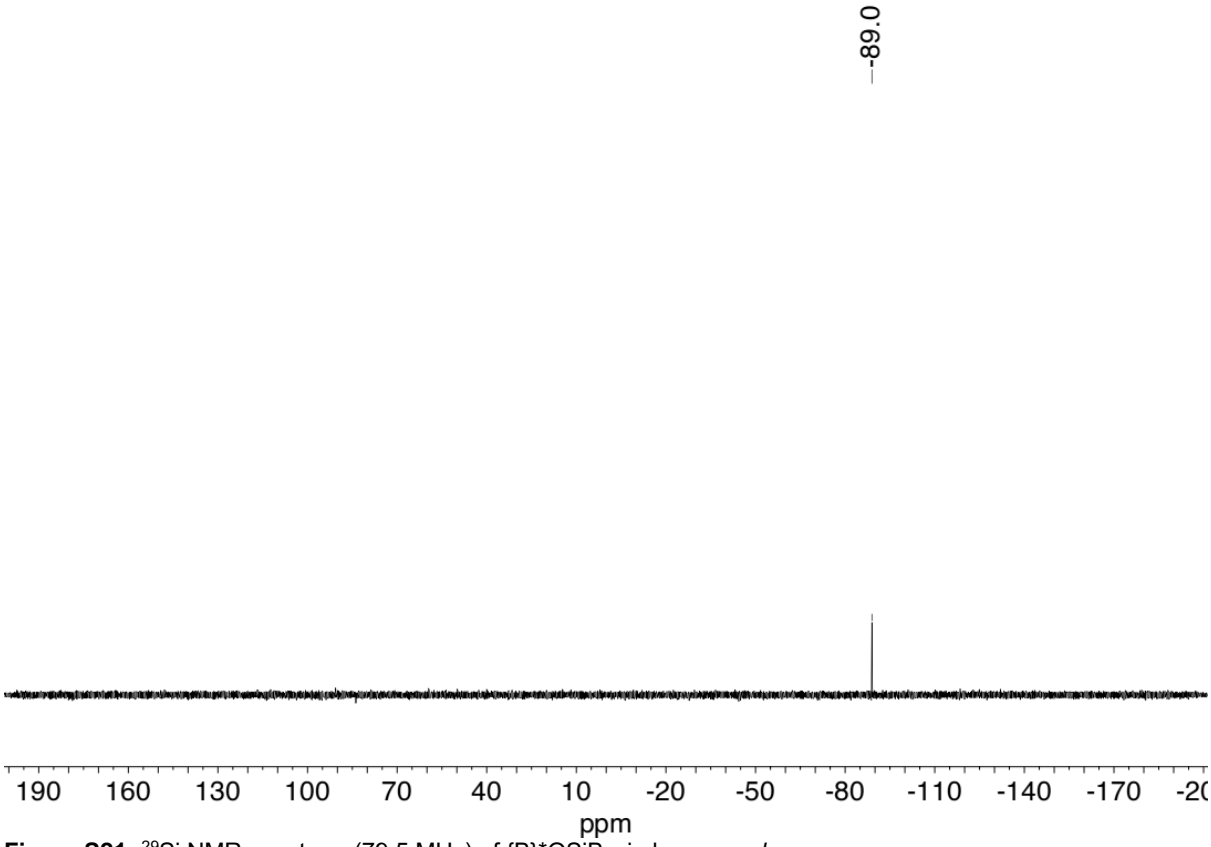


Figure S21: ^{29}Si NMR spectrum (79.5 MHz) of {B}*$OSiBr_3$ in benzene-d_6.

1.3.7 NMR Spectra of {B}*OSiBr

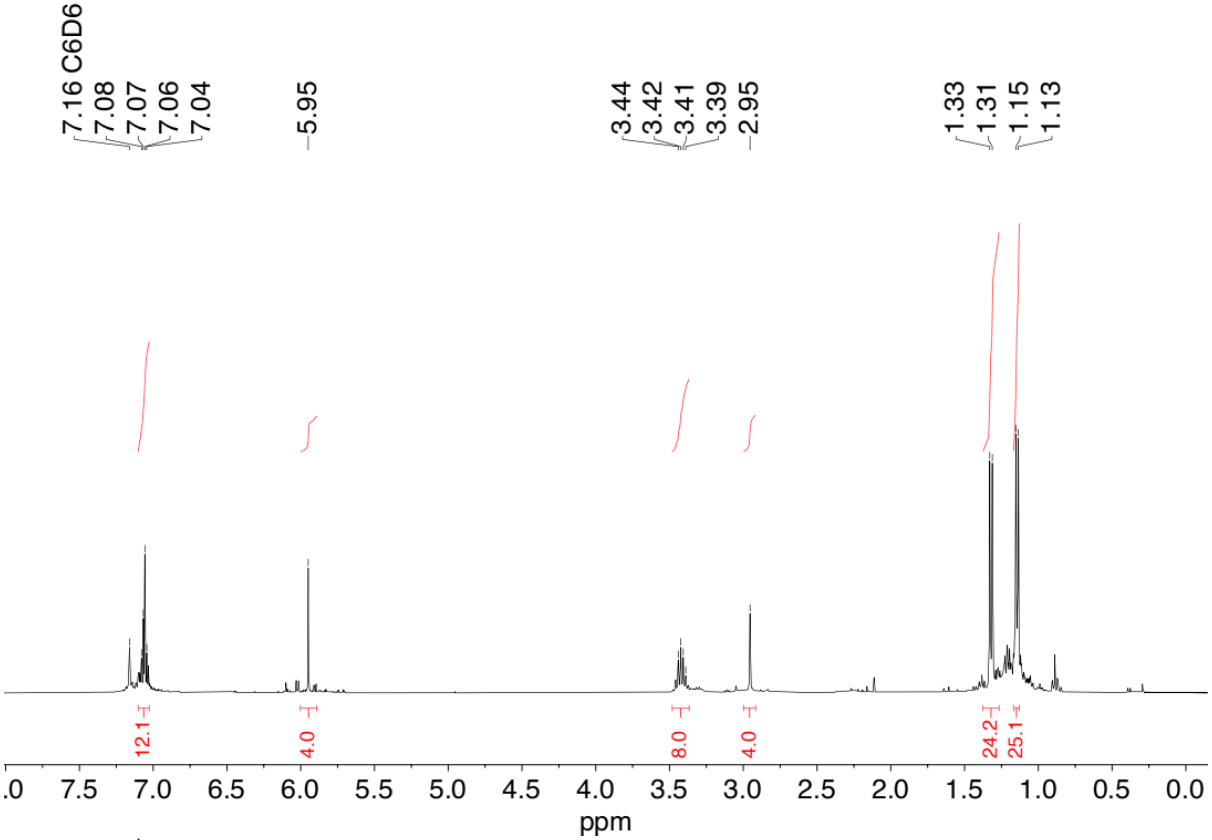


Figure S22 ^{1}H NMR spectrum (400.1 MHz) of {B}*OSiBr in benzene-d_6

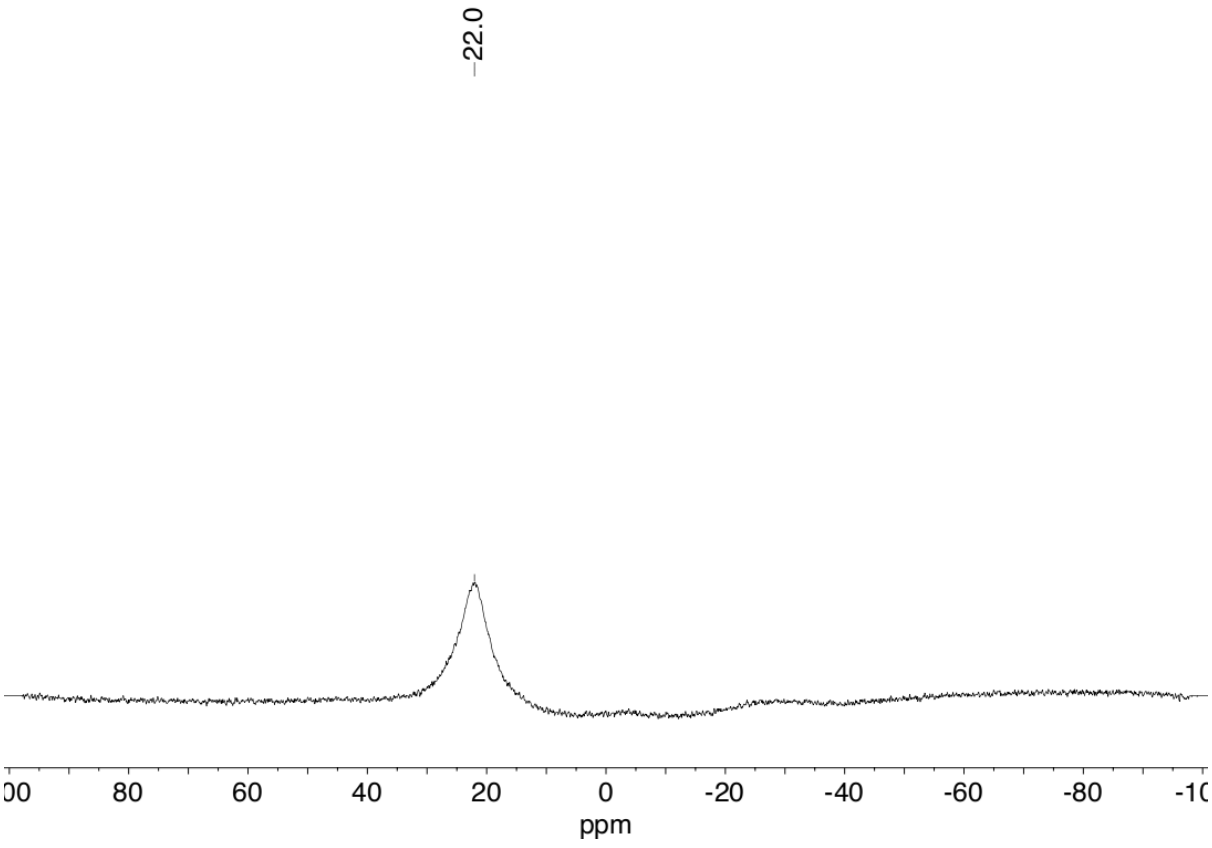


Figure S23: ^{11}B NMR spectrum (128.4 MHz) of {B}*OSiBr in benzene-d_6.

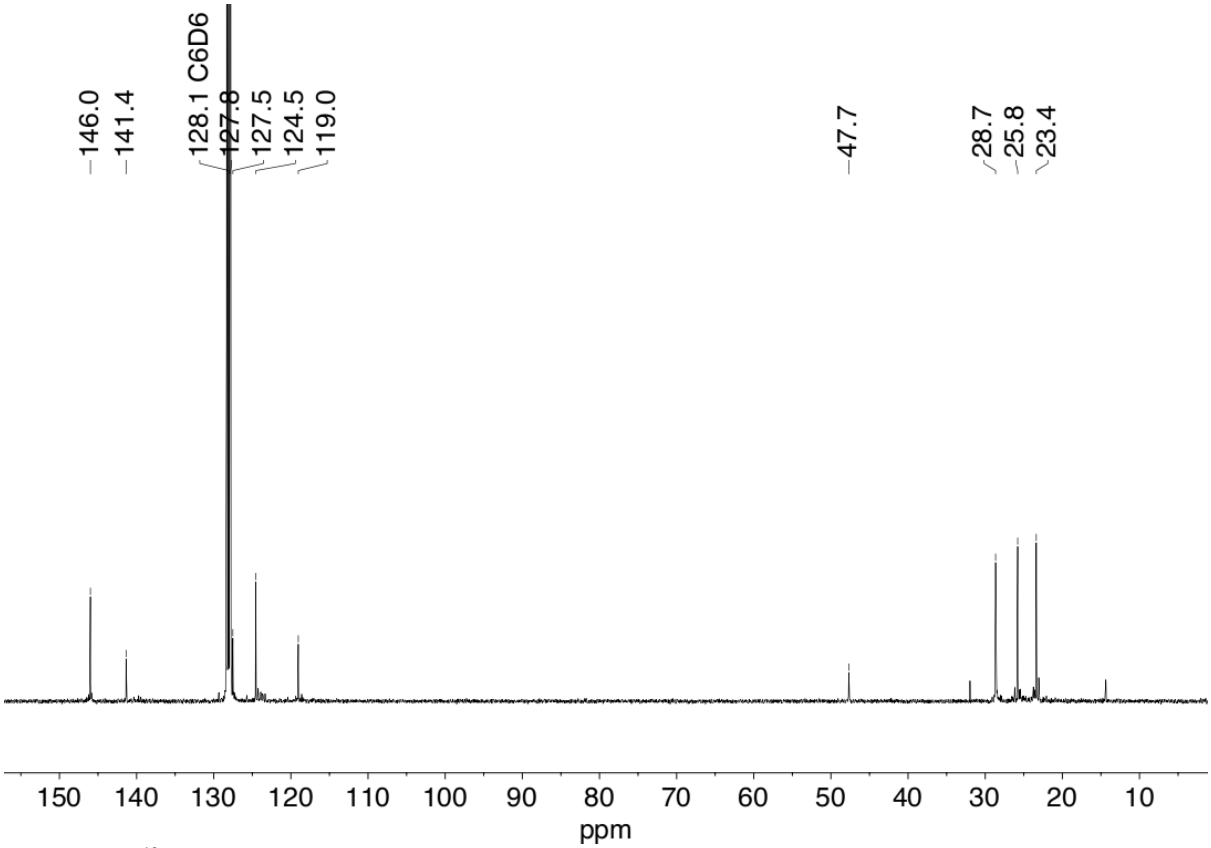


Figure S24: ^{13}C NMR spectrum (100.6MHz) of {B}*OSiBr in benzene-d_6.

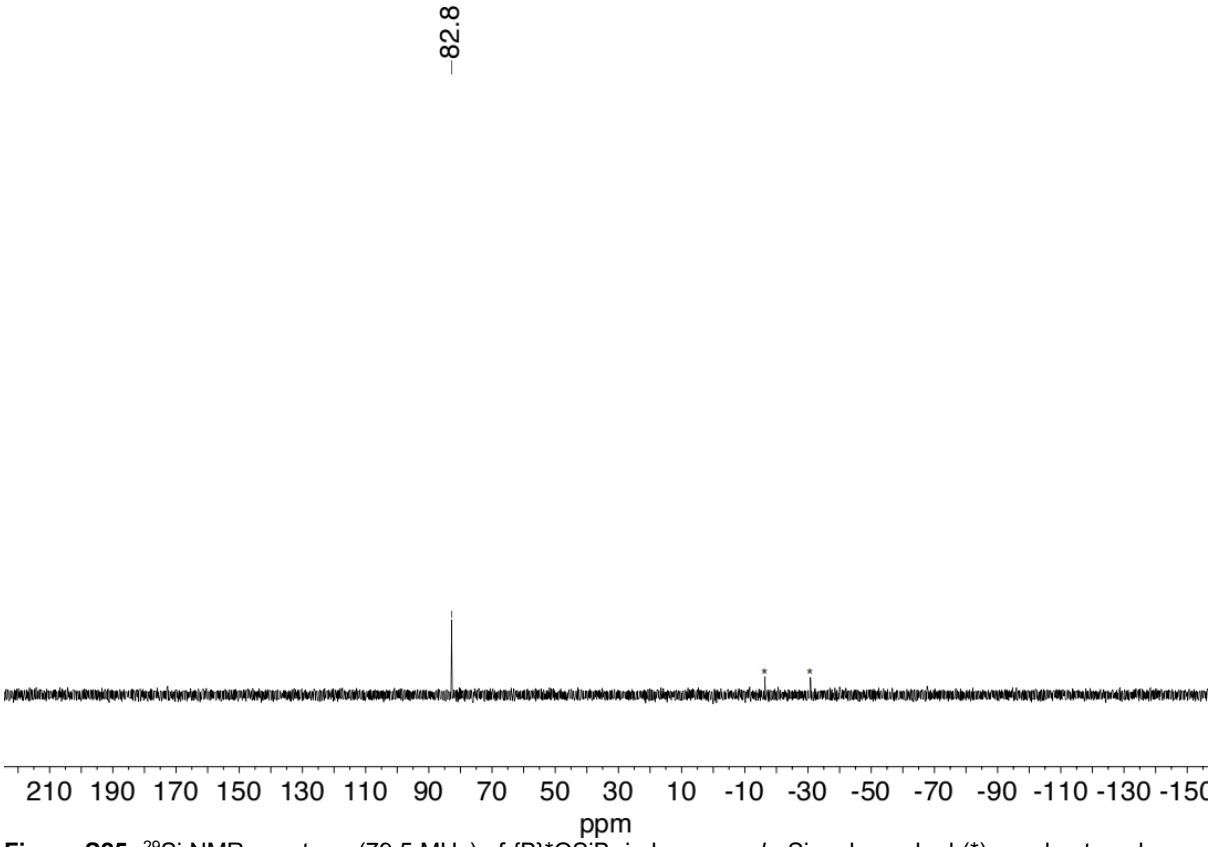


Figure S25: ^{29}Si NMR spectrum (79.5 MHz) of {B}*OSiBr in benzene-d_6. Signals marked (*) are due to unknown impurities.

1.3.8 NMR Spectra of 1

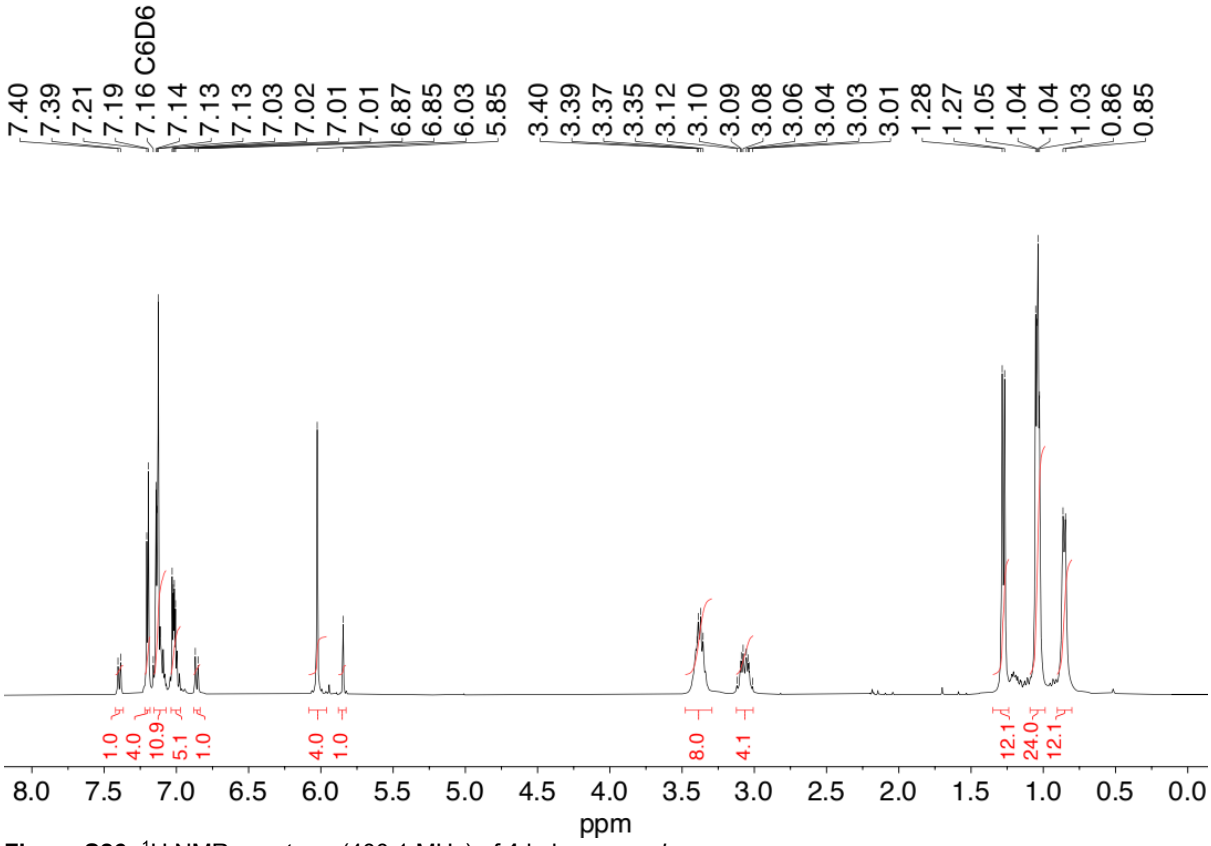


Figure S26: ^{1}H NMR spectrum (400.1 MHz) of **1** in benzene-d_6.

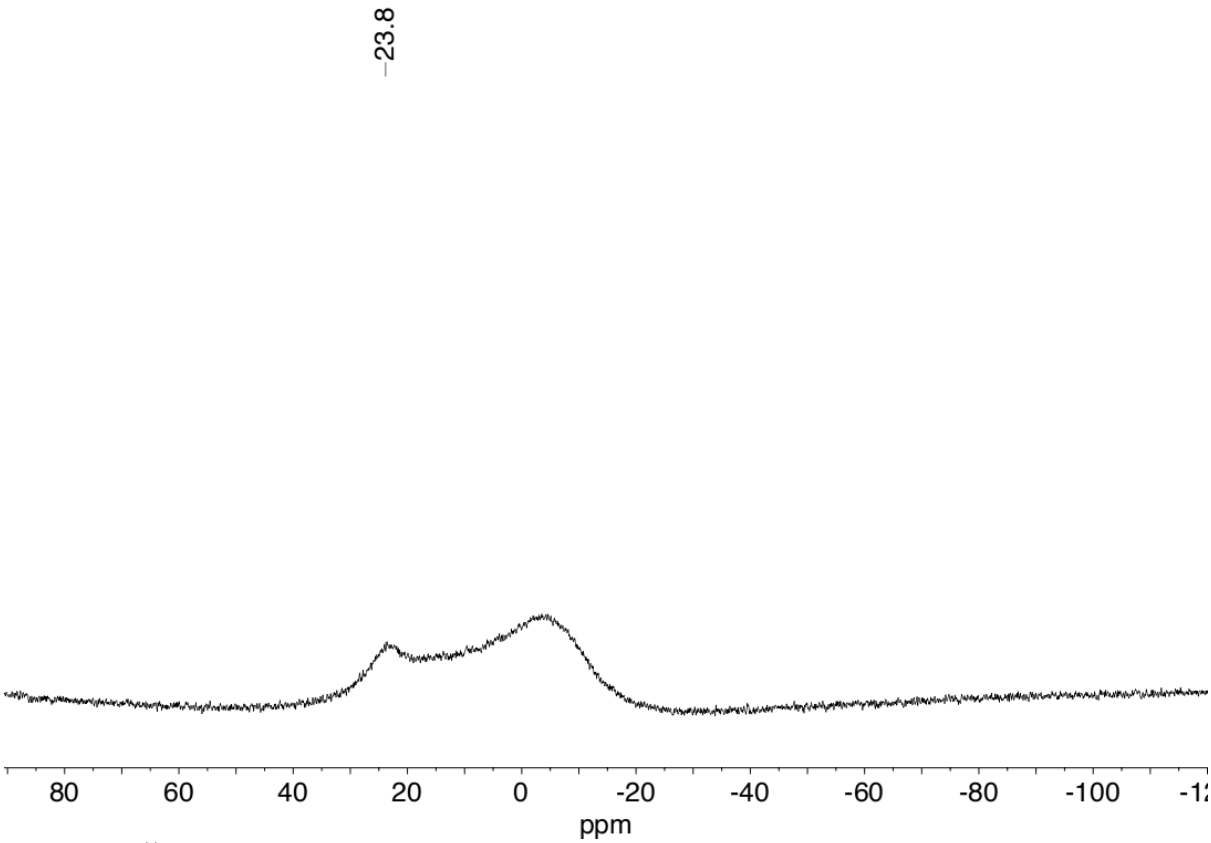


Figure S27: ^{11}B NMR spectrum (128.4 MHz) of **1** in benzene-d_6.

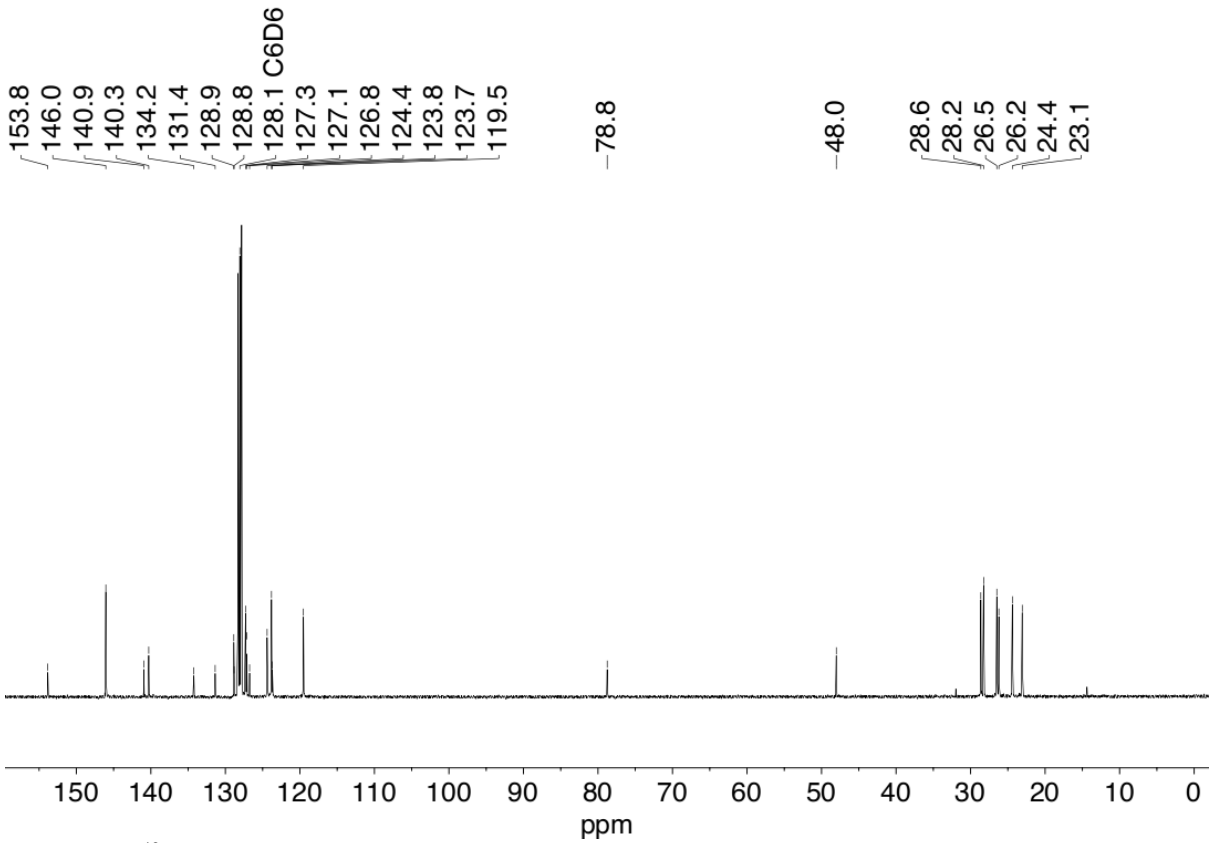


Figure S28: ^{13}C NMR spectrum (100.6 MHz) of **1** in benzene-d_6.

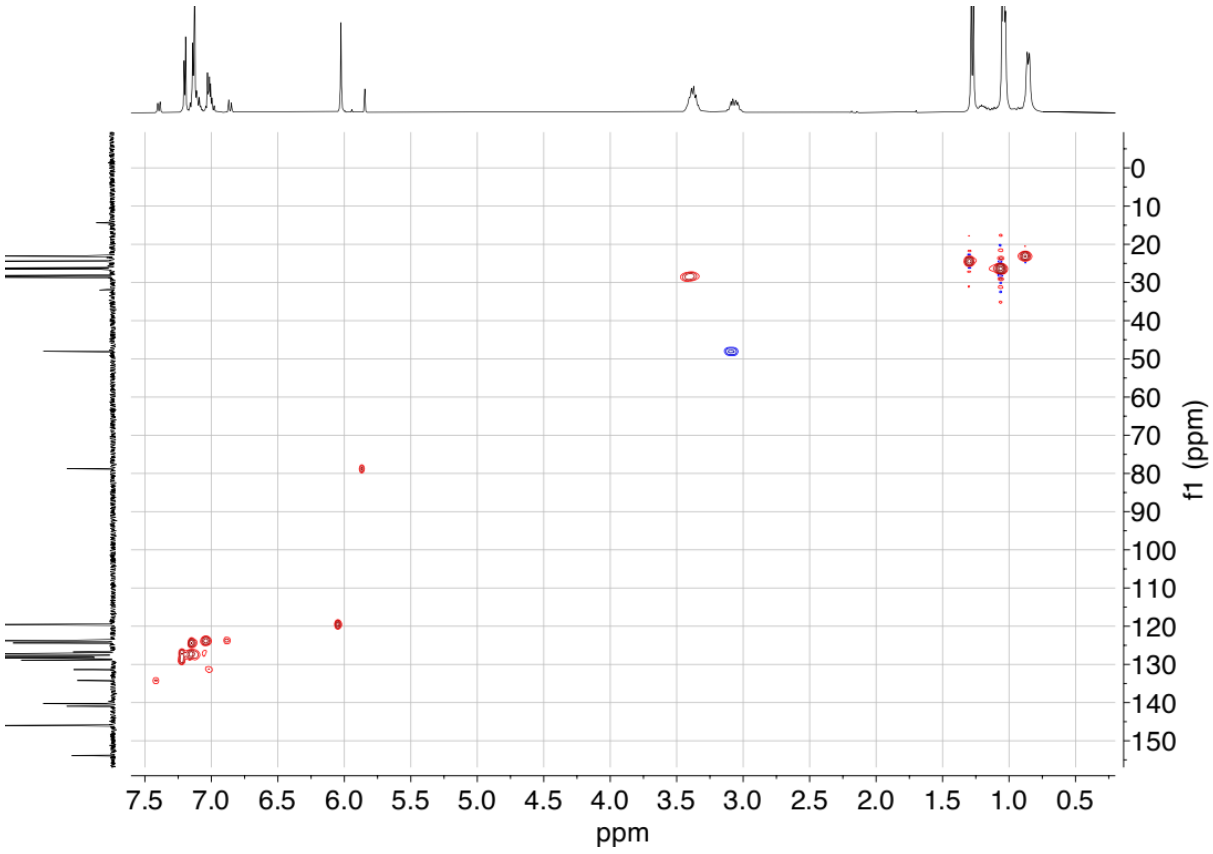


Figure S29: (^{1}H,^{13}C) HSQC spectrum of **1** – overview.

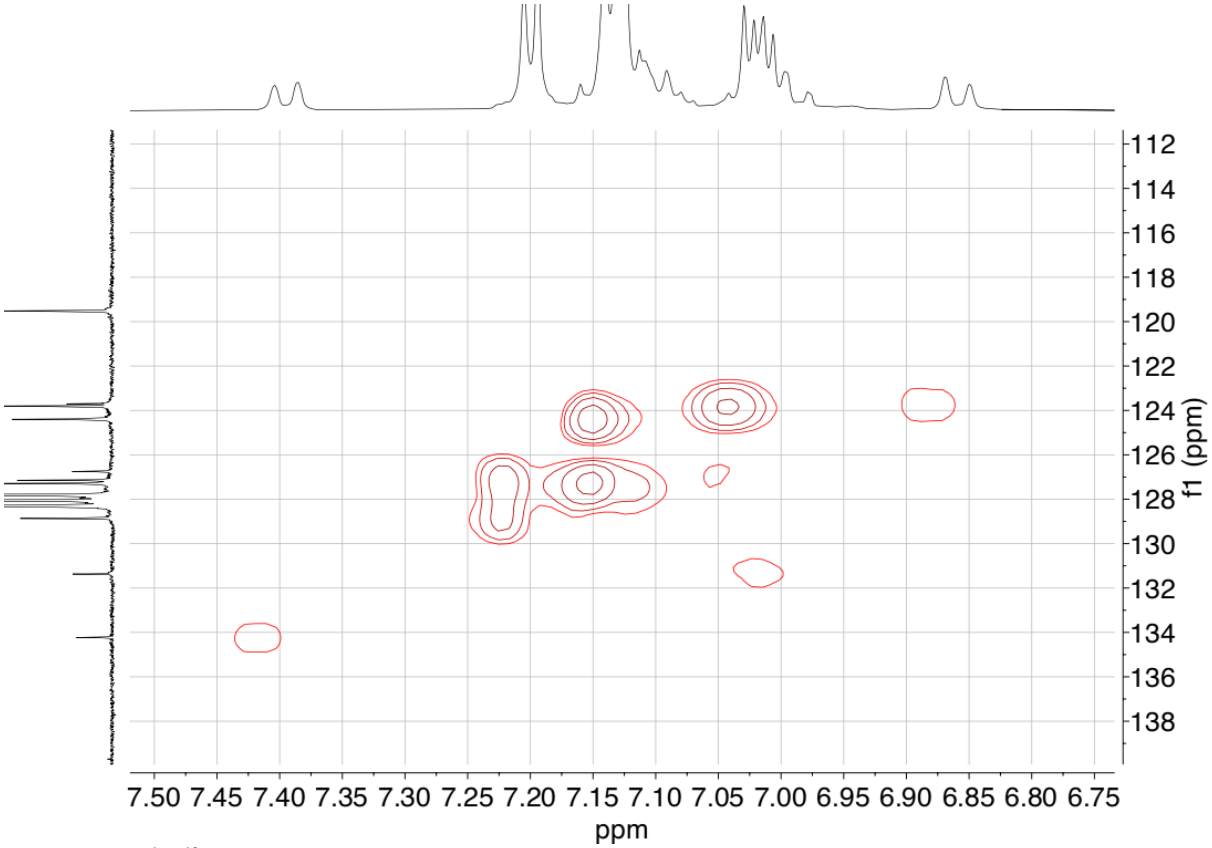


Figure S30: (^{1}H,^{13}C) HSQC spectrum of **1** – aromatic signals.

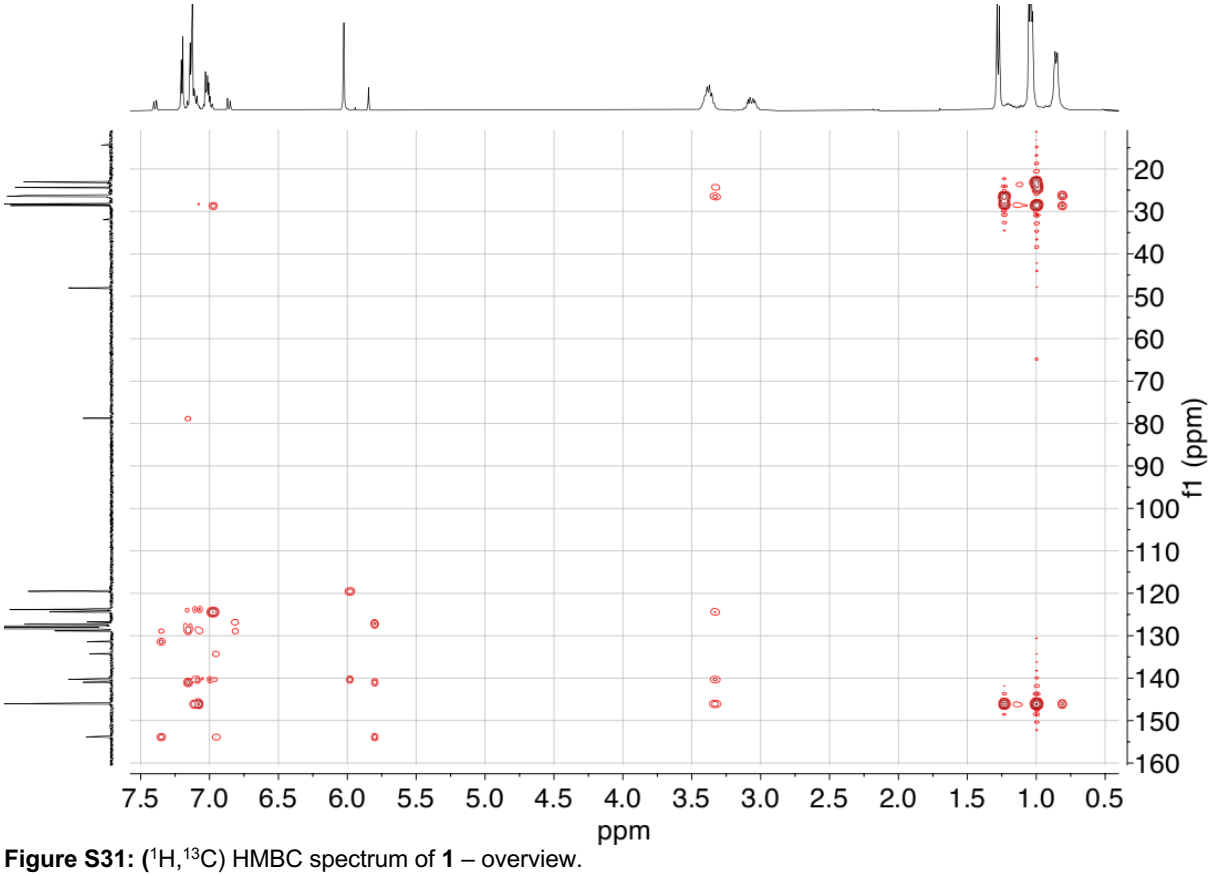


Figure S31: (^{1}H,^{13}C) HMBC spectrum of **1** – overview.

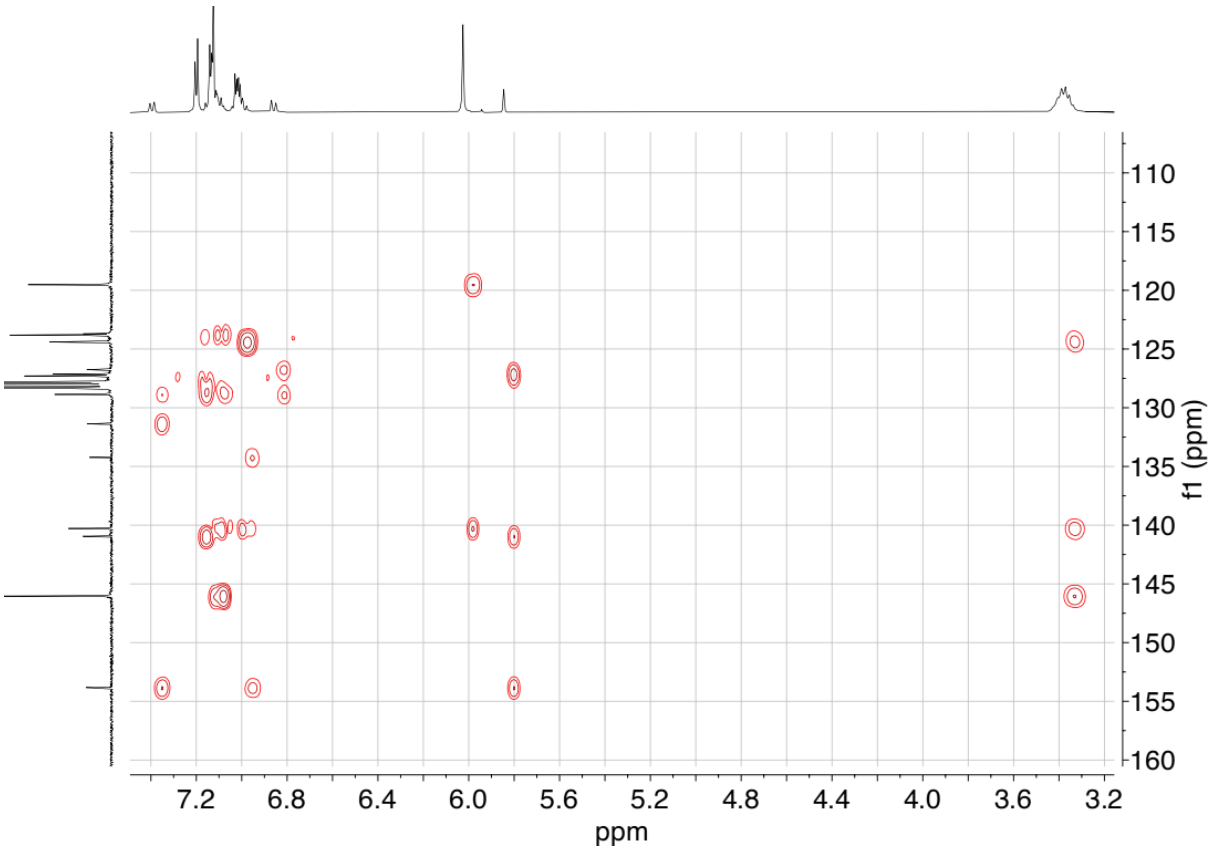


Figure S32: (^{1}H,^{13}C) HMBC spectrum of **1**.

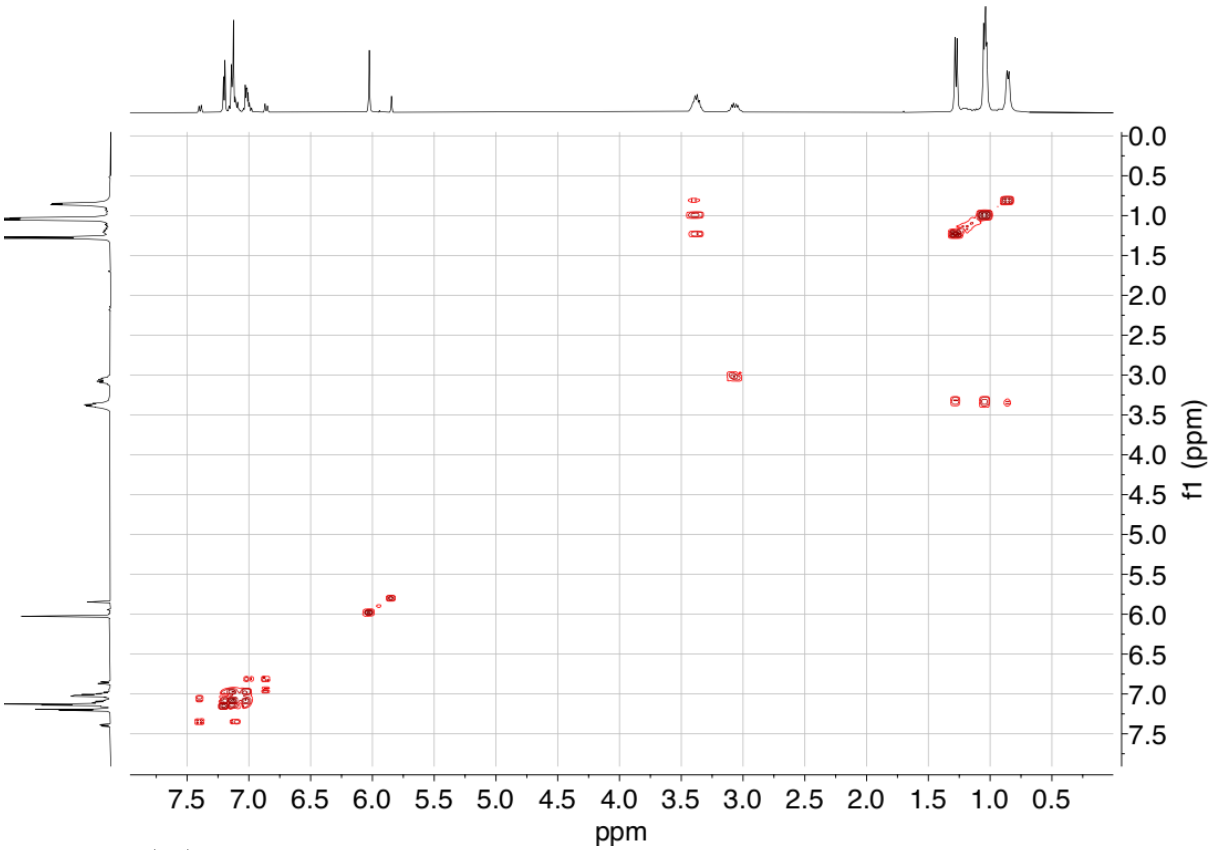


Figure S33: (^{1}H,^{1}H) COSY spectrum – overview.

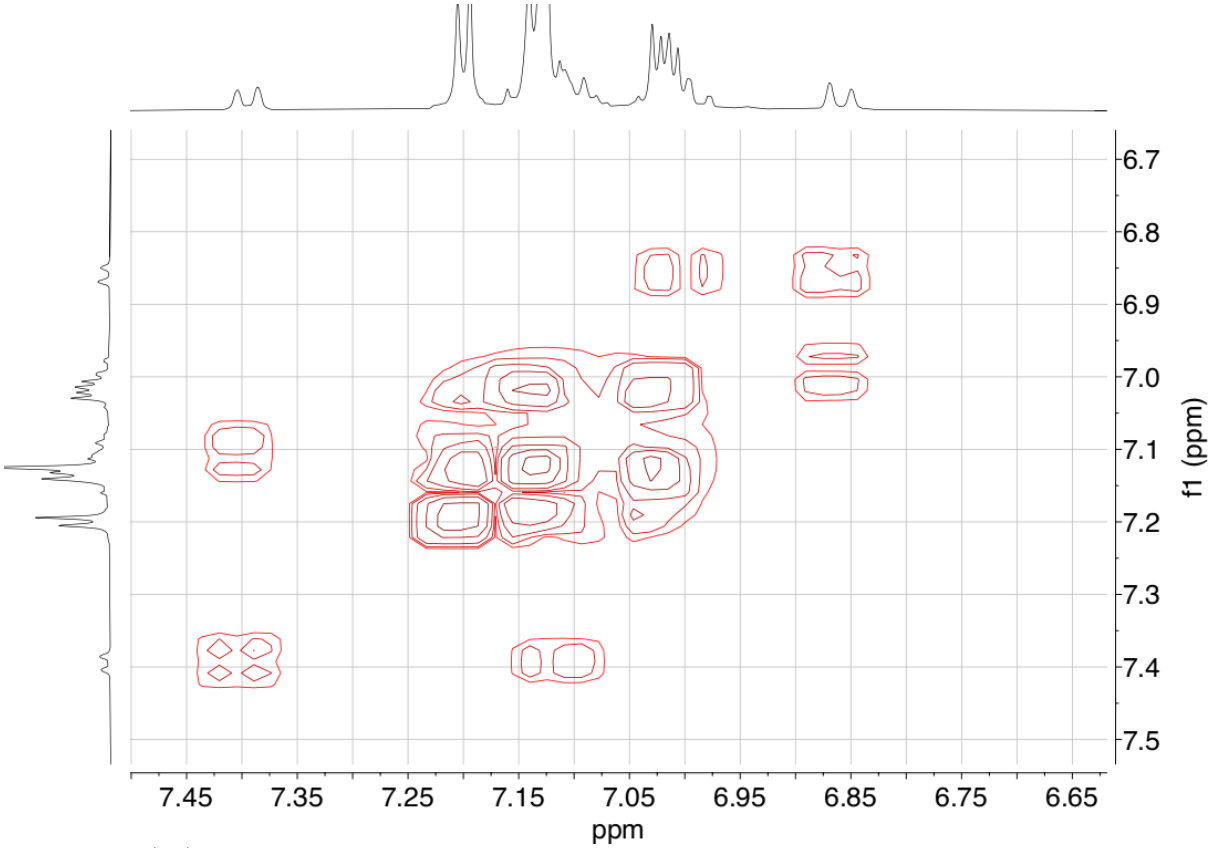


Figure S34: (^{1}H,^{1}H) COSY spectrum – aromatic region.

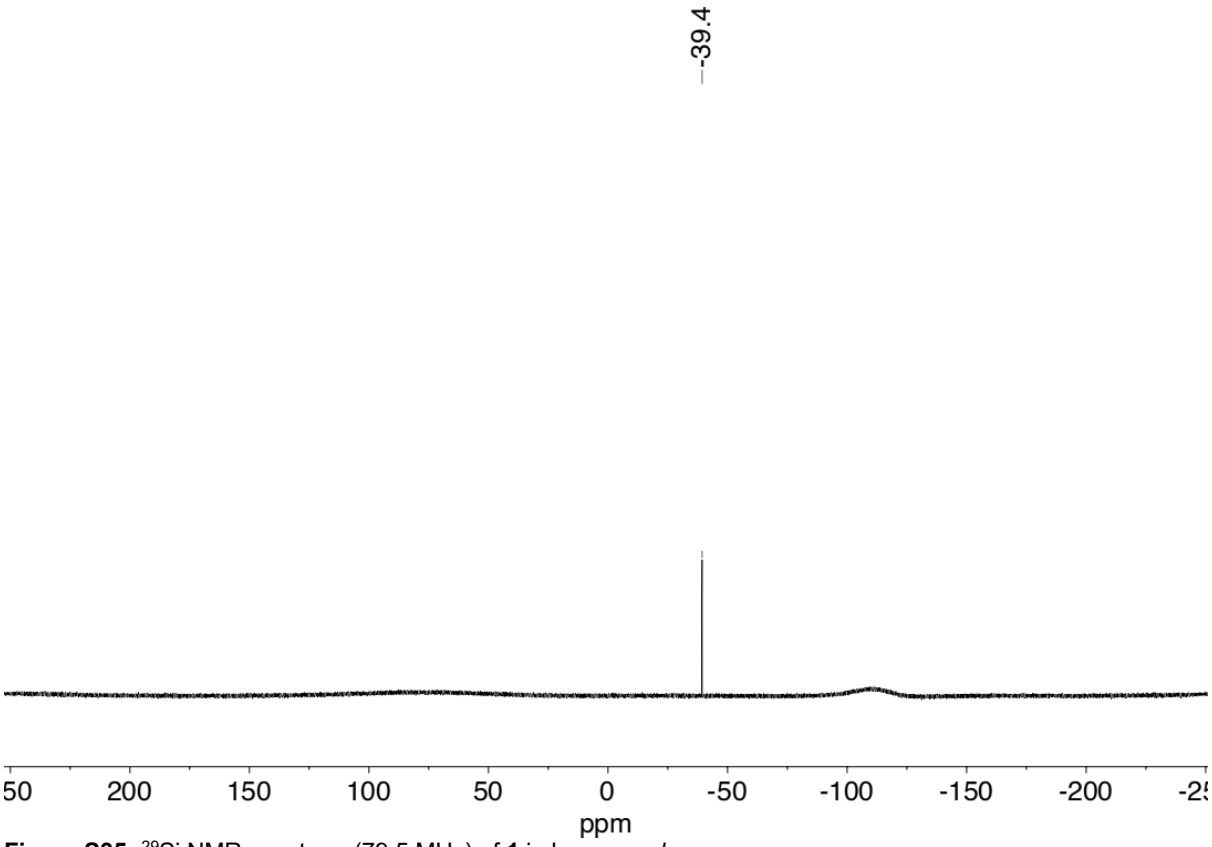


Figure S35: ^{29}Si NMR spectrum (79.5 MHz) of **1** in benzene-d_6.

1.3.9 NMR spectra of {B}*OGeCl

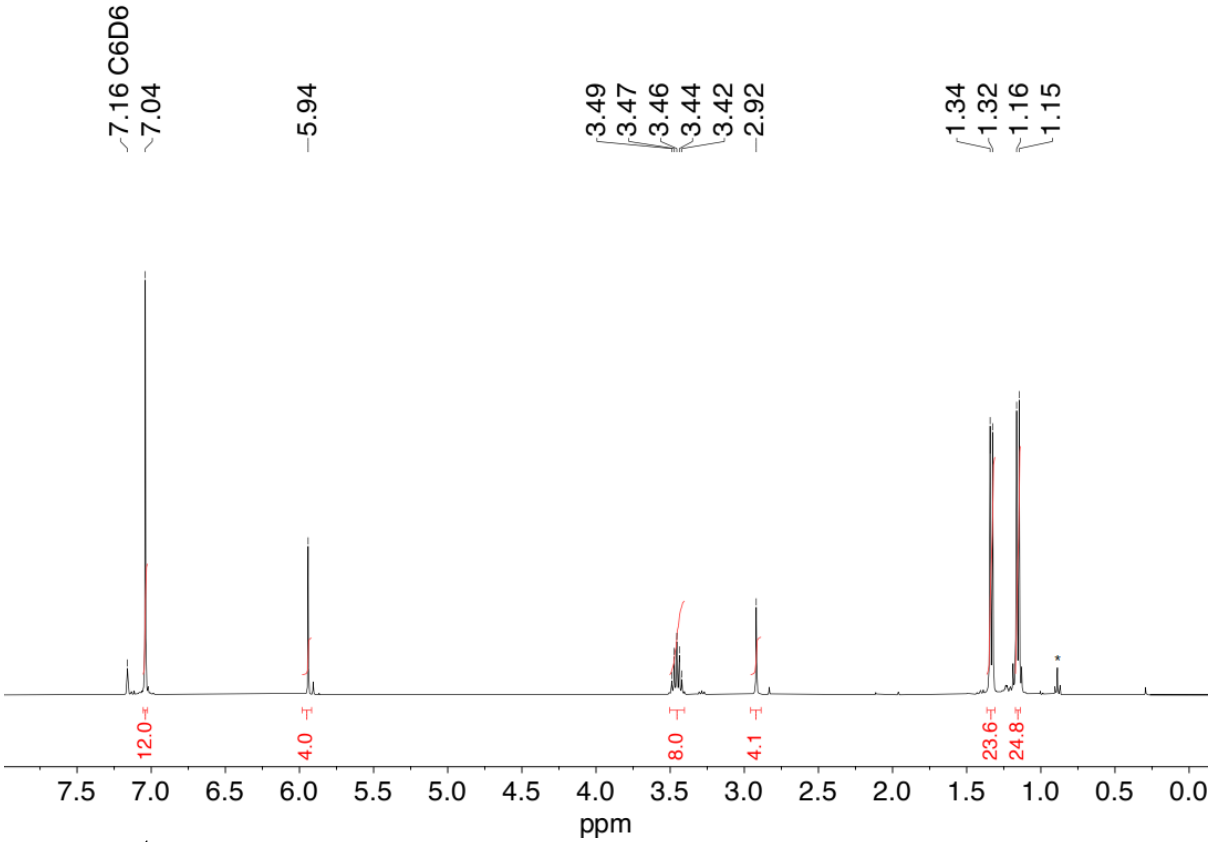


Figure S36: ^{1}H NMR spectrum (400.1 MHz) of {B}*OGeCl in benzene-d_6

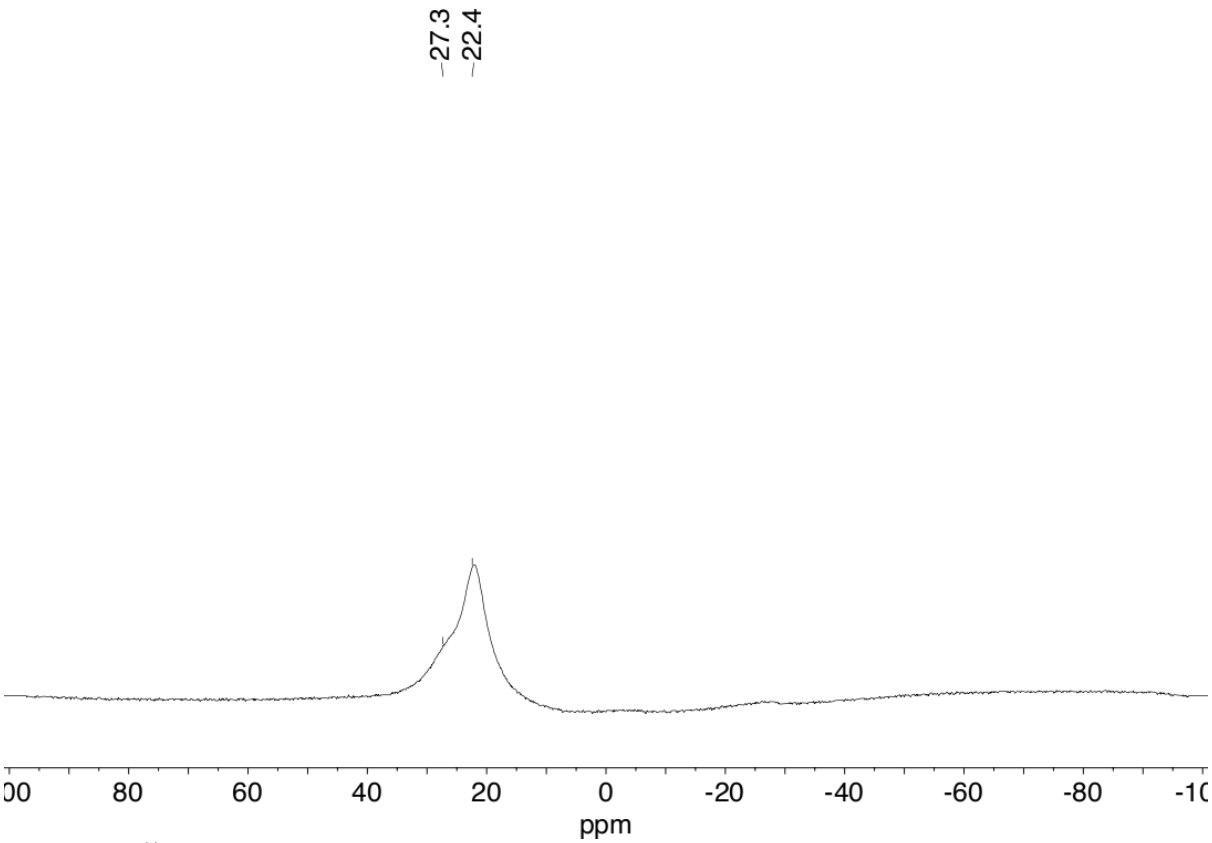


Figure S37: ^{11}B NMR spectrum (128.4 MHz) of {B}*OGeCl in benzene-d_6.

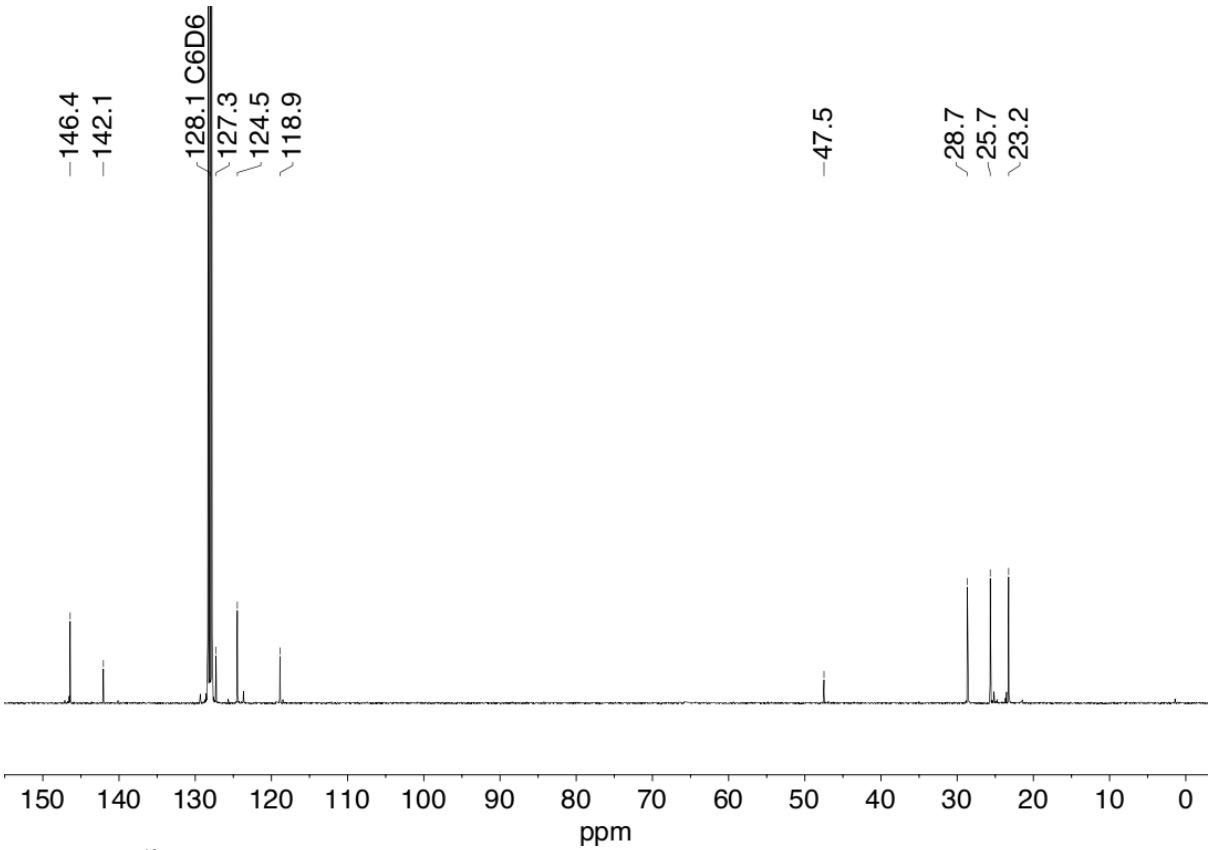


Figure S38: ^{13}C NMR spectrum (100.6 MHz) of {B}*OGeCl in benzene-d_6.

1.3.10 NMR spectra of {B}*OSnCl

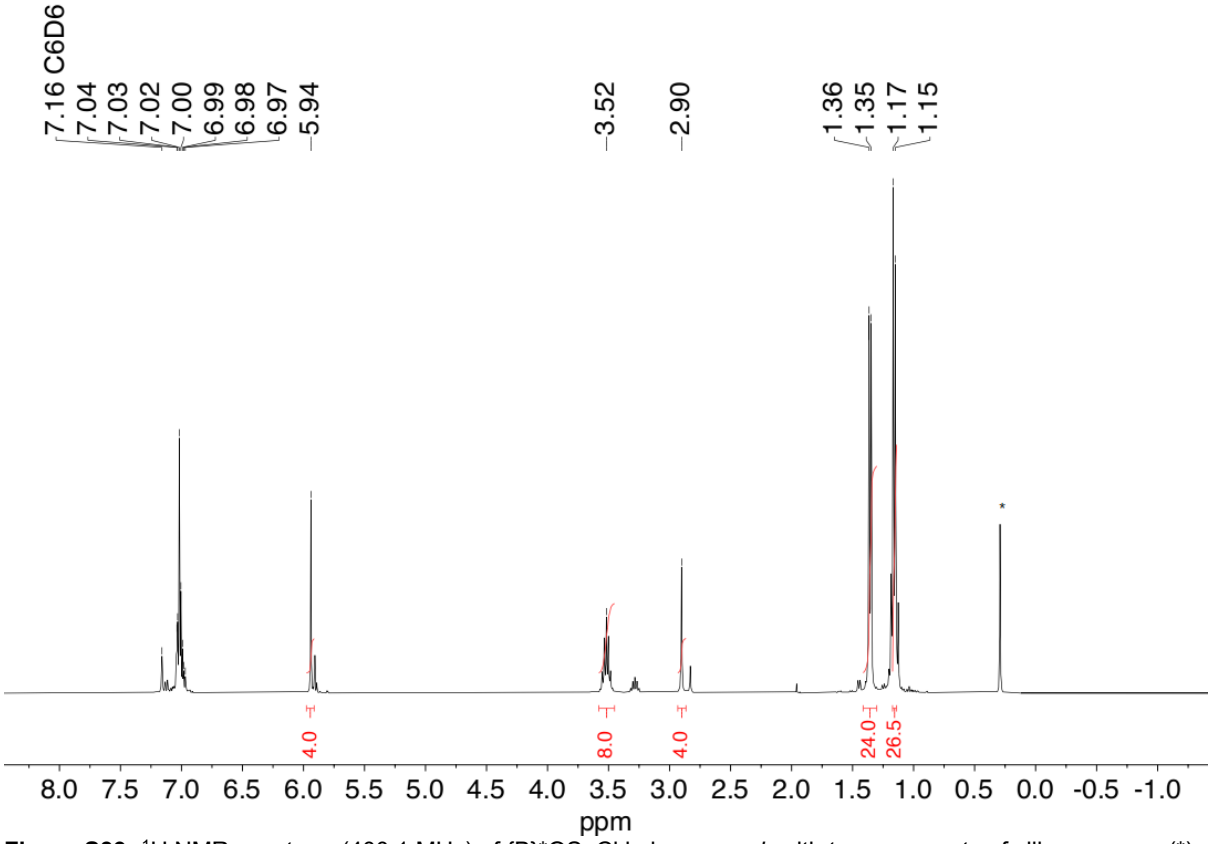


Figure S39: ^{1}H NMR spectrum (400.1 MHz) of {B}*OSnCl in benzene-d_6 with trace amounts of silicon grease (*).

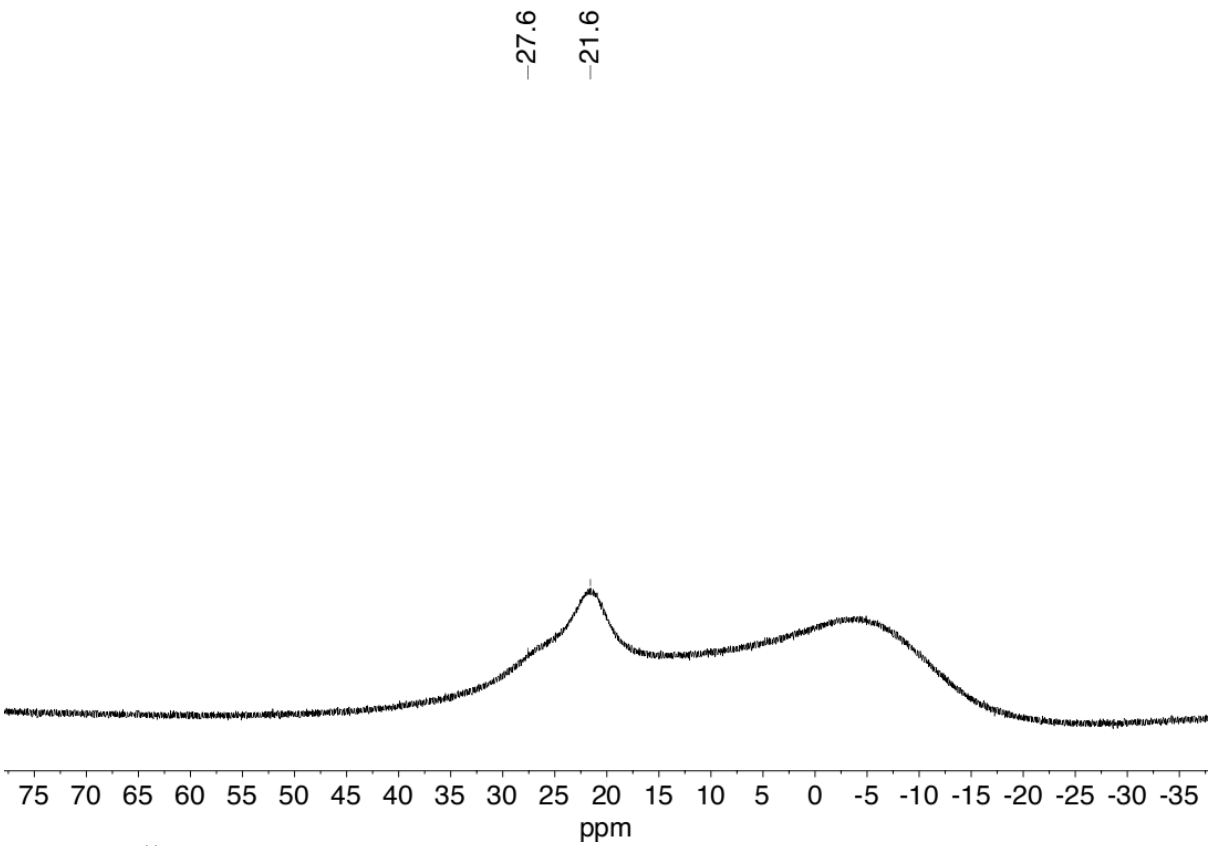


Figure S40: ^{11}B NMR spectrum (128.4 MHz) of {B}*OSnCl in benzene-d_6.

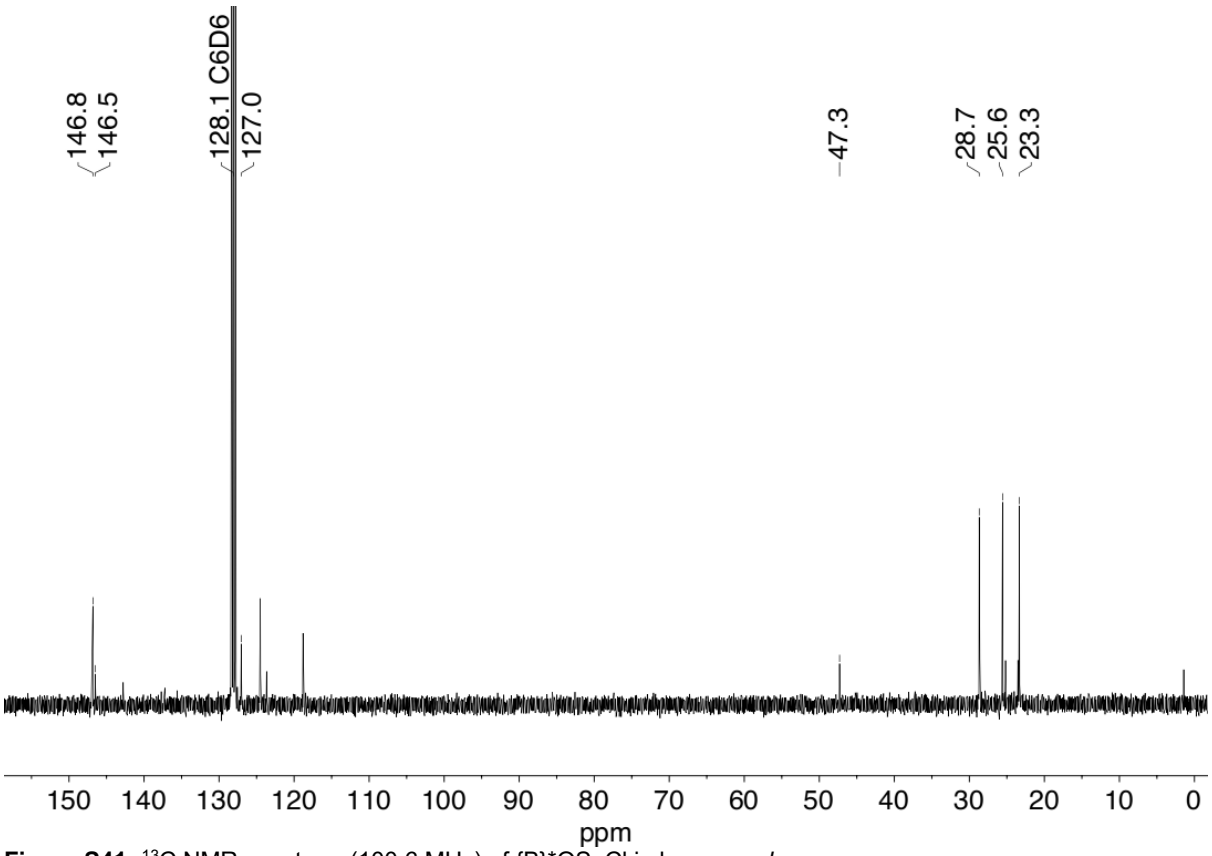


Figure S41: ^{13}C NMR spectrum (100.6 MHz) of {B}*OSnCl in benzene-d_6.

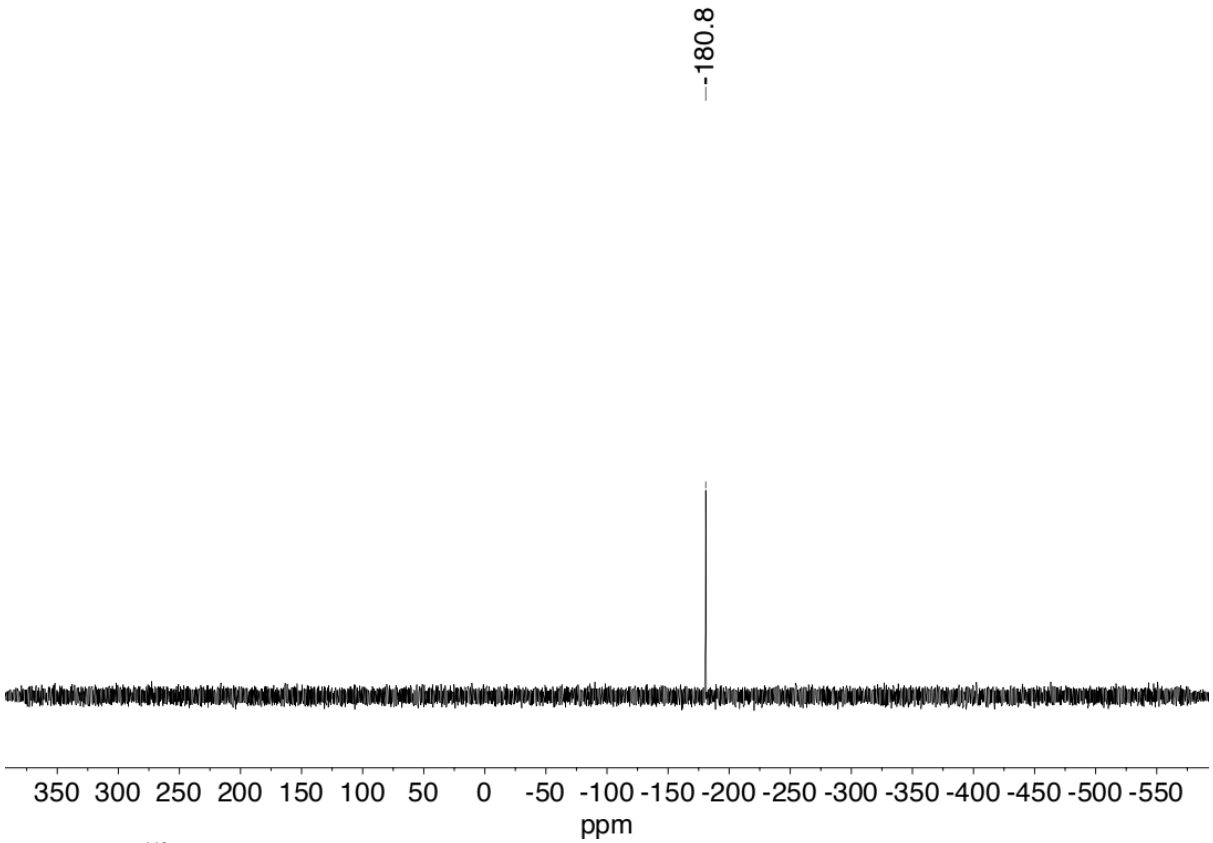


Figure S42: ^{119}Sn NMR (149.2 MHz) spectrum of {B}*OSnCl in benzene-d_6.

1.4 X-Ray Crystallographic Details

1.4.1 General information

For the data collection, single crystals were embedded in inert oil and mounted on nylon loops or micro mounts. Geometric and intensity data were collected on a Rigaku Xtalab Synergy Dualflex with a graphite monochromator with Cu Kα (1.54180 Å) or Mo Kα (0.71073 Å) (**{B}***OH, **{B}***OK, **{B}***$OSiCl_3$, **{B}***$OSiBr_3$, **{B}***OSnCl), the MX1 beamline of the Australian Synchrotron (λ = 0.71090 Å; **{B}***$OSiHCl_2$), the MX2 beamline of the Australian Synchrotron (λ = 0.71073; **{B}***Br) or a Stoe IPDS2 equipped with a 2-circle goniometer and an area detector (**{B}***OSnCl and **1**). After absorption correction and data reduction the structures were solved with direct methods and refined using alternating cycles of least-square refinements against F^2 (SHELX-16).[S5] Several attempts to get good quality single crystals of **{B}***Br failed because of twinning problems. Finally, a tiny fragment was suitable to get an acceptable data set which shows minor artificial modulation and a rather high residual electron density. In the molecular structures of **{B}***OK, **{B}***$OSiHCl_2$, **{B}***$OSiCl_3$, **{B}***$OSiBr_3$, **{B}***OK, **{B}***OGeCl and **{B}***OSnCl are disordered *i*Pr groups which were modelled adequately. The collected data are summarized in Table S1 and included in the CIF files.

Table S1: Crystallographic data for new compounds.

Compound	**{B}***Br	**{B}***OH	**{B}***OK · C_6H_6
Empirical formula	$C_{54}H_{76}B_3BrN_6$	$C_{54}H_{77}B_3N_6O$	$C_{54}H_{76}B_3KN_6O$, C_6H_6
Formula weight	921.54	858.64	974.84
Temperature/K	100(2)	123(2)	123.00(10)
Crystal system	monoclinic	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/n$	C2/c
a/Å	13.321(3)	10.6749(2)	25.1162(6)
b/Å	20.663(4)	37.7910(7)	13.2745(3)
c/Å	19.283(4)	13.3221(3)	18.3072(4)
α/°	90	90	90
β/°	100.62(3)	107.410(2)	110.891(2)
γ/°	90	90	90
Volume/Å^3	5216.7(19)	5128.13(19)	5702.5(2)
Z	4	4	4
ρ_{calc}g/cm^3	1.173	1.112	1.135
μ/mm^{-1}	0.829	0.497	1.144
F(000)	1968.0	1864	2104
Crystal size/mm^3	0.01 × 0.01 × 0.01	0.08 × 0.07 × 0.02	0.21 × 0.2 × 0.15
Radiation	Synchrotron (λ = 0.71090)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2Θ range for data collection/°	2.916 to 51.998	7.338 to 160.414	7.534 to 160.542
Index ranges	-16 ≤ h ≤ 16, -25 ≤ k ≤ 25, -23 ≤ l ≤ 23	-13 ≤ h ≤ 11, -47 ≤ k ≤ 47, -13 ≤ l ≤ 17	-26 ≤ h ≤ 32, -16 ≤ k ≤ 15, -23 ≤ l ≤ 23
Reflections collected	65586	46250	25377
Independent reflections	10214 [R_{int} = 0.0625, R_{sigma} = 0.0339]	10878 [R_{int} = 0.0573, R_{sigma} = 0.0494]	6077 [R_{int} = 0.0597, R_{sigma} = 0.0440]
Data/restraints/parameters	10214/0/593	10878/3/649	6077/6/371
Goodness-of-fit on F^2	1.059	1.046	1.053
Final R indexes [I>=2σ (I)]	R_1 = 0.0735, wR_2 = 0.2287	R_1 = 0.0739, wR_2 = 0.2041	R_1 = 0.0513, wR_2 = 0.1421
Final R indexes [all data]	R_1 = 0.0763, wR_2 = 0.2318	R_1 = 0.0834, wR_2 = 0.2142	R_1 = 0.0539, wR_2 = 0.1446
Largest diff. peak/hole / e Å^{-3}	2.12/-0.99	0.97/-0.44	0.23/-0.48

Table S1 (continued): Crystallographic data for new compounds.

Compound	**{B}***$OSiHCl_2 \cdot (C_6H_{14})_{0.5}$	**{B}***$OSiCl_3$	**{B}***$OSiBr_3$
Empirical formula	$C_{54}H_{77}B_3Cl_2N_6OSi$, $0.5(C_6H_{14})$	$C_{108}H_{152}B_6Cl_6N_{12}O_2Si_2$	$C_{108}H_{152}B_6Br_6N_{12}O_2Si_2$
Formula weight	1000.72	1984.15	2250.91
Temperature/K	100(2)	123(2)	123(2)
Crystal system	monoclinic	orthorhombic	orthorhombic
Space group	$P2_1/n$	$P2_12_12_1$	$P2_12_12_1$
a/Å	11.120(2)	19.47230(10)	19.58760(10)
b/Å	40.840(8)	23.17940(10)	23.29940(10)
c/Å	12.690(3)	24.88890(10)	24.94380(10)
α/°	90	90	90
β/°	90.71(3)	90	90
γ/°	90	90	90
Volume/$Å^3$	5763(2)	11233.76(9)	11383.84(9)
Z	4	4	4
$\rho_{calc}g/cm^3$	1.153	1.173	1.313
μ/mm^{-1}	0.177	1.998	3.144
F(000)	2156	4240	4672
Crystal size/mm^3	0.7 × 0.7 × 0.1	0.18 × 0.11 × 0.04	0.233 × 0.2 × 0.1
Radiation	Synchrotron (λ = 0.7109)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2Θ range for data collection/°	1.994 to 51.998	6.912 to 160.804	6.878 to 160.738
Index ranges	-13 ≤ h ≤ 13, -50 ≤ k ≤ 50, -15 ≤ l ≤ 15	-11 ≤ h ≤ 24, -29 ≤ k ≤ 29, -31 ≤ l ≤ 29	-25 ≤ h ≤ 23, -29 ≤ k ≤ 29, -22 ≤ l ≤ 31
Reflections collected	137192	66695	236655
Independent reflections	11291 [R_{int} = 0.0368, R_{sigma} = 0.0151]	22991 [R_{int} = 0.0462, R_{sigma} = 0.0480]	24733 [R_{int} = 0.0583, R_{sigma} = 0.0250]
Data/restraints/parameters	11291/0/678	22991/24/1307	24733/0/1287
Goodness-of-fit on F^2	1.026	1.061	1.036
Final R indexes [I>=2σ (I)]	R_1 = 0.0475, wR_2 = 0.1319	R_1 = 0.0442, wR_2 = 0.1175	R_1 = 0.0349, wR_2 = 0.0958
Final R indexes [all data]	R_1 = 0.0508, wR_2 = 0.1359	R_1 = 0.0477, wR_2 = 0.1200	R_1 = 0.0358, wR_2 = 0.0967
Largest diff. peak/hole / e $Å^{-3}$	1.06/-0.61	0.47/-0.34	0.49/-0.62
Flack parameter		-0.010(8)	0.228(4)

Table S1 (continued): Crystallographic data for new compounds.

Compound	**{B}***OGeCl · $(C_6H_6)_{1.25}$	**{B}***OSnCl	**(1)**
Empirical formula	$C_{54}H_{76}B_3ClGeN_6O$, 1.25(C_6H_6)	$C_{54}H_{76}B_3ClN_6OSn$	$C_{67}H_{86}B_3BrN_6O_2Si$
Formula weight	1063.31	1011.80	1147.84
Temperature/K	100(2)	123.00(10)	100(2)
Crystal system	triclinic	monoclinic	monoclinic
Space group	P-1	$P2_1/n$	$P2_1$
a/Å	16.4864(6)	30.8728(4)	11.4979(4)
b/Å	16.4582(5)	16.2163(2)	20.9867(6)
c/Å	44.1370(14)	33.9145(6)	13.7765(5)
α/°	95.160(3)	90	90
β/°	97.087(3)	106.314(2)	104.384(3)
γ/°	89.930(3)	90	90
Volume/Å^3	11835.7(7)	16295.4(4)	3220.10(19)
Z	8	12	2
ρ_{calc}g/cm^3	1.193	1.237	1.184
μ/mm^{-1}	0.607	0.562	0.704
F(000)	4532	6384	1220
Crystal size/mm^3	0.18 × 0.14 × 0.08	0.216 × 0.164 × 0.104	0.17 × 0.1 × 0.06
Radiation	MoKα (λ = 0.71073)	Mo Kα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.484 to 50.234	6.312 to 62.086	3.052 to 51.828
Index ranges	-18 ≤ h ≤ 19, -19 ≤ k ≤ 18, -52 ≤ l ≤ 51	-41 ≤ h ≤ 41, -22 ≤ k ≤ 22, -48 ≤ l ≤ 45	-14 ≤ h ≤ 11, -25 ≤ k ≤ 25, -16 ≤ l ≤ 16
Reflections collected	73606	224156	19502
Independent reflections	40545 [R_{int} = 0.0624, R_{sigma} = 0.0561]	46657 [R_{int} = 0.0771, R_{sigma} = 0.0705]	12070 [R_{int} = 0.0773, R_{sigma} = 0.0622]
Data/restraints/parameters	40545/5/2658	46657/0/1861	12070/1/741
Goodness-of-fit on F^2	1.059	1.027	1.04
Final R indexes [I>=2σ (I)]	R_1 = 0.0835, wR_2 = 0.2218	R_1 = 0.0477, wR_2 = 0.1120	R_1 = 0.0680, wR_2 = 0.1708
Final R indexes [all data]	R_1 = 0.1061, wR_2 = 0.2418	R_1 = 0.0960, wR_2 = 0.1335	R_1 = 0.0805, wR_2 = 0.1843
Largest diff. peak/hole / e Å^{-3}	0.68/-1.14	0.96/-0.86	0.67/-0.91
Flack parameter			0.132(12)

1.4.2 Plots of molecular structures

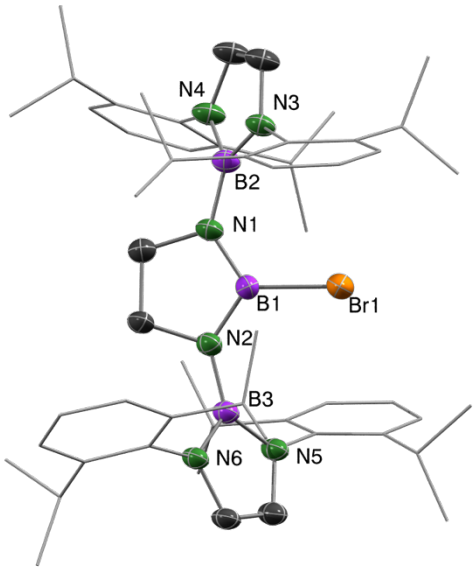


Figure S43: The molecular structure of **{B}***Br in the solid state with 50 % thermal ellipsoids, Dipp groups are shown as wire frame and hydrogen atoms are omitted for clarity.

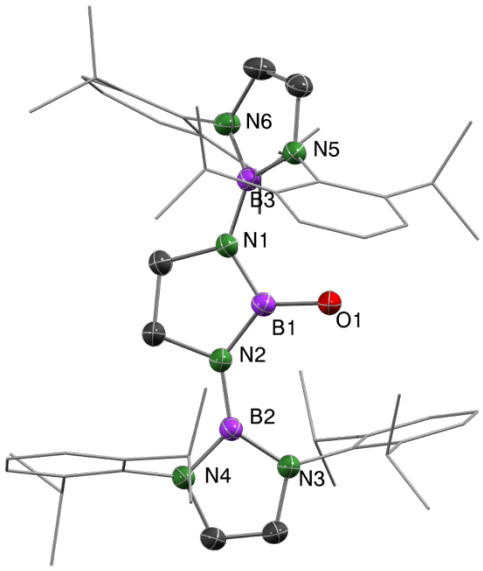


Figure S44: The molecular structure of **{B}***OH in the solid state with 50 % thermal ellipsoids, Dipp groups are shown as wire frame and hydrogen atoms are omitted for clarity. Note that there is a disorder in two of the *i*Pr groups.

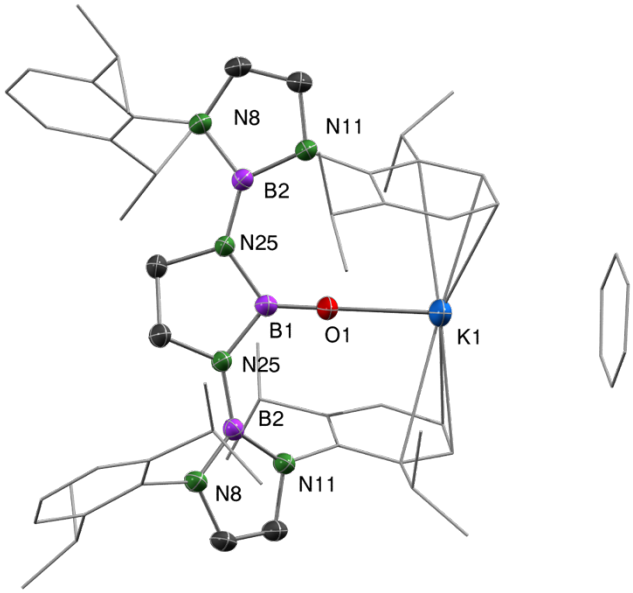


Figure S45: The molecular structure of **{B}***OK in the solid state with 50 % thermal ellipsoids, Dipp groups are shown as wire frame and hydrogen atoms are omitted for clarity. Note that there is a disorder in one *i*Pr group.

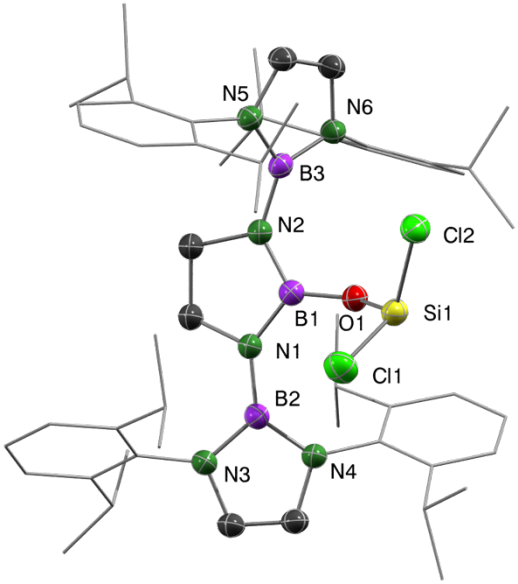


Figure S46: The molecular structure of {B}*OSiHCl$_2$ in the solid state with 50 % thermal ellipsoids, Dipp groups are shown as wire frame and hydrogen atoms and an embedded *n*-hexane molecule are omitted for clarity. Note that there is a disorder in one *i*Pr group.

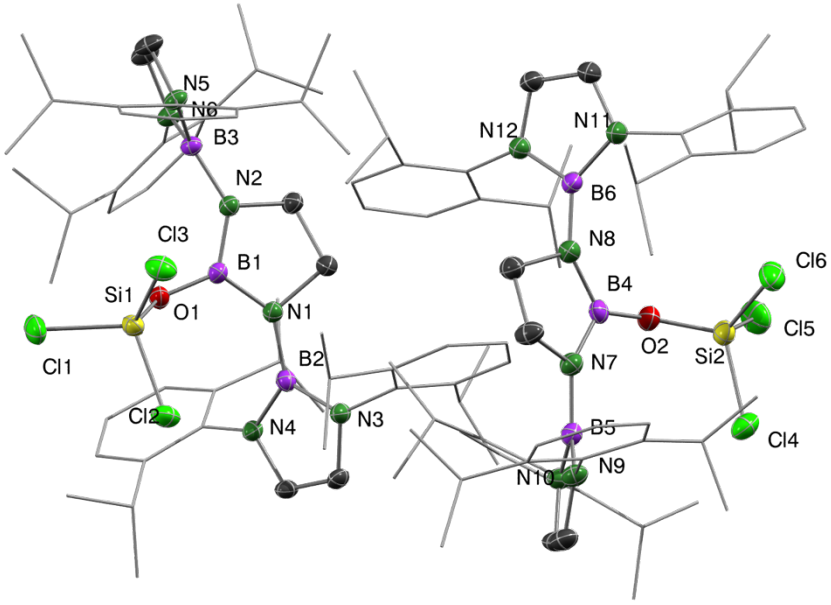


Figure S47: The molecular structure of {B}*OSiCl$_3$ in the solid state with 50 % thermal ellipsoids, Dipp groups are shown as wire frame and hydrogen atoms are omitted for clarity. Note that there is a disorder in two of the *i*Pr groups.

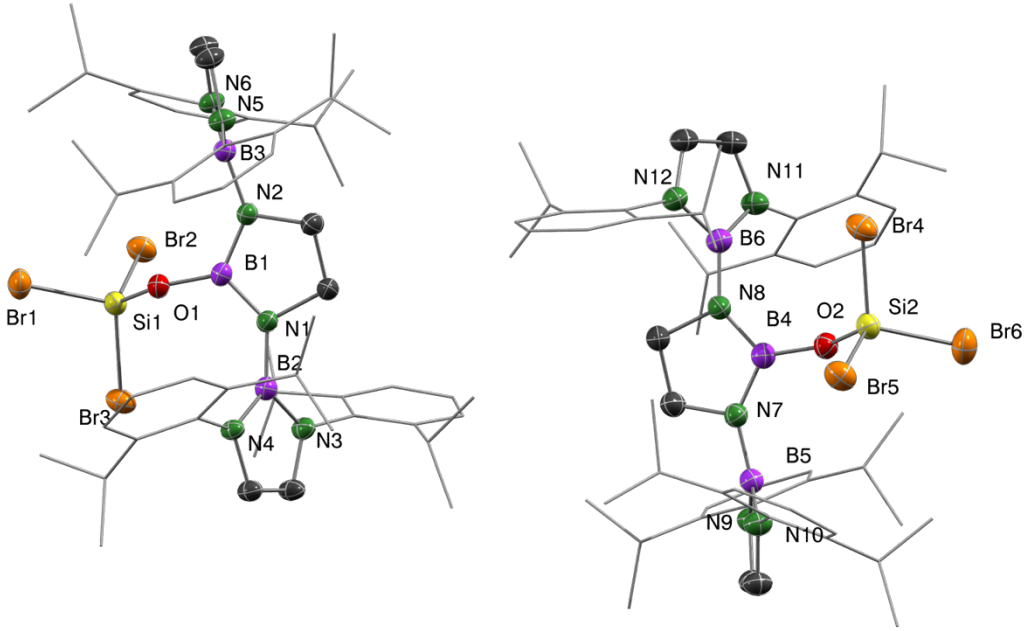


Figure S48: The molecular structure of {B}*OSiBr$_3$ in the solid state with 50 % thermal ellipsoids, Dipp groups are shown as wire frame and hydrogen atoms are omitted for clarity. Note that there is a disorder in one *i*Pr group not shown.

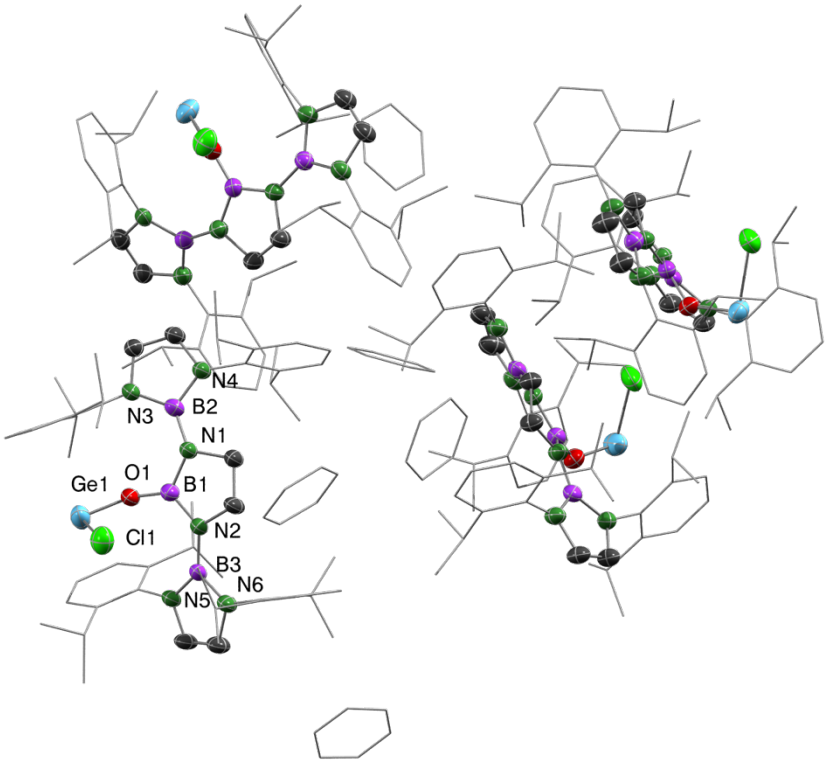


Figure S49: The molecular structure of **{B}***OGeCl in the solid state with 50 % thermal ellipsoids. Four independent molecules are shown together with five benzene molecules in the asymmetric unit. For clarity Dipp groups are shown as wire frame, hydrogen atoms are omitted and only the hetero atoms of one molecule are labelled. Note that there is a disorder in one of the *i*Pr groups.

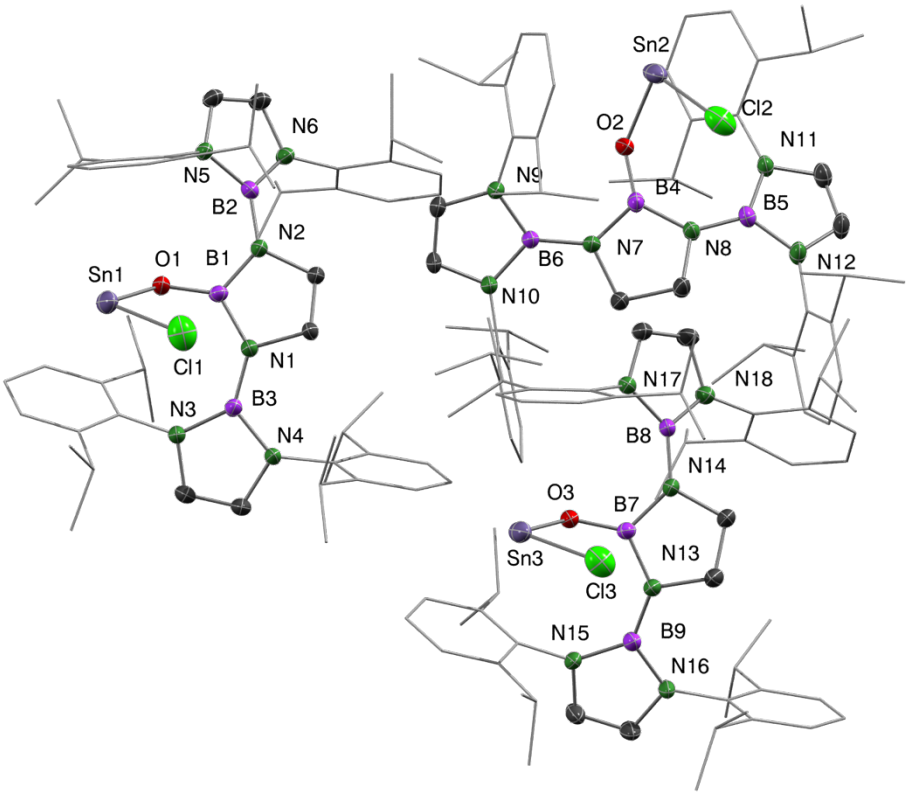


Figure S50: The molecular structure of **{B}***OSnCl in the solid state with 50 % thermal ellipsoids, Dipp groups are shown as wire frame, hydrogen atoms and one *n*-hexane molecule are ommited for clarity. Note that there is a disorder in one of the *i*Pr groups.

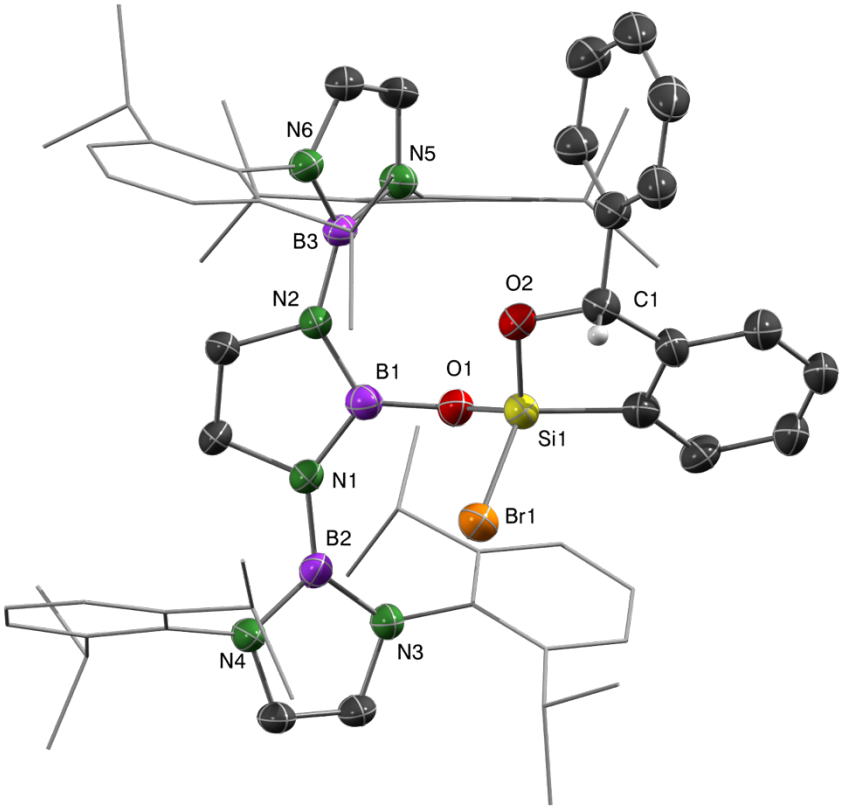


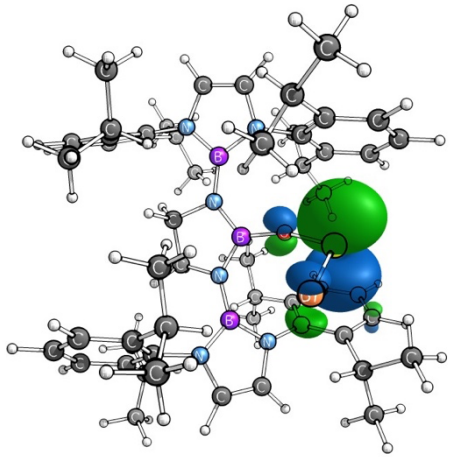
Figure S51: The molecular structure of **1** in the solid state with 50 % thermal ellipsoids, Dipp groups are shown as wire frame. Except the hydrogen atom at C1 all others are omitted for clarity.

2 Computational Details

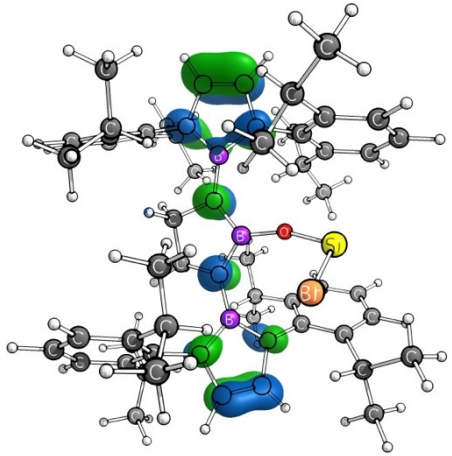
The geometries of **{B}***OSiBr, **{B}***OGeCl and **{B}***OSnCl were optimized in the gas phase with Gaussian16 (Revision C.01)[S6] and checked for imaginary frequencies to confirm the geometries as minima on the energy hypersurface. Therefore, the PBE1PBE[S7–10] functional was employed with the def2-SVP[S11] basis set. Grimmes Dispersion correction was used including Becke-Johnson damping.[S10,S11] To compare the silylene with more compounds the frontier orbitals were also calculated on the same level of theory as Kira *et. al.* used for in their recent review (B3PW91/6–31+G(d,p)).[S18–S21] Single point calculations were performed with the def2-TZVP[S11] basis set and ECP[S19] was used for the Sn atom. Pictures were generated with the ChemCraft program.[S20] We used the online tool SambVca to study the steric demand and determine the buried volume.[S21]

2.1 Frontier Orbitals calculated with the PBE1PBE method

{B}*OSiBr

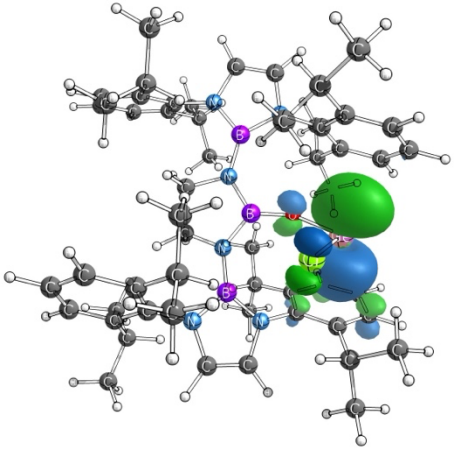


LUMO: –1.45 eV

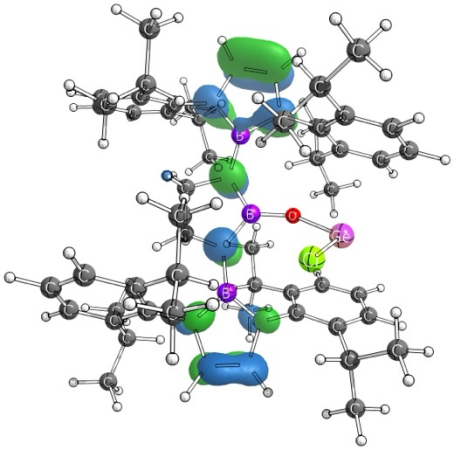


HOMO: –5.24 eV

{B}*OGeCl

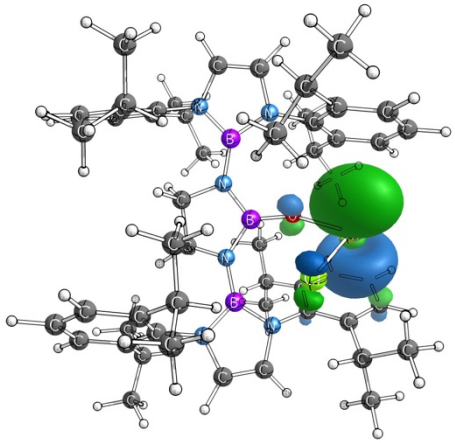


LUMO: –1.39 eV

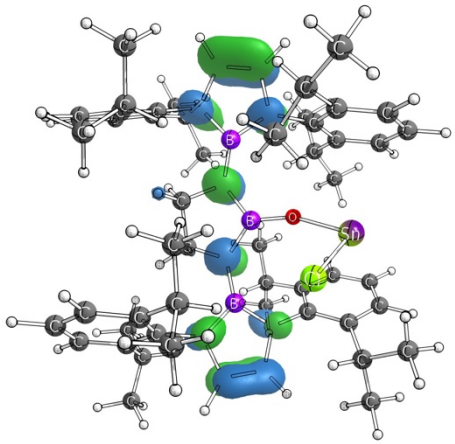


HOMO: –5.15 eV

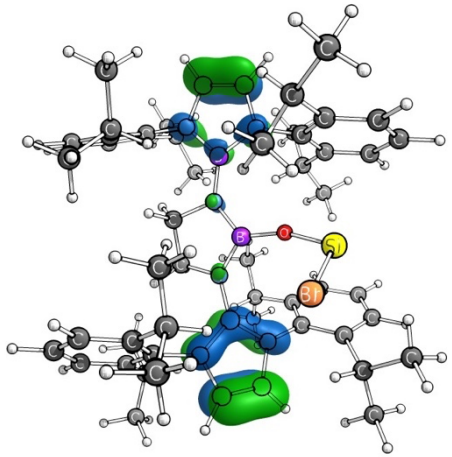
{B}*OSnCl



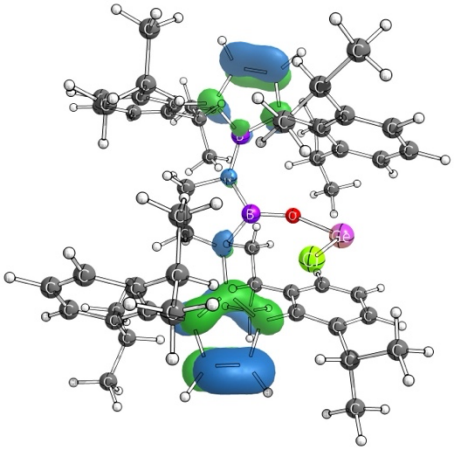
LUMO: –1.61 eV



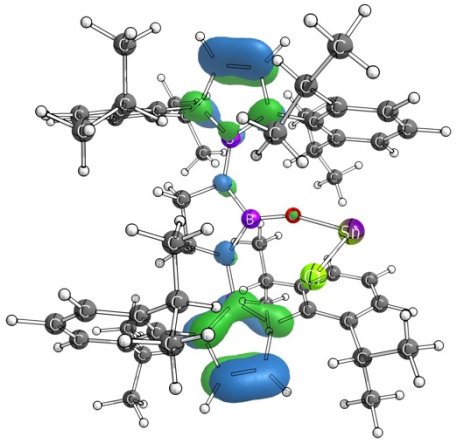
HOMO: –5.06 eV



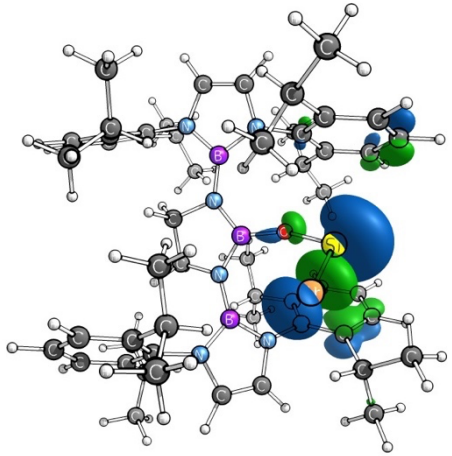
HOMO–1: –5.56 eV



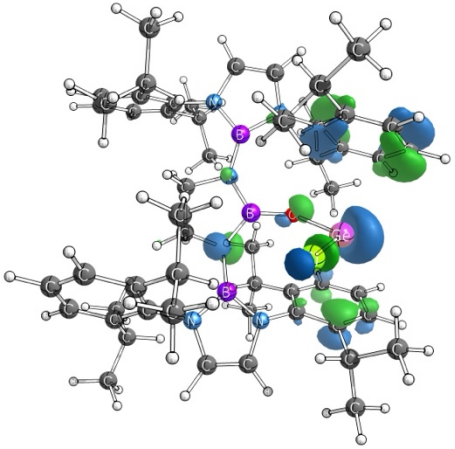
HOMO–1: –5.50 eV



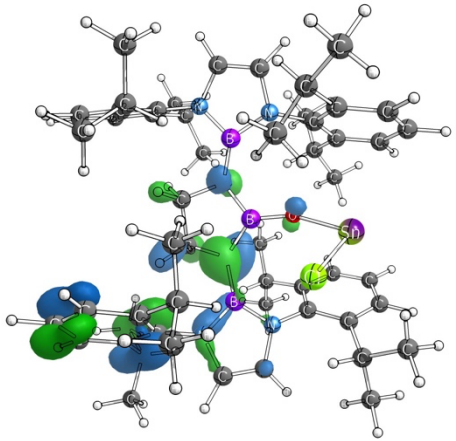
HOMO–1: –5.40 eV



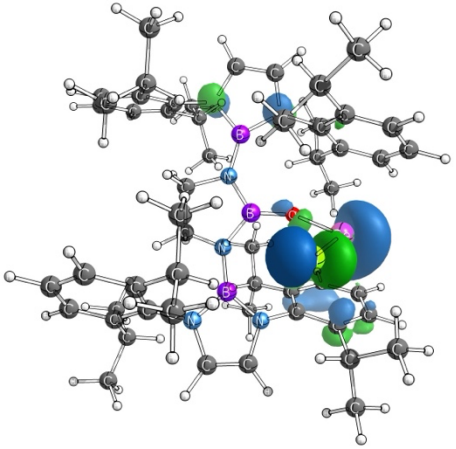
HOMO–2: –6.49 eV



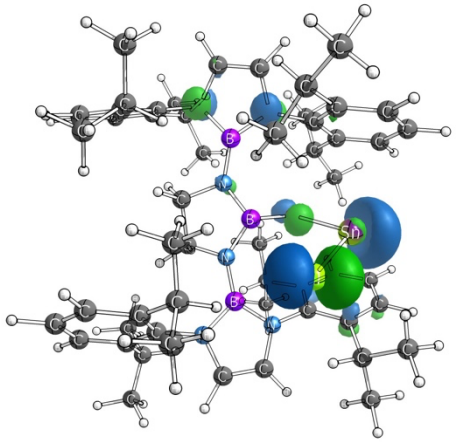
HOMO–2: –6.62 eV



HOMO–2: –6.56 eV



HOMO–11: –7.49 eV



HOMO–11: –7.52 eV

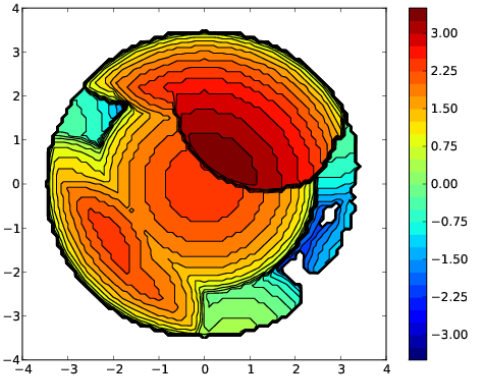
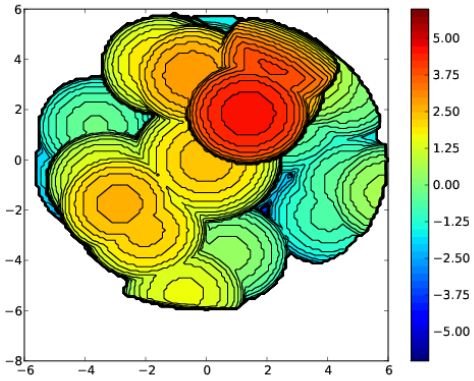
2.2 Comparison of frontier orbitals

In the recent review article of Kira *et. al.* frontier orbitals of isolable silylenes were compared and discussed.[S15] For that purposed they model compounds where they simplified some of the bulky groups. We used the same method for a single point calculation on the previous optimized structure to obtain more comparable data which is listed in the following table.

	PBE1PBE	B3PW91
LUMO	–1.45 eV	–1.65 eV
lone pair	–6.49 eV	–6.34 eV
ΔE	5.04 eV	4.69 eV

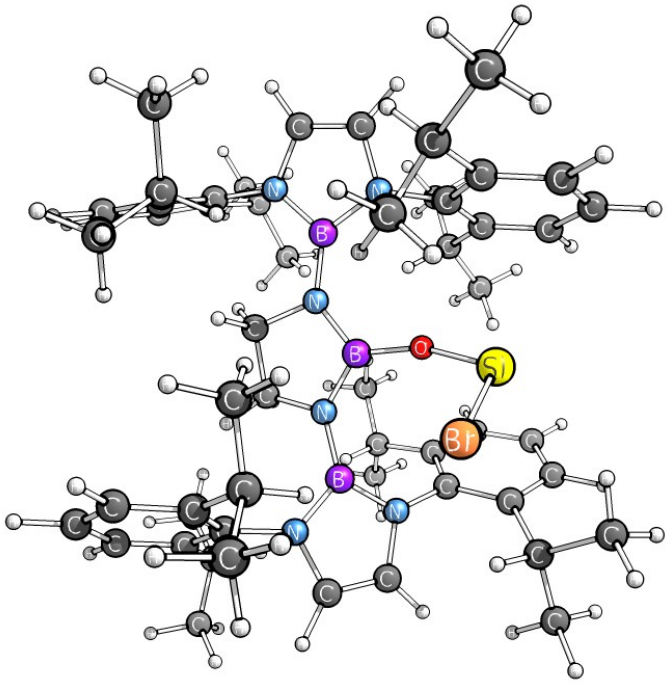
2.3 Burried Volume

We used the computed structure of **{B}***OSiBr and measured steric shielding of the boryloxy ligand (**{B}***$^{-}$) on the silicon centre. For this purpose, the z-axis was defined by the oxygen and the silicon atom. The N,B,N moiety of the centred heterocycle was used to define the xz-plane. The bromine atom was omitted. The measurement was performed for spheres with radii of 3.5 and 6.0 respectively.

	Sphere 3.5	Sphere 6.0
		
$\%V_{free}$	20.4	39.2
$\%V_{Buried}$	79.6	60.8

2.4 Cartesian coordinates for the computed structures

{B}*OSiBr:



O	0.383413028	-1.579520115	-0.094070007
N	-1.403429103	0.104034008	0.257221018
N	-2.944107211	-1.963653139	-0.243916017
N	-3.975316287	0.033714002	0.143932011
N	0.855365063	0.812827060	0.352189025
N	3.384455243	0.160400011	0.674414046
N	2.920299209	2.195052158	-0.259477019
C	-2.158412153	-3.128575225	-0.475286034
C	-1.630558117	-3.824727275	0.619369045
C	-4.938874353	-0.946374067	-0.098845007
H	-5.989386434	-0.711059052	-0.078383006
C	-4.333048309	-2.119119155	-0.331598024
H	-4.765068340	-3.081465220	-0.546827041
C	-4.401528317	1.362025095	0.427474031
C	-1.349652095	-4.801822346	-1.986698142
H	-1.226867088	-5.187529372	-2.989926214
C	-2.011898144	-3.590954261	-1.791576128
C	4.574041328	0.847406063	0.409277029
H	5.532500407	0.427619031	0.649237047
C	-0.857547062	-5.525317407	-0.913994066
H	-0.353696025	-6.467606454	-1.084382076
C	-2.776507198	-3.581889259	-4.216501301
H	-1.842106131	-3.940519284	-4.649702334
H	-3.260045233	-2.964793215	-4.972304359
H	-3.412715245	-4.447262318	-4.034170290
C	-4.828782350	1.669765119	1.727204124
C	-2.538521182	-2.771809200	-2.952744215

H	-3.500349252	-2.351163167	-2.645588191
C	1.713865121	3.446412247	-1.977101142
C	-4.382735317	2.320016165	-0.595507045
C	-5.231082379	2.976022214	1.987899141
H	-5.562463375	3.244948234	2.982198215
C	3.372903240	-1.063314074	1.396712098
C	-1.759913125	-3.261573237	2.018764145
H	-1.645429120	-2.175078157	1.933236137
C	2.661093190	-1.129587079	2.611625188
C	0.027112002	1.915954139	0.855694063
H	0.315423022	2.882314205	0.446367032
H	0.131979009	1.984970145	1.945821141
C	2.625280189	-2.339084167	3.296521235
H	2.081663148	-2.394019174	4.232232307
C	-4.792272343	0.619956045	2.820619202
H	-5.060829362	-0.337613024	2.365503172
C	1.671634120	2.244231161	-2.888964206
H	2.151586153	1.417088100	-2.368749172
C	-0.985442070	-5.033371360	0.373562027
H	-0.569926040	-5.594258408	1.200016089
C	4.094549293	-2.186528155	0.930099068
C	4.299616309	2.044342144	-0.135377010
H	4.979584356	2.812647205	-0.461695033
C	-4.790807347	3.613000261	-0.283341020
H	-4.779253344	4.375908317	-1.050729075
C	3.019600220	4.511055323	1.480607108
H	3.303816240	3.479477252	1.698758121
C	2.348674171	3.410351246	-0.727770051
C	1.123815078	4.641428336	-2.380280171
H	0.626530046	4.682787337	-3.342657241
C	5.017299364	-2.153412153	-0.273624020
H	4.756188344	-1.285916093	-0.882337064
C	2.396069175	4.544203325	0.100590007
C	2.461291176	2.496649180	-4.168799301
H	2.474664178	1.602141114	-4.791542343
H	3.493490252	2.770255202	-3.952477282
H	2.021309144	3.303508238	-4.757030344
C	2.028420148	0.076330005	3.278398237
H	2.058268148	0.917019065	2.586407188
C	-3.945598285	1.948747142	-1.997836143
H	-3.189485230	1.161400083	-1.908926136
C	3.281322238	-3.460110249	2.825698203
H	3.232526232	-4.392659317	3.372556243
C	4.020459292	-3.369700241	1.664016121
H	4.562549328	-4.236566306	1.308705095
C	-1.606205116	-1.597274117	-3.245059235
H	-1.412603100	-0.995800069	-2.355882169

H	-2.032353147	-0.938484066	-4.003531287
H	-0.643458045	-1.950638141	-3.618073261
B	-0.022382002	-0.292545021	0.140594010
C	-1.395672101	1.561388110	0.470523034
H	-2.098014153	1.865627134	1.244668092
H	-1.690104121	2.082655149	-0.445928032
C	-3.314024238	3.101689221	-2.763190199
H	-4.039410288	3.882000282	-2.995369214
H	-2.915641211	2.744963196	-3.712246269
H	-2.494305179	3.562545258	-2.210123158
C	-5.209601376	3.939705283	0.994406073
H	-5.522729413	4.951452357	1.217472085
C	1.810674130	5.719343421	-0.358170026
H	1.840435132	6.603459483	0.267852019
C	-3.142036224	-3.529665253	2.610650189
H	-3.328870237	-4.602265330	2.681106192
H	-3.936446281	-3.088440221	2.010475145
H	-3.214055232	-3.115638222	3.616731262
C	4.910884354	-3.392455244	-1.158136081
H	5.338017396	-4.270103305	-0.672435050
H	5.463100398	-3.237638233	-2.084087150
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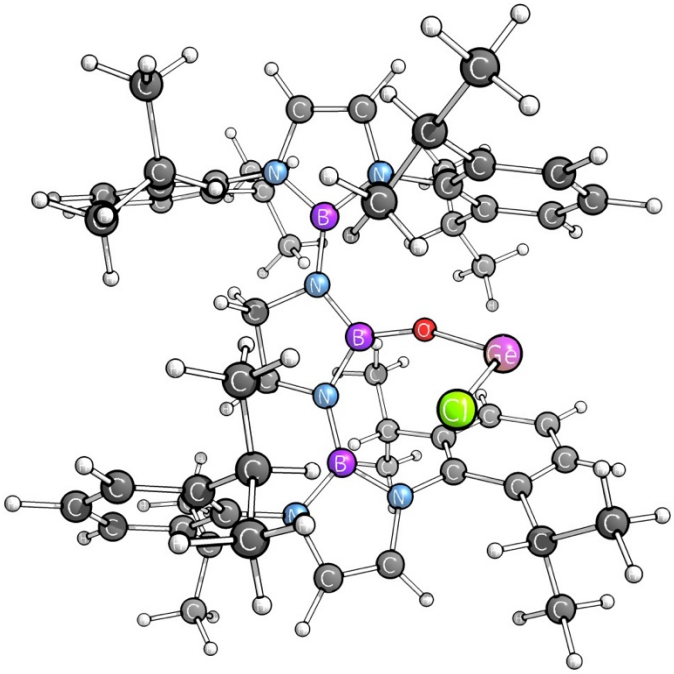

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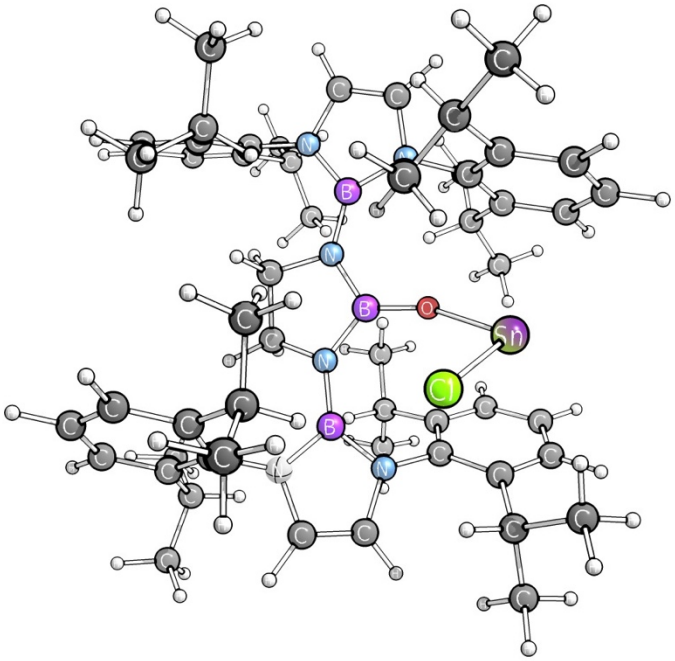

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C	-5.991353000	0.190482000	3.856926000
H	-5.902400000	-0.646378000	4.563863000
H	-7.018370000	0.187913000	3.464709000
H	-5.863102000	1.112737000	4.443984000
C	-3.540831000	0.144722000	3.330727000
H	-3.345500000	1.140749000	3.760441000
H	-2.767272000	-0.047199000	2.572991000
H	-3.401183000	-0.594125000	4.134894000

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