Electronic Supplementary Material (ESI) for ChemComm.

Transborylation of alkenylboranes with diboranes

Paula Dominguez-Molano,[a] Gerard Bru,[a] Oriol Salvado,[a] Ricardo J. Maza,[a] Jorge J. Carbó[a] and Elena Fernández*[a] Department Química Física i Inorgánica. University Rovira i Virgili, C/Marcel·lí Domingo s/n, 43007 Tarragona, Spain*

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General Information

Solvents and reagents: Solvents and reagents were obtained from commercial suppliers and dried and/or purified (if needed) by standard procedures. Tetrahydrofuran was dried by distillation from sodium benzophenone ketyl. Lithium 2,2,6,6-tetramethylpiperidide and vinyl boranes **16**, **18** and **20**, were purchased from Sigma-Aldrich Inc. Diboron reagents were purchased from Ally Chem and used without further purification. All reactions were conducted in oven and flame-dried glassware under an inert atmosphere of argon, using Schlenk-type techniques. *Flash chromatography* was performed on standard silica gel (Merck Kieselgel 60 F254 400-630 mesh). *Thin layer chromatography* was performed on Merck Kieselgel 60 F254 which was developed using standard visualizing agents: UV fluorescence (254 and 366 nm) or potassium permanganate/Δ. *NMR spectr*a were recorded at a Varian Goku 400 or a Varian Mercury 400 spectrometer. ^{1}H NMR and ^{13}C{^{1}H} NMR chemical shifts (δ) are reported in ppm with the solvent resonance as the internal standard ($CHCl_3$: 7.26 ppm (^{1}H)) and ($CDCl_3$: 77.16 ppm (^{13}C). ^{11}B{^{1}H} NMR chemical shifts (δ) are reported in ppm relative to $(CH_3)_2O\cdots BF_3$. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, hept = heptuplet, br = broad, m = multiplet), coupling constants (Hz) and integration. *High resolution mass spectra (HRMS)* were recorded using a 6210 Time of Flight (TOF) mass spectrometer from Agilent Technologies (Waldbronn, Germany) with an ESI interface and it was performed at the Servei de Recursos Científics i Tècnics (Universitat Rovira i Virgili, Tarragona) or using a BIOTOF II Time of Flight (TOF) mass spectrometer from Bruker with an APCI interface or EI interface and it was performed at the Unidade de Espectrometría de Masas e Proteómica (Universidade de Santiago de Compostela, Santiago de Compostela). GC-MS analyses were performed on a HP6890 gas chromatograph and an Agilent Technologies 5973 Mass selective detector (Waldbronn, Germany) equipped with an achiral capillary column HP-5 (30m, 0.25mm i. d., 0.25μm thickness) using He as the carrier gas.

General Procedure for the preparation of chiral diboron compound (22b).

This procedure was adapted from a previous methodology described by W. Tang et al.[1] An oven-dried Schlenk flask with a magnetic stirring bar was charged with activated molecular sieves (4 Å), tetrahydroxy diboron (1 equiv, 1 mmol) and (S,S)-(−)-Hydrobenzoin (2 equiv, 2 mmol) in THF (2 mL). The reaction mixture was stirring at 70ºC for 16h and the crude mixture was filtered through a pad of Celite®. The solvents were removed under vacuum to obtain a white solid that was crystallized in ethyl acetate. The white solid was filtered and washed with cold ethyl acetate to obtain the product (**22b**) (54%, 240 mg).

General procedure for the preparation of *E*-alkenyl pinacolboranes

A Schlenk-tube equipped with a magnetic stir bar was charged with bis(pinacolboryl)methane (0.5 mmol, 1 equiv) and LiTMP (0.6 mmol, 1.2 equiv) in dry THF as solvent (2 mL). The mixture was stirred during 30 min at 0 °C. Then, the aldehyde (0.8 mmol, 1.6 equiv) was added. The reaction was stirred during 10 min at 0 °C, followed by 16 h at room temperature. The solvent was gently concentrated at the rotary evaporator and the NMR yield was calculated by comparison to an internal standard (naphthalene). The crude residue was purified by silica gel flash chromatography to afford the desired product.

General procedure for the preparation of *Z*-alkenyl pinacolboranes

A Schlenk-tube equipped with a magnetic stir bar was charged with $HC(SiMe_3)(Bpin)_2$ (0.5 mmol, 1 equiv) and LiTMP (0.6 mmol, 1.2 equiv) in dry THF as solvent (2 mL). The mixture was stirred during 30 min at 0 °C. Then, the aldehyde (0.8 mmol, 1.6 equiv) was added. The reaction was stirred during 10 min at 0 °C, followed by 16 h at room temperature. The solvent was gently concentrated at the Schlenk line. Next, a solution of 3 mL of dichloromethane containing CF_3COOH (3 mmol, 8 equiv) was added and the reaction was stirred for 16 h at room temperature. The solvent was gently concentrated at the rotary evaporator and the NMR yield was calculated by comparison to an internal standard (naphthalene). The crude residue was purified by silica gel flash chromatography to afford the desired product.

General procedure for the preparation of 1,1-diborylalkenes

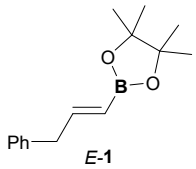
A Schlenk-tube equipped with a magnetic stir bar was charged with $Cu(OAc)_2$ (10 mol%, 36 mg, 0.2 mmol), KF (1 equiv, 116 mg, 2 mmol) in dry toluene as solvent (2.5 mL). Then, P^nBu_3 (81 mg, 99 µL, 0.4 mmol), arylacetylene (204 mg, 0.22 mL, 2 mmol), and HBpin (512 mg, 0.58 mL, 4 mmol) were added in this order. The mixture was stirred during 15 min at 40°C. The reaction mixture was then diluted with Et_2O and filtered through a plug of celite in air with copious washing (Et_2O). The solvent was gently concentrated at the rotary evaporator and the NMR yield was calculated through comparison to an internal standard (naphthalene). The crude residue was purified by silica gel flash chromatography to afford the desired product.

General procedure for transborylation of alkenylboranes with diboron reagents

A Schlenk-tube equipped with a magnetic stir bar was charged with alkenylborane (0.3 mmol, 1 equiv), diboron reagent (0.6 mmol, 2 equiv) in dry MeOH as solvent (2 mL). The mixture was stirred during 16 h at 90 °C. The solvent was gently concentrated at the rotary evaporator and the NMR yield was calculated by comparison to an internal standard (naphthalene). The crude residue was purified by silica gel flash chromatography to afford the desired product.

Characterizarion data for alkenyl pinacolboranes

(*E*)-4,4,5,5-Tetramethyl-2-(3-phenylprop-1-en-1-yl)-1,3,2-dioxaborolane (*E*-1)[2]



E-**1**

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded *E*-**1** (61%, 75 mg) as a pale yellowish oil.

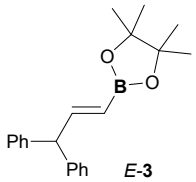
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.24 – 7.13 (m, 2H), 7.15 – 7.04 (m, 3H), 6.68 (dt, J = 17.8, 6.3 Hz, 1H), 5.37 (dt, J = 17.8, 1.7 Hz, 1H), 3.39 (dd, J = 6.3, 1.7 Hz, 2H), 1.16 (s, 12H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 152.47, 139.10, 128.95, 128.46, 126.18, 83.12, 42.30, 24.82.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 29.58.

HRMS (ESI) for **$C_{15}H_{25}NBO_2$ [M+NH_4^+]$^+$:** calculated: 262.1979, found: 262.1978.

(*E*)-2-(3,3-Diphenylprop-1-en-1-yl)-4,4,6-trimethyl-1,3,2-dioxaborinane (*E*-3)



E-**3**

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded *E*-**3** (94%, 151 mg) as a pale yellowish oil.

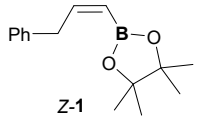
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.33 – 7.25 (m, 5H), 7.23 – 7.16 (m, 5H), 7.05 (dd, J = 17.9, 6.9 Hz, 1H), 5.40 (dd, J = 17.9, 1.5 Hz, 1H), 4.80 (dd, J = 6.9, 1.5 Hz, 1H), 1.26 (s, 12H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 154.58, 142.65, 130.07, 128.80, 128.40, 126.42, 83.20, 56.86, 24.82.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 30.23.

HRMS (ESI) for **$C_{21}H_{29}NBO_2$ [M+NH_4^+]$^+$:** calculated: 338.2291, found: 338.2299.

(*Z*)-4,4,5,5-Tetramethyl-2-(3-phenylprop-1-en-1-yl)-1,3,2-dioxaborolane (*Z*-1)



Z-**1**

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded *Z*-**1** (36%, 44 mg) as a pale yellowish oil.

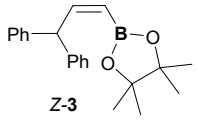
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.33 – 7.25 (m, 2H), 7.26 – 7.13 (m, 3H), 6.55 (dt, J = 14.3, 7.5 Hz, 1H), 5.43 (dt, J = 13.3, 1.4 Hz, 1H), 3.76 (dt, J = 7.6, 0.9 Hz, 2H), 1.30 (s, 12H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 152.69, 140.67, 128.64, 128.42, 125.92, 83.03, 38.67, 24.88.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 30.01.

HRMS (ESI) for **$C_{15}H_{25}NBO_2$ [M+NH_4^+]$^+$:** calculated: 262.1979, found: 262.1978.

(*Z*)-2-(3,3-Diphenylprop-1-en-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (*Z*-3)

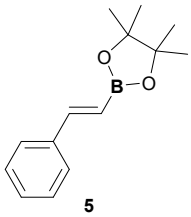


Z-**3**

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded *Z*-**3** (71%, 114 mg) as a pale yellowish oil.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.34 – 7.25 (m, 5H), 7.25 – 7.17 (m, 5H), 6.85 (dd, J = 13.2, 10.4 Hz, 1H), 5.65 (dd, J = 10.3, 0.6 Hz, 1H), 5.52 (dd, J = 13.2, 0.6 Hz, 1H), 1.28 (s, 12H).
^{13}C NMR ($CDCl_3$, 100 MHz) δ 155.14, 144.26, 128.42, 128.39, 126.15, 83.12, 51.99, 30.93, 24.90.
^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 30.09.
HRMS (ESI) for **$C_{21}H_{29}NBO_2$ [M+NH_4^+]$^+$:** calculated: 338.2302, found: 338.2291.

(*E*)-4,4,5,5-Tetramethyl-2-(2-phenylethenyl)-1,3,2-dioxaborolane (5)

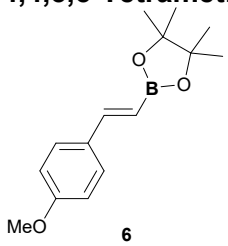


5

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded **5** (68%, 79 mg) as a pale yellowish oil.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.52 – 7.45 (m, 2H), 7.40 (d, J = 18.5 Hz, 1H), 7.38 – 7.26 (m, 3H), 6.17 (d, J = 18.4 Hz, 1H), 1.32 (s, 12H).
^{13}C NMR ($CDCl_3$, 100 MHz) δ 149.52, 128.90, 128.58, 127.07, 83.37, 24.83.
^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 30.16.
HRMS (ESI) for **$C_{14}H_{20}BO_2$ [M+H^+]$^+$:** calculated: 231.1556, found: 231.1555.

(*E*)-4,4,5,5-Tetramethyl-2-(4-methoxystyryl)-1,3,2-dioxaborolane (6)

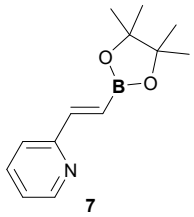


6

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded **6** (73%, 95 mg) as a pale yellowish oil.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.40 – 7.34 (m, 2H), 7.28 (d, J = 18.4 Hz, 1H), 6.83 – 6.77 (m, 2H), 5.94 (d, J = 18.4 Hz, 1H), 3.75 (s, 3H), 1.24 (s, 12H).
^{13}C NMR ($CDCl_3$, 100 MHz) δ 160.30, 149.07, 130.42, 128.48, 113.98, 113.33, 83.23, 55.30, 24.82.
^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 30.21.
HRMS (ESI) for **$C_{15}H_{22}BO_3$ [M+H^+]$^+$:** calculated: 261.1662, found: 261.1667.

(*E*)-2-(2-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)vinyl)pyridine (7)[3]



7

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded **7** (40%, 47 mg) as a pale yellowish oil.

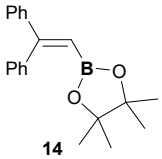
^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.60 (dd, J = 4.8, 1.8 Hz, 1H), 7.65 (dt, J = 7.7, 1.8 Hz, 1H), 7.45 (d, J = 18.3 Hz, 1H), 7.40 (dt, J = 7.9, 1.1 Hz, 1H), 7.17 (dd, J = 7.5, 4.8 Hz, 1H), 6.63 (d, J = 18.3 Hz, 1H), 1.31 (s, 12H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 155.47, 149.76, 148.79, 136.45, 123.08, 122.23, 83.48, 24.80.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 29.97.

HRMS (ESI) for **$C_{13}H_{19}BNO_2$ [M+H$^+$]$^+$:** calculated: 230.1467, found: 230.1472.

2-(2,2-Diphenylvinyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (14)



14

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded **14** (61% , 94 mg) as a pale yellowish oil.

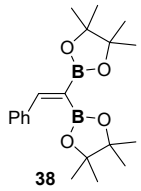
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.33 – 7.24 (m, 10H), 5.99 (s, 1H), 1.15 (s, 12H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 129.85, 128.29, 128.02, 127.99, 127.60, 127.54, 83.16, 24.62.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 29.66.

HRMS (ESI) for **$C_{20}H_{24}BO_2$ [M+H$^+$]$^+$:** calculated: 307.1869, found: 307.1877.

2,2'-(2-phenylethene-1,1-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (38)



38

Purified by flash column chromatography (pentane:ethyl ether = 10:1) yielded **38** (58%, 68 mg) as a pale yellowish oil.

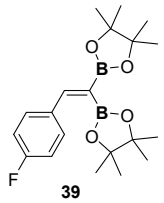
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.71 (s, 1H), 7.51 – 7.44 (m, 2H), 7.34 – 7.27 (m, 3H), 1.31 (s, 12H), 1.28 (s, 12H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 155.18, 139.60, 128.45, 128.18, 128.12, 83.63, 83.22, 24.89, 24.66.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 30.84.

HRMS (ESI) for **$C_{20}H_{30}B_2O_4$ [M+H]$^+$:** calculated: 371.2568, found: 371.2567.

2,2'-(2-(4-fluorophenyl)ethene-1,1-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (39)



39

Purified by flash column chromatography (pentane:ethyl ether = 10:1) yielded **39** (44%, 56 mg) as a pale yellowish oil.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.66 (s, 1H), 7.49 – 7.43 (m, 2H), 6.98 (t, *J* = 8.7 Hz, 2H), 1.31 (s, 12H), 1.27 (s, 12H).

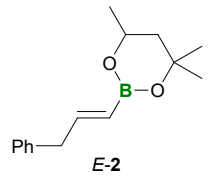
^{13}C NMR ($CDCl_3$, 100 MHz) δ 153.84, 129.96, 129.88, 115.20, 114.99, 83.69, 83.27, 24.87, 24.66.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 30.86.

HRMS (ESI) for **$C_{20}H_{29}B_2FO_4$ [M+H]$^+$:** calculated: 375.2210, found: 375.2215.

Characterization data for transborylated alkenylboranes

(*E*)-4,4,6-Trimethyl-2-(3-phenylprop-1-en-1-yl)-1,3,2-dioxaborinane (*E*-2)



E-**2**

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded *E*-**2** (89%, 65 mg) as a pale yellowish oil.

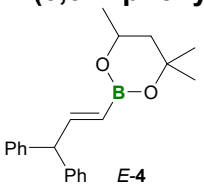
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.26 – 7.17 (m, 2H), 7.11 (dt, J = 6.4, 1.2 Hz, 3H), 6.57 (dt, J = 17.6, 6.4 Hz, 1H), 5.30 (d, J = 17.6 Hz, 1H), 4.18 – 4.05 (m, 1H), 3.37 (d, J = 6.4 Hz, 2H), 1.69 (dd, J = 13.9, 3.0 Hz, 1H), 1.41 (dd, J = 13.9, 11.6 Hz, 1H), 1.20 (s, 6H), 1.17 (d, J = 6.2 Hz, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 149.01, 139.77, 128.96, 128.40, 126.01, 70.68, 64.65, 45.97, 42.07, 31.25, 28.12, 23.17.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 26.18.

HRMS (ESI) for **$C_{15}H_{25}NBO_2$ [M+NH_4^+]$^+$:** calculated: 262.1978, found: 262.1998.

(*E*)-2-(3,3-Diphenylprop-1-en-1-yl)-4,4,6-trimethyl-1,3,2-dioxaborinane (*E*-4)



E-**4**

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded *E*-**4** (77%, 74 mg) as a pale yellowish oil.

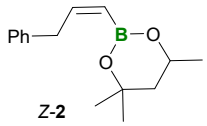
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.39 – 7.29 (m, 4H), 7.25 (m, 6H), 7.01 (dd, J = 17.6, 6.8 Hz, 1H), 5.37 (dd, J = 17.7, 1.5 Hz, 1H), 4.83 (dd, J = 6.9, 1.5 Hz, 1H), 4.26 (m, 1H), 1.82 (dd, J = 13.9, 2.9 Hz, 1H), 1.66 – 1.48 (m, 1H), 1.34 (s, 6H), 1.20 (d, J = 2.2 Hz, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 151.43, 143.17, 132.43, 130.08, 128.86, 128.35, 128.30, 126.27, 70.71, 64.67, 56.62, 45.98, 31.25, 28.16.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 25.79.

HRMS (ESI) for **$C_{21}H_{26}BO_2$ [M+H^+]$^+$:** calculated: 320.7415, found: 320.7442.

(*Z*)-4,4,6-Trimethyl-2-(3-phenylprop-1-en-1-yl)-1,3,2-dioxaborinane (*Z*-2)



Z-**2**

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded ***Z*-2** (69%, 51 mg) as a pale yellowish oil.

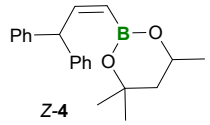
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.25 – 7.15 (m, 4H), 7.15 – 7.07 (m, 1H), 6.33 (dt, J = 13.5, 7.6 Hz, 1H), 5.25 (d, J = 13.5 Hz, 1H), 4.20 (m, 1H), 3.68 (d, J = 7.6, 2H), 1.74 (dd, J = 13.9, 2.9 Hz, 1H), 1.53 – 1.42 (m, 1H), 1.26 (d, 6H), 1.22 (d, J = 2.2 Hz, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 149.70, 141.38, 128.67, 128.34, 125.73, 70.88, 64.78, 45.96, 37.98, 31.36, 28.25, 24.88, 23.25.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 26.23.

HRMS (ESI) for **$C_{15}H_{25}NBO_2$ [M+NH_4^+]$^+$:** calculated: 262.1978, found: 262.1998.

(*S*,*Z*)-2-(3,3-Diphenylprop-1-en-1-yl)-4,4,6-trimethyl-1,3,2-dioxaborinane (*Z*-4)



Z-**4**

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded *Z*-**4** (32%, 31 mg) as a pale yellowish oil.

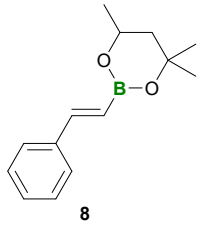
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.35 – 7.27 (m, 5H), 7.27 – 7.16 (m, 4H), 6.74 (dd, J = 13.4, 10.2 Hz, 1H), 5.76 (d, J = 10.2 Hz, 1H), 5.44 (d, J = 13.4 Hz, 1H), 4.27 (m, 1H), 1.81 (dd, J = 13.9, 2.9 Hz, 1H), 1.57 – 1.48 (m, 1H), 1.34 (s, 3H), 1.31 (d, J = 6.2 Hz, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 152.24, 128.33, 125.98, 70.97, 64.82, 51.18, 45.85, 31.35, 30.94, 28.25, 23.23.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 26.29.

HRMS (ESI) for **$C_{21}H_{29}NBO_2$ [M+NH_4^+]$^+$:** calculated: 338.2302, found: 338.2291.

(*E*)-4,4,6-Trimethyl-2-(2-phenylethenyl)-1,3,2-dioxaborinane (8)[4]



8

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded **8** (62%, 43 mg) as a pale yellowish oil.

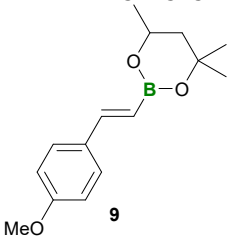
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.50 – 7.43 (m, 2H), 7.33 – 7.20 (m, 4H), 6.09 (d, J = 18.2 Hz, 1H), 4.26 (m, 1H), 1.80 (dd, J = 13.9, 2.9 Hz, 1H), 1.54 (dd, J = 12.7, 12.6 Hz, 1H), 1.33 (s, 3H), 1.32 (s, 3H), 1.30 (d, J = 6.2 Hz, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 146.49, 138.02, 128.45, 128.29, 126.97, 70.90, 64.85, 46.03, 31.29, 28.17, 23.21.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 26.24.

HRMS (ESI) for **$C_{14}H_{20}BO_2$ [M+H^+]$^+$:** calculated: 231.1556, found: 231.1569.

(*E*)-2-(4-Methoxystyryl)-4,4,6-trimethyl-1,3,2-dioxaborinane (9)



9

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded **9** (80%, 62 mg) as a pale yellowish oil.

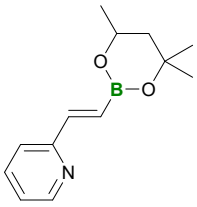
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.48 – 7.38 (m, 2H), 7.31 – 7.21 (d, J = 18.2 Hz, 1H), 6.88 – 6.81 (m, 2H), 5.95 (d, J = 18.2 Hz, 1H), 4.27 (m, 1H), 3.81 (s, 3H), 1.82 (dd, J = 13.9, 2.9 Hz, 1H), 1.60 – 1.49 (m, 2H), 1.34 (s, 3H), 1.33 (s, 3H), 1.31 (d, J = 6.2 Hz, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.83, 146.04, 130.93, 128.29, 113.85, 70.83, 64.80, 55.28, 46.02, 31.31, 28.17, 23.24.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 26.25.

HRMS (ESI) for **$C_{15}H_{22}BO_3$ [M+H]$^+$:** calculated:261.1662, found:261.1658.

(*E*)-2-(2-(4,4,6-Trimethyl-1,3,2-dioxaborinan-2-yl)vinyl)pyridine (10)



10

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded **10** (56%, 39 mg) as a pale yellowish oil.

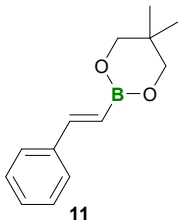
^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.57 (dd, J = 4.8, 1.8 Hz, 1H), 7.63 (t, J = 7.7, 1.9 Hz, 1H), 7.47 (dd, J = 8.0, 1.1 Hz, 1H), 7.39 (d, J = 18.2 Hz, 1H), 7.13 (ddd, J = 7.5, 4.8, 1.2 Hz, 1H), 6.48 (d, J = 18.2 Hz, 1H), 4.28 (m, 1H), 1.82 (dd, J = 13.9, 3.0 Hz, 1H), 1.55 (dd, J = 13.9, 11.6 Hz, 1H), 1.33 (s, 6H), 1.30 (d, J = 6.2 Hz, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 156.35, 149.53, 146.37, 136.27, 122.55, 121.19, 70.97, 64.92, 45.99, 31.23, 28.14, 23.16.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 26.47.

HRMS (ESI) for **$C_{13}H_{19}NBO_2$ [M+H$^+$]$^+$:** calculated: 230.1467, found: 230.1474.

(*E*)-5,5-Dimethyl-2-(2-phenylethenyl)-1,3,2-dioxaborinane (11)



11

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded **11** (68%, 44 mg) as a pale yellowish oil.

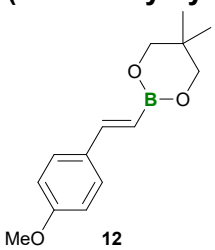
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.52 – 7.46 (m, 2H), 7.38 – 7.23 (m, 4H), 6.11 (d, J = 18.3 Hz, 1H), 3.70 (s, 4H), 1.01 (s, 6H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 147.13, 137.80, 128.52, 127.01, 72.22, 31.87, 21.89.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 26.48.

HRMS (ESI) for **$C_{26}H_{35}B_2O_4$ [2M+H$^+$]$^+$:** calculated: 432.2817, found: 432.2643.

(*E*)-2-(4-Methoxystyryl)-5,5-dimethyl-1,3,2-dioxaborinane (12)



12

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded **12** (64%, 47 mg) as a pale yellowish oil.

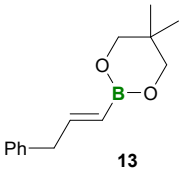
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.47 – 7.39 (m, 2H), 7.28 (d, J = 17.3 Hz, 1H), 6.92 – 6.80 (m, 2H), 5.95 (d, J = 18.2 Hz, 1H), 3.81 (s, 3H), 3.69 (s, 4H), 0.98 (s, 6H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 160.01, 146.66, 130.69, 128.36, 113.92, 72.20, 55.30, 31.88, 24.83, 21.90.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 25.98.

HRMS (ESI) for **$C_{14}H_{20}BO_3$ [M+H]$^+$:** calculated: 247.1506, found: 247.1507.

(*E*)-5,5-Dimethyl-2-(3-phenylprop-1-en-1-yl)-1,3,2-dioxaborinane (13)



13

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded **13** (48%, 33 mg) as a pale yellowish oil.

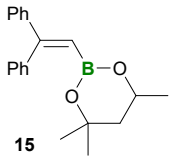
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.31 – 7.25 (m, 2H), 7.19 (t, J = 7.5 Hz, 3H), 6.67 (dt, J = 17.6, 6.4 Hz, 1H), 5.39 (dt, J = 17.6, 1.6 Hz, 1H), 3.62 (s, 4H), 3.46 (dd, J = 6.5, 1.6 Hz, 2H), 0.96 (s, 6H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 149.74, 139.59, 128.86, 128.42, 126.05, 72.08, 42.07, 31.77, 21.87.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 25.82.

HRMS (ESI) for **$C_{14}H_{23}NBO_2$ $[M+NH_4^+]^+$:** calculated: 262.1978, found: 262.1978.

2-(2,2-diphenylvinyl)-4,4,6-trimethyl-1,3,2-dioxaborinane (15)



15

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded **15** (92%, 84 mg) as a pale yellowish oil.

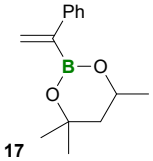
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.35 – 7.20 (m, 10H), 6.00 (s, 1H), 4.09 (m, 1H), 1.69 (dd, J = 13.9, 3.0 Hz, 1H), 1.47 – 1.33 (m, 1H), 1.17 (s, 3H), 1.08 (s, 4H), 1.06 (d, J = 6.2 Hz, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 157.10, 143.37, 142.60, 129.72, 127.88, 127.84, 127.61, 127.43, 127.05, 70.87, 64.83, 45.77, 30.89, 27.80, 22.89.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 26.14.

HRMS (ESI) for **$C_{20}H_{27}NBO_2$ $[M+NH_4^+]^+$:** calculated: 472.2830, found: 472.2834.

4,4,6-Trimethyl-2-(1-phenylvinyl)-1,3,2-dioxaborinane (17)



17

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded **17** (80%, 55 mg) as a pale yellowish oil.

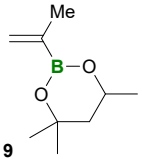
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.52 – 7.40 (m, 2H), 7.35 – 7.25 (m, 2H), 7.26 – 7.17 (m, 1H), 5.98 (d, J = 3.5 Hz, 1H), 5.90 (d, J = 3.5 Hz, 1H), 4.29 (m, 1H), 1.84 (dd, J = 13.9, 3.0 Hz, 1H), 1.62 – 1.54 (m, 1H), 1.33 (s, 6H), 1.30 (d, J = 6.2 Hz, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 142.64, 128.79, 127.83, 127.58, 126.44, 71.19, 65.13, 45.91, 31.23, 28.13, 23.16.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 26.39.

HRMS (ESI) for **$C_{14}H_{23}NBO_2$ $[M+NH_4^+]^+$:** calculated: 248.1822, found: 248.1831.

4,4,6-Trimethyl-2-(prop-1-en-2-yl)-1,3,2-dioxaborinane (19)



19

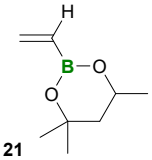
Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded **19** (15%, 8 mg) as a pale yellowish oil.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 5.65 (m, 1H), 5.52 – 5.46 (m, 1H), 4.21 (m, 1H), 1.77 (d, J = 17.1 Hz, 1H), 1.70 (s, 3H), 1.53 – 1.42 (m, 1H), 1.29 (s, 6H), 1.26 (d, J = 6.2 Hz, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 126.70, 70.60, 64.67, 45.89, 31.26, 28.13, 24.79, 23.18, 20.92.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 26.01.

4,4,6-Trimethyl-2-vinyl-1,3,2-dioxaborinane (21)



21

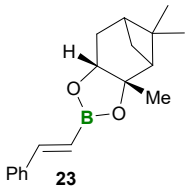
Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded **21** (30%,14 mg) as a pale yellowish oil.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.04 (dd, J = 18.7, 5.1 Hz, 1H), 5.86 (dd, J = 13.4, 5.0 Hz, 1H), 5.77 (dd, J = 18.8, 13.4 Hz, 1H), 4.22 (m, 1H), 1.79 (dd, J = 13.9, 3.0 Hz, 1H), 1.58 – 1.49 (m, 1H), 1.30 (s, 6H), 1.27 (d, J = 6.2 Hz, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 133.76, 70.76, 64.71, 45.96, 31.21, 28.10, 23.13.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 25.84.

(3a*R*,4*S*,6*S*,7a*R*)-3a,5,5-Trimethyl-2-((*E*)-styryl)hexahydro-4,6-methanobenzo[*d*][1,3,2] dioxaborole (23)



23

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded **23** (88%, 74 mg) as a pale yellowish oil.

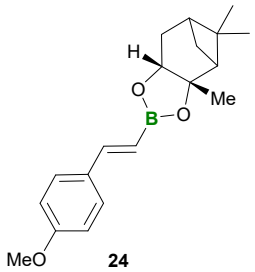
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.53 – 7.46 (m, 2H), 7.41 (d, J = 18.5 Hz, 1H), 7.39 – 7.25 (m, 3H), 6.20 (d, J = 18.4 Hz, 1H), 4.38 (dd, J = 8.7, 1.9 Hz, 1H), 2.45 – 2.33 (m, 1H), 2.30 – 2.19 (m, 1H), 2.12 (t, J = 6.0, 4.8 Hz, 1H), 1.98 – 1.90 (m, 2H), 1.46 (s, 3H), 1.31 (s, 3H), 1.21 (d, J = 10.9 Hz, 1H), 0.88 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 149.61, 137.65, 129.02, 128.71, 128.10, 127.19, 85.96, 78.00, 51.55, 39.68, 38.33, 35.68, 28.81, 27.25, 26.60, 24.18.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 29.25.

HRMS (ESI) for **$C_{36}H_{46}B_2O_4$ [2M$^+$]$^+$:** calculated: 564.3582, found: 564.3583.

(3a*S*,4*S*,6*S*,7a*R*)-2-((*E*)-4-Methoxystyryl)-3a,5,5-trimethylhexahydro-4,6-methanobenzo[*d*][1,3,2]dioxaborole (24)



24

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded **24** (72%, 68 mg) as a pale yellowish oil.

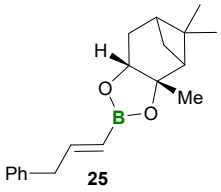
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.48 – 7.40 (m, 2H), 7.36 (d, J = 18.4 Hz, 1H), 6.90 – 6.83 (m, 2H), 6.03 (d, J = 18.4 Hz, 1H), 4.36 (dd, J = 8.7, 1.9 Hz, 1H), 3.82 (s, 3H), 2.39 (m, 1H), 2.30 – 2.17 (m, 1H), 2.11 (dd, J = 6.1, 4.9 Hz, 1H), 1.98 – 1.86 (m, 2H), 1.45 (s, 3H), 1.31 (s, 3H), 1.26 – 1.16 (m, 1H), 0.87 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 160.29, 149.01, 130.47, 130.30, 128.46, 113.98, 85.70, 77.80, 65.86, 55.30, 51.45, 39.57, 38.20, 35.59, 28.69, 27.12, 26.47, 24.04, 15.29.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 29.88.

HRMS (ESI) for **$C_{19}H_{26}BO_3$ [M+H$^+$]$^+$:** calculated: 313.1975, found: 313.1987.

(3a*S*,4*S*,6*S*,7a*R*)-3a,5,5-Trimethyl-2-((*E*)-3-phenylprop-1-en-1-yl)hexahydro-4,6-methanobenzo[*d*][1,3,2]dioxaborole (25)



25

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded **25** (80%, 71 mg) as a pale yellowish oil.

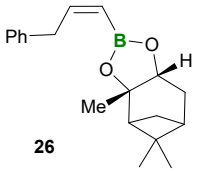
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.40 – 7.31 (m, 2H), 7.31 – 7.22 (m, 3H), 6.84 (dt, J = 17.8, 6.4 Hz, 1H), 5.55 (dt, J = 17.8, 1.6 Hz, 1H), 4.36 (dd, J = 8.7, 1.9 Hz, 1H), 3.56 (m, 2H), 2.41 (ddt, J = 14.0, 8.7, 2.2 Hz, 1H), 2.35 – 2.22 (m, 1H), 2.12 (dd, J = 6.1, 4.9 Hz, 1H), 2.01 – 1.89 (m, 2H), 1.46 (s, 3H), 1.36 (s, 3H), 1.22 (d, J = 10.9 Hz, 1H), 0.92 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 152.33, 139.14, 128.91, 128.45, 126.16, 85.59, 77.70, 51.37, 42.31, 39.52, 38.15, 35.48, 28.64, 27.10, 26.44, 24.01.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 29.57.

HRMS (ESI) for **$C_{19}H_{29}NBO_2$ [M+NH_4^+]$^+$:** calculated: 314.2291, found: 314.2302.

(3a*S*,7a*R*)-3a,5,5-trimethyl-2-((*Z*)-3-phenylprop-1-en-1-yl)hexahydro-4,6-methanobenzo[d][1,3,2]dioxaborole (26)



26

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded **26** (80%, 71 mg) as a pale yellowish oil.

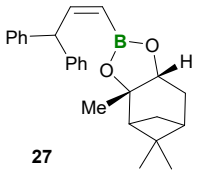
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.36 – 7.24 (m, 3H), 7.24 – 7.15 (m, 3H), 6.57 (dt, J = 13.3, 7.6 Hz, 1H), 5.47 (dt, J = 13.3, 1.4 Hz, 1H), 4.35 (dd, J = 8.7, 1.8 Hz, 1H), 3.84 – 3.70 (m, 2H), 2.44 – 2.31 (m, 1H), 2.30 – 2.19 (m, 1H), 2.10 (dd, J = 6.1, 4.8 Hz, 1H), 1.98 – 1.87 (m, 2H), 1.31 (s, 3H), 1.25 – 1.18 (m, 1H), 0.87 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 152.60, 140.64, 128.64, 128.43, 125.92, 85.43, 77.58, 51.40, 39.61, 38.70, 38.14, 35.62, 28.72, 27.11, 26.53, 24.03.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 29.48.

HRMS (ESI) for **$C_{19}H_{29}NBO_2$ [M+NH_4^+]$^+$:** calculated: 314.2289, found: 314.2294.

(3a*S*,7a*R*)-2-((*Z*)-3,3-diphenylprop-1-en-1-yl)-3a,5,5-trimethylhexahydro-4,6-methanobenzo[d][1,3,2]dioxaborole (27)



27

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded **27** (74%, 83 mg) as a pale yellowish oil.

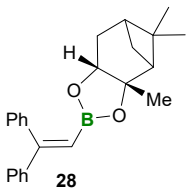
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.13 – 7.06 (m, 4H), 7.06 – 6.96 (m, 6H), 6.67 (dd, *J* = 13.2, 10.3 Hz, 1H), 5.45 (d, *J* = 10.3 Hz, 1H), 5.36 (d, *J* = 13.2 Hz, 1H), 4.14 (dd, *J* = 8.6, 1.8 Hz, 1H), 2.22 – 2.11 (m, 1H), 2.06 – 1.95 (m, 1H), 1.90 (dd, *J* = 6.1, 4.9 Hz, 1H), 1.76 – 1.65 (m, 2H), 1.23 (s, 3H), 1.11 (s, 3H), 0.95 (d, *J* = 10.9 Hz, 1H), 0.67 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 155.09, 144.26, 144.20, 128.44, 128.41, 126.17, 85.53, 77.63, 52.10, 51.39, 39.60, 38.14, 35.60, 28.69, 27.12, 26.50, 24.91, 24.04.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 28.79.

HRMS (ESI) for **$C_{25}H_{30}BO_2$ [M+H^+]$^+$:** calculated: 373.3210, found: 373.3204.

(3a*S*,4*S*,6*S*,7a*R*)-2-(2,2-diphenylvinyl)-3a,5,5-trimethylhexahydro-4,6-methanobenzo[*d*][1,3,2]dioxaborole (28)



28

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded **28** (78%, 84 mg) as a pale yellowish oil.

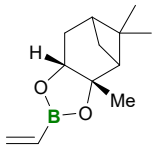
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.36 – 7.20 (m, 10H), 6.01 (s, 1H), 4.15 (dd, *J* = 8.7, 2.0 Hz, 1H), 2.24 – 2.09 (m, 2H), 1.95 (t, *J* = 5.5 Hz, 1H), 1.83 (tt, J = 5.9, 3.1 Hz, 1H), 1.63 (ddd, *J* = 14.5, 3.4, 2.1 Hz, 1H), 1.26 (s, 3H), 1.23 (s, 3H), 1.10 (d, *J* = 10.7 Hz, 1H), 0.77 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.96, 143.09, 141.92, 132.42, 129.83, 128.08, 128.03, 127.96, 127.63, 127.57, 85.44, 77.73, 65.87, 51.25, 39.47, 38.13, 35.22, 28.44, 27.08, 26.51, 24.00, 15.30.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 29.89.

HRMS (ESI) for **$C_{24}H_{28}BO_2$ [M+H$^+$]$^+$:** calculated: 359.2191, found: 259.2182.

(3aS,7aR)-3a,5,5-trimethyl-2-vinylhexahydro-4,6 methanobenzo[d][1,3,2]dioxaborole(29)



29

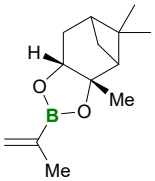
Purified by flash column chromatography (pentane:diethyl ether = 200:1) yielded **29** (51%, 32 mg) as a pale yellowish oil.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.16 (dd, *J* = 19.4, 4.2 Hz, 1H), 6.03 (dd, *J* = 13.6, 4.3 Hz, 1H), 5.89 (dd, *J* = 19.4, 13.7 Hz, 1H), 4.32 (dd, *J* = 8.8, 1.9 Hz, 1H), 2.40 – 2.31 (m, 1H), 2.28 – 2.16 (m, 1H), 2.10 – 2.03 (m, 1H), 1.95 – 1.85 (m, 2H), 1.41 (s, 3H), 1.29 (s, 3H), 1.15 (d, *J* = 11.0 Hz, 1H), 0.85 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 137.13, 85.92, 77.95, 53.56, 51.48, 39.66, 38.31, 35.60, 28.75, 27.24, 26.56, 24.16.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 29.35.

(3aS,7aR)-3a,5,5-trimethyl-2-(prop-1-en-2-yl)hexahydro-4,6-methanobenzo[d] [1,3,2]dioxaborole (30)



30

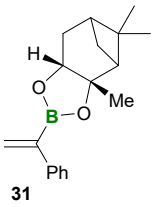
Purified by flash column chromatography (pentane:diethyl ether = 200:1) yielded **30** (71%, 47 mg) as a pale yellowish oil.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 5.78 – 5.72 (m, 1H), 5.67 – 5.60 (m, 1H), 4.32 (dd, *J* = 8.7, 1.9 Hz, 1H), 2.40 – 2.30 (m, 1H), 2.27 – 2.16 (m, 1H), 2.11 – 2.03 (m, 1H), 1.94 – 1.85 (m, 2H), 1.84 (t, *J* = 1.5 Hz, 3H), 1.41 (s, 2H), 1.29 (s, 2H), 0.85 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 130.08, 86.03, 78.13, 51.50, 39.66, 38.30, 35.70, 28.81, 27.24, 26.59, 24.94, 24.16, 21.44.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 29.52.

(3aS,7aR)-3a,5,5-trimethyl-2-(1-phenylvinyl)hexahydro-4,6-methanobenzo[d][1,3,2]dioxaborole (31)



31

Purified by flash column chromatography (pentane:diethyl ether = 200:1) yielded **31** (93%, 79 mg) as a pale yellowish oil.

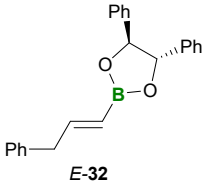
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.53 – 7.45 (m, 2H), 7.37 – 7.29 (m, 2H), 7.28 – 7.20 (m, 2H), 6.08 (d, *J* = 2.0 Hz, 2H), 4.41 (dd, *J* = 8.8, 1.9 Hz, 1H), 2.44 – 2.34 (m, 1H), 2.32 – 2.21 (m, 1H), 2.16 – 2.09 (m, 1H), 2.01 – 1.90 (m, 2H), 1.46 (s, 3H), 1.31 (s, 3H), 1.25 (d, *J* = 10.9 Hz, 1H), 0.88 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 141.67, 131.11, 128.33, 127.32, 127.16, 86.34, 78.38, 51.52, 39.69, 38.32, 35.70, 28.83, 27.25, 26.74, 24.18.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 30.04.

HRMS (ESI) for **$C_{18}H_{24}BO_2$ [M+H$^+$]$^+$:** calculated: 283.1869; found: 283.1854.

(4*R*,5*R*)-4,5-diphenyl-2-((*E*)-3-phenylprop-1-en-1-yl)-1,3,2-dioxaborolane (*E*-32)



E-**32**

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded ***E*-32** (76%, 78 mg) as a pale yellowish oil.

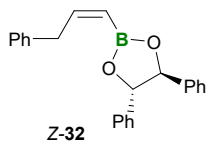
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.39 – 7.23 (m, 12H), 7.24 – 7.14 (m, 3H), 6.96 (dtd, *J* = 17.9, 6.5, 1.3 Hz, 1H), 5.63 (dq, *J* = 17.8, 1.6 Hz, 1H), 5.13 (s, 2H), 3.54 (dd, *J* = 6.4, 1.6 Hz, 2H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 154.15, 140.32, 138.93, 128.92, 128.77, 128.55, 128.32, 126.30, 125.85, 86.42, 42.40.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 29.37.

HRMS (ESI) for **$C_{23}H_{25}NBO_2$ [M+NH$_4^+$]$^+$:** calculated: 358.1978, found: 358.1997.

(4R,5R)-4,5-diphenyl-2-((Z)-3-phenylprop-1-en-1-yl)-1,3,2-dioxaborolane (*Z*-32)



Z-**32**

Purified by flash column chromatography (hexane:diethyl ether =100:1) yielded ***Z*-32** (74%, 76 mg) as a pale yellowish oil.

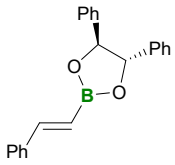
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.45 – 7.24 (m, 15H), 7.24 – 7.17 (m, 1H), 6.76 (dt, *J* = 13.3, 7.6 Hz, 1H), 5.67 (dt, *J* = 13.3, 1.4 Hz, 1H), 5.24 (s, 2H), 3.89 (dd, *J* = 7.6, 1.4 Hz, 2H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 154.54, 140.43, 140.32, 128.80, 128.65, 128.50, 128.33, 126.05, 125.80, 86.28, 38.89.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 30.84.

HRMS (ESI) for **$C_{23}H_{25}NBO_2$ [M+NH_4^+]$^+$:** calculated: 358.1978, found: 358.1955.

(4*R*,5*R*)-4,5-diphenyl-2-((*E*)-styryl)-1,3,2-dioxaborolane (33)



33

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded **33** (65%, 64 mg) as a pale yellowish oil.

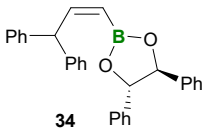
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.63 (d, *J* = 18.5 Hz, 1H), 7.56 (dd, *J* = 8.2, 1.5 Hz, 2H), 7.44 – 7.32 (m, 13H), 6.37 (d, *J* = 18.4 Hz, 1H), 5.26 (s, 2H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 151.07, 149.53, 140.32, 137.32, 129.25, 128.83, 128.69, 128.40, 127.26, 125.87, 86.59, 83.37, 65.87.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 30.55.

HRMS (ESI) for **$C_{22}H_{24}NBO_2$ [M+NH_4^+]$^+$:** calculated: 324.2215, found: 324.2221.

(4*R*,5*R*)-2-((*Z*)-3,3-diphenylprop-1-en-1-yl)-4,5-diphenyl-1,3,2-dioxaborolane (34)



34

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded **34** (80%, 101 mg) as a pale yellowish oil.

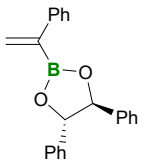
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.39 – 7.13 (m, 21H), 7.03 (dd, *J* = 13.3, 10.4 Hz, 1H), 5.78 – 5.70 (m, 2H), 5.18 (s, 2H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 198.56, 196.78, 156.97, 144.10, 144.05, 132.45, 130.11, 129.71, 128.82, 128.56, 128.54, 128.52, 128.42, 128.35, 128.32, 128.04, 126.35, 125.81, 86.37, 52.43.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 30.08.

HRMS (ESI) for **$C_{29}H_{25}BO_2Na$ [M+Na^+]$^+$:** calculated: 439.1845, found: 439.1853.

(4S,5S)-4,5-diphenyl-2-(1-phenylvinyl)-1,3,2-dioxaborolane (35)



35

Purified by flash column chromatography (pentane:diethyl ether = 100:1) yielded **35** (47%, 46 mg) as a white solid.

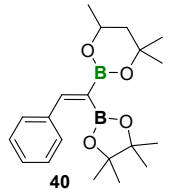
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.67 – 7.61 (m, 2H), 7.44 – 7.34 (m, 12H), 7.32 – 7.26 (m, 1H), 6.36 (d, *J* = 2.8 Hz, 1H), 6.28 (d, *J* = 2.9 Hz, 1H), 5.31 (s, 2H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 141.24, 140.40, 133.08, 128.96, 128.53, 128.46, 127.40, 127.37, 125.98, 87.07.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 31.76.

HRMS (ESI) for **$C_{22}H_{23}NBO_2$ [M+NH_4^+]$^+$:** calculated: 344.1822; found: 344.1834.

(*Z*)-4,4,6-trimethyl-2-(2-phenyl-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)vinyl)-1,3,2-dioxaborinane (40)



40

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded **40** (65%, 48 mg) as a pale yellowish oil.

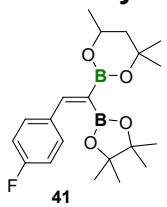
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.66 (s, 1H), 7.53 – 7.41 (m, 2H), 7.32 – 7.19 (m, 3H), 4.26 (m, 1H), 1.76 (dd, *J* = 13.8, 3.0 Hz, 1H), 1.53 (dd, *J* = 13.9, 4.6 Hz, 1H), 1.31 (s, 12H), 1.30 (s, 6H), 1.27 – 1.24 (d, *J* = 11.3, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 152.57, 140.16, 128.09, 128.02, 127.91, 83.39, 70.85, 64.86, 45.86, 31.28, 28.19, 24.86, 24.74, 23.11.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 26.11.

HRMS (ESI) for **$C_{20}H_{30}B_2O_4$ [M+H]$^+$:** calculated: 357.2409, found: 357.2410.

(*Z*)-2-(2-(4-fluorophenyl)-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)vinyl)-4,4,6-trimethyl-1,3,2-dioxaborinane (41)



41

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded **41** (64%, 57 mg) as a pale yellowish oil.

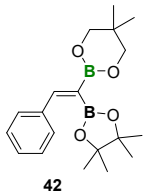
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.61 (s, 1H), 7.47 – 7.40 (m, 2H), 6.97 (m, 2H), 4.24 (m, 1H), 1.76 (dd, *J* = 13.9, 3.0 Hz, 1H), 1.55 – 1.48 (m, 2H), 1.31 (s, 12H), 1.30 (s, 6H), 1.28 – 1.24 (m, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 151.21, 129.78, 129.70, 115.05, 114.83, 83.46, 70.90, 64.89, 45.85, 31.26, 28.18, 24.85, 24.74, 23.09.

^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 26.10.

HRMS (ESI) for **$C_{20}H_{29}B_2FO_4$ [M+H]$^+$:** calculated: 375.2313, found: 375.2316.

(*Z*)-5,5-dimethyl-2-(2-phenyl-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)vinyl)-1,3,2-dioxaborinane (42)



42

Purified by flash column chromatography (hexane:diethyl ether = 100:1) yielded **42** (22%, 10 mg) as a pale yellowish oil.

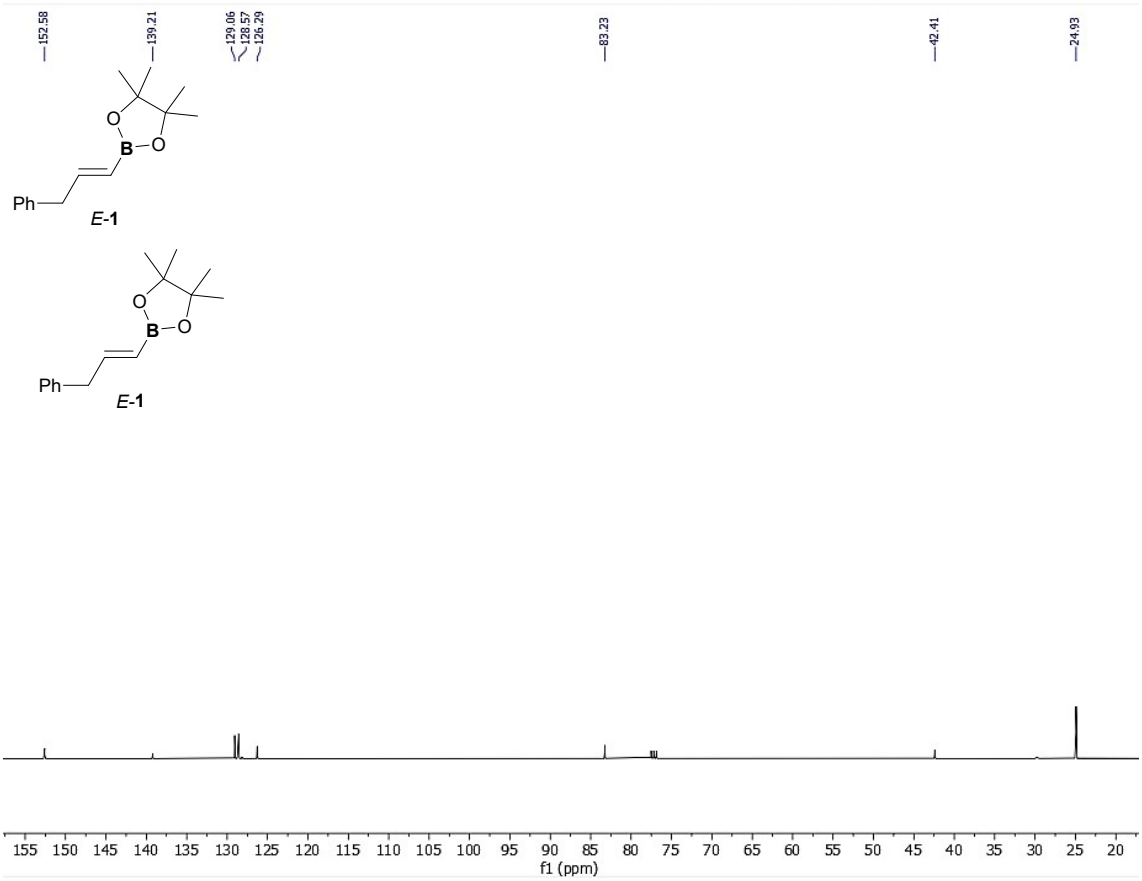
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.67 (s, 1H), 7.51 – 7.46 (m, 2H), 7.33 – 7.22 (m, 3H), 3.67 (s, 4H), 1.30 (s, 12H), 0.98 (s, 6H).

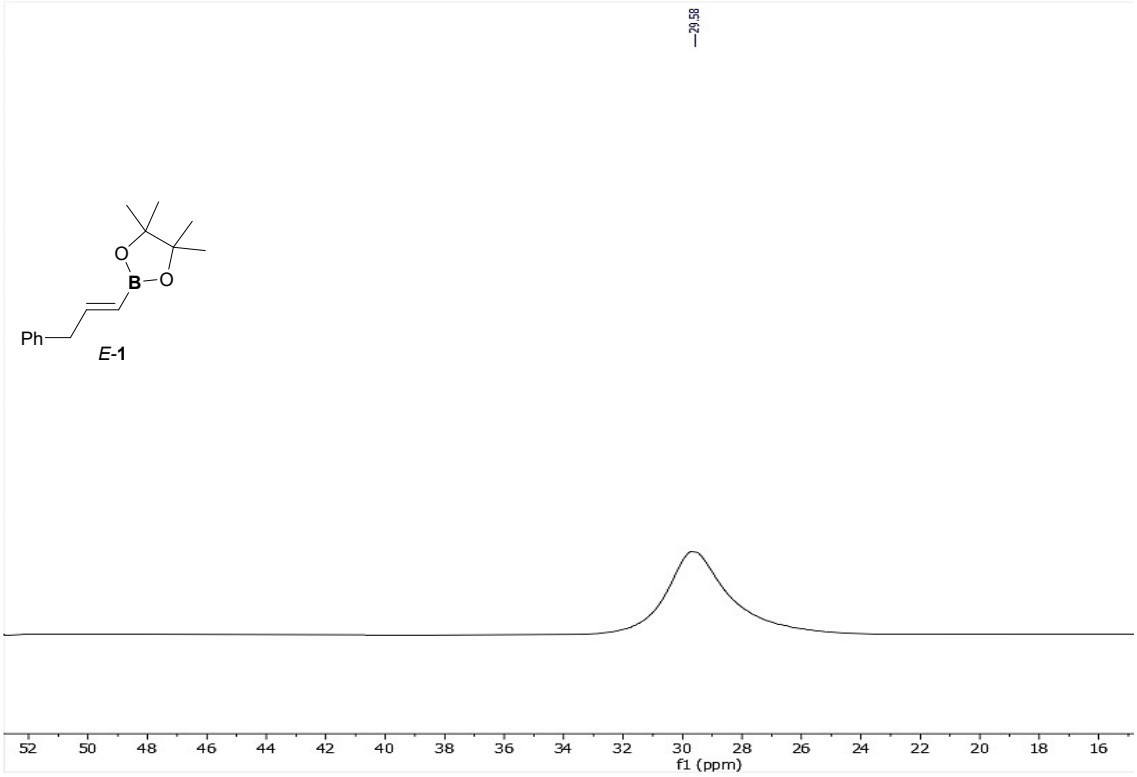
^{13}C NMR ($CDCl_3$, 100 MHz) δ 155.19, 152.97, 139.89, 128.14, 128.07, 83.49, 72.26, 31.81, 24.72, 21.99.

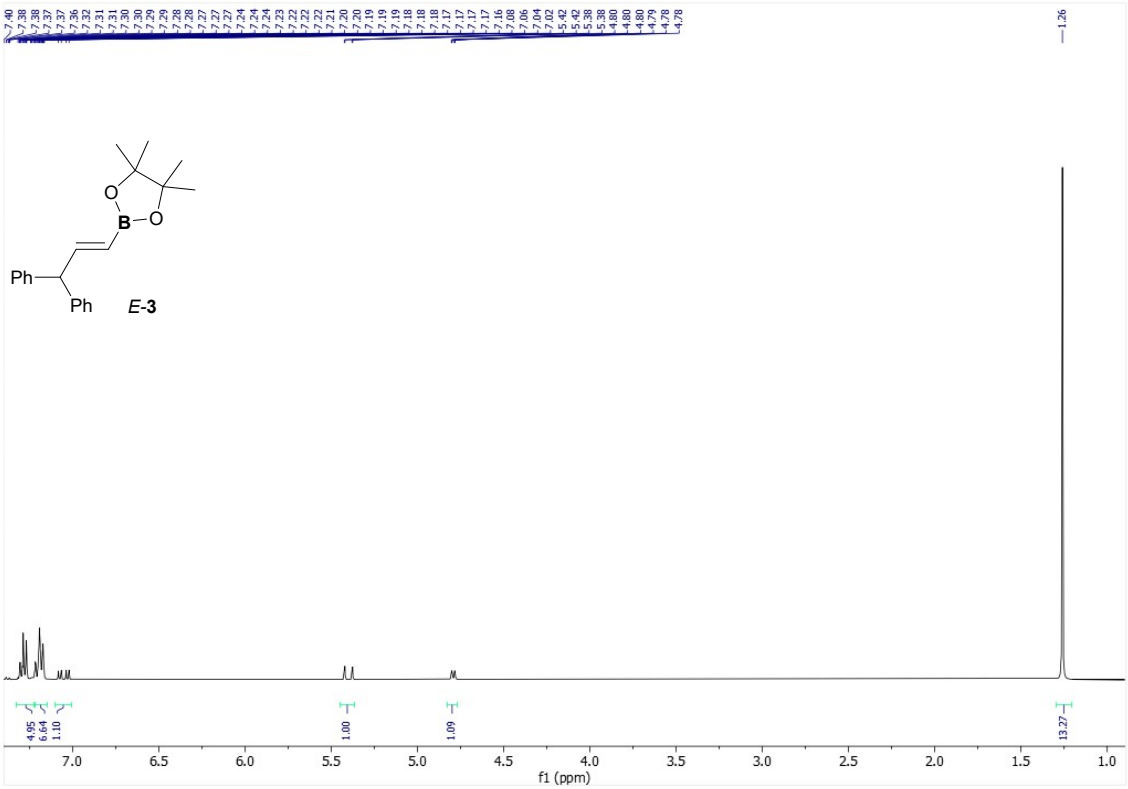
^{11}B NMR ($CDCl_3$, 128.3 MHz) δ 26.52.

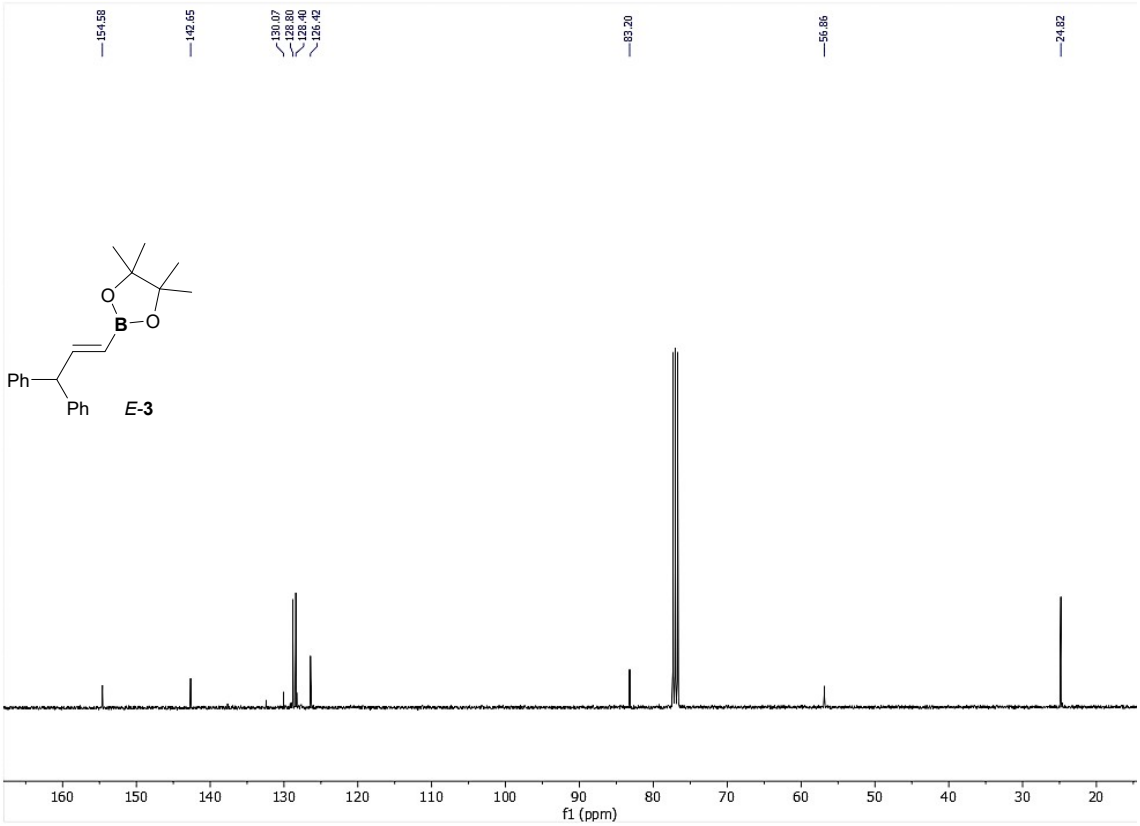
HRMS (ESI) for **$C_{19}H_{28}B_2O_4$ [M+H]$^+$:** calculated: 343.2261, found: 343.2270.

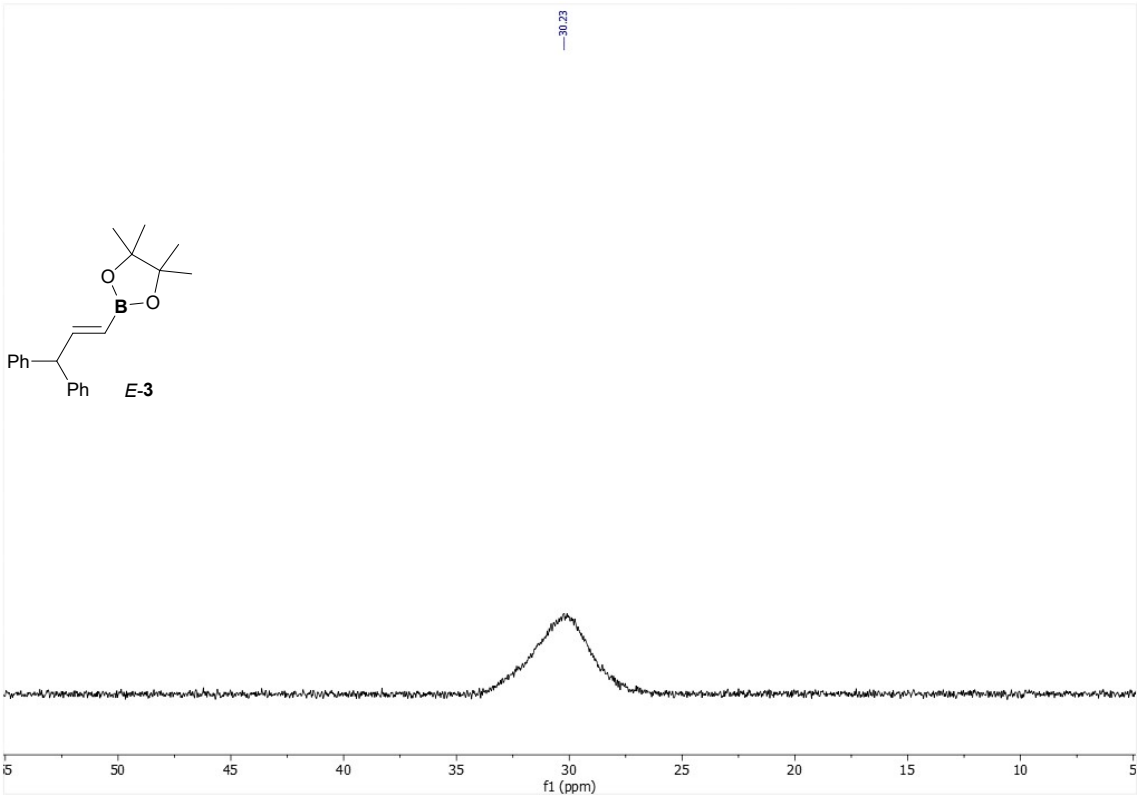
^{1}H, ^{13}C, ^{11}B Spectra for alkenyl pinacolboranes

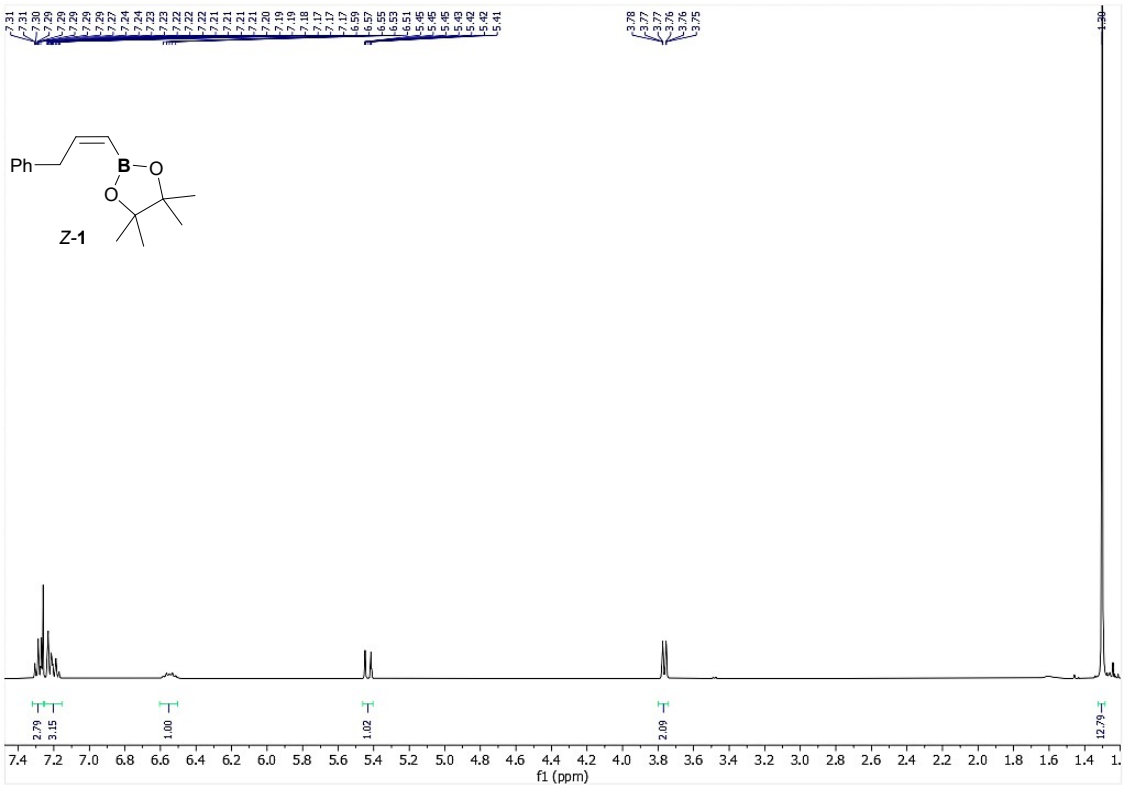


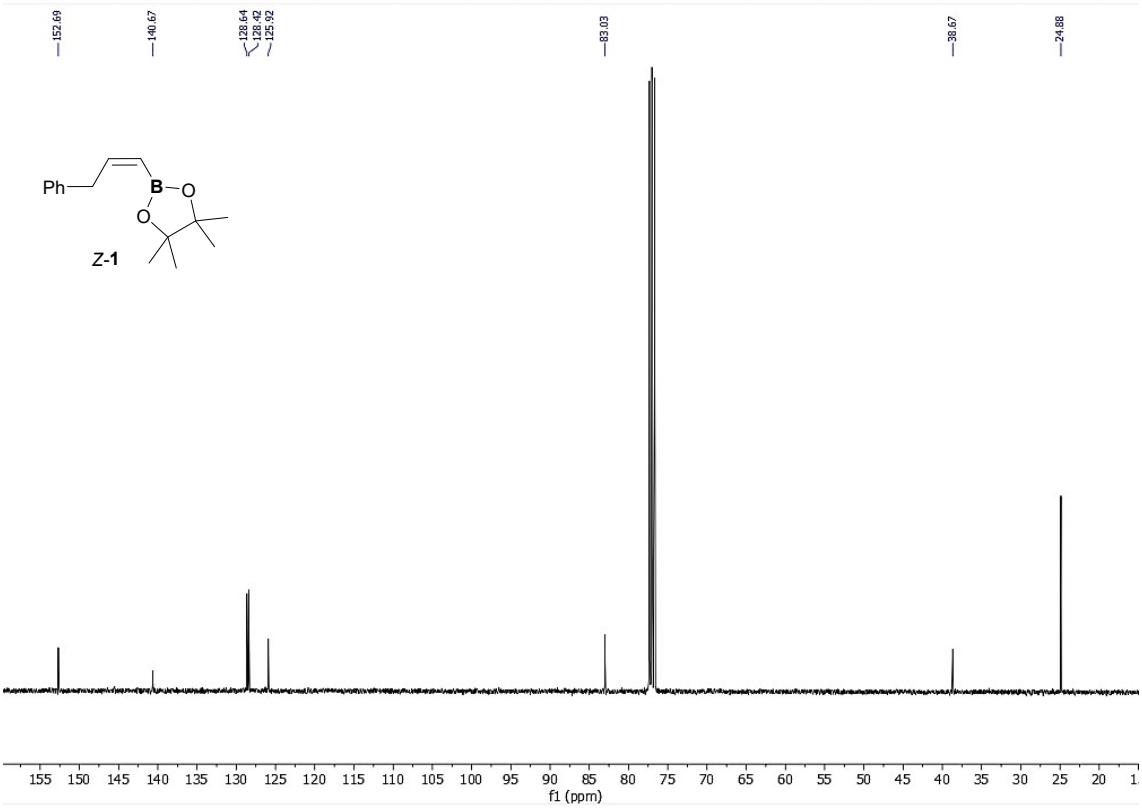



Ph
Ph
E-3
f1 (ppm)


Ph
Ph
E-3
f1 (ppm)


30.23
O
B
O
Ph
Ph
E-3
50
45
40
35
30
25
20
15
10
f1 (ppm)


Ph
B
O
O
Z-1
2.79
3.15
1.00
1.02
2.09
12.79
7.4
7.2
7.0
6.8
6.6
6.4
6.2
6.0
5.8
5.6
5.4
5.2
5.0
4.8
4.6
4.4
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
f1 (ppm)


152.69
140.67
128.64
128.42
125.92
83.03
38.67
24.88
Ph
B
O
O
Z-1
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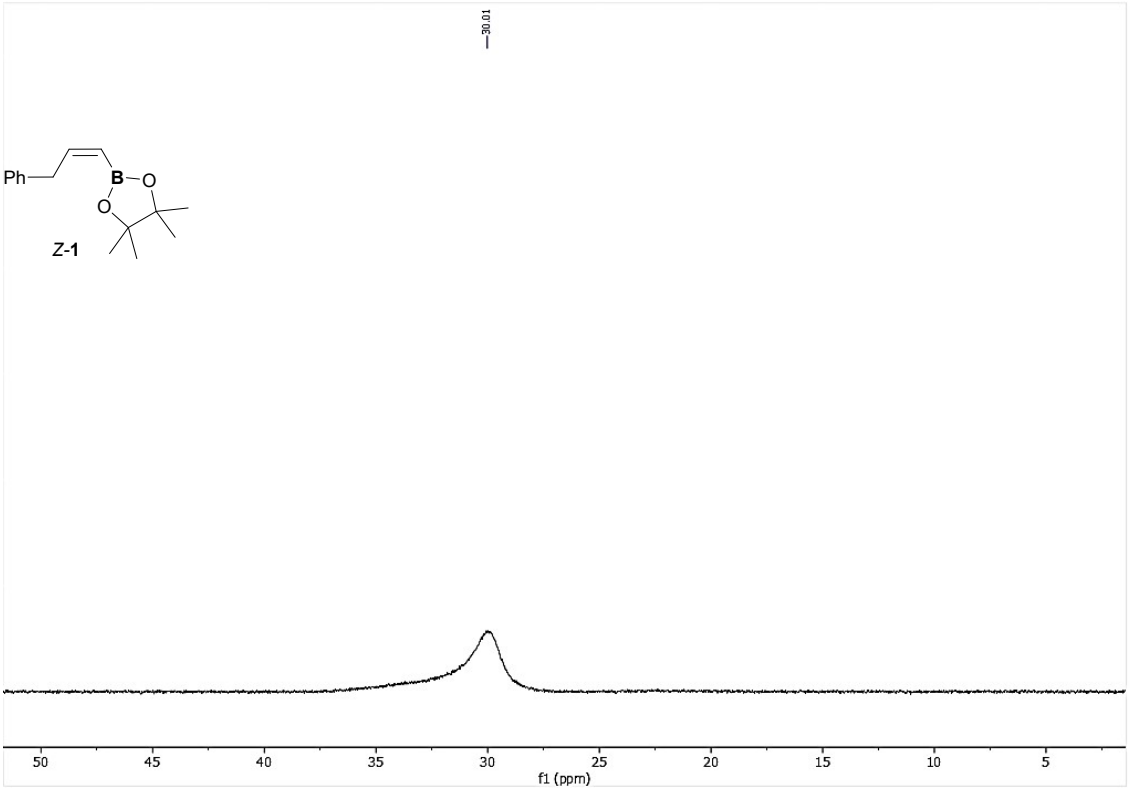
f1 (ppm)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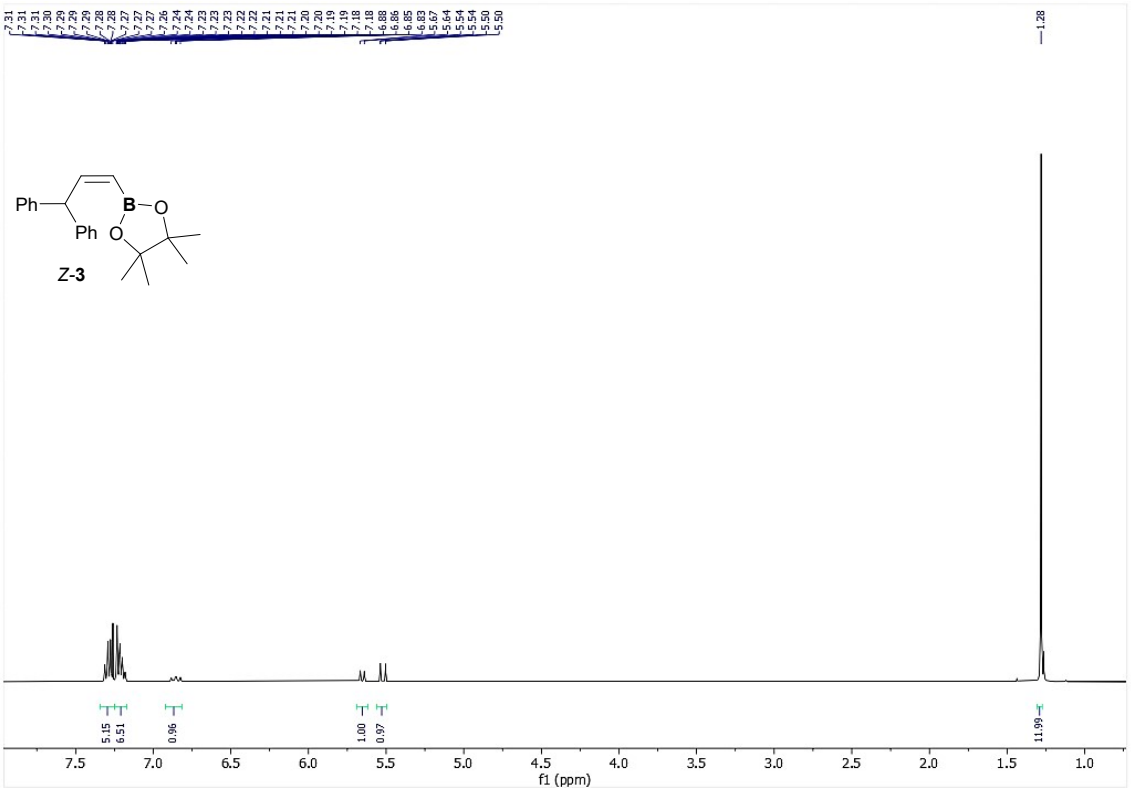
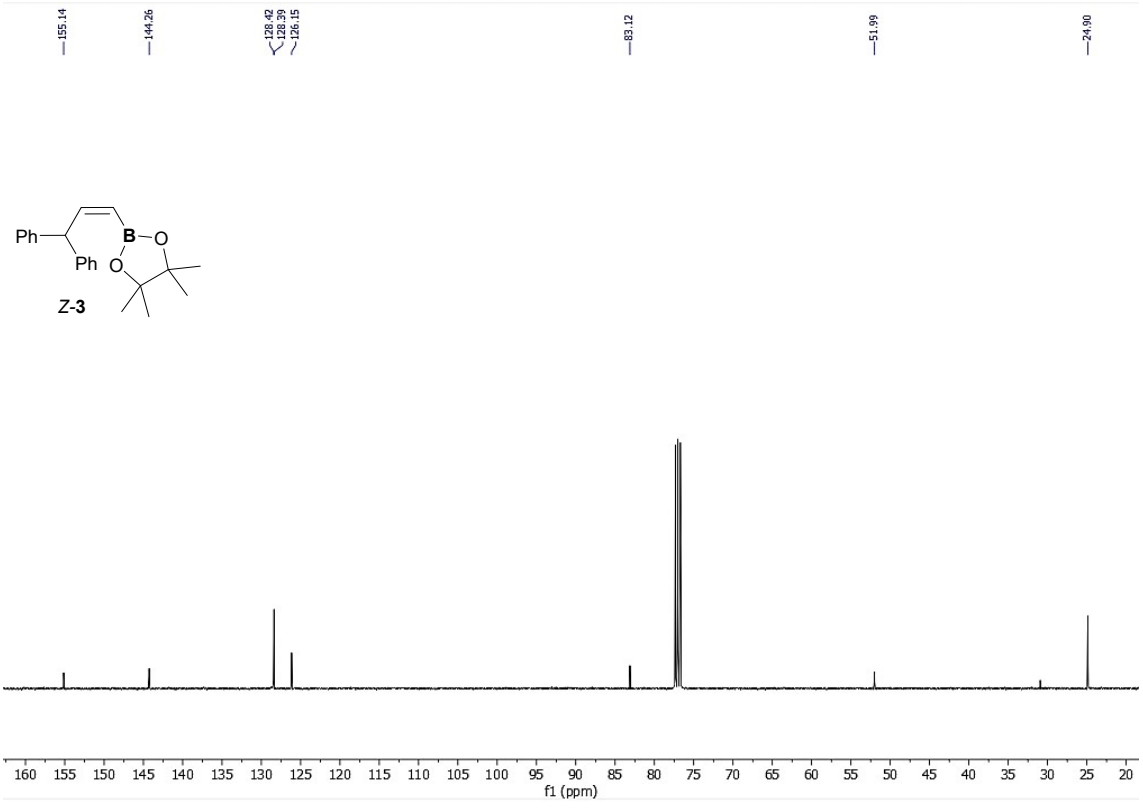
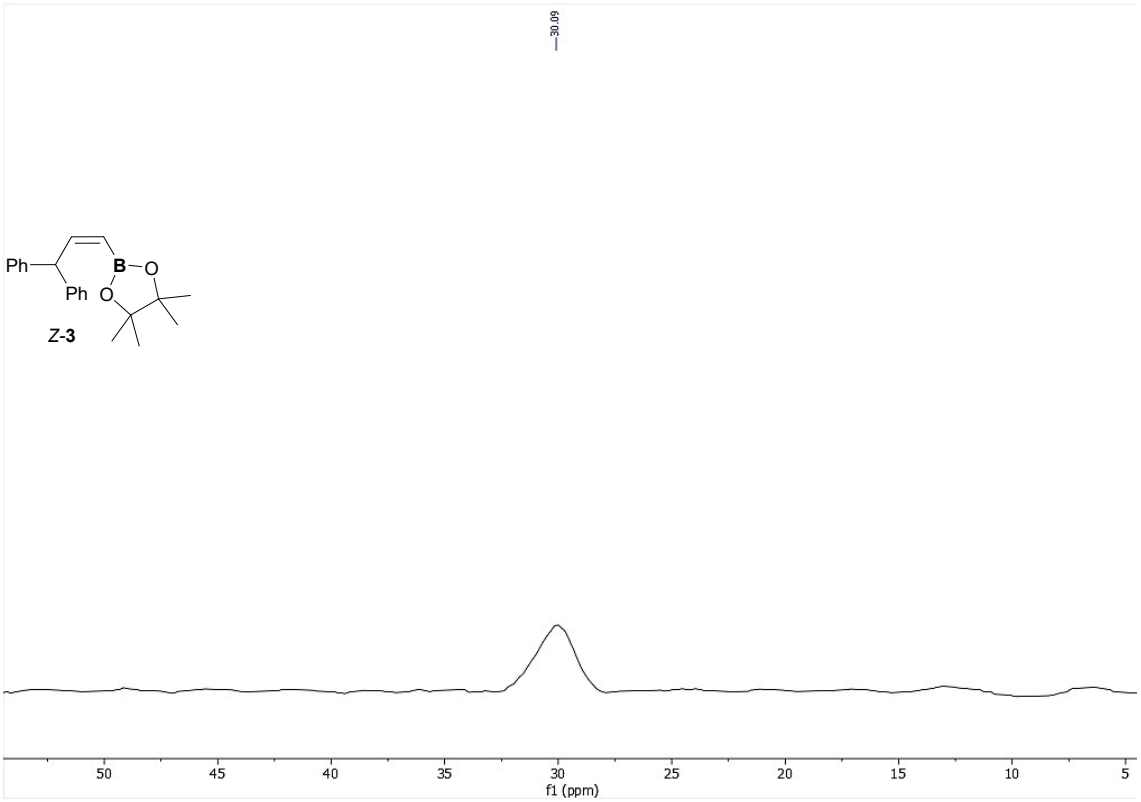
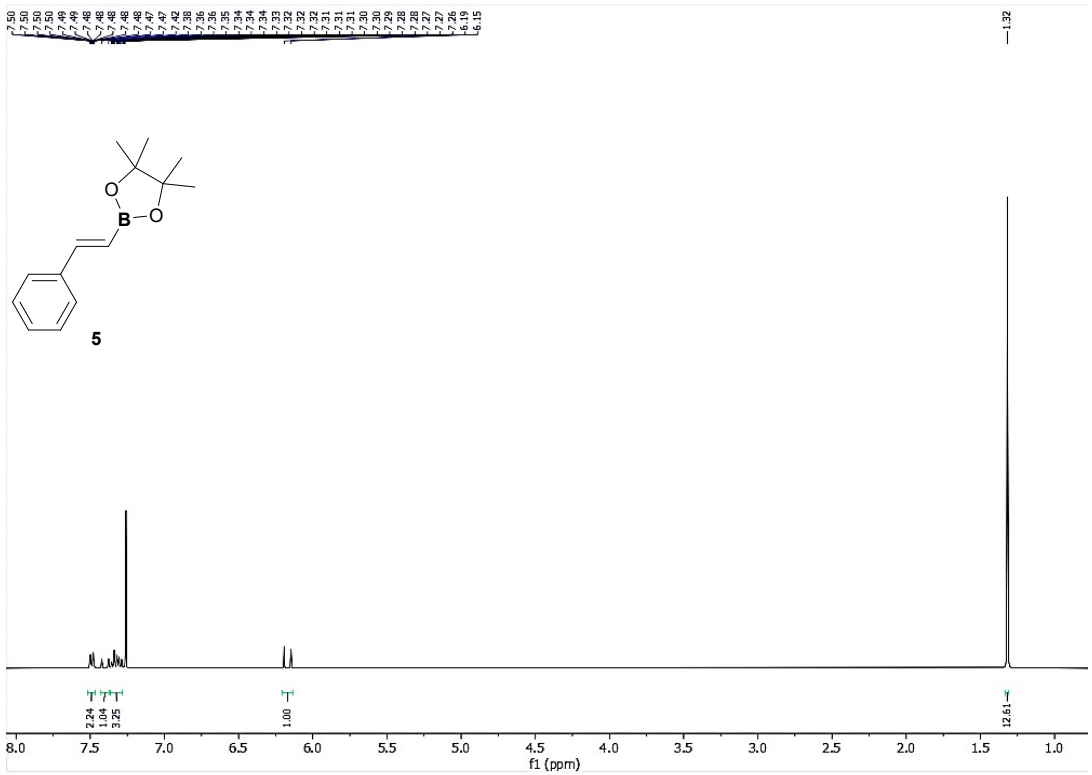
B
O
O
Z-1
50 45 40 35 30 25 20 15 10 5
f1 (ppm)


Ph
B
O
Ph
O
Z-3
1.28
5.15
6.51
0.96
1.00
0.97
11.99
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)

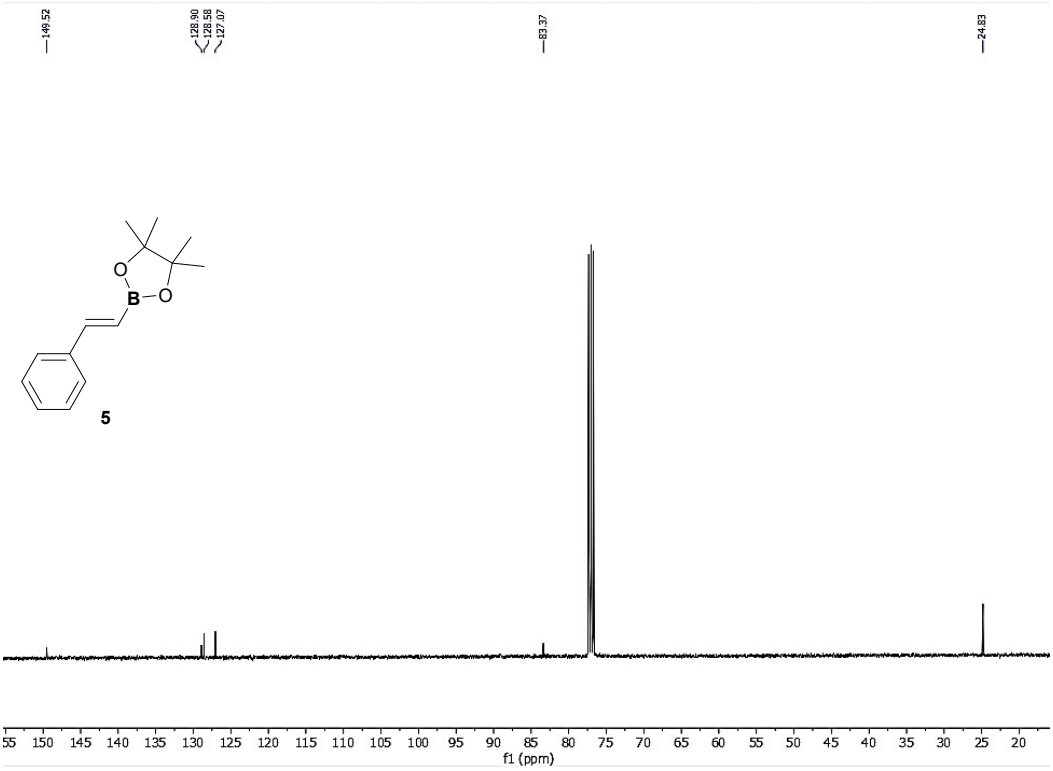

155.14
144.26
128.42
128.39
126.15
83.12
51.99
24.90
Ph
B
O
Ph
O
Z-3
160
155
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
f1 (ppm)

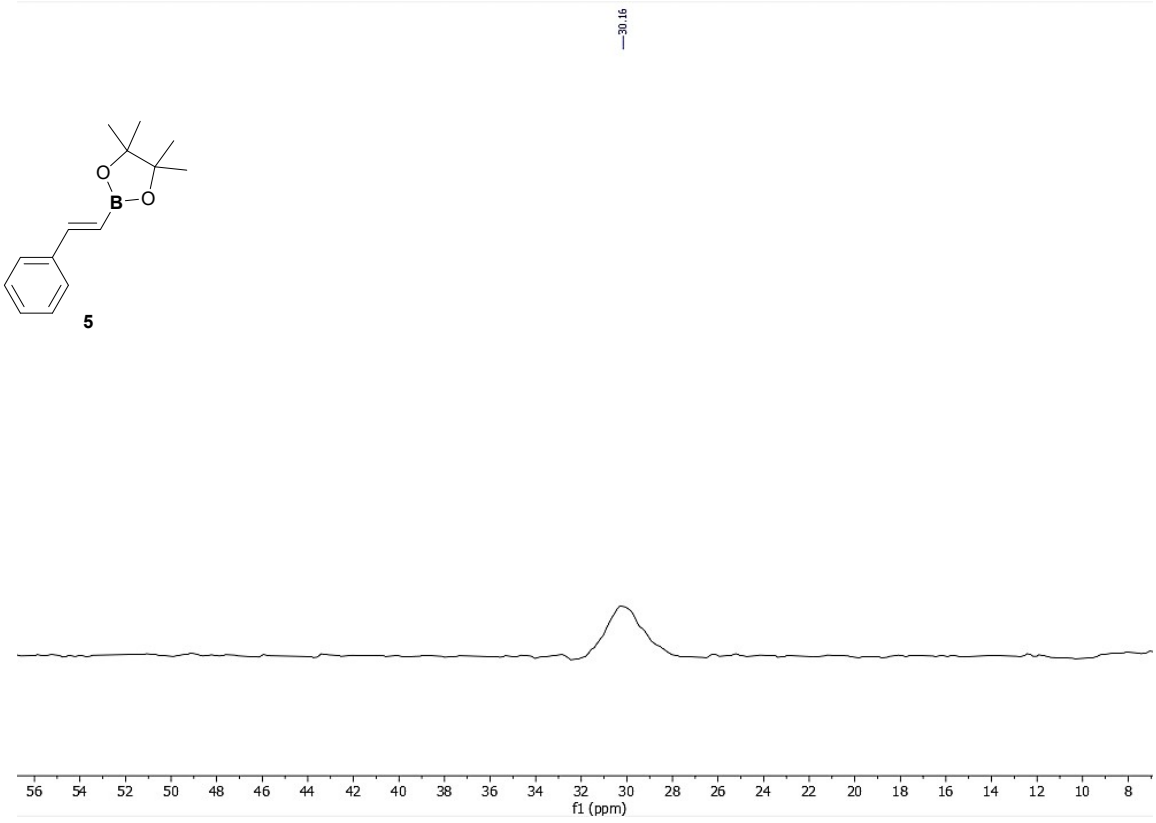

30.09
Ph
Ph
B
O
O
50
45
40
35
30
25
20
15
10
5
f1 (ppm)

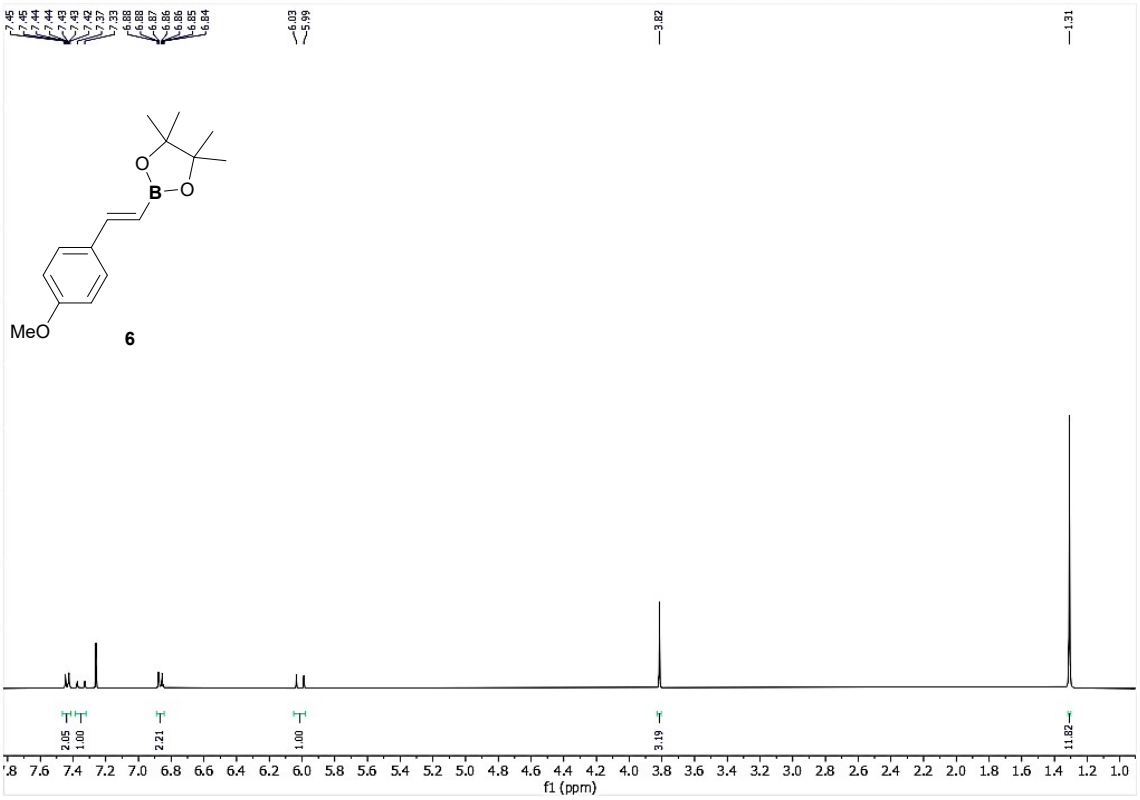
Z-**3**

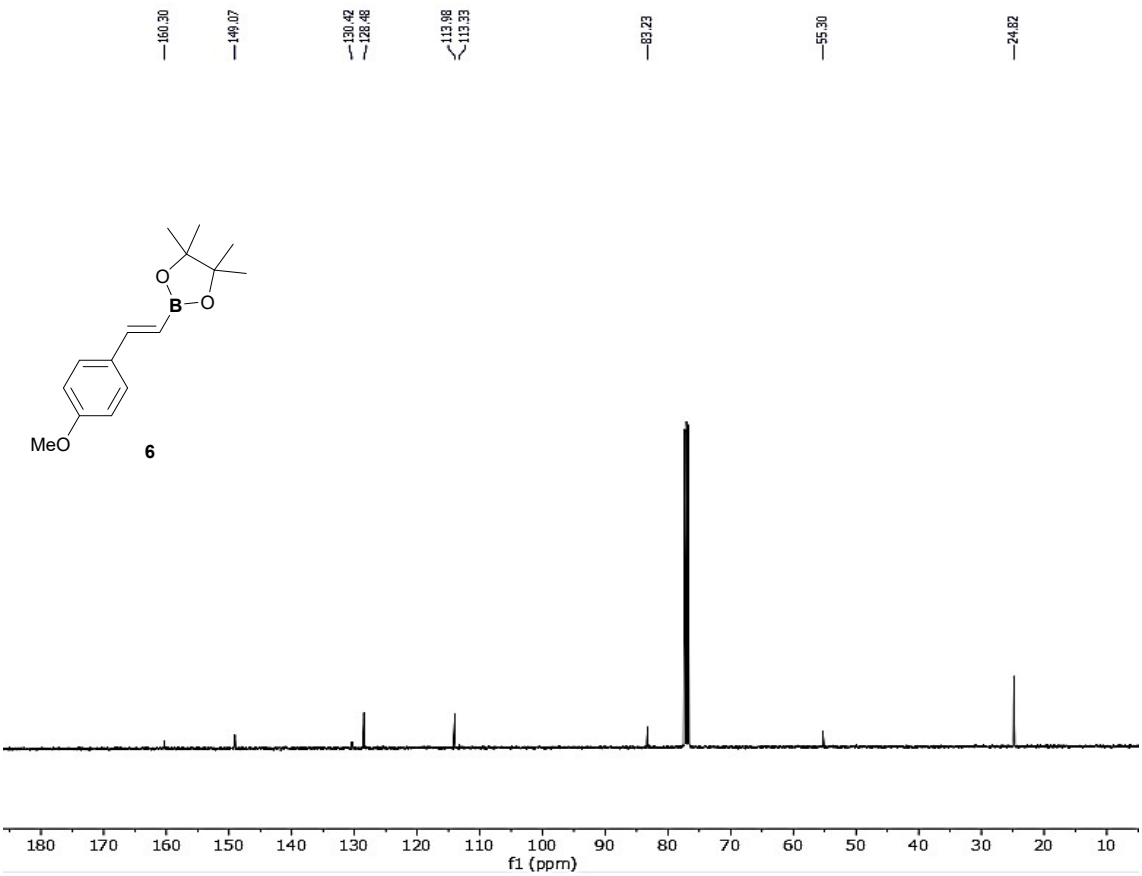

1.32
O
B
O
2.24
1.04
3.25
1.00
12.61
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)

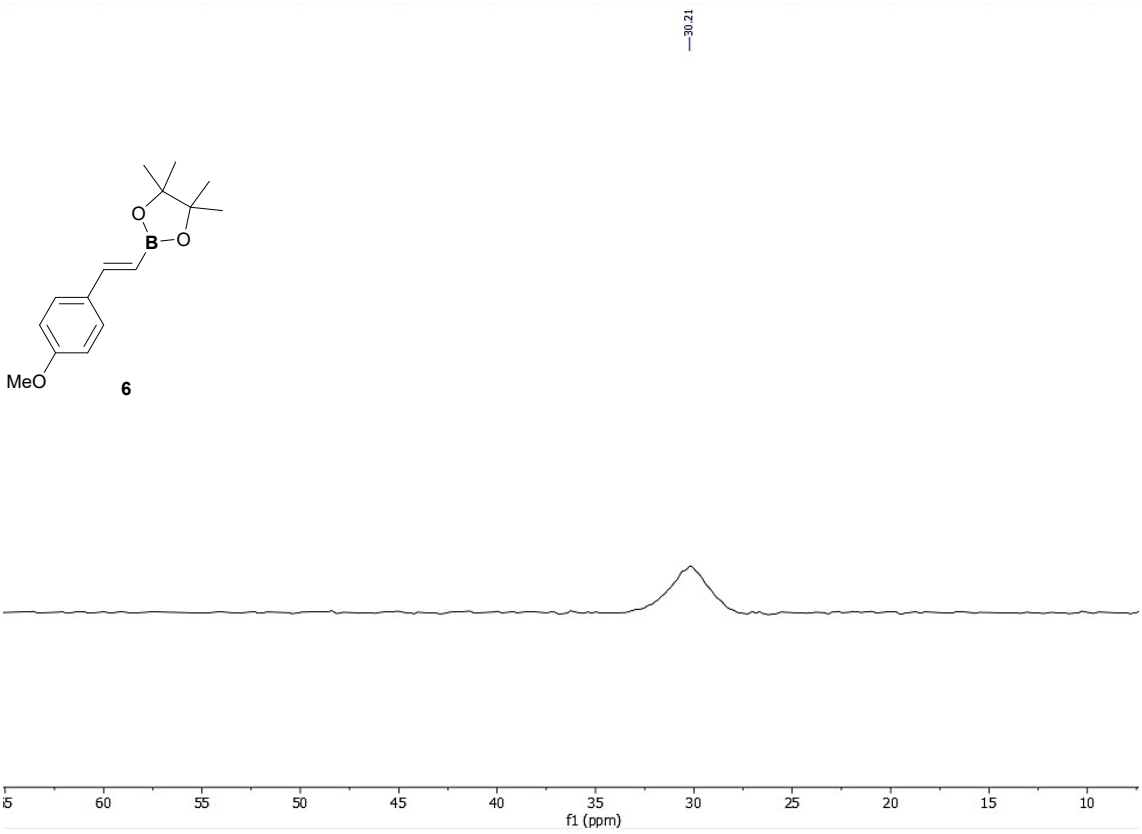
5

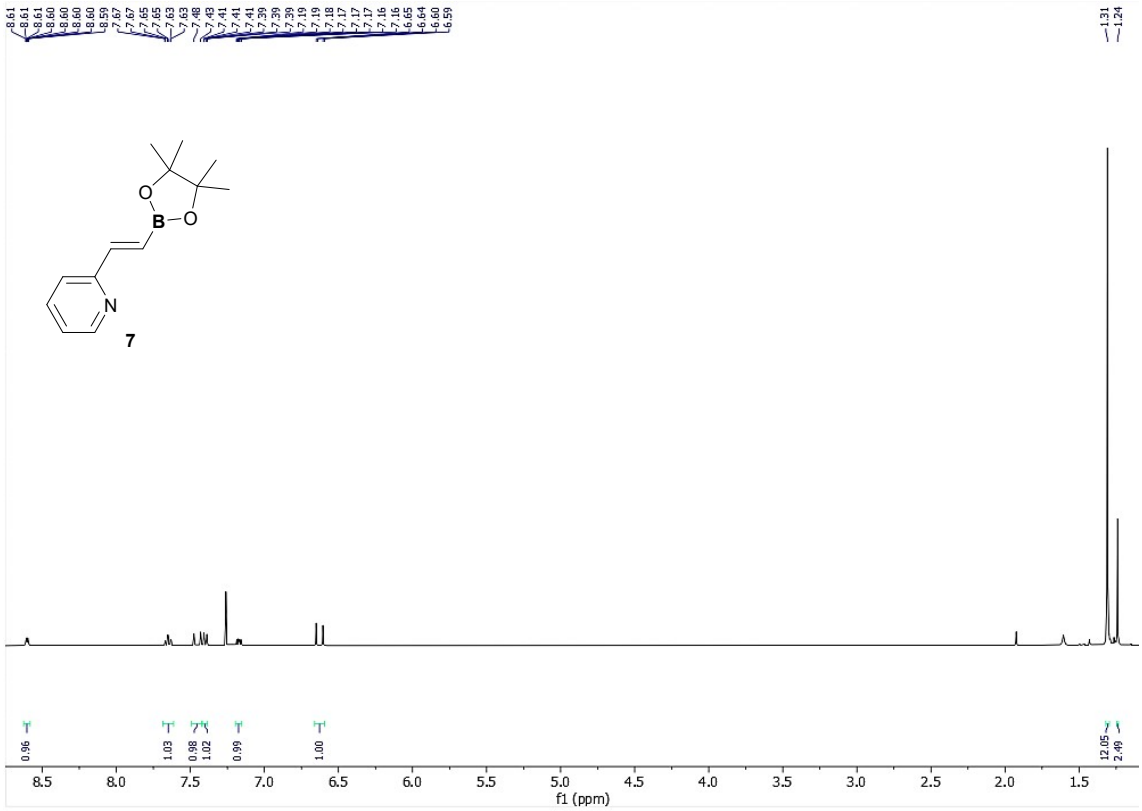

149.52
128.90
128.58
127.07
83.37
24.83
O
B
O
5
55 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20
f1 (ppm)

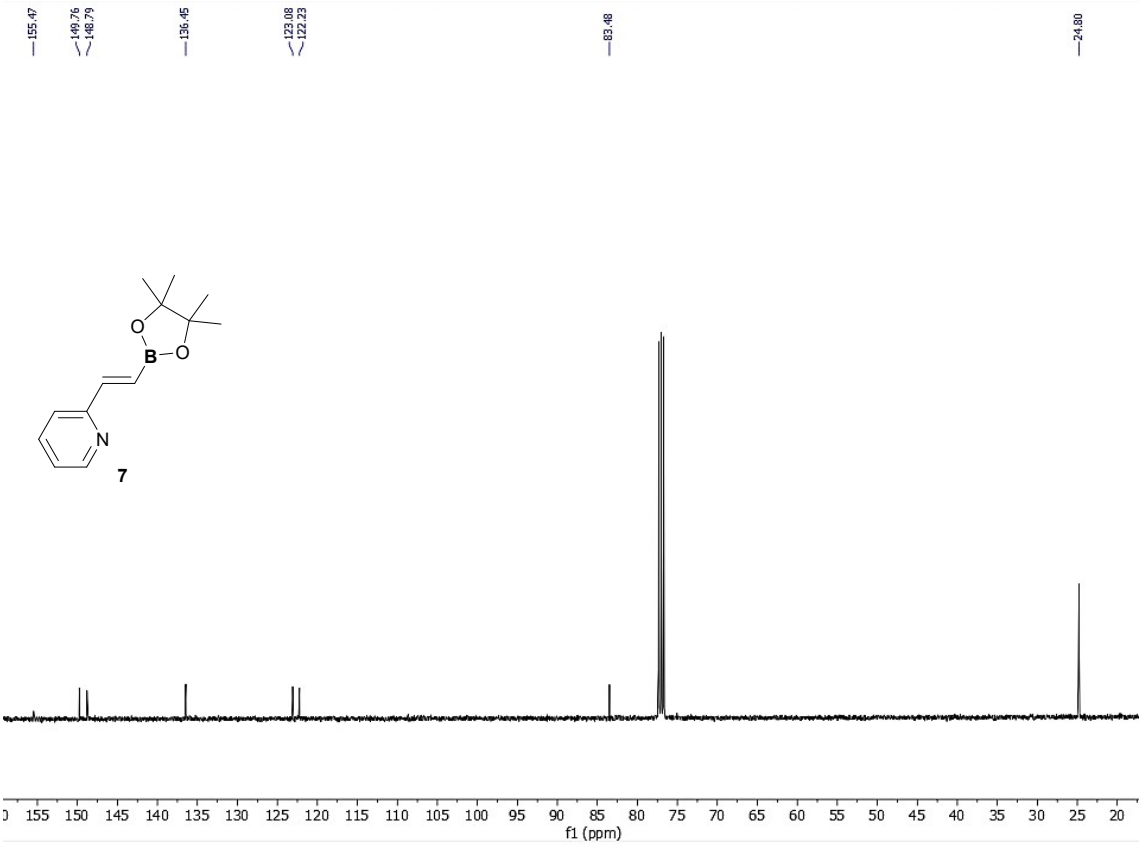

30.16
O
B
O
5
56 54 52 50 48 46 44 42 40 38 36 34 32 30 28 26 24 22 20 18 16 14 12 10 8
f1 (ppm)

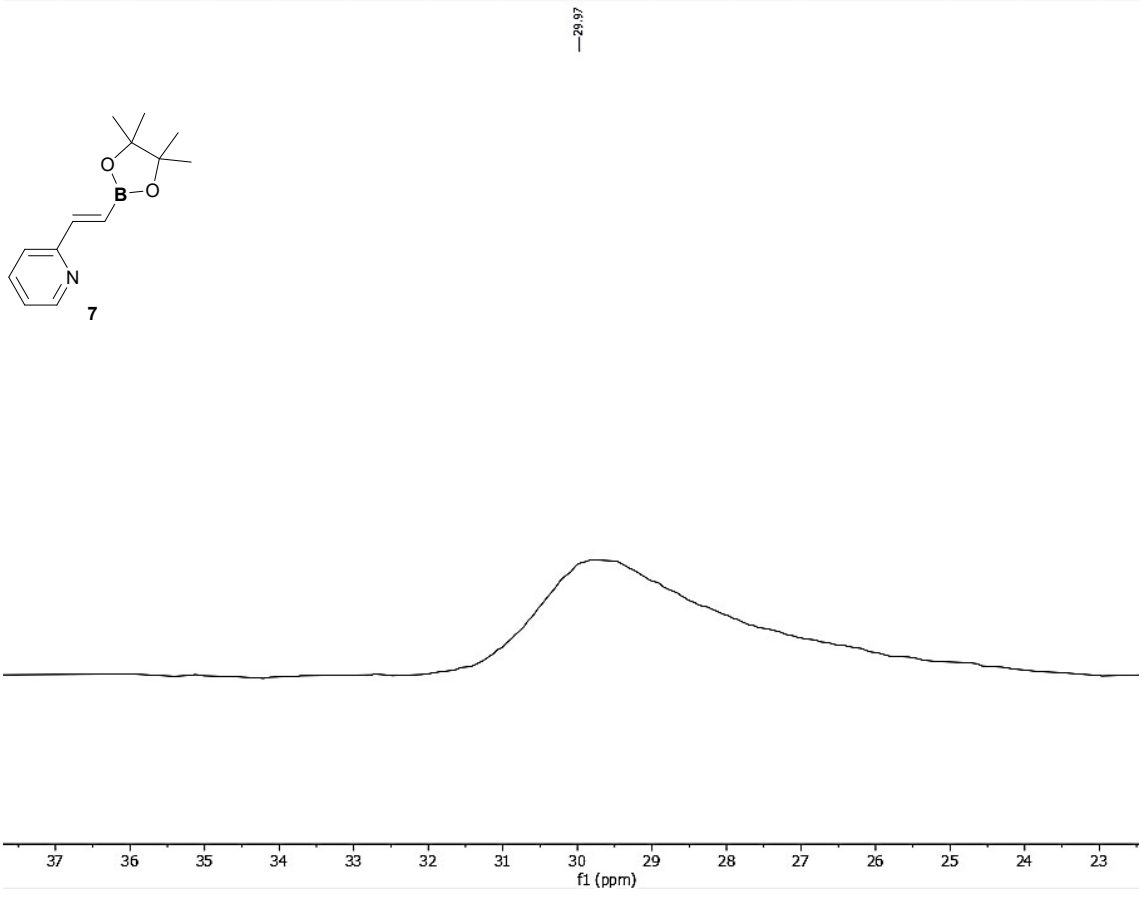

7.45
7.45
7.44
7.44
7.43
7.43
7.42
7.37
7.33
6.88
6.88
6.87
6.86
6.86
6.85
6.84
6.03
5.99
3.82
1.31
O
B
O
MeO
6
2.05
1.00
2.21
1.00
3.19
11.82
f1 (ppm)

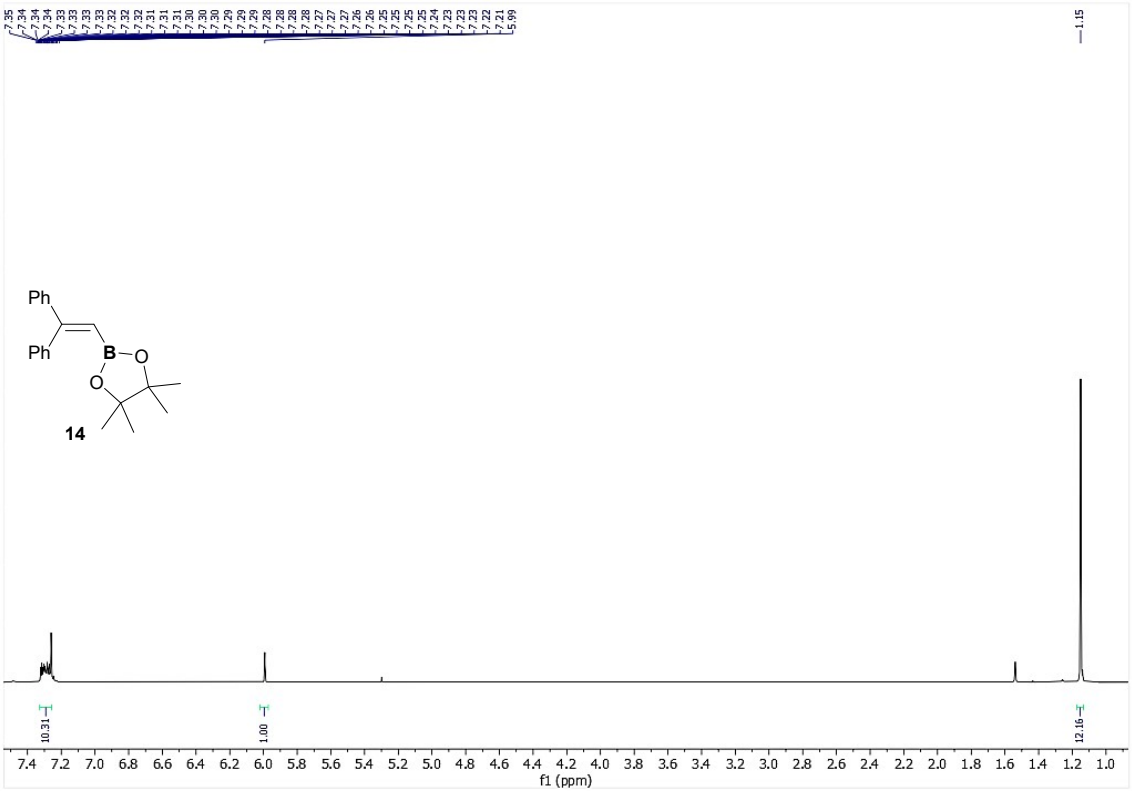

160.30
149.07
130.42
128.48
113.98
113.33
83.23
55.30
24.82
O
B
O
MeO
6
f1 (ppm)

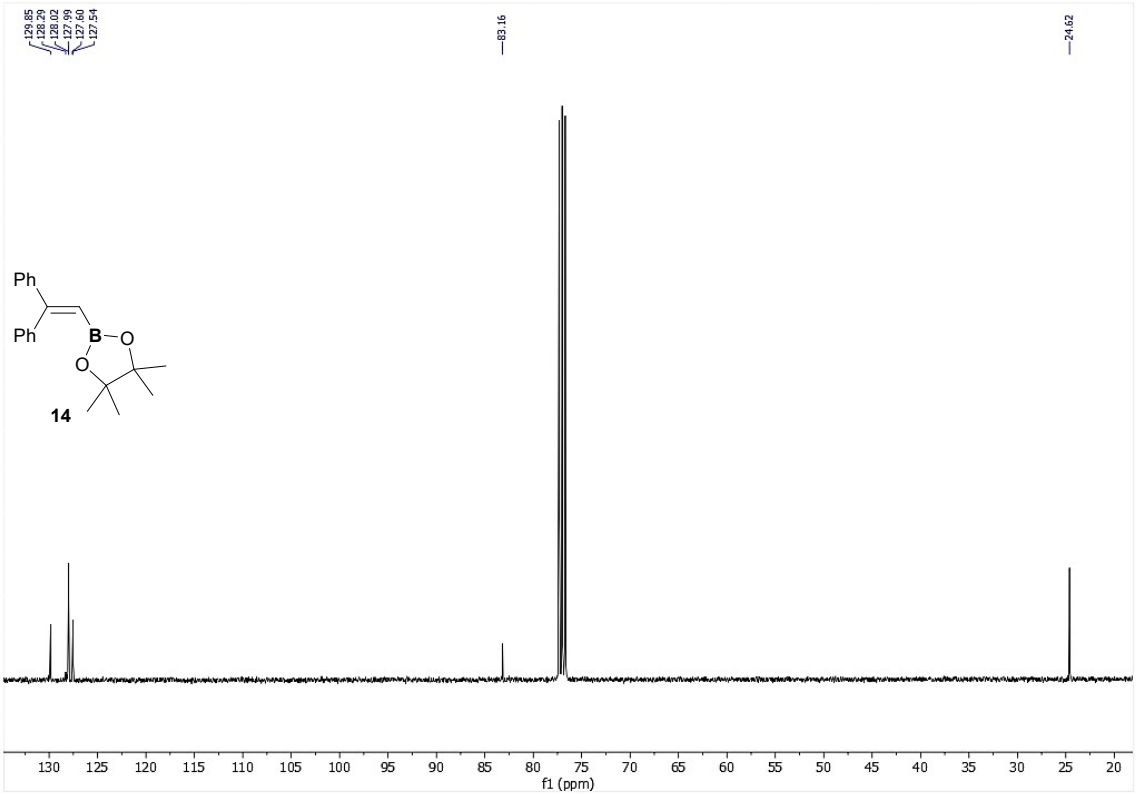

30.21
O
B
O
MeO
6
f1 (ppm)

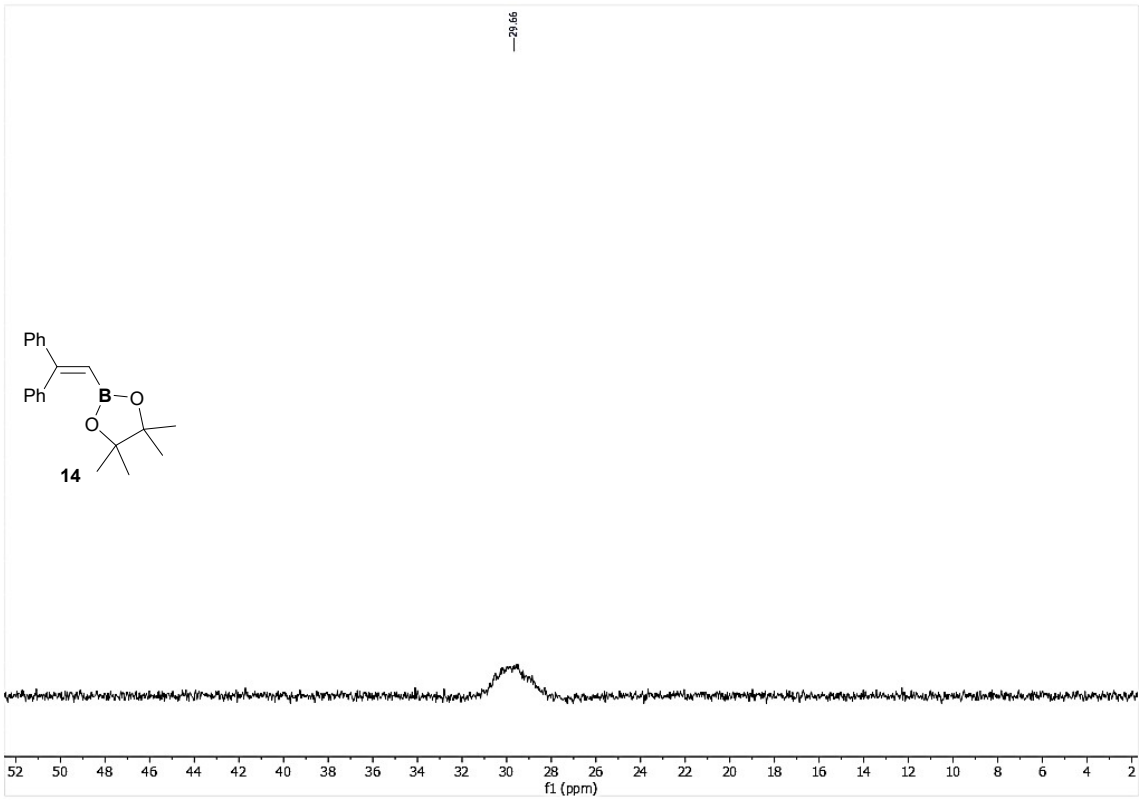

8.61
8.60
7.67
7.65
7.63
7.48
7.43
7.41
7.39
7.19
7.18
7.17
7.16
6.65
6.64
6.60
6.59
1.31
1.24
O
B
O
N
7
0.96
1.03
0.98
1.02
0.99
1.00
12.05
2.49
f1 (ppm)

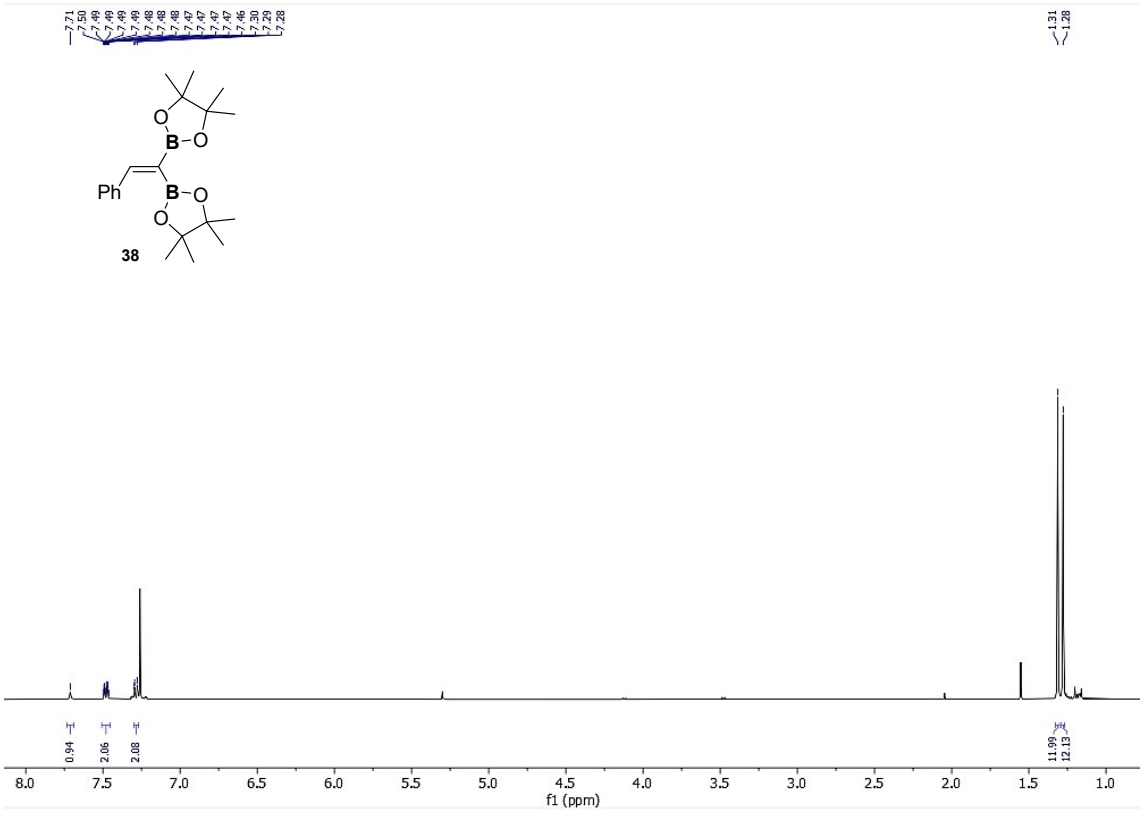

155.47
149.76
148.79
136.45
123.08
122.23
83.48
24.80
O
B
O
N
7
155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20
f1 (ppm)

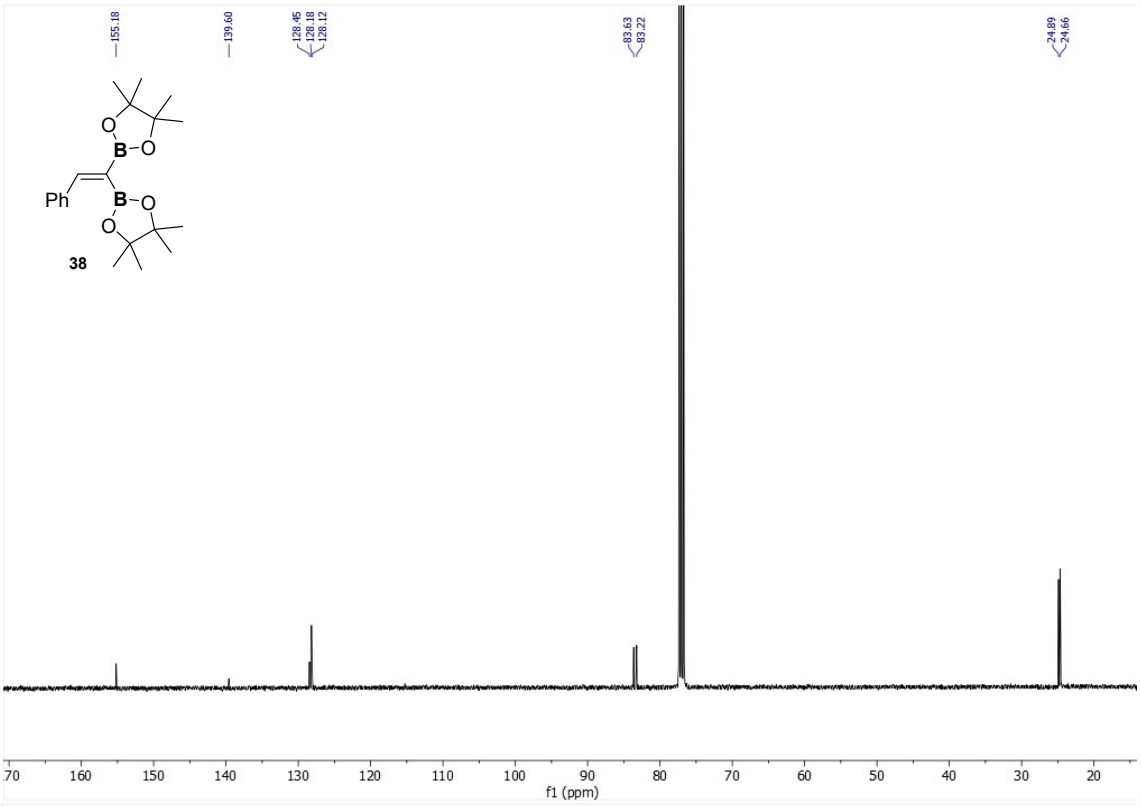

29.97
O
B
O
N
7
37 36 35 34 33 32 31 30 29 28 27 26 25 24 23
f1 (ppm)

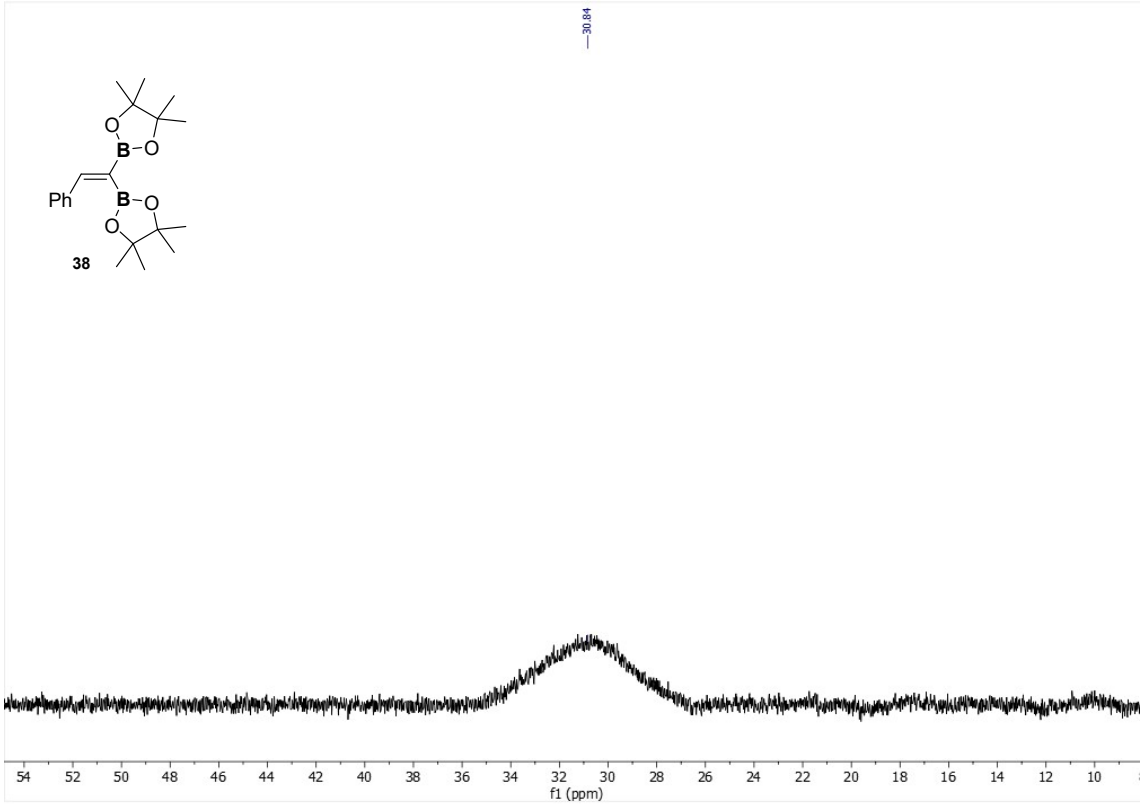

Ph
Ph
B
O
O
14
1.15
10.31
1.00
12.16
f1 (ppm)

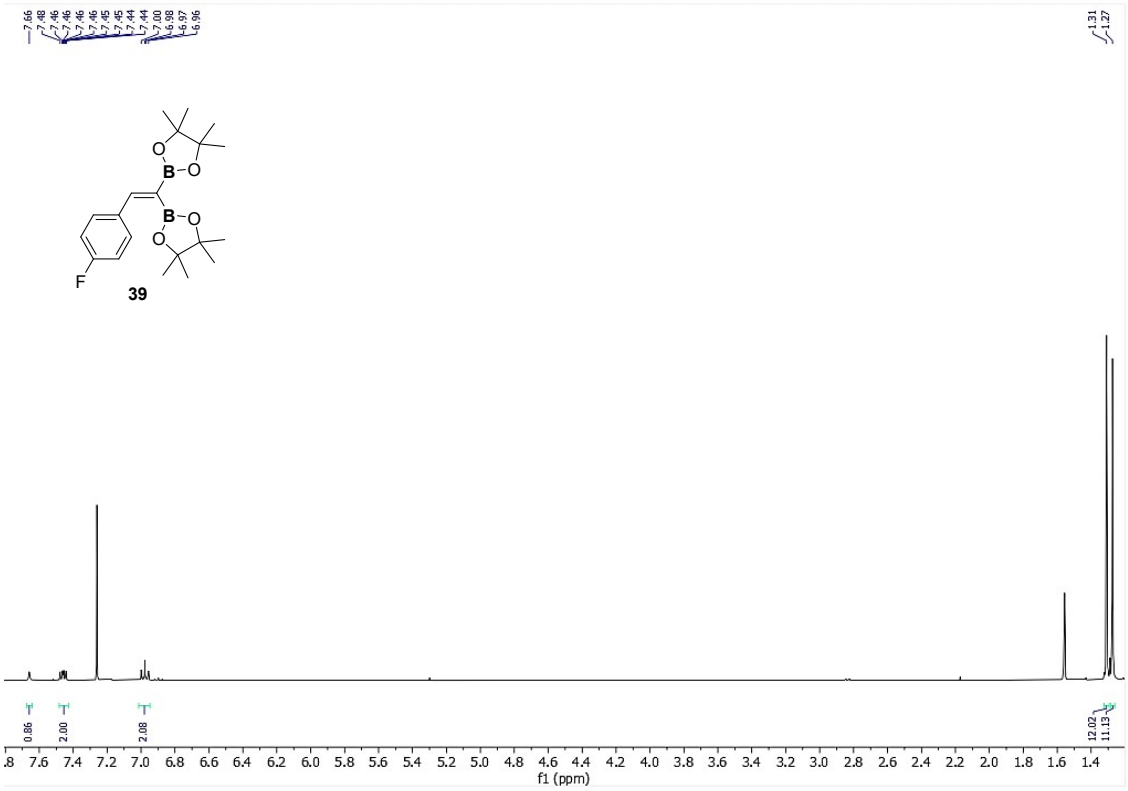

129.85
128.29
128.02
127.99
127.60
127.54
83.16
24.62
Ph
Ph
B
O
O
14
f1 (ppm)

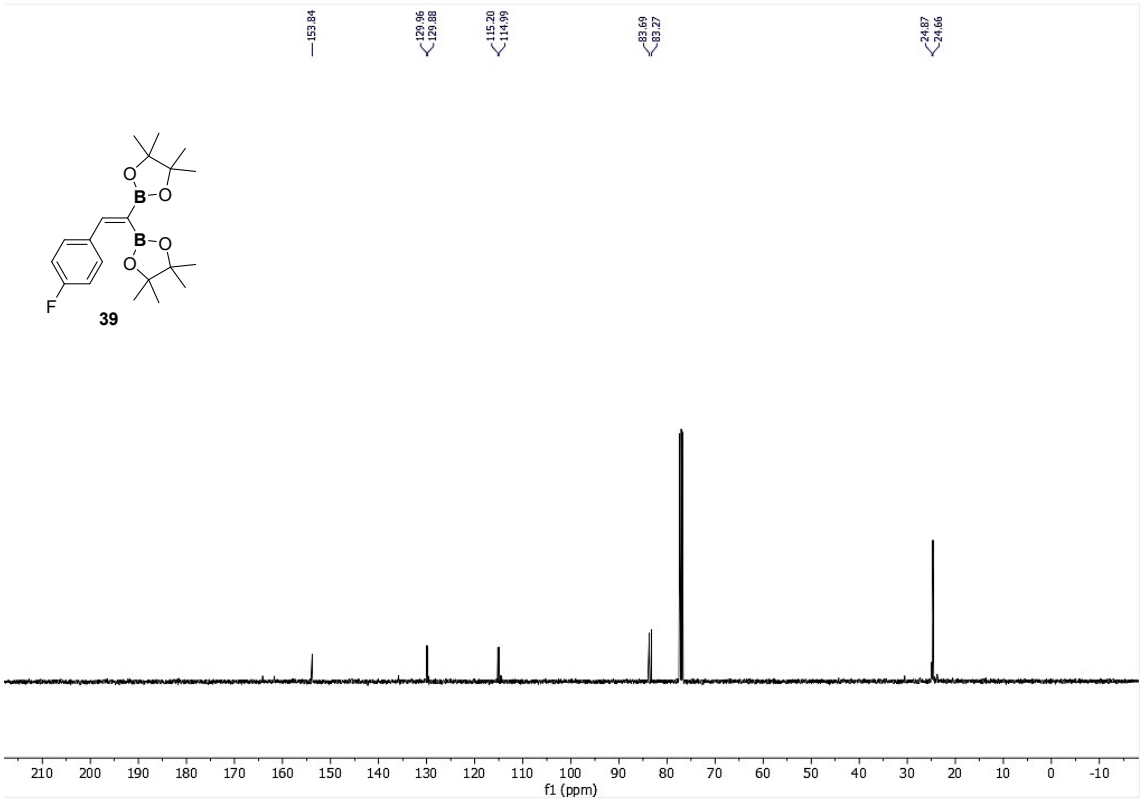

29.66
Ph
Ph
B
O
O
14
52 50 48 46 44 42 40 38 36 34 32 30 28 26 24 22 20 18 16 14 12 10 8 6 4 2
f1 (ppm)

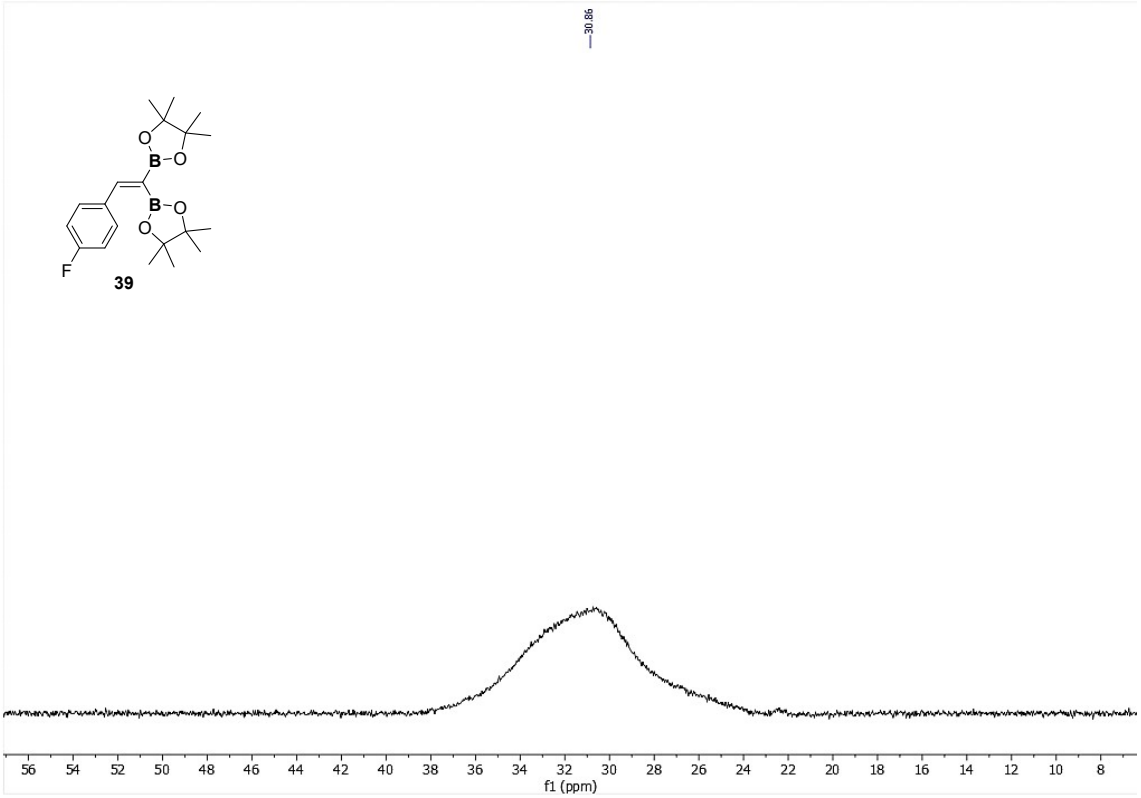

7.71
7.50
7.49
7.49
7.49
7.49
7.48
7.48
7.48
7.48
7.47
7.47
7.47
7.47
7.46
7.30
7.29
7.28
1.31
1.28
O
B
O
Ph
B
O
O
38
0.94
2.06
2.08
11.99
12.13
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
f1 (ppm)


155.18
139.60
128.45
128.18
128.12
83.63
83.22
24.89
24.66
Ph
B
O
38
f1 (ppm)

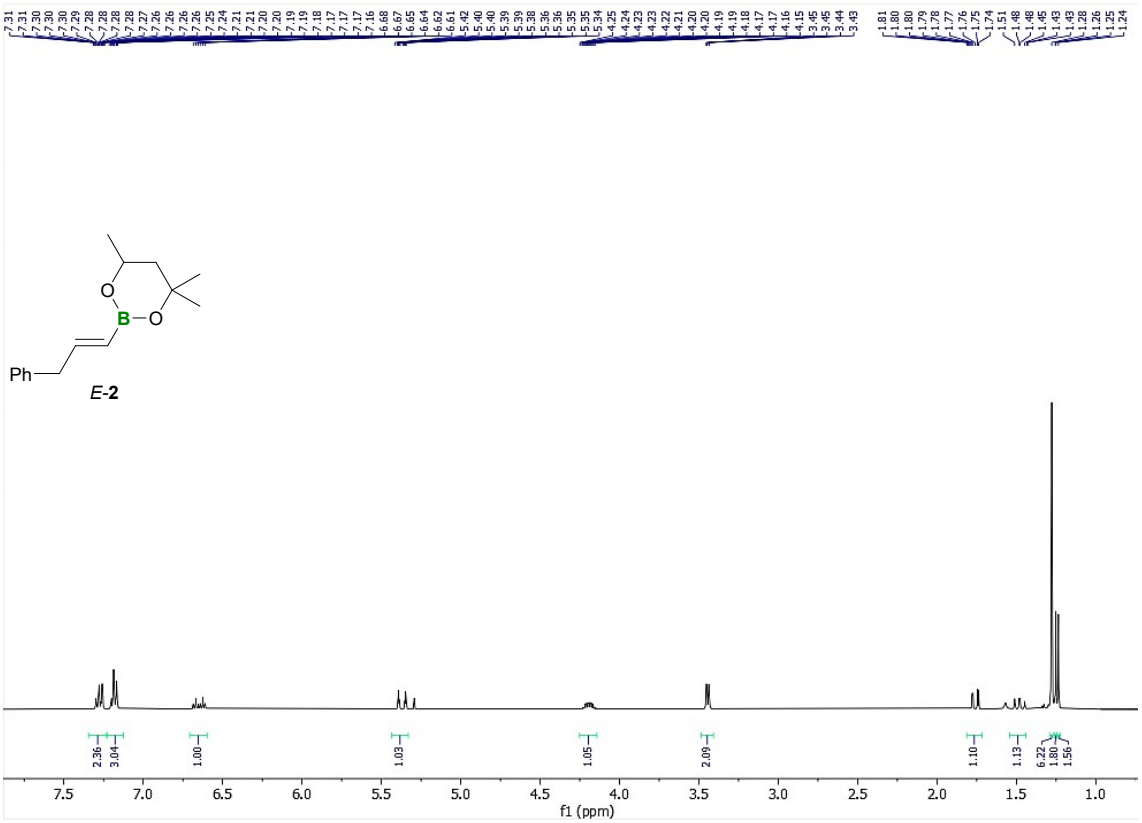

30.84
Ph
B
O
38
f1 (ppm)

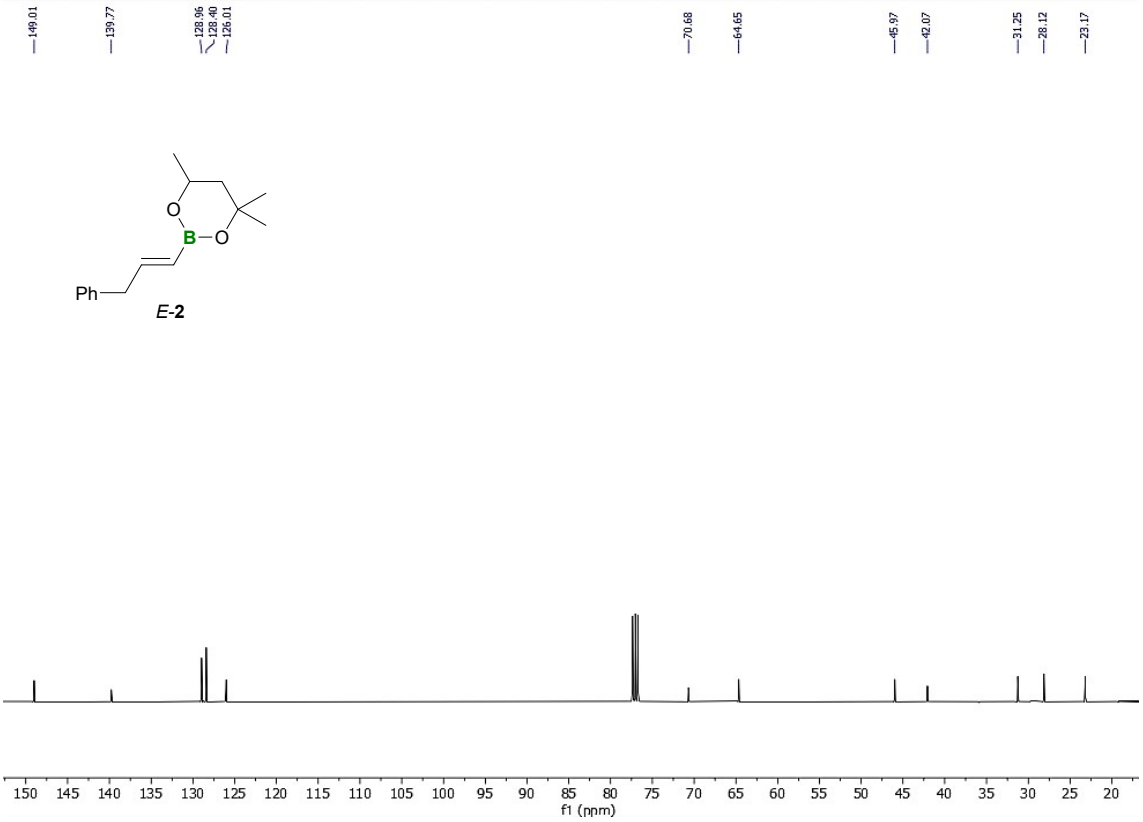

7.66
7.48
7.46
7.46
7.46
7.46
7.45
7.45
7.44
7.44
7.00
6.98
6.97
6.96
1.31
1.27
O
B–O
B–O
O
F
39
0.86
2.00
2.08
12.02
11.13
f1 (ppm)

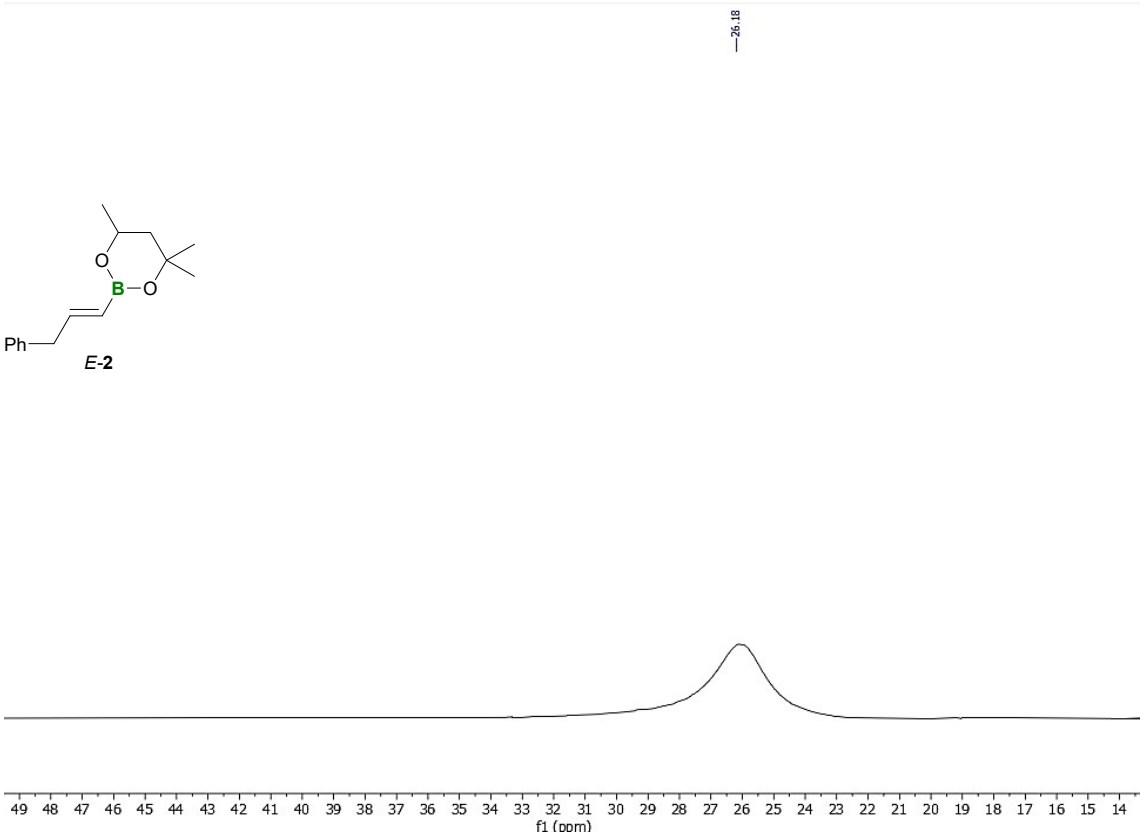

153.84
129.96
129.88
115.20
114.99
83.69
83.27
24.87
24.66
O
B–O
B–O
O
F
39
f1 (ppm)



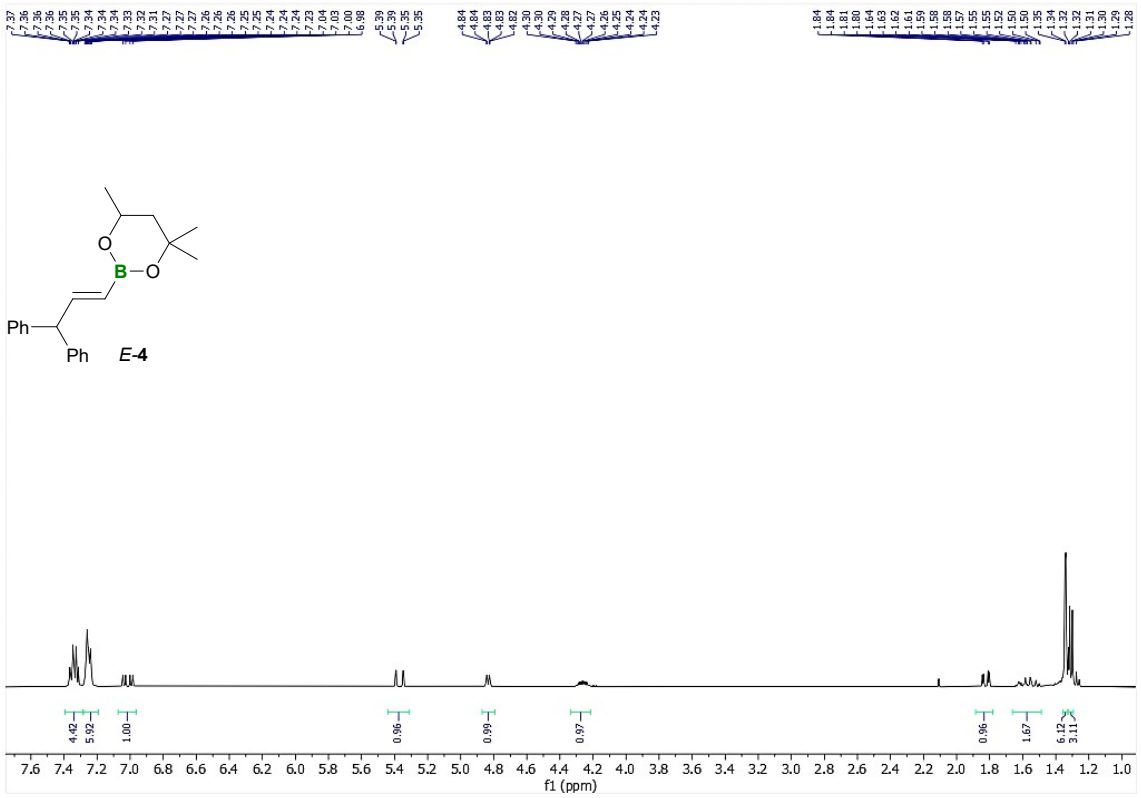
^{1}H, ^{13}C, ^{11}B Spectra for transborylated alkenylboranes


O
B
O
Ph
E-2
2.36
3.04
1.00
1.03
1.05
2.09
1.10
1.13
6.22
1.80
1.56
f1 (ppm)

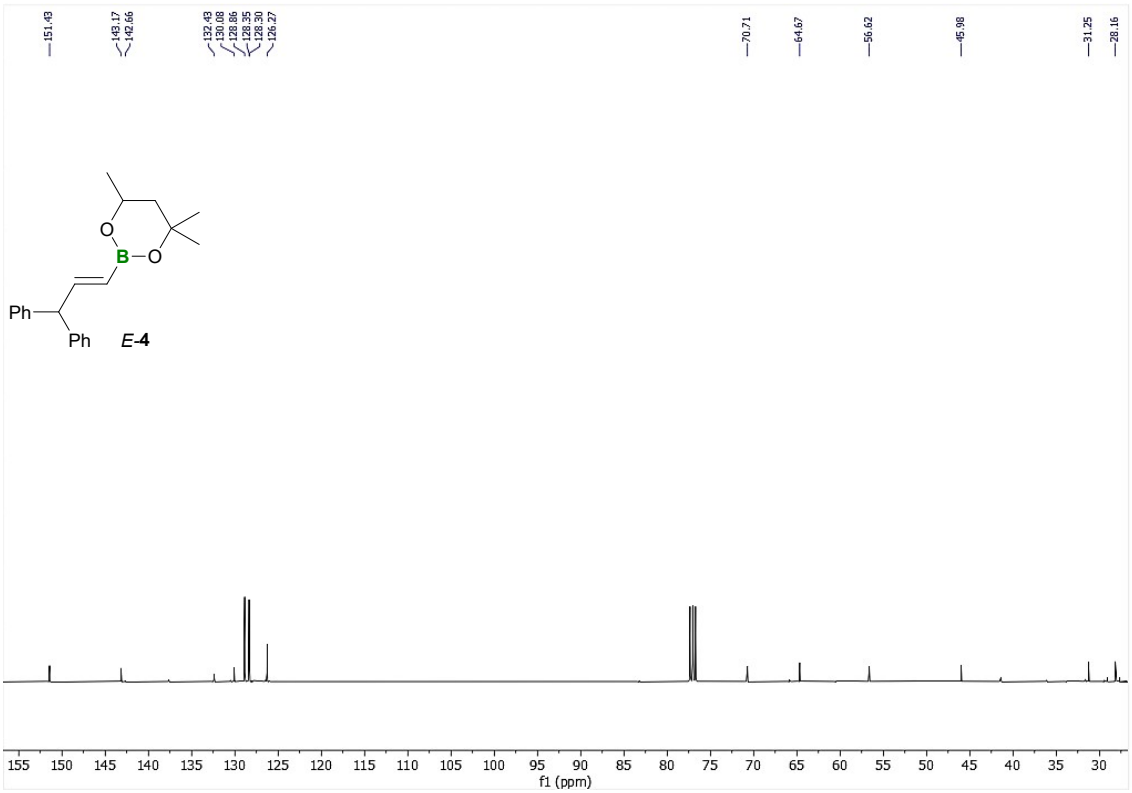

149.01
139.77
128.96
128.40
126.01
70.68
64.65
45.97
42.07
31.25
28.12
23.17
O
B
O
Ph
E-2
f1 (ppm)

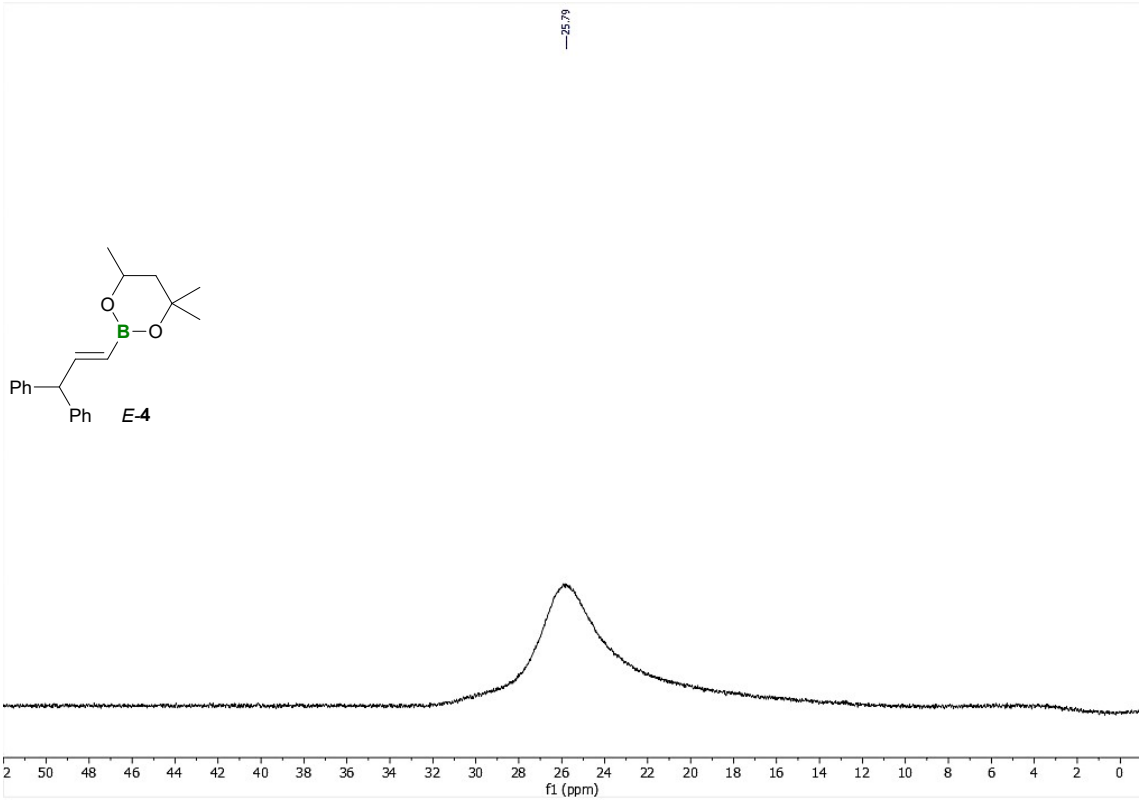

26.18
O
B
O
Ph
49 48 47 46 45 44 43 42 41 40 39 38 37 36 35 34 33 32 31 30 29 28 27 26 25 24 23 22 21 20 19 18 17 16 15 14
f1 (ppm)

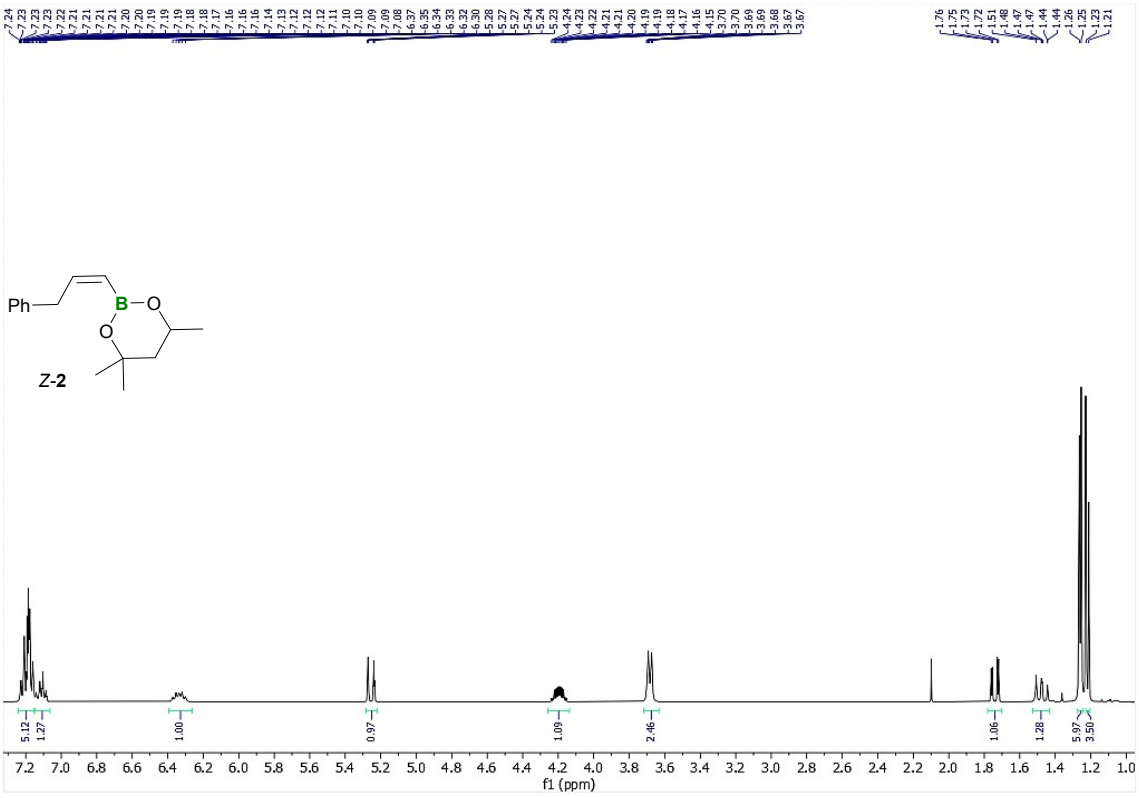
E-**2**

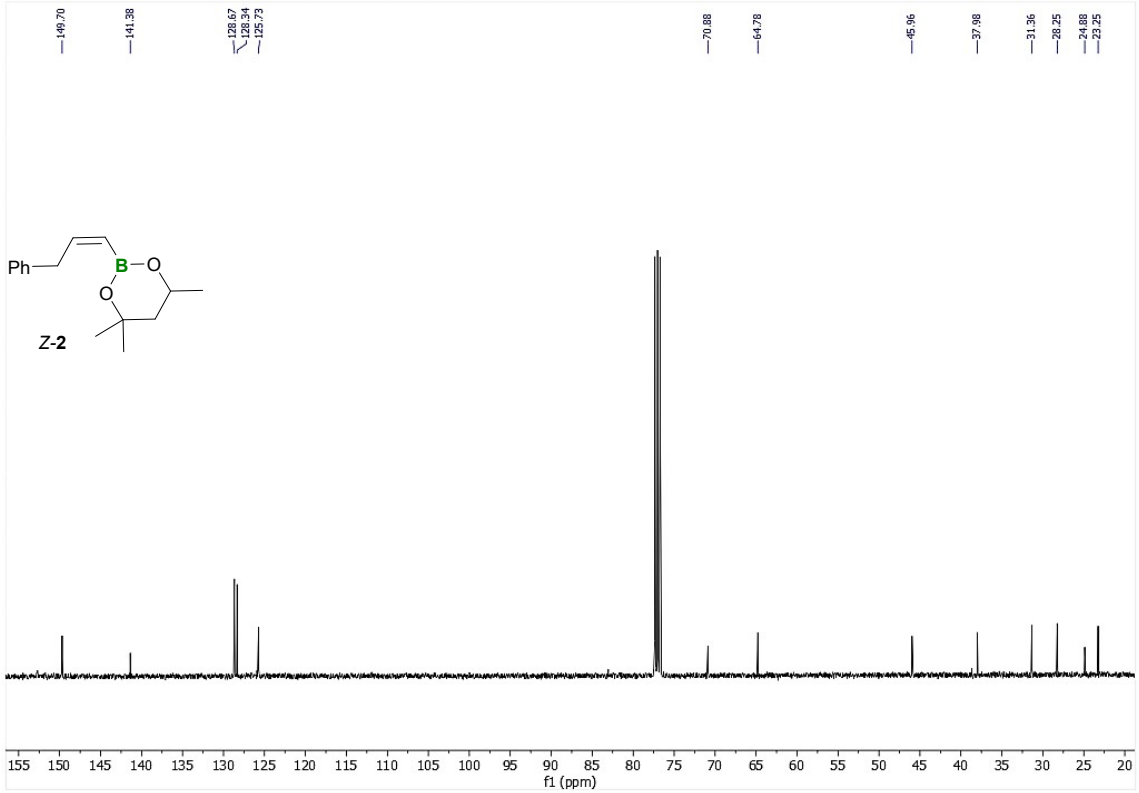

O
B
O
Ph
Ph
4.42
5.92
1.00
0.96
0.99
0.97
0.96
1.67
6.12
3.11
7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0
f1 (ppm)

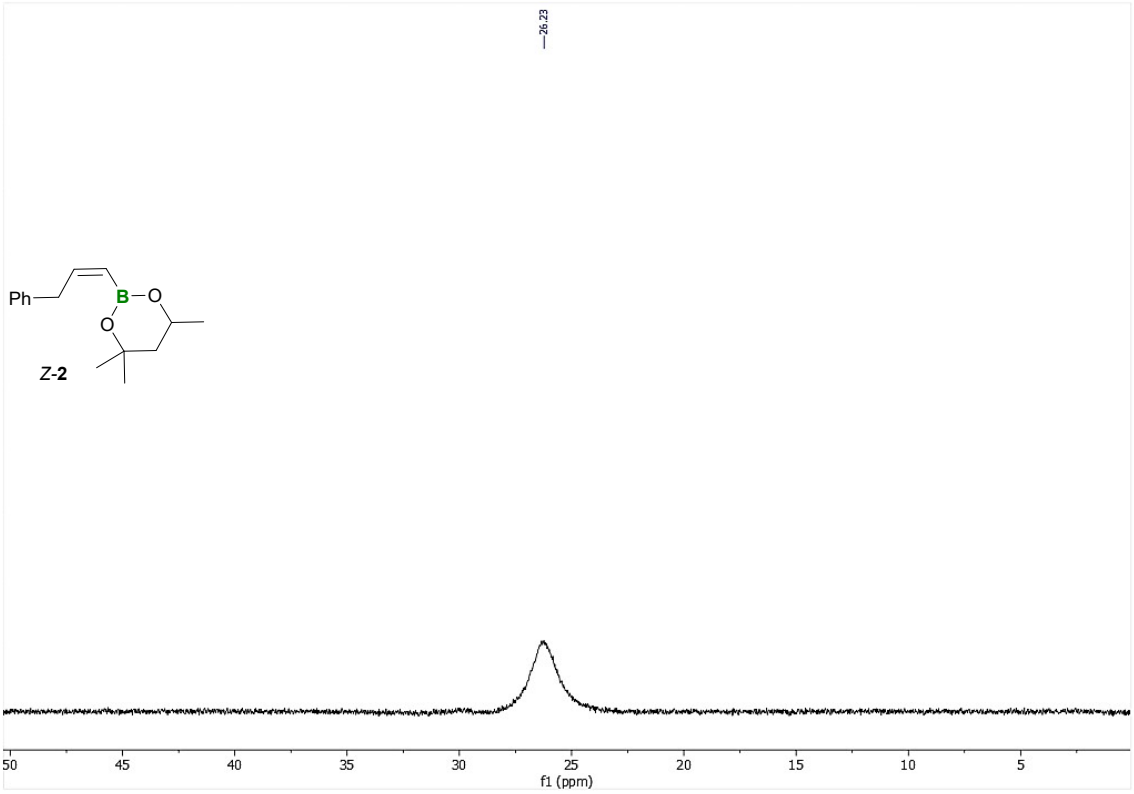
E-**4**

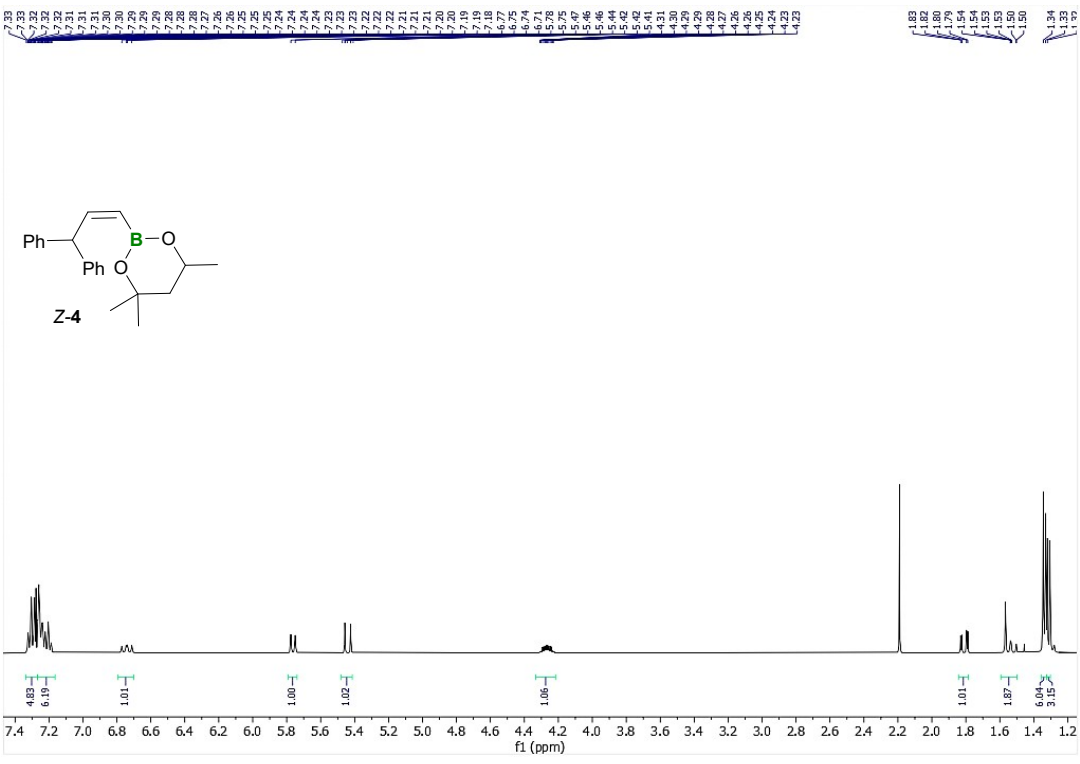

151.43
143.17
142.66
132.43
130.08
128.86
128.35
128.30
126.27
70.71
64.67
56.62
45.98
31.25
28.16
O
B
O
Ph
Ph
E-4
155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30
f1 (ppm)

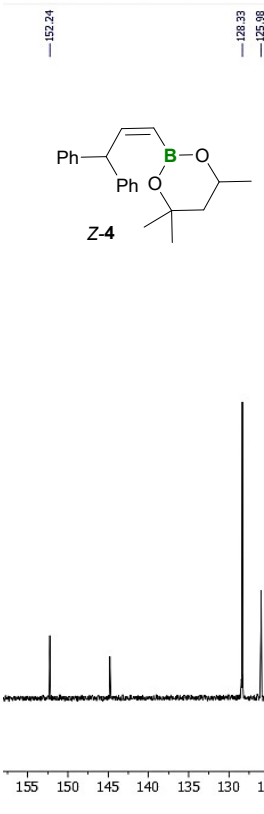

25.79
O
B
O
Ph
Ph
E-4
2 50 48 46 44 42 40 38 36 34 32 30 28 26 24 22 20 18 16 14 12 10 8 6 4 2 0
f1 (ppm)

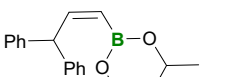

Ph
B
O
O
Z-2
5.12
1.27
1.00
0.97
1.09
2.46
1.06
1.28
5.97
3.50
f1 (ppm)

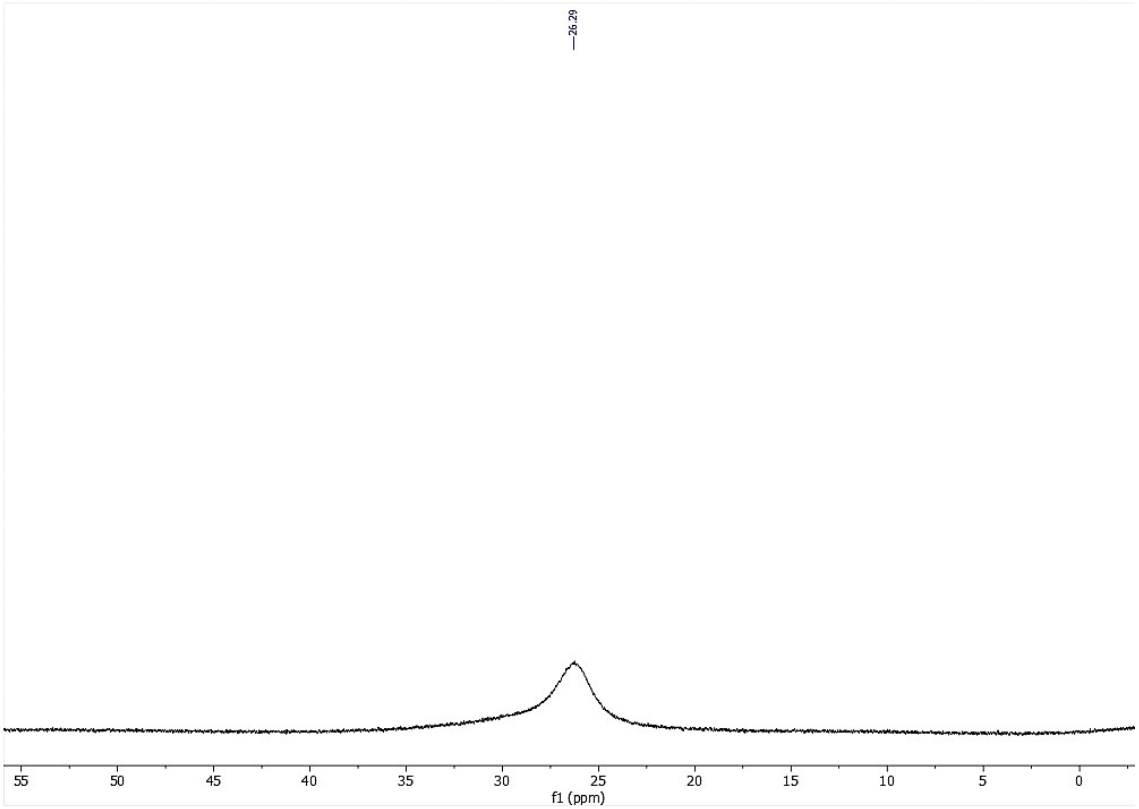

149.70
141.38
128.67
128.34
125.73
70.88
64.78
45.96
37.98
31.36
28.25
24.88
23.25
Ph
B
O
O
Z-2
f1 (ppm)

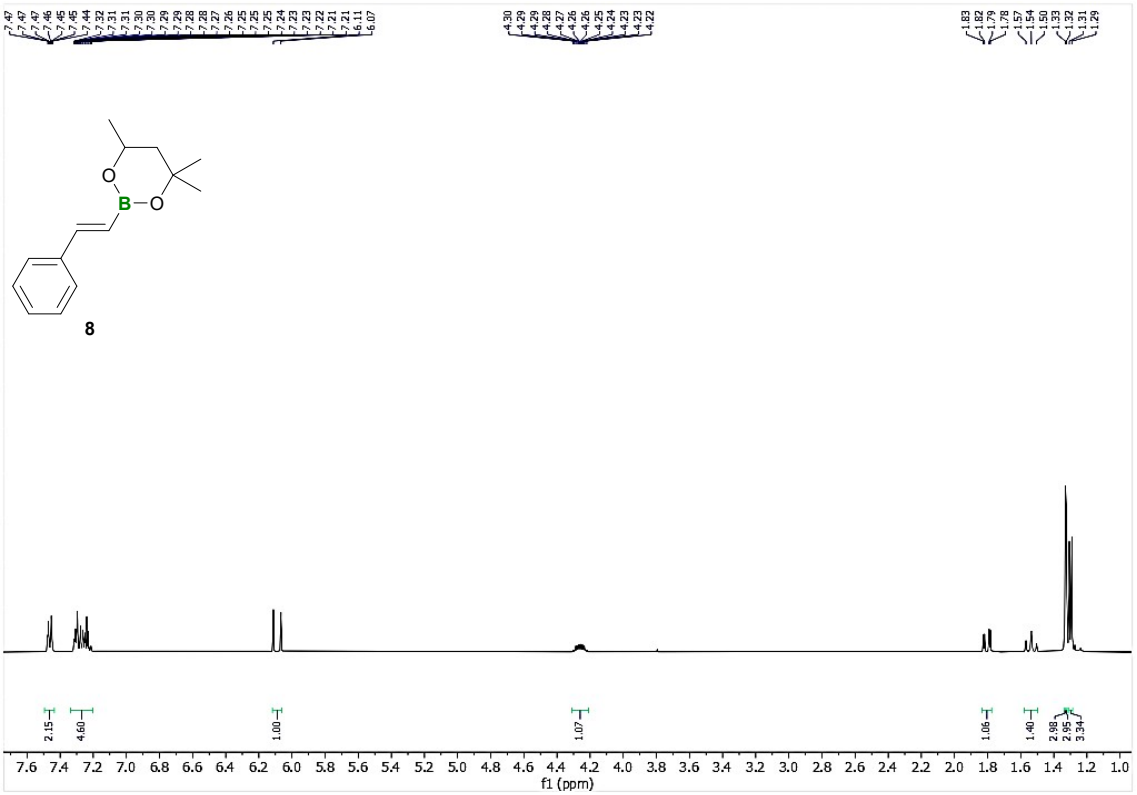

26.23
Ph
B
O
O
Z-2
50
45
40
35
30
25
20
15
10
5
f1 (ppm)

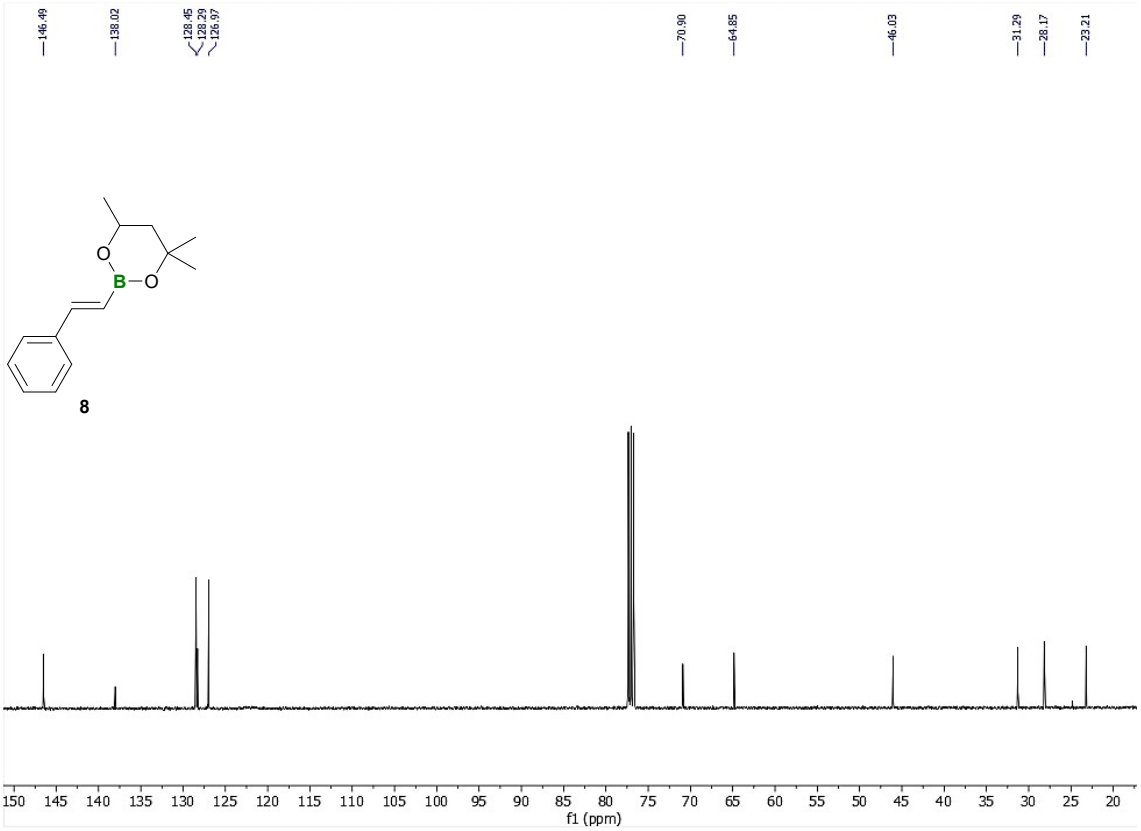

Ph
B
O
Ph
O
Z-4
4.83
6.19
1.01
1.00
1.02
1.06
1.01
1.87
6.04
3.15
7.4
7.2
7.0
6.8
6.6
6.4
6.2
6.0
5.8
5.6
5.4
5.2
5.0
4.8
4.6
4.4
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
f1 (ppm)

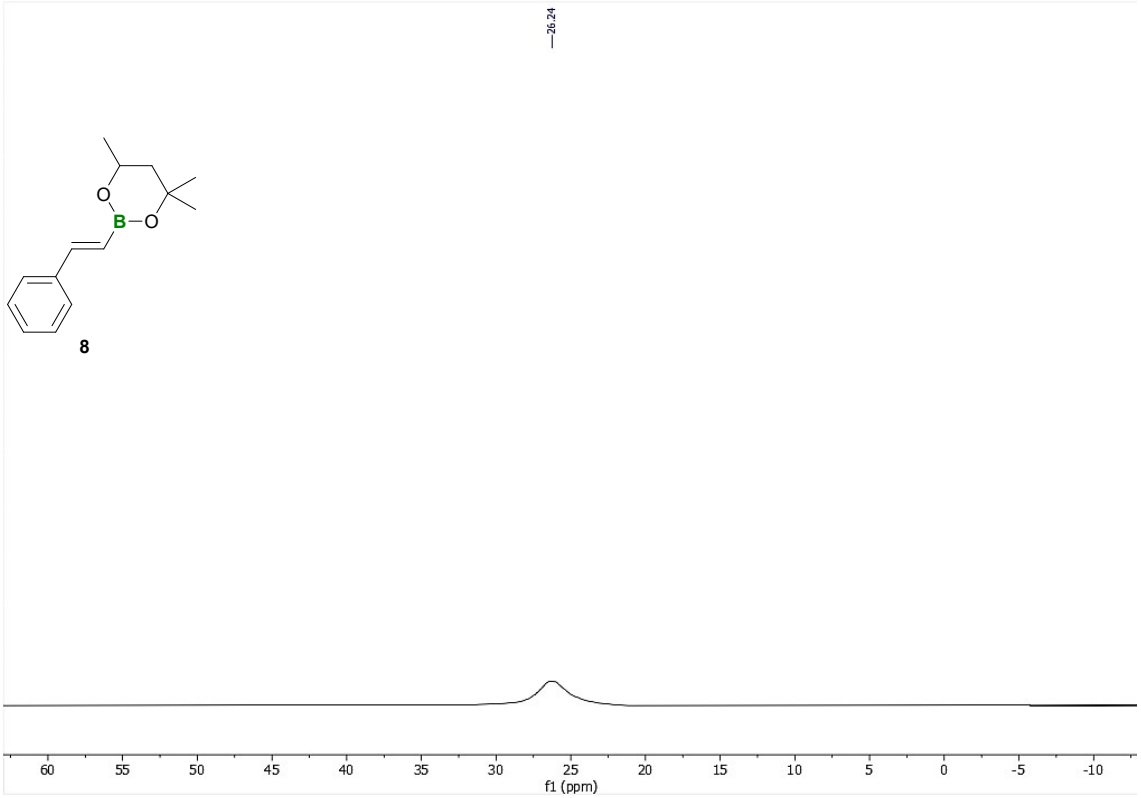

152.24
128.33
125.98
Ph
B
O
Ph
O
Z-4
155
150
145
140
135
130

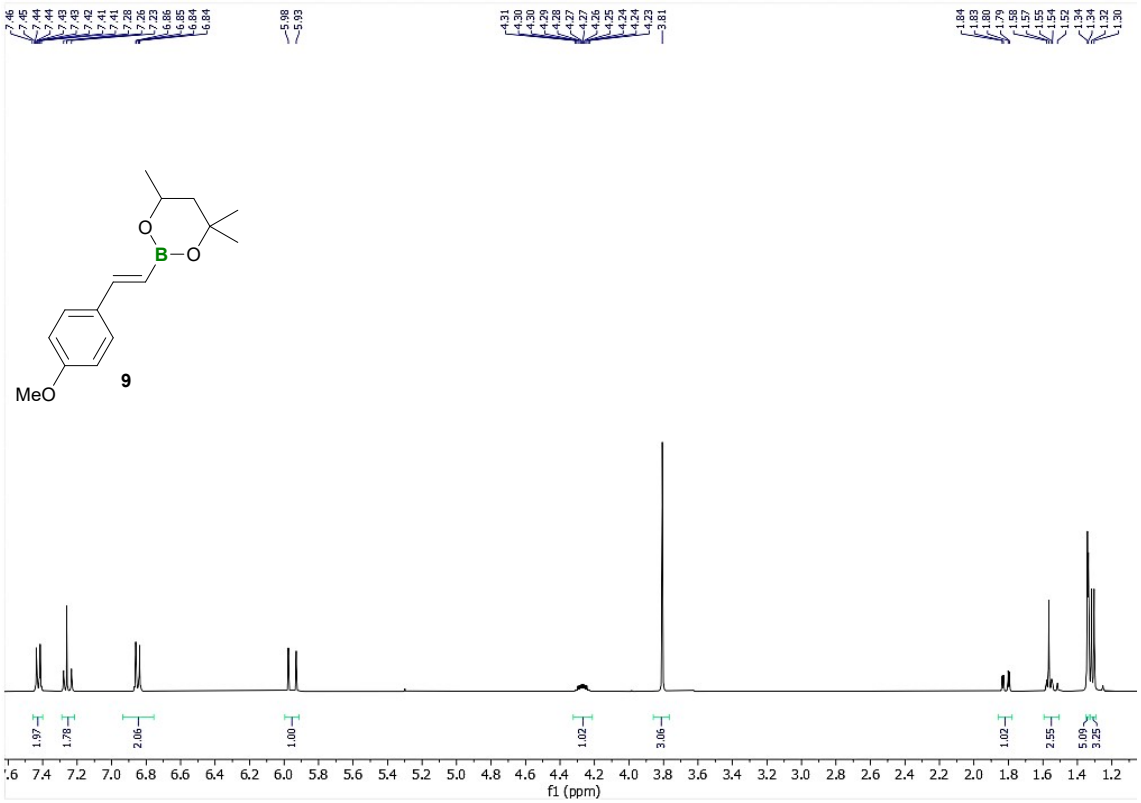

Ph
B
O
Ph
O

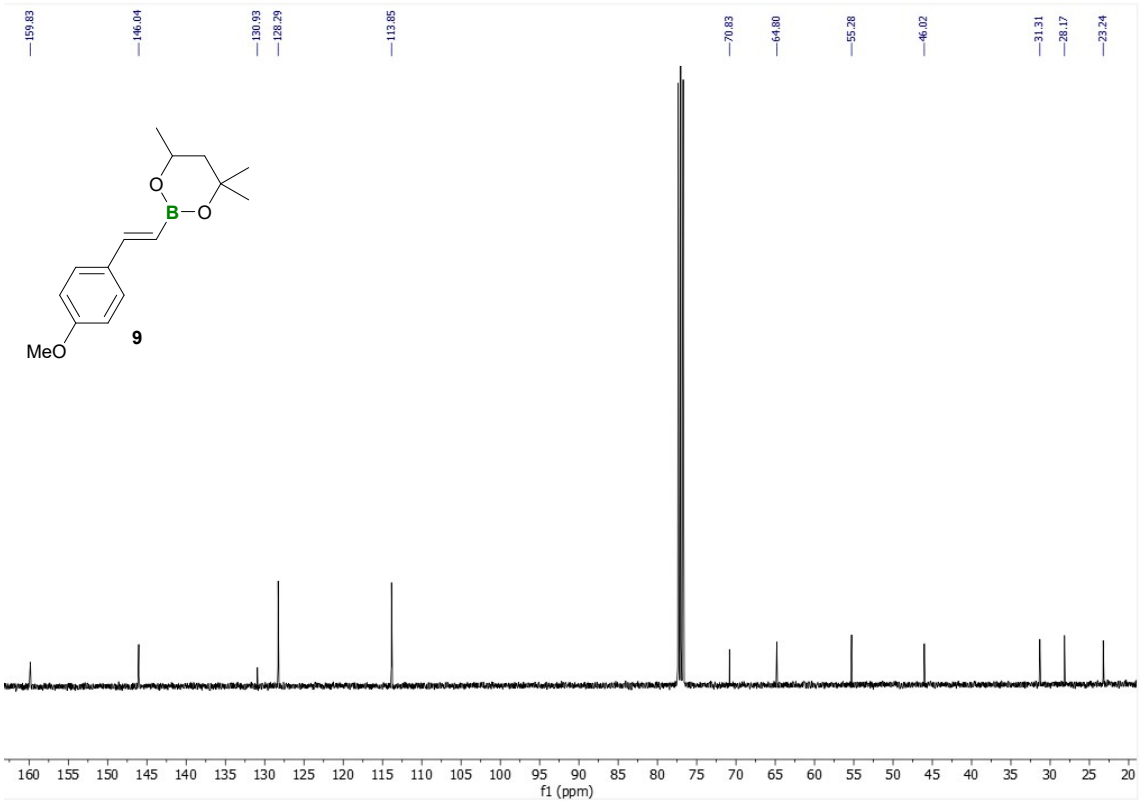

26.29
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)

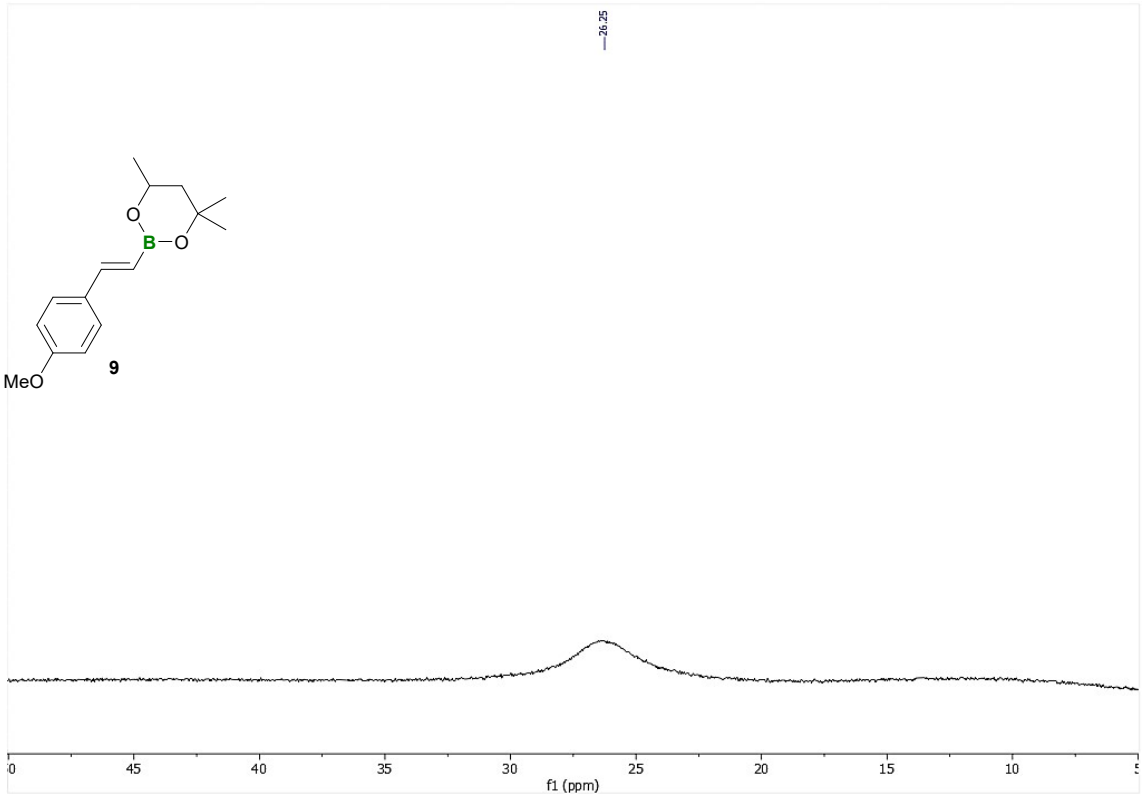

O
B
O
8
2.15
4.60
1.00
1.07
1.06
1.40
2.98
2.95
3.34
7.6
7.4
7.2
7.0
6.8
6.6
6.4
6.2
6.0
5.8
5.6
5.4
5.2
5.0
4.8
4.6
4.4
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
f1 (ppm)


146.49
138.02
128.45
128.29
126.97
70.90
64.85
46.03
31.29
28.17
23.21
O
B
O
8
150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20
f1 (ppm)

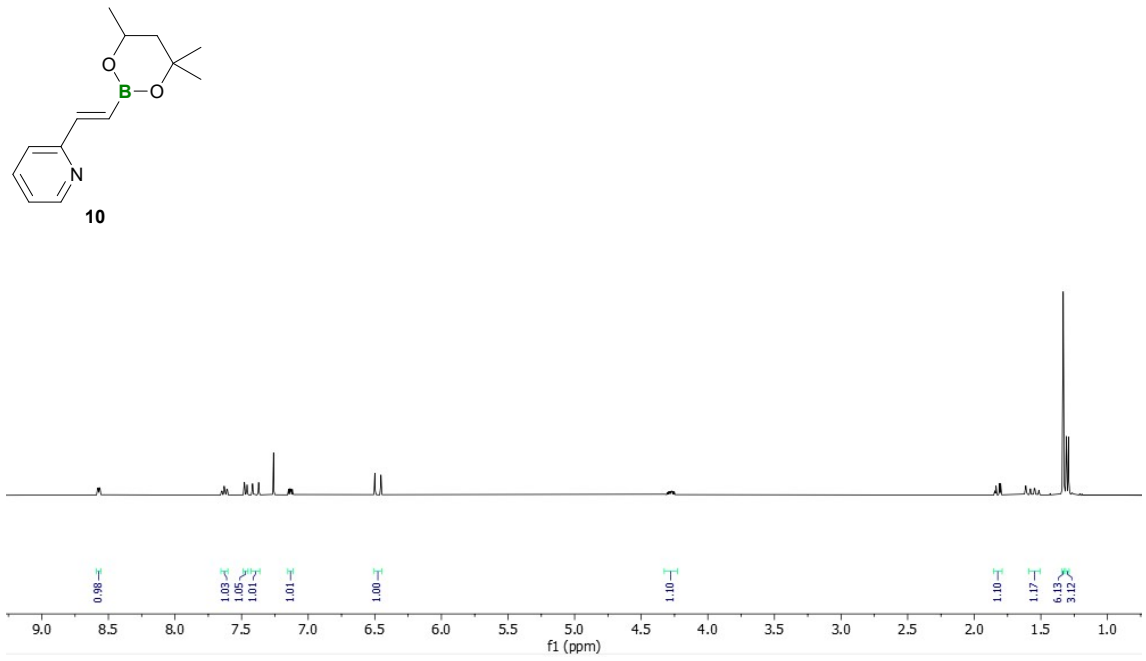

26.24
O
B
O
8
60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10
f1 (ppm)


O
B—O
MeO
9
1.97
1.78
2.06
1.00
1.02
3.06
1.02
2.55
5.09
3.25
f1 (ppm)

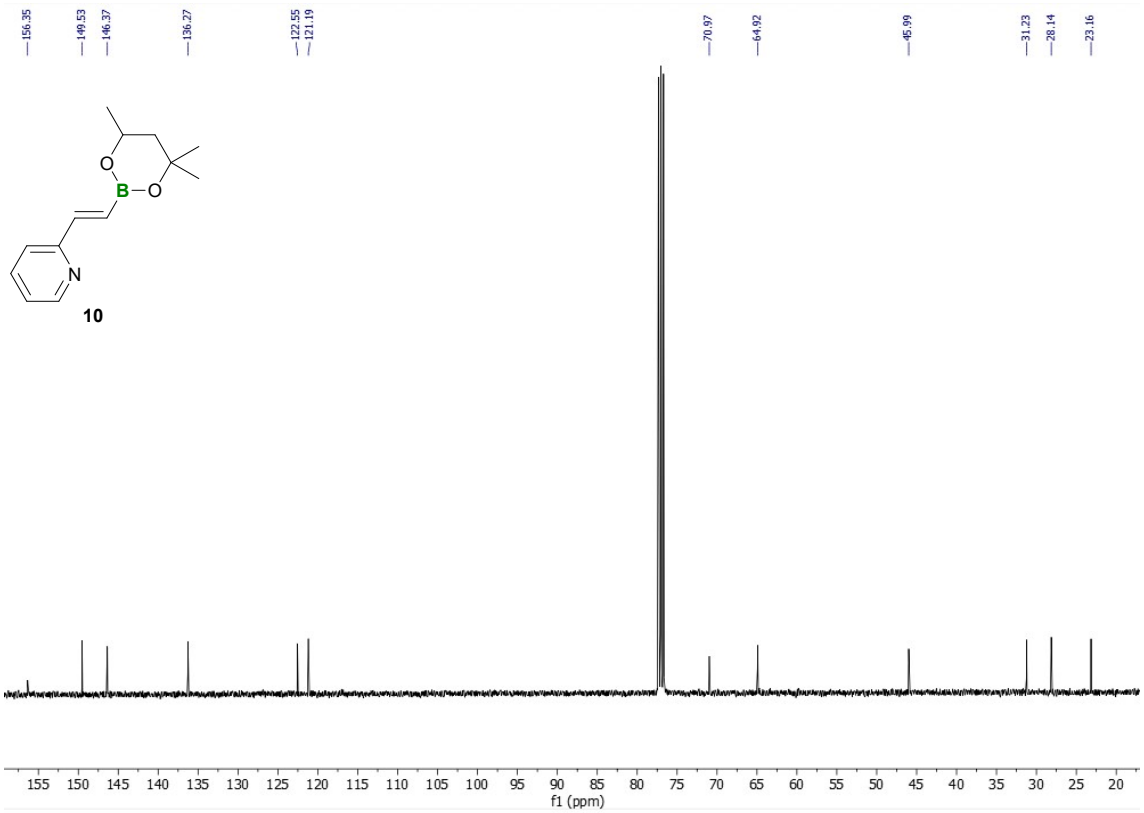

159.83
146.04
130.93
128.29
113.85
70.83
64.80
55.28
46.02
31.31
28.17
23.24
O
B—O
MeO
9
f1 (ppm)

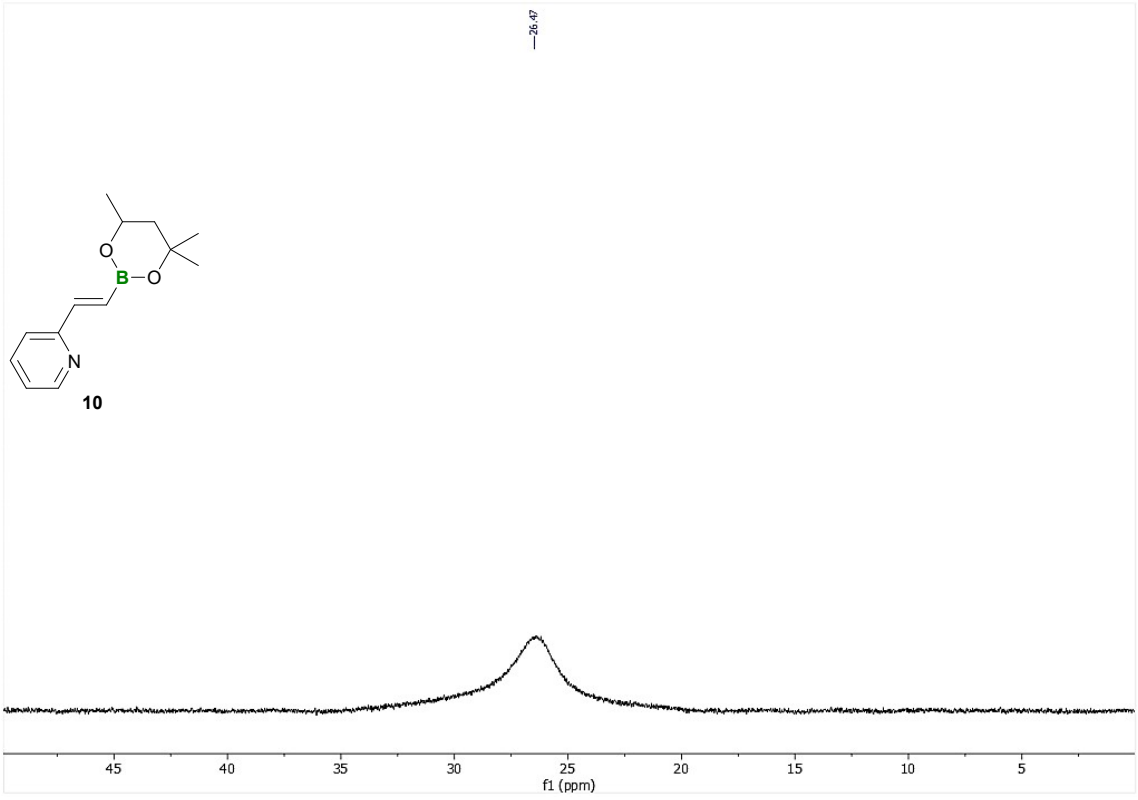


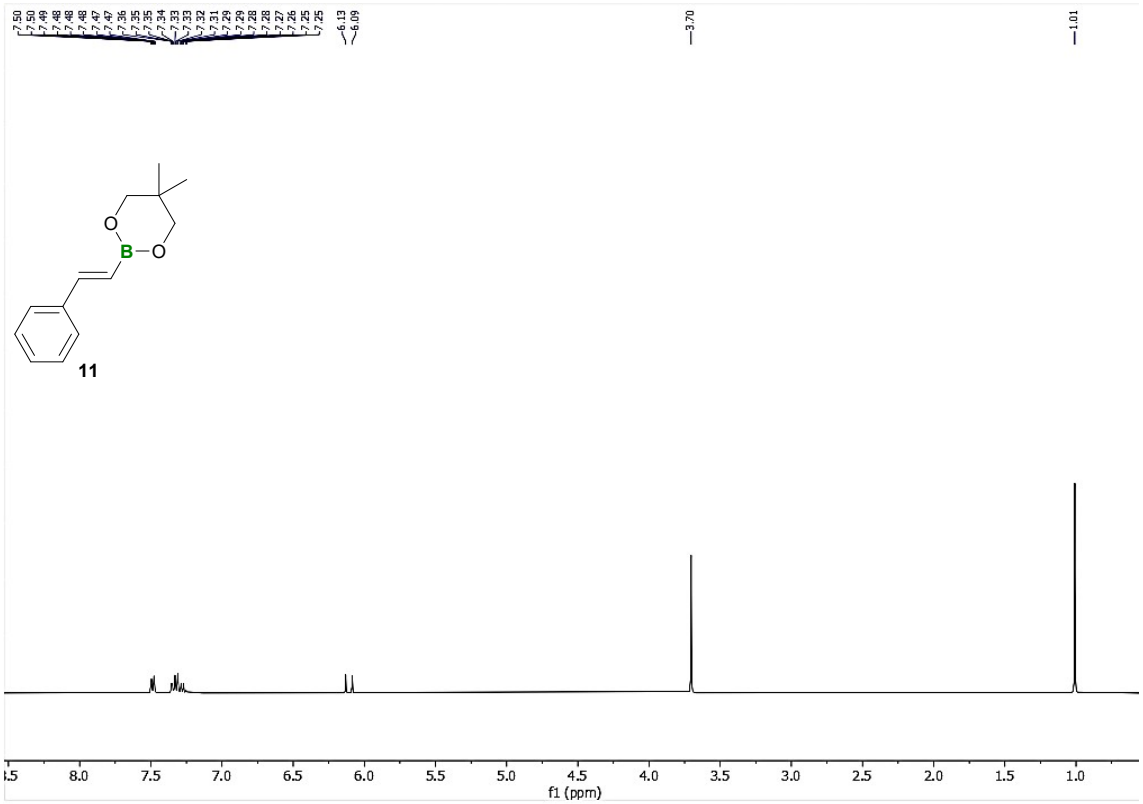
9

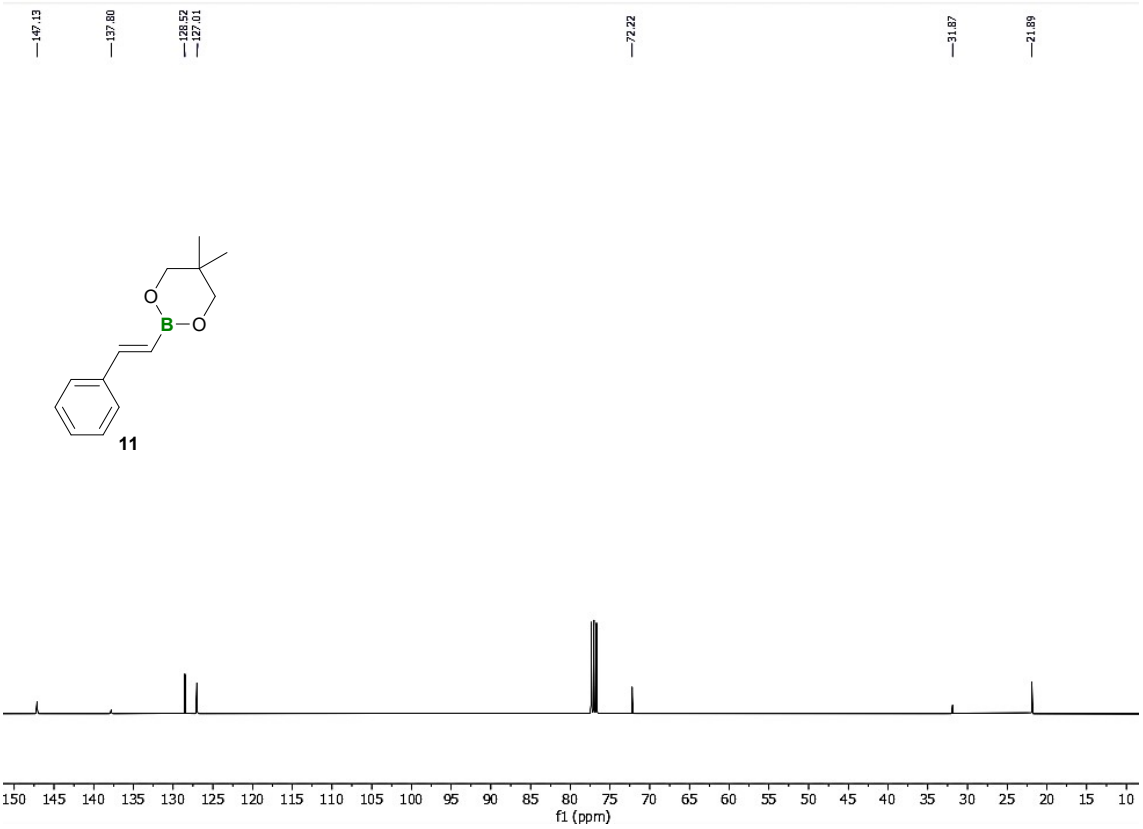


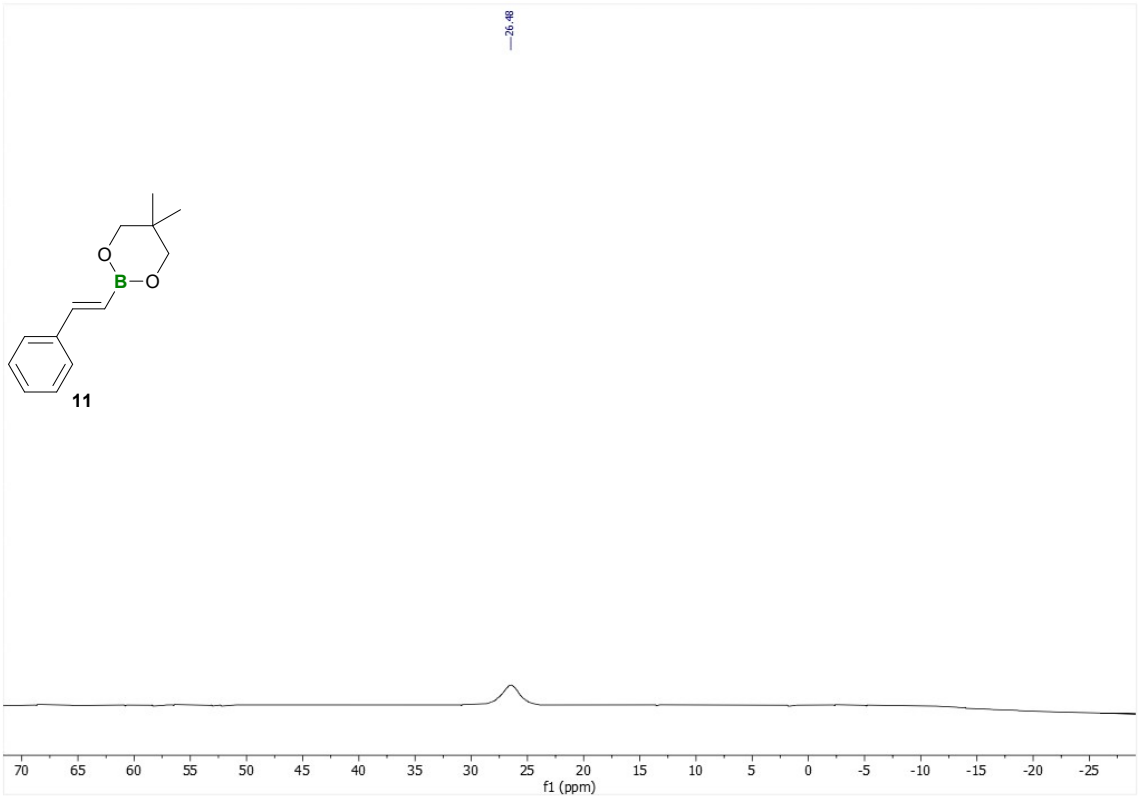
10

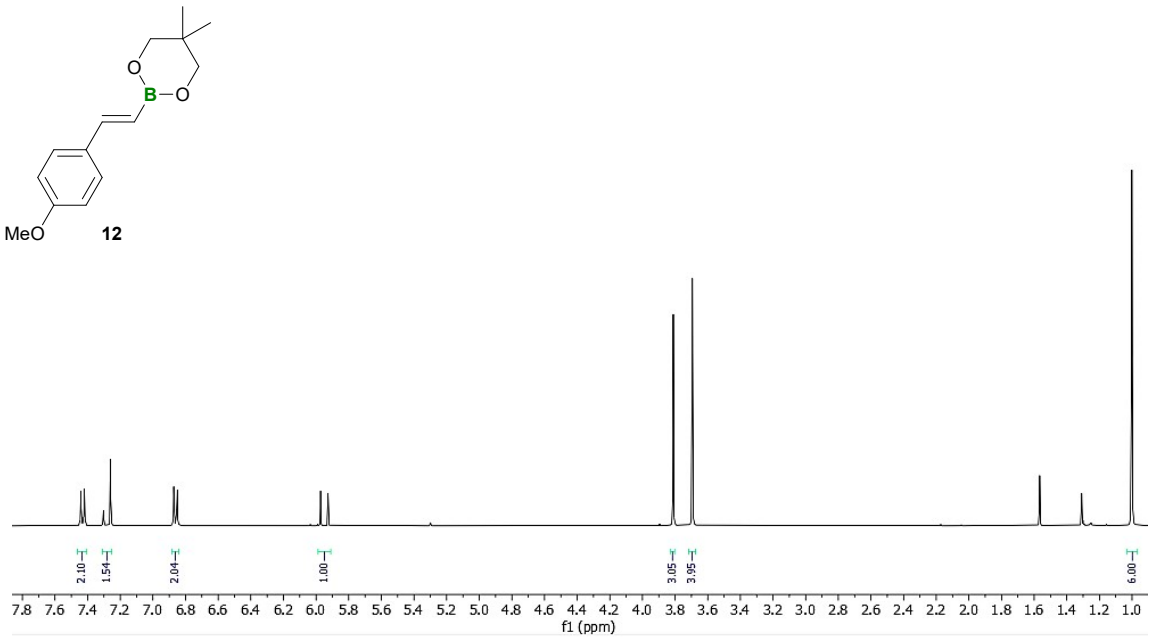

156.35
149.53
146.37
136.27
122.55
121.19
70.97
64.92
45.99
31.23
28.14
23.16
O
B
O
N
10
155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20
f1 (ppm)

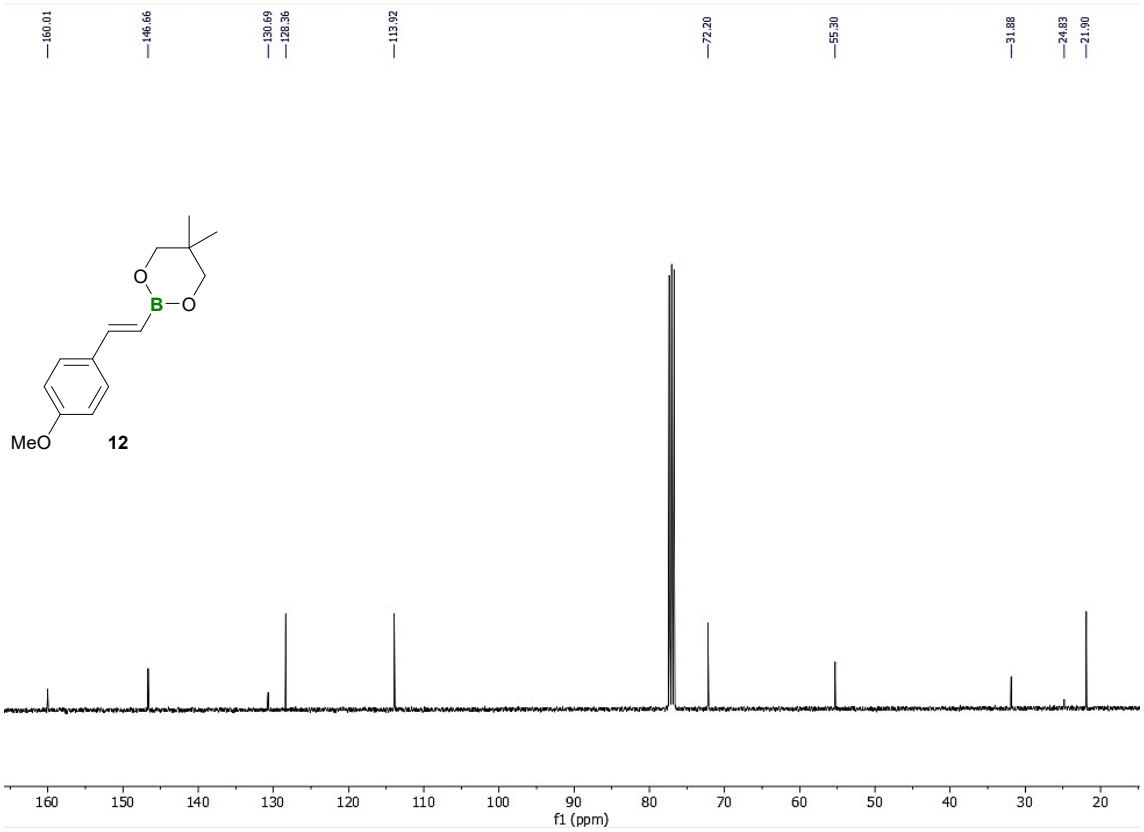

26.47
O
B
O
N
10
45 40 35 30 25 20 15 10 5
f1 (ppm)

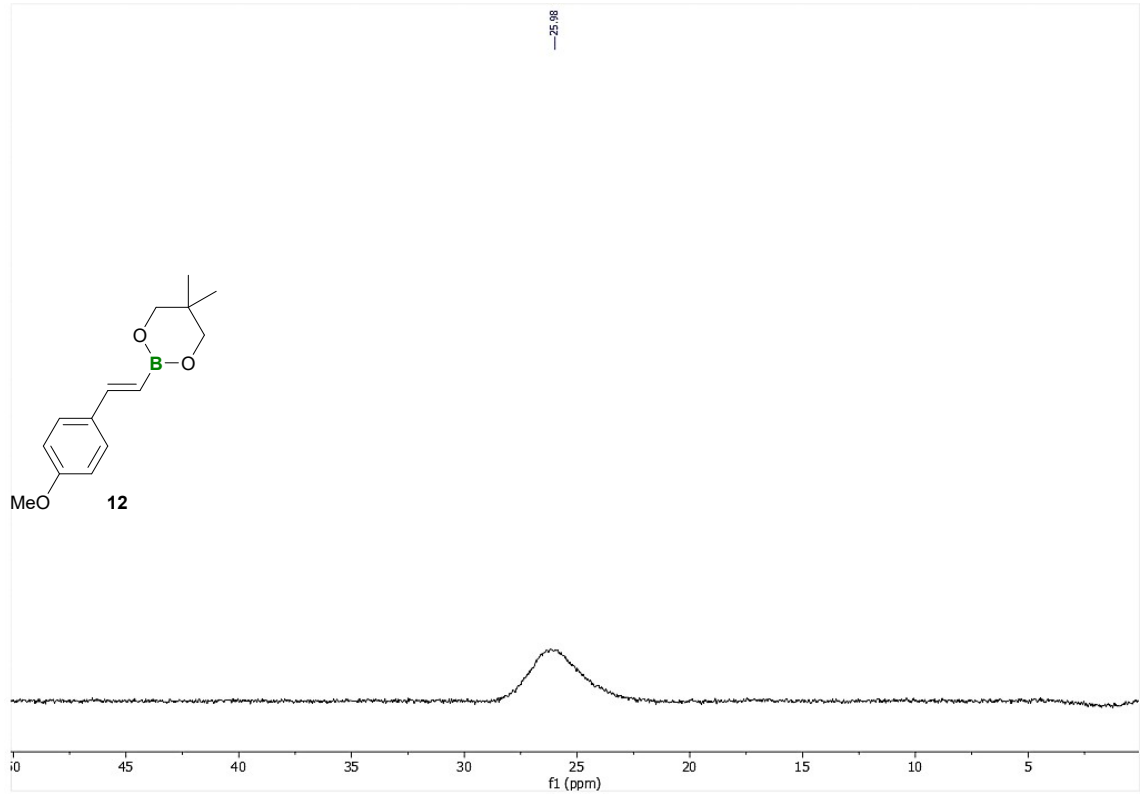

7.50
7.50
7.49
7.48
7.48
7.48
7.47
7.47
7.36
7.35
7.35
7.34
7.33
7.33
7.32
7.31
7.29
7.29
7.28
7.28
7.27
7.26
7.25
7.25
6.13
6.09
3.70
1.01
O
B—O
11
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)

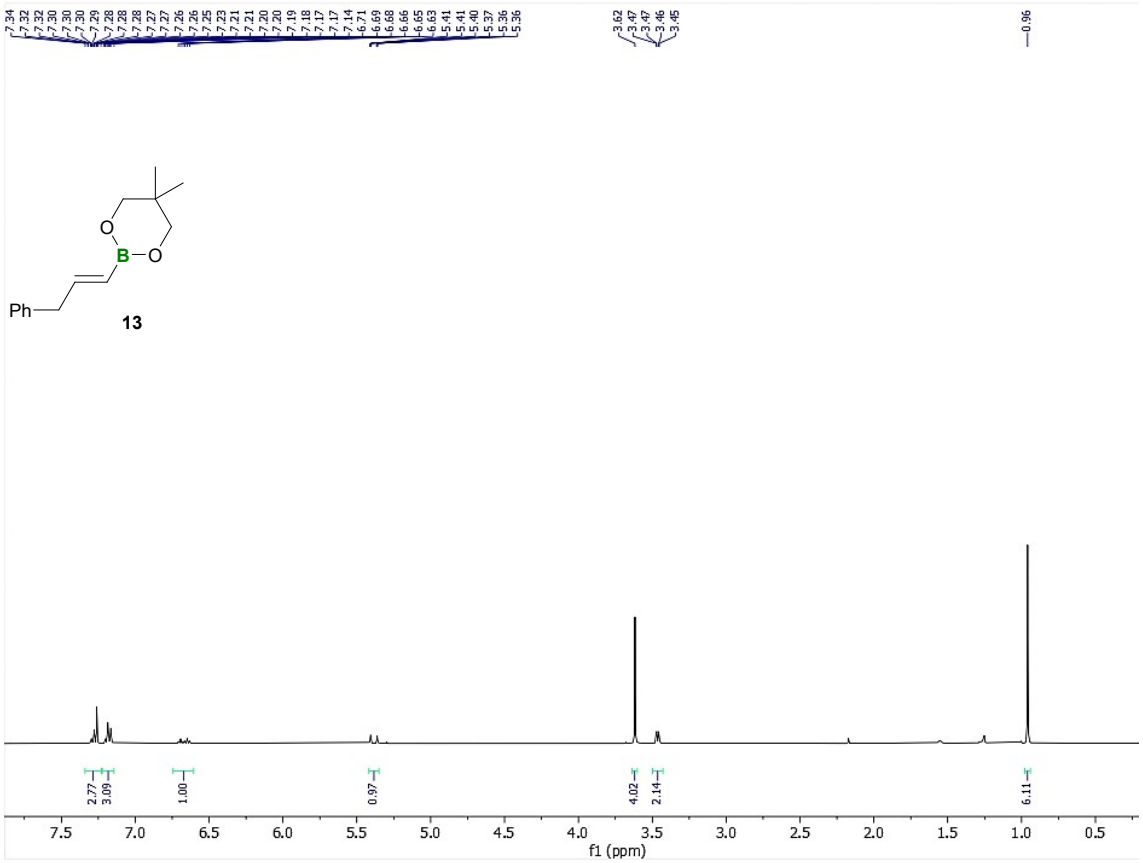

147.13
137.80
128.52
127.01
72.22
31.87
21.89
O
B—O
11
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
f1 (ppm)

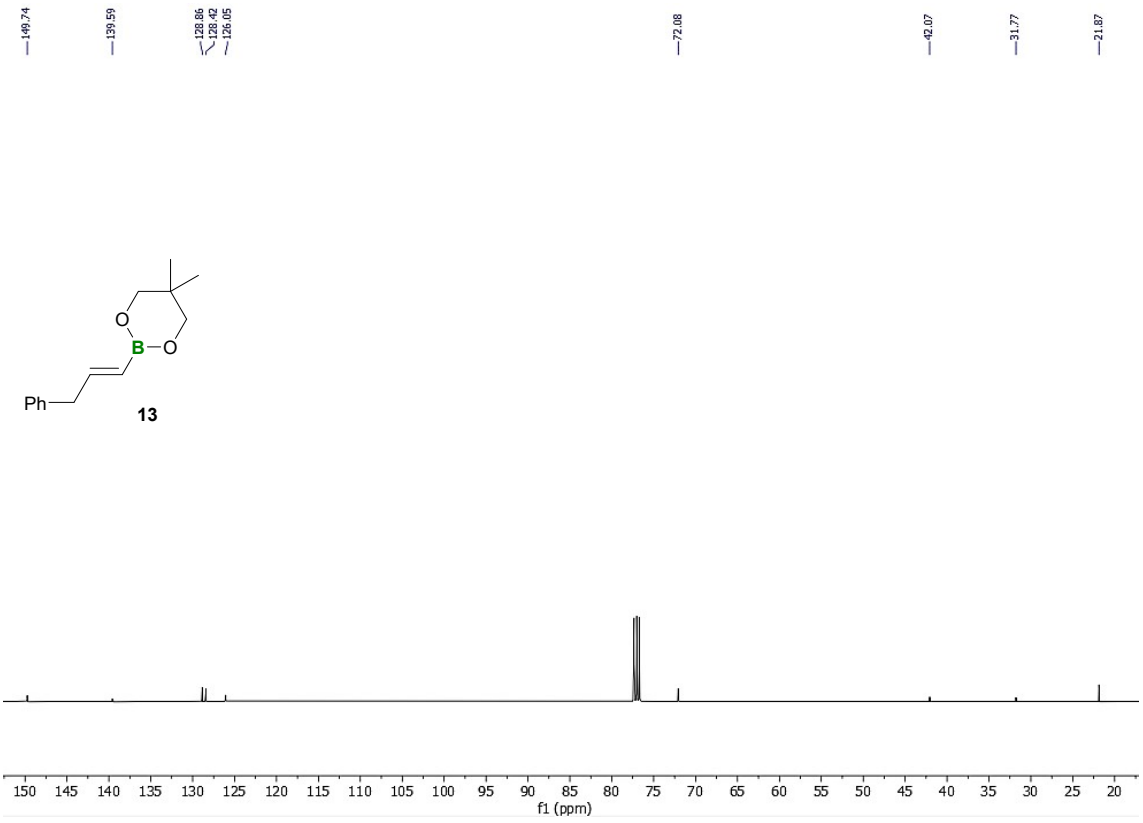

26.48
O
B—O
11
70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25
f1 (ppm)

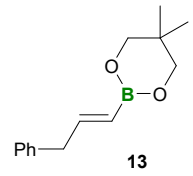

O
B—O
MeO
12
2.10
1.54
2.04
1.00
3.05
3.95
6.00
7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0
f1 (ppm)


160.01
146.66
130.69
128.36
113.92
72.20
55.30
31.88
24.83
21.90
O
B
O
MeO
12
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)


25.98
O
B
O
MeO
12
45
40
35
30
25
20
15
10
5
f1 (ppm)

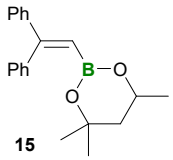

7.34 7.32 7.32 7.30 7.30 7.30 7.29 7.28 7.28 7.28 7.27 7.27 7.26 7.26 7.25 7.23 7.21 7.21 7.20 7.20 7.19 7.18 7.17 7.17 7.14 6.71 6.69 6.68 6.68 6.66 6.65 6.63 5.41 5.41 5.40 5.37 5.36 5.36
3.62 3.47 3.47 3.47 3.46 3.45
0.96
O
B
O
Ph
13
2.77 3.09 1.00 0.97 4.02 2.14 6.11
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


149.74 139.59 128.86 128.42 126.05 72.08 42.07 31.77 21.87
O
B
O
Ph
13
150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20
f1 (ppm)

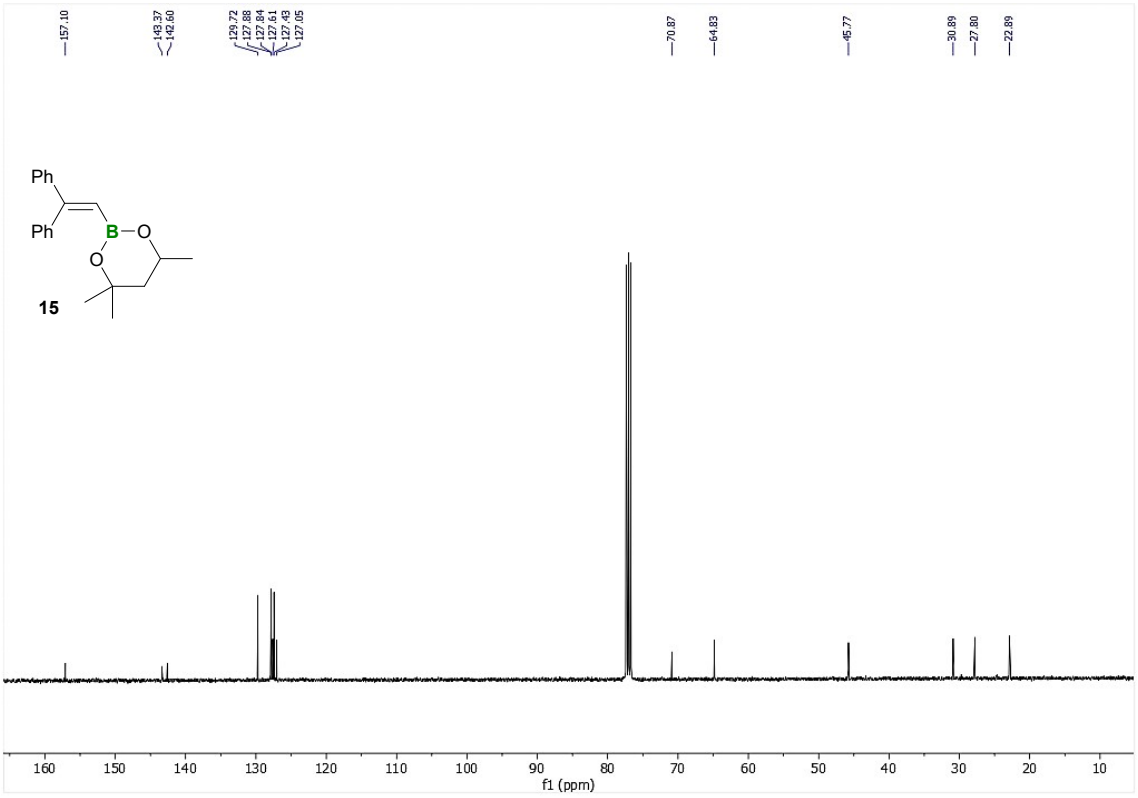

O
B
O
Ph

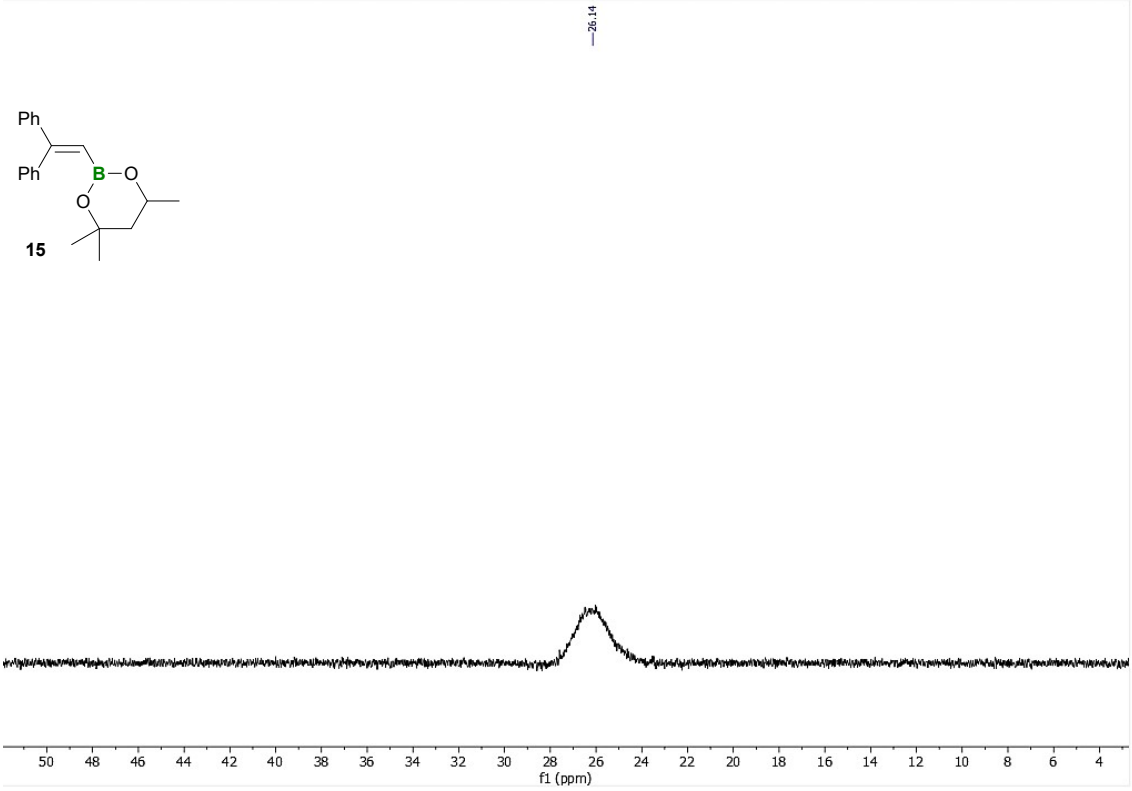
13

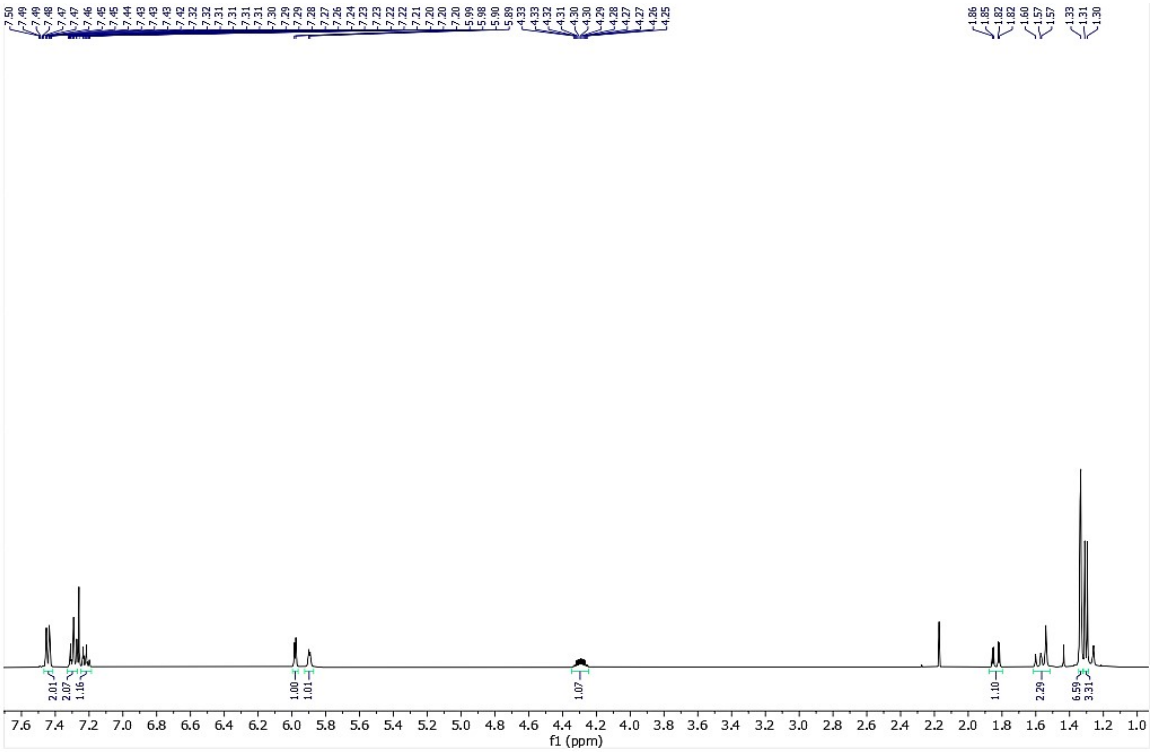
25.82
50 49 48 47 46 45 44 43 42 41 40 39 38 37 36 35 34 33 32 31 30 29 28 27 26 25 24 23 22 21 20 19 18 17 16 15 14
f1 (ppm)
7.31
7.31
7.30
7.30
7.29
7.29
7.28
7.28
7.28
7.28
7.27
7.27
7.26
7.26
7.26
7.25
7.25
7.24
7.24
7.24
6.00
4.13
4.12
4.11
4.11
4.10
4.09
4.08
4.08
4.07
4.06
4.05
4.05
1.71
1.70
1.67
1.67
1.43
1.42
1.42
1.39
1.39
1.38
1.36
1.36
1.33
1.17
1.08
1.07
1.05
9.87
1.00
1.04
1.05
1.27
2.91
2.89
2.92
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

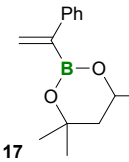

Ph
Ph
B
O
O

15

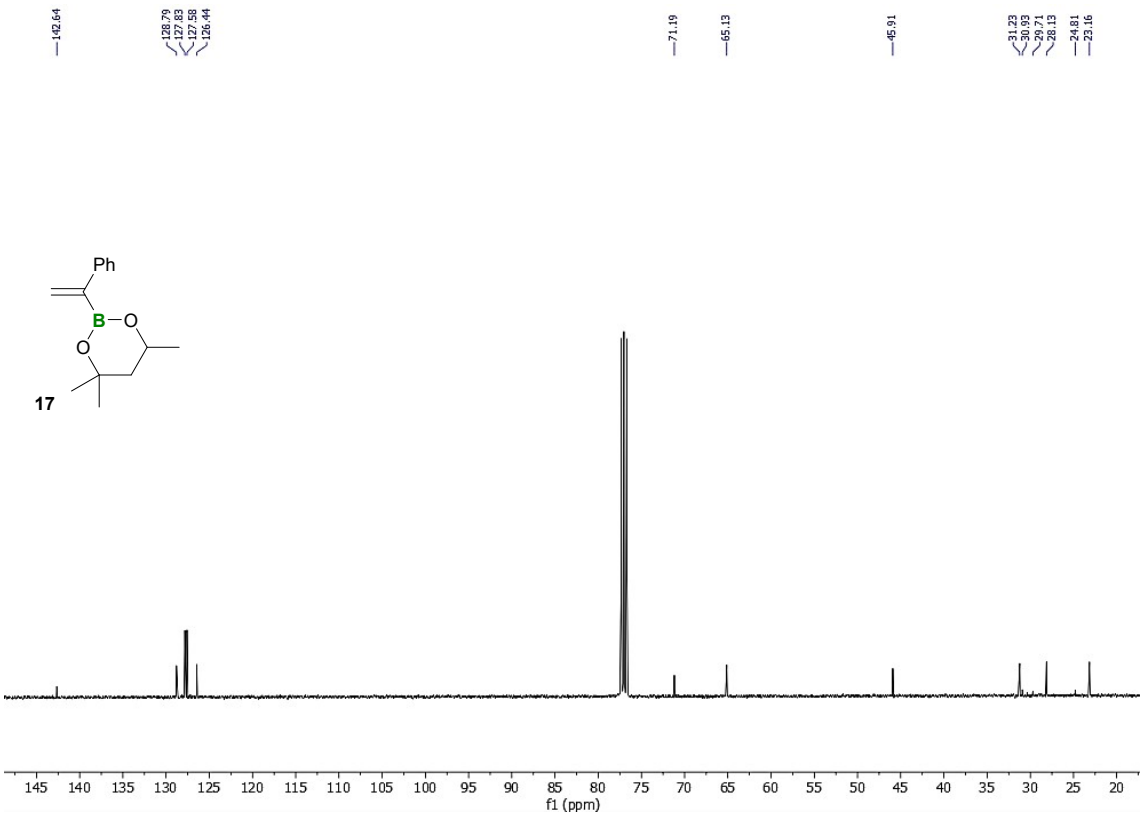

157.10
143.37
142.60
129.72
127.88
127.84
127.61
127.43
127.05
70.87
64.83
45.77
30.89
27.80
22.89
Ph
Ph
B
O
O
15
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


26.14
Ph
Ph
B
O
O
15
50
48
46
44
42
40
38
36
34
32
30
28
26
24
22
20
18
16
14
12
10
8
6
4
f1 (ppm)

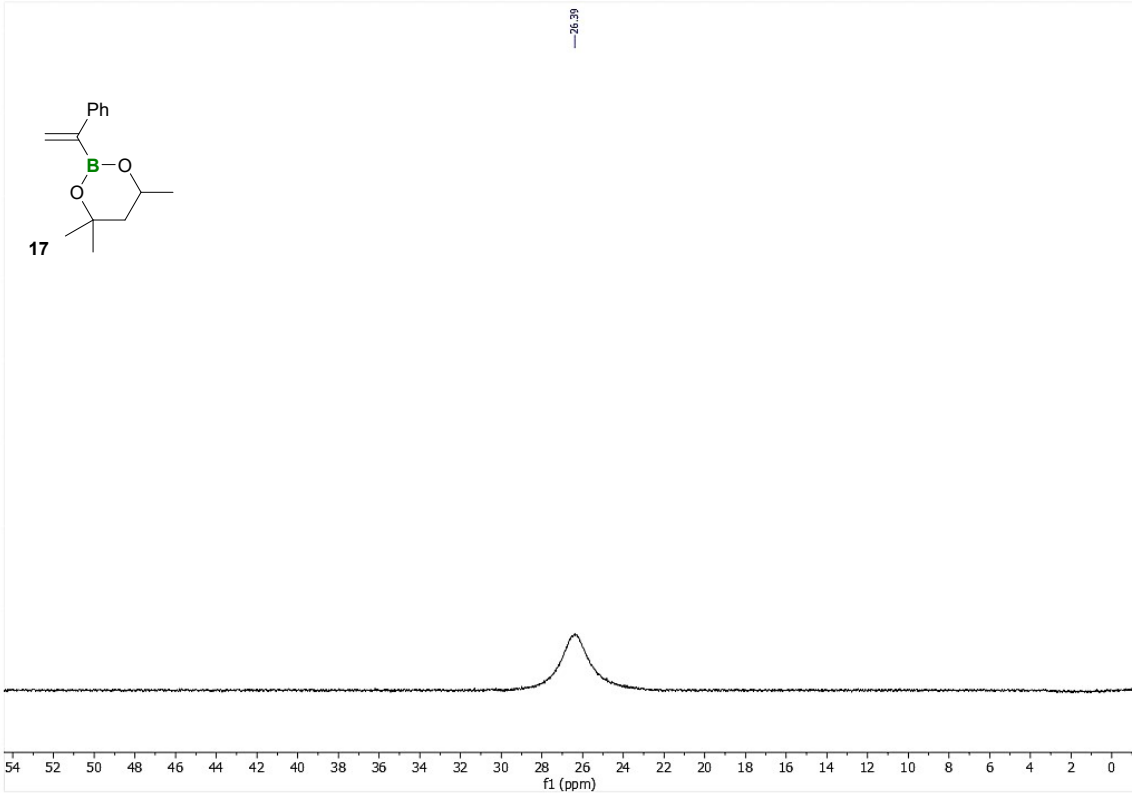


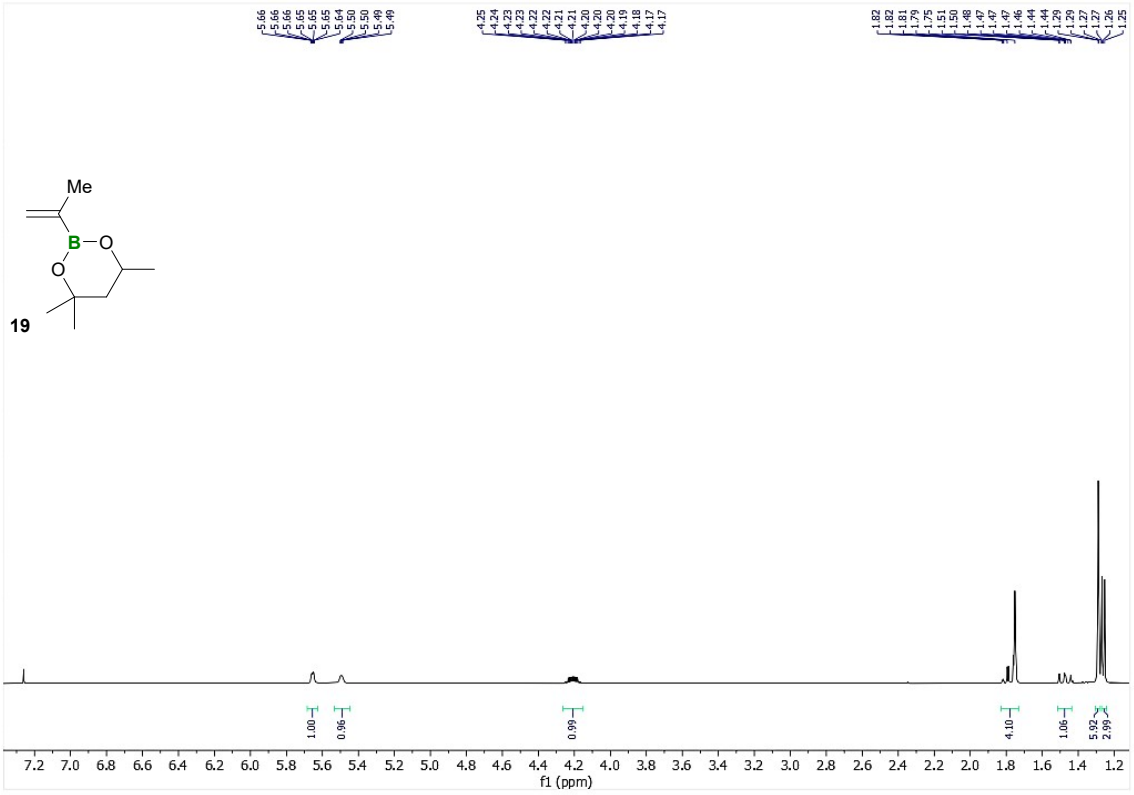


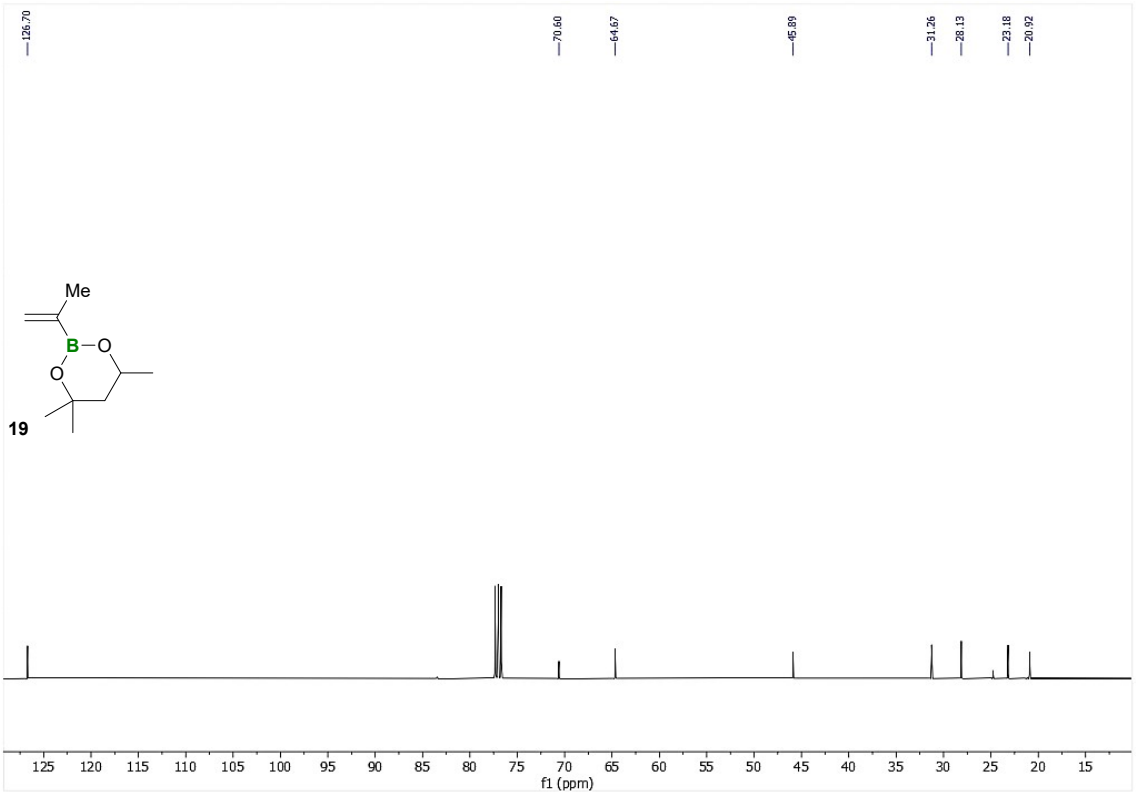
17

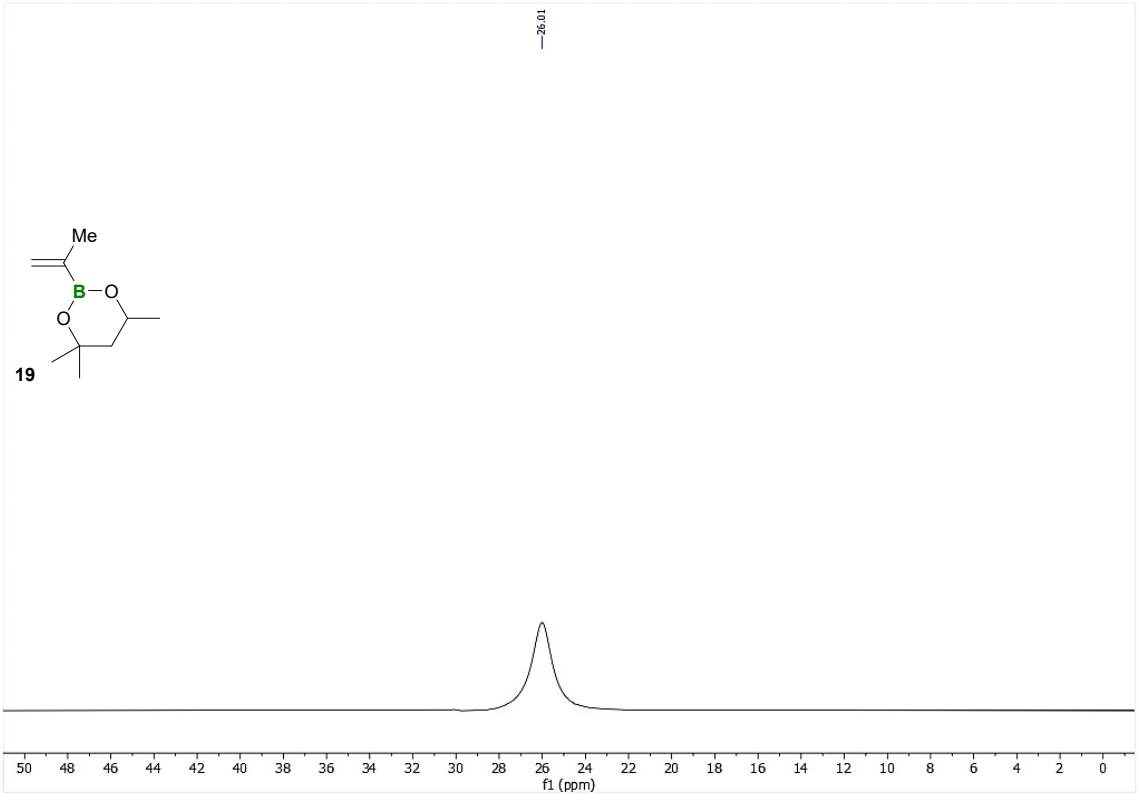


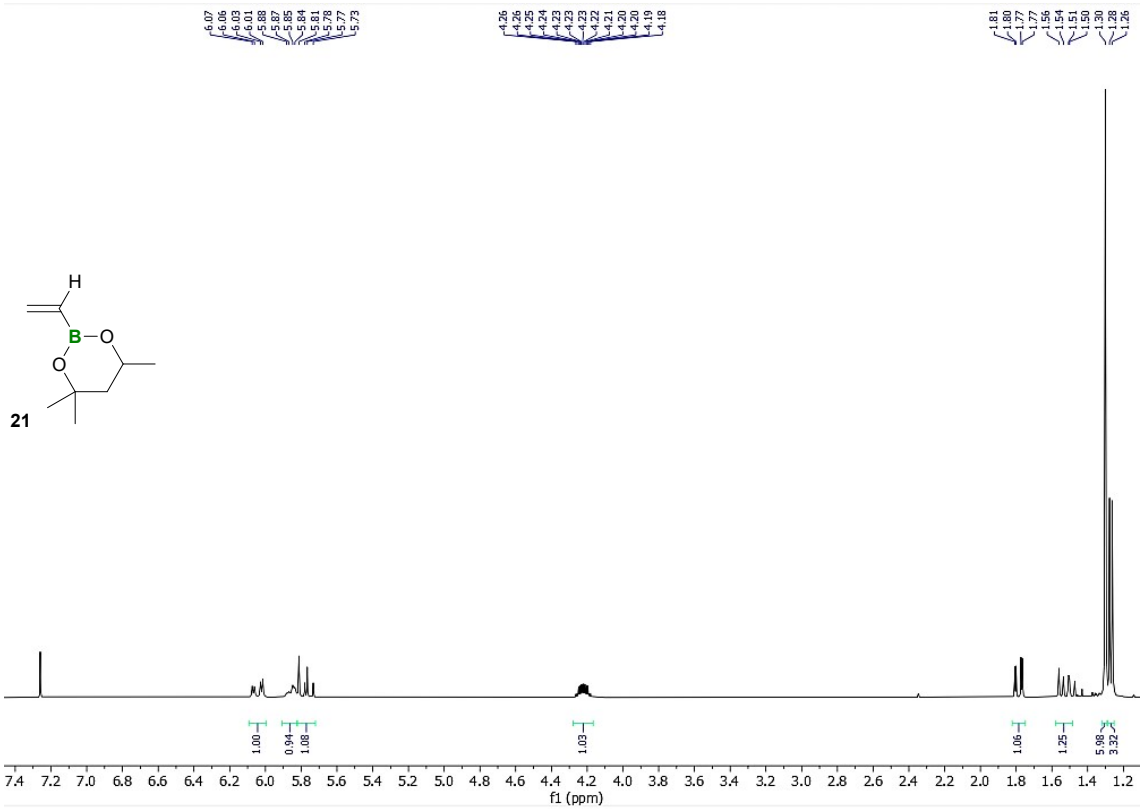
17

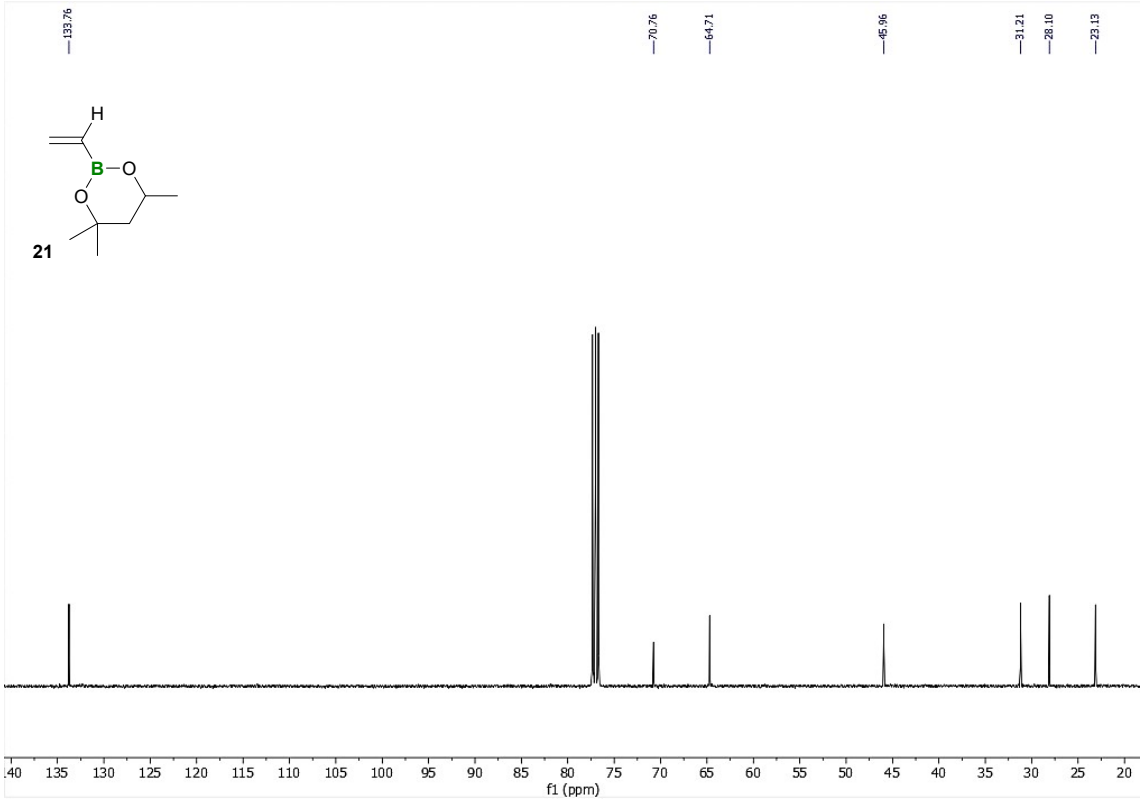

26.39
Ph
B
O
O
17
54 52 50 48 46 44 42 40 38 36 34 32 30 28 26 24 22 20 18 16 14 12 10 8 6 4 2 0
f1 (ppm)

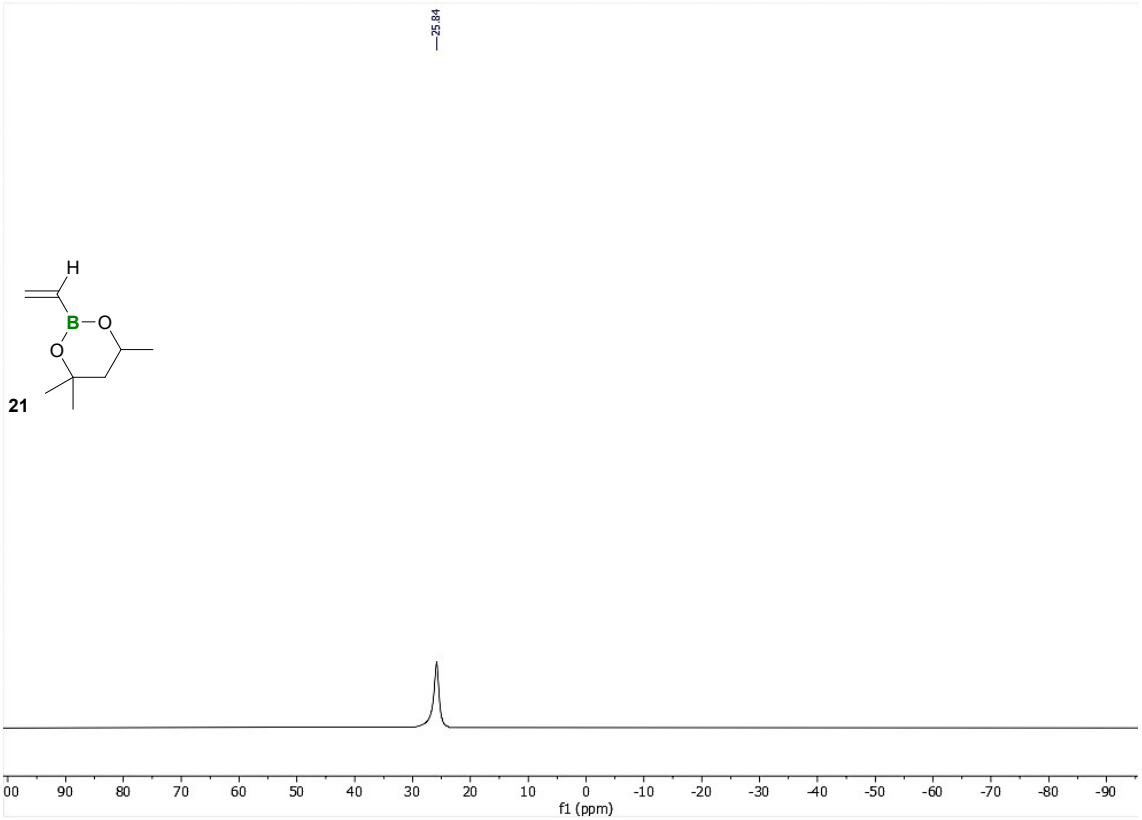

5.66 5.66 5.66 5.65 5.65 5.65 5.64 5.50 5.50 5.49 5.49
4.25 4.24 4.23 4.23 4.22 4.22 4.21 4.21 4.20 4.20 4.20 4.19 4.18 4.17 4.17
1.82 1.82 1.81 1.79 1.75 1.51 1.50 1.48 1.47 1.47 1.47 1.46 1.44 1.29 1.29 1.27 1.27 1.26 1.25
Me
B
O
O
19
1.00 0.96 0.99 4.10 1.06 5.92 2.99
7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2
f1 (ppm)

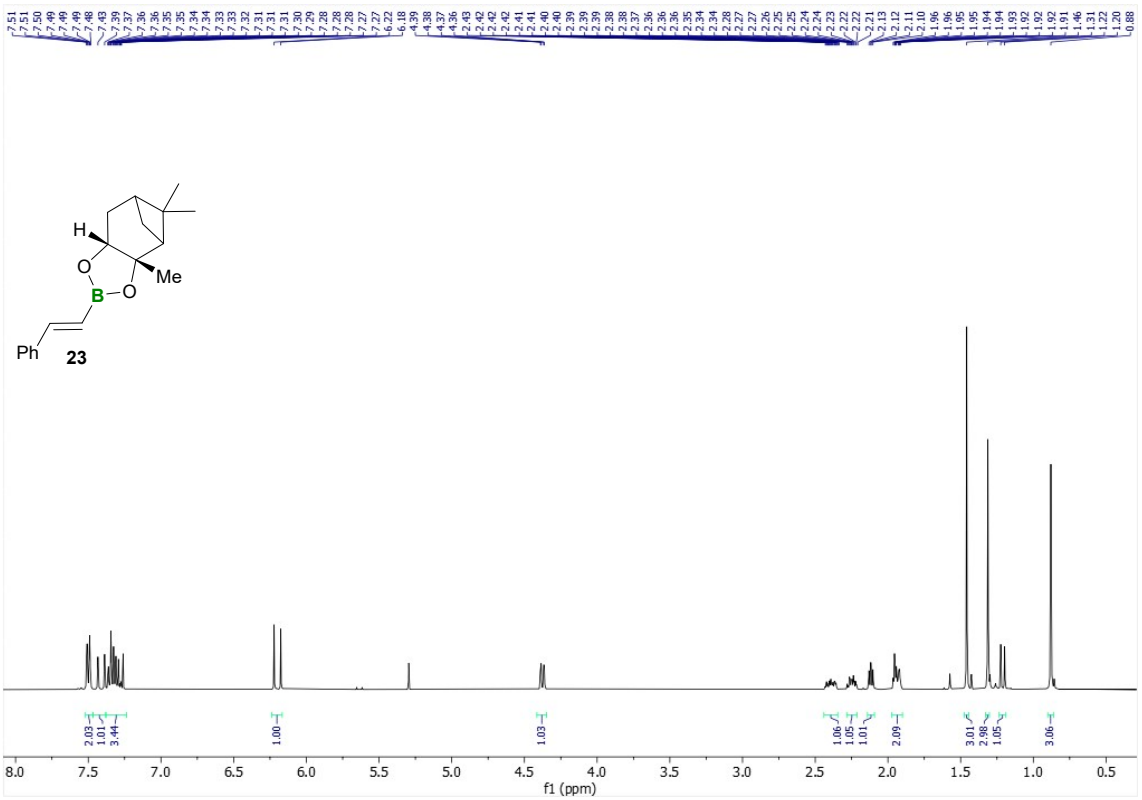

126.70
70.60
64.67
45.89
31.26
28.13
23.18
20.92
Me
B
O
O
19
125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15
f1 (ppm)

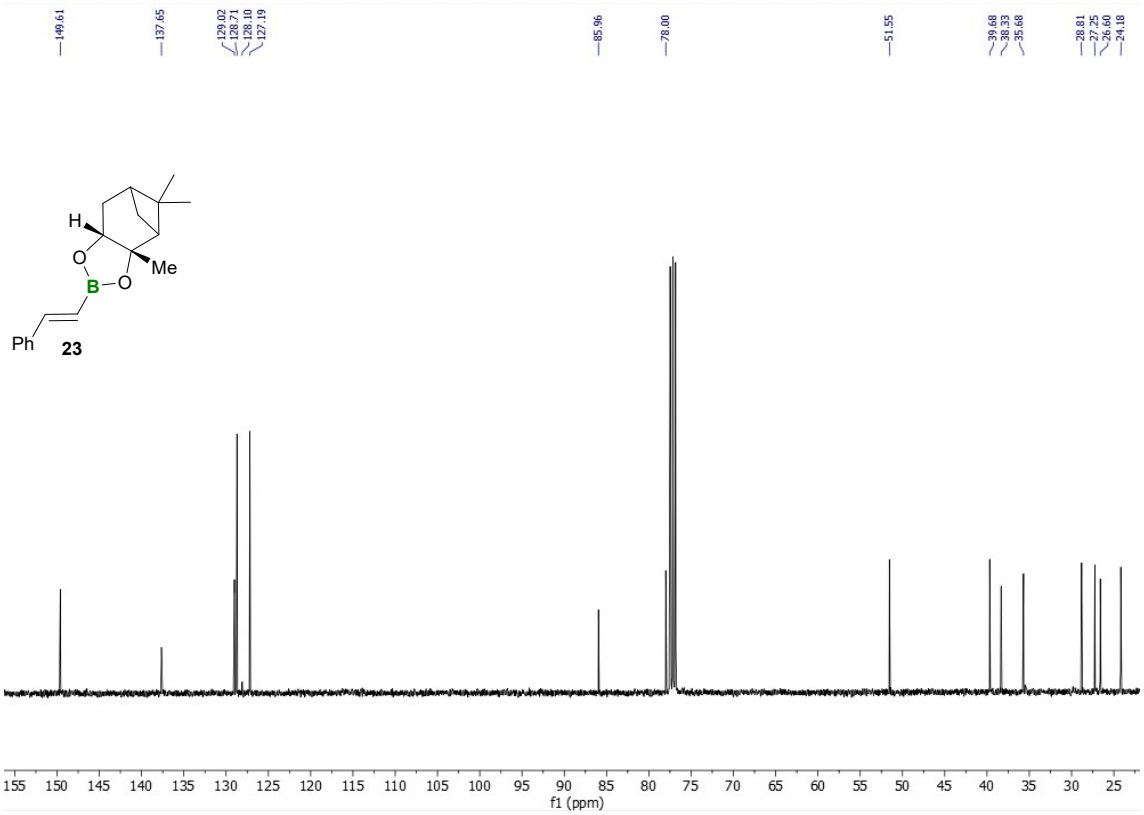

26.01
Me
B
O
O
19
50 48 46 44 42 40 38 36 34 32 30 28 26 24 22 20 18 16 14 12 10 8 6 4 2 0
f1 (ppm)

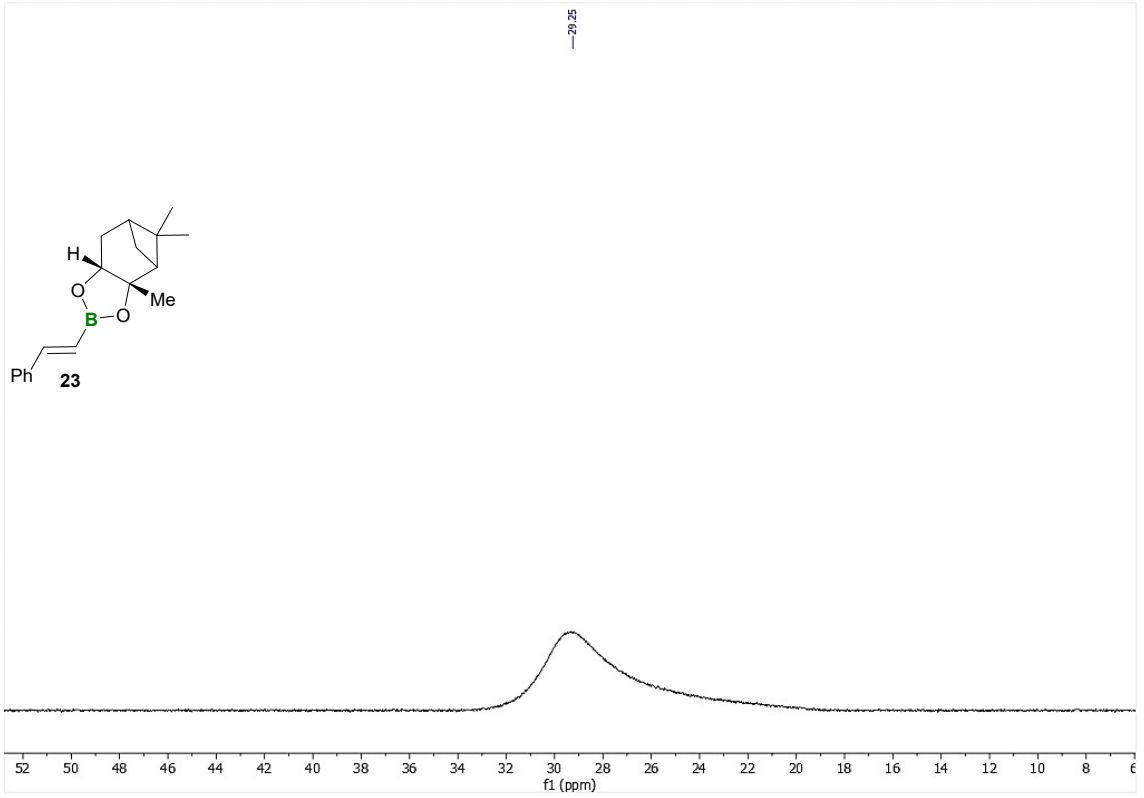

6.07
6.06
6.03
6.01
5.88
5.87
5.85
5.84
5.81
5.78
5.77
5.73
4.26
4.26
4.25
4.24
4.23
4.23
4.23
4.22
4.21
4.20
4.20
4.19
4.18
1.81
1.80
1.77
1.77
1.56
1.54
1.51
1.50
1.30
1.28
1.26
H
B
O
O
21
1.00
0.94
1.08
1.03
1.06
1.25
5.98
3.32
7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2
f1 (ppm)

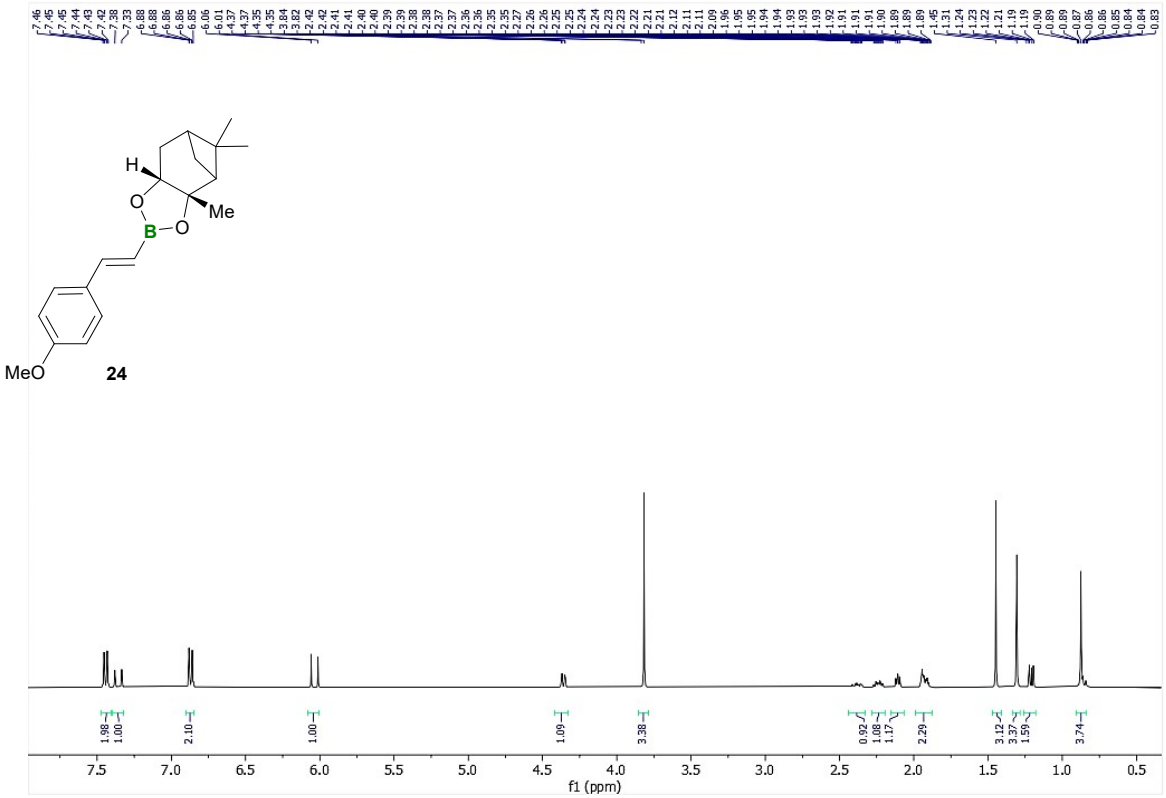

133.76
70.76
64.71
45.96
31.21
28.10
23.13
H
B
O
O
21
140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20
f1 (ppm)

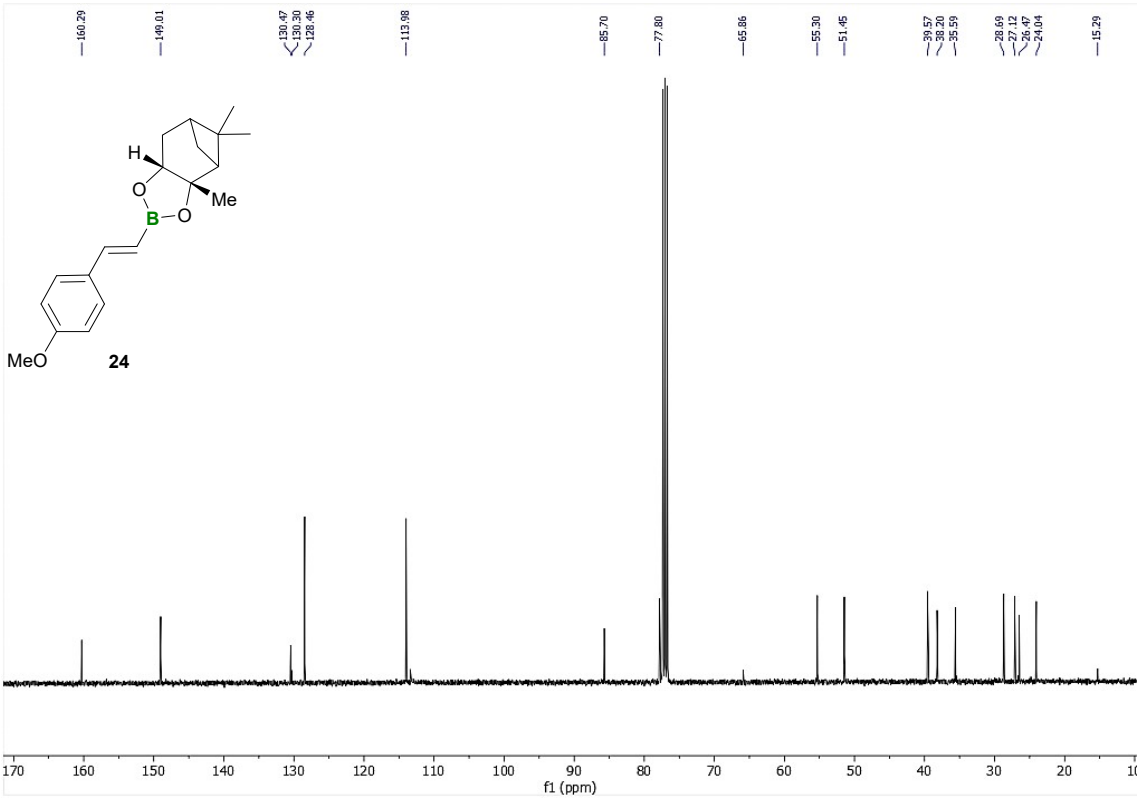

25.84
H
B
O
O
21
00 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90
f1 (ppm)

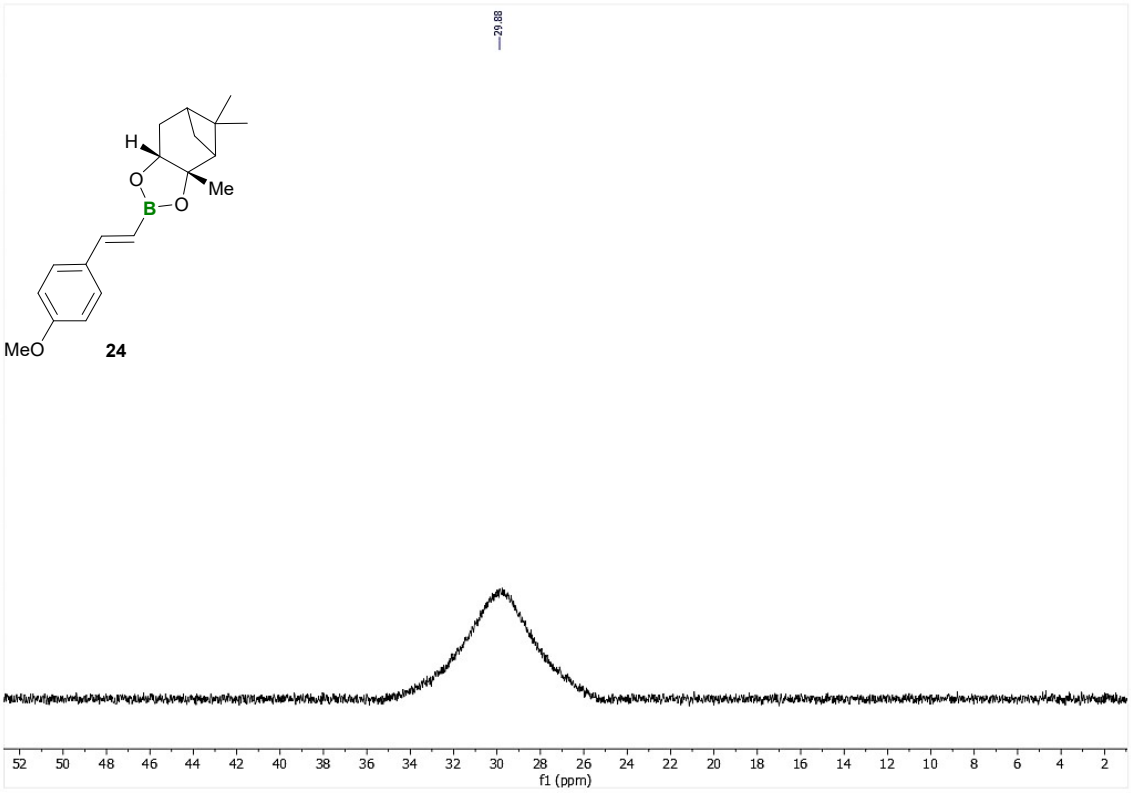

H
O
Me
B
O
Ph
23
2.03
1.01
3.44
1.00
1.03
1.06
1.05
1.01
2.09
3.01
2.98
1.05
3.06
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

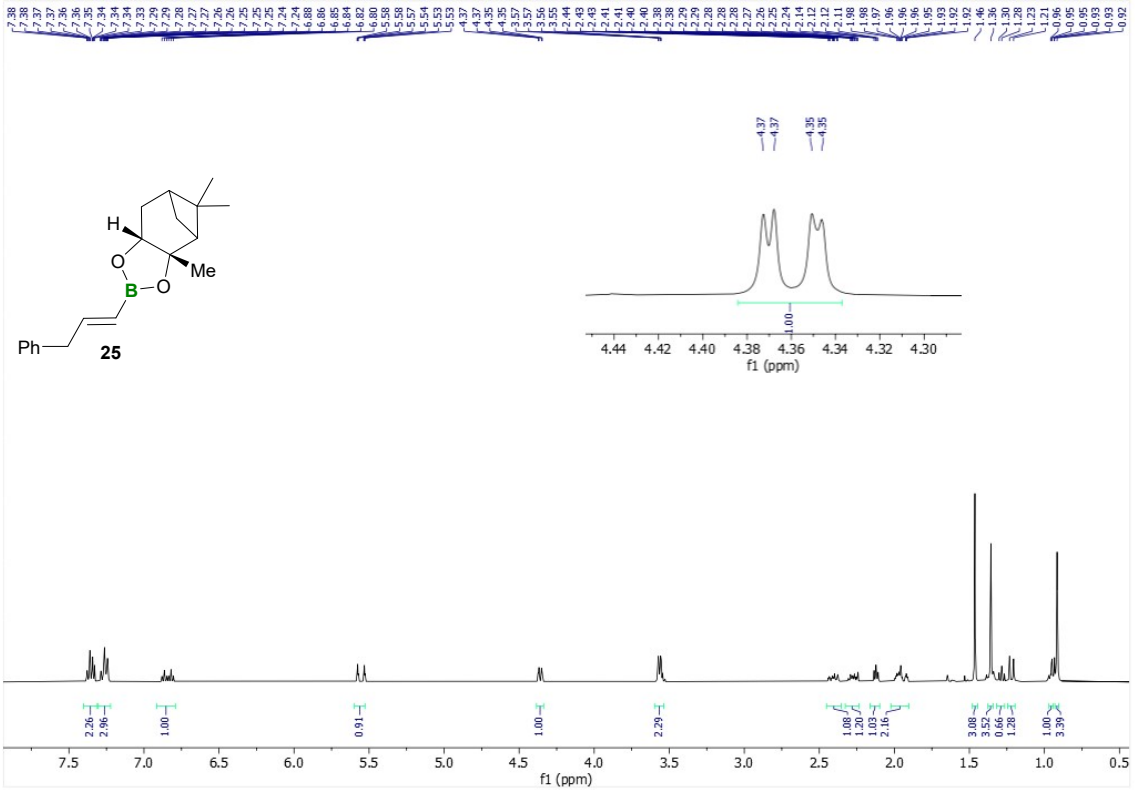

149.61
137.65
129.02
128.71
128.10
127.19
85.96
78.00
51.55
39.68
38.33
35.68
28.81
27.25
26.60
24.18
H
O
Me
B
O
Ph
23
155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25
f1 (ppm)

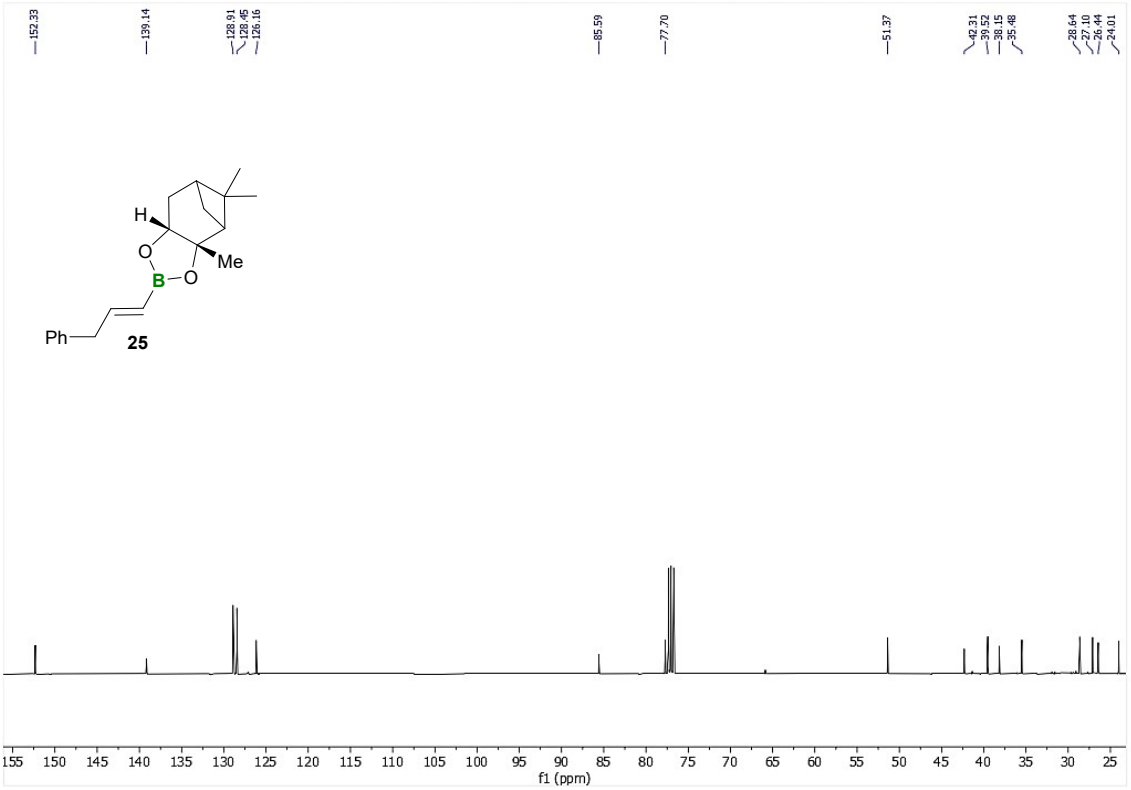

29.25
H
O
Me
B
O
Ph
23
52 50 48 46 44 42 40 38 36 34 32 30 28 26 24 22 20 18 16 14 12 10 8
f1 (ppm)

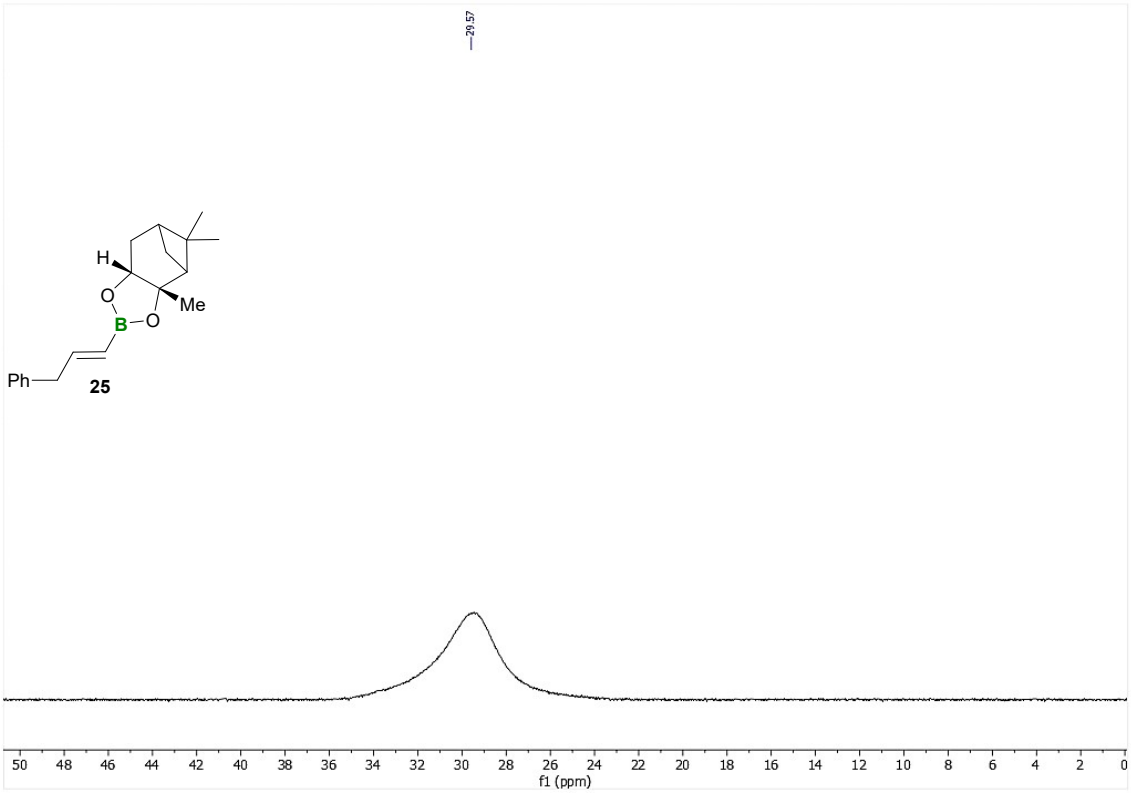

H
O
Me
B
O
MeO
24
1.98
1.00
2.10
1.00
1.09
3.38
0.92
1.08
1.17
2.29
3.12
3.37
1.59
3.74
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

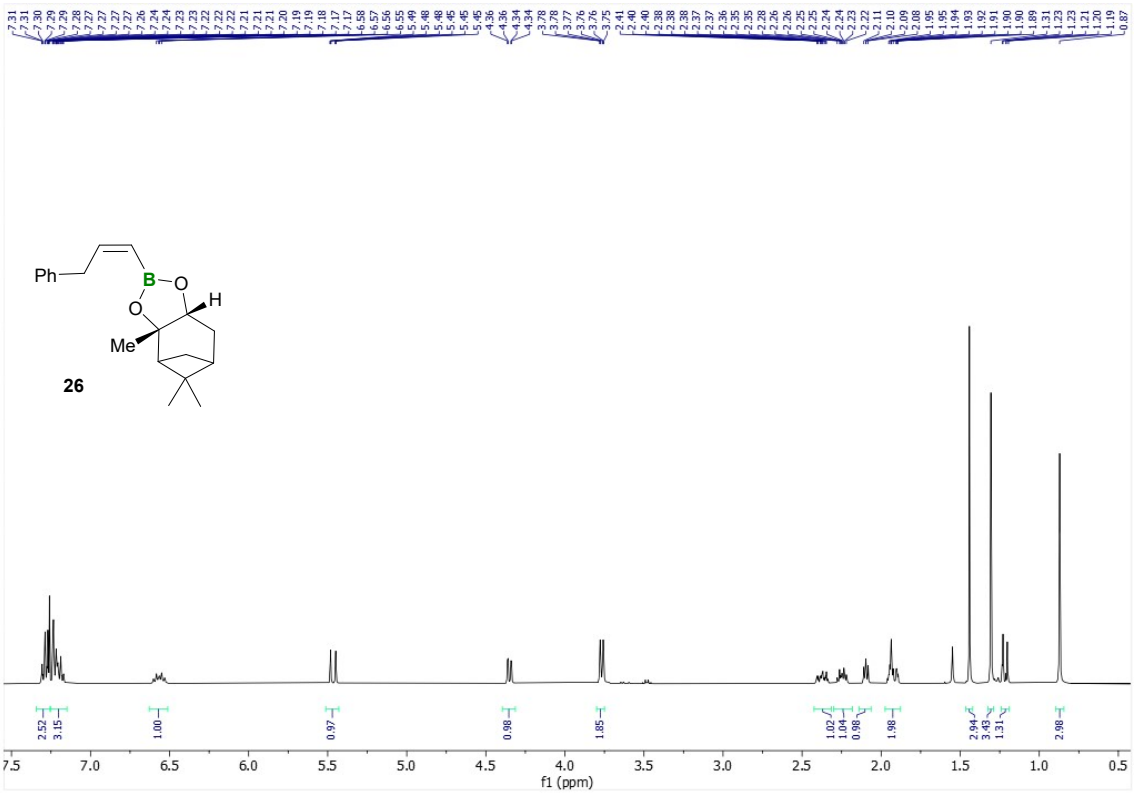

160.29
149.01
130.47
130.30
128.46
113.98
85.70
77.80
65.86
55.30
51.45
39.57
38.20
35.59
28.69
27.12
26.47
24.04
15.29
H
O
Me
B
O
MeO
24
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

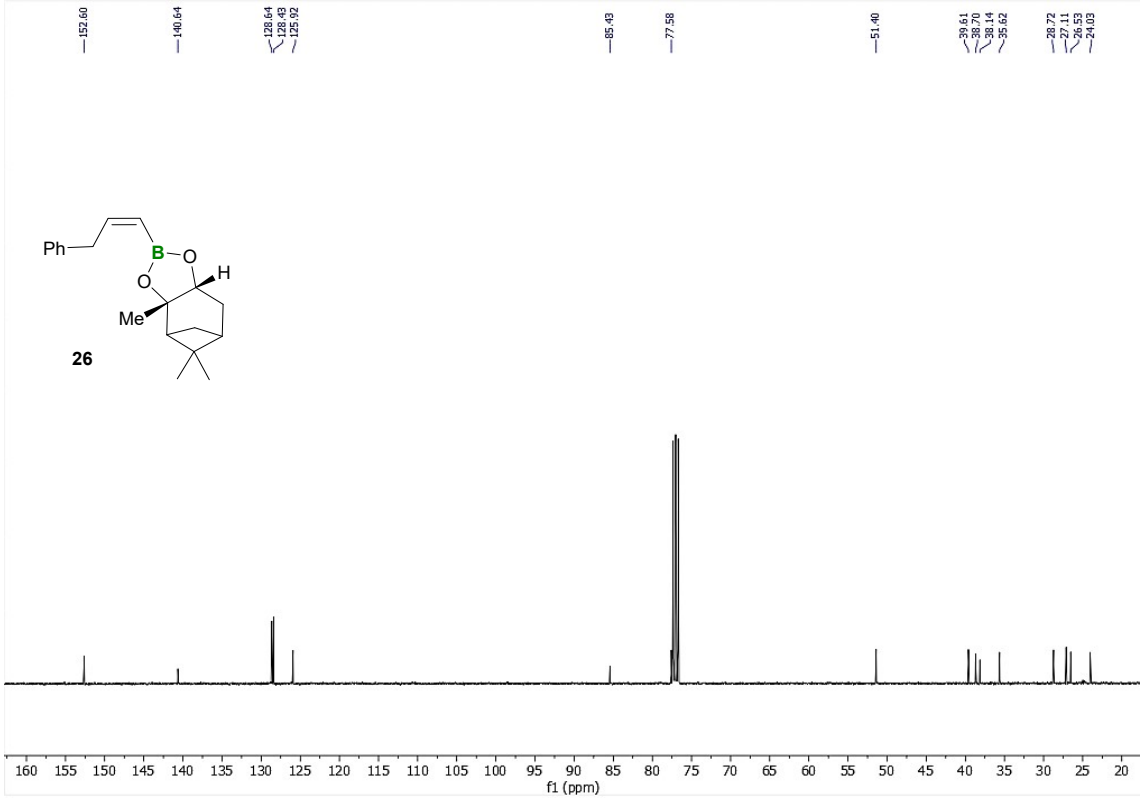

29.88
H
O
B
O
Me
MeO
24
52 50 48 46 44 42 40 38 36 34 32 30 28 26 24 22 20 18 16 14 12 10 8 6 4 2
f1 (ppm)

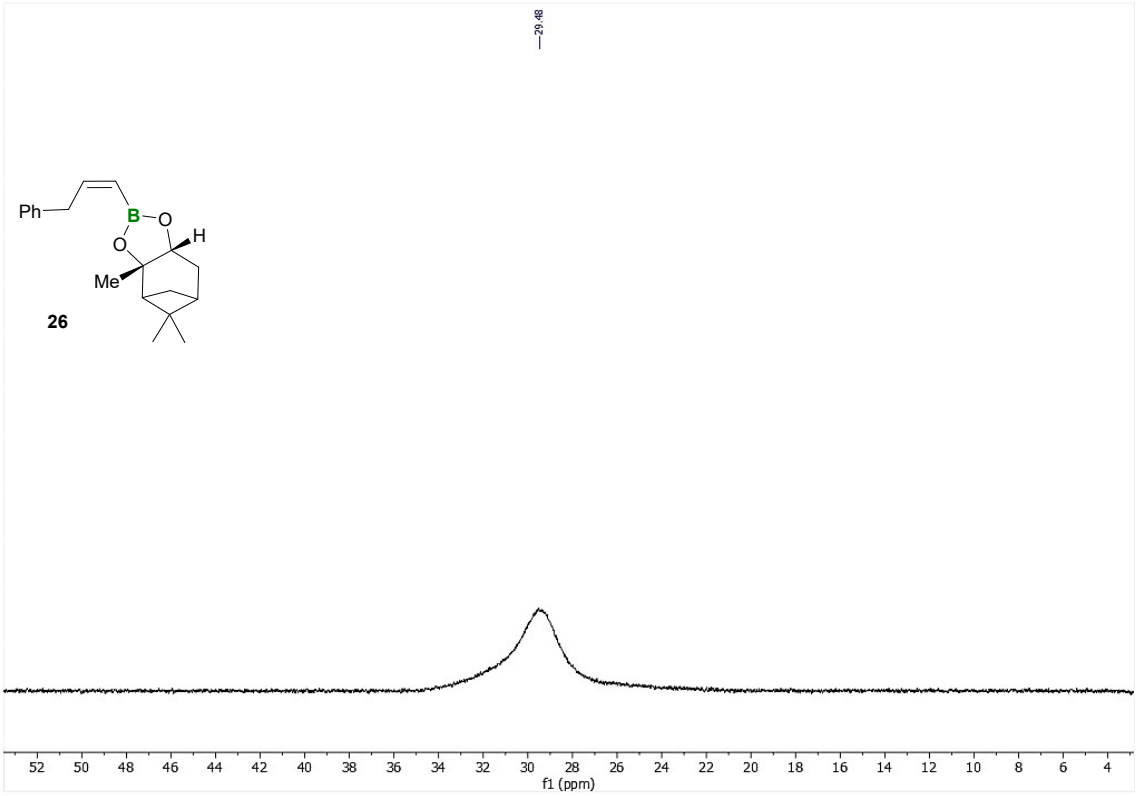

H
O
B
O
Me
Ph
25
4.44 4.42 4.40 4.38 4.36 4.34 4.32 4.30
f1 (ppm)
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

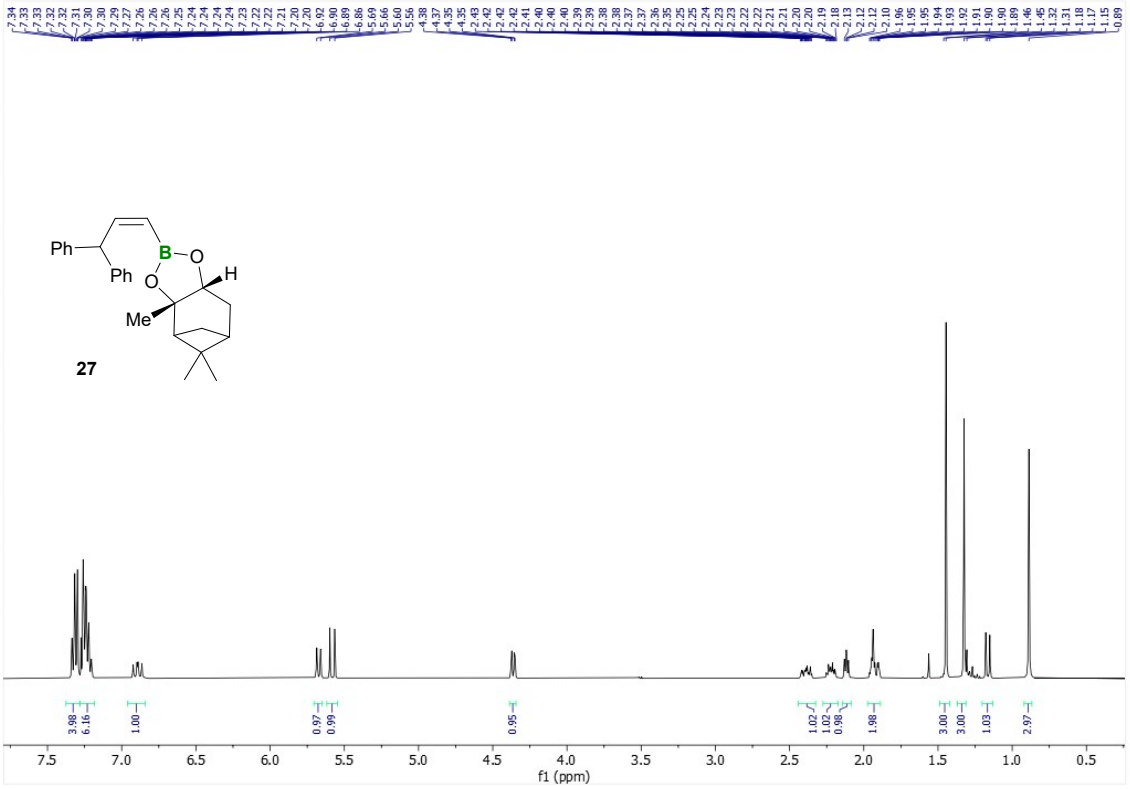

152.33
139.14
128.91
128.45
126.16
85.59
77.70
51.37
42.31
39.52
38.15
35.48
28.64
27.10
26.44
24.01
H
O
Me
B
O
Ph
25
155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25
f1 (ppm)

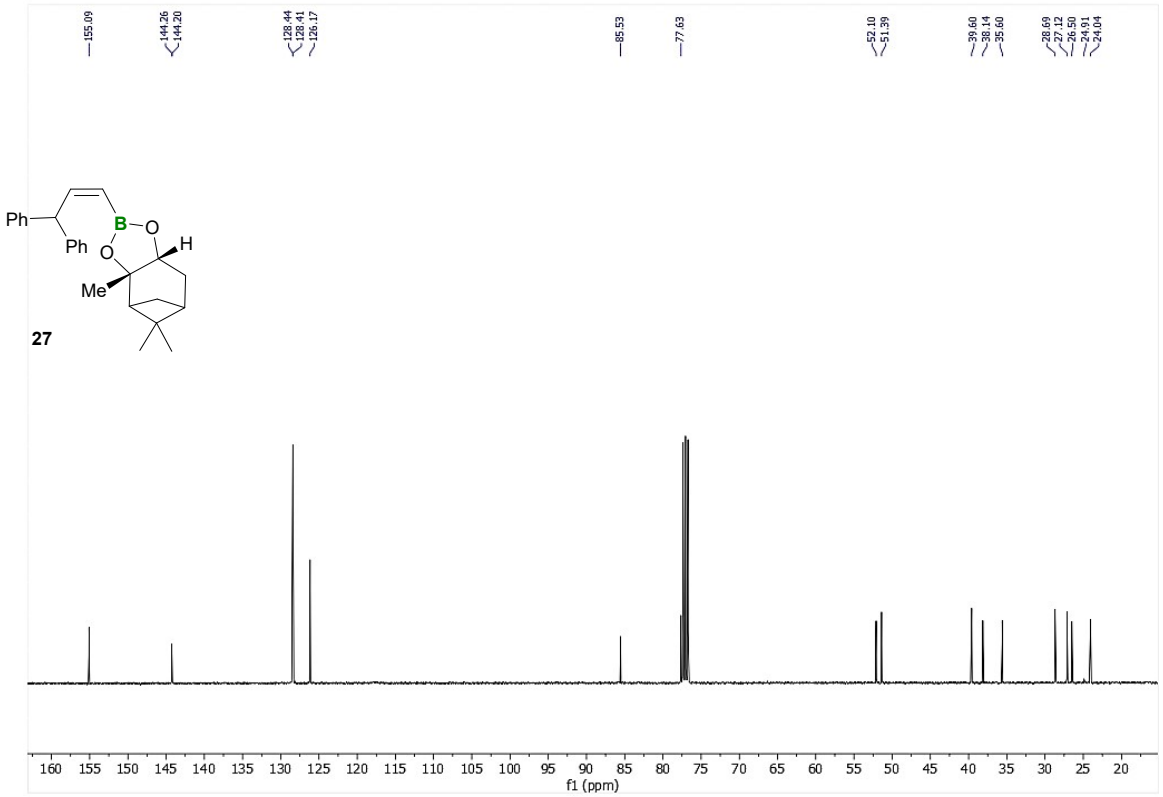

29.57
H
O
Me
B
O
Ph
25
50 48 46 44 42 40 38 36 34 32 30 28 26 24 22 20 18 16 14 12 10 8 6 4 2 0
f1 (ppm)

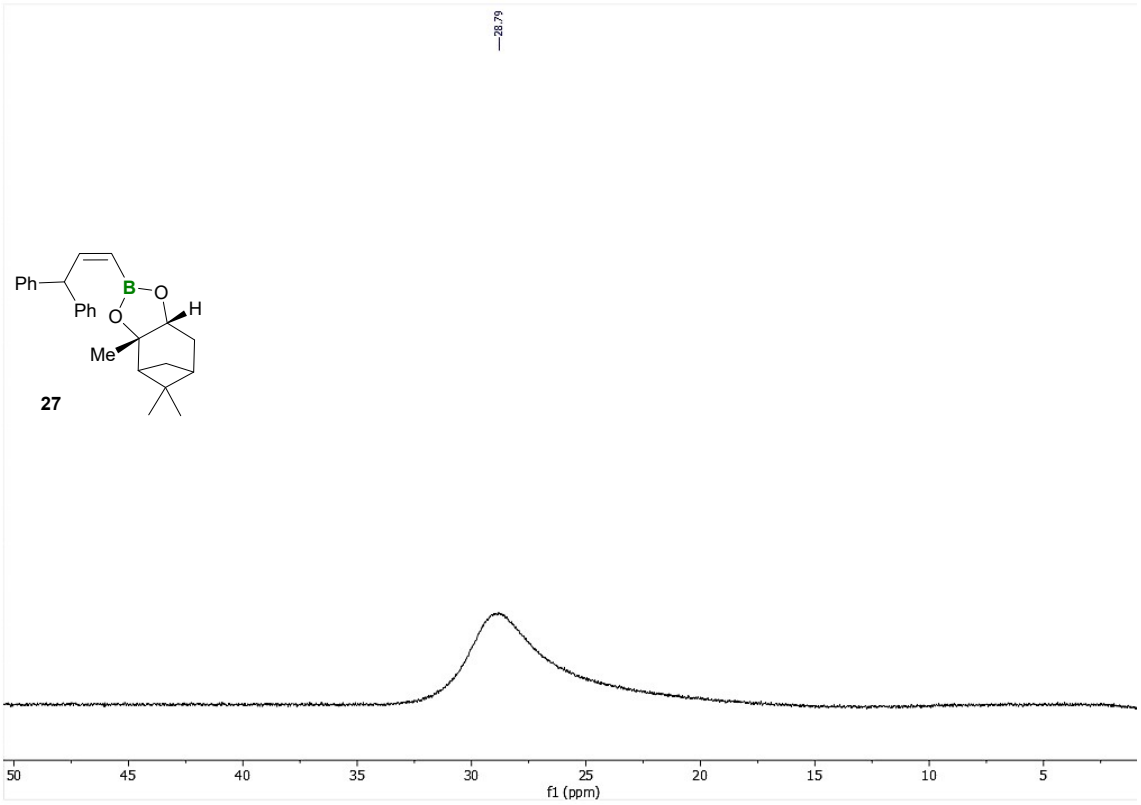

Ph
B
O
O
H
Me
26
2.52
3.15
1.00
0.97
0.98
1.85
1.02
1.04
0.98
1.98
2.94
3.43
1.31
2.98
f1 (ppm)

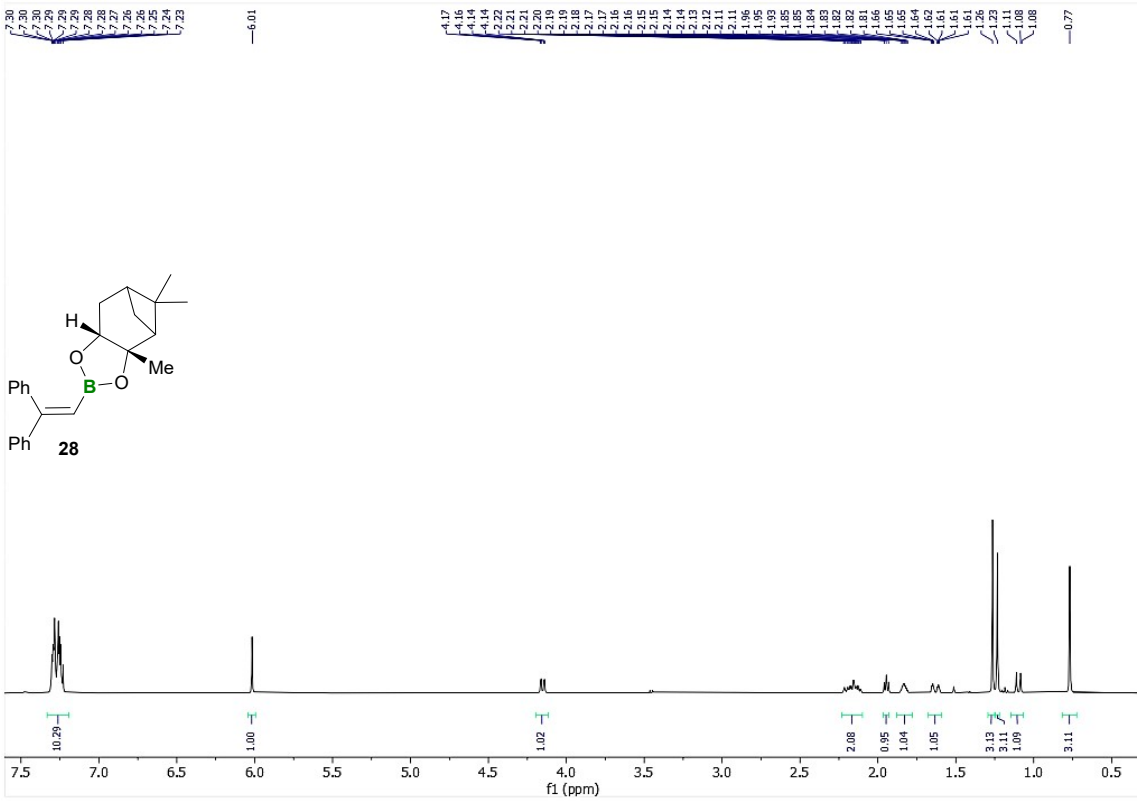

152.60
140.64
128.64
128.45
125.92
85.43
77.58
51.40
39.61
38.70
38.14
35.62
28.72
27.11
26.53
24.03
Ph
B
O
O
H
Me
26
f1 (ppm)

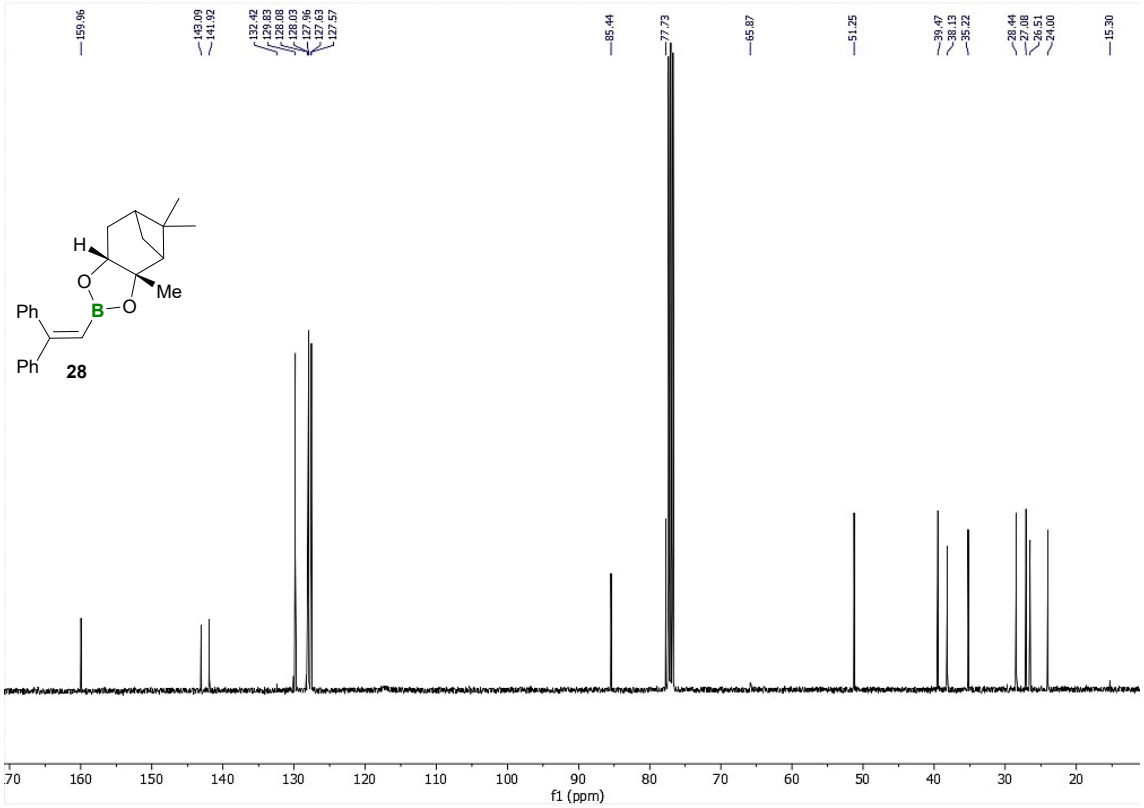

29.48
Ph
B
O
O
H
Me
26
52 50 48 46 44 42 40 38 36 34 32 30 28 26 24 22 20 18 16 14 12 10 8 6 4
f1 (ppm)

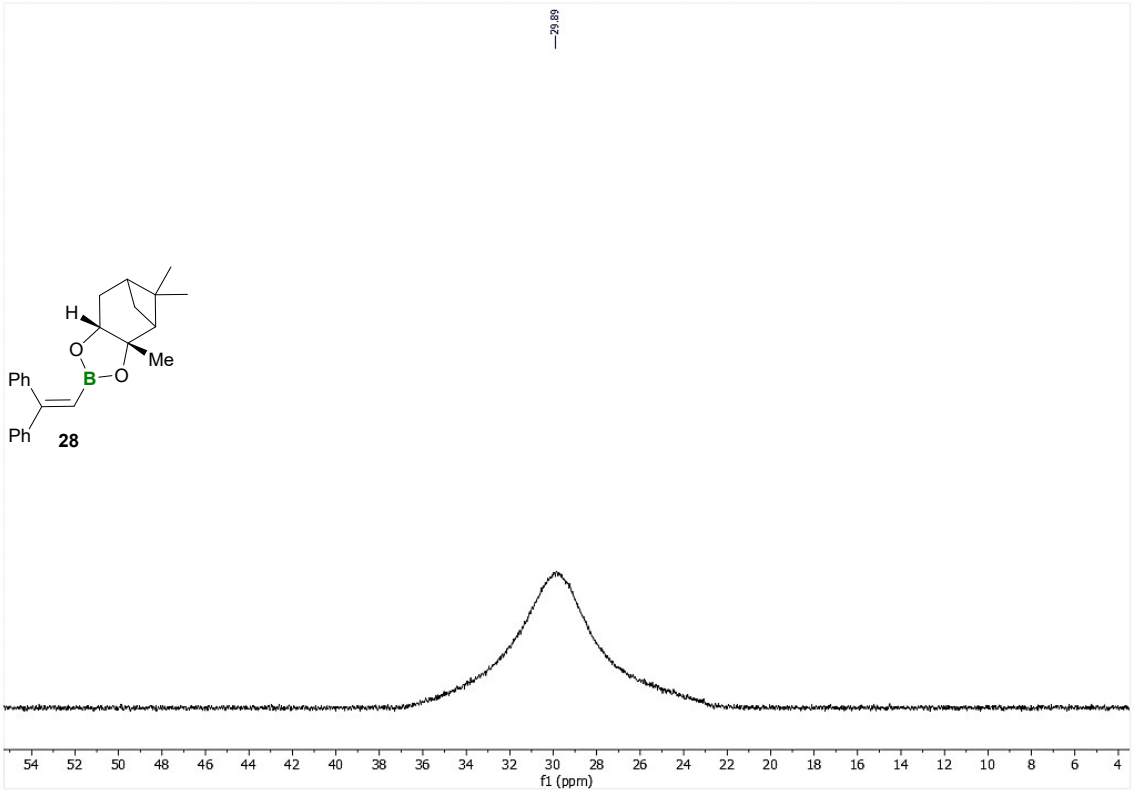

Ph
Ph
B
O
O
H
Me
27
3.98
6.16
1.00
0.97
0.99
0.95
1.02
1.02
0.98
1.98
3.00
3.00
1.03
2.97
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

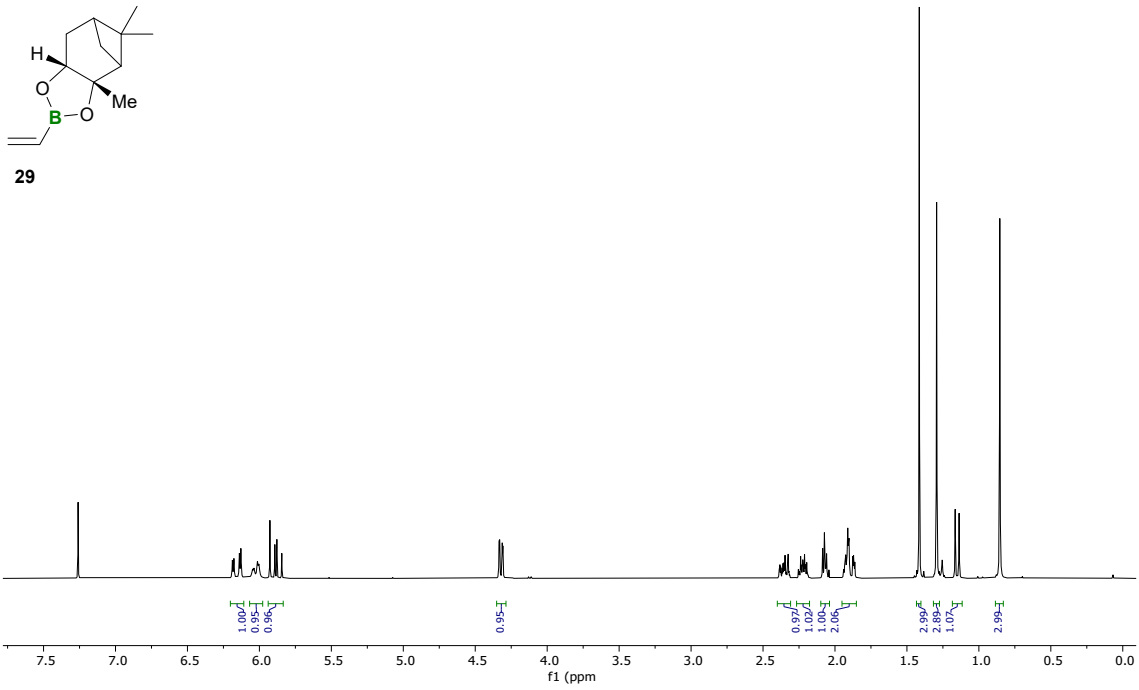

155.09
144.26
144.20
128.44
128.41
126.17
85.53
77.63
52.10
51.39
39.60
38.14
35.60
28.69
27.12
26.50
24.01
24.04
Ph
Ph
B
O
O
H
Me
27
160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20
f1 (ppm)

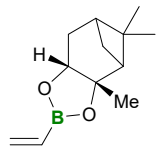

28.79
Ph
Ph
B
O
O
H
Me
27
50 45 40 35 30 25 20 15 10 5
f1 (ppm)


H
O
Me
Ph
B
O
Ph
28
10.29
1.00
1.02
2.08
0.95
1.04
1.05
3.13
3.11
1.09
3.11
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


159.96
143.09
141.92
132.42
129.83
128.08
128.03
127.96
127.63
127.57
85.44
77.73
65.87
51.25
39.47
38.13
35.22
28.44
27.08
26.51
24.00
15.30
H
O
Me
Ph
B
O
Ph
28
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

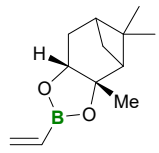

29.89
H
O
B
O
Me
Ph
Ph
28
f1 (ppm)


H
O
B
O
Me
29
1.00
0.95
0.96
0.95
0.97
1.02
1.00
2.06
2.99
2.89
1.07
2.99
f1 (ppm)

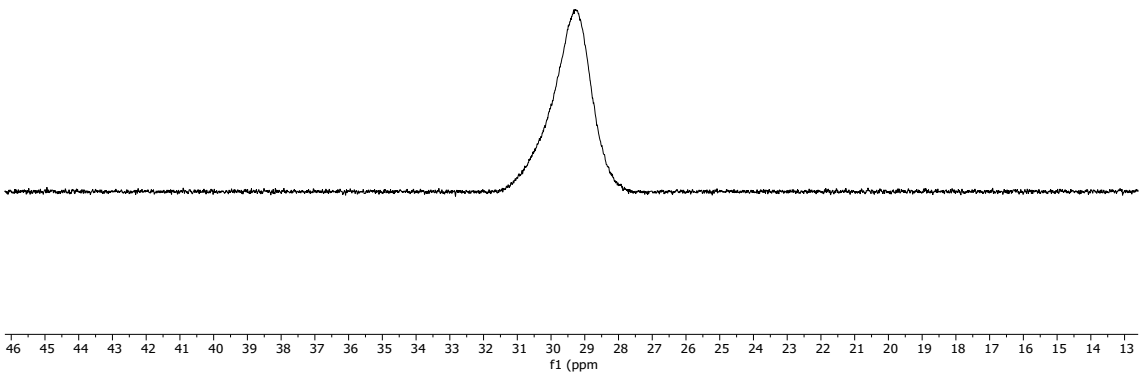

H
O
B
O
Me

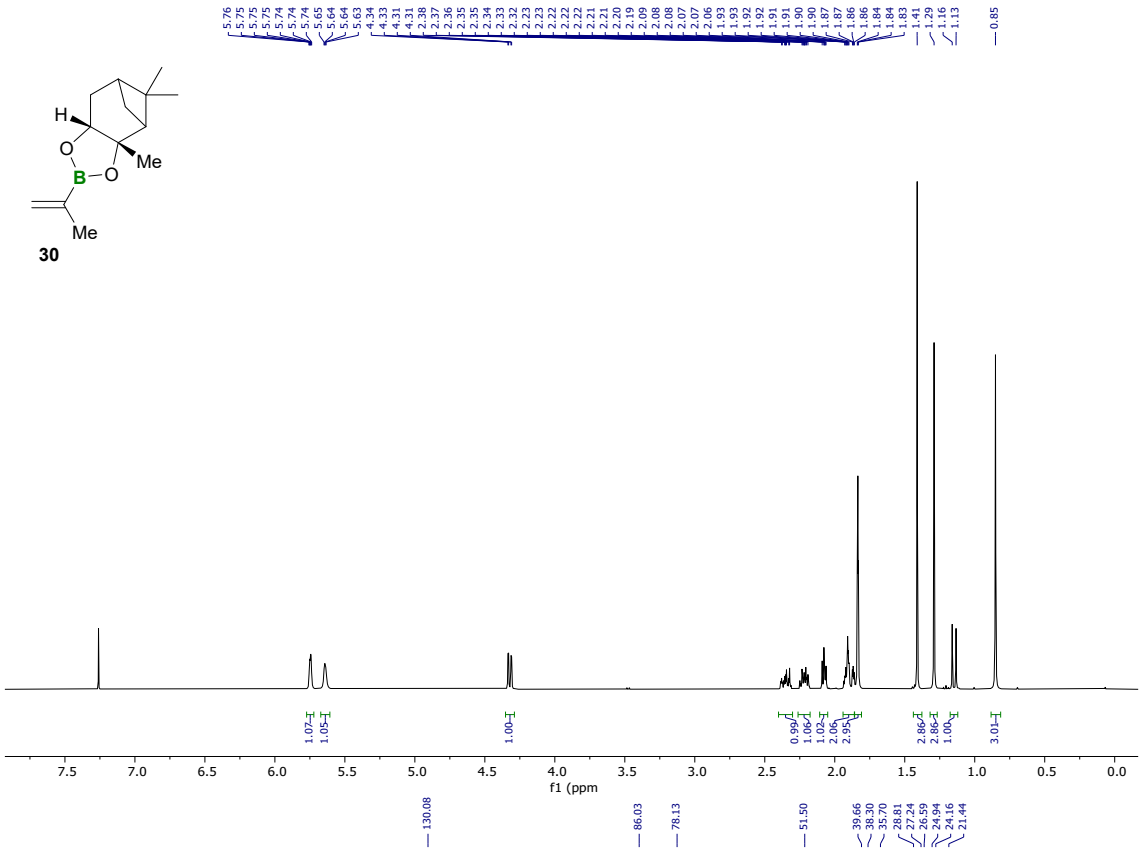
29

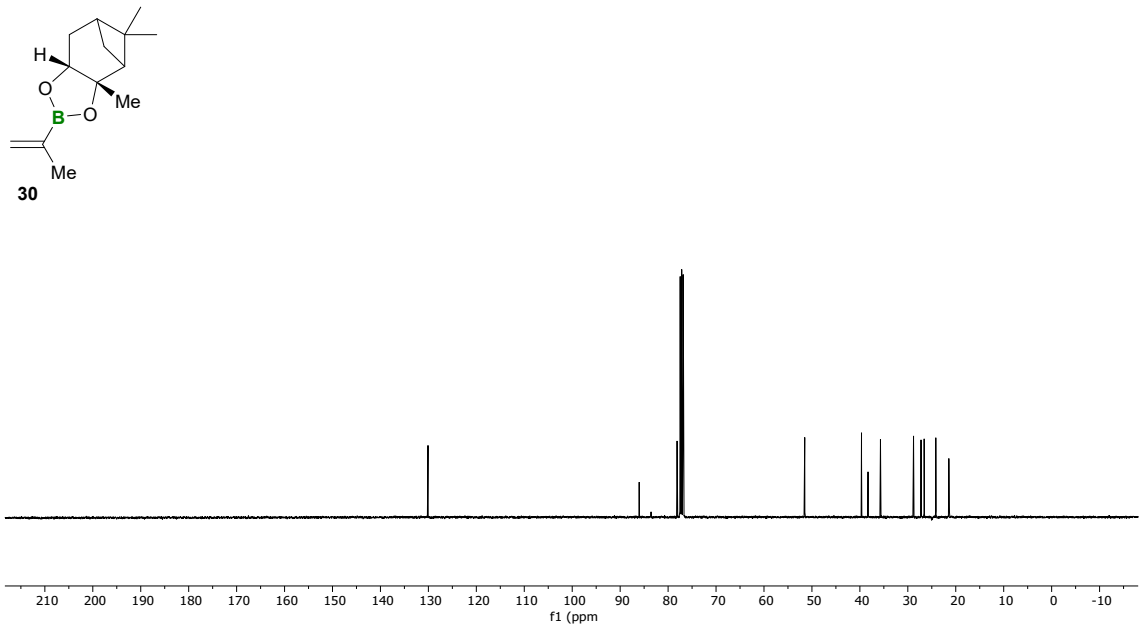
137.13
105.92
77.95
53.56
51.49
39.66
38.31
35.60
28.75
27.24
26.56
24.16
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm
29.35

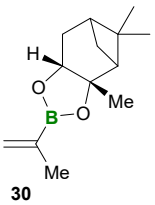

H
O
B
O
Me

29

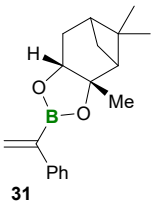

46 45 44 43 42 41 40 39 38 37 36 35 34 33 32 31 30 29 28 27 26 25 24 23 22 21 20 19 18 17 16 15 14 13
f1 (ppm


H
O
B
O
Me
Me
30
f1 (ppm)

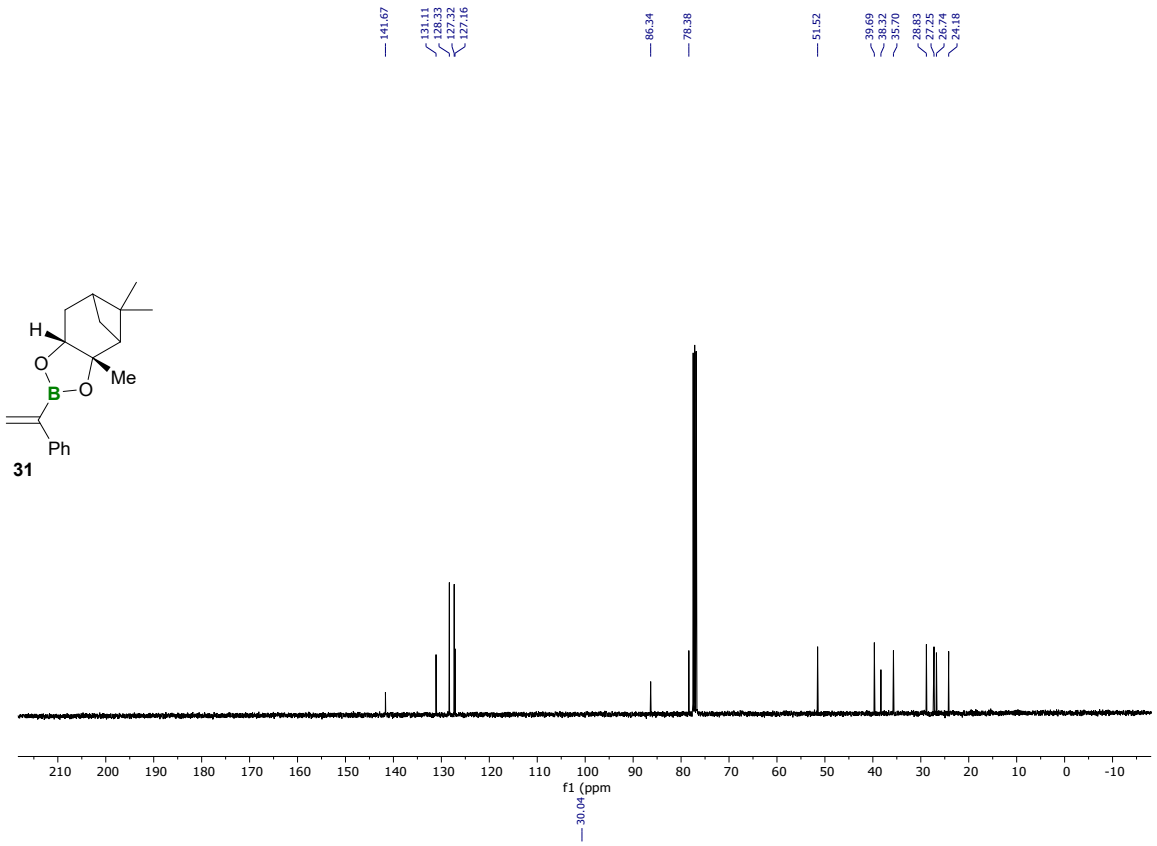

H
O
B
O
Me
Me
30
f1 (ppm)

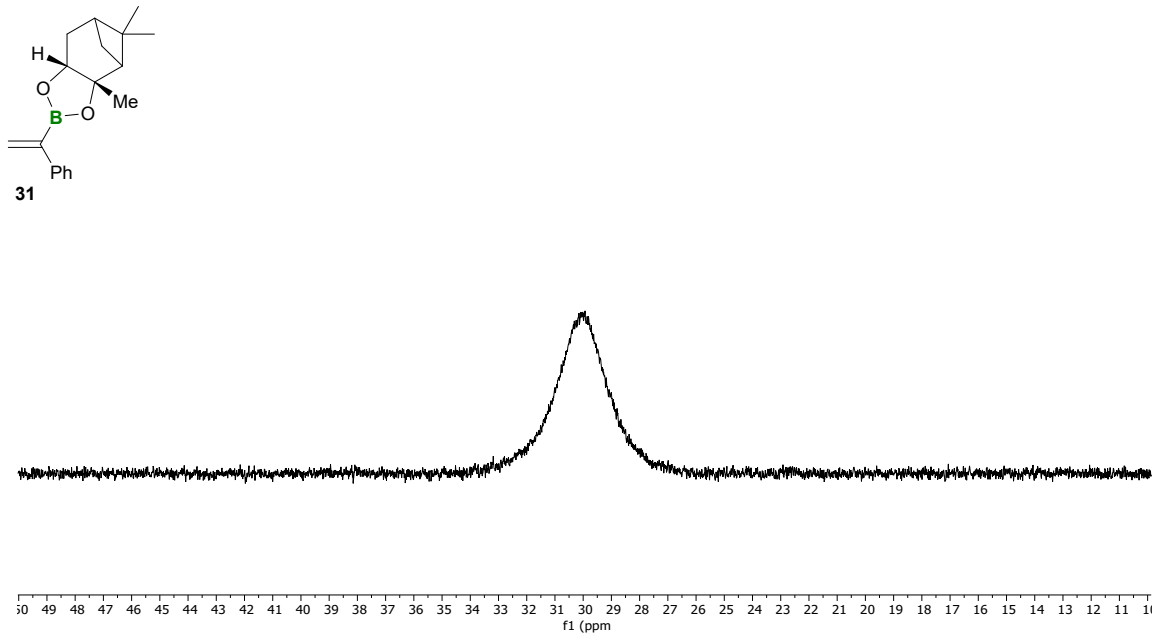


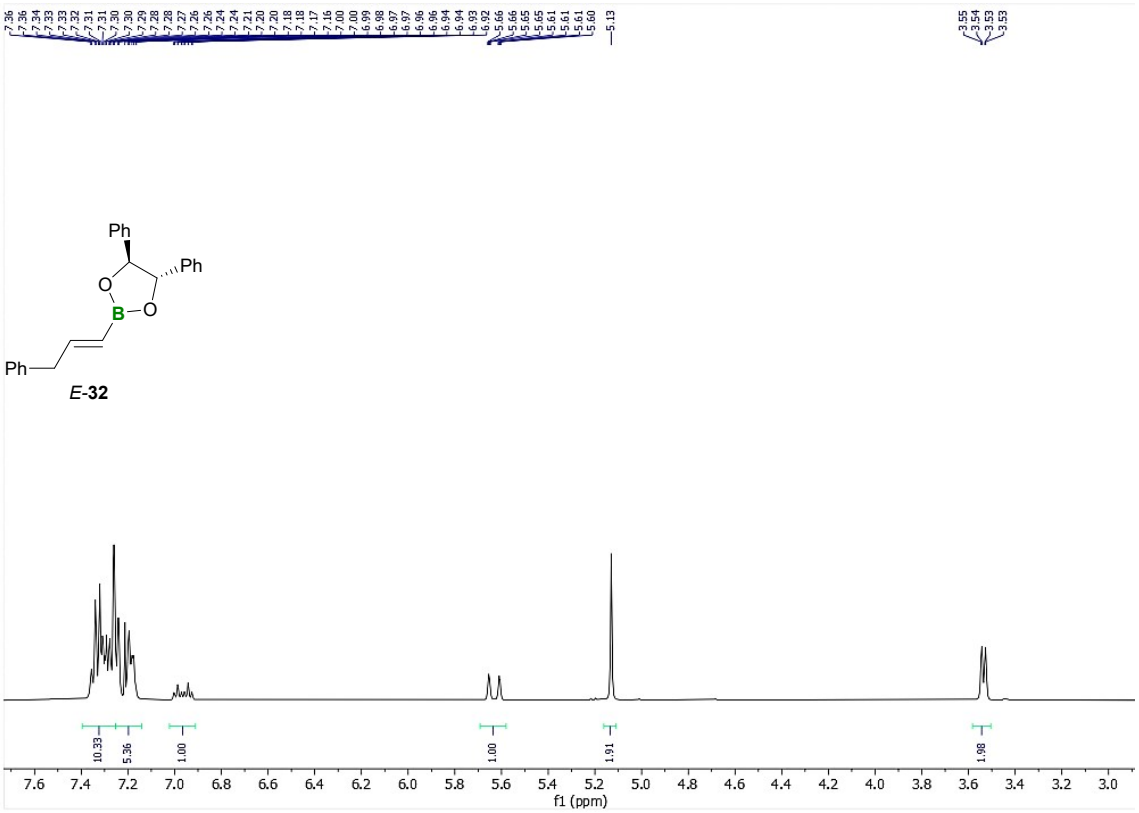
30



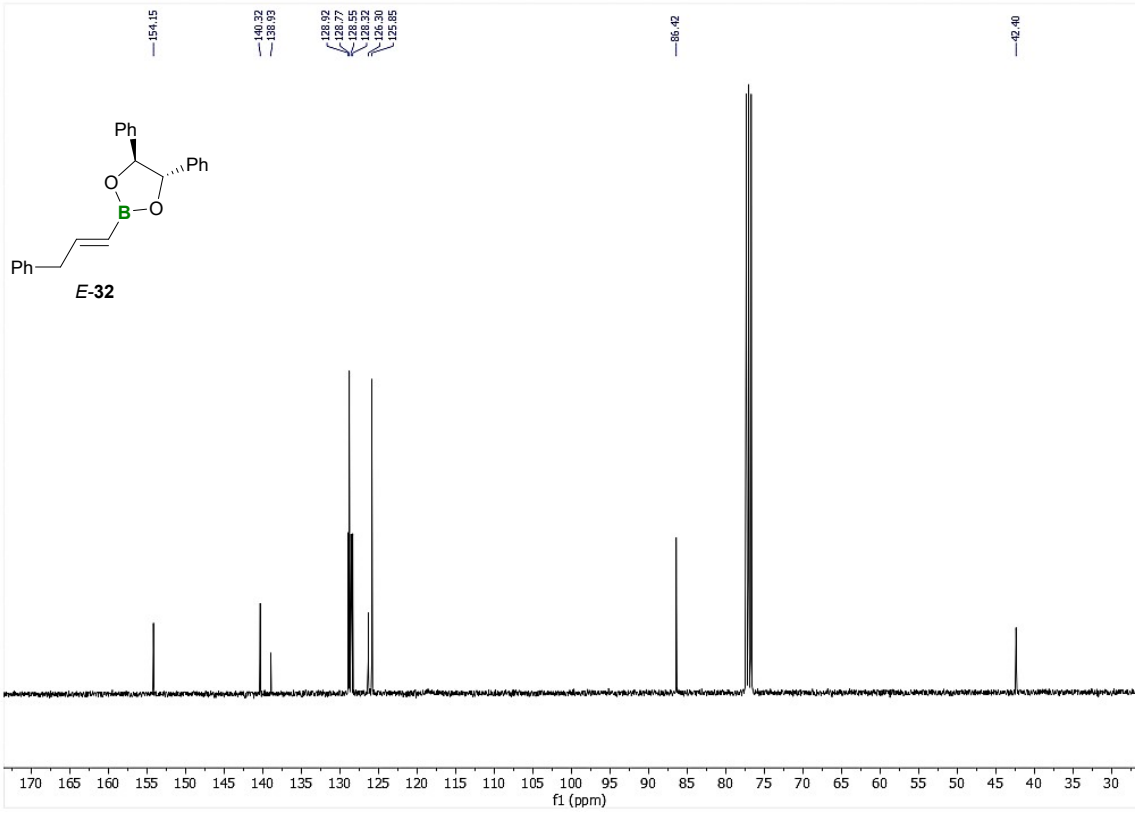
31


141.67
131.11
128.33
127.32
127.16
86.34
78.38
51.52
39.69
38.22
35.70
28.83
27.25
26.74
24.18
H
O
B
O
Me
Ph
31
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm
30.04

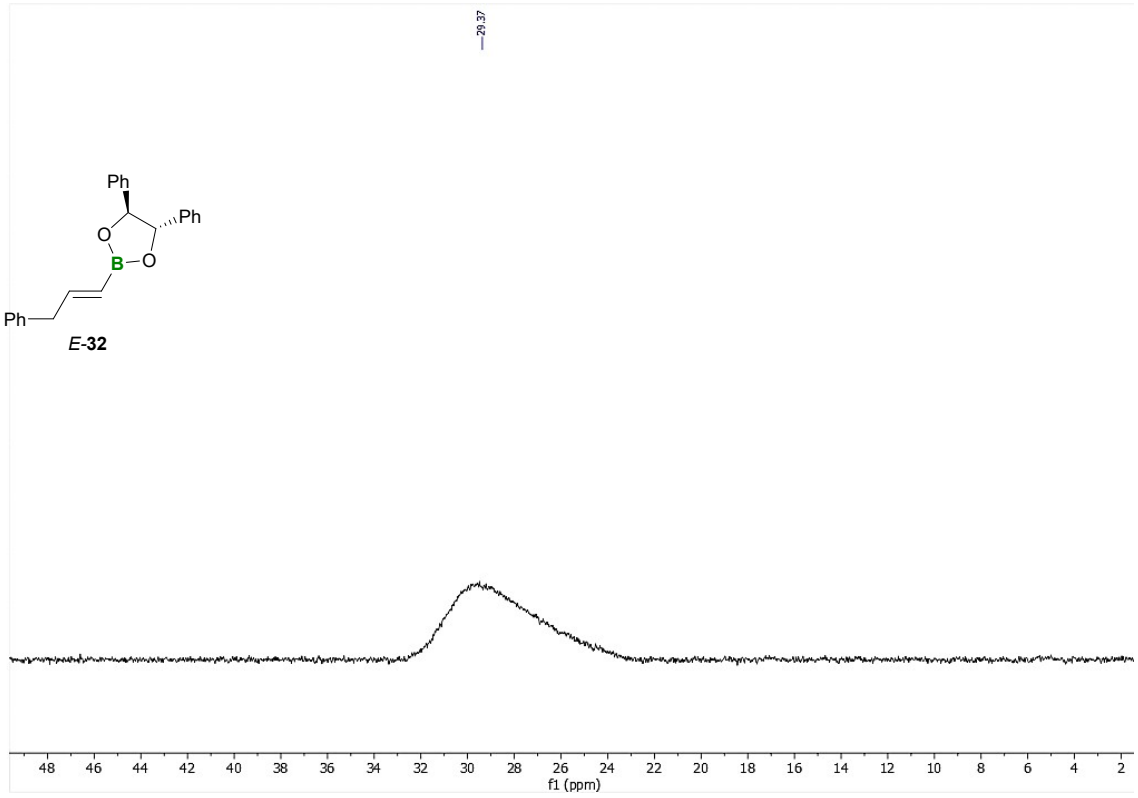

H
O
B
O
Me
Ph
31
50 49 48 47 46 45 44 43 42 41 40 39 38 37 36 35 34 33 32 31 30 29 28 27 26 25 24 23 22 21 20 19 18 17 16 15 14 13 12 11
f1 (ppm


Ph
Ph
O
B
O
Ph
10.33
5.36
1.00
1.00
1.91
1.98
f1 (ppm)

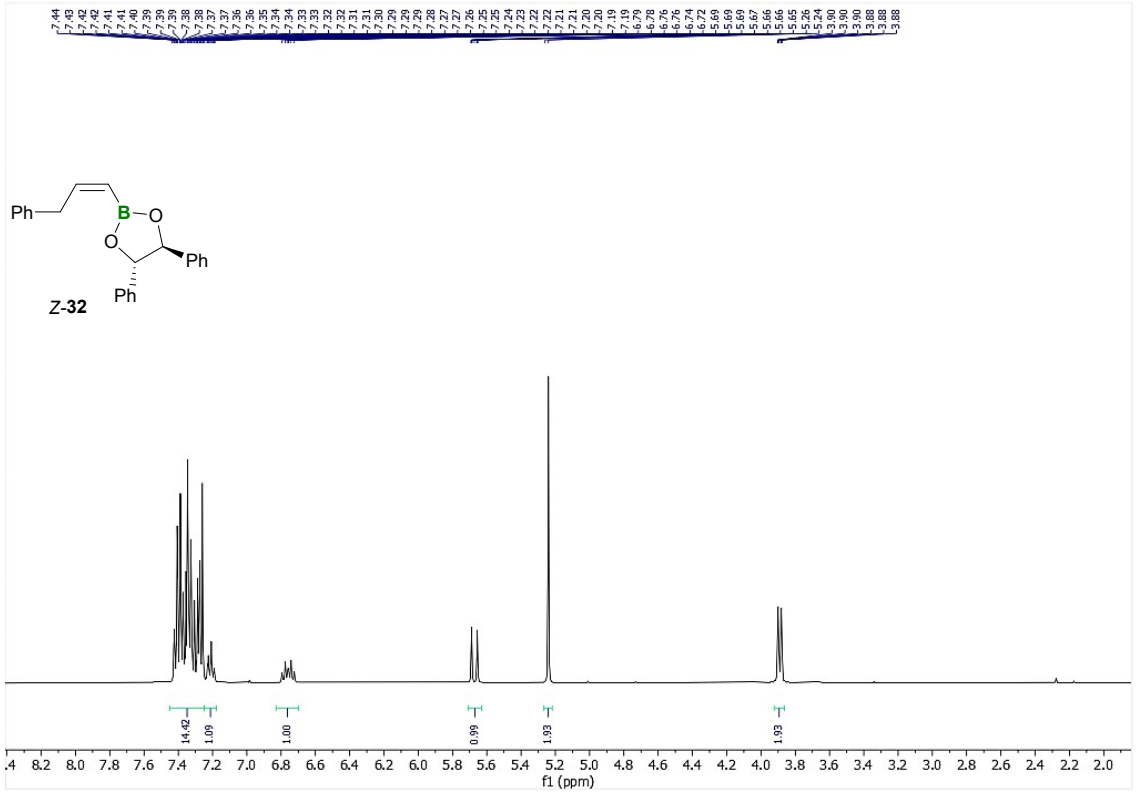
E-**32**


154.15
140.32
138.93
128.92
128.77
128.55
128.32
126.30
125.85
86.42
42.40
Ph
Ph
O
B
O
Ph
f1 (ppm)

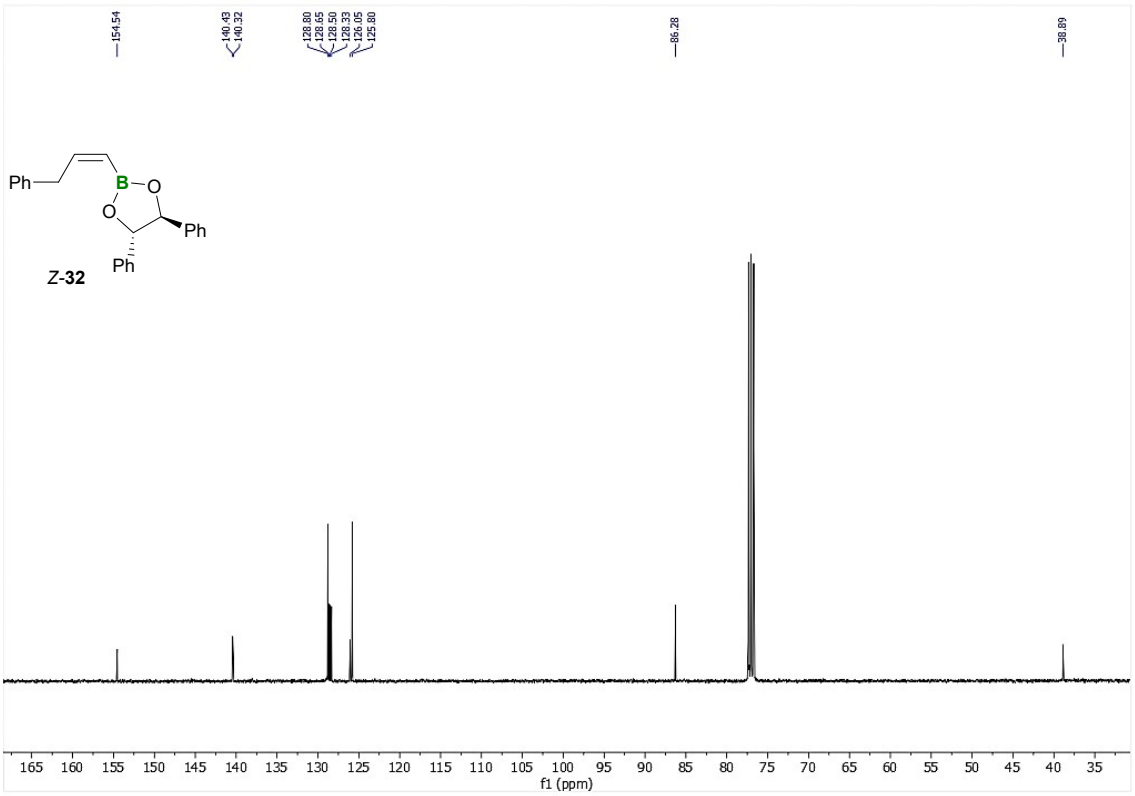
E-**32**

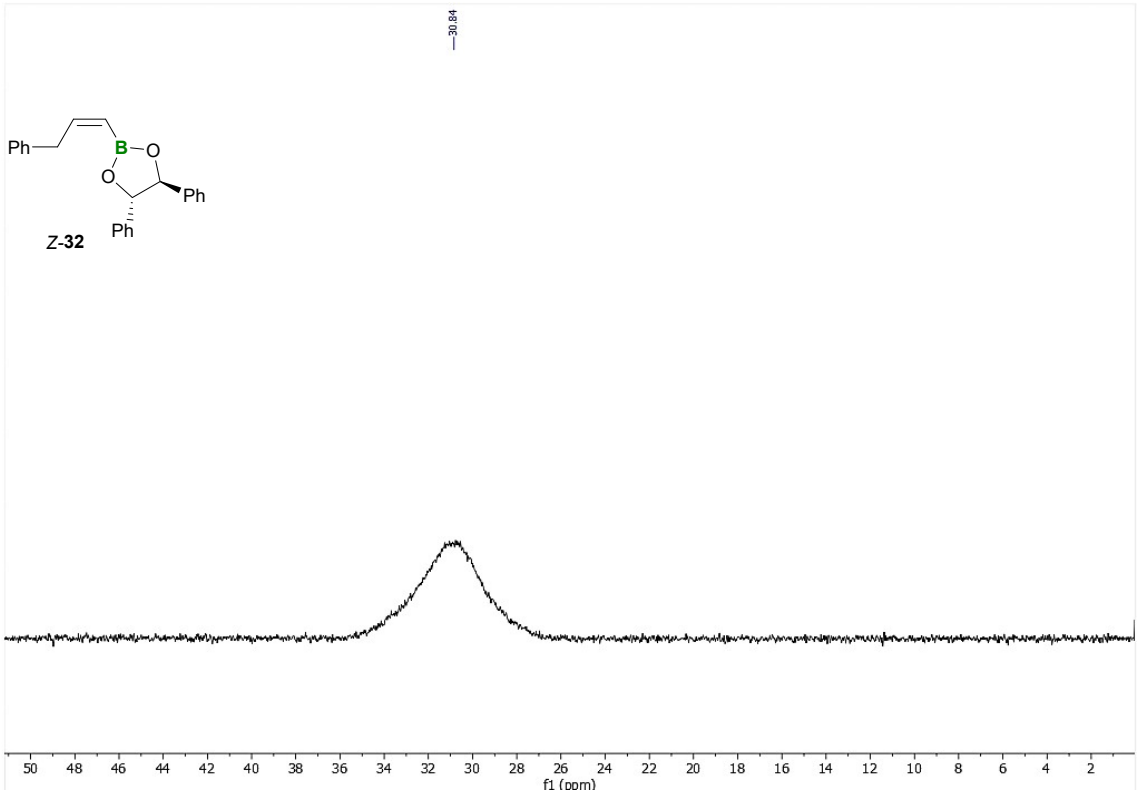

29.37
Ph
Ph
O
B
O
Ph
48 46 44 42 40 38 36 34 32 30 28 26 24 22 20 18 16 14 12 10 8 6 4 2
f1 (ppm)

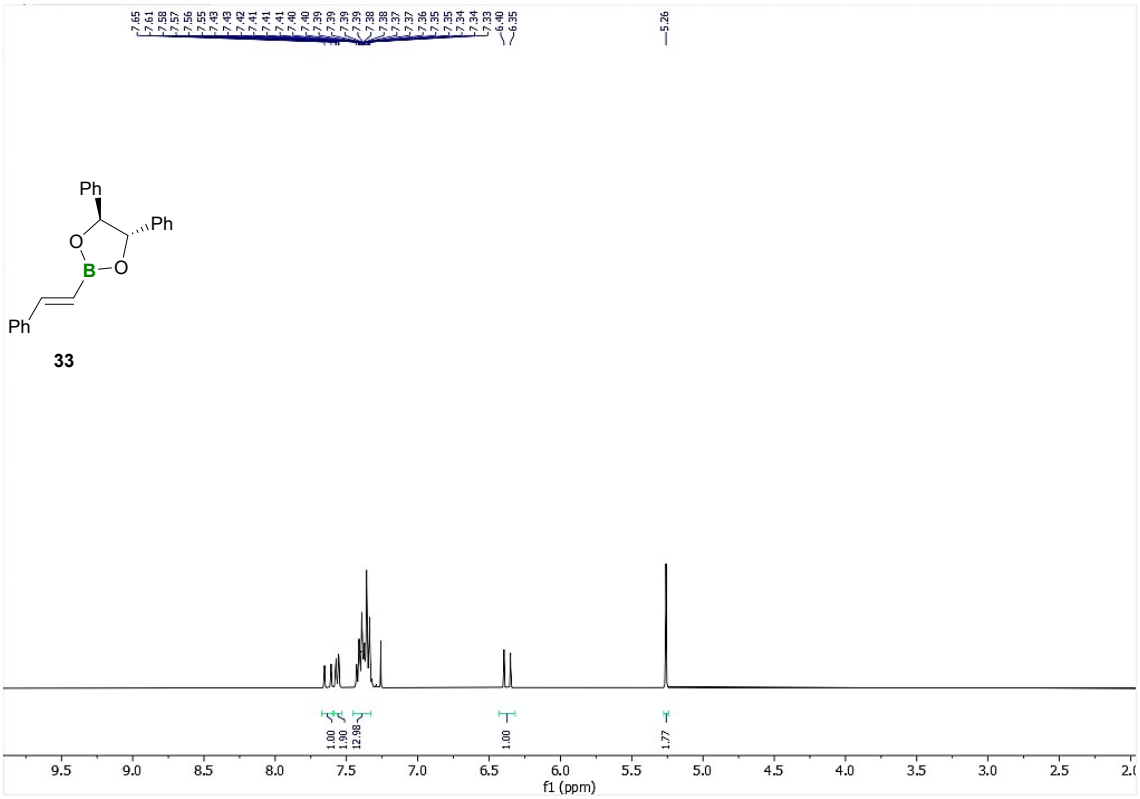
E-**32**

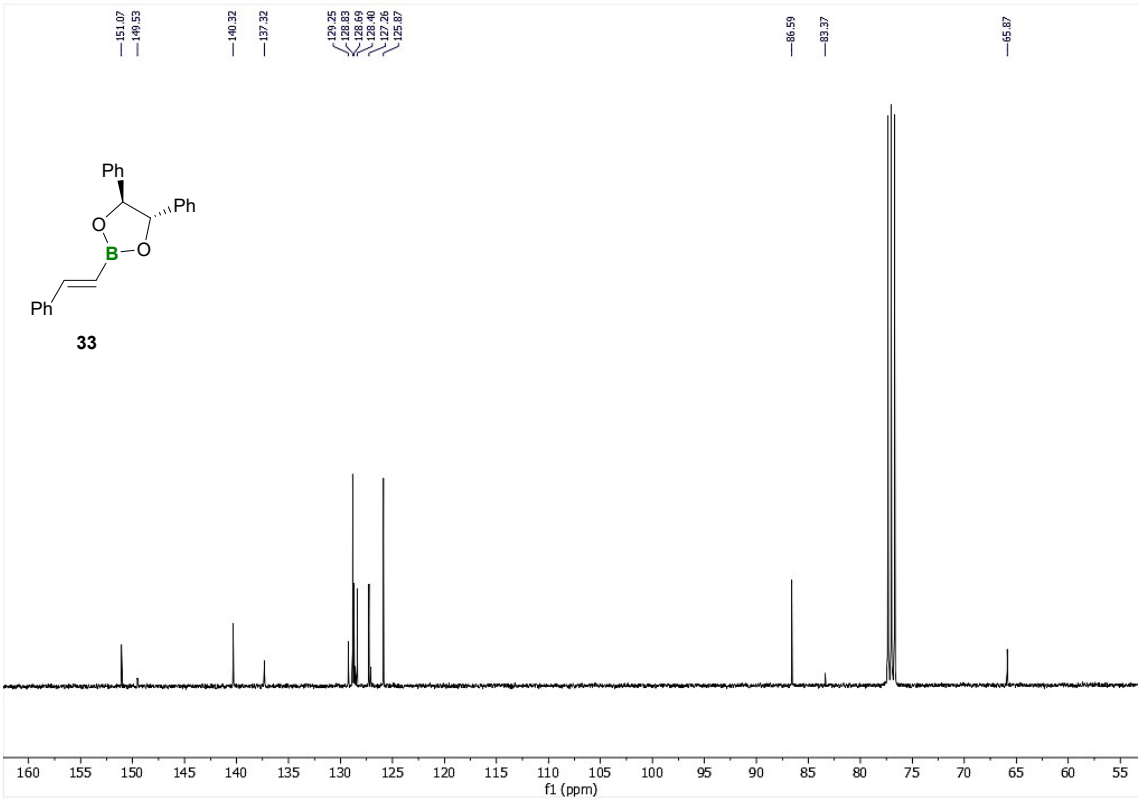

Ph
B
O
O
Ph
Ph
14.42
1.09
1.00
0.99
1.93
1.93
f1 (ppm)

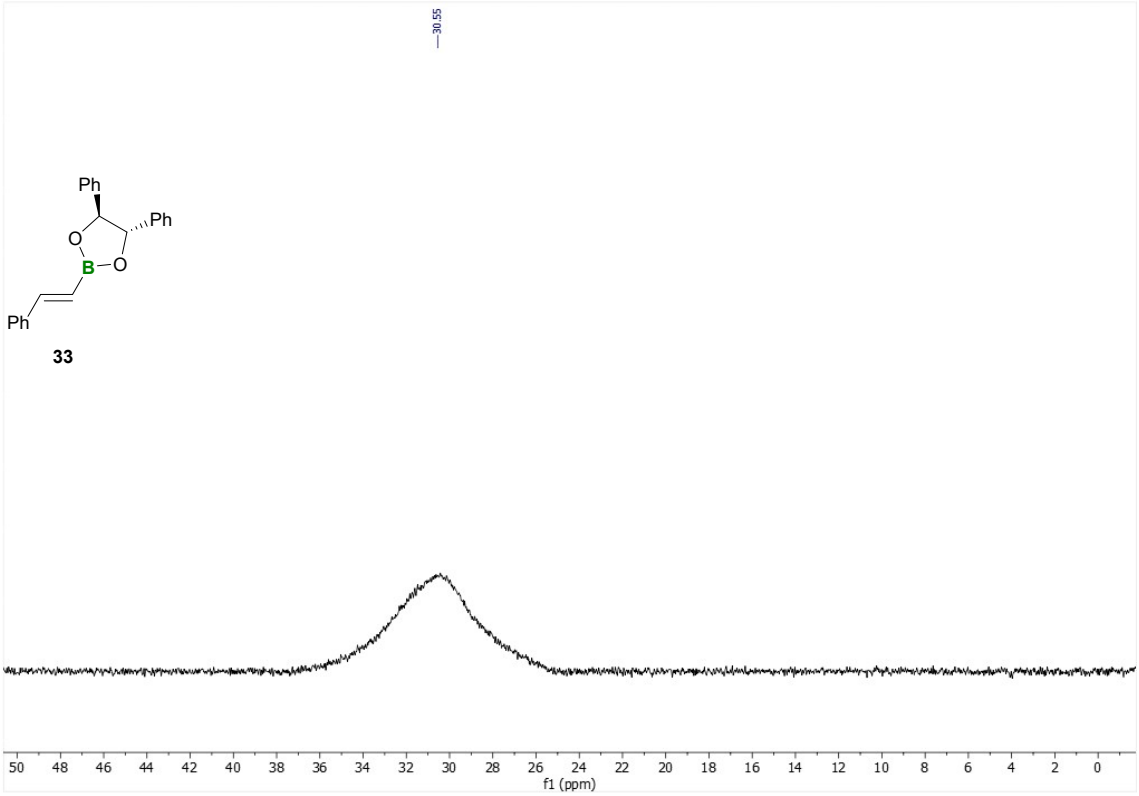
Z-**32**


154.54
140.43
140.32
128.80
128.65
128.50
128.33
126.05
125.80
86.28
38.89
Ph
B
O
O
Ph
Ph
Z-32
165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35
f1 (ppm)

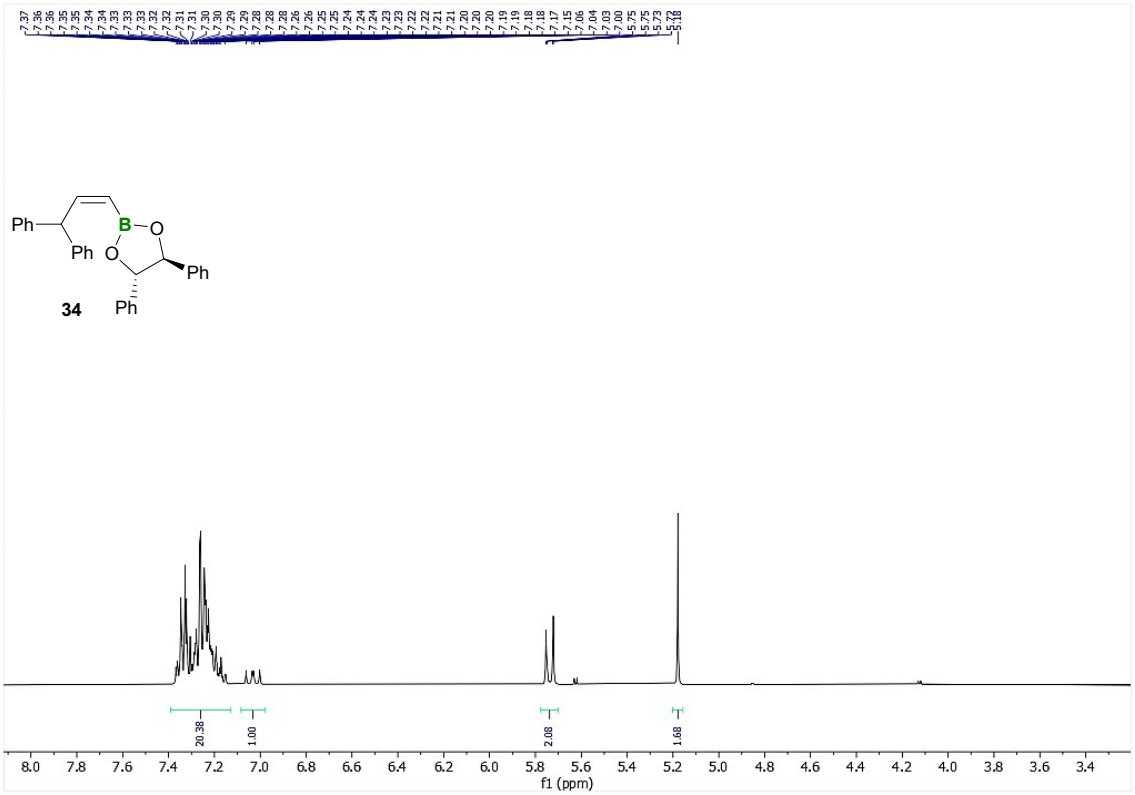

30.84
Ph
B
O
O
Ph
Ph
Z-32
50 48 46 44 42 40 38 36 34 32 30 28 26 24 22 20 18 16 14 12 10 8 6 4 2
f1 (ppm)


Ph
Ph
O
B
O
Ph
33
7.65
7.61
7.58
7.57
7.56
7.55
7.43
7.42
7.41
7.41
7.41
7.40
7.40
7.39
7.39
7.39
7.39
7.38
7.38
7.37
7.37
7.36
7.35
7.35
7.34
7.34
7.33
6.40
6.35
5.26
1.00
1.90
12.98
1.00
1.77
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
f1 (ppm)

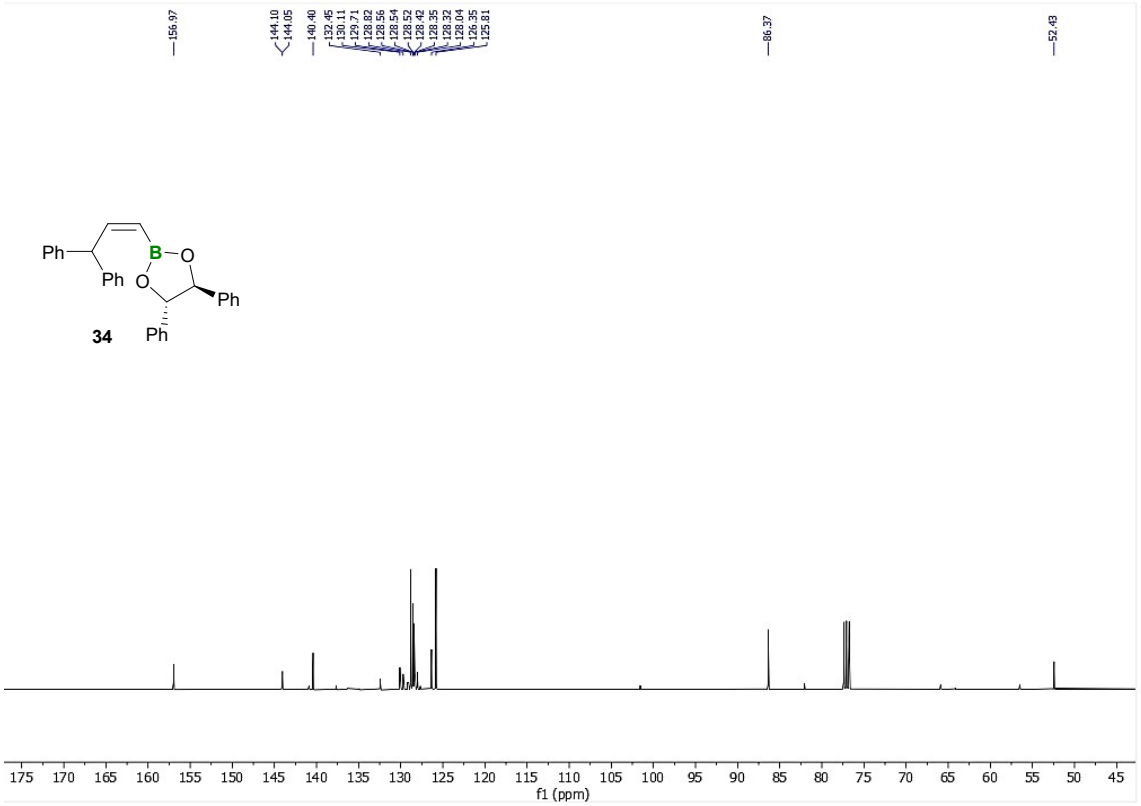

Ph
Ph
O
B
O
Ph
33
151.07
149.53
140.32
137.32
129.25
128.83
128.69
128.40
127.26
125.87
86.59
83.37
65.87
160
155
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
f1 (ppm)

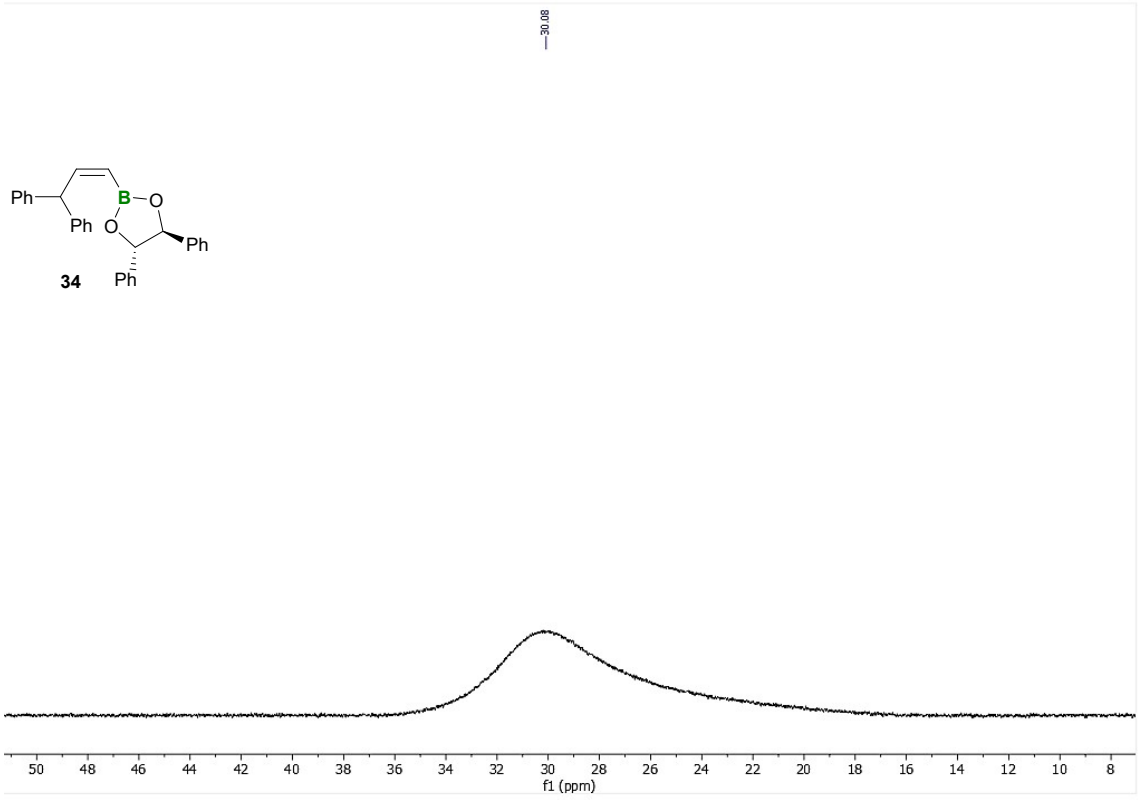

30.55
Ph
Ph
O
B
O
Ph
50 48 46 44 42 40 38 36 34 32 30 28 26 24 22 20 18 16 14 12 10 8 6 4 2 0
f1 (ppm)

33


Ph
B
O
Ph
O
Ph
Ph
20.38
1.00
2.08
1.68
8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4
f1 (ppm)

34


156.97
144.10
144.05
140.40
132.45
130.11
129.71
128.82
128.56
128.54
128.53
128.42
128.35
128.32
128.04
126.35
125.81
86.37
52.43
Ph
Ph
B
O
O
Ph
Ph
34
175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45
f1 (ppm)


30.08
Ph
Ph
B
O
O
Ph
Ph
34
50 48 46 44 42 40 38 36 34 32 30 28 26 24 22 20 18 16 14 12 10 8
f1 (ppm)


7.64
7.64
7.64
7.63
7.62
7.62
7.44
7.44
7.43
7.43
7.42
7.42
7.42
7.41
7.41
7.40
7.40
7.40
7.39
7.39
7.38
7.37
7.36
7.35
7.35
7.34
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7.31
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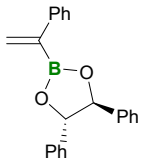
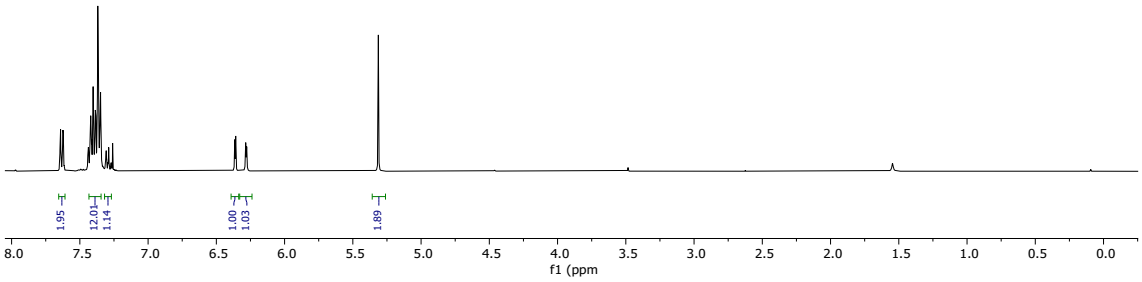
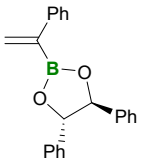
7.29
7.26
6.37
6.36
6.28
6.28
5.31


Ph
B
O
O
Ph
Ph

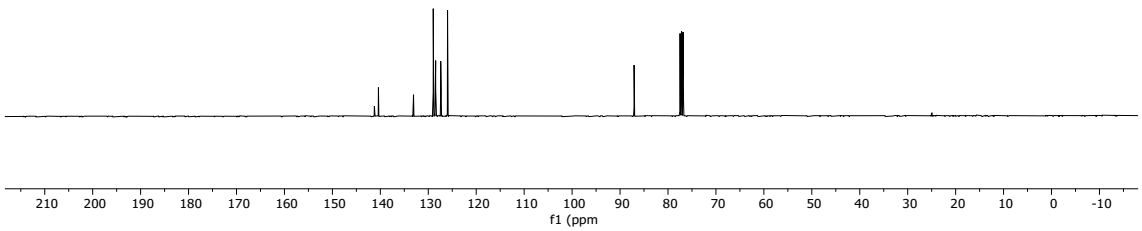
35


1.95
12.01
1.14
1.00
1.03
1.89
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm


141.24
140.40
133.08
129.95
128.53
128.46
127.40
127.37
125.98
87.07


Ph
B
O
O
Ph
Ph

35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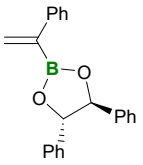
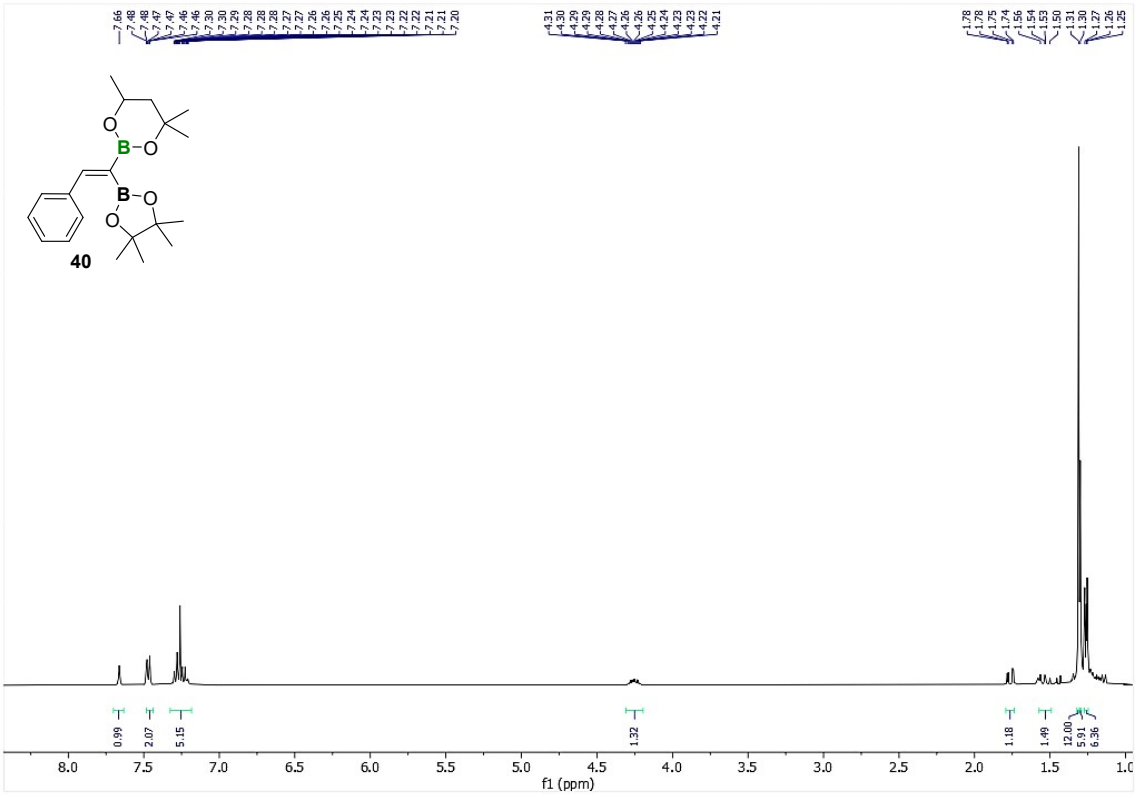
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm


Ph
B
O
O
Ph
Ph

35

31.76
52
50
48
46
44
42
40
38
36
34
32
30
28
26
24
22
20
18
16
14
12
10
f1 (ppm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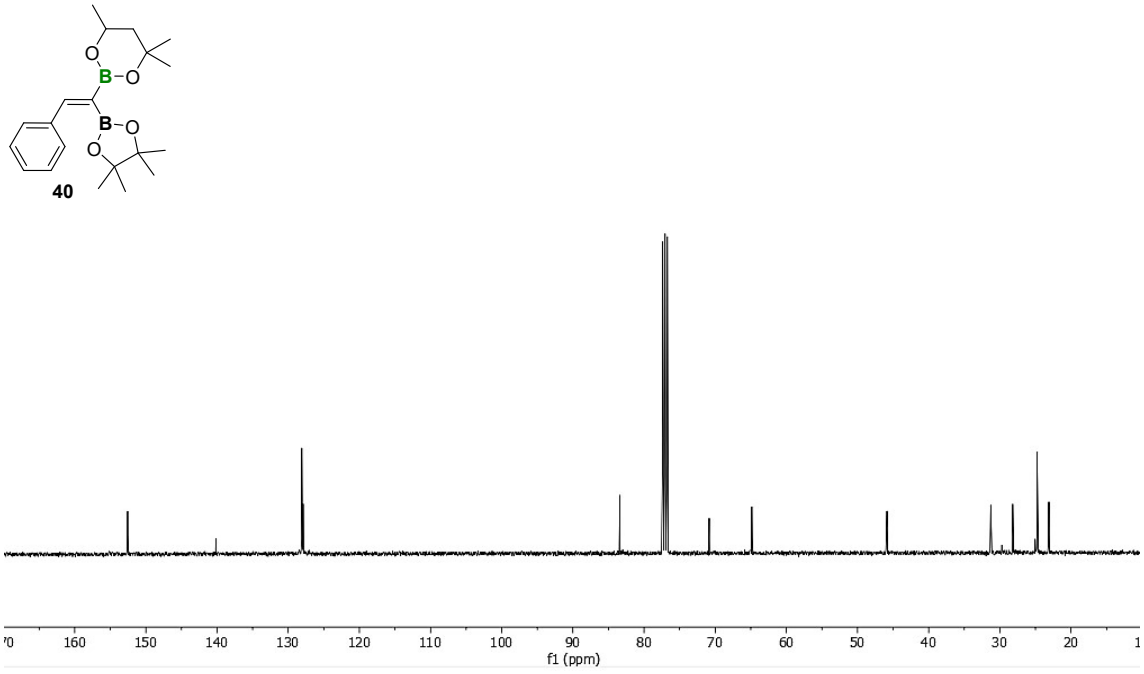
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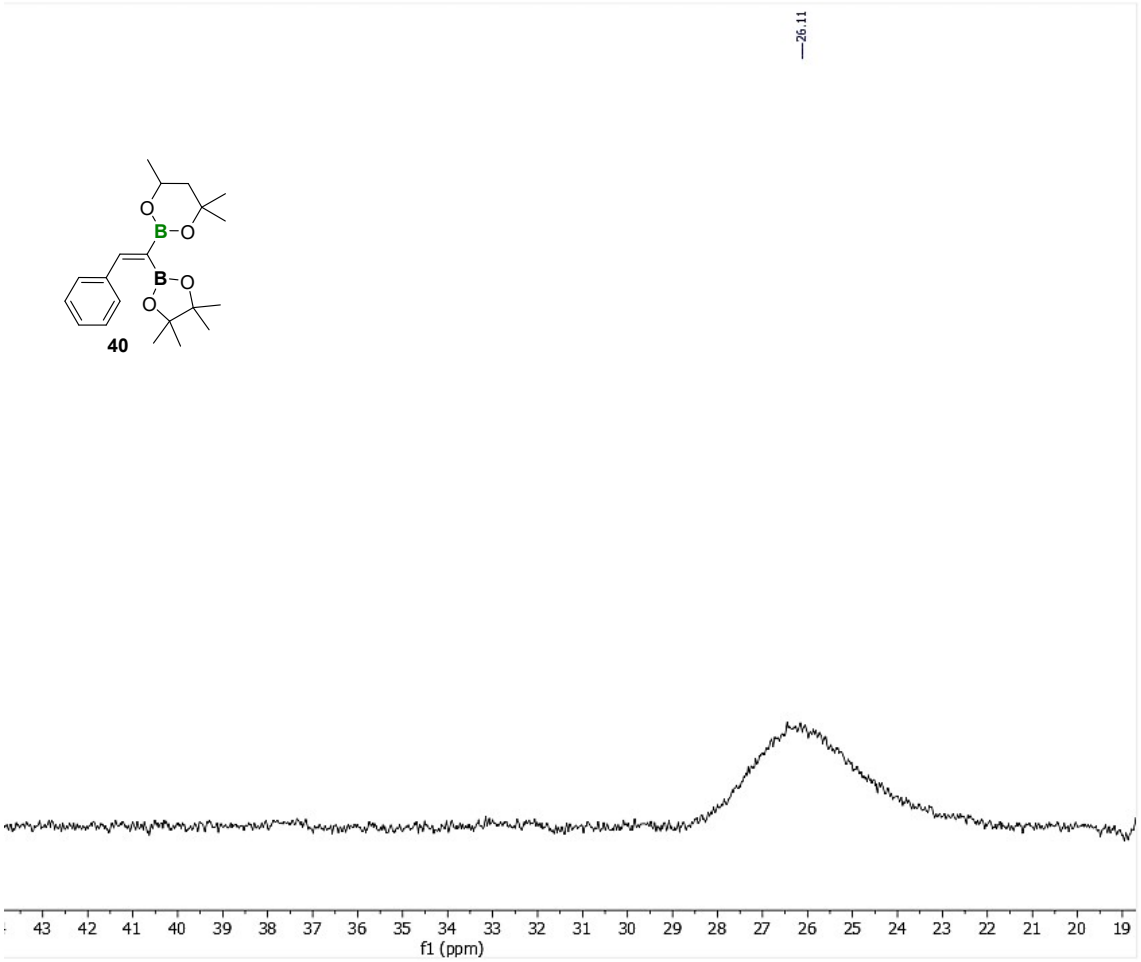
f1 (ppm)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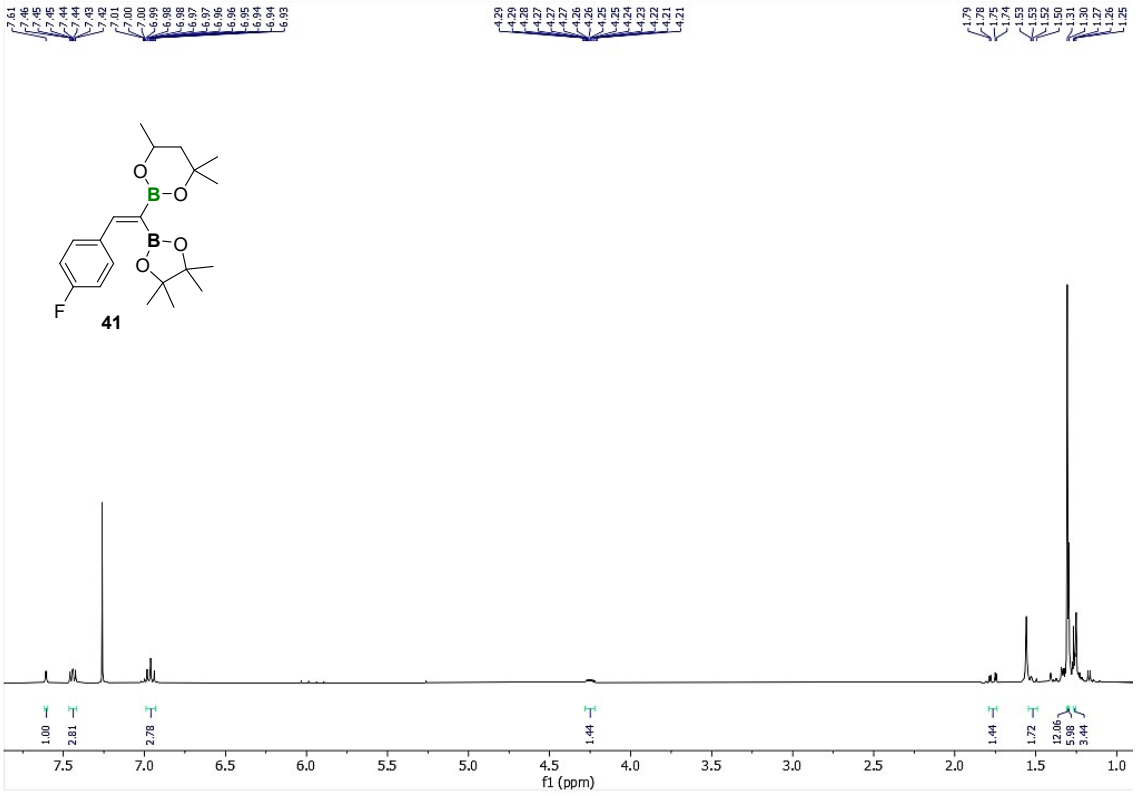
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2.78
1.44
1.44
1.72
12.06
5.98
3.44
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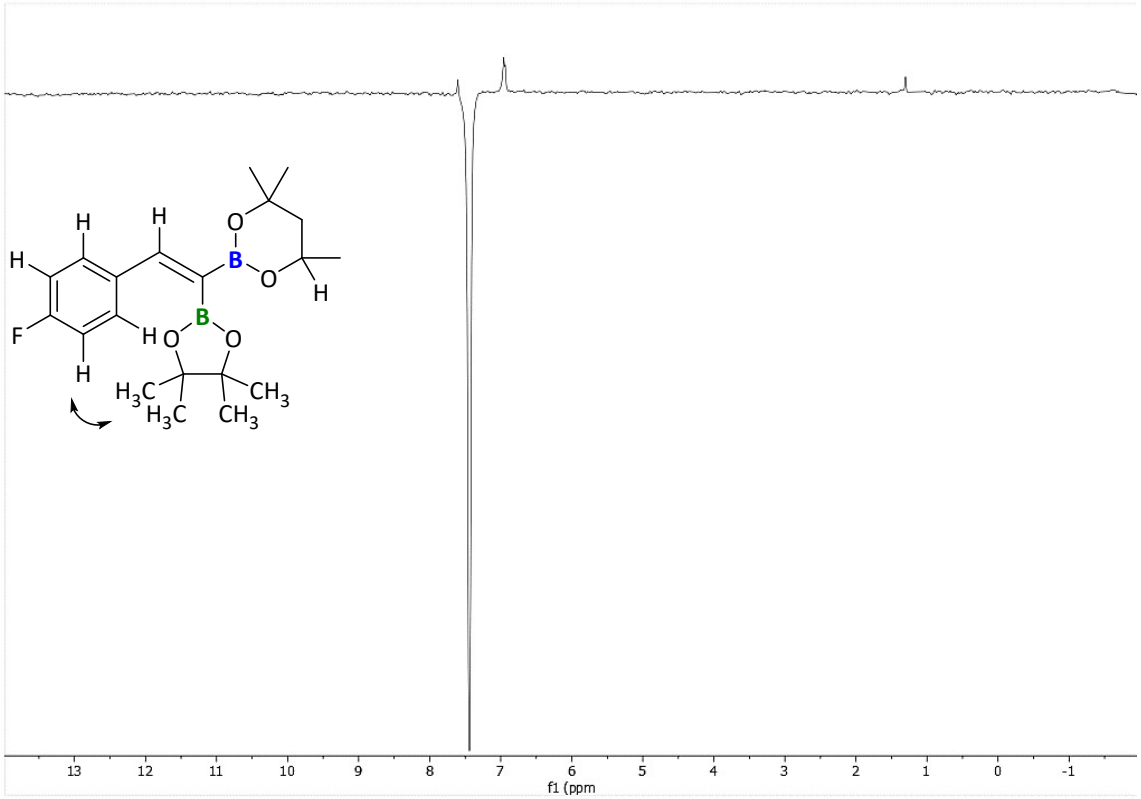
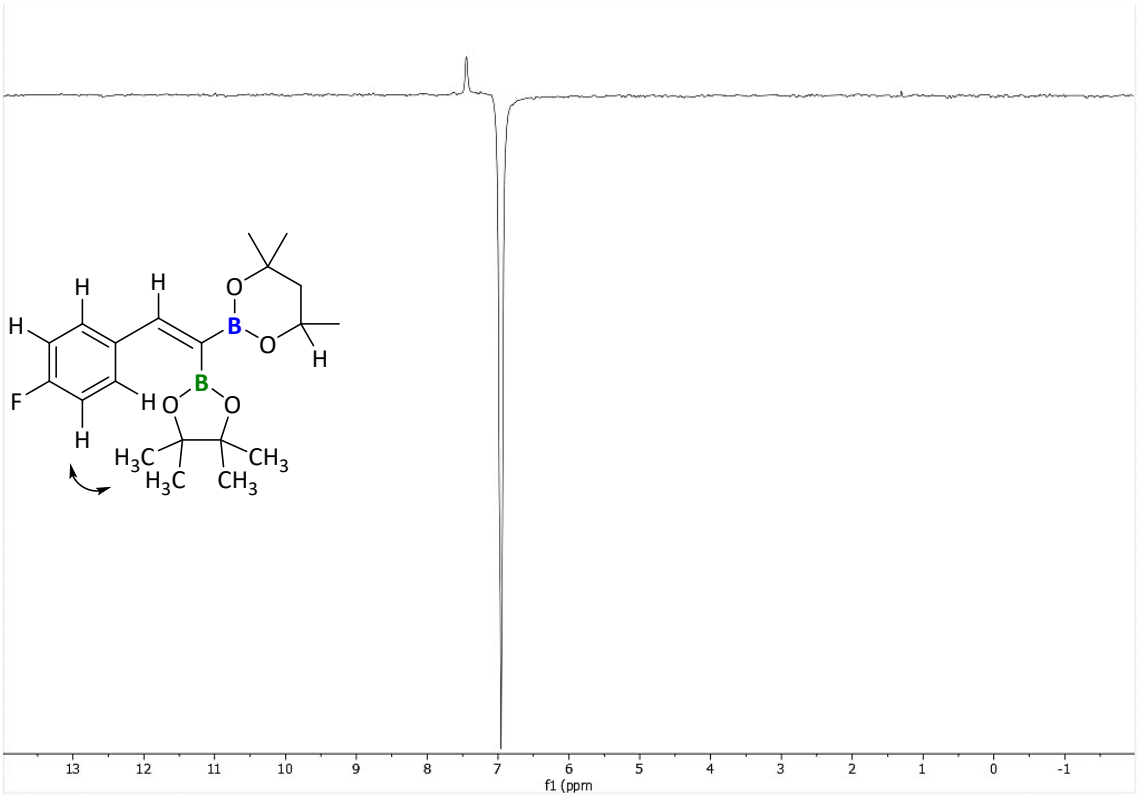
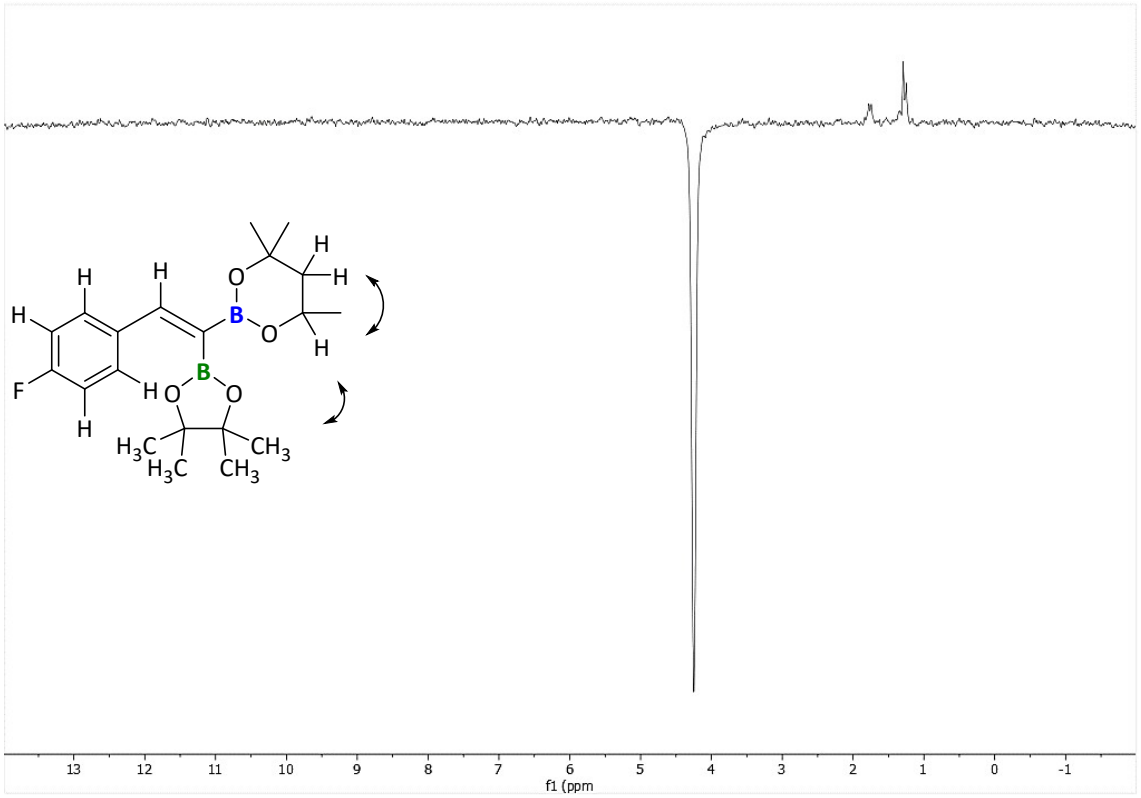
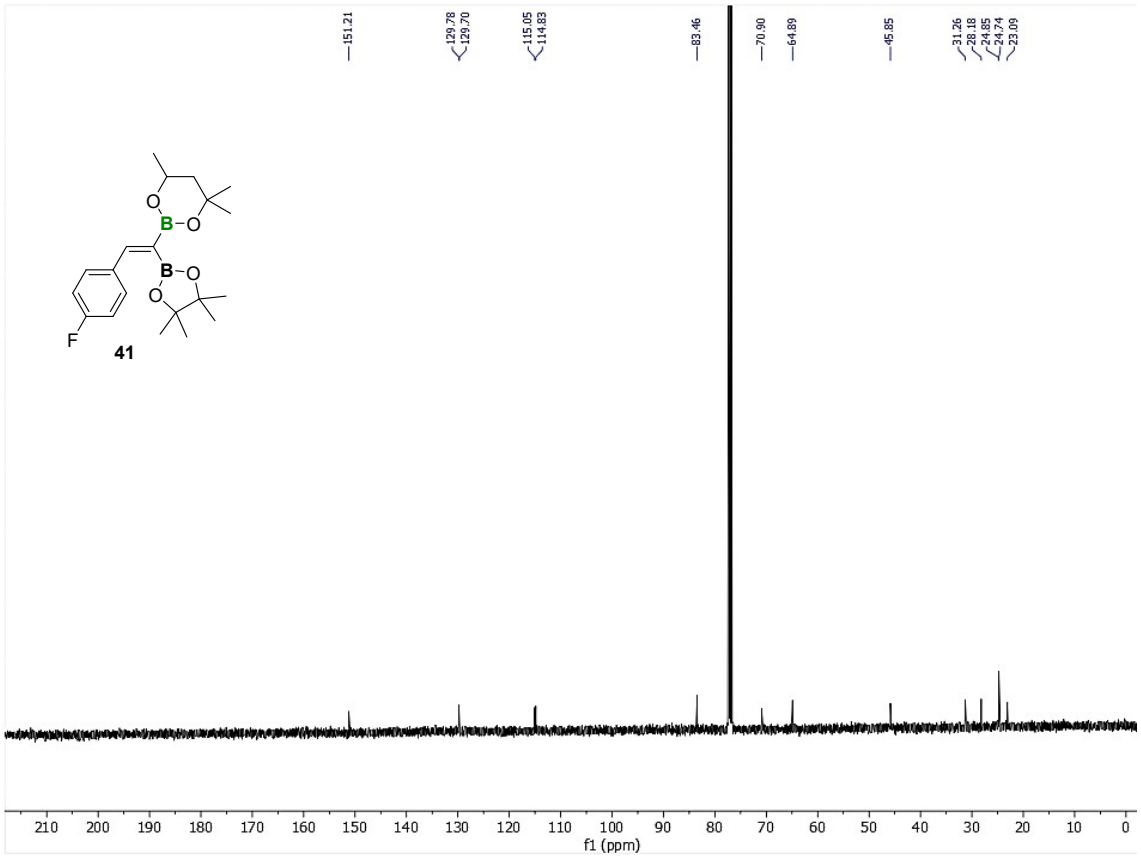

H
H
O
B
O
H
H
F
H
O
B
O
H
H3C
CH3
H3C
CH3
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)


H
H
O
B
O
H
H
F
H
O
B
O
H
H3C
CH3
H3C
CH3
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)


H
H
O
H
H
B
O
H
F
B
H
O
O
H
H3C
CH3
H3C
CH3
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)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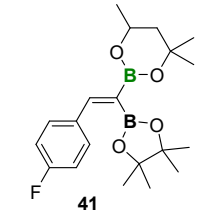
129.78
129.70
115.05
114.83
83.46
70.90
64.89
45.85
31.26
28.18
24.85
24.74
23.09
O
B–O
B–O
O
F
41
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



41

26.10
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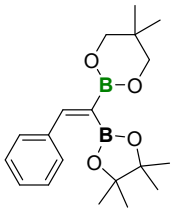
f1 (ppm)



42

7.67
7.49
7.49
7.48
7.48
7.47
7.47
7.47
7.46
7.31
7.30
7.30
7.29
7.29
7.29
7.28
7.28
7.28
7.27
7.27
7.27
7.26
7.25
7.25
7.24
7.24
3.67
1.30
0.98
1.00
2.81
5.59
4.68
13.71
6.59
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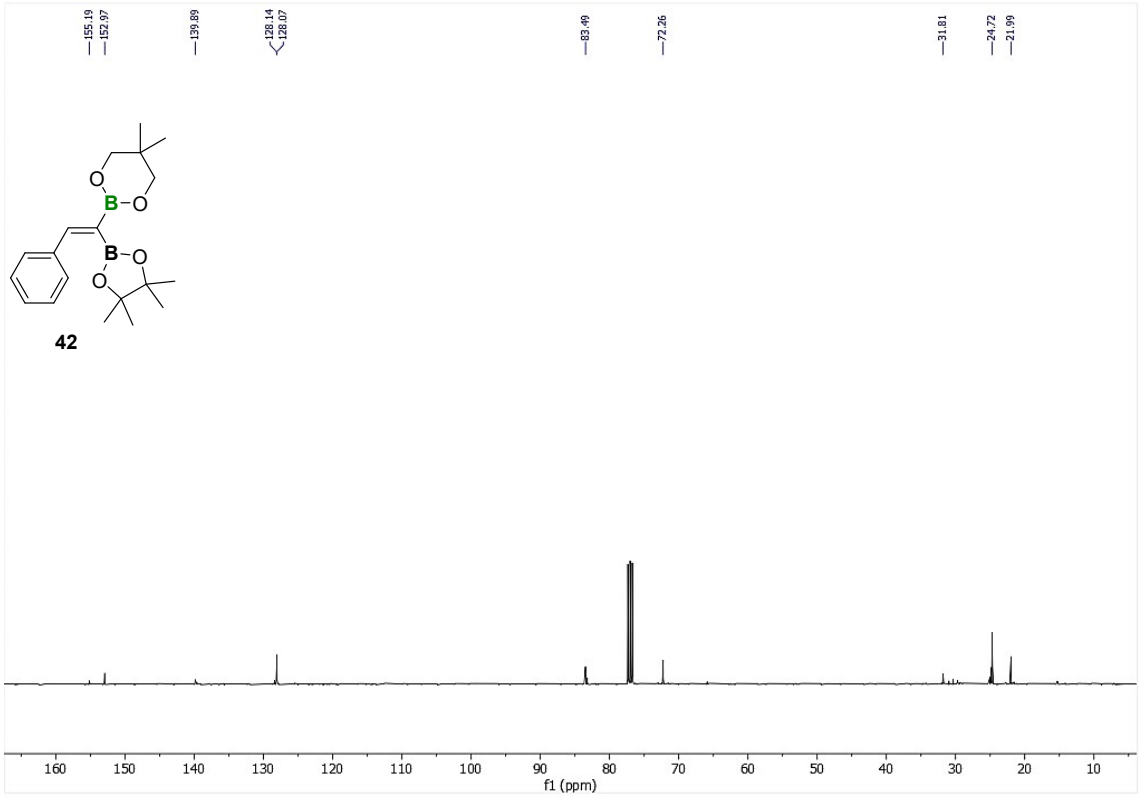
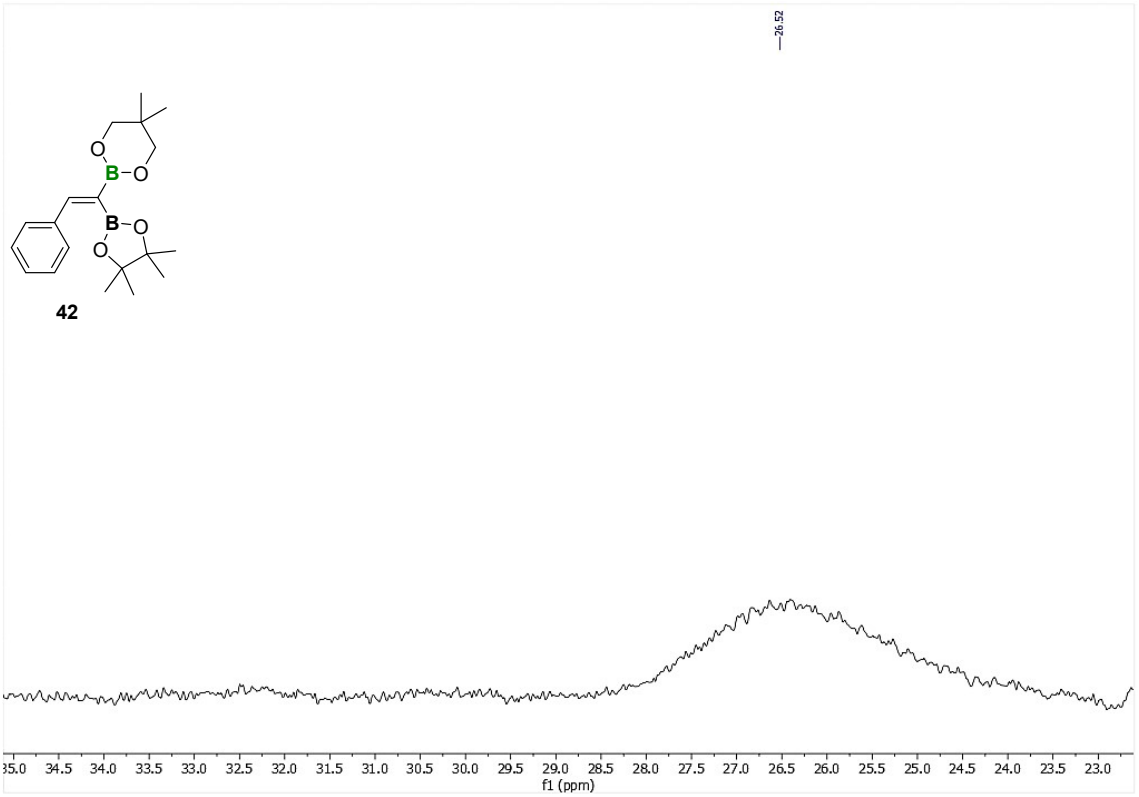
f1 (ppm)


155.19
152.97
139.89
128.14
128.07
83.49
72.26
31.81
24.72
21.99
B
O
42
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


26.52
B
O
42
35.0
34.5
34.0
33.5
33.0
32.5
32.0
31.5
31.0
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28.0
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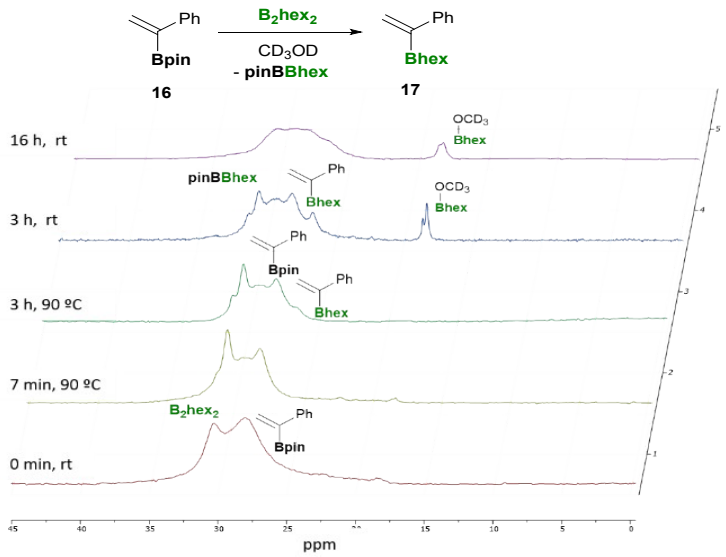
27.0
26.5
26.0
25.5
25.0
24.5
24.0
23.5
23.0
f1 (ppm)

Evolution by ^{11}B NMR spectra along the reaction between 16 and B_2hex_2



The evolution of the ^{11}B NMR spectra along the reaction between 4,4,5,5-tetramethyl-2-(1-phenylvinyl)-1,3,2-dioxaborolane (**16**) and B_2hex_2

Mass spectra from the MS analysis for mixed diboron and *gem*-diborylalkanes formed along the transborylation

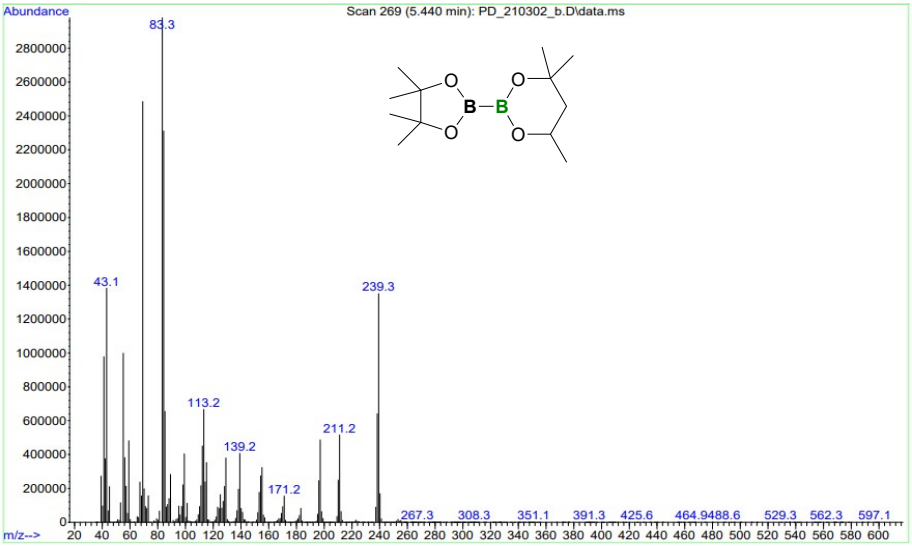


Figure S1. Mass spectra from the MS analysis for pinB–Bhex.

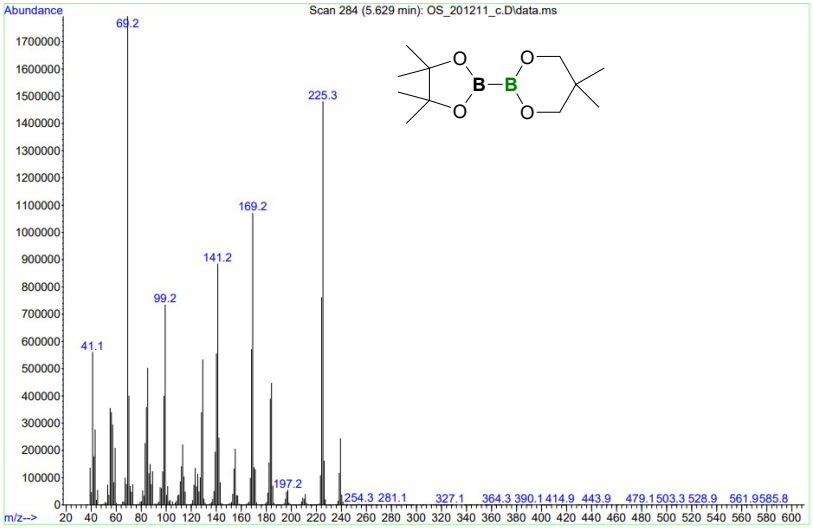


Figure S2. Mass spectra from the MS analysis for pinB–Bneo.

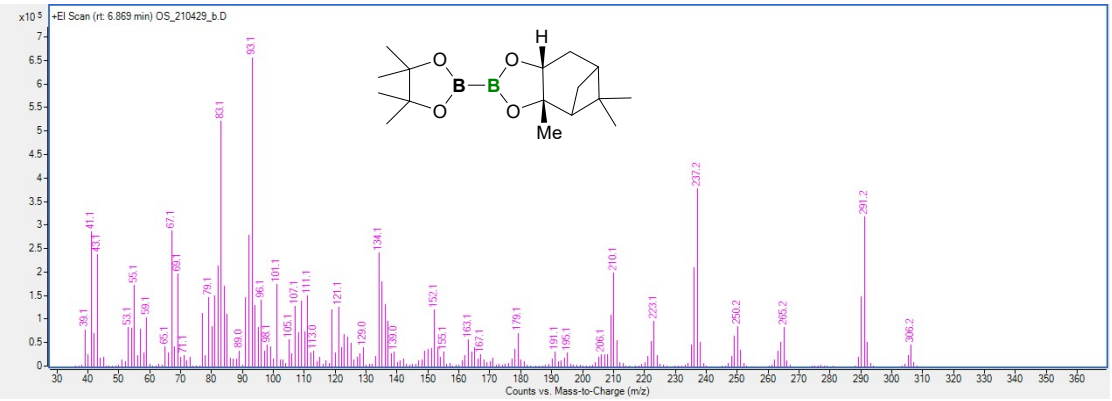


Figure S3. Mass spectra from the MS analysis for Bpin–Bpai.

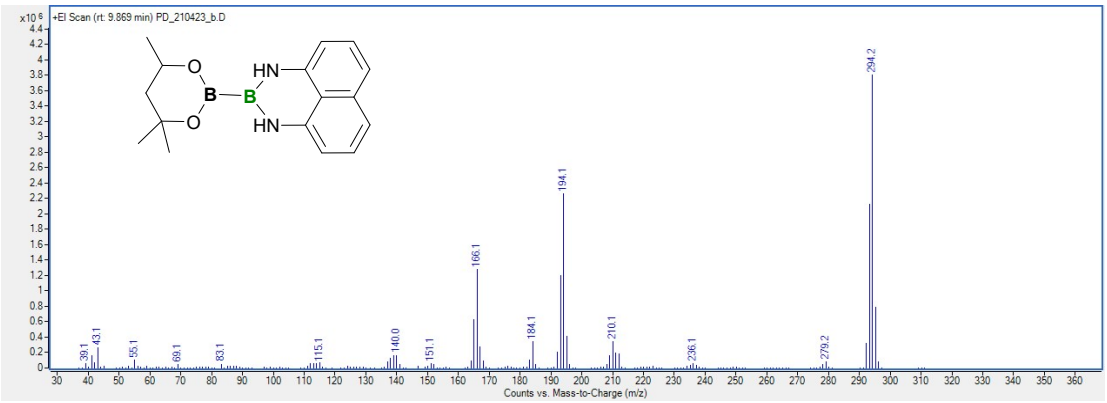


Figure S4. Mass spectra from the MS analysis for hexB–Bdan.

Computational details

Geometry optimizations and transition state searches were performed with Gaussian 16 package,[5] within the framework of Density Functional Theory (DFT)[6] by using the ωB97X-D functional[7] and 6-31G(d,p) basis set.[8] To check our methodology, we have reevaluated the thermodynamics of the overall transborylation reaction between *E*-**1** and B_2neo_2 using a larger basis set, 6-311++G(d,p). At this level, the computed, reaction free energy gives the same value, -0.8 kcal·mol^{-1}, further supporting the selected methodology. Solvent effects were included in geometry optimizations and energy calculations using the IEF-PCM implicit solvation model[9] as implemented in Gaussian16. The dielectric constants were 32.613 for methanol (MeOH), 26.726 for 2,2,2-trifluoroethanol (TFE) and 19.264 for 2-propanol (iPrOH). All minima were characterized by the lack of imaginary frequencies whereas only one imaginary frequency was identified for transition-state structures, which is associated to the normal mode of vibration connecting reactants and products. Free energy corrections were calculated at a concentration of 1 M and a temperature of 298.15 K. A data set collection of computational results is available in the ioChem-BD repository[10] and can be accessed via https://doi.org/10.19061/iochem-bd-2-57.

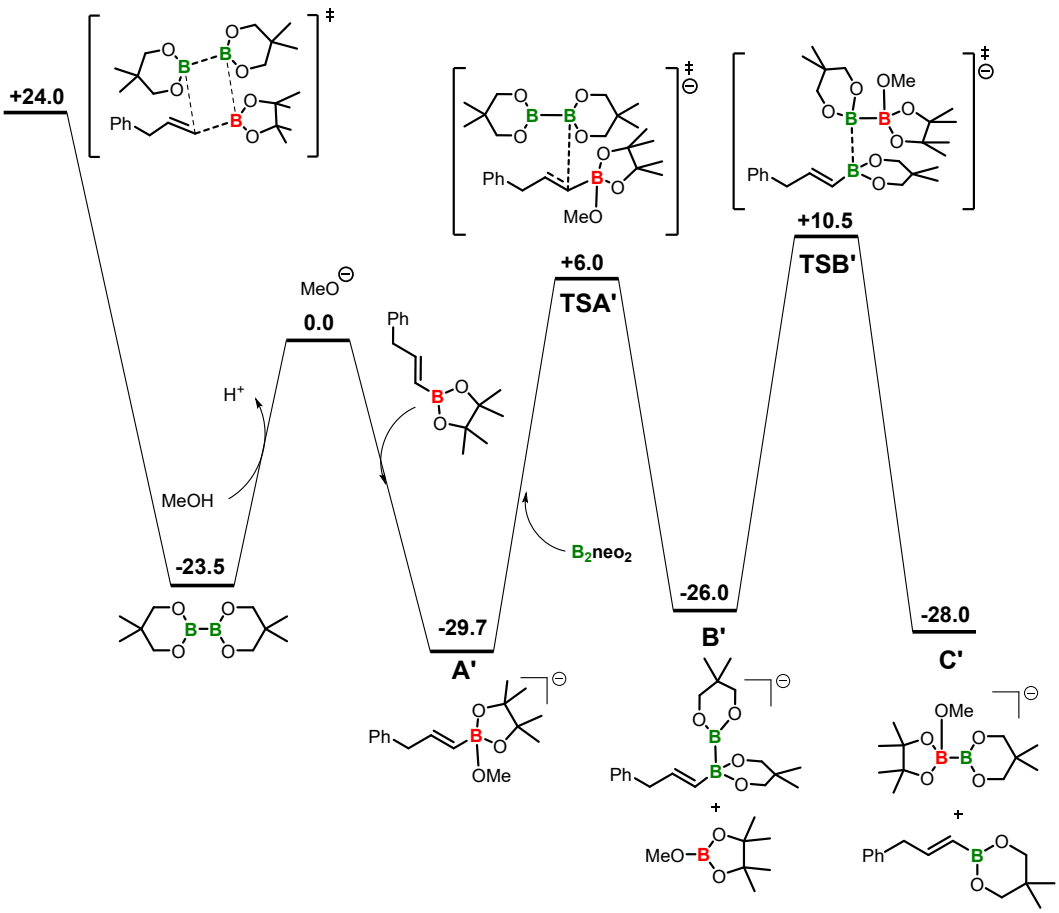


Figure S4: Free-energy profile in kcal·mol^{-1} for the transborylation of *E*-**1** with Bneo-Bneo via direct B-B/C-B metathesis with the unactivated diboron (left), and via methoxide coordination to the boron atom of the alkenylborane (right).

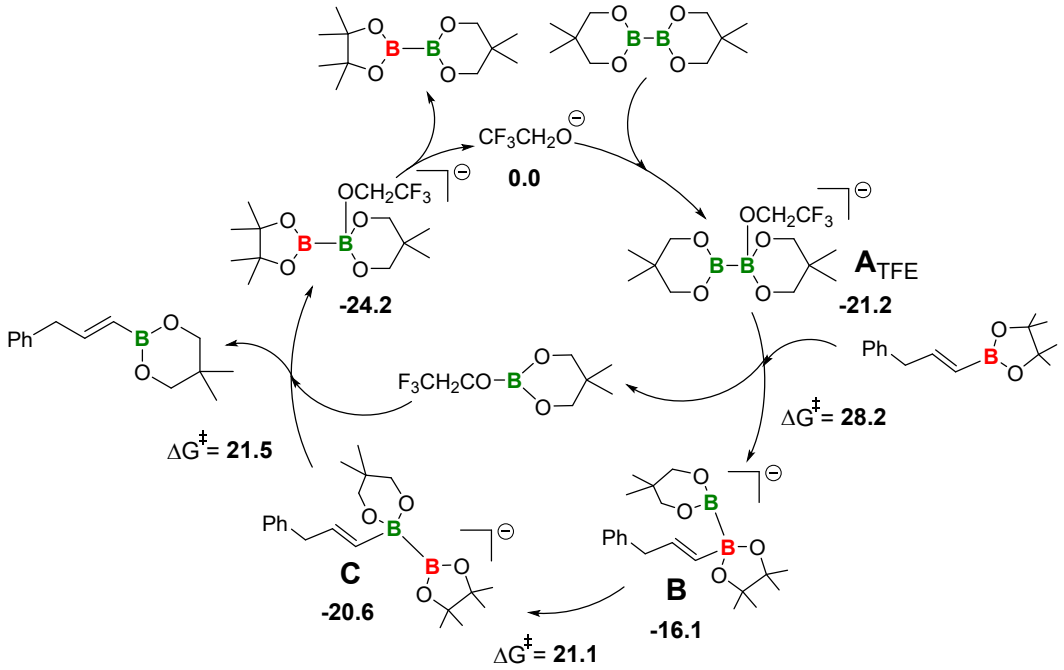


Figure S5: Suggested mechanism for the transborylation of *E*-**1** with Bneo-Bneo in the presence of CF_3CH_2OH (TFE). Relative free energies and barriers in kcal·mol^{-1}.

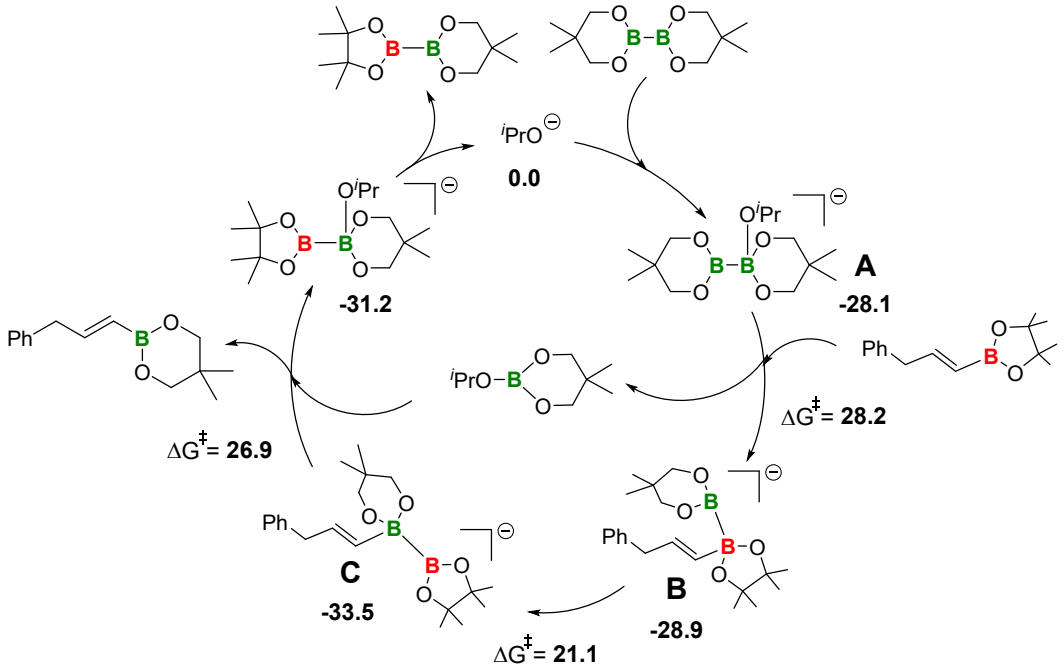


Figure S6. Suggested mechanism for the transborylation of *E*-**1** with Bneo-Bneo in the presence of ^{i}PrOH. Relative free energies and barriers in kcal·mol^{-1}.

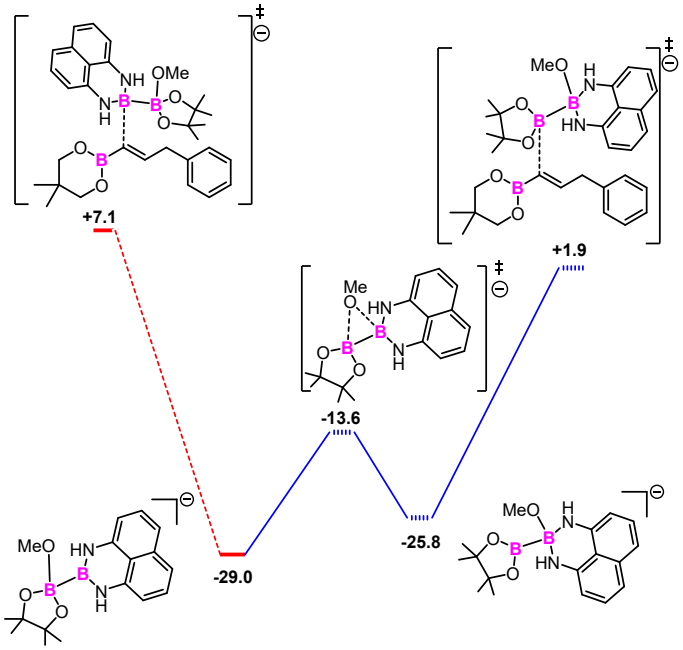


Figure S7. Free-energy profile (kcal·mol^{-1}) of two possible paths for the regioselective transborylation of vinylboronic ester **13** with Bpin-Bdan in MeOH.

Cartesian coordinates and electronic energies in a.u. of computed structures

Calculations in MeOH

E-**1**

Electronic Energy: -759.451277

C	-0.536910	-0.339162	0.125553
H	-1.215369	0.502286	-0.010994
C	-1.054876	-1.570077	0.215772
H	-0.378896	-2.414252	0.355591
C	-2.512553	-1.950584	0.145455
H	-2.634117	-2.676108	-0.669249
C	2.977783	1.003961	0.090287
C	3.191158	-0.457558	0.616552
B	0.988341	-0.084544	0.213170
O	1.545730	1.170022	0.216961
O	1.927127	-1.085232	0.299043
C	3.355800	-0.531085	2.135200
H	3.297409	-1.576852	2.447199
H	4.322587	-0.130404	2.450803
H	2.564347	0.023118	2.647645
C	4.311611	-1.224362	-0.070054
H	5.268103	-0.714735	0.079754
H	4.389875	-2.226642	0.359262
H	4.132640	-1.323786	-1.141865
C	3.313781	1.163222	-1.393049
H	2.956420	2.137866	-1.734723
H	4.392132	1.111890	-1.564347
H	2.827508	0.390473	-1.995081
C	3.676336	2.082186	0.905475
H	4.758688	1.922308	0.898246
H	3.475013	3.063922	0.468833
H	3.331196	2.090178	1.940631
H	-2.764682	-2.498217	1.062658
C	-3.462033	-0.794197	-0.044974
C	-3.797710	-0.351386	-1.326747
C	-3.992512	-0.118189	1.056396
C	-4.647604	0.736872	-1.505534
H	-3.388600	-0.865860	-2.192353
C	-4.843065	0.970561	0.882983
H	-3.736306	-0.449710	2.059270
C	-5.173519	1.401201	-0.399832
H	-4.900671	1.065058	-2.508915
H	-5.249228	1.481733	1.750319
H	-5.838079	2.248293	-0.537093

MeO$^-$

Electronic Energy: -115.145738

O	-2.745245	0.113637	-0.000042
C	-1.415051	0.113713	-0.000027
H	-0.901459	-0.364183	0.899599
H	-0.901581	-0.425732	-0.863995
H	-0.901222	1.131508	-0.035536

A

Electronic Energy: -858.925288

B	1.170694	0.438704	-1.058760

B	-0.004123	-0.837886	-0.805971
O	0.658960	1.719434	-0.476890
O	2.416322	0.010247	-0.363632
O	-0.179439	-1.840857	-1.752079
O	-0.686875	-0.932537	0.401225
C	-1.524527	-2.036247	0.701301
C	-1.010406	-2.962253	-1.502489
C	-1.087548	-3.316042	-0.015332
C	3.393476	1.007034	-0.274975
C	1.625336	2.726006	-0.414934
H	-2.559804	-1.795316	0.419656
H	-1.505805	-2.184966	1.788267
H	-2.021982	-2.757667	-1.881852
H	-0.610015	-3.809146	-2.073726
H	3.784264	1.273167	-1.274138
H	4.245051	0.621053	0.310458
C	-2.131538	-4.412154	0.201736
H	-1.848196	-5.327696	-0.328078
H	-2.222188	-4.655475	1.265609
H	-3.117891	-4.102602	-0.160213
C	0.280641	-3.781221	0.499904
H	0.227272	-4.016705	1.568021
H	0.603220	-4.683077	-0.030920
H	1.049020	-3.015655	0.361853
O	1.545064	0.648788	-2.490675
C	0.534029	1.154574	-3.295759
H	0.851651	1.137035	-4.348739
H	-0.398377	0.564606	-3.222558
H	0.266072	2.196182	-3.047718
C	2.868695	2.295339	0.385953
H	1.183345	3.620978	0.055132
H	1.958203	3.025533	-1.426946
C	2.477220	2.017014	1.839193
H	3.340075	1.666455	2.418416
H	2.093712	2.924351	2.321576
H	1.699331	1.251914	1.876099
C	3.937907	3.384748	0.321953
H	3.576165	4.318007	0.769531
H	4.840993	3.083070	0.865807
H	4.226314	3.599103	-0.713878

Bneo-OMe

Electronic Energy: -487.006650

C	-2.406233	2.214421	-1.861062
C	-1.897074	3.390852	0.242047
C	-2.518479	3.565805	-1.147158
H	-2.930848	2.246791	-2.821444
H	-1.350937	1.986947	-2.061515
H	-2.051306	4.290232	0.846626
H	-0.815784	3.226878	0.149716
B	-2.952857	1.222627	0.262322
O	-2.970678	1.149651	-1.104782
O	-2.464930	2.297384	0.955690
C	-3.986918	3.995833	-1.031533
H	-4.587409	3.269120	-0.477723
H	-4.063177	4.957171	-0.513903
H	-4.430577	4.108248	-2.025714

C	-1.723929	4.616140	-1.926388
H	-2.137502	4.743413	-2.931718
H	-1.768583	5.585919	-1.420941
H	-0.671193	4.331774	-2.024953
O	-3.480274	0.151304	0.919729
C	-3.544680	0.106815	2.334512
H	-4.587878	-0.012320	2.640594
H	-2.975536	-0.756082	2.691893
H	-3.140822	1.013646	2.790299

B_2neop_2

Electronic Energy: --743.714845

B	0.880307	0.411191	0.541993
B	-0.082877	-1.004295	0.374077
O	0.663262	1.466659	-0.303430
O	1.855471	0.440696	1.503145
O	-1.142652	-0.987361	-0.493230
O	0.245826	-2.121050	1.095653
C	-0.523915	-3.313633	0.965138
C	-1.949953	-2.149453	-0.664727
C	-1.171625	-3.444961	-0.416607
C	2.679185	1.593780	1.656441
C	1.456397	2.646401	-0.198858
C	2.860136	2.362754	0.344331
C	3.671276	1.533844	-0.660380
H	3.788632	2.082058	-1.600426
H	4.668939	1.322350	-0.262914
H	3.191976	0.577707	-0.887951
C	3.572318	3.687361	0.626455
H	4.570490	3.508151	1.038495
H	3.689664	4.265971	-0.295335
H	3.013231	4.298266	1.342758
H	-1.298285	-3.316907	1.742733
H	0.147142	-4.157702	1.155421
H	-2.802547	-2.087826	0.023472
H	-2.340935	-2.127155	-1.687262
H	3.647634	1.254516	2.038473
H	2.228412	2.247553	2.413883
C	-2.142779	-4.627422	-0.411489
H	-2.635702	-4.725537	-1.383930
H	-1.610579	-5.562558	-0.210148
H	-2.917995	-4.505946	0.352158
C	-0.102067	-3.648338	-1.497887
H	0.459309	-4.569099	-1.310664
H	-0.568112	-3.728640	-2.485001
H	0.612605	-2.821393	-1.531379
H	1.514787	3.090091	-1.198211
H	0.939006	3.358701	0.456314

TSA

Electronic Energy: -1618.356769

C	-0.788241	-2.893226	-0.407548
C	-0.552666	-2.363855	-1.867961
B	-0.347949	-0.603365	-0.369570
O	-0.647182	-0.953959	-1.712373
O	-0.321681	-1.828705	0.414889

C	2.937204	2.516091	0.257650
C	0.680087	2.953073	-0.585787
C	2.025663	3.624396	-0.282216
H	3.957083	2.900951	0.401277
H	2.561502	2.191852	1.239859
H	-0.021201	3.688812	-1.005961
H	0.244239	2.595218	0.358537
B	1.808205	0.922922	-1.255670
O	3.016572	1.411667	-0.609670
O	0.806062	1.903350	-1.505621
C	2.619894	4.240516	-1.552087
H	2.770868	3.477276	-2.318904
H	1.952272	5.008110	-1.960115
H	3.586614	4.711418	-1.339716
C	1.836472	4.696925	0.790376
H	2.794816	5.154987	1.059902
H	1.174845	5.493801	0.432855
H	1.396001	4.275831	1.701160
C	-1.245364	0.545492	0.272346
H	-1.010565	0.888880	1.282387
C	-2.348597	1.032118	-0.299837
C	-3.313034	1.996813	0.339492
H	-2.892047	2.347833	1.290844
H	-3.447145	2.885106	-0.291114
C	-4.674669	1.375191	0.596788
C	-4.771886	0.134176	1.235557
C	-5.853022	2.017964	0.213374
C	-6.011506	-0.443612	1.489822
H	-3.859169	-0.381598	1.521552
C	-7.098023	1.442485	0.463759
H	-5.796351	2.980132	-0.289575
C	-7.181620	0.209470	1.104120
H	-6.065774	-1.407620	1.986950
H	-8.002377	1.957950	0.154567
H	-8.149613	-0.241978	1.298041
C	2.045371	-0.456956	2.727958
C	2.977715	-2.153740	1.233360
B	1.586197	-0.382764	0.315124
O	1.450860	0.149501	1.595898
O	2.467506	-1.446735	0.123601
O	2.083281	0.199349	-2.444823
C	3.347537	-0.360240	-2.654973
H	4.129129	0.407123	-2.758285
H	3.641187	-1.034560	-1.842289
H	3.314701	-0.939223	-3.586064
C	-0.020582	-4.166171	-0.066240
H	-0.227353	-4.455739	0.969048
H	-0.323579	-4.993405	-0.717174
H	1.054547	-4.011883	-0.170446
C	-2.276176	-3.087285	-0.081486
H	-2.714059	-3.927493	-0.629545
H	-2.377765	-3.286237	0.989694
H	-2.843106	-2.180631	-0.311129
C	-1.618157	-2.808096	-2.869385
H	-1.378764	-2.408224	-3.859502
H	-1.653700	-3.900139	-2.945907
H	-2.608928	-2.445234	-2.587818

C	0.830001	-2.724404	-2.419713
H	0.904560	-3.797472	-2.628096
H	0.987776	-2.175244	-3.351033
H	1.612597	-2.428881	-1.720398
C	3.325356	-1.230748	2.403027
H	3.870592	-2.700052	0.903528
H	2.231815	-2.894434	1.559388
H	1.314273	-1.141570	3.181978
H	2.257709	0.333406	3.459290
C	4.455735	-0.275534	2.003289
H	4.662528	0.436228	2.810419
H	5.375522	-0.837904	1.805974
H	4.195045	0.283575	1.101607
C	3.736764	-2.063335	3.618065
H	4.641217	-2.642033	3.402109
H	3.950720	-1.417166	4.476362
H	2.947450	-2.764454	3.910718
H	-2.619256	0.689939	-1.300122

B

Electronic Energy: -1131.371170

C	3.413844	-0.573439	0.943277
C	3.748197	-0.664244	-0.583677
B	1.480034	-0.091402	-0.310460
O	2.709549	0.081167	-1.172247
O	2.013177	-0.682556	0.964724
C	0.380201	-1.101898	-0.970398
H	0.110775	-0.941242	-2.025072
C	-0.329475	-2.041589	-0.334114
H	-0.123115	-2.228870	0.722552
C	-1.457738	-2.859720	-0.925661
H	-1.447592	-2.755144	-2.016906
H	-1.317421	-3.925060	-0.700278
C	-2.806237	-2.418516	-0.393393
C	-3.510585	-1.385712	-1.019408
C	-3.349559	-2.983973	0.762952
C	-4.720571	-0.927988	-0.506405
H	-3.097131	-0.929750	-1.915501
C	-4.559429	-2.528549	1.283135
H	-2.817167	-3.790067	1.261959
C	-5.249629	-1.497498	0.650366
H	-5.249208	-0.123283	-1.008735
H	-4.964310	-2.981436	2.183291
H	-6.192951	-1.142262	1.053241
C	-0.561936	3.329706	-1.071902
C	-0.828605	2.819936	1.303986
B	0.601338	1.402868	-0.094637
O	0.316106	2.222072	-1.183663
O	0.049652	1.719395	1.142154
C	-1.610142	3.137376	0.026829
H	0.020871	4.239218	-0.865044
H	-1.052413	3.467885	-2.043881
H	-1.520047	2.579526	2.121541
H	-0.252946	3.706014	1.609467
C	-2.406863	4.428914	0.213705
H	-2.949321	4.685414	-0.702428
H	-3.142013	4.317300	1.017699

H	-1.752800	5.270327	0.467047
C	-2.551251	1.978637	-0.323696
H	-2.010116	1.037626	-0.451799
H	-3.292097	1.828031	0.468695
H	-3.090027	2.186225	-1.254705
C	4.023080	-1.688658	1.793280
H	5.116057	-1.700103	1.712441
H	3.764826	-1.538851	2.847166
H	3.641639	-2.666126	1.489144
C	3.827131	0.788061	1.530357
H	3.375900	0.893553	2.521996
H	4.912900	0.890279	1.634249
H	3.456724	1.600008	0.898232
C	3.694560	-2.117482	-1.087551
H	3.723245	-2.111500	-2.182192
H	4.538064	-2.717268	-0.727850
H	2.760186	-2.589283	-0.773639
C	5.093593	-0.051016	-0.972537
H	5.919828	-0.532007	-0.436480
H	5.268709	-0.180604	-2.046044
H	5.114700	1.019414	-0.755295

TSB

Electronic Energy: -1131.338495

C	3.878626	-0.494556	0.799160
C	3.846544	-0.465735	-0.767511
B	1.985352	0.632601	0.052030
O	2.923163	0.583304	-1.036746
O	2.572907	-0.071953	1.164285
C	0.380717	-0.388657	-0.531881
H	0.327805	-0.550885	-1.616504
C	-0.296263	-1.238160	0.243283
H	-0.279226	-1.076267	1.324578
C	-1.136802	-2.411061	-0.214026
H	-0.912288	-2.636672	-1.262036
H	-0.872829	-3.303142	0.370914
C	-2.622094	-2.147078	-0.065869
C	-3.461981	-2.123276	-1.180107
C	-3.179000	-1.881758	1.189865
C	-4.818905	-1.832987	-1.050828
H	-3.046249	-2.323830	-2.164115
C	-4.531440	-1.585549	1.324765
H	-2.542683	-1.898819	2.070876
C	-5.358376	-1.557832	0.202313
H	-5.453018	-1.816747	-1.932172
H	-4.942552	-1.377681	2.308115
H	-6.413992	-1.327135	0.306077
C	-0.951136	3.122844	-0.750002
C	-1.554364	1.751502	1.230873
B	0.597452	1.494894	0.084096
O	0.123117	2.266416	-1.037572
O	-0.146295	1.673348	1.289681
C	-2.117555	2.403117	-0.062902
H	-0.625252	3.958749	-0.105488
H	-1.300760	3.563664	-1.694489
H	-1.988036	0.745424	1.340624
H	-1.873702	2.340522	2.102144

C	-3.208761	3.416513	0.294874
H	-3.632961	3.873779	-0.606439
H	-4.026826	2.928623	0.836836
H	-2.815973	4.218240	0.930601
C	-2.701339	1.342020	-1.001967
H	-1.943728	0.606262	-1.276799
H	-3.522647	0.802631	-0.517539
H	-3.089972	1.806976	-1.916472
C	4.152456	-1.871995	1.399039
H	5.121769	-2.260944	1.068355
H	4.171231	-1.803496	2.491320
H	3.375798	-2.586556	1.118269
C	4.874378	0.518585	1.381827
H	4.710221	0.591894	2.461101
H	5.915233	0.225164	1.211702
H	4.713183	1.508589	0.945708
C	3.313945	-1.772127	-1.373168
H	3.139307	-1.616411	-2.442208
H	4.027416	-2.594419	-1.258441
H	2.364468	-2.055421	-0.914028
C	5.184317	-0.126404	-1.420376
H	5.950505	-0.860210	-1.147804
H	5.078414	-0.138275	-2.509719
H	5.532390	0.865565	-1.124958

C

Electronic Energy: -1131.377597

C	4.048800	-0.820106	0.822528
C	3.998282	-1.027112	-0.724705
B	2.153282	0.162740	-0.042095
O	2.997877	-0.074530	-1.126440
O	2.710668	-0.380559	1.113309
C	-0.383121	-0.422945	-0.639779
H	-0.420782	-0.657411	-1.713916
C	-1.101530	-1.229969	0.148713
H	-1.111773	-1.032437	1.223966
C	-2.015452	-2.336676	-0.310400
H	-1.828001	-2.540575	-1.373331
H	-1.812561	-3.271694	0.228088
C	-3.484812	-1.987476	-0.130731
C	-3.959154	-0.719571	-0.484822
C	-4.395668	-2.917235	0.375304
C	-5.304515	-0.393868	-0.343731
H	-3.253818	0.017090	-0.861146
C	-5.744356	-2.595521	0.520867
H	-4.044900	-3.905677	0.662054
C	-6.204236	-1.331695	0.161190
H	-5.651524	0.596452	-0.624284
H	-6.434668	-3.332772	0.919956
H	-7.253305	-1.077470	0.276769
C	-0.740277	2.530745	-1.260837
C	-1.130957	2.001906	1.125703
B	0.561308	0.831563	-0.158243
O	0.511994	1.920411	-1.190145
O	0.108034	1.356559	1.170145
C	-1.182266	3.137840	0.084906
H	-1.944251	1.292152	0.886686

H	-1.351479	2.418527	2.123201
C	-0.228711	4.265662	0.485858
H	-0.235160	5.069634	-0.260293
H	-0.518528	4.699313	1.450633
H	0.790789	3.883901	0.571418
C	-2.612020	3.665573	-0.029071
H	-3.307137	2.868068	-0.318565
H	-2.956660	4.079476	0.925926
H	-2.680631	4.460819	-0.780802
C	4.348224	-2.078845	1.626932
H	5.326080	-2.488154	1.353509
H	4.367400	-1.840395	2.694165
H	3.590605	-2.847569	1.463904
C	4.998789	0.303933	1.245206
H	4.830222	0.531356	2.301294
H	6.046635	0.017304	1.117505
H	4.811594	1.213352	0.667304
C	3.481790	-2.412861	-1.123627
H	3.285072	-2.420929	-2.199119
H	4.210321	-3.197513	-0.900410
H	2.546230	-2.644353	-0.605934
C	5.301890	-0.729854	-1.453779
H	6.100524	-1.389482	-1.099413
H	5.173471	-0.899544	-2.526568
H	5.615543	0.305521	-1.308121
H	-1.521942	1.809297	-1.576569
H	-0.713102	3.325598	-2.025518

TSC

Electronic Energy: -1618.365905

C	0.391735	-3.210969	0.120683
C	-0.228222	-3.593710	-1.228426
C	-0.058816	-2.370080	-2.138639
H	1.479273	-3.102618	0.004228
H	0.208752	-4.004145	0.859541
H	1.012084	-2.190759	-2.308148
H	-0.521316	-2.566270	-3.116427
B	-0.370255	-0.903482	-0.253904
O	-0.658083	-1.221405	-1.599521
O	-0.143988	-2.015584	0.637432
C	2.563077	2.787467	-0.208630
C	0.173539	2.810128	-0.755127
C	1.418853	3.702118	-0.663477
H	3.520066	3.326432	-0.257662
H	2.390058	2.502361	0.838344
H	-0.690339	3.401940	-1.090121
H	-0.064341	2.422201	0.246643
B	1.501525	0.947793	-1.474171
O	2.686457	1.628296	-0.998196
O	0.352310	1.754977	-1.661254
C	1.733820	4.324987	-2.026593
H	1.917710	3.548878	-2.773152
H	0.897728	4.942400	-2.374684
H	2.623043	4.962820	-1.965822
C	1.196590	4.794431	0.382522
H	2.097568	5.405266	0.509316
H	0.380992	5.461576	0.082193

H	0.940363	4.365003	1.357594
C	-1.366669	0.143710	0.406853
H	-1.170807	0.463897	1.433279
C	-2.461025	0.623404	-0.187114
H	-2.682531	0.316639	-1.210368
C	-3.454050	1.568214	0.436090
H	-3.105413	1.844477	1.440142
H	-3.504096	2.500713	-0.141544
C	-4.854051	0.989206	0.536834
C	-5.047785	-0.323922	0.977343
C	-5.977813	1.751098	0.209261
C	-6.327623	-0.857620	1.094176
H	-4.178805	-0.929942	1.219152
C	-7.261804	1.221407	0.323217
H	-5.846121	2.771622	-0.141771
C	-7.441454	-0.085892	0.767256
H	-6.456559	-1.879712	1.437746
H	-8.121730	1.830193	0.060375
H	-8.440279	-0.502122	0.853993
C	2.423782	-0.199045	2.419172
C	3.396739	-0.972065	1.462458
B	1.561372	-0.206688	0.265703
O	1.518880	0.441008	1.505804
O	2.615493	-1.127914	0.269809
C	3.808104	-2.353438	1.961274
H	4.461939	-2.829183	1.224403
H	4.358456	-2.279131	2.904997
H	2.939646	-2.997397	2.111938
C	4.644892	-0.170761	1.083474
H	5.307731	-0.021643	1.940942
H	5.196454	-0.722157	0.316143
H	4.365795	0.797185	0.662503
C	3.094246	0.867007	3.279424
H	2.338026	1.379807	3.880996
H	3.820294	0.413584	3.962261
H	3.608230	1.613398	2.670895
C	1.585162	-1.120667	3.308869
H	2.200773	-1.641081	4.048578
H	0.847995	-0.513824	3.843734
H	1.043999	-1.846611	2.698698
O	1.745156	0.155588	-2.622248
C	2.990510	-0.461266	-2.792293
H	3.819753	0.256320	-2.726711
H	3.164323	-1.239007	-2.037899
H	3.012003	-0.923647	-3.786310
C	0.527863	-4.783846	-1.818126
H	0.461183	-5.656021	-1.158063
H	0.111113	-5.068599	-2.790628
H	1.588635	-4.548815	-1.960787
C	-1.712719	-3.932126	-1.059866
H	-2.168328	-4.174779	-2.026743
H	-1.841418	-4.796651	-0.398652
H	-2.256196	-3.087089	-0.629580

[BpinBneop-OMe]$^-$

Electronic Energy: -898.247459

B	0.911091	0.402384	1.066072

B	-0.121195	-0.902719	0.529511
O	0.486673	1.657675	0.377596
O	2.312876	0.056709	0.716301
O	-0.738379	-0.990325	-0.716083
O	-0.401798	-2.049057	1.270093
C	-1.411054	-2.810875	0.585240
C	-1.246699	-2.324886	-0.890277
C	3.219175	1.111387	0.873726
C	1.373758	2.721711	0.559912
C	2.801765	2.375564	0.099231
C	2.808497	2.094291	-1.405323
H	2.491296	2.979114	-1.970445
H	3.812929	1.817956	-1.748122
H	2.125583	1.274423	-1.636659
C	3.751929	3.525563	0.429455
H	4.779731	3.285406	0.132683
H	3.458688	4.441228	-0.097465
H	3.755166	3.743350	1.503948
H	4.211278	0.782598	0.521885
H	3.331444	1.387532	1.938143
H	1.009887	3.594304	-0.008111
H	1.421513	3.027099	1.622254
C	-2.539516	-2.270730	-1.694015
H	-2.330155	-1.921422	-2.709070
H	-2.991354	-3.265412	-1.764176
H	-3.263905	-1.590271	-1.242654
C	-0.186930	-3.113230	-1.665213
H	-0.524777	-4.127947	-1.894463
H	0.018998	-2.597715	-2.607086
H	0.747248	-3.174350	-1.099848
C	-2.760676	-2.423484	1.196614
H	-3.581176	-3.007925	0.770373
H	-2.727404	-2.610388	2.273419
H	-2.969503	-1.360961	1.042482
C	-1.154650	-4.296867	0.801885
H	-1.291412	-4.545868	1.858049
H	-1.858423	-4.898495	0.217743
H	-0.138475	-4.574303	0.515807
O	0.883974	0.593307	2.548190
C	-0.340587	0.989728	3.068934
H	-0.285858	1.022602	4.166628
H	-0.652123	1.988632	2.719347
H	-1.158608	0.294004	2.801125

13

Electronic Energy: -720.133445

C	-0.928180	3.535981	0.931596
C	-2.007587	3.903582	-0.091285
C	-2.125670	2.720503	-1.057311
H	-1.278786	2.709616	1.563313
H	-0.712427	4.389075	1.583148
H	-2.540294	1.850030	-0.532843
H	-2.799892	2.967509	-1.883885
B	0.283913	2.571273	-0.925538
O	-0.872391	2.354903	-1.626201
O	0.295629	3.151592	0.315019
C	1.632433	2.156559	-1.587674

H	1.615520	1.705827	-2.580144
C	2.816697	2.332672	-0.990893
H	2.839454	2.782606	0.002167
C	4.175882	1.973699	-1.539400
H	4.793983	2.880830	-1.537145
H	4.659873	1.290149	-0.829784
C	4.163398	1.362165	-2.918202
C	4.227236	2.169542	-4.056545
C	4.048081	-0.020040	-3.084951
C	4.183373	1.610763	-5.331122
H	4.313009	3.246917	-3.941216
C	4.003631	-0.583994	-4.357326
H	3.993327	-0.659638	-2.207870
C	4.071596	0.230809	-5.485110
H	4.238229	2.253251	-6.204490
H	3.917610	-1.660536	-4.468016
H	4.039484	-0.206983	-6.477779
C	-3.341981	4.103232	0.630437
H	-3.274012	4.930749	1.343644
H	-4.134889	4.342336	-0.085237
H	-3.639350	3.204111	1.179964
C	-1.622427	5.181990	-0.847724
H	-2.391694	5.435700	-1.583822
H	-1.526094	6.022078	-0.152774
H	-0.672614	5.076828	-1.379219

A’

Electronic Energy: -874.665462

C	0.989509	0.864128	-0.160877
H	1.169576	1.931270	-0.352545
C	1.894344	0.261029	0.614718
H	1.776602	-0.806053	0.814785
C	3.141887	0.886333	1.188928
H	3.136091	1.964229	0.980185
H	3.169240	0.776090	2.280955
C	4.403878	0.271476	0.610089
C	4.583034	0.215702	-0.776710
C	5.402202	-0.259118	1.428476
C	5.728163	-0.348553	-1.328189
H	3.803003	0.610711	-1.422264
C	6.551602	-0.828930	0.881261
H	5.278336	-0.229391	2.508200
C	6.718777	-0.875359	-0.499419
H	5.847946	-0.382158	-2.407039
H	7.314383	-1.239187	1.536348
H	7.611140	-1.320720	-0.928153
C	-0.430641	-0.952257	-2.957444
C	0.041592	-1.985365	-1.877322
B	-0.273395	0.117042	-0.875147
O	-0.132746	0.286061	-2.352375
O	-0.278802	-1.343713	-0.662892
C	1.559073	-2.224153	-1.937772
H	1.861688	-2.785765	-1.048130
H	1.855089	-2.797748	-2.822824
H	2.095302	-1.272404	-1.929687
C	-0.676235	-3.333810	-1.940136
H	-0.533362	-3.814392	-2.914589

H	-0.277160	-4.004694	-1.172065
H	-1.747917	-3.218098	-1.763332
C	-1.943547	-1.043817	-3.218962
H	-2.245562	-0.181854	-3.822981
H	-2.219842	-1.954614	-3.761370
H	-2.492648	-1.003630	-2.275787
C	0.310041	-1.054772	-4.290962
H	0.191261	-2.049443	-4.735544
H	-0.090923	-0.320406	-4.997617
H	1.376891	-0.855224	-4.166269
O	-1.578732	0.617802	-0.372368
C	-1.817196	1.976522	-0.551921
H	-2.856497	2.208608	-0.280126
H	-1.167774	2.617447	0.071436
H	-1.668633	2.293312	-1.597877

Bpin-OMe

Electronic Energy: -526.323704

C	-2.363054	-3.237113	-1.116638
C	-1.627300	-3.322142	0.268288
B	-0.306449	-2.322410	-1.266394
O	-1.554009	-2.279613	-1.838375
O	-0.254785	-3.040787	-0.096256
O	0.752369	-1.697821	-1.836595
C	2.008207	-1.727793	-1.172261
H	2.689376	-1.077781	-1.723412
H	1.922225	-1.366875	-0.143098
H	2.418996	-2.741918	-1.155800
C	-2.063487	-2.229707	1.244856
H	-1.378916	-2.221864	2.096654
H	-2.036426	-1.242824	0.774099
H	-3.075302	-2.409817	1.616876
C	-1.690972	-4.685698	0.939135
H	-1.160769	-4.652434	1.894491
H	-2.730483	-4.963604	1.136709
H	-1.233827	-5.459052	0.319746
C	-3.792634	-2.722210	-1.043952
H	-3.834961	-1.712351	-0.632765
H	-4.229732	-2.703506	-2.045721
H	-4.402779	-3.381262	-0.419226
C	-2.312619	-4.549557	-1.899737
H	-2.957603	-5.307645	-1.448173
H	-2.657823	-4.366309	-2.920267
H	-1.293557	-4.943926	-1.948693

TSA'

Electronic Energy: -1618.347513

B	0.100137	-1.093421	-0.908529
C	-0.047646	4.195279	0.079038
C	-1.612350	3.806194	-1.762882
C	-0.185484	4.261378	-1.443065
H	0.981589	4.430189	0.377292
H	-0.705443	4.945930	0.541037
H	-1.735561	3.689968	-2.847241
H	-2.324230	4.575162	-1.429937
B	-1.294243	2.096740	-0.036831

O	-0.364530	2.913750	0.592789
O	-1.951945	2.570300	-1.157502
C	0.843107	3.341908	-2.114181
H	0.713401	2.294193	-1.825242
H	0.750610	3.404803	-3.204347
H	1.859561	3.651260	-1.845608
C	0.008983	5.703498	-1.914528
H	1.021025	6.052211	-1.683346
H	-0.130516	5.778154	-2.998192
H	-0.702402	6.383720	-1.433663
C	-0.140753	-0.464194	0.780912
H	-0.309325	-1.300817	1.469739
C	0.959084	0.257322	1.102790
H	1.223221	1.110962	0.479036
C	1.878391	0.010880	2.261909
H	1.685980	-0.988761	2.670078
C	-3.261998	-1.217503	0.607516
C	-3.364868	0.567463	2.318628
B	-1.654605	0.539863	0.644308
O	-2.713162	-0.130249	-0.086850
O	-1.982113	0.571003	2.097704
C	-4.024011	-0.756736	1.874994
H	-3.945344	-1.756977	-0.064161
H	-2.472091	-1.927583	0.886628
H	-3.552945	0.729623	3.390541
H	-3.850693	1.401280	1.780159
C	-5.502086	-0.505302	1.567339
H	-6.021754	-1.441669	1.334306
H	-6.013324	-0.040924	2.419389
H	-5.604464	0.163481	0.705628
C	-3.879434	-1.821675	2.964793
H	-2.833100	-1.902282	3.278125
H	-4.483189	-1.575036	3.845956
H	-4.200855	-2.805354	2.601678
H	1.613494	0.724717	3.054953
C	3.347272	0.168107	1.926334
C	3.874743	-0.441418	0.782033
C	4.199585	0.906664	2.749487
C	5.226920	-0.313252	0.476349
H	3.209595	-1.006954	0.131377
C	5.553613	1.032525	2.445124
H	3.800486	1.389531	3.637966
C	6.071849	0.421974	1.306213
H	5.623594	-0.789080	-0.415939
H	6.201653	1.611245	3.096411
H	7.125809	0.520769	1.065162
O	1.382057	-1.810432	-0.806874
O	-0.878723	-2.108330	-1.219671
O	0.137192	0.027837	-1.808636
C	-0.867579	0.136768	-2.781957
H	-0.769607	-0.637991	-3.559323
H	-1.865847	0.064793	-2.341462
H	-0.771422	1.116872	-3.263287
C	1.236140	-3.062718	-1.448632
C	-0.271232	-3.388078	-1.182355
C	2.221293	-4.054560	-0.836379
H	3.246294	-3.757807	-1.081289

H	2.128910	-4.081400	0.251375
H	2.058834	-5.064698	-1.227547
C	1.545801	-2.901414	-2.944191
H	2.545586	-2.469399	-3.050152
H	1.526897	-3.858787	-3.474882
H	0.831943	-2.223005	-3.418559
C	-0.495009	-4.014014	0.200644
H	-1.567116	-4.016762	0.417925
H	-0.131496	-5.045690	0.244989
H	0.007537	-3.432179	0.977300
C	-0.924458	-4.271581	-2.242479
H	-0.413943	-5.237676	-2.318778
H	-1.968890	-4.460480	-1.975006
H	-0.908354	-3.789600	-3.222247

B’

Electronic Energy: -1092.049743

C	0.787215	2.538085	1.363774
C	0.528052	2.922145	-1.036342
C	1.573659	2.726076	0.063797
H	1.468846	2.273776	2.182257
H	0.300256	3.486494	1.634232
H	1.016937	2.983397	-2.016967
H	-0.001695	3.872218	-0.872725
B	-0.755162	1.143201	0.054541
O	-0.194266	1.518921	1.272289
O	-0.409765	1.860161	-1.086482
C	2.438757	1.496007	-0.236496
H	1.842010	0.586686	-0.342327
H	2.997069	1.639213	-1.167853
H	3.164357	1.321242	0.564929
C	2.451617	3.973686	0.172123
H	3.184693	3.861853	0.978116
H	3.002530	4.140840	-0.759526
H	1.854939	4.868970	0.378453
C	-0.614682	-1.563416	-0.147070
H	-0.778833	-2.342096	-0.907751
C	0.488612	-1.710852	0.595475
H	0.723351	-0.951233	1.345713
C	1.517979	-2.812348	0.480144
H	1.206357	-3.525871	-0.291766
C	-3.689525	-1.115539	-1.120051
C	-3.775274	0.088531	1.036218
B	-1.691776	-0.327763	-0.046897
O	-2.569375	-0.301026	-1.273852
O	-2.561649	-0.581872	1.159637
C	-4.665779	-0.547808	-0.061398
H	-4.214497	-1.206550	-2.085368
H	-3.404826	-2.141614	-0.819060
H	-4.310872	0.065705	1.999698
H	-3.613997	1.156390	0.788043
C	-5.568448	0.522830	-0.676793
H	-6.277644	0.085518	-1.389590
H	-6.147933	1.045665	0.094188
H	-4.963999	1.265746	-1.208293
C	-5.505778	-1.687710	0.518142
H	-4.866770	-2.382932	1.073568

H	-6.273369	-1.308875	1.203173
H	-6.012767	-2.252101	-0.274296
H	1.591023	-3.367914	1.424769
C	2.879705	-2.243403	0.140233
C	3.219921	-1.964418	-1.186475
C	3.792661	-1.910937	1.143295
C	4.438183	-1.372105	-1.503753
H	2.513222	-2.207047	-1.976219
C	5.012224	-1.312699	0.832556
H	3.543190	-2.120365	2.180654
C	5.339388	-1.041074	-0.493213
H	4.684639	-1.165629	-2.541018
H	5.708276	-1.061340	1.627353
H	6.289706	-0.577119	-0.738337

TSB'

Electronic Energy: -1618.342293

B	-2.147566	-0.290290	0.842155
C	-1.090867	3.303371	1.125583
C	-1.177994	2.966273	-1.304346
C	-0.629397	3.889893	-0.210256
H	-0.658816	3.874499	1.956757
H	-2.185896	3.378229	1.197858
H	-0.717554	3.213395	-2.269364
H	-2.259291	3.139659	-1.400838
B	-0.895517	1.070636	0.223654
O	-0.716764	1.950191	1.287394
O	-0.970742	1.587430	-1.066314
C	0.900045	3.969468	-0.253120
H	1.350118	2.996643	-0.050560
H	1.244110	4.313819	-1.234773
H	1.265157	4.676871	0.499938
C	-1.227765	5.286453	-0.395249
H	-0.864012	5.968917	0.380214
H	-0.943271	5.703980	-1.367267
H	-2.321728	5.265392	-0.342783
C	1.581698	0.458155	-0.217814
H	1.542964	1.031763	-1.146082
C	2.664575	0.610065	0.551310
H	2.739434	0.040091	1.478116
C	3.839391	1.496208	0.231676
H	3.984537	2.235454	1.030201
C	0.733079	-2.544846	-1.221663
C	0.111512	-2.704033	1.196076
B	0.414132	-0.617400	0.047341
O	0.033485	-1.330631	-1.133308
O	0.710284	-1.427263	1.168307
C	0.377942	-3.530832	-0.090627
H	0.504112	-3.005103	-2.192378
H	1.822320	-2.358813	-1.202718
H	0.518539	-3.236725	2.066125
H	-0.966229	-2.597273	1.343194
C	-0.896642	-4.302516	-0.445448
H	-0.741196	-4.941317	-1.323134
H	-1.209502	-4.946268	0.385963
H	-1.701326	-3.590314	-0.648732
C	1.552142	-4.495000	0.105456

H	2.440338	-3.958026	0.457326
H	1.307180	-5.266409	0.844050
H	1.812522	-5.000470	-0.832422
H	3.622336	2.064871	-0.682160
C	5.134924	0.727039	0.042570
C	6.328808	1.171167	0.614870
C	5.161249	-0.438212	-0.730198
C	7.520429	0.475894	0.417635
H	6.325862	2.072081	1.223322
C	6.348437	-1.135695	-0.931151
H	4.234984	-0.800067	-1.168599
C	7.534452	-0.680667	-0.357213
H	8.437402	0.837266	0.873334
H	6.347973	-2.038562	-1.534528
H	8.460713	-1.225605	-0.510262
O	-2.580229	-1.441848	0.106992
O	-3.165854	0.744249	0.599717
O	-1.840456	-0.544931	2.216470
C	-2.880859	-1.085826	2.979814
H	-3.701933	-0.368050	3.133013
H	-3.310933	-1.985761	2.515438
H	-2.489708	-1.365118	3.965568
C	-3.546576	-1.081381	-0.859692
C	-4.179042	0.234230	-0.259711
C	-4.538443	-2.236371	-1.004087
H	-4.024672	-3.104723	-1.428250
H	-4.958931	-2.530395	-0.039975
H	-5.360295	-1.968753	-1.676867
C	-2.854425	-0.862557	-2.210033
H	-2.321344	-1.779250	-2.474016
H	-3.580928	-0.635747	-2.998201
H	-2.118051	-0.061979	-2.140475
C	-5.412007	-0.036785	0.612198
H	-5.687385	0.887857	1.128540
H	-6.270260	-0.367207	0.018556
H	-5.197836	-0.794779	1.369131
C	-4.536317	1.287226	-1.305634
H	-5.309326	0.916871	-1.987615
H	-4.922621	2.183289	-0.809127
H	-3.660691	1.569124	-1.891003

[BneopBpin-OMe]$^{-}$

Electronic Energy: -898.243857

B	0.432781	0.602582	1.024417
B	-1.019900	-0.374519	0.931553
O	0.373783	1.963513	0.737438
O	1.680868	0.014074	1.202064
O	-1.362305	-0.606352	-0.506940
O	-0.786525	-1.747960	1.472924
C	-1.322907	-2.679055	0.561996
C	-1.127818	-1.960955	-0.815985
C	2.881830	0.742931	1.014675
C	1.546966	2.736172	0.549320
C	2.717341	1.900011	0.026626
C	2.411443	1.368634	-1.379899
H	2.286901	2.198968	-2.083101
H	3.233446	0.740153	-1.738931

H	1.497046	0.769439	-1.398533
C	3.990516	2.746506	0.004910
H	4.844391	2.153452	-0.339314
H	3.878272	3.597511	-0.675143
H	4.228647	3.137310	1.000090
H	3.645631	0.042262	0.654325
H	3.225502	1.136177	1.982509
H	1.309100	3.540502	-0.158414
H	1.831932	3.208316	1.500833
C	-2.104184	-2.412191	-1.902636
H	-1.892953	-1.884489	-2.838756
H	-2.014118	-3.487530	-2.094786
H	-3.136691	-2.195564	-1.619243
C	0.310913	-2.108380	-1.341100
H	0.539115	-3.129860	-1.664699
H	0.438814	-1.442606	-2.201401
H	1.024266	-1.806584	-0.569747
C	-2.809058	-2.918571	0.881862
H	-3.252589	-3.700699	0.255550
H	-2.893203	-3.230995	1.928115
H	-3.375080	-1.992471	0.760132
C	-0.570153	-4.003621	0.692116
H	-0.776324	-4.455889	1.668121
H	-0.880446	-4.715922	-0.081113
H	0.508755	-3.852292	0.612204
O	-2.218563	0.272194	1.531648
C	-2.101073	0.581588	2.879413
H	-3.002687	1.108738	3.222714
H	-1.979991	-0.313791	3.513820
H	-1.234673	1.235931	3.094452

Calculations in ^{i}PrOH

***E*-1$_{iPr}$**

Electronic Energy: -759.450973

C	-0.536896	-0.338331	0.124271
H	-1.215325	0.503064	-0.012537
C	-1.054467	-1.569313	0.215161
H	-0.378066	-2.413109	0.355293
C	-2.512096	-1.950249	0.145242
H	-2.633804	-2.676008	-0.669257
C	2.977931	1.004121	0.090791
C	3.190706	-0.457797	0.616284
B	0.988336	-0.083916	0.212176
O	1.546125	1.170452	0.216778
O	1.926948	-1.084887	0.297963
C	3.354813	-0.532076	2.135001
H	3.295731	-1.577959	2.446459
H	4.321608	-0.131912	2.451314
H	2.563304	0.022165	2.647310
C	4.311416	-1.224412	-0.070204
H	5.267995	-0.715090	0.080331
H	4.389187	-2.226997	0.358467
H	4.132864	-1.323237	-1.142129
C	3.314809	1.164187	-1.392282
H	2.957602	2.139028	-1.733497

H	4.393244	1.112762	-1.563186
H	2.828592	0.391916	-1.994958
C	3.676389	2.081655	0.907015
H	4.758748	1.921563	0.900252
H	3.475384	3.063715	0.470989
H	3.330649	2.089095	1.941965
H	-2.763938	-2.497754	1.062633
C	-3.461923	-0.794182	-0.045182
C	-3.800660	-0.353819	-1.326959
C	-3.989588	-0.115969	1.056105
C	-4.650856	0.734115	-1.505781
H	-3.393509	-0.869920	-2.192518
C	-4.840385	0.972540	0.882661
H	-3.730748	-0.445409	2.058986
C	-5.173991	1.400634	-0.400117
H	-4.906291	1.060454	-2.509166
H	-5.244245	1.485516	1.750010
H	-5.838736	2.247574	-0.537431

^{i}PrO^{-}

Electronic Energy: -193.764169

C	0.329502	-2.083099	-1.994816
H	0.291964	-3.182971	-2.308871
C	1.729114	-1.615732	-2.493916
H	2.558124	-2.250951	-2.148637
H	1.740231	-1.602389	-3.590474
H	1.915708	-0.588437	-2.150601
C	0.380874	-2.156280	-0.439679
H	-0.577060	-2.531457	-0.059750
H	1.182171	-2.802610	-0.052176
H	0.524176	-1.146342	-0.030403
O	-0.673742	-1.333005	-2.455889

A_{iPr}

Electronic Energy: -937.544014

B	1.285127	0.255472	-1.034443
B	0.247157	-1.117505	-0.736896
O	0.815726	1.419048	-0.223480
O	2.693812	-0.077761	-0.698676
O	0.665022	-2.393692	-1.097511
O	-1.032035	-0.958911	-0.213494
C	-1.927769	-2.049970	-0.090250
C	-0.191510	-3.516811	-0.994462
C	-1.211041	-3.382820	0.139279
C	3.558956	1.018617	-0.760415
C	1.666685	2.525801	-0.266414
H	-2.539894	-2.118319	-1.001858
H	-2.605687	-1.835133	0.745308
H	-0.723900	-3.654292	-1.947252
H	0.434662	-4.404179	-0.837649
H	3.636784	1.407931	-1.791376
H	4.569238	0.693794	-0.458936
C	-2.219241	-4.530322	0.064402
H	-1.718502	-5.495344	0.196282
H	-2.974391	-4.434867	0.851808
H	-2.736447	-4.546205	-0.901036
C	-0.506744	-3.389411	1.501432

H	-1.235551	-3.275361	2.310796
H	0.024782	-4.334719	1.653578
H	0.219694	-2.576913	1.584848
O	1.303460	0.620427	-2.498401
C	0.179975	1.226725	-3.063247
H	-0.344276	1.830035	-2.303776
C	3.108964	2.178218	0.147703
H	1.273926	3.305588	0.408162
H	1.700384	2.968373	-1.280016
C	3.140525	1.736775	1.612840
H	4.157431	1.459975	1.916735
H	2.798836	2.542799	2.273584
H	2.489704	0.872059	1.756732
C	4.017990	3.388191	-0.061749
H	3.696415	4.234475	0.556971
H	5.054596	3.153740	0.208091
H	4.009551	3.715408	-1.108164
C	0.645184	2.164317	-4.177314
C	-0.811814	0.188382	-3.605763
H	-0.312450	-0.461968	-4.333002
H	-1.196896	-0.434671	-2.793320
H	-1.665195	0.668070	-4.099009
H	-0.195543	2.690762	-4.642608
H	1.342449	2.907709	-3.778271
H	1.166521	1.594648	-4.955573

Bneo-O^{i}Pr in ^{i}PrOH

Electronic Energy: -565.629402

C	-2.256315	2.233144	-1.834002
C	-1.999793	3.449162	0.291427
C	-2.611121	3.536627	-1.110205
H	-2.757482	2.189130	-2.806448
H	-1.173626	2.189883	-2.011284
H	-2.309470	4.305611	0.898855
H	-0.904319	3.461700	0.223045
B	-2.692583	1.139495	0.265828
O	-2.649466	1.078849	-1.101394
O	-2.402480	2.271378	0.981801
C	-4.133370	3.710652	-1.023284
H	-4.614127	2.885017	-0.491319
H	-4.381569	4.637383	-0.496448
H	-4.569591	3.761521	-2.025742
C	-1.989424	4.716444	-1.860388
H	-2.395503	4.784847	-2.874465
H	-2.209444	5.658030	-1.347623
H	-0.901706	4.616066	-1.935617
O	-3.066756	-0.004357	0.905785
C	-3.243824	-0.025107	2.325777
H	-2.468535	0.596599	2.788724
C	-4.612769	0.541752	2.679356
H	-5.401170	-0.051897	2.205974
H	-4.767233	0.523463	3.762112
H	-4.698299	1.576510	2.337026
C	-3.074418	-1.465520	2.780678
H	-3.178961	-1.536209	3.866862
H	-3.834577	-2.102371	2.317390
H	-2.087676	-1.843995	2.501638

B_2neop_2 in ^{i}PrOH

Electronic Energy: -743.714372

B	0.975280	0.353728	0.488245
B	-0.059650	-0.986315	0.184939
O	1.318490	0.648549	1.780867
O	1.418994	1.102910	-0.568842
O	-0.402854	-1.281296	-1.107650
O	-0.503377	-1.735360	1.242116
C	-1.359222	-2.853379	1.022022
C	-1.256292	-2.387034	-1.390259
C	-1.136199	-3.502360	-0.347340
C	2.275093	2.220690	-0.348510
C	2.171648	1.754429	2.063765
C	2.051815	2.869725	1.020779
C	0.666432	3.525875	1.088196
H	0.505926	3.977944	2.072018
H	0.580416	4.313879	0.333421
H	-0.138745	2.806709	0.914738
C	3.139541	3.916761	1.269807
H	3.087582	4.712403	0.519802
H	3.013294	4.376872	2.255005
H	4.140054	3.473955	1.227020
H	-2.400730	-2.519315	1.112274
H	-1.167164	-3.574449	1.823390
H	-2.291993	-2.026710	-1.434737
H	-0.987906	-2.761181	-2.383738
H	2.083483	2.941800	-1.149948
H	3.316542	1.886345	-0.438420
C	-2.223934	-4.549434	-0.596169
H	-2.097751	-5.009663	-1.581318
H	-2.171916	-5.344984	0.153930
H	-3.224448	-4.106632	-0.553361
C	0.249197	-4.158450	-0.415062
H	0.335338	-4.946570	0.339577
H	0.409588	-4.610358	-1.398977
H	1.054373	-3.439284	-0.241600
H	1.902819	2.128571	3.057127
H	3.207375	1.394239	2.108670

TSA_{iPr}

Electronic Energy: -1696.973260

C	0.388852	-2.151290	-1.973807
C	0.765214	-2.865756	-0.624971
B	0.472308	-0.577410	-0.273391
O	0.503869	-1.875366	0.361591
O	0.590164	-0.775244	-1.671111
C	-0.445549	3.040564	0.013648
C	-2.625672	2.574230	1.017796
C	-1.746810	3.707908	0.476992
H	0.240657	3.796861	-0.395848
H	0.052031	2.592341	0.887549
H	-3.624883	2.958160	1.271111
H	-2.167540	2.197544	1.944136
B	-1.666249	1.077275	-0.723478
O	-0.677906	2.081865	-0.978985

O	-2.792060	1.521133	0.102890
C	-2.433798	4.416196	-0.693684
H	-2.644807	3.711608	-1.501690
H	-3.379338	4.869325	-0.374036
H	-1.795244	5.212213	-1.094042
C	-1.451334	4.701589	1.600206
H	-0.815481	5.518242	1.240625
H	-2.376394	5.144501	1.986582
H	-0.935468	4.215639	2.436119
C	1.453926	0.483158	0.390496
H	1.337164	0.713645	1.451702
C	2.496995	1.018092	-0.246563
H	2.644545	0.785529	-1.302596
C	3.546432	1.900407	0.376788
H	3.254998	2.129985	1.410284
C	-3.168762	-1.805698	1.512865
C	-1.939381	-0.345345	3.050424
B	-1.421245	-0.319277	0.664253
O	-2.358918	-1.325248	0.464990
O	-1.127973	0.078802	1.970286
C	-2.480289	-1.766778	2.879923
H	-4.092899	-1.207591	1.555412
H	-3.457881	-2.836621	1.269484
H	-1.339359	-0.277851	3.966775
H	-2.784720	0.351992	3.157824
C	-3.506976	-2.055688	3.976715
H	-3.930268	-3.058666	3.854816
H	-3.930268	-3.058666	3.854816
H	-3.039832	-2.009210	4.966458
H	-4.332345	-1.335354	3.957327
C	-1.338052	-2.786729	2.940694
H	-0.592948	-2.586972	2.167350
H	-0.850036	-2.752472	3.921868
H	-1.725903	-3.801510	2.793382
C	1.296734	-2.519490	-3.146483
H	1.247845	-3.593284	-3.357225
H	0.969137	-1.984842	-4.043070
H	2.336635	-2.249375	-2.951238
C	-1.068787	-2.380942	-2.383318
H	-1.299329	-1.734852	-3.233125
H	-1.233029	-3.424048	-2.676367
H	-1.746627	-2.106228	-1.574876
C	2.258721	-3.205194	-0.526572
H	2.478044	-3.529741	0.495069
H	2.546805	-4.008677	-1.211962
H	2.869883	-2.323491	-0.740060
C	-0.067881	-4.105598	-0.313643
H	0.033964	-4.858550	-1.102609
H	0.268969	-4.551124	0.627645
H	-1.120119	-3.836968	-0.205235
O	-2.100340	0.464751	-1.933013
C	-3.395648	0.678389	-2.432669
H	-3.772578	1.658397	-2.102417
H	3.606648	2.860650	-0.151717
C	4.924674	1.262324	0.377961
C	5.089031	-0.062193	0.797396
C	6.055139	1.974262	-0.027665

C	6.347672	-0.654627	0.817530
H	4.213176	-0.630172	1.099285
C	7.318332	1.385029	-0.011158
H	5.945538	3.002537	-0.363289
C	7.469275	0.067681	0.412404
H	6.453887	-1.684156	1.146440
H	8.183955	1.955908	-0.333751
H	8.451434	-0.394615	0.423399
C	-3.314976	0.681006	-3.956673
C	-4.365854	-0.389600	-1.929817
H	-4.030845	-1.380352	-2.254691
H	-4.387579	-0.379776	-0.839324
H	-5.376586	-0.216008	-2.317514
H	-4.297057	0.864692	-4.405591
H	-2.948291	-0.287043	-4.315747
H	-2.624059	1.455843	-4.301631

B_{iPr}

Electronic Energy: -1131.368766

C	3.355511	-0.662538	0.955815
C	3.691410	-0.793108	-0.568078
B	1.447101	-0.125686	-0.320408
O	2.690265	-0.011649	-1.173890
O	1.951355	-0.699071	0.974511
C	0.329964	-1.123627	-0.969380
H	0.056274	-0.958455	-2.022046
C	-0.383158	-2.059614	-0.331502
H	-0.171091	-2.251858	0.722980
C	-1.523112	-2.862289	-0.919880
H	-1.515347	-2.750294	-2.010914
H	-1.396004	-3.931049	-0.703920
C	-2.867812	-2.410856	-0.384105
C	-3.442916	-1.223845	-0.850204
C	-3.540503	-3.126546	0.607765
C	-4.653368	-0.764959	-0.342527
H	-2.923443	-0.650437	-1.613866
C	-4.753771	-2.670869	1.122909
H	-3.109349	-4.051632	0.982475
C	-5.314819	-1.488366	0.649515
H	-5.079849	0.160312	-0.718756
H	-5.260360	-3.242300	1.895051
H	-6.259423	-1.132202	1.048652
C	-0.559404	3.283922	-1.205771
C	-0.521773	3.074086	1.229481
B	0.635818	1.414464	-0.155246
O	0.238186	2.115851	-1.291460
O	0.267768	1.905414	1.092129
C	-1.454293	3.295116	0.036134
H	0.090588	4.171288	-1.193678
H	-1.172511	3.338789	-2.114447
H	-1.105659	2.977355	2.153662
H	0.135692	3.948218	1.345513
C	-2.145840	4.653018	0.161949
H	-2.797973	4.837032	-0.698482
H	-2.764699	4.690290	1.064718
H	-1.418036	5.469922	0.216172
C	-2.497727	2.173907	-0.038523

H	-2.032077	1.186879	-0.092926
H	-3.142826	2.188149	0.846501
H	-3.133301	2.294847	-0.922688
C	3.904705	-1.795909	1.823026
H	4.995969	-1.864750	1.745586
H	3.652306	-1.618689	2.874025
H	3.473788	-2.756408	1.530761
C	3.835916	0.684200	1.526050
H	3.383931	0.828145	2.512592
H	4.925041	0.731570	1.635389
H	3.510545	1.504778	0.880733
C	3.576606	-2.250885	-1.049284
H	3.604573	-2.262111	-2.143979
H	4.395215	-2.878970	-0.680203
H	2.623598	-2.679308	-0.729252
C	5.064692	-0.246735	-0.959968
H	5.866560	-0.756293	-0.413224
H	5.237460	-0.400497	-2.030602
H	5.133379	0.824824	-0.758408

TSB_{iPr}

Electronic Energy: -1131.336089

C	3.876840	-0.493973	0.800802
C	3.848046	-0.467652	-0.765906
B	1.986675	0.633490	0.048086
O	2.926427	0.581393	-1.038938
O	2.570877	-0.070967	1.162196
C	0.380886	-0.388806	-0.536822
H	0.327918	-0.549254	-1.621712
C	-0.296512	-1.238355	0.237891
H	-0.278347	-1.077602	1.319334
C	-1.138504	-2.410077	-0.220065
H	-0.916438	-2.633354	-1.269112
H	-0.873441	-3.303670	0.362190
C	-2.623447	-2.146557	-0.067927
C	-3.466395	-2.122207	-1.179828
C	-3.177198	-1.882015	1.189364
C	-4.822996	-1.832247	-1.046827
H	-3.053081	-2.321674	-2.165070
C	-4.529278	-1.586091	1.328008
H	-2.538430	-1.898929	2.068575
C	-5.359232	-1.557926	0.207841
H	-5.459339	-1.815320	-1.926569
H	-4.937684	-1.378512	2.312563
H	-6.414586	-1.327255	0.314508
C	-0.951173	3.122451	-0.752220
C	-1.550526	1.752428	1.230613
B	0.598813	1.495450	0.079508
O	0.121302	2.265222	-1.041812
O	-0.142797	1.674033	1.286442
C	-2.116600	2.403831	-0.062126
H	-0.623403	3.958497	-0.108735
H	-1.302805	3.563105	-1.696125
H	-1.984551	0.746541	1.341619
H	-1.868083	2.341817	2.102397
C	-3.206438	3.417932	0.297671
H	-3.632580	3.874964	-0.602907

H	-4.023553	2.930821	0.841839
H	-2.811687	4.219852	0.931978
C	-2.702983	1.342580	-0.999337
H	-1.945918	0.606934	-1.275875
H	-3.523143	0.803363	-0.512705
H	-3.093791	1.807199	-1.913123
C	4.149333	-1.870530	1.403413
H	5.119018	-2.260630	1.074923
H	4.166212	-1.800110	2.495595
H	3.372450	-2.584902	1.122767
C	4.871340	0.520264	1.383904
H	4.704573	0.595279	2.462661
H	5.912787	0.227136	1.216353
H	4.709933	1.509366	0.945887
C	3.315263	-1.774722	-1.370054
H	3.141365	-1.620051	-2.439309
H	4.028034	-2.597482	-1.253602
H	2.365245	-2.056422	-0.911052
C	5.187506	-0.130736	-1.416570
H	5.952312	-0.865360	-1.142005
H	5.083406	-0.143112	-2.506077
H	5.536095	0.861073	-1.121228

C_{iPr}

Electronic Energy: -1131.375132

C	4.041904	-0.830407	0.823346
C	3.992715	-1.038030	-0.723962
B	2.151095	0.158281	-0.044316
O	2.996351	-0.082987	-1.127629
O	2.705797	-0.385809	1.112143
C	-0.387952	-0.416728	-0.642209
H	-0.426636	-0.651173	-1.716283
C	-1.106801	-1.222361	0.147347
H	-1.115213	-1.024873	1.222554
C	-2.020432	-2.329752	-0.310815
H	-1.834182	-2.532847	-1.374154
H	-1.815035	-3.264919	0.226621
C	-3.490450	-1.984466	-0.129477
C	-3.967039	-0.714990	-0.474431
C	-4.400139	-2.920000	0.367978
C	-5.313337	-0.393397	-0.333000
H	-3.262476	0.025733	-0.844064
C	-5.749720	-2.602498	0.513802
H	-4.047541	-3.909802	0.647801
C	-6.211832	-1.336984	0.163106
H	-5.662014	0.598370	-0.606323
H	-6.439026	-3.344336	0.906158
H	-7.261664	-1.085930	0.278948
C	-0.728696	2.542030	-1.262278
C	-1.122182	2.013616	1.123512
B	0.562154	0.833645	-0.161203
O	0.518763	1.922948	-1.192879
O	0.112199	1.360655	1.167392
C	-1.165531	3.151371	0.084274
H	-1.940186	1.309565	0.882951
H	-1.340727	2.430152	2.121554
C	-0.203011	4.271260	0.486151

H	-0.204057	5.076400	-0.258841
H	-0.488796	4.705628	1.451862
H	0.813651	3.881708	0.570327
C	-2.591135	3.690372	-0.028392
H	-3.292588	2.898681	-0.318598
H	-2.932266	4.105673	0.927301
H	-2.653988	4.487127	-0.779101
C	4.335624	-2.089989	1.628768
H	5.312258	-2.503387	1.356810
H	4.354211	-1.851023	2.695886
H	3.574980	-2.855626	1.465355
C	4.995787	0.290172	1.246829
H	4.825709	0.519117	2.302336
H	6.042883	-0.000393	1.121256
H	4.812698	1.199809	0.668031
C	3.472257	-2.422413	-1.122756
H	3.277045	-2.430265	-2.198535
H	4.197523	-3.209683	-0.897792
H	2.534859	-2.649632	-0.606557
C	5.298512	-0.745534	-1.451216
H	6.094637	-1.407374	-1.095100
H	5.171218	-0.915388	-2.524109
H	5.614929	0.289064	-1.305933
H	-1.516101	1.826603	-1.577964
H	-0.696487	3.337295	-2.026484

TSC_{iPr}

Electronic Energy: -1696.986041

C	0.053621	-3.079060	0.183264
C	-0.439605	-3.440411	-1.222387
C	-0.134199	-2.232055	-2.117514
H	1.149263	-2.986837	0.180206
H	-0.212652	-3.876594	0.891885
H	0.950325	-2.122083	-2.234371
H	-0.561305	-2.402679	-3.116904
B	-0.562793	-0.746653	-0.240533
O	-0.674672	-1.034949	-1.620616
O	-0.519695	-1.882816	0.653655
C	2.285518	2.835502	0.264394
C	0.188427	2.803538	-0.995566
C	1.370296	3.701705	-0.608353
H	3.217975	3.373740	0.487410
H	1.781058	2.627094	1.219251
H	-0.507083	3.355526	-1.644219
H	-0.365221	2.530007	-0.085279
B	1.628647	0.878816	-1.091093
O	2.632270	1.624191	-0.359664
O	0.599078	1.653105	-1.685197
C	2.112989	4.180852	-1.858886
H	2.476095	3.331075	-2.441993
H	1.451721	4.776415	-2.498835
H	2.971945	4.804803	-1.586202
C	0.867921	4.894854	0.204005
H	1.702763	5.521652	0.537364
H	0.199273	5.521765	-0.396414
H	0.316315	4.567325	1.092403
C	-1.626509	0.324005	0.273744

H	-1.530407	0.706616	1.292587
C	-2.675488	0.738518	-0.440875
H	-2.798862	0.365541	-1.458715
C	-3.747386	1.677886	0.045121
H	-3.467819	2.058648	1.036539
H	-3.817928	2.552553	-0.614701
C	-5.118446	1.029860	0.134345
C	-5.261735	-0.256572	0.663773
C	-6.266178	1.704536	-0.287790
C	-6.516332	-0.848289	0.775133
H	-4.372893	-0.795785	0.979736
C	-7.524883	1.116350	-0.179430
H	-6.173285	2.702813	-0.708385
C	-7.654655	-0.163276	0.353659
H	-6.605938	-1.848402	1.188860
H	-8.404039	1.657651	-0.516092
H	-8.633624	-0.625084	0.436527
C	1.665355	-0.128559	2.931037
C	2.786553	-0.936427	2.187006
B	1.238317	-0.147438	0.655021
O	0.972182	0.519301	1.855622
O	2.250177	-1.089547	0.868625
C	3.057895	-2.321009	2.765915
H	3.831563	-2.818862	2.173920
H	3.413626	-2.250692	3.799223
H	2.160826	-2.942762	2.744877
C	4.103690	-0.167306	2.051746
H	4.586229	-0.010402	3.021184
H	4.783167	-0.747686	1.420140
H	3.932978	0.793946	1.562487
C	2.183096	0.937062	3.891149
H	1.338267	1.467733	4.339937
H	2.766675	0.483527	4.699174
H	2.809029	1.668012	3.375366
C	0.646029	-1.019396	3.646905
H	1.091789	-1.547753	4.495067
H	-0.165098	-0.388949	4.023979
H	0.215585	-1.737798	2.945764
O	2.188798	-0.049093	-2.006012
C	3.542550	-0.434614	-1.882415
H	3.885830	-0.255048	-0.859529
C	0.326249	-4.660032	-1.734770
H	0.147586	-5.532415	-1.095965
H	0.011399	-4.920739	-2.751506
H	1.405274	-4.469635	-1.754311
C	-1.945477	-3.722913	-1.200805
H	-2.308739	-3.968324	-2.205370
H	-2.173750	-4.569116	-0.542413
H	-2.498860	-2.851448	-0.841367
C	3.660119	-1.927896	-2.162641
H	4.705829	-2.251308	-2.117951
H	3.090294	-2.488014	-1.416174
H	3.268109	-2.168567	-3.157562
C	4.396198	0.398581	-2.836475
H	4.064303	0.254062	-3.870939
H	4.298667	1.458466	-2.585220
H	5.454104	0.120229	-2.771496

[BpinBneop-O^{i}Pr]$^{-}$ in ^{i}PrOH

Electronic Energy: -976.866670

B	0.992471	0.617756	1.067176
B	-0.074022	-0.445620	0.180455
O	0.833983	2.006711	0.536004
O	2.388674	0.143828	0.892433
O	-0.838779	-0.112195	-0.934031
O	-0.289485	-1.784490	0.507888
C	-1.399418	-2.277980	-0.260553
C	-1.407139	-1.310939	-1.487849
C	3.363216	1.036738	1.348147
C	1.795854	2.907413	0.998123
C	3.232473	2.432969	0.712422
C	3.464458	2.348209	-0.798000
H	3.360332	3.335060	-1.265212
H	4.471467	1.974768	-1.020401
H	2.736444	1.673707	-1.253034
C	4.236737	3.391275	1.350784
H	5.266296	3.055463	1.178912
H	4.140857	4.399185	0.929903
H	4.084154	3.464347	2.434012
H	4.359696	0.624470	1.116471
H	3.313889	1.157859	2.446201
H	1.633160	3.885820	0.514978
H	1.704829	3.069275	2.088225
C	-2.788950	-0.998365	-2.048165
H	-2.697860	-0.317491	-2.899227
H	-3.280414	-1.912670	-2.396226
H	-3.425878	-0.523756	-1.299473
C	-0.480913	-1.769574	-2.617828
H	-0.877620	-2.647872	-3.135275
H	-0.379863	-0.958151	-3.343630
H	0.515167	-2.008420	-2.234673
C	-2.650350	-2.143971	0.612807
H	-3.538276	-2.541323	0.112468
H	-2.497360	-2.704091	1.539303
H	-2.832293	-1.098089	0.877045
C	-1.163973	-3.743659	-0.602621
H	-1.169300	-4.342534	0.312507
H	-1.956251	-4.118792	-1.258535
H	-0.202840	-3.889610	-1.098915
O	0.714808	0.594274	2.537589
C	-0.599230	0.859202	2.933241
H	-1.242040	1.019715	2.048828
C	-1.153273	-0.345693	3.695127
H	-1.106392	-1.228098	3.051681
H	-0.548869	-0.535721	4.589941
H	-2.192722	-0.190712	4.006931
C	-0.657535	2.135038	3.773540
H	-0.307258	2.986416	3.183519
H	-1.675264	2.345739	4.121908
H	-0.007459	2.035138	4.650601

13$_{iPr}$

Electronic Energy: -720.132794

C	-0.932455	3.531409	0.890076
C	-1.957859	3.957681	-0.165300
C	-2.061848	2.809647	-1.174442
H	-1.329145	2.695248	1.480120
H	-0.723837	4.358394	1.576543
H	-2.520544	1.933863	-0.697738
H	-2.692286	3.100251	-2.021072
B	0.333732	2.591089	-0.941901
O	-0.794014	2.429285	-1.700205
O	0.307221	3.134564	0.314086
C	1.700430	2.149672	-1.550571
H	1.718874	1.732840	-2.559088
C	2.861026	2.250839	-0.892406
H	2.862403	2.656460	0.120018
C	4.203342	1.820573	-1.416563
H	4.098277	1.479085	-2.452875
H	4.883794	2.680280	-1.427430
C	4.814767	0.718264	-0.571395
C	4.139590	-0.495882	-0.411526
C	6.045860	0.887196	0.063414
C	4.685533	-1.518440	0.356982
H	3.174825	-0.633926	-0.892721
C	6.596027	-0.134312	0.836060
H	6.581195	1.826359	-0.048489
C	5.917722	-1.340348	0.984646
H	4.148873	-2.455581	0.468532
H	7.555133	0.014838	1.322373
H	6.344266	-2.136709	1.586243
C	-3.317365	4.166253	0.505472
H	-3.261398	4.968390	1.248099
H	-4.072963	4.447763	-0.234727
H	-3.658838	3.257285	1.011466
C	-1.511622	5.250346	-0.861392
H	-2.242476	5.546408	-1.620444
H	-1.426660	6.064702	-0.135058
H	-0.542362	5.139979	-1.355241

Calculations in TFE

***E*-1$_{TFE}$**

Electronic Energy: -759.451179

C	-0.536926	-0.338824	0.125309
H	-1.215414	0.502592	-0.011204
C	-1.054709	-1.569799	0.215551
H	-0.378561	-2.413845	0.355349
C	-2.512354	-1.950485	0.145307
H	-2.633930	-2.676070	-0.669346
C	2.977820	1.004040	0.090529
C	3.191003	-0.457618	0.616523
B	0.988319	-0.084258	0.213022
O	1.545867	1.170237	0.217110
O	1.927021	-1.085073	0.298788
C	3.355503	-0.531462	2.135184
H	3.296930	-1.577284	2.446955
H	4.322292	-0.130937	2.451007
H	2.564031	0.022702	2.647636
C	4.311471	-1.224393	-0.070113

H	5.268009	-0.714872	0.079836
H	4.389604	-2.226762	0.359016
H	4.132544	-1.323650	-1.141943
C	3.313956	1.163550	-1.392760
H	2.956611	2.138252	-1.734267
H	4.392318	1.112189	-1.564032
H	2.827649	0.390943	-1.994941
C	3.676458	2.082039	0.905957
H	4.758803	1.922028	0.898825
H	3.475276	3.063874	0.469484
H	3.331186	2.089923	1.941066
H	-2.764415	-2.498090	1.062558
C	-3.461973	-0.794216	-0.045128
C	-3.798744	-0.352269	-1.326890
C	-3.991432	-0.117418	1.056233
C	-4.648738	0.735896	-1.505678
H	-3.390360	-0.867317	-2.192497
C	-4.842056	0.971251	0.882822
H	-3.734279	-0.448220	2.059101
C	-5.173635	1.401006	-0.399985
H	-4.902647	1.063424	-2.509062
H	-5.247388	1.483074	1.750164
H	-5.838254	2.248053	-0.537242

$CF_3CH_2O^-$ in TFE

Electronic Energy: -452.121682

C	-2.415610	0.828560	-0.038340
C	-1.943693	1.620371	-1.266155
H	-2.264630	0.940235	-2.116191
H	-0.822025	1.450401	-1.232710
O	-2.369750	2.872013	-1.293216
F	-1.999798	1.372773	1.129657
F	-1.964294	-0.456766	-0.033029
F	-3.764418	0.748699	0.048952

A_{TFE}

Electronic Energy: -1195.890633

B	1.241615	0.305653	-0.963370
B	0.074201	-0.954256	-0.645185
O	0.653499	1.612832	-0.552347
O	2.490451	0.021900	-0.224683
O	-0.356148	-1.801275	-1.657745
O	-0.409105	-1.143671	0.641648
C	-1.320853	-2.185936	0.949187
C	-1.274177	-2.853216	-1.405872
C	-1.168828	-3.394680	0.022044
C	3.414596	1.074255	-0.244651
C	1.565279	2.676202	-0.576440
H	-2.348040	-1.800036	0.881002
H	-1.149410	-2.483626	1.990990
H	-2.296807	-2.492369	-1.586160
H	-1.073766	-3.651870	-2.130548
H	3.793704	1.252069	-1.266850
H	4.280268	0.797015	0.378882
C	-2.301837	-4.388644	0.281445
H	-2.225049	-5.247979	-0.392931

H	-2.259071	-4.764788	1.308998
H	-3.282931	-3.925710	0.130537
C	0.188475	-4.074835	0.240934
H	0.271433	-4.442350	1.269058
H	0.302754	-4.928404	-0.435388
H	1.020150	-3.388640	0.060336
O	1.649479	0.383060	-2.421501
C	0.677510	0.815846	-3.292910
H	0.010946	0.008777	-3.642149
H	0.040144	1.603992	-2.864097
C	2.815567	2.393662	0.275875
H	1.064082	3.582803	-0.199397
H	1.894142	2.892821	-1.608305
C	2.421655	2.242506	1.747100
H	3.299513	2.023144	2.366737
H	1.962500	3.163229	2.126722
H	1.705815	1.425968	1.860496
C	3.826508	3.526830	0.107511
H	3.409458	4.480046	0.453196
H	4.736590	3.331914	0.686959
H	4.116479	3.648440	-0.942718
C	1.326849	1.408384	-4.521925
F	2.093481	2.481219	-4.239415
F	2.119986	0.528514	-5.164484
F	0.396205	1.818559	-5.412560

Bneo-OCH_2CF_3 in TFE

Electronic Energy: -823.964597

C	1.184243	2.604723	2.305080
C	1.007635	3.441522	-0.006695
C	1.446737	3.821532	1.410736
H	1.280280	4.227097	-0.717754
H	-0.080916	3.311579	-0.042747
B	1.989013	1.296893	0.465694
O	1.809236	1.422873	1.809535
O	1.623749	2.235135	-0.453177
C	2.934884	4.198043	1.428892
H	3.572828	3.391719	1.057275
H	3.110663	5.076807	0.800698
H	3.255301	4.438012	2.447369
C	0.600519	4.998274	1.901703
H	0.886604	5.278824	2.920047
H	0.748177	5.872205	1.259742
H	-0.466449	4.752867	1.902846
O	2.589249	0.130051	0.050666
C	3.003041	-0.005475	-1.281793
H	2.927705	-1.054727	-1.574997
H	2.412340	0.604774	-1.969560
C	4.455605	0.412780	-1.412411
F	5.268430	-0.348915	-0.664622
F	4.858416	0.309837	-2.689378
F	4.643834	1.687956	-1.025810
H	1.574902	2.779105	3.312182
H	0.104842	2.424982	2.386132

B_2neop_2 in TFE

Electronic Energy: -743.714667

B	0.975370	0.353692	0.488279
B	-0.059747	-0.986290	0.184977
O	1.318170	0.648595	1.780988
O	1.419449	1.102612	-0.568830
O	-0.403315	-1.281014	-1.107565
O	-0.503070	-1.735451	1.242237
C	-1.359029	-2.853663	1.022201
C	-1.256962	-2.386892	-1.390066
C	-1.136253	-3.502307	-0.347339
C	2.275747	2.220475	-0.348329
C	2.171437	1.754628	2.064021
C	2.051870	2.869675	1.020764
C	0.666425	3.525796	1.087562
H	0.505614	3.978044	2.071244
H	0.580721	4.313668	0.332625
H	-0.138753	2.806629	0.913948
C	3.139459	3.916822	1.270012
H	3.087665	4.712285	0.519820
H	3.012765	4.377032	2.255095
H	4.139982	3.474034	1.227653
H	-2.400457	-2.519586	1.112829
H	-1.166598	-3.574812	1.823381
H	-2.292619	-2.026501	-1.433998
H	-0.988902	-2.760816	-2.383693
H	2.084480	2.941429	-1.149960
H	3.317110	1.885864	-0.437762
C	-2.223868	-4.549567	-0.595996
H	-2.097838	-5.009558	-1.581265
H	-2.171395	-5.345174	0.153997
H	-3.224427	-4.106940	-0.552799
C	0.249255	-4.158142	-0.415618
H	0.335714	-4.946382	0.338850
H	0.409345	-4.609863	-1.399659
H	1.054446	-3.438919	-0.242300
H	1.902253	2.128920	3.057207
H	3.207052	1.394286	2.109260

TSA_{TFE}

Electronic Energy: -1955.321415

C	0.490230	1.967220	2.023530
C	1.194174	2.716643	0.842187
B	0.711352	0.532040	0.220031
O	0.919158	1.876565	-0.275217
O	0.601555	0.602825	1.631038
C	-0.359700	-3.018008	-0.278578
C	-2.202974	-2.356198	-1.744009
C	-1.580754	-3.561402	-1.031560
H	0.129955	-3.829922	0.278245
H	0.371405	-2.643432	-1.011515
H	-3.135490	-2.648992	-2.246586
H	-1.502351	-2.001268	-2.514582
B	-1.548171	-0.959946	0.193296
O	-0.704989	-2.016131	0.638200
O	-2.508580	-1.309585	-0.855121
C	-2.586566	-4.183419	-0.057809
H	-2.946114	-3.441807	0.658887

H	-3.451078	-4.583526	-0.600130
H	-2.127526	-5.007406	0.500303
C	-1.131018	-4.592091	-2.066690
H	-0.668337	-5.457115	-1.578892
H	-1.982301	-4.955384	-2.653186
H	-0.399392	-4.165732	-2.762288
C	1.724871	-0.540309	-0.373417
H	1.753181	-0.698614	-1.453432
C	2.647009	-1.160796	0.365167
H	2.652340	-1.001494	1.444702
C	3.749629	-2.036453	-0.168535
H	3.581954	-2.213253	-1.239250
C	-2.560022	2.052675	-2.059290
C	-1.107405	0.673846	-3.469890
B	-1.010901	0.462925	-1.042125
O	-1.940649	1.490955	-0.921739
O	-0.505912	0.147112	-2.300282
C	-1.639982	2.096224	-3.281900
H	-3.459372	1.466140	-2.302055
H	-2.887516	3.066827	-1.797701
H	-0.357404	0.653019	-4.270092
H	-1.933853	0.012577	-3.772266
C	-2.449167	2.505514	-4.513830
H	-2.862085	3.512104	-4.387411
H	-1.815846	2.514448	-5.407374
H	-3.282556	1.818023	-4.695810
C	-0.482327	3.075416	-3.055082
H	0.118864	2.782548	-2.190672
H	0.164871	3.108300	-3.939130
H	-0.867485	4.087257	-2.883329
C	1.179886	2.136478	3.374797
H	1.222692	3.192449	3.662218
H	0.616767	1.599648	4.144183
H	2.196368	1.737387	3.357412
C	-0.987552	2.345011	2.155325
H	-1.477094	1.640622	2.831444
H	-1.100276	3.358801	2.554552
H	-1.485063	2.276026	1.186242
C	2.719871	2.771386	1.005024
H	3.159960	3.127104	0.068337
H	3.024130	3.450998	1.807243
H	3.123108	1.775762	1.210365
C	0.659835	4.117866	0.566335
H	0.791494	4.762972	1.441694
H	1.206576	4.565012	-0.269710
H	-0.399234	4.092576	0.305481
O	-2.210264	-0.387450	1.334008
C	-3.470410	0.164524	1.226837
H	-3.449949	1.261230	1.277959
H	-3.989368	-0.123318	0.307289
H	3.733175	-3.020483	0.317304
C	5.126931	-1.424294	0.023600
C	5.345845	-0.072852	-0.264045
C	6.203969	-2.189267	0.475914
C	6.606582	0.495343	-0.109712
H	4.509798	0.534550	-0.599799
C	7.468707	-1.624798	0.632815

H	6.050791	-3.239757	0.710472
C	7.674702	-0.279402	0.340042
H	6.755484	1.546750	-0.337350
H	8.292172	-2.236919	0.988317
H	8.657940	0.163479	0.464717
C	-4.308381	-0.318836	2.388012
F	-5.542435	0.228020	2.351137
F	-4.470307	-1.656497	2.386202
F	-4.470307	-1.656497	2.386202
F	-3.770945	0.005394	3.580510

B_{TFE}

Electronic Energy: -1131.370475

C	3.357236	-0.663223	0.956210
C	3.693724	-0.788283	-0.567996
B	1.448599	-0.122630	-0.319026
O	2.691914	-0.005493	-1.171618
O	1.952782	-0.699625	0.974362
C	0.331936	-1.119370	-0.971190
H	0.059046	-0.952003	-2.023765
C	-0.382382	-2.056758	-0.336609
H	-0.172093	-2.251804	0.717777
C	-1.521563	-2.858239	-0.928067
H	-1.514947	-2.741035	-2.018530
H	-1.392569	-3.927750	-0.717150
C	-2.866047	-2.411049	-0.388340
C	-3.446341	-1.225866	-0.852573
C	-3.532906	-3.128623	0.606192
C	-4.656148	-0.770198	-0.340284
H	-2.931966	-0.651376	-1.618867
C	-4.745527	-2.676293	1.125797
H	-3.097859	-4.052562	0.979231
C	-5.311667	-1.495327	0.654443
H	-5.086703	0.153723	-0.715132
H	-5.247712	-3.249172	1.899719
H	-6.255783	-1.141877	1.057078
C	-0.554023	3.291649	-1.198623
C	-0.537512	3.064558	1.235418
B	0.634843	1.416281	-0.150942
O	0.246447	2.125112	-1.285530
O	0.254408	1.897201	1.096603
C	-1.459676	3.292923	0.035500
H	0.094650	4.179629	-1.174804
H	-1.159185	3.351707	-2.112198
H	-1.129253	2.960628	2.153744
H	0.118296	3.938164	1.363387
C	-2.153943	4.649130	0.164799
H	-2.798603	4.838386	-0.700076
H	-2.780802	4.679161	1.062271
H	-1.427628	5.466411	0.231298
C	-2.501123	2.171114	-0.055969
H	-2.033686	1.185081	-0.112972
H	-3.153835	2.178534	0.823521
H	-3.129298	2.297167	-0.944646
C	3.905813	-1.799823	1.819497
H	4.997052	-1.868476	1.742362
H	3.652981	-1.626446	2.871055

H	3.475072	-2.759248	1.523479
C	3.837642	0.681165	1.531681
H	3.386866	0.820946	2.519404
H	4.926775	0.728273	1.640344
H	3.511823	1.504458	0.890013
C	3.580370	-2.244325	-1.054454
H	3.609561	-2.251817	-2.149154
H	4.399096	-2.873016	-0.686847
H	2.627499	-2.674737	-0.736775
C	5.066750	-0.239514	-0.957410
H	5.868594	-0.750299	-0.411882
H	5.240374	-0.389776	-2.028407
H	5.134941	0.831424	-0.752329

TSB_{TFE}

Electronic Energy: -1131.337722

C	3.878005	-0.494435	0.799692
C	3.847018	-0.466309	-0.766993
B	1.985816	0.632994	0.050781
O	2.924277	0.582805	-1.037413
O	2.572252	-0.071578	1.163624
C	0.380815	-0.388556	-0.533479
H	0.327819	-0.550112	-1.618199
C	-0.296273	-1.238126	0.241506
H	-0.278792	-1.076704	1.322862
C	-1.137297	-2.410606	-0.216086
H	-0.913611	-2.635353	-1.264464
H	-0.872930	-3.303234	0.367881
C	-2.622483	-2.146831	-0.066571
C	-3.463412	-2.122938	-1.180017
C	-3.178329	-1.881751	1.189682
C	-4.820242	-1.832816	-1.049487
H	-3.048495	-2.323152	-2.164436
C	-4.530663	-1.585695	1.325841
H	-2.541182	-1.898701	2.070087
C	-5.358625	-1.557911	0.204163
H	-5.455115	-1.816416	-1.930287
H	-4.940866	-1.377906	2.309592
H	-6.414164	-1.327268	0.308904
C	-0.951204	3.122737	-0.750624
C	-1.553145	1.751482	1.230683
B	0.597935	1.495188	0.082661
O	0.122535	2.266140	-1.038885
O	-0.145166	1.673657	1.288663
C	-2.117287	2.403243	-0.062654
C	-3.208062	3.416806	0.295915
H	-3.632826	3.874192	-0.605092
H	-4.025862	2.929066	0.838436
H	-2.814667	4.218457	0.931376
C	-2.701889	1.342219	-1.001275
H	-1.944415	0.606582	-1.276785
H	-3.522784	0.802765	-0.516197
H	-3.091270	1.807186	-1.915467
C	4.151235	-1.871667	1.400356
H	5.120621	-2.261085	1.070352
H	4.169409	-1.802628	2.492611
H	3.374413	-2.586050	1.119579

C	4.873461	0.518896	1.382597
H	4.708470	0.592675	2.461712
H	5.914476	0.225473	1.213275
H	4.712302	1.508666	0.945957
C	3.314293	-1.772846	-1.372266
H	3.139927	-1.617379	-2.441366
H	4.027487	-2.595340	-1.257026
H	2.364617	-2.055601	-0.913207
C	5.185374	-0.127796	-1.419092
H	5.951066	-0.861927	-1.145900
H	5.080081	-0.139756	-2.508492
H	5.533661	0.864084	-1.123625
H	-1.986608	0.745286	1.340454
H	-1.872193	2.340250	2.102264
H	-1.301476	3.563558	-1.694898
H	-0.624781	3.958653	-0.106364

C_{TFE}

Electronic Energy: -1131.376803

C	-4.046814	-0.823257	-0.822766
C	-3.997108	-1.029923	0.724593
B	-2.152692	0.161208	0.042833
O	-2.997699	-0.076790	1.126812
O	-2.709152	-0.382633	-1.112785
C	0.384673	-0.421381	0.640174
H	0.422710	-0.655953	1.714270
C	1.103219	-1.227870	-0.148753
H	1.112818	-1.030305	-1.223986
C	2.017209	-2.334682	0.310005
H	1.830019	-2.538537	1.373009
H	1.813816	-3.269714	-0.228315
C	3.486753	-1.986411	0.130109
C	3.961444	-0.717804	0.481081
C	4.397598	-2.917975	-0.372638
C	5.307094	-0.393193	0.340241
H	3.256088	0.020133	0.854828
C	5.746553	-2.597383	-0.517931
H	4.046533	-3.907006	-0.657015
C	6.206780	-1.332822	-0.161311
H	5.654340	0.597743	0.618333
H	6.436826	-3.336076	-0.914441
H	7.256085	-1.079442	-0.276692
C	0.736925	2.533637	1.261282
C	1.128188	2.005177	-1.125130
B	-0.561599	0.831905	0.159036
O	-0.513959	1.920798	1.190989
O	-0.109439	1.357642	-1.169349
C	1.177350	3.141531	-0.084638
H	1.942891	1.297034	-0.885861
H	1.348034	2.421918	-2.122754
C	0.221300	4.267208	-0.485753
H	0.225819	5.071194	0.260421
H	0.510372	4.701496	-1.450481
H	-0.797353	3.883239	-0.571546
C	2.605968	3.672403	0.028888
H	3.302808	2.876570	0.318851
H	2.949691	4.086377	-0.926422

H	2.672977	4.468304	0.780092
C	-4.344624	-2.082473	-1.627105
H	-5.322345	-2.492604	-1.354339
H	-4.363130	-1.844229	-2.694393
H	-3.586373	-2.850430	-1.463417
C	-4.997610	0.299815	-1.246319
H	-4.828328	0.527214	-2.302293
H	-6.045346	0.012375	-1.119317
H	-4.811498	1.209490	-0.668487
C	-3.479934	-2.415276	1.124020
H	-3.284084	-2.423099	2.199676
H	-4.207563	-3.200614	0.900153
H	-2.543651	-2.645758	0.607205
C	-5.301428	-0.733438	1.452772
H	-6.099400	-1.393755	1.098117
H	-5.173488	-0.902644	2.525694
H	-5.615694	0.301692	1.306695
H	1.520284	1.813869	1.576836
H	0.708384	3.328498	2.025957

TSC_{TFE}

Electronic Energy: -1955.329549

C	0.164300	-2.852476	1.350336
C	-0.086348	-3.609078	0.040622
C	0.196186	-2.609723	-1.087844
H	1.237894	-2.632410	1.439652
H	-0.124153	-3.475819	2.208833
H	1.257518	-2.330043	-1.065125
H	0.004329	-3.082143	-2.061848
B	-0.666844	-0.805195	0.255968
O	-0.608365	-1.463633	-0.996717
O	-0.570612	-1.654394	1.427941
C	1.716003	3.186976	-0.046542
C	-0.405710	2.686281	-1.165979
C	0.677159	3.762559	-1.015855
H	2.592245	3.847009	0.009930
H	1.273949	3.121879	0.956934
H	-1.179883	3.023115	-1.868853
H	-0.893204	2.527234	-0.193314
B	1.242371	0.960853	-0.981928
O	2.171701	1.911316	-0.438041
O	0.117075	1.475460	-1.652853
C	1.317764	4.075767	-2.371344
H	1.776625	3.182383	-2.801463
H	0.567559	4.447751	-3.078256
H	2.092806	4.843193	-2.265309
C	0.065056	5.026236	-0.411255
H	0.832376	5.789613	-0.241039
H	-0.687642	5.453629	-1.082751
H	-0.419124	4.814200	0.548497
C	-1.890396	0.200447	0.417369
H	-1.964322	0.765838	1.350334
C	-2.859057	0.380396	-0.482708
H	-2.816452	-0.169879	-1.423777
C	-4.041539	1.298288	-0.320472
H	-3.942711	1.845277	0.626770
H	-4.044272	2.056024	-1.115268

C	-5.377738	0.577355	-0.338622
C	-5.542521	-0.629203	0.348665
C	-6.475498	1.107731	-1.020261
C	-6.771049	-1.283047	0.360857
H	-4.689608	-1.056851	0.868793
C	-7.707701	0.457085	-1.011868
H	-6.363770	2.041518	-1.565813
C	-7.860081	-0.741603	-0.319981
H	-6.878363	-2.219493	0.900188
H	-8.547733	0.885598	-1.550335
H	-8.817996	-1.252332	-0.314383
C	1.365338	0.854471	3.169108
C	2.591696	0.039775	2.626673
B	0.974829	0.227980	0.974930
O	0.610637	1.129034	1.977980
O	2.095181	-0.498115	1.392363
C	3.028827	-1.115781	3.520555
H	3.867363	-1.641471	3.054421
H	3.359467	-0.748877	4.497781
H	2.218957	-1.832157	3.670657
C	3.802306	0.910902	2.282806
H	4.255698	1.346474	3.178090
H	4.552310	0.287251	1.787093
H	3.518622	1.704899	1.589539
C	1.729198	2.175752	3.837261
H	0.816481	2.691902	4.148814
H	2.342582	2.003591	4.727790
H	2.277081	2.832209	3.158591
C	0.454930	0.041670	4.093630
H	0.951066	-0.208724	5.035936
H	-0.433218	0.638454	4.322654
H	0.126306	-0.871084	3.592151
O	1.888205	-0.043470	-1.757896
C	3.193301	-0.394723	-1.442313
H	3.841537	0.478768	-1.301545
H	3.251604	-1.003023	-0.531463
C	0.882888	-4.786406	-0.062495
H	0.739482	-5.486656	0.768176
H	0.727611	-5.339077	-0.995769
H	1.924267	-4.445754	-0.041800
C	-1.535516	-4.100529	-0.028493
H	-1.726471	-4.613972	-0.977866
H	-1.746182	-4.804349	0.784895
H	-2.233960	-3.263719	0.052407
C	3.769714	-1.200384	-2.580731
F	5.046356	-1.543045	-2.308773
F	3.780304	-0.520178	-3.741543
F	3.096884	-2.344575	-2.807095

[BpinBneop-OCH$_2$CF$_3$]$^-$ in TFE

Electronic Energy: -1235.212431

B	0.987480	0.275559	1.007549
B	-0.047699	-1.011776	0.452330
O	0.447161	1.565065	0.497039
O	2.372413	0.050331	0.553003
O	-0.543510	-1.152636	-0.838955
O	-0.510938	-2.053291	1.251385

C	-1.529953	-2.770026	0.530896
C	-1.176406	-2.440449	-0.955217
C	3.231066	1.134391	0.780466
C	1.287464	2.659141	0.744940
C	2.700817	2.446311	0.173159
C	2.632662	2.325099	-1.351132
H	2.234558	3.243242	-1.799528
H	3.628226	2.146665	-1.774864
H	1.982836	1.493656	-1.631564
C	3.607025	3.608527	0.576229
H	4.626716	3.460713	0.201610
H	3.236142	4.555684	0.167382
H	3.661078	3.711538	1.666263
H	4.214832	0.902643	0.341282
H	3.389784	1.297119	1.861297
H	0.841603	3.559194	0.291416
H	1.377171	2.850024	1.828848
C	-2.375520	-2.327897	-1.887749
H	-2.035733	-2.098352	-2.901582
H	-2.927471	-3.272705	-1.920661
H	-3.057264	-1.536905	-1.570081
C	-0.142672	-3.399772	-1.551216
H	-0.568739	-4.390874	-1.731408
H	0.206280	-2.995951	-2.505368
H	0.722028	-3.505257	-0.889988
C	-2.878218	-2.191097	0.968913
H	-3.715960	-2.723959	0.510126
H	-2.965362	-2.281680	2.055106
H	-2.952403	-1.131259	0.709140
C	-1.459661	-4.247581	0.893484
H	-1.718665	-4.382591	1.947384
H	-2.169899	-4.824917	0.292959
H	-0.458916	-4.652993	0.734133
O	1.053164	0.330306	2.519950
C	-0.137940	0.624574	3.143565
H	-0.738180	1.362788	2.590417
H	-0.775881	-0.261214	3.306242
C	0.134310	1.227290	4.501455
F	0.853742	0.411616	5.296385
F	-1.019304	1.492662	5.153900
F	0.813891	2.389222	4.425131

13_{TFE}

Electronic Energy: -720.132992

C	-0.932307	3.530864	0.890233
C	-1.957601	3.957736	-0.164992
C	-2.062006	2.810101	-1.174524
H	-1.329118	2.694555	1.479920
H	-0.723491	4.357565	1.576954
H	-2.520772	1.934242	-0.698121
H	-2.692393	3.101167	-2.021006
B	0.333676	2.590812	-0.942198
O	-0.794100	2.429593	-1.700543
O	0.307421	3.133864	0.313958
C	1.700237	2.148939	-1.551107
H	1.718315	1.731169	-2.559254
C	2.861258	2.250751	-0.893722

H	2.863305	2.657497	0.118275
C	4.203317	1.819882	-1.418035
H	4.097881	1.477648	-2.454049
H	4.883897	2.679453	-1.429584
C	4.814596	0.718068	-0.572071
C	4.140138	-0.496625	-0.412861
C	6.044881	0.888001	0.064172
C	4.685854	-1.518674	0.356604
H	3.176185	-0.635653	-0.895417
C	6.594808	-0.132983	0.837757
H	6.579687	1.827508	-0.047272
C	5.917122	-1.339509	0.985848
H	4.149778	-2.456213	0.467593
H	7.553208	0.016944	1.325209
H	6.343493	-2.135426	1.588145
C	-3.316994	4.166324	0.505971
H	-3.260661	4.968073	1.248979
H	-4.072504	4.448367	-0.234103
H	-3.658594	3.257162	1.011502
C	-1.511179	5.250596	-0.860631
H	-2.242168	5.547097	-1.619373
H	-1.425925	6.064580	-0.133930
H	-0.542026	5.140288	-1.354779

Direct B-B/C-B metathesis

TSA-DIRECT in MeOH

Electronic Energy: -1503.116681

C	-1.922827	2.626651	1.379628
C	-1.929128	3.657567	0.247121
C	-2.250584	2.896577	-1.043434
H	-2.927993	2.186058	1.480384
H	-1.676340	3.110640	2.331236
H	-3.318901	2.635369	-1.051533
H	-2.062465	3.532334	-1.916387
B	-0.927230	1.040637	-0.117355
O	-1.499882	1.704087	-1.213943
O	-0.972896	1.603436	1.165329
C	-0.566230	4.352504	0.143425
H	-0.587826	5.119041	-0.638195
H	-0.309546	4.839674	1.090020
H	0.227310	3.642083	-0.099222
C	-3.027616	4.691817	0.504117
H	-2.808547	5.268548	1.408395
H	-3.100559	5.395195	-0.331851
H	-4.005366	4.215600	0.632870
C	-3.636567	-1.647043	1.046329
C	-3.460013	-1.857366	-1.394144
C	-4.432788	-1.537109	-0.255963
H	-4.236934	-1.313188	1.898033
H	-3.348210	-2.691478	1.224149
H	-3.936858	-1.695227	-2.365834
H	-3.150655	-2.909267	-1.338726
B	-1.834250	-0.580914	-0.157407
O	-2.454390	-0.849750	1.026100
O	-2.296322	-1.038471	-1.353316

C	-5.003308	-0.122025	-0.418214
H	-4.215283	0.636049	-0.433981
H	-5.563183	-0.040371	-1.354971
H	-5.681327	0.114958	0.407509
C	-5.564021	-2.566645	-0.247576
H	-6.256204	-2.371932	0.577592
H	-6.133500	-2.520230	-1.181028
H	-5.177533	-3.584847	-0.134771
C	0.900591	0.943282	-0.674424
H	0.930151	1.036813	-1.758397
C	1.818660	1.573190	0.067599
H	1.776389	1.462057	1.149849
C	2.989324	2.336101	-0.483300
H	2.788262	2.643677	-1.513615
H	3.172756	3.234613	0.114403
C	4.198273	1.418693	-0.435374
C	4.450289	0.541516	-1.493581
C	5.009939	1.360013	0.698001
C	5.493164	-0.376690	-1.420481
H	3.815530	0.571702	-2.375109
C	6.053065	0.439994	0.775247
H	4.819422	2.033976	1.528935
C	6.295710	-0.432466	-0.282420
H	5.677661	-1.050979	-2.250900
H	6.675531	0.404467	1.663808
H	7.107205	-1.150539	-0.222017
C	0.840301	-2.678744	-0.254900
C	1.300201	-2.075988	1.120048
B	0.235926	-0.464870	-0.108980
O	0.510374	-1.508894	-1.019890
O	0.531534	-0.868111	1.211311
C	2.783965	-1.696647	1.137440
H	2.984161	-1.103538	2.033866
H	3.424084	-2.583293	1.162304
H	3.058353	-1.093301	0.269214
C	0.979556	-2.947336	2.328328
H	1.471970	-3.921122	2.243317
H	1.343112	-2.462023	3.238341
H	-0.095358	-3.105144	2.433118
C	-0.412515	-3.551713	-0.138262
H	-0.806339	-3.740353	-1.140245
H	-0.186713	-4.512132	0.333022
H	-1.189174	-3.058149	0.450484
C	1.926356	-3.442777	-1.002793
H	2.282647	-4.288133	-0.405988
H	1.523076	-3.835027	-1.940618
H	2.774841	-2.797365	-1.237953

***E*-2 in MeOH**

Electronic Energy: -720.133087

C	-1.265172	-1.020839	3.128611
C	0.251641	0.916172	3.209874
B	0.622690	-0.872933	1.626837
O	1.000626	0.335050	2.147837
O	-0.478466	-1.555282	2.068167
C	1.463889	-1.499499	0.472158
H	1.149848	-2.455265	0.048953

C	2.563751	-0.923816	-0.027241
C	3.427212	-1.490220	-1.120536
H	2.975977	-2.414075	-1.500600
H	3.467853	-0.782740	-1.957200
C	4.839837	-1.767606	-0.640093
C	5.056489	-2.656738	0.417387
C	5.942634	-1.147332	-1.228597
C	6.344042	-2.925122	0.869714
H	4.203717	-3.137225	0.889940
C	7.234774	-1.411966	-0.777325
H	5.790330	-0.451270	-2.049213
C	7.439302	-2.302038	0.272813
H	6.494288	-3.619980	1.690245
H	8.080888	-0.920314	-1.247419
H	8.444577	-2.509011	0.625833
H	2.899082	0.027362	0.387957
C	-1.225082	0.509980	3.174593
H	-2.291644	-1.372532	2.982631
H	-0.899592	-1.432705	4.077960
H	0.700463	0.611046	4.163837
H	0.351383	2.003010	3.123453
C	-1.920398	1.106095	1.943367
H	-2.972644	0.806022	1.917275
H	-1.879085	2.199379	1.974334
H	-1.456191	0.780038	1.008590
C	-1.913865	0.995810	4.451773
H	-1.876980	2.087756	4.517613
H	-2.966359	0.695410	4.459878
H	-1.435678	0.584502	5.346751

A2-Bpin in MeOH

Electronic Energy: -1046.592698

C	-2.816945	-2.843931	-0.817539
C	-3.693177	-1.824824	-0.011788
B	-1.396291	-1.389146	0.369507
O	-1.565863	-2.194306	-0.882681
O	-2.782310	-1.281310	0.918479
B	-0.804169	0.205074	-0.029512
C	-3.317810	-3.116275	-2.236169
H	-2.676626	-3.859607	-2.721594
H	-4.341082	-3.508717	-2.227821
H	-3.298610	-2.207804	-2.842579
C	-2.665791	-4.184370	-0.078459
H	-3.592912	-4.768175	-0.079722
H	-1.891260	-4.772369	-0.581558
H	-2.345237	-4.014256	0.951187
C	-4.227915	-0.695460	-0.908434
H	-5.005924	-1.041227	-1.597214
H	-4.659529	0.084811	-0.272581
H	-3.415462	-0.249289	-1.487923
C	-4.865626	-2.458942	0.736933
H	-5.442571	-1.684185	1.252991
H	-5.541068	-2.979666	0.048678
H	-4.513811	-3.172413	1.485245
N	-1.649924	1.321062	0.295237
N	0.404572	0.606951	-0.705546
C	-1.394898	2.644185	0.004176

C	-0.173041	2.953654	-0.673179
C	-2.269354	3.667447	0.339944
C	0.135120	4.305780	-0.994796
C	0.737145	1.910454	-1.033397
C	-1.953902	4.999503	0.017666
H	-3.196758	3.430389	0.852934
C	1.351901	4.590079	-1.670016
C	-0.786272	5.324018	-0.631139
C	1.914108	2.230450	-1.694118
H	-2.653620	5.784442	0.291186
C	2.209486	3.569828	-2.005383
H	1.590343	5.620552	-1.915894
H	-0.553740	6.356432	-0.874523
H	2.605738	1.439471	-1.969347
H	3.138003	3.794507	-2.522856
H	1.076006	-0.089194	-0.992698
H	-2.531736	1.104070	0.740535
O	-0.608456	-2.111771	1.405612
C	0.739385	-2.287016	1.114342
H	1.204285	-2.928660	1.875784
H	0.902317	-2.768682	0.134597
H	1.304561	-1.336866	1.099434

A2-Bdan in MeOH

Electronic Energy: -1046.565504

C	3.651979	-0.661750	-0.675314
C	3.766774	0.820888	-0.193948
B	1.629816	0.048343	0.164059
O	2.407185	-1.078608	-0.081172
O	2.385321	1.198370	-0.036332
B	-0.032822	0.030877	0.668510
C	4.768227	-1.579628	-0.194649
H	4.606759	-2.590716	-0.578804
H	5.738745	-1.229088	-0.559889
H	4.803609	-1.631018	0.895026
C	3.491743	-0.787677	-2.192458
H	4.421052	-0.548406	-2.717128
H	3.214497	-1.816970	-2.435122
H	2.702010	-0.126518	-2.560266
C	4.428190	0.956127	1.180138
H	5.500390	0.745410	1.134841
H	4.293112	1.980157	1.538367
H	3.968336	0.278961	1.905700
C	4.434835	1.763615	-1.185941
H	4.472611	2.773913	-0.769028
H	5.461162	1.442439	-1.390181
H	3.888302	1.804555	-2.129865
N	-0.791073	1.274291	0.190110
N	-0.776171	-1.162057	0.032722
C	-2.140545	1.298545	0.013337
C	-2.846230	0.056422	-0.167630
C	-2.869364	2.492159	-0.039070
C	-4.251832	0.061641	-0.401764
C	-2.121396	-1.187743	-0.162961
C	-4.254529	2.478352	-0.256186
H	-2.347297	3.435911	0.097607
C	-4.924950	-1.171846	-0.616150

C	-4.946579	1.301354	-0.431402
C	-2.828337	-2.373042	-0.396448
H	-4.788958	3.425373	-0.284016
C	-4.212745	-2.350146	-0.616211
H	-5.997552	-1.166497	-0.788466
H	-6.019372	1.303096	-0.602649
H	-2.290231	-3.317742	-0.395535
H	-4.730946	-3.291152	-0.787260
H	-0.335020	-2.069954	0.025168
H	-0.380057	2.179754	0.365831
O	-0.141561	0.010664	2.171422
C	0.466353	-1.062997	2.812549
H	1.551502	-1.128111	2.609639
H	0.338834	-0.966793	3.899419
H	0.037123	-2.037408	2.517232

BpinBdan in MeOH

Electronic Energy: -931.378852

C	-2.768186	-2.935038	-0.729546
C	-4.085816	-2.170313	-0.362993
B	-2.353804	-0.702941	-0.547515
O	-1.886107	-1.855123	-1.128237
O	-3.585855	-0.868197	0.034122
B	-1.499758	0.768801	-0.548341
C	-2.900464	-3.917145	-1.883977
H	-1.937465	-4.399960	-2.069382
H	-3.629282	-4.695498	-1.638943
H	-3.216536	-3.419274	-2.802020
C	-2.112573	-3.617589	0.471395
H	-2.689172	-4.486927	0.797894
H	-1.113034	-3.954455	0.185509
H	-2.012547	-2.927931	1.314137
C	-5.004631	-1.941074	-1.563515
H	-5.473432	-2.873404	-1.888778
H	-5.792946	-1.240220	-1.277755
H	-4.456157	-1.512764	-2.407064
C	-4.871924	-2.771495	0.792581
H	-5.768804	-2.174837	0.978214
H	-5.186223	-3.790700	0.548689
H	-4.282063	-2.798075	1.710163
N	-2.055133	1.966266	-0.018946
N	-0.184834	0.880206	-1.078609
C	-1.387266	3.186180	-0.000733
C	-0.068644	3.235187	-0.550248
C	-1.958270	4.329469	0.525680
C	0.645355	4.465752	-0.551271
C	0.542806	2.065395	-1.098754
C	-1.242278	5.541984	0.519717
H	-2.959795	4.287443	0.942763
C	1.954397	4.499169	-1.101364
C	0.025121	5.619478	-0.002161
C	1.818381	2.136399	-1.626138
H	-1.709663	6.428342	0.938050
C	2.515726	3.359742	-1.622201
H	2.500174	5.437608	-1.102641
H	0.568987	6.559026	-0.002469
H	2.278629	1.245537	-2.042458

H	3.516876	3.393325	-2.041312
H	0.279094	0.074191	-1.470619
H	-2.984897	1.969517	0.373600

TS-Bpin-to-Bdan in MeOH

Electronic Energy: -1046.565504

C	4.406966	2.427119	0.050034
C	5.083352	1.231450	0.119686
C	4.375332	0.007257	-0.015783
C	2.964803	0.040552	-0.210858
C	2.279997	1.300434	-0.277696
C	3.017782	2.475469	-0.148236
H	6.111401	-1.275367	0.185579
H	4.953488	3.361308	0.152219
H	6.158311	1.206091	0.272817
C	5.036416	-1.249553	0.032625
C	2.234563	-1.184833	-0.366680
H	2.505405	3.432500	-0.196862
C	2.926114	-2.393275	-0.318970
C	4.316059	-2.411207	-0.119088
H	2.378022	-3.324321	-0.435143
H	4.827000	-3.370094	-0.082994
N	0.926059	1.303567	-0.484287
N	0.881678	-1.122392	-0.577587
B	0.073138	0.100064	-0.386899
C	-3.774491	-0.641925	-0.474291
C	-3.733675	0.839927	0.033485
B	-1.586306	0.106786	-0.303418
O	-2.424641	1.256741	-0.353460
O	-2.413226	-1.056081	-0.373073
C	-3.851094	0.946474	1.559689
H	-3.628251	1.975661	1.856432
H	-4.858501	0.698833	1.908627
H	-3.127910	0.291527	2.049757
C	-4.762561	1.760162	-0.615942
H	-5.780435	1.404967	-0.422959
H	-4.672401	2.768208	-0.199710
H	-4.615820	1.825113	-1.695978
C	-4.650497	-1.571923	0.359705
H	-5.691392	-1.230875	0.363038
H	-4.627078	-2.581175	-0.062778
H	-4.299226	-1.627757	1.392014
C	-4.178358	-0.746054	-1.950076
H	-3.996926	-1.768282	-2.294741
H	-5.236503	-0.513975	-2.105727
H	-3.576933	-0.068358	-2.562416
O	-0.683379	0.095261	1.275893
C	-0.625278	-1.096962	2.000403
H	-1.071912	-0.960675	2.998370
H	-1.179045	-1.911017	1.507600
H	0.411799	-1.440496	2.144593
H	0.418981	-2.016467	-0.637456
H	0.495036	2.215080	-0.465975

TSA2-Bdan in MeOH

Electronic Energy: -1766.698129

C	-1.176137	-1.097353	2.773827
C	0.312514	0.860058	2.417611
B	0.040317	-0.700103	0.631416
O	0.297644	0.636506	1.032861
O	-0.440665	-1.567669	1.665362
C	-2.814725	-3.097873	-0.599346
C	-3.820749	-1.961835	-0.196563
B	-1.700939	-1.076989	-0.447726
O	-1.636880	-2.368489	-0.969232
O	-2.948881	-0.872964	0.147442
C	1.168585	-1.427049	-0.232910
H	0.980706	-2.447023	-0.578347
C	2.350295	-0.879080	-0.532955
C	3.460057	-1.544599	-1.304033
H	3.118751	-2.528327	-1.652197
H	3.697753	-0.961102	-2.203331
C	4.731909	-1.716344	-0.493228
C	4.676729	-2.210817	0.813691
C	5.981411	-1.403819	-1.032691
C	5.838324	-2.396355	1.556961
H	3.707831	-2.441464	1.248351
C	7.147863	-1.586443	-0.292194
H	6.042441	-1.011864	-2.044901
C	7.080291	-2.084784	1.005950
H	5.774644	-2.781991	2.570108
H	8.109403	-1.335352	-0.729802
H	7.987056	-2.225863	1.585807
B	-1.231799	0.590153	-1.518215
H	2.555025	0.138887	-0.196743
C	-0.978324	0.402865	3.105624
H	-2.244304	-1.293771	2.605615
H	-0.859322	-1.707576	3.630378
H	1.169843	0.344817	2.885611
H	0.450565	1.937012	2.582205
C	-2.161092	1.227956	2.591878
H	-3.087117	0.921596	3.092570
H	-2.003952	2.295098	2.782320
H	-2.286981	1.085232	1.519212
C	-0.842339	0.585900	4.619918
H	-0.733791	1.645475	4.877134
H	-1.730874	0.207378	5.137448
H	0.029078	0.049097	5.011632
C	-3.258779	-3.939678	-1.790978
H	-2.494680	-4.689908	-2.014188
H	-4.194666	-4.463711	-1.571386
H	-3.402073	-3.323713	-2.680814
C	-2.431411	-4.015248	0.564409
H	-3.276273	-4.627646	0.892940
H	-1.631326	-4.684029	0.233442
H	-2.051339	-3.432126	1.405159
C	-4.695506	-1.483253	-1.358663
H	-5.403377	-2.253863	-1.677459
H	-5.266542	-0.609519	-1.029775
H	-4.071748	-1.180415	-2.202208
C	-4.700249	-2.287936	1.004990
H	-5.333008	-1.426988	1.239221
H	-5.352866	-3.139488	0.786645

H	-4.105327	-2.523798	1.889250
N	-1.991755	1.698465	-0.890214
N	0.138404	1.025604	-1.874225
C	-1.458134	2.885190	-0.483346
C	-0.085929	3.171161	-0.783164
C	-2.210310	3.839722	0.200323
C	0.490285	4.406418	-0.375609
C	0.711754	2.197805	-1.467115
C	-1.631854	5.057724	0.589851
H	-3.248314	3.624941	0.438758
C	1.859831	4.657933	-0.662344
C	-0.315800	5.351071	0.315511
C	2.051365	2.484775	-1.722806
H	-2.244756	5.780709	1.122752
C	2.608638	3.708323	-1.317268
H	2.300489	5.601236	-0.352519
H	0.122506	6.295782	0.624287
H	2.662054	1.749268	-2.239496
H	3.657083	3.902012	-1.530547
H	0.807317	0.320629	-2.147663
H	-2.931746	1.506611	-0.577585
O	-1.993466	-0.028436	-2.587258
C	-1.316576	-0.822395	-3.524477
H	-0.778917	-1.649900	-3.044894
H	-2.055301	-1.253959	-4.208130
H	-0.602034	-0.229987	-4.113678

TSA2-Bpin in MeOH

Electronic Energy: -1766.689245

C	-0.898364	-1.045610	2.614890
C	1.121609	0.398597	2.713243
B	0.437353	-0.426571	0.593726
O	0.969670	0.674348	1.345916
O	-0.244450	-1.403378	1.421859
C	1.308088	3.082071	-1.098870
C	0.068007	3.613366	-0.259438
B	-0.363737	1.509805	-1.173876
O	1.028009	1.708690	-1.314106
O	-0.916260	2.592579	-0.416725
C	1.461029	-1.202133	-0.362905
H	1.174517	-2.187344	-0.751307
C	2.689248	-0.779755	-0.669856
C	3.694298	-1.522904	-1.508723
H	3.246273	-2.458591	-1.869306
H	3.946788	-0.935659	-2.401658
C	4.979408	-1.840884	-0.765395
C	4.939032	-2.325553	0.545696
C	6.226088	-1.673578	-1.372487
C	6.110282	-2.641911	1.227448
H	3.974646	-2.443359	1.032445
C	7.402176	-1.987661	-0.694159
H	6.277028	-1.290995	-2.388882
C	7.348262	-2.474151	0.609293
H	6.057476	-3.016941	2.245227
H	8.361198	-1.847797	-1.183929
H	8.262916	-2.716908	1.141135
B	-1.295027	-0.158555	-0.413873

O	-1.103964	1.246806	-2.383120
C	-0.432804	0.548464	-3.397795
H	0.385222	1.144757	-3.822456
H	0.000666	-0.394655	-3.038864
H	-1.149014	0.312798	-4.191882
H	3.011558	0.189655	-0.291436
C	-0.221509	0.114535	3.397492
H	-1.944546	-0.781294	2.402353
H	-0.914281	-1.949539	3.238135
H	1.797918	-0.459425	2.870095
H	1.591482	1.273252	3.184805
C	-1.095765	1.371705	3.349520
H	-2.093806	1.169437	3.754354
H	-0.647646	2.182687	3.935571
H	-1.196267	1.721828	2.320918
C	0.017613	-0.293590	4.853740
H	0.499642	0.514729	5.415348
H	-0.929280	-0.527361	5.352977
H	0.658273	-1.180383	4.916549
C	2.646944	3.182471	-0.371167
H	3.436162	2.779675	-1.013935
H	2.899557	4.221152	-0.133835
H	2.619385	2.592024	0.545528
C	1.432320	3.741047	-2.480856
H	1.665754	4.808290	-2.416287
H	2.238734	3.246130	-3.030287
H	0.511034	3.614819	-3.056281
C	0.364340	3.785561	1.230533
H	1.081666	4.593744	1.405323
H	-0.565698	4.039033	1.749300
H	0.745904	2.853163	1.641589
C	-0.524991	4.924126	-0.785351
H	-1.391372	5.196386	-0.174842
H	0.201028	5.741562	-0.723108
H	-0.858686	4.832479	-1.820733
N	-1.595705	-1.380348	-1.134773
N	-2.455138	0.400121	0.228847
C	-2.826946	-1.991178	-1.171810
C	-3.918607	-1.374347	-0.481940
C	-3.042316	-3.185144	-1.850067
C	-5.206867	-1.979828	-0.500269
C	-3.718386	-0.148502	0.224476
C	-4.317380	-3.775662	-1.858233
H	-2.216571	-3.658650	-2.373418
C	-6.273037	-1.341357	0.188182
C	-5.382090	-3.199664	-1.205643
C	-4.785269	0.443228	0.886514
H	-4.457332	-4.709763	-2.395578
C	-6.054513	-0.160940	0.858403
H	-7.257683	-1.799223	0.175282
H	-6.362766	-3.665752	-1.220141
H	-4.629469	1.372799	1.426216
H	-6.875678	0.320291	1.382651
H	-2.363440	1.322195	0.631576
H	-0.851758	-1.898314	-1.574989

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