Supplementary Information (SI) for Polymer Chemistry.

Supporting Information

Modulating the Radical Polymerization Behavior of Alkenyl Boronates via Boronate Tuning

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I. General Reagent Information

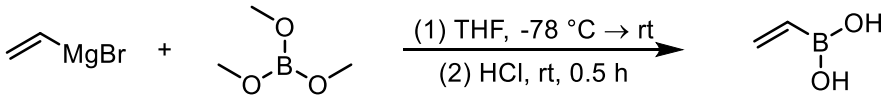
Trimethyl borate (99%, Adamas), vinylmagnesium bromide (1.0 M solution in THF, Adamas), 3,4-diethylhexane-3,4-diol (95%, Adamas), (1S,2S,3R,5S)-(+)-pinanediol (98%+, Adamas), benzpinacol (95%+, Adamas), isopropenylmagnesium bromide (1.0 M solution in THF, Adamas), 2,2-dimethyl-1,3-propanediol (99%, Adamas), 2-methyl-2-propyl-1,3-propanediol (97%+, Adamas), 2-butyl-2-ethyl-1,3-propanediol (98%, Adamas), 3-methyl-1,3-butanediol (99%, Adamas), 3-methyl-1,3-butanediol (99%, Adamas), 2-ethyl-1,3-hexanediol (98%+, Adamas), 2,2,4-trimethyl-1,3-pentanediol (98%, Adamas), 2,2-azobis(2-methylpropionitrile) (98%, TCI), 2-cyano-2-propyl dodecyl trithiocarbonate (CPDT, 97%, Adamas), toluene (99.5%, Sinoreagent), tetrahydrofuran (THF, 99.5% anhydrous, Adamas), dichloromethane (DCM, 99.9% anhydrous, Adamas), diethyl ether (Et_2O, 99.7%, Sinoreagent), *N,N*-dimethylacrylamide (DMAA, 98%+, Adamas), tert-butyl acrylate (*t*BA, 99%, Adamas), methyl methacrylate (MMA, 99%, Adamas), styrene (St, 99%, Adamas), acrylonitrile (AN, 98%, TCI), *N*-phenylmaleimide (NPMI, 98%+, Adamas), vinyl acetate (VAc, 98%, Energy Chemical), maleic anhydride (MAH, 99%+, Adamas) were used as received. All other reagents were obtained from TCI, Energy Chemical and Adamas and used as received.

II. General Analytical Information

^{1}H, ^{11}B and ^{13}C NMR spectra were recorded on Bruker Avance 400 (400 MHz) at room temperature using $CDCl_3$ as a solvent. Chemical shifts were quoted in parts per million (ppm) referenced to the appropriate solvent peak. Gel permeation chromatography (GPC) was performed in THF solution at 35 °C with an elution rate of 1.0 mL min^{-1} on an Agilent 1260 HPLC system equipped with a G7110B pump and a G7162A refractive index detector. The molecular weights were determined using PLgel MIXED-A column and PLgel MIXED-C column based on linear poly(methyl methacrylate) (PMMA) as standards. Thermogravimetric analysis (TGA) experiments were carried out on samples (2.00~5.00 mg) from 50 ºC to 800 ºC at a heating rate of 20 ºC/min in a N_2 atmosphere using a PE Pyris1 TGA. Differential scanning calorimetry (DSC) experiments were conducted using a TA Instruments DSC Q2000 under N_2 flow. Matrix-assisted laser desorption ionization-time of flight (MALDI-TOF) mass spectrometry was obtained on AB SCIEX 5800 MALDI-TOF mass spectrometer.

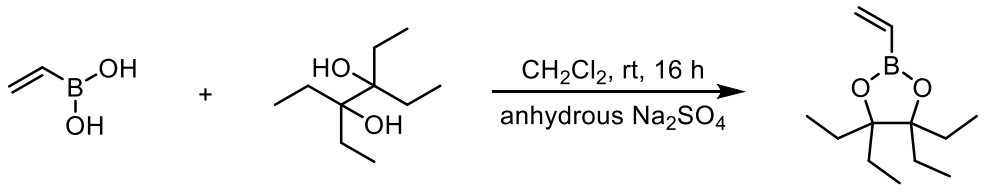
III. Synthesis of Reagents

Synthesis of Vinyl Boronic Acid



The vinyl boronic acid was synthesized with some modification according to the previously reported procedure.[1] Trimethyl borate (12.5 g, 120 mmol) was dissolved in 50.0 mL dry THF and cooled to -78.0 ℃, and a 1.0 M solution of vinylmagnesium bromide in THF (100 mL, 100 mmol) was added to it dropwise. The resulting white slurry was allowed to stir and warmed to room temperature overnight. The reaction was then quenched with the addition of 50.0 mL of 20% HCl aqueous solution and stirred for 0.5 h. It was then extracted with diethyl ether for 2 times, and the combined organic layer was washed with brine, dried with Na_2SO_4 to remove traces of water. The solvent was then removed under reduced pressure but not allowed to become completely concentrated (to around 40 mL).

Synthesis of Vinyl Boronic Acid Ethyl Pinacol Ester (VB_{epin})



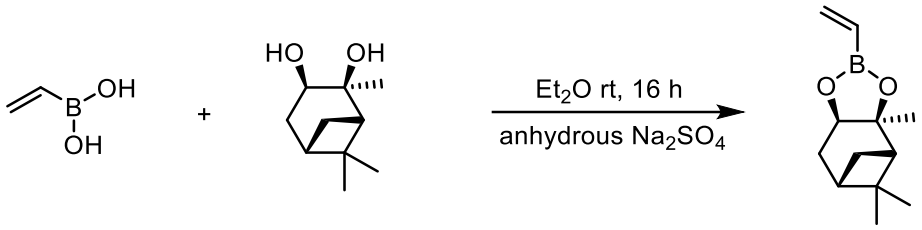
The VB_{epin} was synthesized with some modification according to the previously reported procedure.[2] At room temperature, 3,4-diethylhexane-3,4-diol (5.22 g, 30.0 mmol) was dissolved in 50.0 mL CH_2Cl_2, and a 2.5 M solution of vinyl boronic acid obtained above in diethyl ether (10.0 mL, 25.0 mmol) was added. Then, anhydrous Na_2SO_4 (5.0 g) was added. The reaction was allowed to stir for 16 h at room temperature,

filtered through a short pad of Celite, and washed with CH_2Cl_2. The filtrate was concentrated in vacuo, and the crude product was purified by chromatography to afford the desired product as a colourless oil (3.27 g, 62.3% yield).

R_f = 0.45 (pure petroleum ether).

^{1}H NMR (400 MHz, Chloroform-*d*): δ 6.22 – 5.78 (m, 3H), 1.76 – 1.59 (m, 9H), 0.91 (t, *J* = 7.5 Hz, 13H). **^{13}C NMR** (101 MHz, Chloroform-*d*): δ 136.92, 88.40, 26.46, 8.90. **^{11}B NMR** (128 MHz, Chloroform-*d*): δ 28.98.

Synthesis of Vinyl Boronic Acid Pinanediol Ester (VB_{pnd})



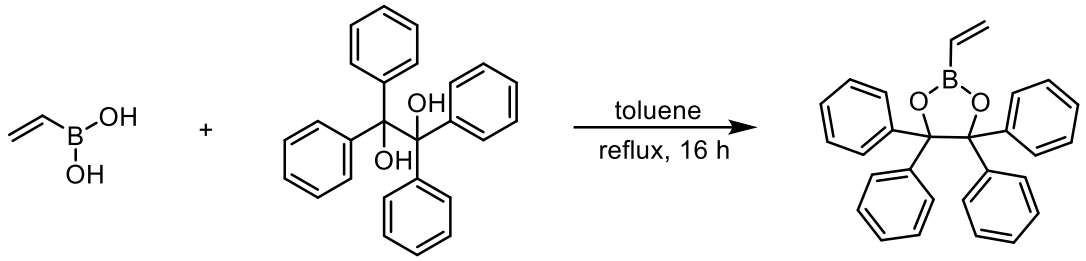
At room temperature, (1S,2S,3R,5S)-(+)-pinanediol (3.40 g, 20.0 mmol) was dissolved in 40.0 mL diethyl ether, and a 2.5 M solution of vinyl boronic acid obtained above in diethyl ether (8.00 mL, 20.0 mmol) was added. Then, anhydrous Na_2SO_4 (4.0 g) was added. The reaction was allowed to stir for 16 h at room temperature, filtered through a short pad of Celite, and washed with diethyl ether. The filtrate was concentrated in vacuo, and the crude product was purified by chromatography to afford the desired product as a colourless oil (1.82 g, 44.2% yield).

R_f = 0.40 (pure petroleum ether).

^{1}H NMR (400 MHz, Chloroform-*d*): δ 6.24 – 5.77 (m, 3H), 4.32 (dd, *J* = 8.8, 1.9 Hz, 1H), 2.43 – 2.28 (m, 1H), 2.28 – 2.15 (m, 1H), 2.12 – 2.01 (m, 1H), 1.98 – 1.82 (m, 2H), 1.41 (s, 3H), 1.29 (s, 3H), 1.14 (d, *J* = 10.9 Hz, 1H), 0.85 (s, 3H). **^{13}C NMR** (101

MHz, Chloroform-*d*): δ 137.11, 85.88, 77.90, 51.44, 39.62, 38.27, 35.57, 28.73, 27.21, 26.53, 24.13. **^{11}B NMR** (128 MHz, Chloroform-*d*): δ 29.17.

Synthesis of Vinyl Boronic Acid Benzpinacol Ester (VB_{Phpin})

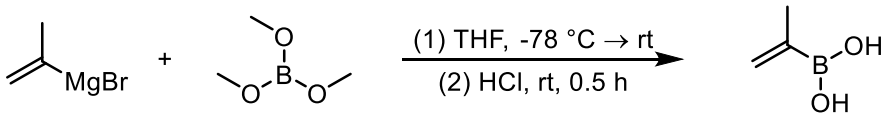


Benzpinacol (7.32 g, 20.0 mmol), a 2.5 M solution of vinyl boronic acid obtained above in diethyl ether (8.00 mL, 20.0 mmol), and 40.0 mL toluene were added to a bottle equipped with a Dean-Stark. After stirring for 16 h at refluxing temperature. Remove the toluene in vacuo, and the crude product was purified by chromatography to afford the desired product as a white solid (4.38 g, 54.5% yield).

R_f = 0.50 (ethyl acetate/petroleum ether = 1/9).

^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.22 – 7.13 (m, 8H), 7.12 – 7.01 (m, 12H), 6.60 – 6.52 (m, 1H), 6.32 – 6.19 (m, 2H). **^{13}C NMR** (101 MHz, Chloroform-*d*): δ 142.66, 139.37, 128.68, 127.38, 127.10. **^{11}B NMR** (128 MHz, Chloroform-*d*): δ 30.42.

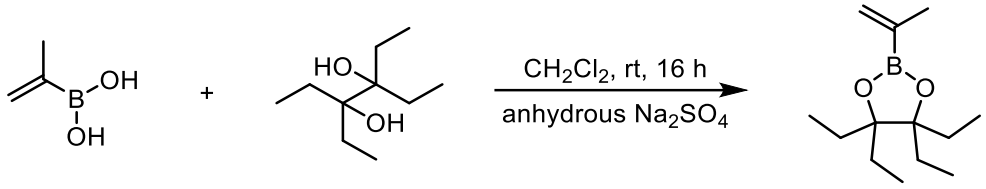
Synthesis of Isopropenyl Boronic Acid



Trimethyl borate (12.5 g, 120 mmol) was dissolved in 50.0 mL dry THF and cooled to -78.0 ℃, and a 1.0 M solution of isopropenylmagnesium bromide in THF (100 mL, 100 mmol) was added to it dropwise. The resulting white slurry was allowed to stir and warmed to room temperature overnight. The reaction was then quenched with the

addition of 50.0 mL of 20% HCl aqueous solution and stirred for 0.5 h. It was then extracted with diethyl ether for 2 times, and the combined organic layer was washed with brine, dried with Na_2SO_4 to remove traces of water. The solvent was then removed under reduced pressure but not allowed to become completely concentrated (to around 40 mL).

Synthesis of Isopropenyl Boronic Acid Ethyl Pinacol Ester (IB_{epin})

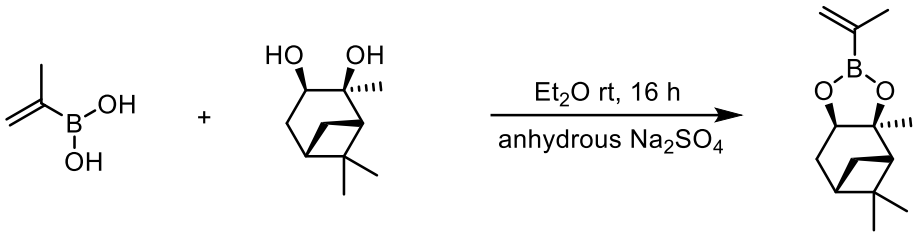


At room temperature, 3,4-diethylhexane-3,4-diol (5.22 g, 30.0 mmol) was dissolved in 50.0 mL CH_2Cl_2, and a 2.5 M solution of isopropenyl boronic acid obtained above in diethyl ether (10.0 mL, 25.0 mmol) was added. Then anhydrous Na_2SO_4 (5.0 g) was added. The reaction was allowed to stir for 16 h at room temperature, filtered through a short pad of Celite, and washed with CH_2Cl_2. The filtrate was concentrated in vacuo, and the crude product was purified by chromatography to afford the desired product as a colourless oil (3.85 g, 68.8% yield).

R_f = 0.50 (pure petroleum ether).

^{1}H NMR (400 MHz, Chloroform-*d*): δ 5.78 – 5.70 (m, 1H), 5.66 – 5.54 (m, 1H), 1.81 (t, *J* = 1.5 Hz, 3H), 1.76 – 1.59 (m, 9H), 0.92 (t, *J* = 7.5 Hz, 13H). **^{13}C NMR** (101 MHz, Chloroform-*d*): δ 129.71, 88.46, 26.49, 21.34, 8.91. **^{11}B NMR** (128 MHz, Chloroform-*d*): δ 29.37.

Synthesis of Isopropenyl Boronic Acid Pinanediol Ester (IB_{pnd})

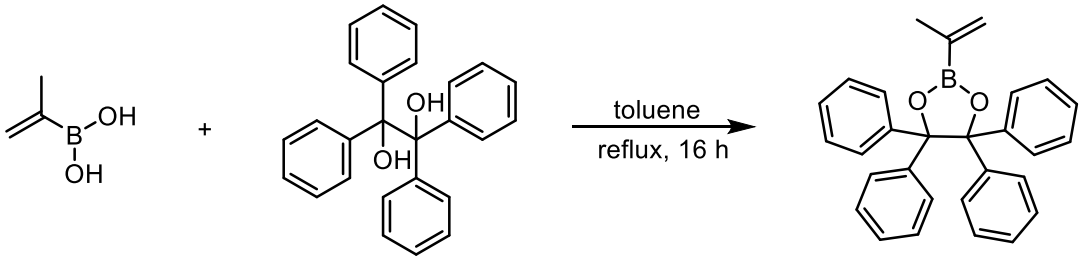


At room temperature, (1S,2S,3R,5S)-(+)-pinanediol (8.50 g, 50.0 mmol) was dissolved in 100.0 mL diethyl ether, and a 2.5 M solution of vinyl boronic acid obtained above in diethyl ether (20.0 mL, 50.0 mmol) was added. Then, anhydrous Na_2SO_4 (10.0 g) was added. The reaction was allowed to stir for 16 h at room temperature, filtered through a short pad of Celite, and washed with diethyl ether. The filtrate was concentrated in vacuo, and the crude product was purified by chromatography to afford the desired product as a colourless oil (8.83 g, 80.3% yield).

R_f = 0.45 (pure petroleum ether).

^{1}H NMR (400 MHz, Chloroform-*d*): δ 5.79 – 5.71 (m, 1H), 5.69 – 5.59 (m, 1H), 4.32 (dd, *J* = 8.7, 1.9 Hz, 1H), 2.43 – 2.28 (m, 1H), 2.28 – 2.16 (m, 1H), 2.12 – 2.04 (m, 1H), 1.95 – 1.85 (m, 2H), 1.84 (t, *J* = 1.5 Hz, 3H), 1.41 (s, 3H), 1.29 (s, 3H), 1.14 (d, *J* = 10.9 Hz, 1H), 0.85 (s, 3H). **^{13}C NMR** (101 MHz, Chloroform-*d*): δ 130.09, 86.03, 51.49, 39.65, 38.29, 35.70, 28.80, 27.24, 26.58, 24.16, 21.44. **^{11}B NMR** (128 MHz, Chloroform-*d*): δ 29.59.

Synthesis of Isopropenyl Boronic Acid Benzpinacol Ester (IB_{Phpin})

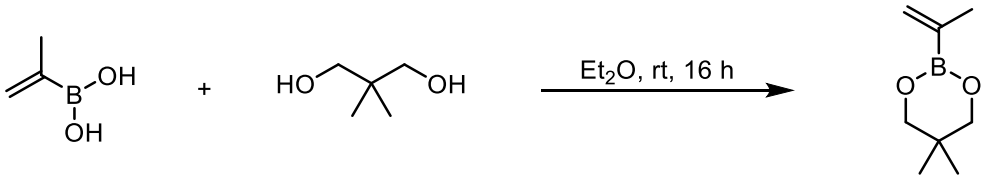


Benzpinacol (7.32 g, 20.0 mmol), a 2.5 M solution of isopropenyl boronic acid obtained above in diethyl ether (8.00 mL, 20.0 mmol), and 40.0 mL toluene were added to a bottle equipped with a Dean-Stark. After stirring for 16 h at refluxing temperature. Remove the toluene in vacuo, and the crude product was purified by chromatography to afford the desired product as a white solid (6.25 g, 75.1% yield).

R_f = 0.35 (pure petroleum ether).

^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.33 – 7.24 (m, 8H), 7.21 – 7.11 (m, 12H), 6.34 – 6.21 (m, 1H), 6.08 – 5.95 (m, 1H), 2.35 – 2.01 (m, 3H). **^{13}C NMR** (101 MHz, Chloroform-*d*): δ 142.69, 132.30, 128.63, 127.34, 127.04, 96.33, 21.46. **^{11}B NMR** (128 MHz, Chloroform-*d*): δ 31.00.

Synthesis of Isopropenyl Boronic Acid Neopentyl Glycol Ester ($IB_{6\text{-}1}$)

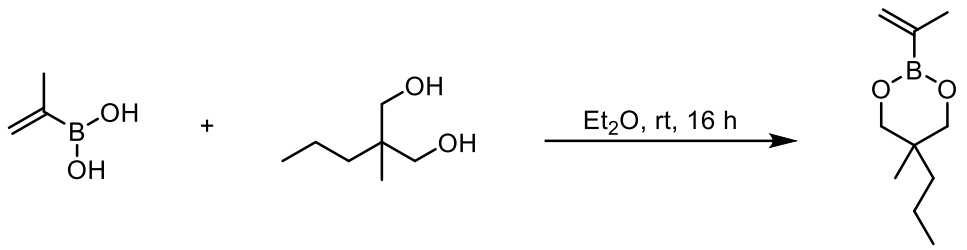


The IB_{neop} was synthesized with some modification according to the previously reported procedure.[3] At room temperature, 2,2-dimethyl-1,3-propanediol (5.20 g, 50.0 mmol) was dissolved in 100.0 mL diethyl ether, and a 2.5 M solution of vinyl boronic acid obtained above in diethyl ether (20.0 mL, 50.0 mmol) was added. The reaction was allowed to stir for 16 h at room temperature, filtered through a short pad of Celite, and washed with diethyl ether. The filtrate was concentrated in vacuo, and the crude product was purified by chromatography to afford the desired product as a colourless oil (3.76 g, 48.8% yield).

R_f = 0.55 (pure petroleum ether).

^{1}H NMR (400 MHz, Chloroform-*d*): δ 5.68 (d, *J* = 2.8 Hz, 1H), 5.54 (s, 1H), 3.64 (s, 4H), 1.77 (s, 3H), 0.97 (s, 6H). **^{13}C NMR** (101 MHz, Chloroform-*d*): δ 127.68, 72.26, 31.77, 21.99, 21.08. **^{11}B NMR** (128 MHz, Chloroform-*d*): δ 26.01.

Synthesis of Isopropenyl Boronic Acid 2-Methyl-2-Propyl-1,3-Propanediol Ester ($IB_{6\text{-}2}$)

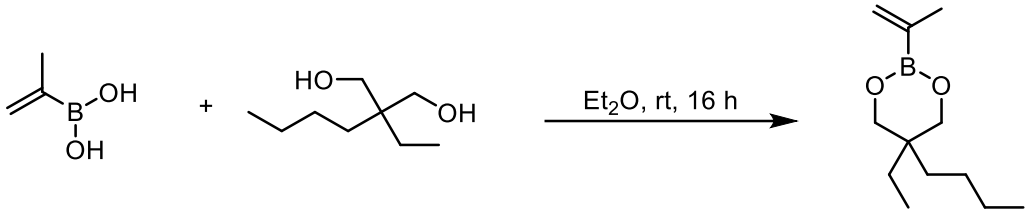


At room temperature, 2-methyl-2-propyl-1,3-propanediol (6.60 g, 50.0 mmol) was dissolved in 100.0 mL diethyl ether, and a 2.5 M solution of vinyl boronic acid obtained above in diethyl ether (20.0 mL, 50.0 mmol) was added. The reaction was allowed to stir for 16 h at room temperature, filtered through a short pad of Celite, and washed with diethyl ether. The filtrate was concentrated in vacuo, and the crude product was purified by chromatography to afford the desired product as a colourless oil (6.96 g, 76.5% yield).

R_f = 0.45 (pure petroleum ether).

^{1}H NMR (400 MHz, Chloroform-*d*): δ 5.67 (d, *J* = 2.3 Hz, 1H), 5.54 (s, 1H), 3.80 – 3.55 (m, 4H), 1.77 (s, 3H), 1.37 – 1.19 (m, 4H), 0.97 – 0.85 (m, 6H). **^{13}C NMR** (101 MHz, Chloroform-*d*): δ 127.65, 71.11, 37.41, 34.39, 21.10, 19.15, 16.56, 14.98. **^{11}B NMR** (128 MHz, Chloroform-*d*): δ 26.03.

Synthesis of Isopropenyl Boronic Acid 2-Butyl-2-Ethyl-1,3-Propanediol Ester (IB$_{6\text{-}3}$)

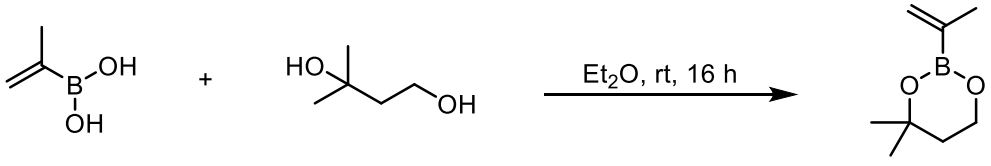


At room temperature, 2-butyl-2-ethyl-1,3-propanediol (8.00 g, 50.0 mmol) was dissolved in 100.0 mL diethyl ether, and a 2.5 M solution of vinyl boronic acid obtained above in diethyl ether (20.0 mL, 50.0 mmol) was added. The reaction was allowed to stir for 16 h at room temperature, filtered through a short pad of Celite, and washed with diethyl ether. The filtrate was concentrated in vacuo, and the crude product was purified by chromatography to afford the desired product as a colourless oil (8.05 g, 76.7% yield).

R$_f$ = 0.45 (pure petroleum ether).

^{1}H NMR (400 MHz, Chloroform-*d*): δ 5.66 (dd, *J* = 3.9, 1.5 Hz, 1H), 5.53 (d, *J* = 1.7 Hz, 1H), 3.71 (s, 4H), 1.76 (s, 3H), 1.40 – 1.16 (m, 8H), 0.90 (t, *J* = 7.1 Hz, 3H), 0.84 (t, *J* = 7.6 Hz, 3H). **^{13}C NMR** (101 MHz, Chloroform-*d*): δ 127.57, 69.61, 36.57, 30.77, 25.00, 23.78, 23.58, 21.11, 14.10, 7.43. **^{11}B NMR** (128 MHz, Chloroform-*d*): δ 26.16.

Synthesis of Isopropenyl Boronic Acid 3-Methyl-1,3-Butanediol Ester (IB$_{6\text{-}4}$)



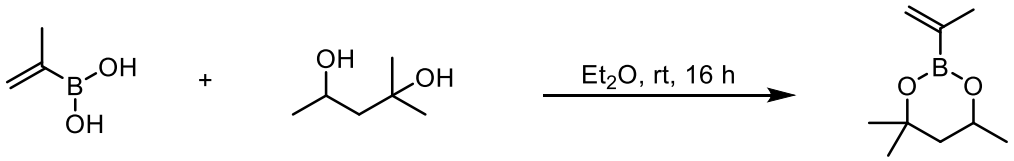
At room temperature, 3-methyl-1,3-butanediol (5.20 g, 50.0 mmol) was dissolved in

100.0 mL diethyl ether, and a 2.5 M solution of vinyl boronic acid obtained above in diethyl ether (20.0 mL, 50.0 mmol) was added. The reaction was allowed to stir for 16 h at room temperature, filtered through a short pad of Celite, and washed with diethyl ether. The filtrate was concentrated in vacuo, and the crude product was purified by chromatography to afford the desired product as a colourless oil (3.05 g, 39.6% yield).

R_f = 0.55 (pure petroleum ether).

^{1}H NMR (400 MHz, Chloroform-*d*): δ 5.64 (s, 1H), 5.50 (s, 1H), 4.19 – 3.94 (m, 2H), 1.83 – 1.77 (m, 2H), 1.74 (s, 3H), 1.30 (s, 6H). **^{13}C NMR** (101 MHz, Chloroform-*d*): δ 126.99, 70.12, 59.16, 38.17, 29.45, 21.02. **^{11}B NMR** (128 MHz, Chloroform-*d*): δ 25.95.

Synthesis of Isopropenyl Boronic Acid 2-Methyl-2,4-Pentanediol Ester ($IB_{6\text{-}5}$)



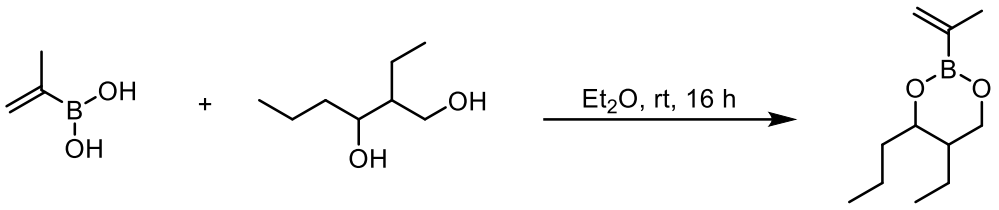
At room temperature, 3-methyl-1,3-butanediol (5.90 g, 50.0 mmol) was dissolved in 100.0 mL diethyl ether, and a 2.5 M solution of vinyl boronic acid obtained above in diethyl ether (20.0 mL, 50.0 mmol) was added. The reaction was allowed to stir for 16 h at room temperature, filtered through a short pad of Celite, and washed with diethyl ether. The filtrate was concentrated in vacuo, and the crude product was purified by chromatography (ethyl acetate/petroleum ether = 0/100) to afford the desired product as a colourless oil (6.78 g, 80.7% yield).

R_f = 0.50 (pure petroleum ether).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 5.65 (d, *J* = 2.9 Hz, 1H), 5.50 (s, 1H), 4.30 –

4.09 (m, 1H), 1.81 – 1.72 (m, 4H), 1.47 (dd, *J* = 13.9, 11.6 Hz, 1H), 1.32 – 1.22 (m, 9H). **^{13}C NMR** (101 MHz, Chloroform-*d*): δ 126.83, 70.73, 64.81, 46.04, 31.40, 28.27, 23.32, 21.05. **^{11}B NMR** (128 MHz, Chloroform-*d*): δ 26.00.

Synthesis of Isopropenyl Boronic Acid 2-Ethyl-1,3-Hexanediol Ester ($IB_{6\text{-}6}$)

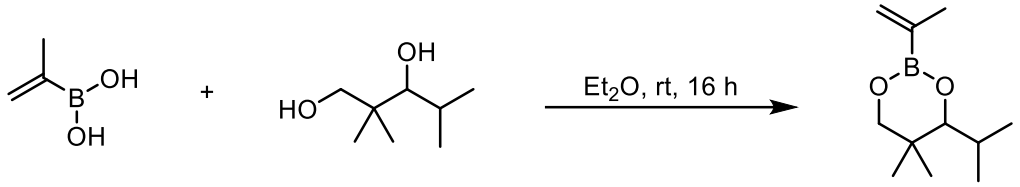


At room temperature, 2-ethyl-1,3-hexanediol (7.30 g, 50.0 mmol) was dissolved in 100.0 mL diethyl ether, and a 2.5 M solution of vinyl boronic acid obtained above in diethyl ether (20.0 mL, 50.0 mmol) was added. The reaction was allowed to stir for 16 h at room temperature, filtered through a short pad of Celite, and washed with diethyl ether. The filtrate was concentrated in vacuo, and the crude product was purified by chromatography to afford the desired product as a colourless oil (6.56 g, 66.9% yield).

R_f = 0.45 (pure petroleum ether).

^{1}H NMR (400 MHz, Chloroform-*d*): δ 5.65 (s, 1H), 5.51 (s, 1H), 4.13 – 3.59 (m, 3H), 1.96 – 1.16 (m, 10H), 1.07 – 0.72 (m, 6H). **^{13}C NMR** (101 MHz, Chloroform-*d*): δ 127.26, 73.45, 64.56, 63.73, 41.73, 41.08, 37.29, 33.86, 22.80, 21.84, 21.06, 19.18, 19.01, 18.37, 14.22, 11.92, 11.44. **^{11}B NMR** (128 MHz, Chloroform-*d*): δ 25.98.

Synthesis of Isopropenyl Boronic Acid 2,2,4-Trimethyl-1,3-Pentanediol Ester (IB_{6-7})



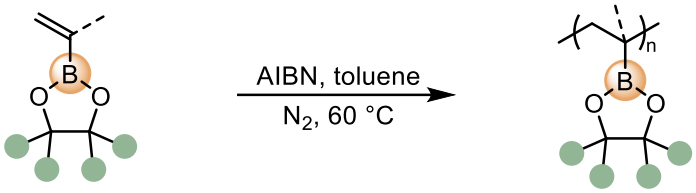
At room temperature, 2,2,4-trimethyl-1,3-pentanediol (7.30 g, 50.0 mmol) was dissolved in 100.0 mL diethyl ether, and a 2.5 M solution of vinyl boronic acid obtained above in diethyl ether (20.0 mL, 50.0 mmol) was added. The reaction was allowed to stir for 16 h at room temperature, filtered through a short pad of Celite, and washed with diethyl ether. The filtrate was concentrated in vacuo, and the crude product was purified by chromatography to afford the desired product as a colourless oil (6.62 g, 67.6% yield).

R_f = 0.45 (pure petroleum ether).

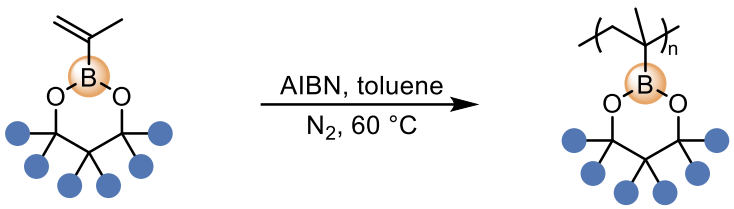
^{1}H NMR (400 MHz, Chloroform-*d*): δ 5.70 (d, *J* = 2.5 Hz, 1H), 5.54 (s, 1H), 3.64 – 3.51 (m, 2H), 3.49 (d, *J* = 3.9 Hz, 1H), 1.96 – 1.83 (m, 1H), 1.78 (s, 3H), 1.04 (d, *J* = 6.9 Hz, 3H), 0.99 – 0.92 (m, 9H). **^{13}C NMR** (101 MHz, Chloroform-*d*): δ 127.39, 83.65, 73.53, 35.00, 29.71, 24.18, 22.91, 21.08, 19.06, 17.70. **^{11}B NMR** (128 MHz, Chloroform-*d*): δ 26.04.

IV. General Procedure of Polymerization

Typical Free Radical Polymerization of Vinyl/Isopropenyl Boronate Monomers.

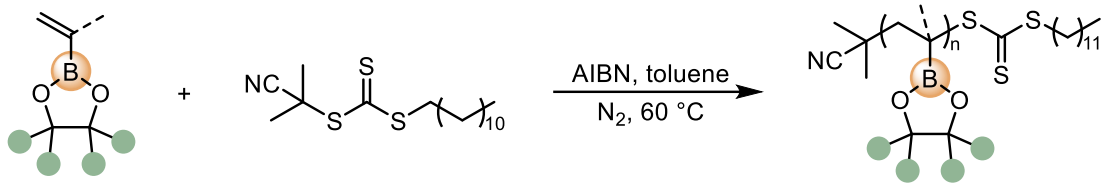


Vinyl boronic acid ethyl pinacol ester (VB_{epin}, 420 mg, 2.00 mmol), AIBN (50.0 mg/mL in toluene, 131 μL, 40.0 μmol), and toluene (69.0 μL) were sealed in a 10 mL Schlenk flask equipped with a magnetic stir bar in the glove box. The reaction mixture was stirred at 60 °C in an oil bath. After 24 h, the polymerization was stopped by removing the reaction mixture from heat and exposing it to air. Homopolymers were precipitated in CH_3OH and filtered to obtain white powders.

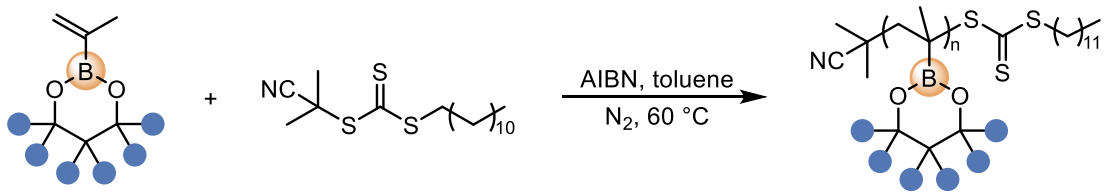


Isopropenyl boronic acid neopentyl glycol ester ($IB_{6\text{-}1}$, 308 mg, 2.00 mmol), AIBN (50.0 mg/mL in toluene, 131 μL, 40.0 μmol), and toluene (69.0 μL) were sealed in a 10 mL Schlenk flask equipped with a magnetic stir bar in the glove box. The reaction mixture was stirred at 60 °C in an oil bath. After 24 h, the polymerization was stopped by removing the reaction mixture from heat and exposing it to air. Homopolymers were precipitated in CH_3OH and filtered to obtain white powders.

Typical RAFT Polymerization of Vinyl/Isopropenyl Boronate Monomers.



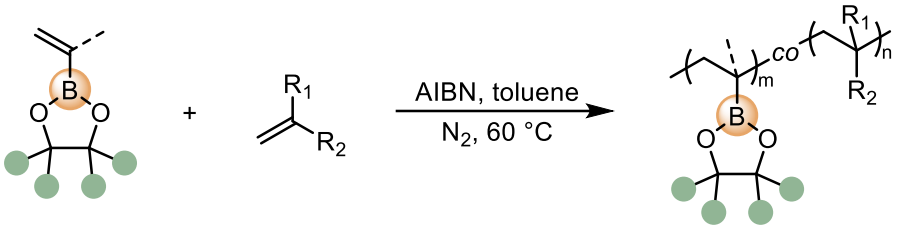
Vinyl boronic acid ethyl pinacol ester (VB_{epin}, 410 mg, 2.00 mmol), AIBN (50.0 mg/mL in toluene, 52.5 μL, 16.0 μmol), chain transfer agent CPDT (50.0 mg/mL in toluene, 138 μL, 20.0 μmol), and toluene (10.0 μL) were sealed in a 10 mL Schlenk flask equipped with a magnetic stir bar in the glove box. The reaction mixture was stirred at 60 °C in an oil bath. The polymerization was monitored by ^{1}H NMR and GPC. After 36 h, the polymerization was stopped by removing the reaction mixture from heat and exposing it to air.



Isopropenyl boronic acid neopentyl glycol ester ($IB_{6\text{-}1}$, 308 mg, 2.00 mmol), AIBN (50.0 mg/mL in toluene, 52.5 μL, 16.0 μmol), chain transfer agent CPDT (50.0 mg/mL in toluene, 138 μL, 20.0 μmol), and toluene (10.0 μL) were sealed in a 10 mL Schlenk flask equipped with a magnetic stir bar in the glove box. The reaction mixture was stirred at 60 °C in an oil bath. The polymerization was monitored by ^{1}H NMR and GPC. After 48 h, the polymerization was stopped by removing the reaction mixture from heat and exposing it to air.

V. General Procedure of Copolymerization

Typical Free Radical Copolymerization of Vinyl/Isopropenyl Boronate Monomers and Other Monomers.



Isopropenyl boronic acid benzpinacol ester (IB_{Phpin}, 166 mg, 0.40 mmol), methyl methacrylate (MMA, 40.0 mg, 0.40 mmol), AIBN (50.0 mg/mL in toluene, 26.3 μL, 8.00 μmol), and toluene (134 μL) were sealed in a 5 mL vial equipped with a magnetic stir bar in the glove box. The reaction mixture was stirred at 60 °C in an oil bath. After 24 h, the polymerization was stopped by removing the reaction mixture from heat and exposing it to air. Copolymers were precipitated in CH_3OH and filtered to obtain white powders.

VI. Analytical Data of the Polymers

Table S1. Free Radical Copolymerization of VB_{Phpin} with Various Types of Monomers[a]

entry	M_2	M_1/M_2/AIBN	M_n[c]	M_w/M_n[c]	$F_{VBPhpin}$[d]
1	DMAA	50:50:1	4100	1.98	0.36
2	*t*-BA	50:50:1	3900	2.10	0.42
3	MMA	50:50:1	9500	2.59	0.35
4[b]	MMA	10:50:1	16500	2.41	0.12
5	St	50:50:1	9900	1.64	0.16
6[b]	St	10:50:1	12000	1.75	0.02
7	AN	50:50:1	4200	1.39	0.35
8	NPMI	50:50:1	2800	1.48	0.12

[a] Reaction conditions: $M_1 = VB_{Phpin}$, $[M_2]_0$ = 1.0 M in THF. Reaction temperature is 60 °C for 24 h under N_2 atmosphere. [b] $[M_2]_0$ = 2.5 M in THF. [c] Determined by GPC in THF, based on linear PMMA as a calibration standard. [d] Calculated by ^{1}H NMR spectroscopy.

Table S2. Free Radical Copolymerization of IB_{Phpin} with MMA and St in Different Feed Ratios[a]

entry	M_2	M_1/M_2/AIBN	M_n[c]	M_w/M_n[c]	$F_{IBPhpin}$[d]
1	MMA	5:50:1	16000	2.71	0.09
2	MMA	10:50:1	20000	2.55	0.16
3	MMA	25:50:1	24200	2.72	0.24
4	MMA	50:50:1	49600	2.97	0.33
5[b]	St	5:50:1	13700	1.59	0.01
6[b]	St	10:50:1	13100	1.62	0.03
7[b]	St	25:50:1	16100	1.68	0.08
8[b]	St	50:50:1	20700	1.82	0.13

[a] Reaction conditions: $M_1 = VB_{Phpin}$, $[M_2]_0$ = 2.5 M in toluene. Reaction temperature is

60 °C for 24 h under N_2 atmosphere. [b] Reaction time is 40 h. [c] Determined by GPC in THF, based on linear PMMA as a calibration standard. [d] Calculated by ^{1}H NMR spectroscopy.

Table S3. Synthesis of Six-Membered Cyclic Alkenyl Boronate Polymers by Radical Polymerization[a]

entry	monomer	conv. (%)[b]	M_n[c]	M_w/M_n[c]	T_d (°C)[d]
1	$IB_{6\text{-}1}$	75	9600	1.61	149
2	$IB_{6\text{-}2}$	83	15300	1.82	211
3	$IB_{6\text{-}3}$	84	20600	1.84	223
4	$IB_{6\text{-}4}$	91	15100	1.86	190
5	$IB_{6\text{-}5}$	91	14400	1.81	221
6	$IB_{6\text{-}6}$	93	21200	1.99	249
7	$IB_{6\text{-}7}$	81	16100	1.85	226

[a] Reaction conditions: $[M]_0:[I]_0 = 50:1$, $[M]_0 = 10.0$ M in toluene. Reaction temperature is 60 °C for 24 h under N_2 atmosphere. [b] Determined by ^{1}H NMR spectroscopy. [c] Determined by GPC in THF, based on linear PMMA as a calibration standard. [d] T_d was measured by thermogravimetric analysis (TGA), indicating the 5% weight-loss temperature.

Table S4. Synthesis of Six-Membered Cyclic Alkenyl Boronate Polymers by RAFT Polymerization[a]

entry	monomer	conv. (%)[b]	M_n[c]	M_w/M_n[c]
1	$IB_{6\text{-}1}$	68	7500	1.22
2	$IB_{6\text{-}2}$	75	11800	1.25
3	$IB_{6\text{-}3}$	73	13000	1.25
4	$IB_{6\text{-}4}$	78	10300	1.26
5	$IB_{6\text{-}5}$	79	10700	1.24
6	$IB_{6\text{-}6}$	86	13400	1.26

7	$IB_{6\text{-}7}$	69	11000	1.25

[a] Reaction conditions: $[M]_0 : [CTA]_0 : [AIBN]_0 = 100 : 1 : 0.8$, $[M]_0 = 10.0$ M in toluene. Reaction temperature is 60 °C for 48 h under N_2 atmosphere. [b] Determined by ^1H NMR spectroscopy. [c] Determined by GPC in THF, based on linear PMMA as a calibration standard.

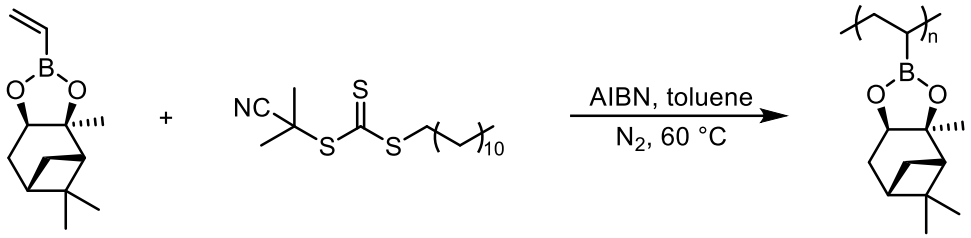


Table S5. Conversion of RAFT Polymerization of VB_{pnd} and GPC-Based Molecular Weight of the Resultant Polymer.[a]

time/h	conv. (%)[b]	M_n[c]	M_w/M_n[c]
6	5	1400	1.15
12	16	2400	1.26
24	47	2600	1.59
36	68	3000	1.48

[a] Reaction conditions: $[M]_0 : [CPDT]_0 : [AIBN]_0 = 100 : 1 : 0.8$, $[M]_0 = 10.0$ M in toluene. Reaction temperature is 60 °C under a N_2 atmosphere. [b] Determined by ^1H NMR spectroscopy. [c] Determined by GPC in THF, based on linear PMMA as a calibration standard.

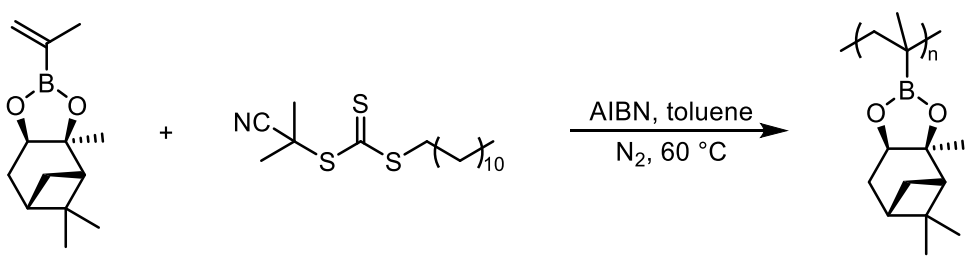


Table S6. Conversion of RAFT Polymerization of IB_{pnd} and GPC-Based Molecular

Weight of the Resultant Polymer.[a]

time/h	conv. (%)[b]	M_n[c]	M_w/M_n[c]
6	5	1600	1.15
12	19	4300	1.22
24	50	8700	1.27
36	65	9700	1.27

[a] Reaction conditions: $[M]_0 : [CPDT]_0 : [AIBN]_0 = 100 : 1 : 0.8$, $[M]_0 = 10.0$ M in toluene. Reaction temperature is 60 °C under a N_2 atmosphere. [b] Determined by ^{1}H NMR spectroscopy. [c] Determined by GPC in THF, based on linear PMMA as a calibration standard.

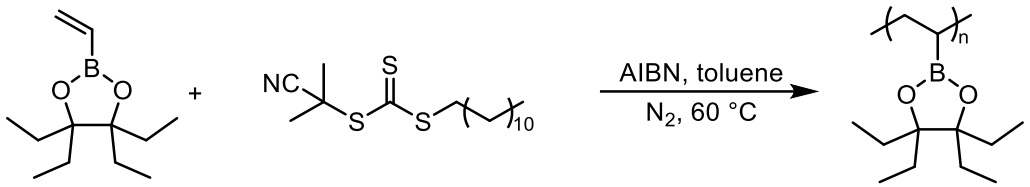


Table S7. Conversion of RAFT Polymerization of VB_{epin} and GPC-Based Molecular Weight of the Resultant Polymer.[a]

time/h	conv. (%)[b]	M_n[c]	M_w/M_n[c]
6	10	1200	1.10
12	19	1800	1.15
24	29	1900	1.30
36	35	2400	1.27

[a] Reaction conditions: $[M]_0 : [CPDT]_0 : [AIBN]_0 = 100 : 1 : 0.8$, $[M]_0 = 10.0$ M in toluene. Reaction temperature is 60 °C under a N_2 atmosphere. [b] Determined by ^{1}H NMR spectroscopy. [c] Determined by GPC in THF, based on linear PMMA as a calibration standard.

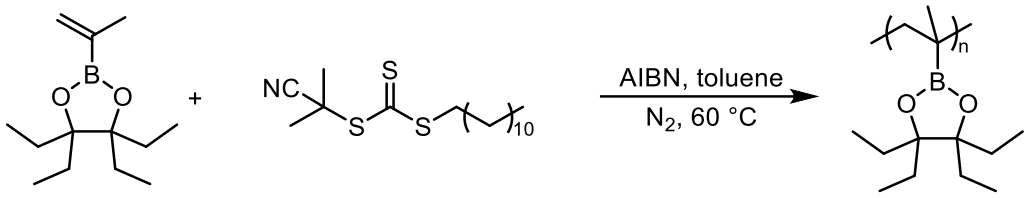


Table S8. Conversion of RAFT Polymerization of IB_{epin} and GPC-Based Molecular Weight of the Resultant Polymer.[a]

time/h	conv. (%)[b]	M_n[c]	M_w/M_n[c]
6	13	1100	1.08
12	21	1700	1.12
24	25	2500	1.17
36	32	2900	1.25

[a] Reaction conditions: $[M]_0 : [CPDT]_0 : [AIBN]_0 = 100 : 1 : 0.8$, $[M]_0 = 10.0$ M in toluene. Reaction temperature is 60 °C under a N_2 atmosphere. [b] Determined by ^1H NMR spectroscopy. [c] Determined by GPC in THF, based on linear PMMA as a calibration standard.

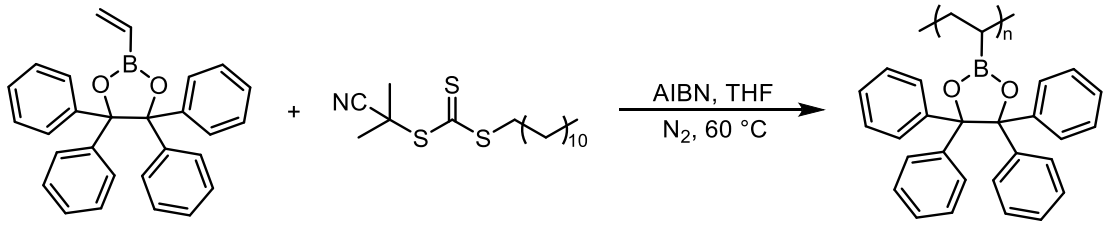


Table S9. Conversion of RAFT Polymerization of VB_{Phpin} and GPC-Based Molecular Weight of the Resultant Polymer.[a]

time/h	conv. (%)[b]	M_n[c]	M_w/M_n[c]
6	5	1600	1.10
12	19	1800	1.18
24	41	2000	1.13
36	56	2100	1.16

[a] Reaction conditions: $[M]_0 : [CPDT]_0 : [AIBN]_0 = 100 : 1 : 0.8$, $[M]_0 = 10.0$ M in toluene.

Reaction temperature is 60 °C under a N_2 atmosphere. [b] Determined by ^{1}H NMR spectroscopy. [c] Determined by GPC in THF, based on linear PMMA as a calibration standard.

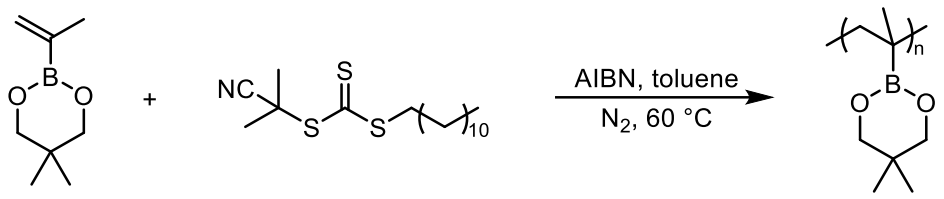


Table S10. Conversion of RAFT Polymerization of $IB_{6\text{-}1}$ and GPC-Based Molecular Weight of the Resultant Polymer.[a]

time/h	conv. (%)[b]	M_n[c]	M_w/M_n[c]
6	8	1400	1.11
12	29	3300	1.13
18	42	4900	1.16
24	53	5300	1.18
48	68	7500	1.22

[a] Reaction conditions: $[M]_0 : [CPDT]_0 : [AIBN]_0 = 100 : 1 : 0.8$, $[M]_0 = 10.0$ M in toluene. Reaction temperature is 60 °C under a N_2 atmosphere. [b] Determined by ^{1}H NMR spectroscopy. [c] Determined by GPC in THF, based on linear PMMA as a calibration standard.

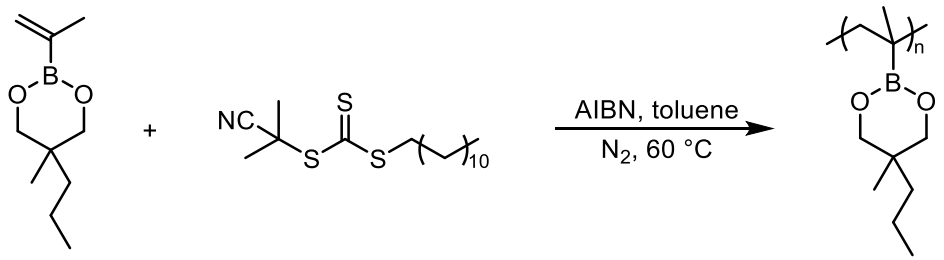


Table S11. Conversion of RAFT Polymerization of $IB_{6\text{-}2}$ and GPC-Based Molecular Weight of the Resultant Polymer.[a]

time/h	conv. (%)[b]	M_n[c]	M_w/M_n[c]
6	18	3200	1.12
12	35	5300	1.16
18	42	7200	1.18
24	54	8500	1.21
48	75	11800	1.25

[a] Reaction conditions: $[M]_0 : [CPDT]_0 : [AIBN]_0 = 100 : 1 : 0.8$, $[M]_0 = 10.0$ M in toluene. Reaction temperature is 60 °C under a N_2 atmosphere. [b] Determined by ^{1}H NMR spectroscopy. [c] Determined by GPC in THF, based on linear PMMA as a calibration standard.

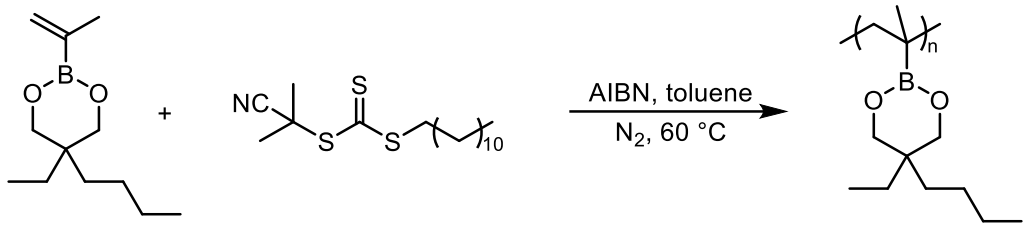


Table S12. Conversion of RAFT Polymerization of $IB_{6\text{-}3}$ and GPC-Based Molecular Weight of the Resultant Polymer.[a]

time/h	conv. (%)[b]	M_n[c]	M_w/M_n[c]
6	15	3500	1.14
12	31	5900	1.16
18	42	8000	1.18
24	54	9500	1.21
48	73	13000	1.25

[a] Reaction conditions: $[M]_0 : [CPDT]_0 : [AIBN]_0 = 100 : 1 : 0.8$, $[M]_0 = 10.0$ M in toluene. Reaction temperature is 60 °C under a N_2 atmosphere. [b] Determined by ^{1}H NMR spectroscopy. [c] Determined by GPC in THF, based on linear PMMA as a calibration standard.

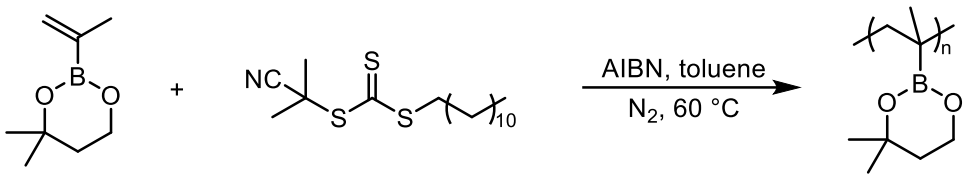


Table S13. Conversion of RAFT Polymerization of $IB_{6\text{-}4}$ and GPC-Based Molecular Weight of the Resultant Polymer.[a]

time/h	conv. (%)[b]	M_n[c]	M_w/M_n[c]
6	12	2200	1.16
12	33	4300	1.14
18	42	5800	1.16
24	52	6900	1.18
48	78	10300	1.26

[a] Reaction conditions: $[M]_0 : [CPDT]_0 : [AIBN]_0 = 100 : 1 : 0.8$, $[M]_0 = 10.0$ M in toluene. Reaction temperature is 60 °C under a N_2 atmosphere. [b] Determined by ^1H NMR spectroscopy. [c] Determined by GPC in THF, based on linear PMMA as a calibration standard.

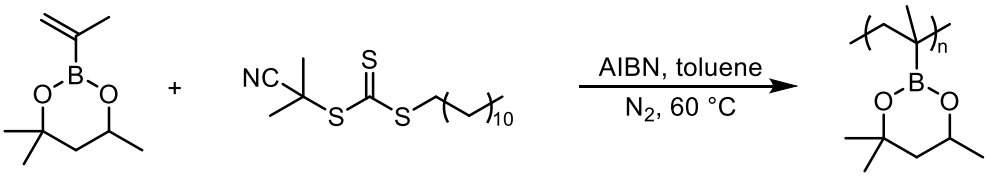


Table S14. Conversion of RAFT Polymerization of $IB_{6\text{-}5}$ and GPC-Based Molecular Weight of the Resultant Polymer.[a]

time/h	conv. (%)[b]	M_n[c]	M_w/M_n[c]
6	7	2000	1.15
12	25	4400	1.14
18	44	6700	1.17
24	53	7500	1.18

48	79	10700	1.24

[a] Reaction conditions: $[M]_0 : [CPDT]_0 : [AIBN]_0 = 100 : 1 : 0.8$, $[M]_0 = 10.0$ M in toluene. Reaction temperature is 60 °C under a N_2 atmosphere. [b] Determined by ^1H NMR spectroscopy. [c] Determined by GPC in THF, based on linear PMMA as a calibration standard.

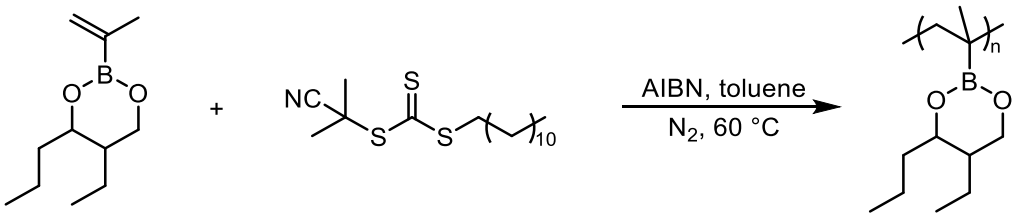


Table S15. Conversion of RAFT Polymerization of $IB_{6\text{-}6}$ and GPC-Based Molecular Weight of the Resultant Polymer.[a]

time/h	conv. (%)[b]	M_n[c]	M_w/M_n[c]
6	17	4200	1.11
12	46	7200	1.17
18	56	9600	1.17
24	62	10000	1.20
48	86	13400	1.26

[a] Reaction conditions: $[M]_0 : [CPDT]_0 : [AIBN]_0 = 100 : 1 : 0.8$, $[M]_0 = 10.0$ M in toluene. Reaction temperature is 60 °C under a N_2 atmosphere. [b] Determined by ^1H NMR spectroscopy. [c] Determined by GPC in THF, based on linear PMMA as a calibration standard.

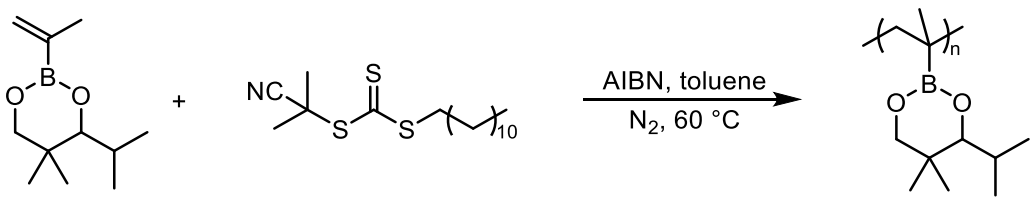


Table S16. Conversion of RAFT Polymerization of $IB_{6\text{-}7}$ and GPC-Based Molecular Weight of the Resultant Polymer.[a]

time/h	conv. (%)[b]	M_n[c]	M_w/M_n[c]
6	7	2000	1.15
12	29	5200	1.18
18	39	6700	1.19
24	50	7400	1.21
48	69	11000	1.25

[a] Reaction conditions: $[M]_0 : [CPDT]_0 : [AIBN]_0 = 100 : 1 : 0.8$, $[M]_0 = 10.0$ M in toluene. Reaction temperature is 60 °C under a N_2 atmosphere. [b] Determined by ^1H NMR spectroscopy. [c] Determined by GPC in THF, based on linear PMMA as a calibration standard.

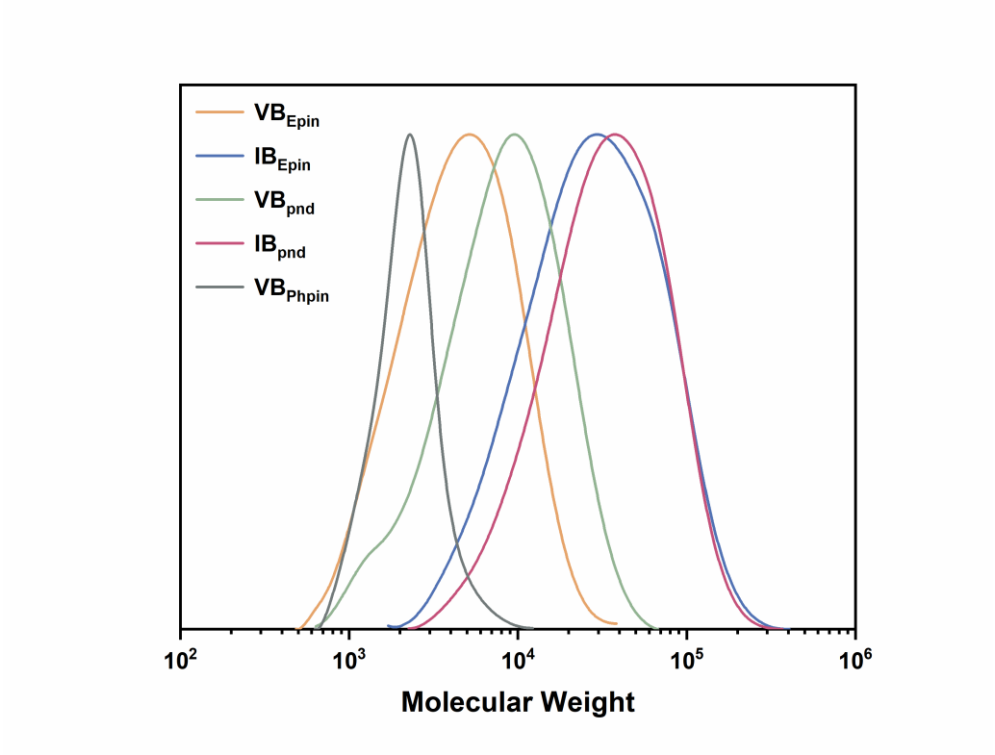


Figure S1. GPC Traces of Homopolymers in Table 1.

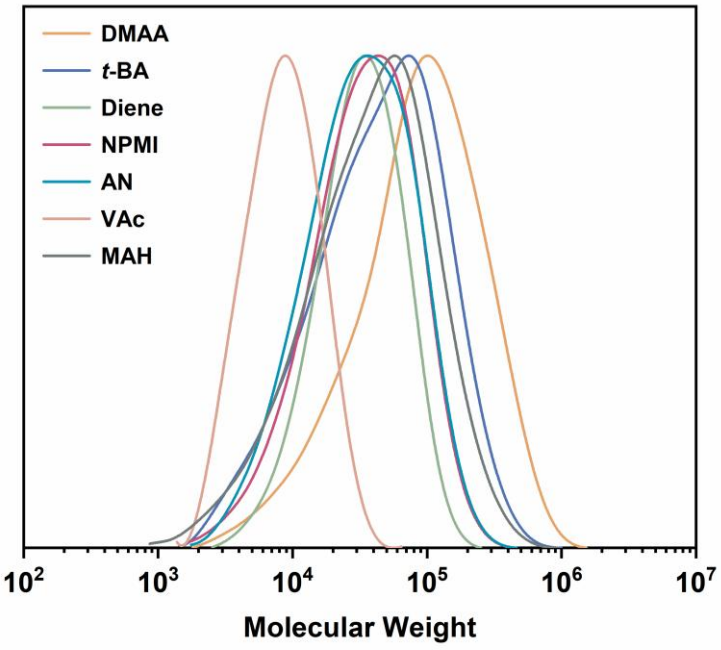


Figure S2. GPC Traces of Copolymers in Table 2.

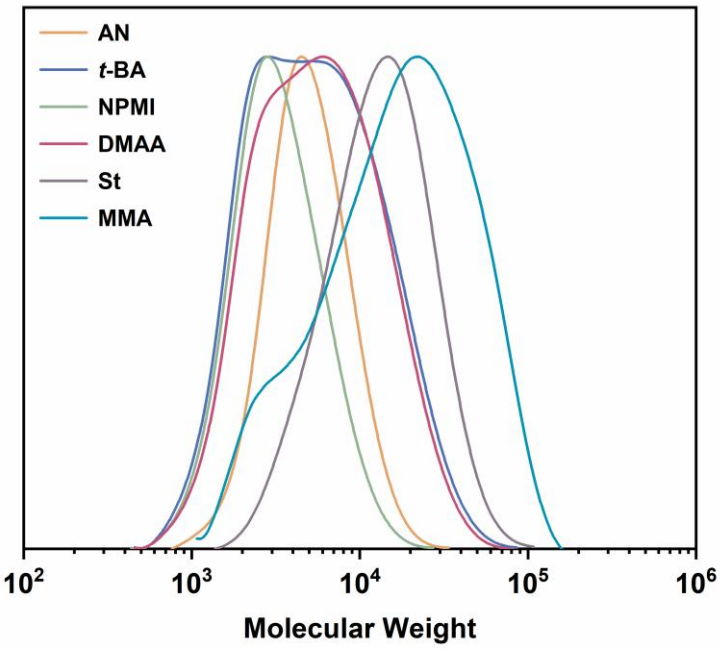


Figure S3. GPC Traces of Copolymers in Table S1.

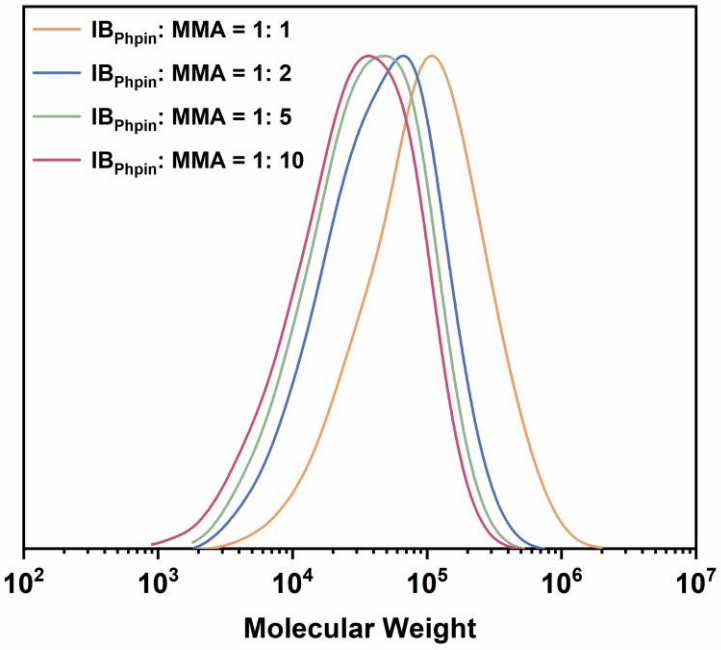


Figure S4. GPC Traces of Copolymers in Table S2.

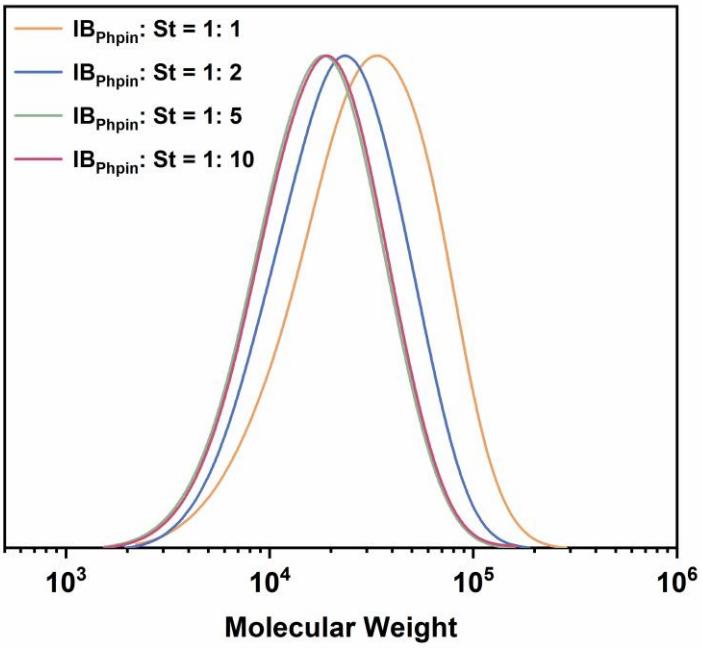


Figure S5. GPC Traces of Copolymers in Table S2.

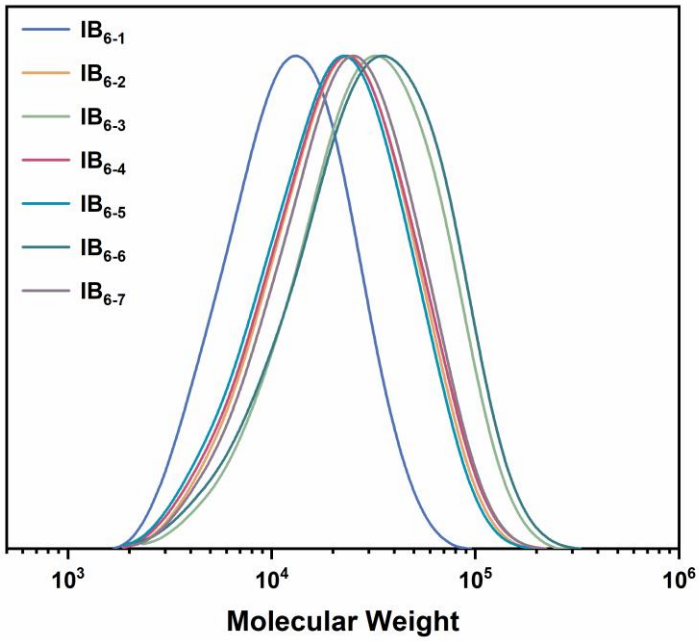


Figure S6. GPC Traces of Homopolymers in Table S3.

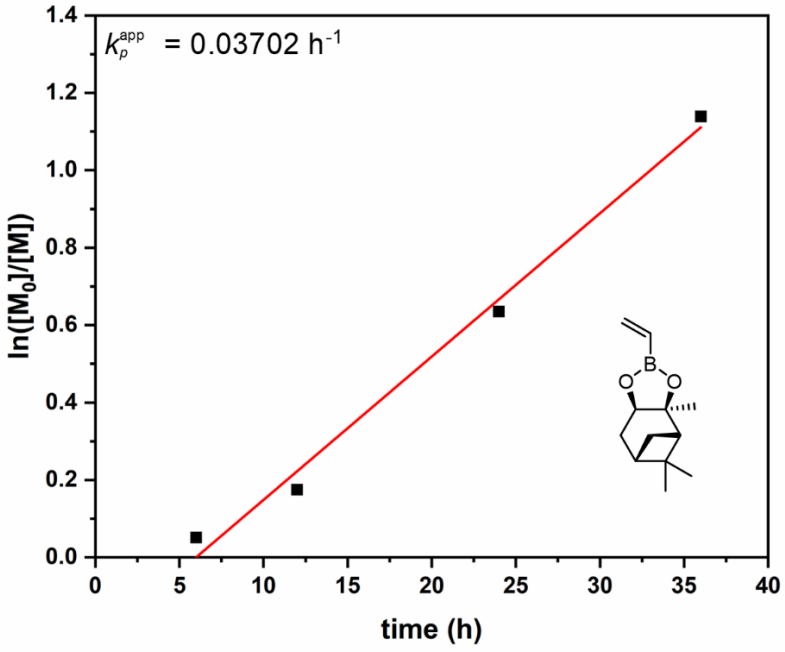


Figure S7. Semilogarithmic Kinetic Plots of RAFT Polymerization of VB_{pnd}.

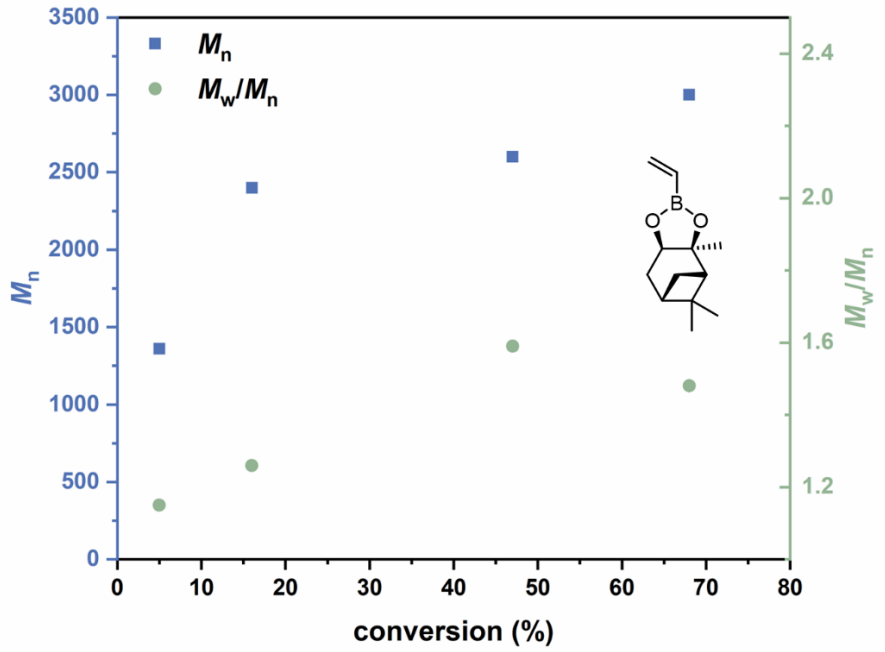


Figure S8. M_n and M_w/M_n as a Function of the VB_{pnd} Conversion.

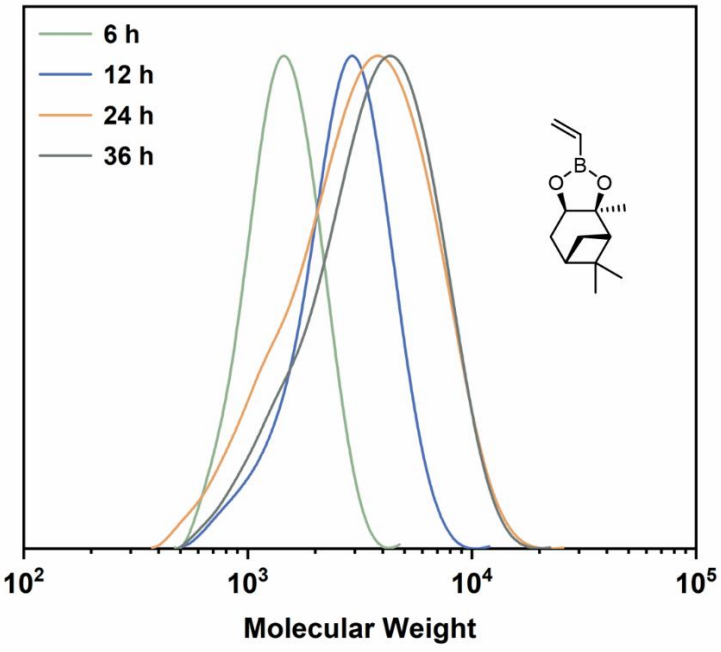


Figure S9. GPC Traces of PVB_{pnd}-CTA at Different Time Intervals.

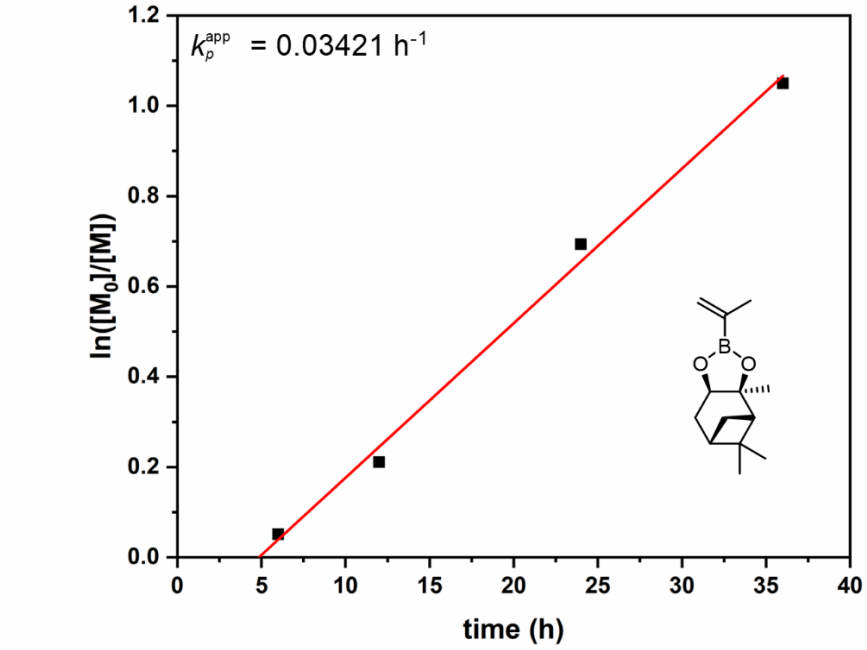


Figure S10. Semilogarithmic Kinetic Plots of RAFT Polymerization of IB_{pnd}.

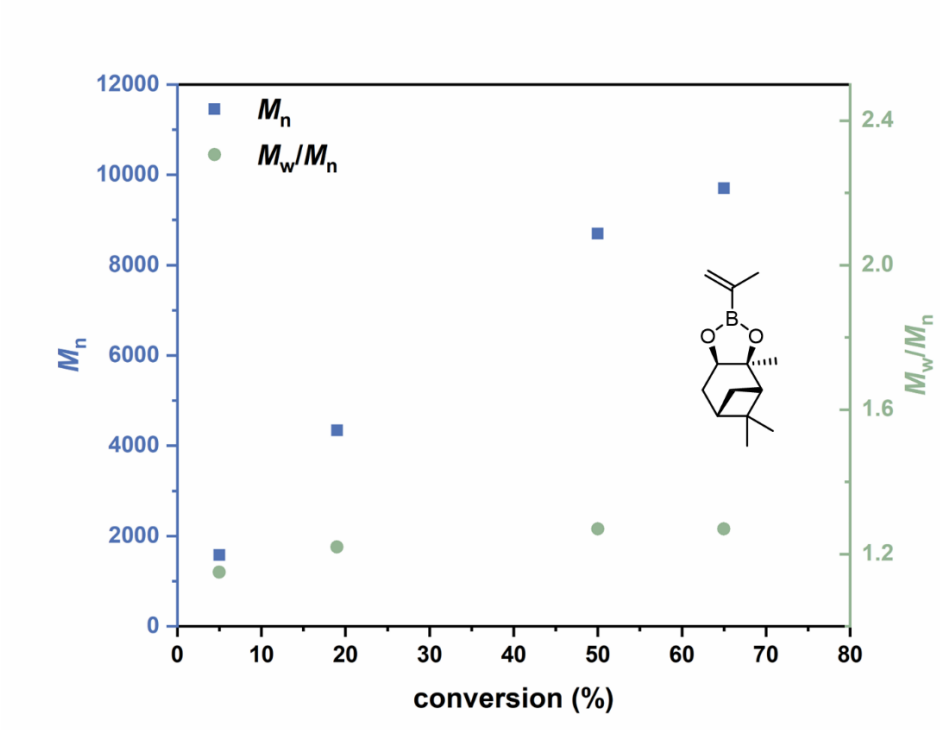


Figure S11. M_n and M_w/M_n as a Function of the IB_{pnd} Conversion.

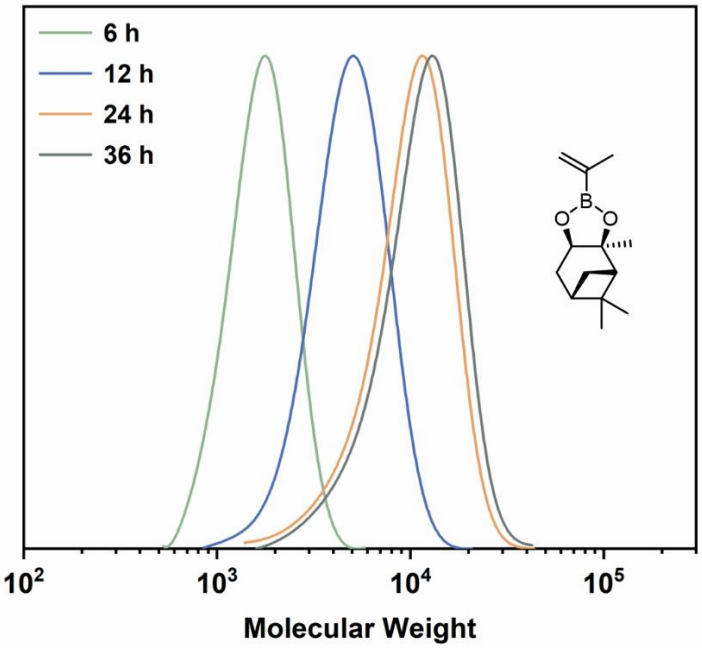


Figure S12. GPC Traces of PIB_{pnd}-CTA at Different Time Intervals.

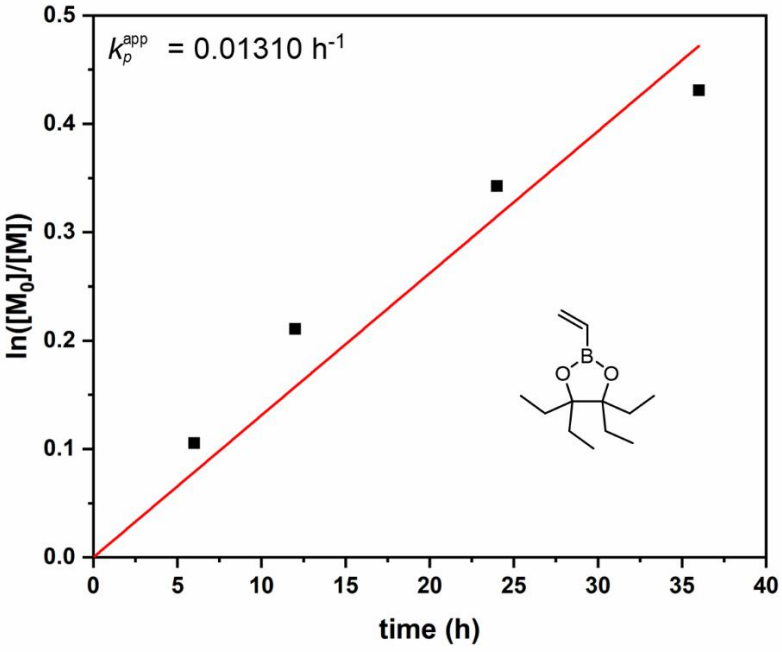


Figure S13. Semilogarithmic Kinetic Plots of RAFT Polymerization of VB_{epin}.

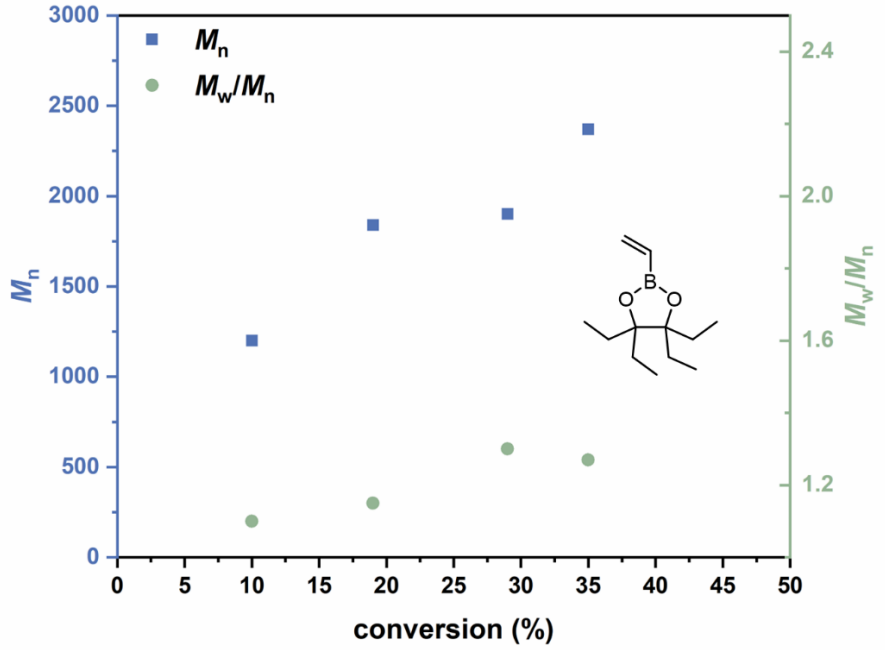


Figure S14. M_n and M_w/M_n as a Function of the VB_{epin} Conversion.

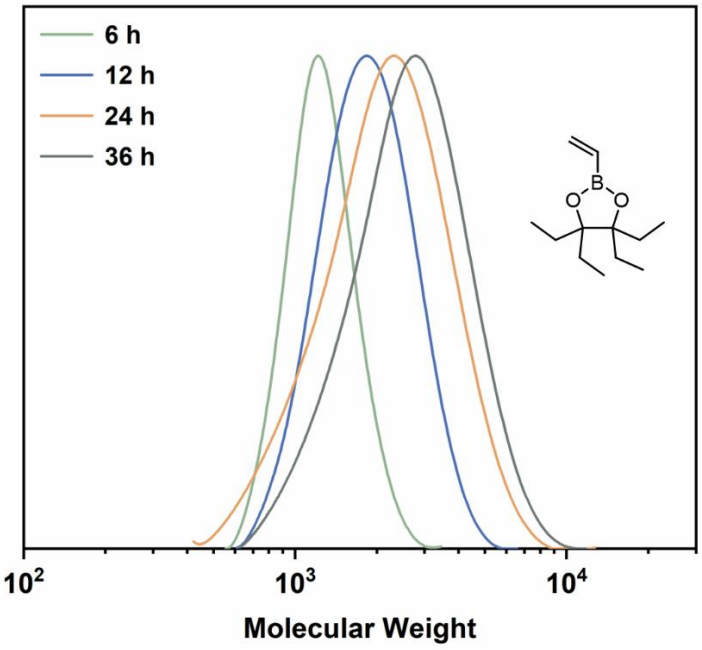


Figure S15. GPC Traces of PVB_{epin}-CTA at Different Time Intervals.

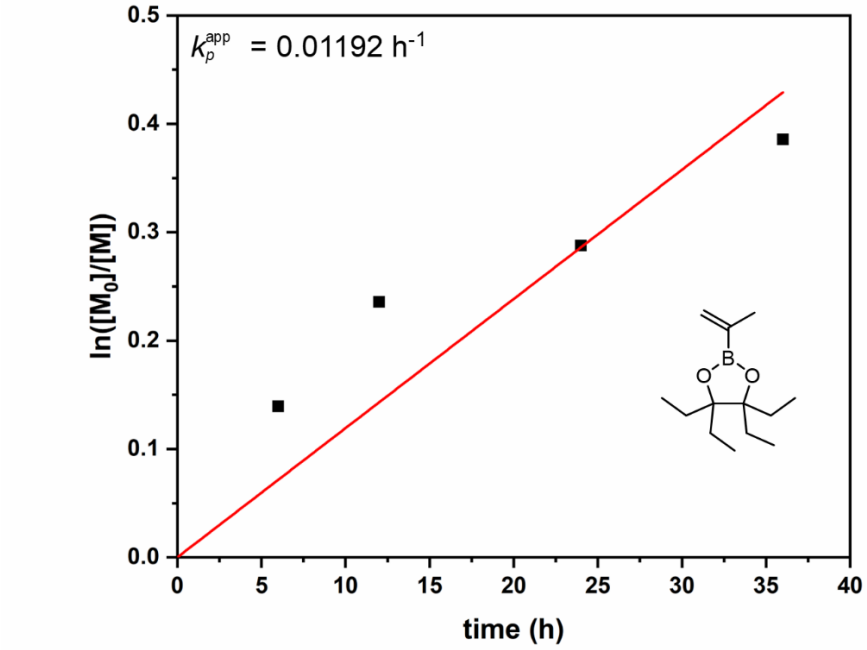


Figure S16. Semilogarithmic Kinetic Plots of RAFT Polymerization of IB_{epin}.

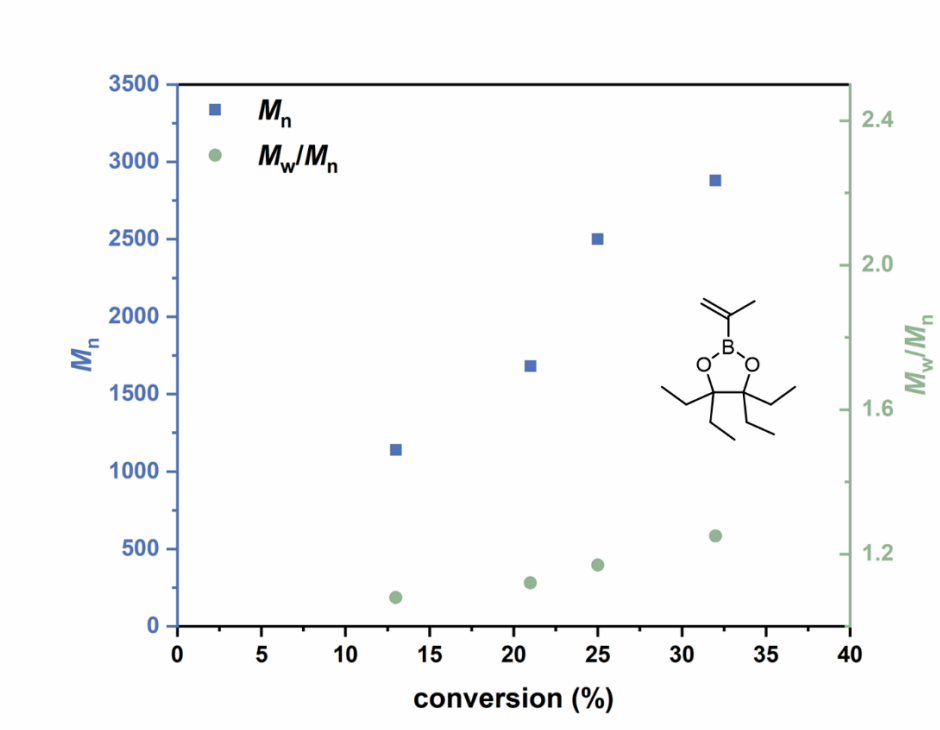


Figure S17. M_n and M_w/M_n as a Function of the IB_{epin} Conversion.

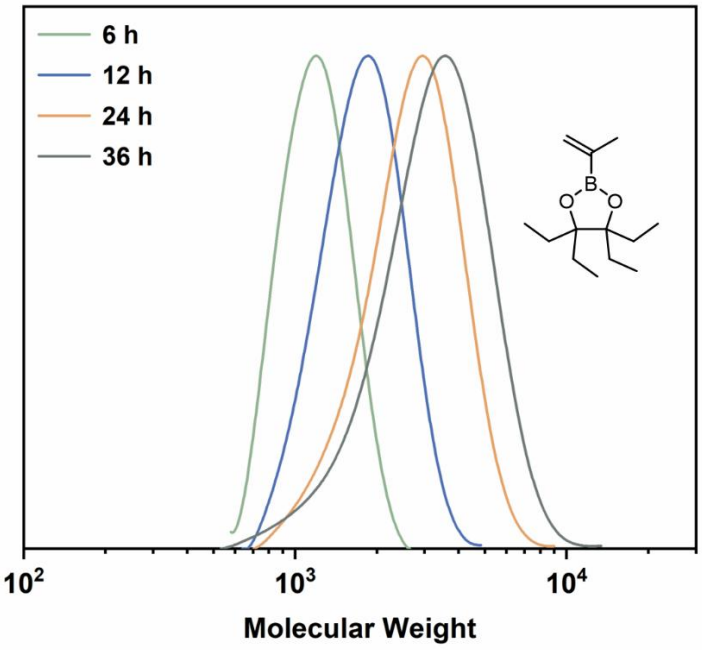


Figure S18. GPC Traces of PIB_{epin}-CTA at Different Time Intervals.

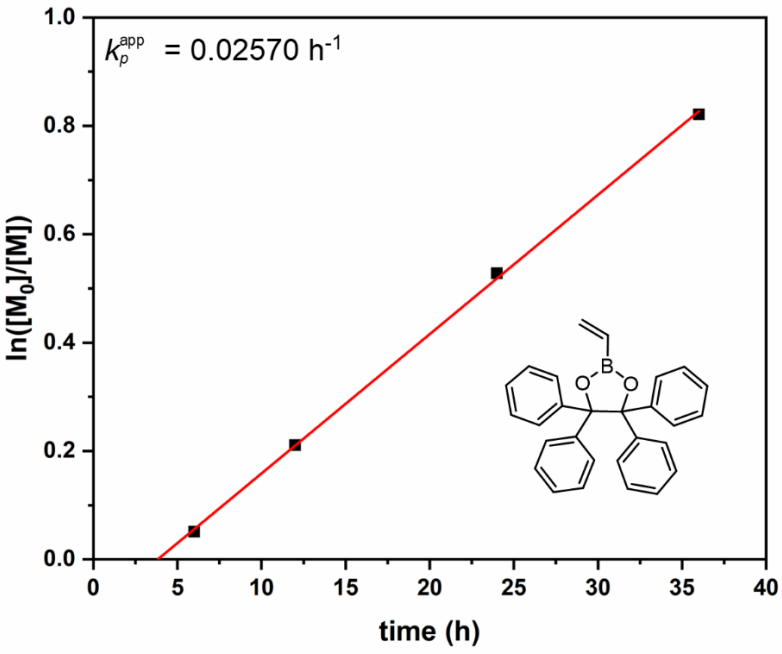


Figure S19. Semilogarithmic Kinetic Plots of RAFT Polymerization of VB_{Phpin}.

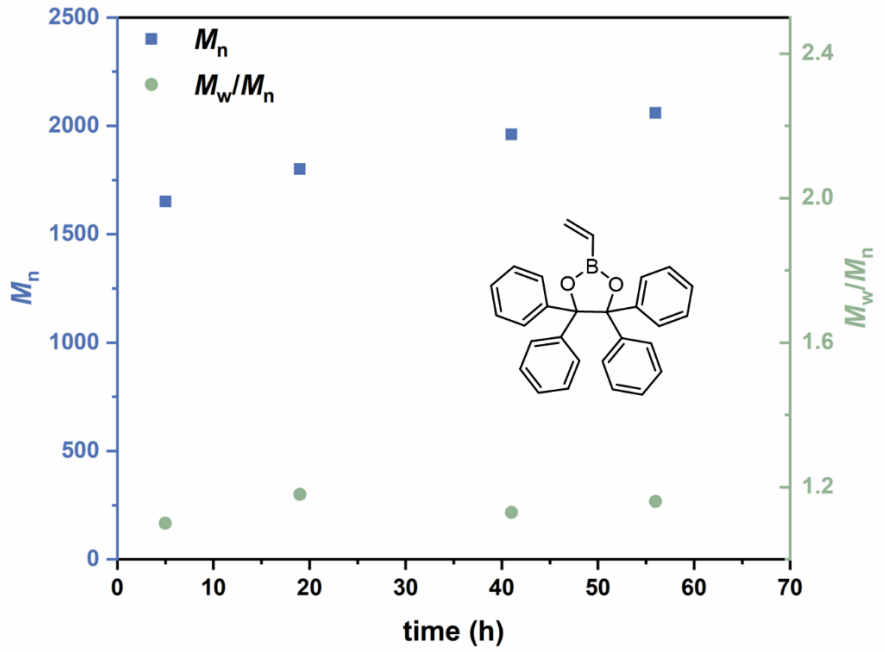


Figure S20. M_n and M_w/M_n as a Function of the VB_{Phpin} Conversion.

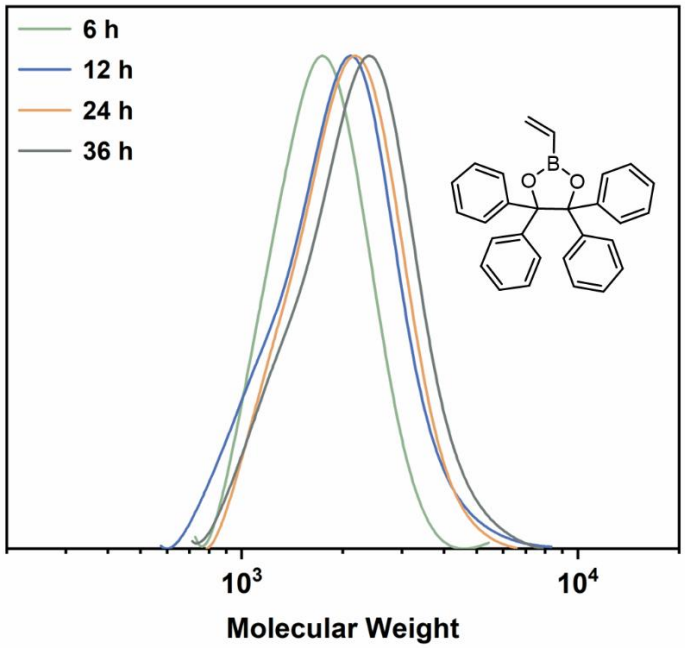


Figure S21. GPC Traces of PVB_{Phpin}-CTA at Different Time Intervals.

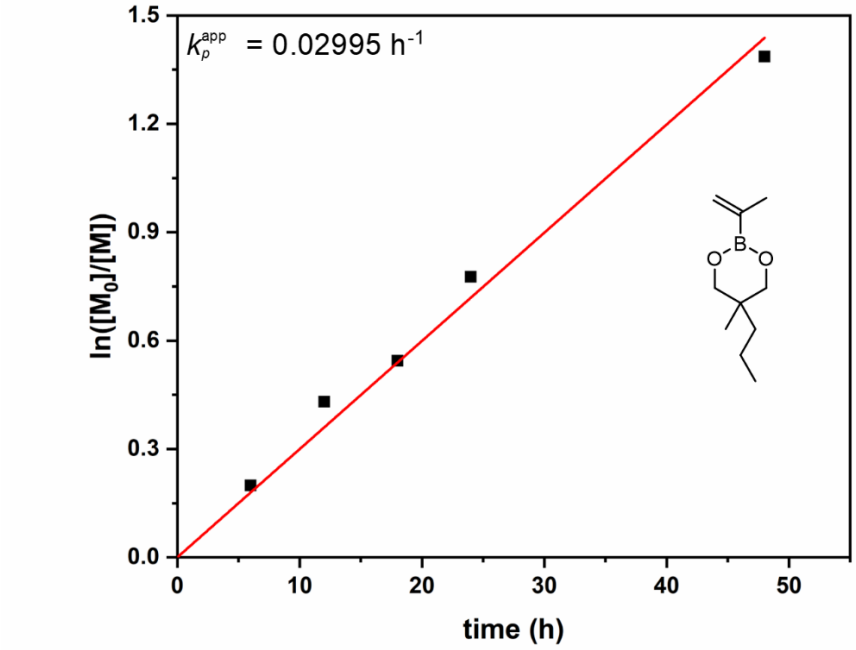


Figure S22. Semilogarithmic Kinetic Plots of RAFT Polymerization of $IB_{6\text{-}2}$.

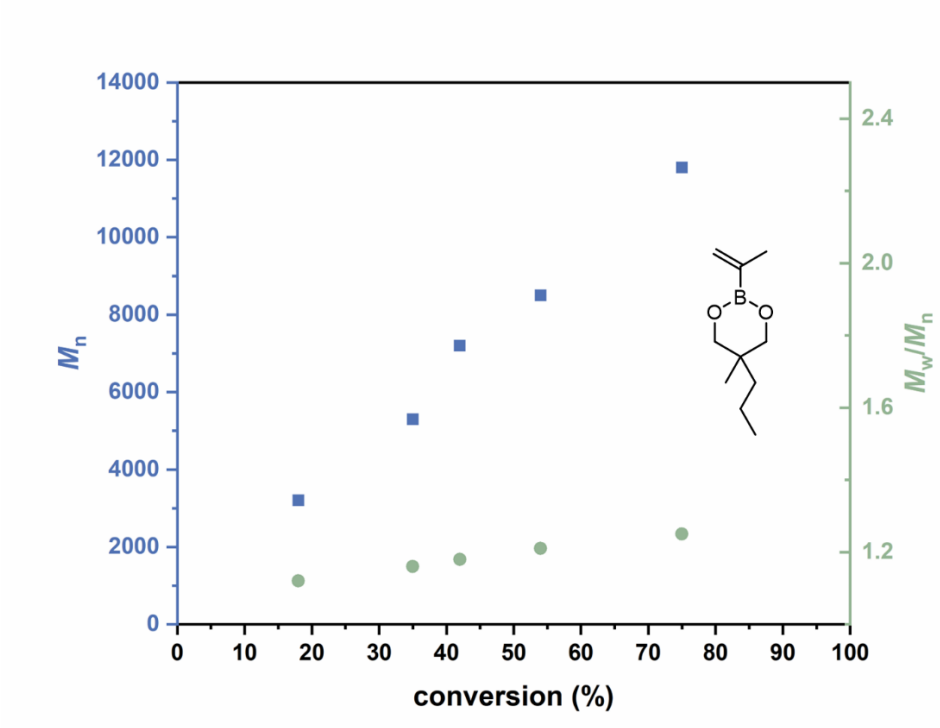


Figure S23. M_n and M_w/M_n as a Function of the $IB_{6\text{-}2}$ Conversion.

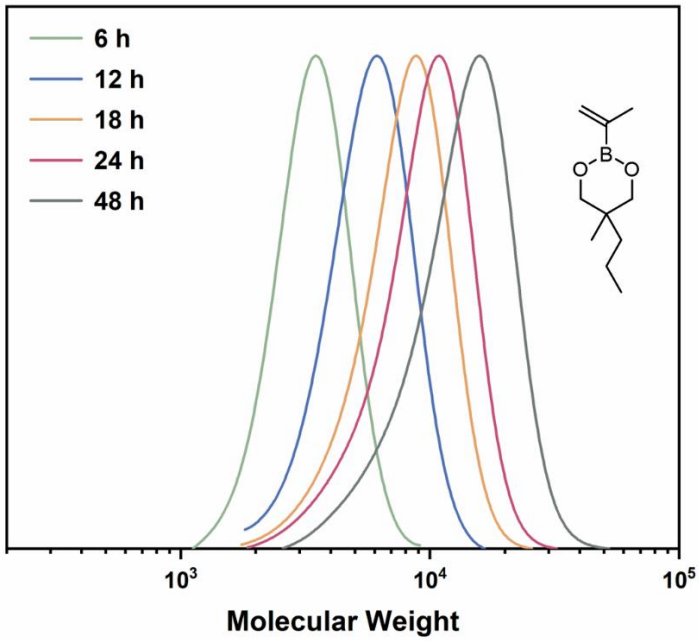


Figure S24. GPC Traces of $PIB_{6\text{-}2}$-CTA at Different Time Intervals.

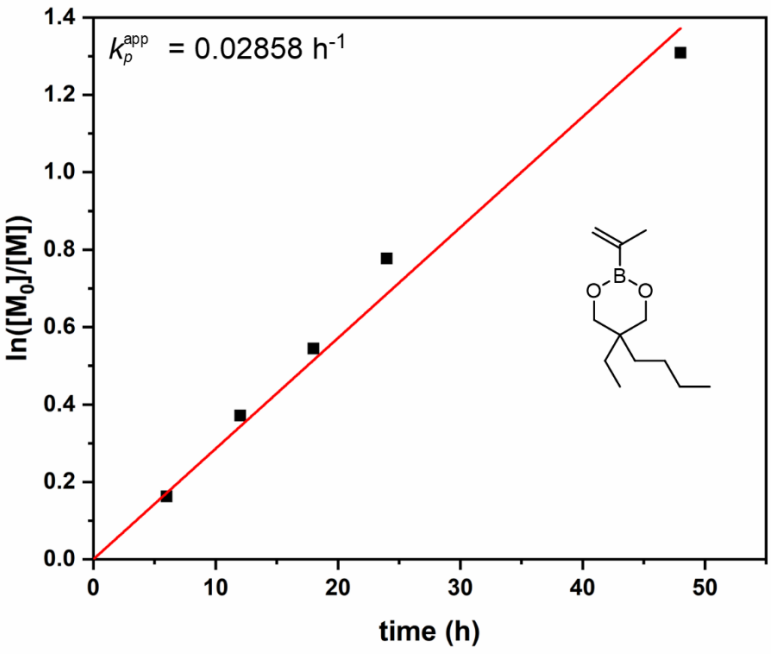


Figure S25. Semilogarithmic Kinetic Plots of RAFT Polymerization of $IB_{6\text{-}3}$.

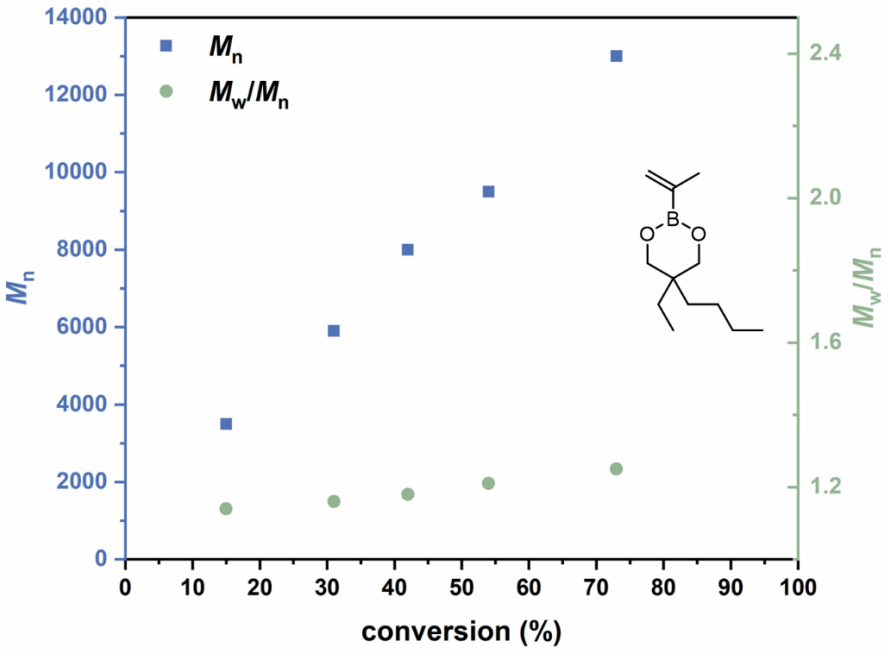


Figure S26. M_n and M_w/M_n as a Function of the $IB_{6\text{-}3}$ Conversion.

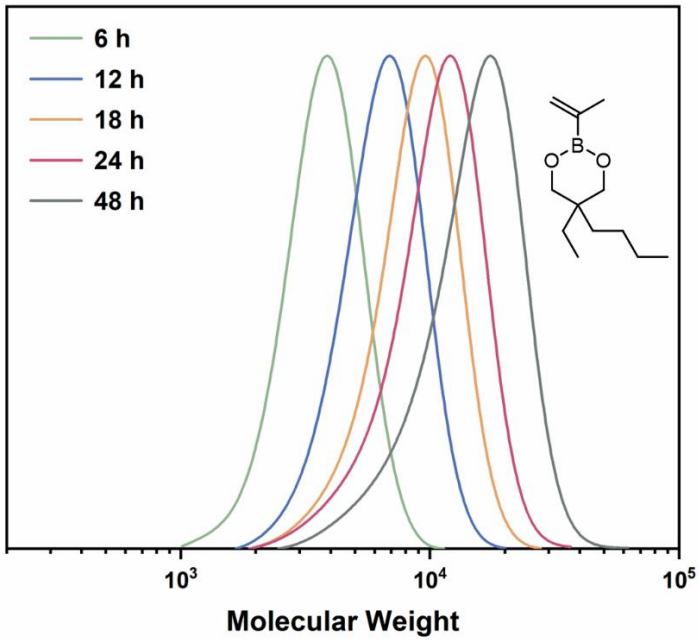


Figure S27. GPC Traces of $PIB_{6\text{-}3}$-CTA at Different Time Intervals.

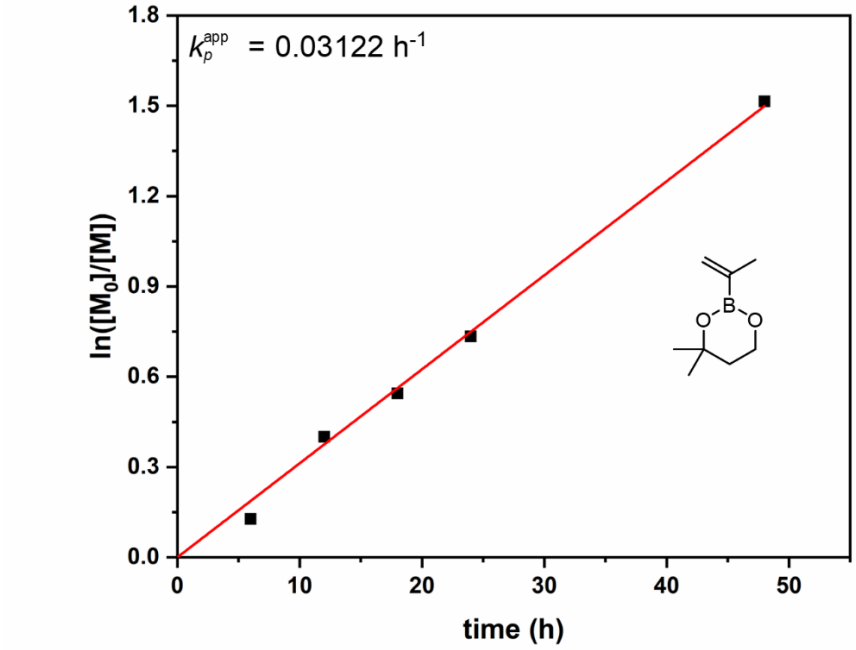


Figure S28. Semilogarithmic Kinetic Plots of RAFT Polymerization of $IB_{6\text{-}4}$.

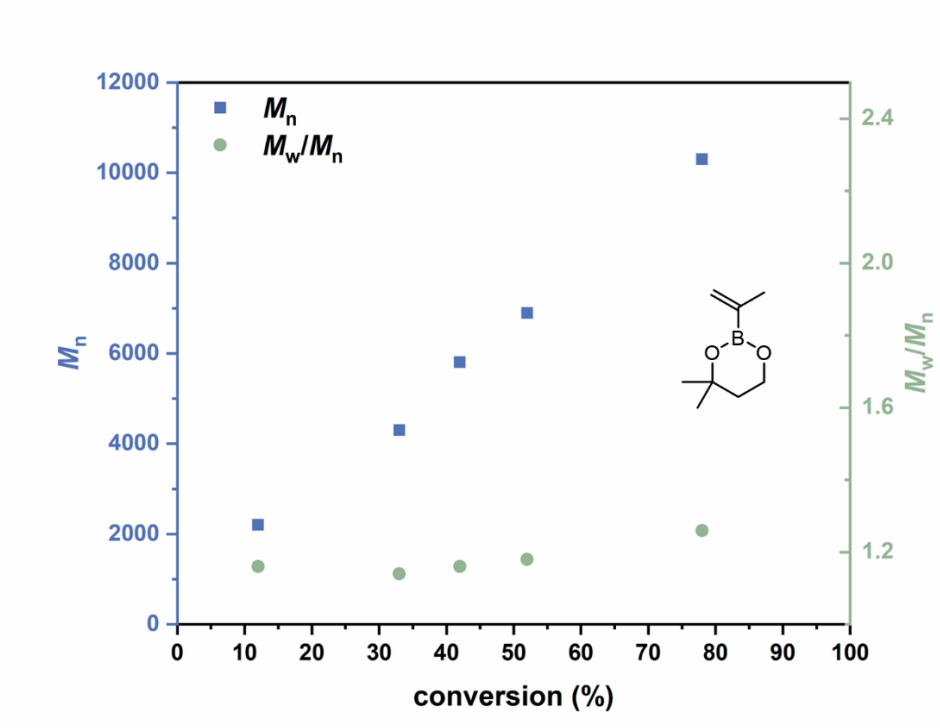


Figure S29. M_n and M_w/M_n as a Function of the $IB_{6\text{-}4}$ Conversion.

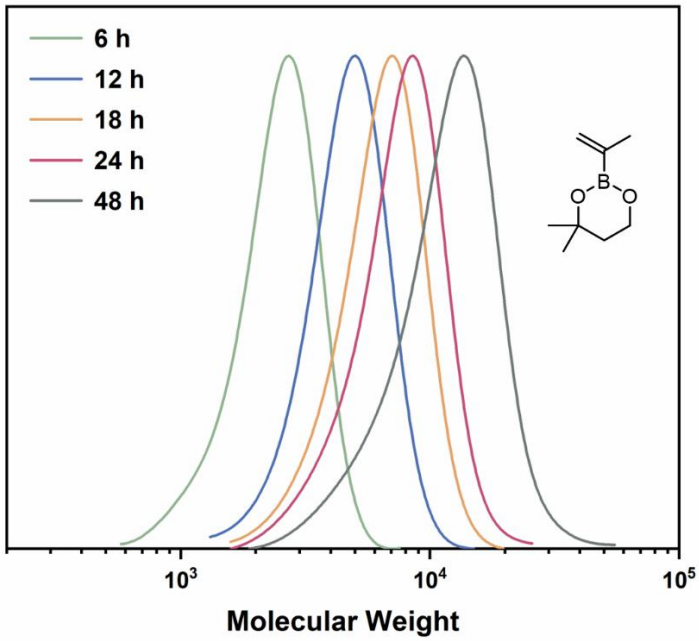


Figure S30. GPC Traces of $PIB_{6\text{-}4}$-CTA at Different Time Intervals.

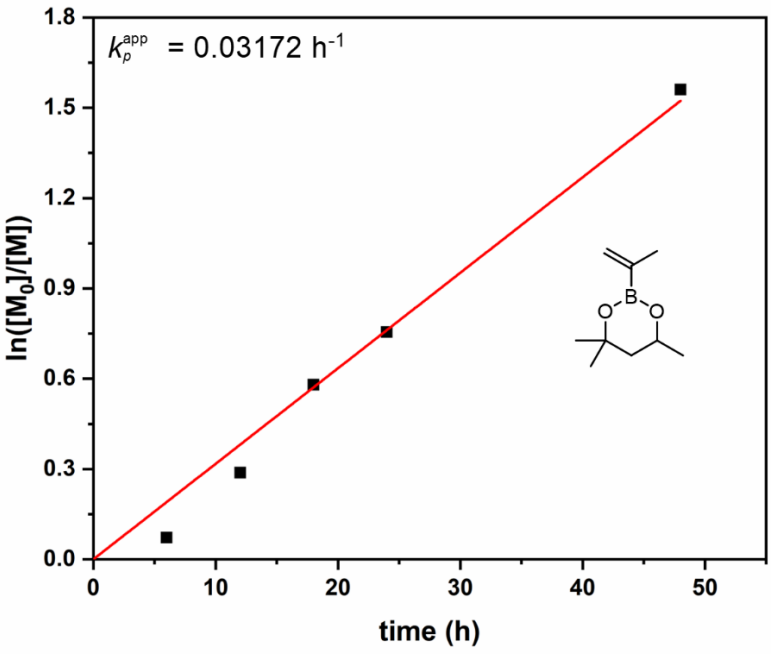


Figure S31. Semilogarithmic Kinetic Plots of RAFT Polymerization of $IB_{6\text{-}5}$.

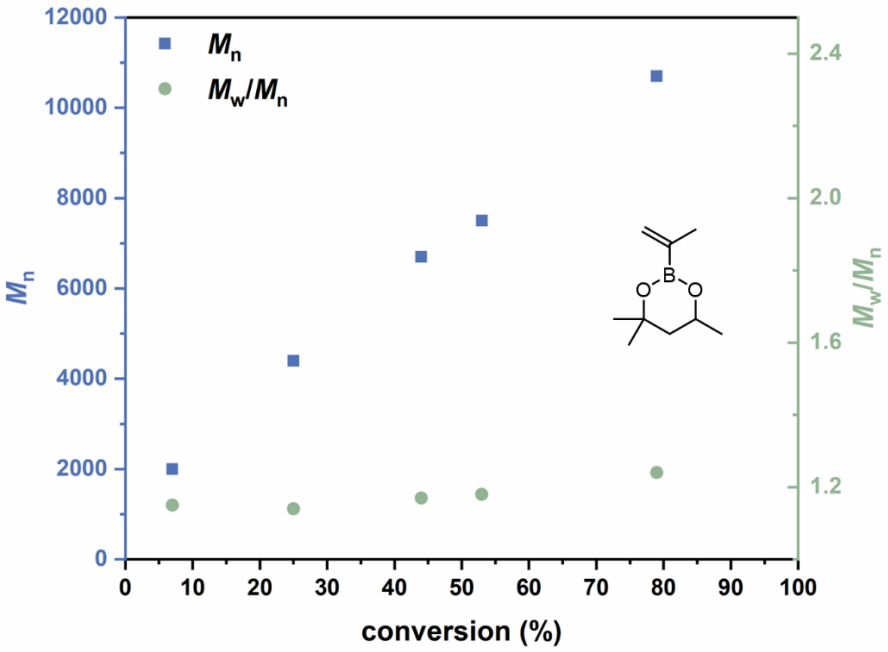


Figure S32. M_n and M_w/M_n as a Function of the $IB_{6\text{-}5}$ Conversion.

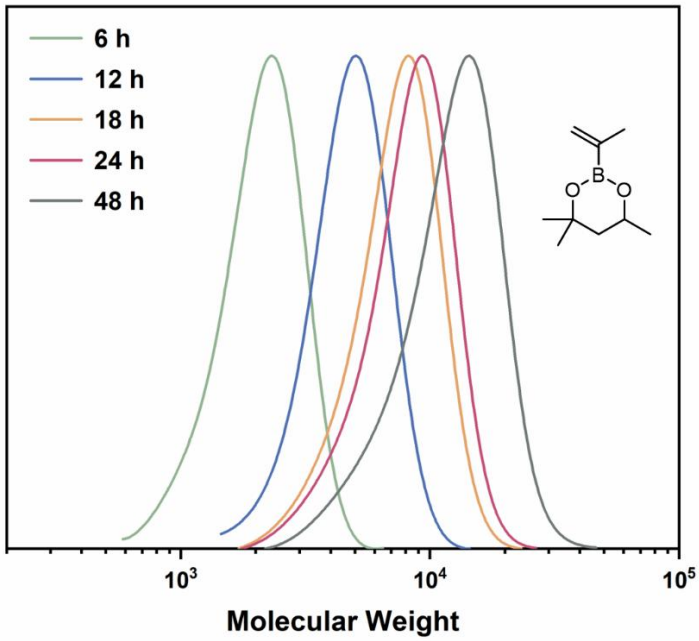


Figure S33. GPC Traces of $PIB_{6\text{-}5}$-CTA at Different Time Intervals.

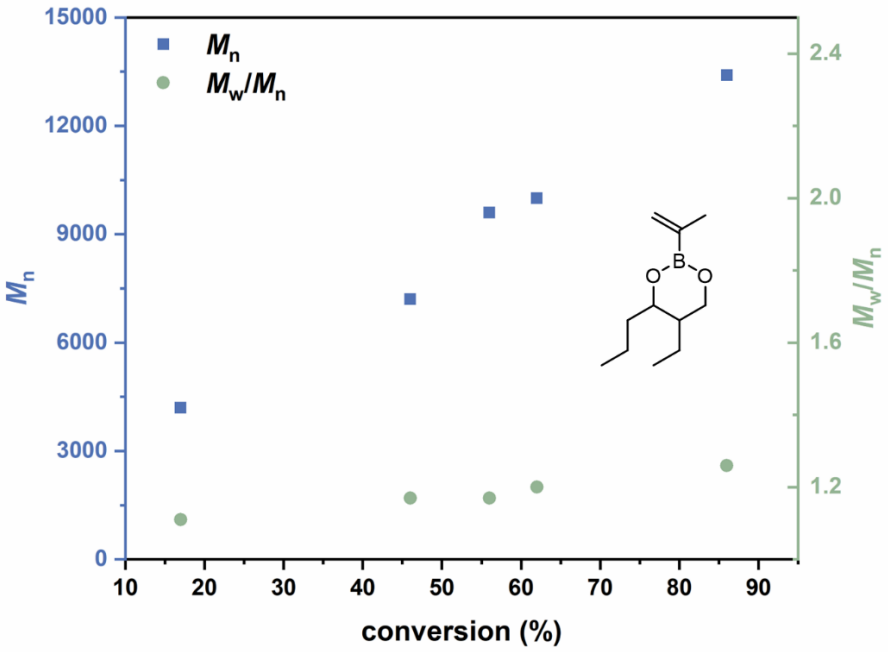


Figure S34. M_n and M_w/M_n as a Function of the $IB_{6\text{-}6}$ Conversion.

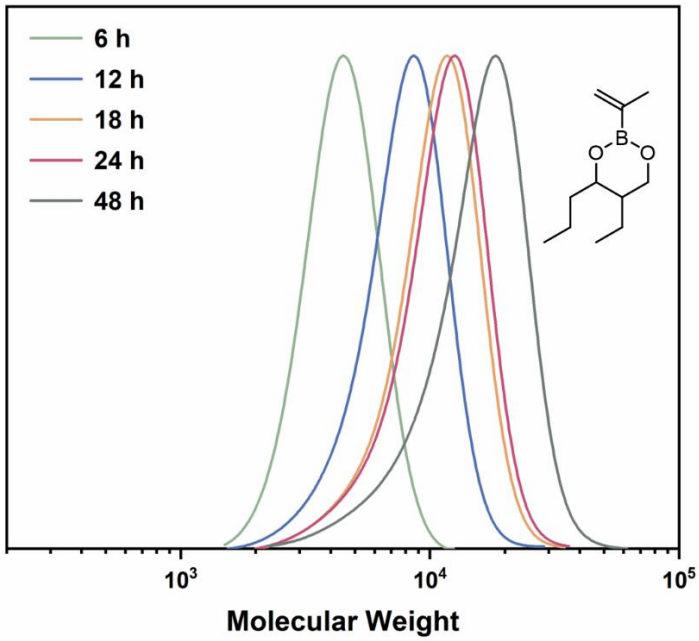


Figure S35. GPC Traces of $PIB_{6\text{-}6}$-CTA at Different Time Intervals.

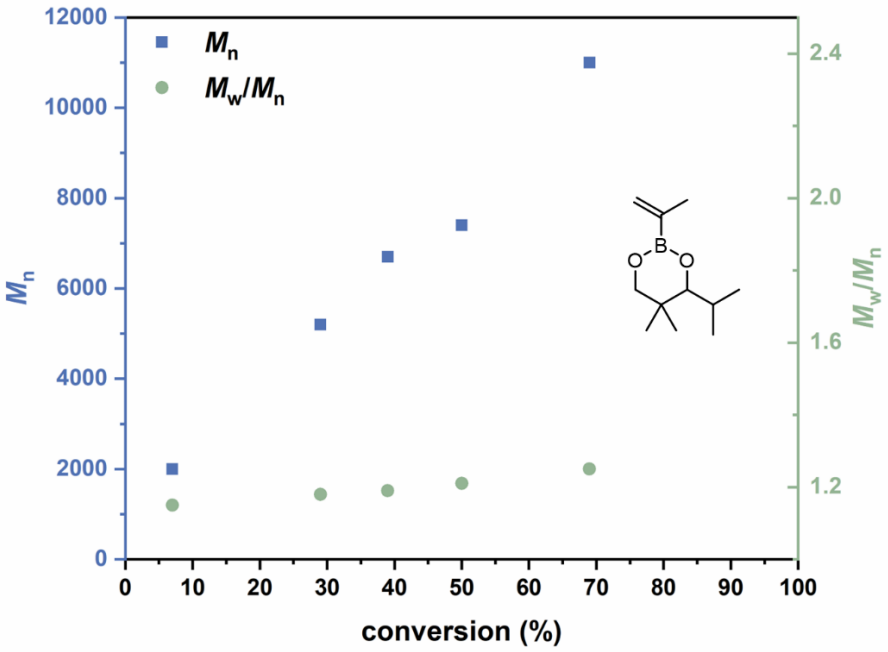


Figure S36. M_n and M_w/M_n as a Function of the $IB_{6\text{-}7}$ Conversion.

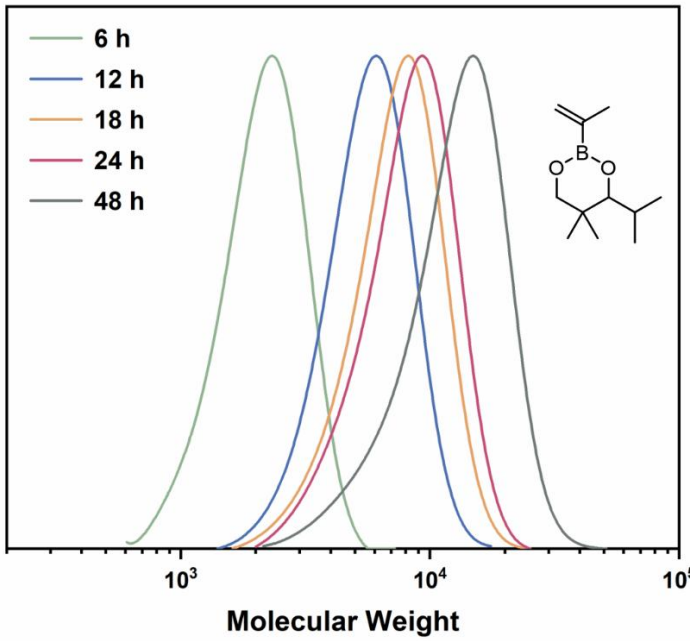


Figure S37. GPC Traces of $PIB_{6\text{-}7}$-CTA at Different Time Intervals.

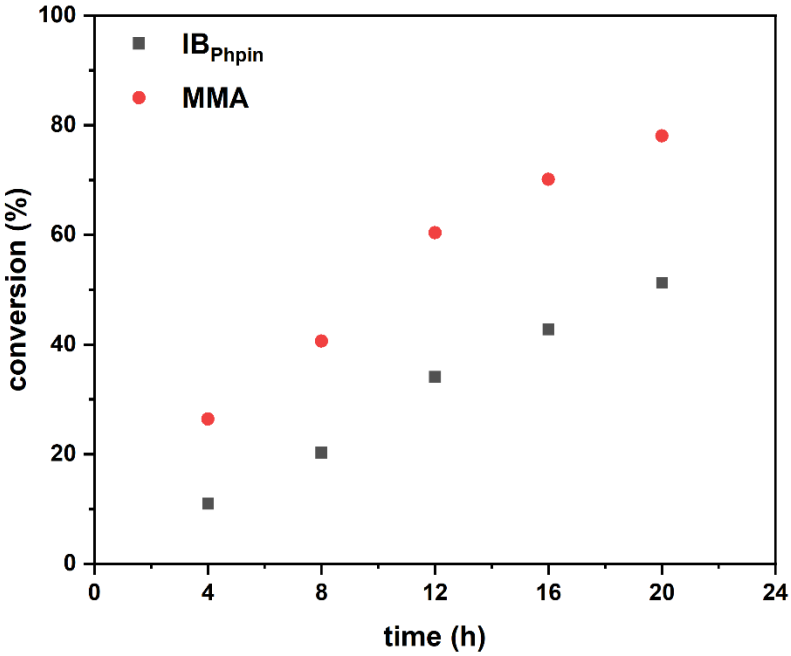


Figure S38. Conversion-Time Correlation of IB_{Phpin} and MMA in Copolymerization.

VII. Copies of Spectroscopic Data

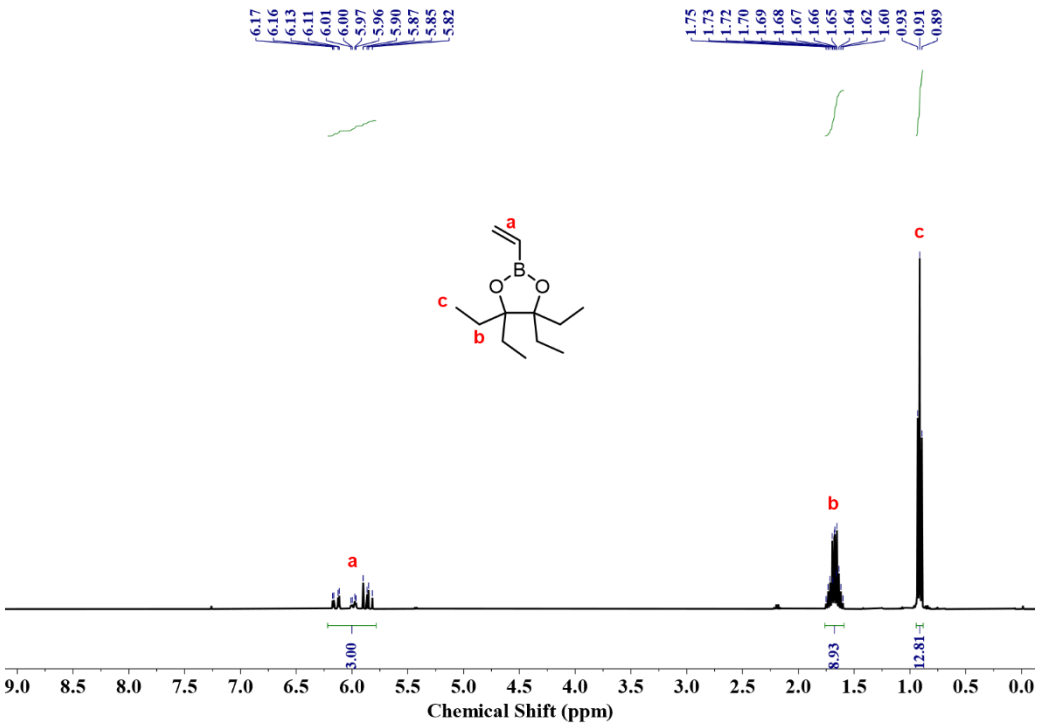


Figure S39. ^{1}H NMR Spectrum of VB_{epin} in $CDCl_3$.

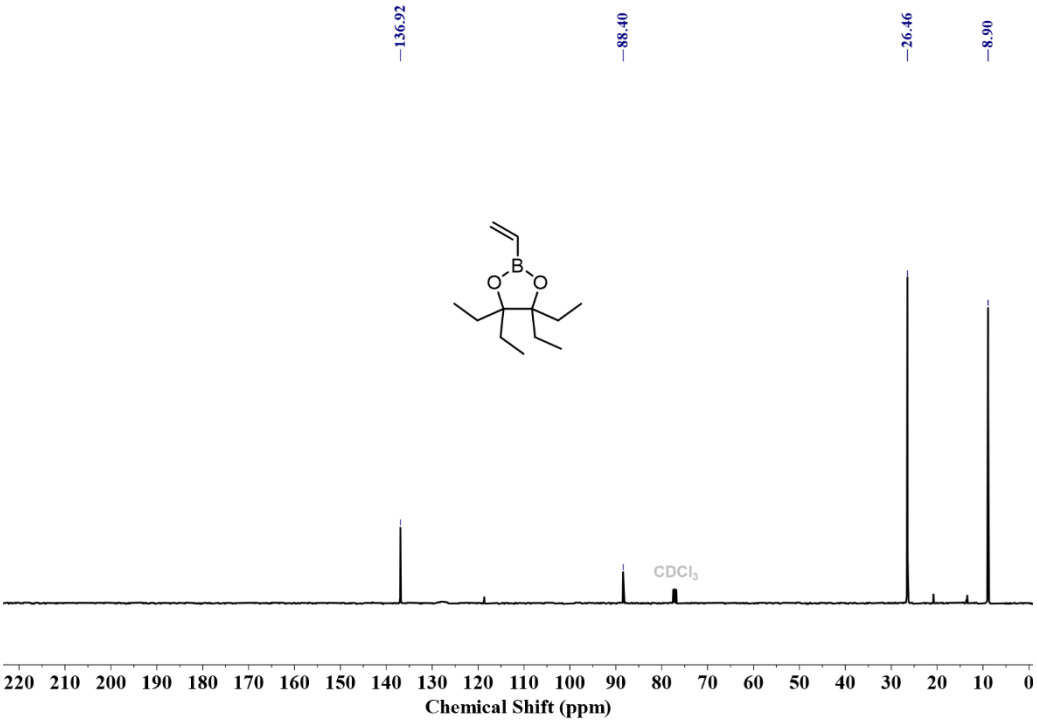


Figure S40. ^{13}C NMR Spectrum of VB_{epin} in $CDCl_3$.

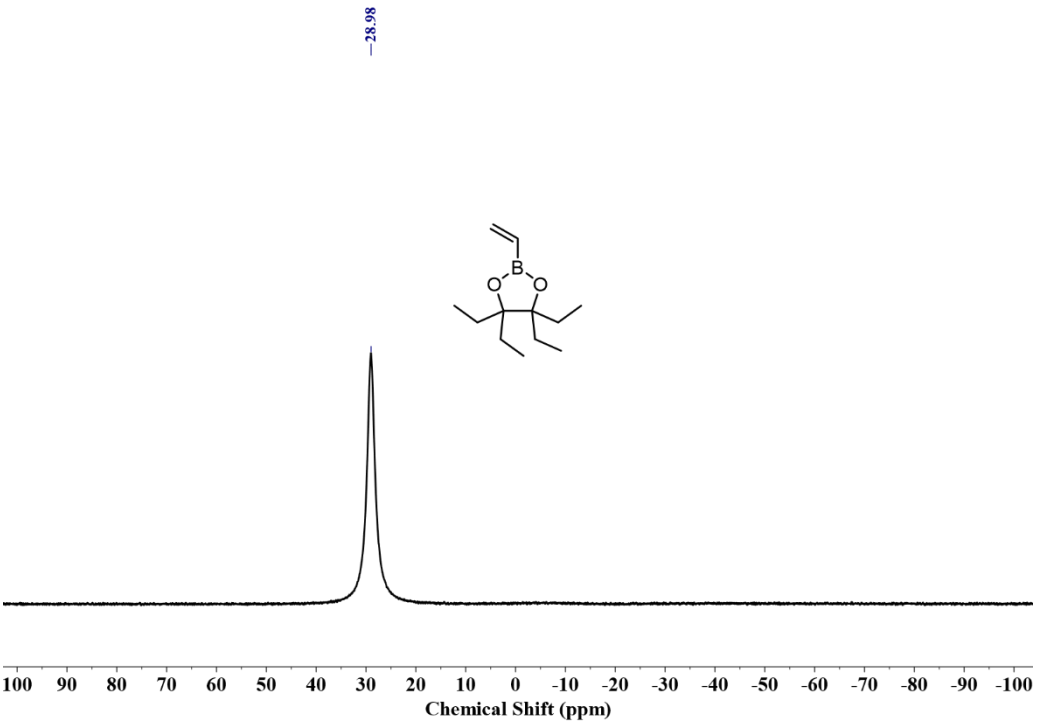


Figure S41. ^{11}B NMR Spectrum of VB_{epin} in $CDCl_3$.

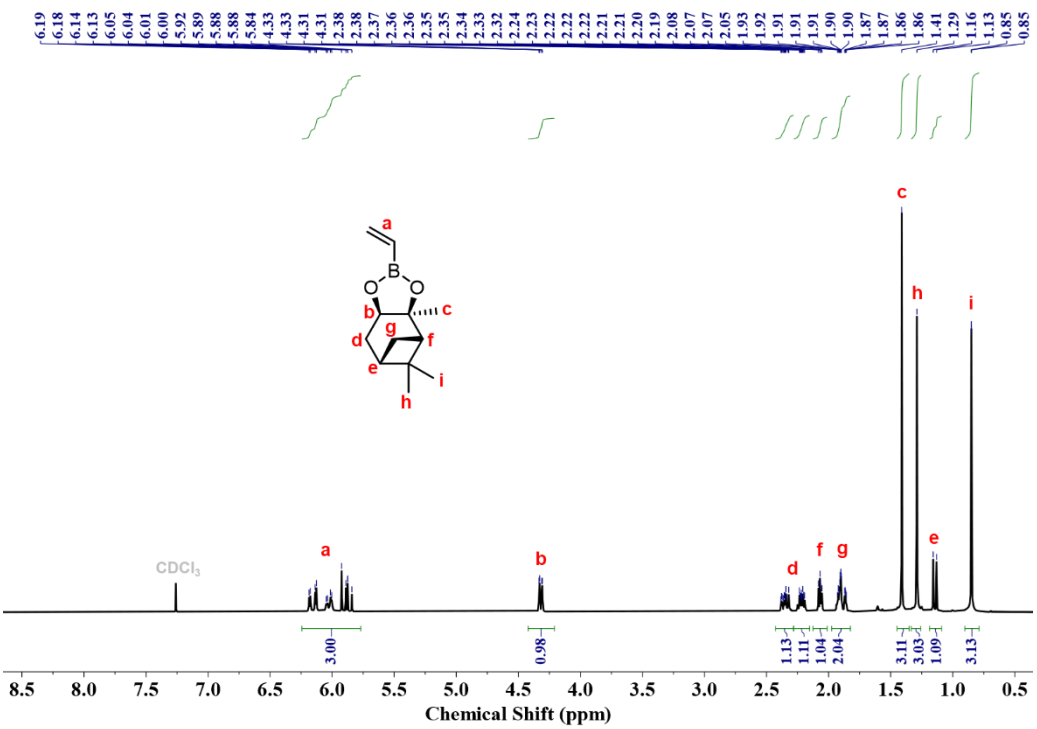


Figure S42. ^{1}H NMR Spectrum of VB_{pnd} in $CDCl_3$.

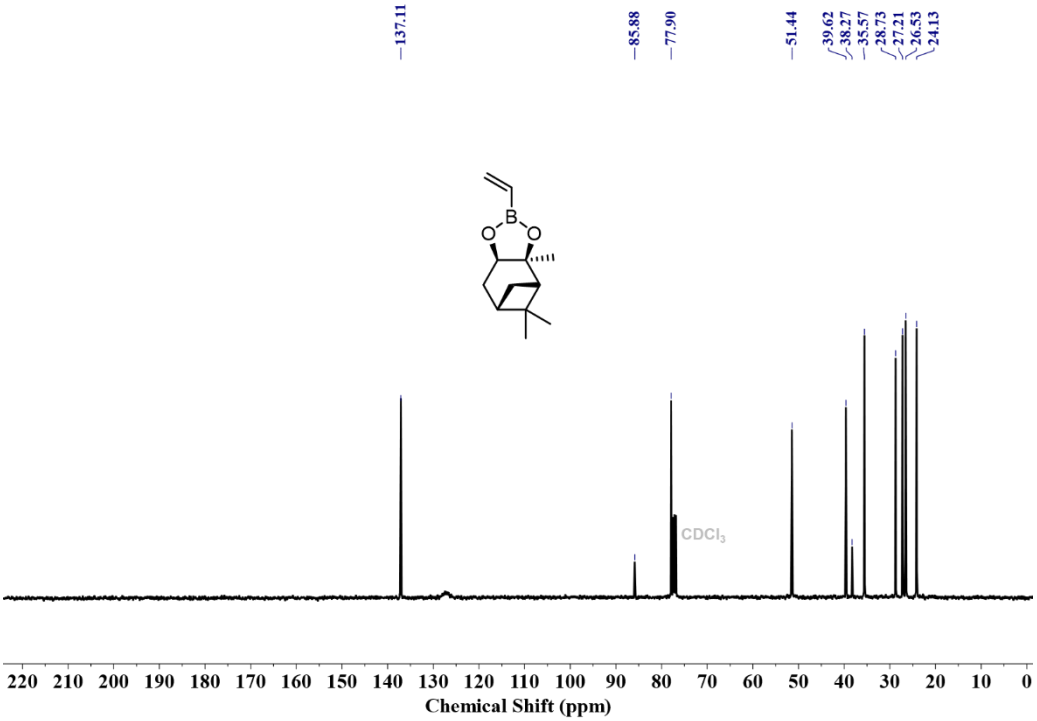


Figure S43. ^{13}C NMR Spectrum of VB_{pnd} in $CDCl_3$.

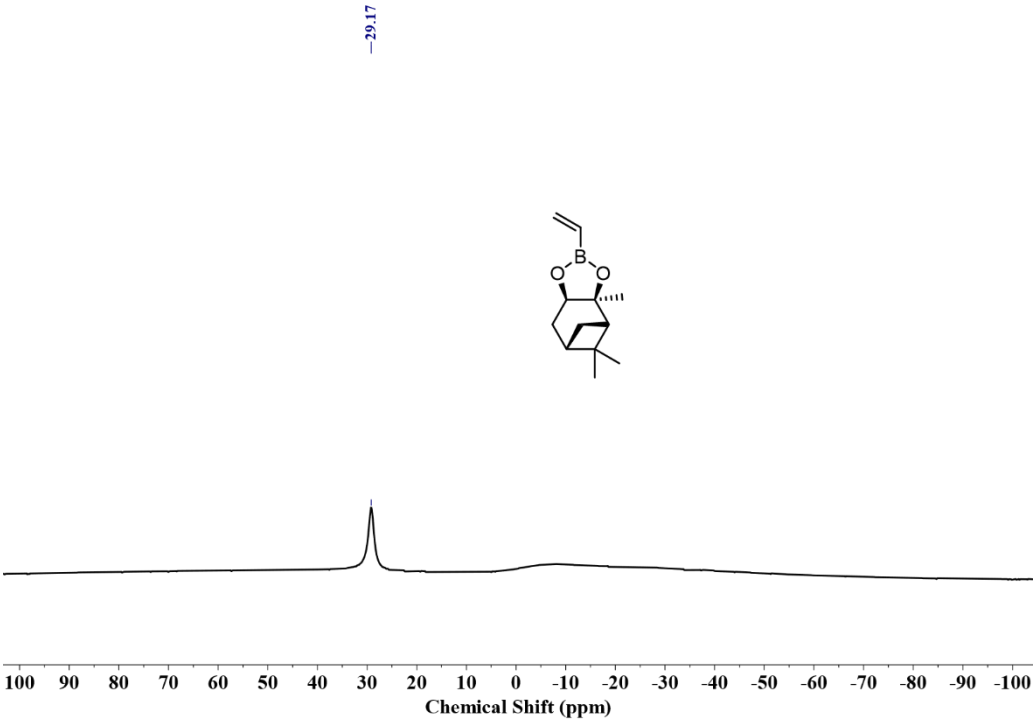


Figure S44. ^{11}B NMR Spectrum of VB_{pnd} in $CDCl_3$.

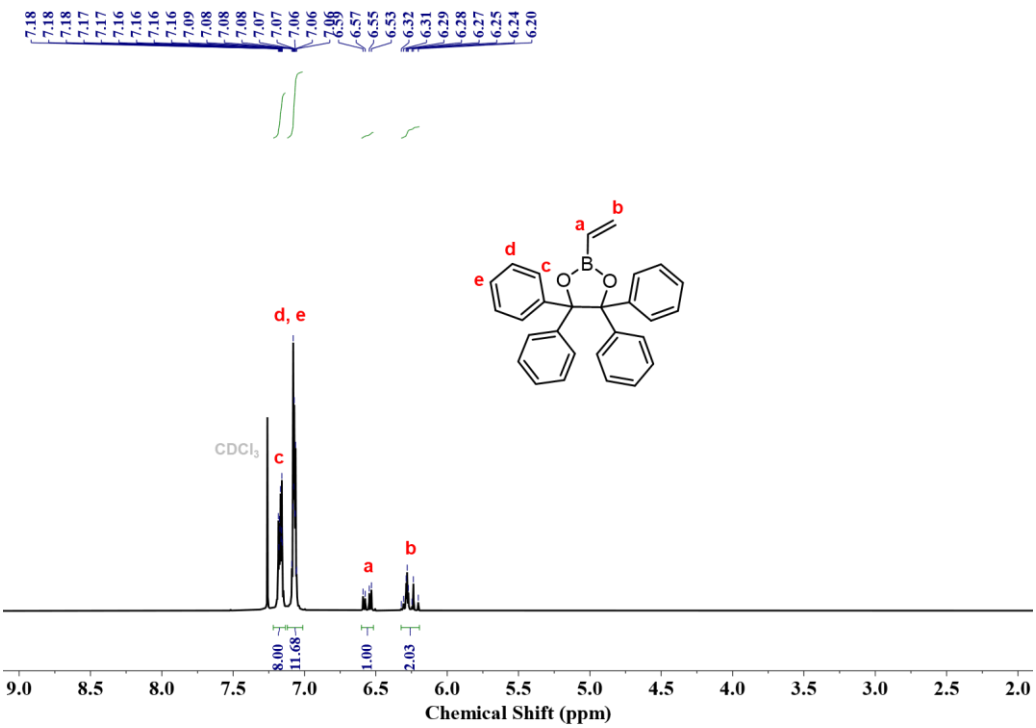


Figure S45. ^{1}H NMR Spectrum of VB_{Phpin} in $CDCl_3$.

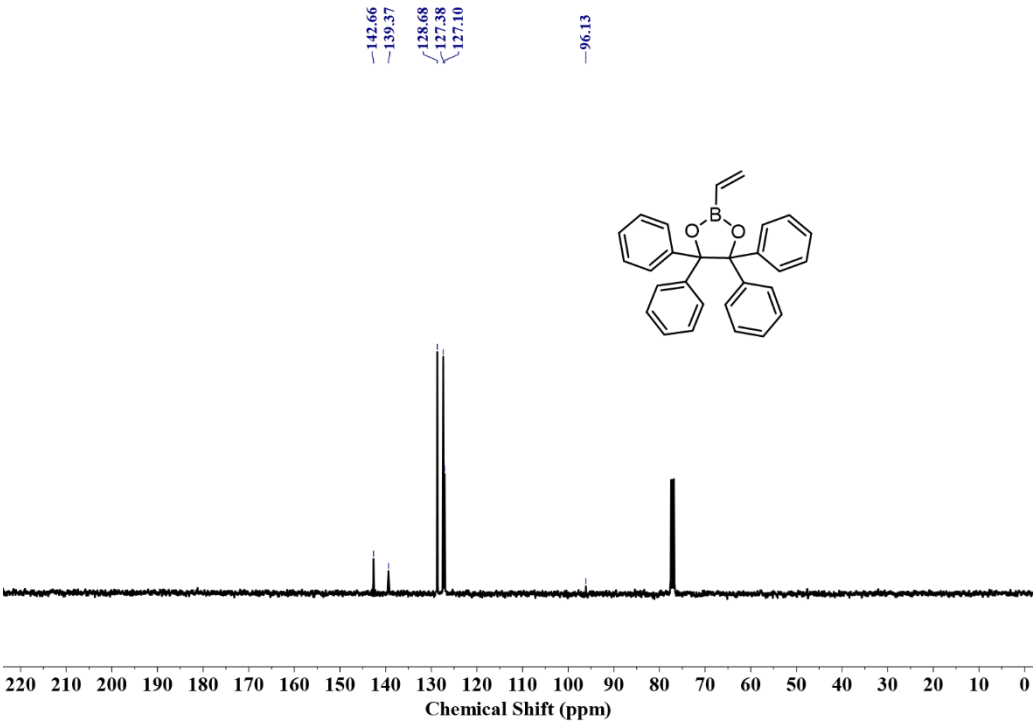


Figure S46. ^{13}C NMR Spectrum of VB_{Phpin} in $CDCl_3$.

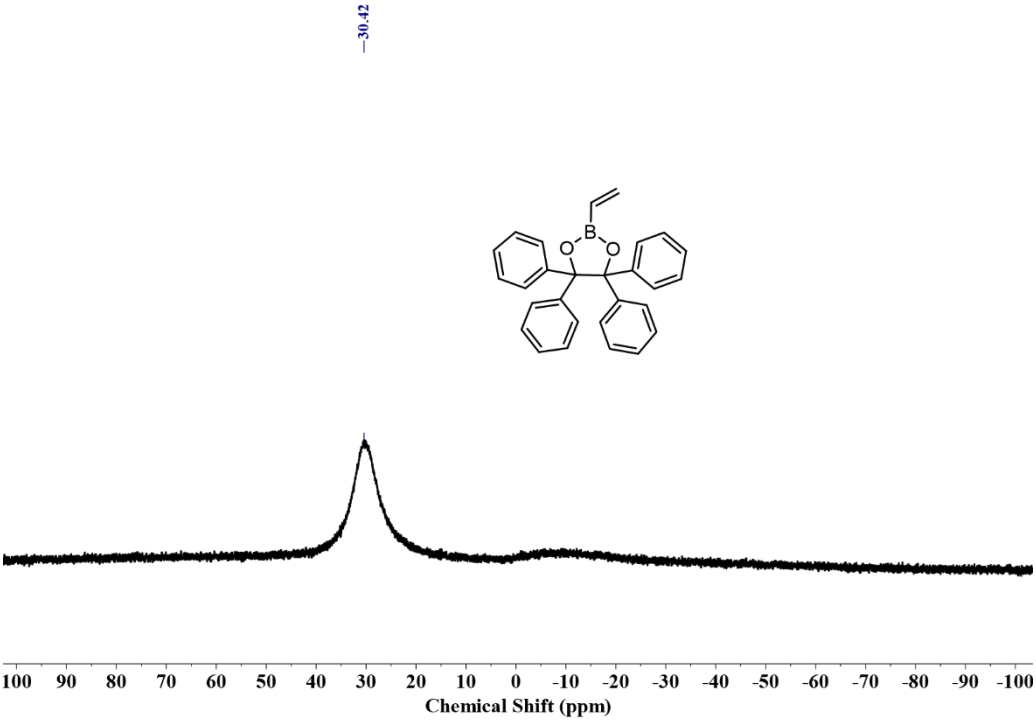


Figure S47. ^{11}B NMR Spectrum of VB_{Phpin} in $CDCl_3$.

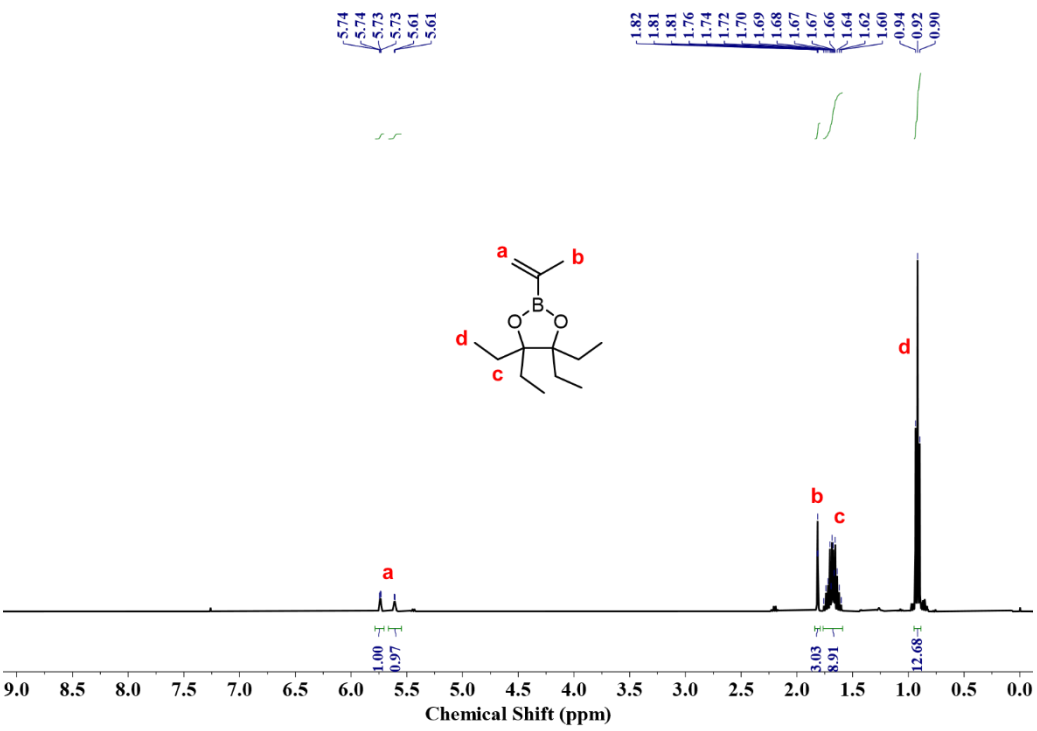


Figure S48. ^{1}H NMR Spectrum of IB_{epin} in $CDCl_3$.

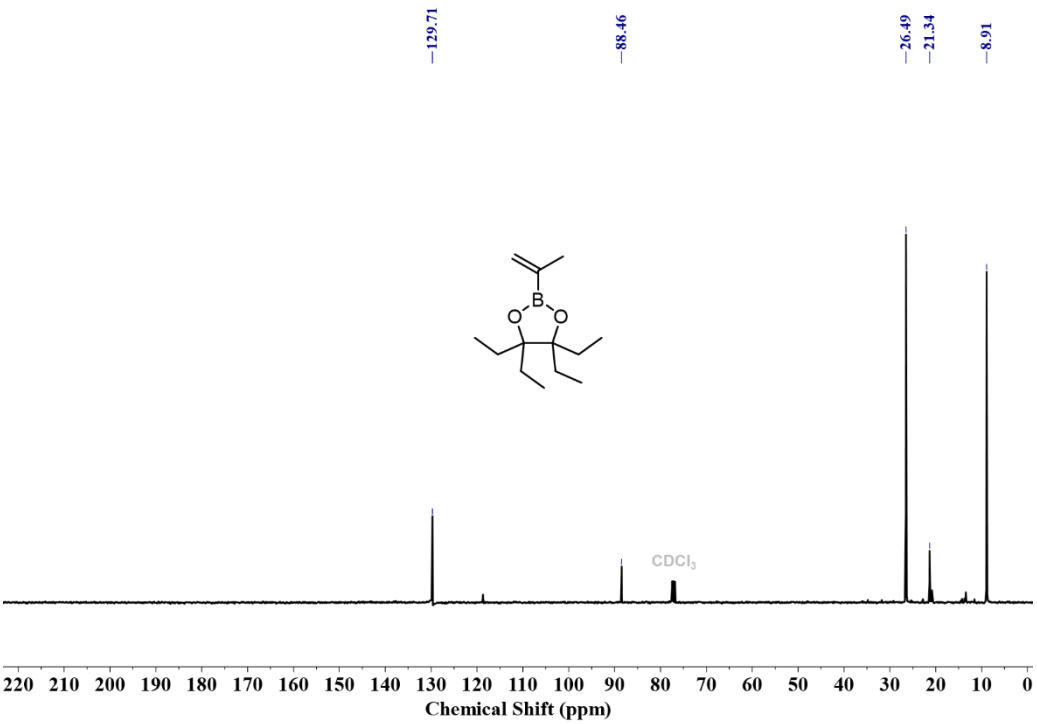


Figure S49. ^{13}C NMR Spectrum of IB_{epin} in $CDCl_3$.

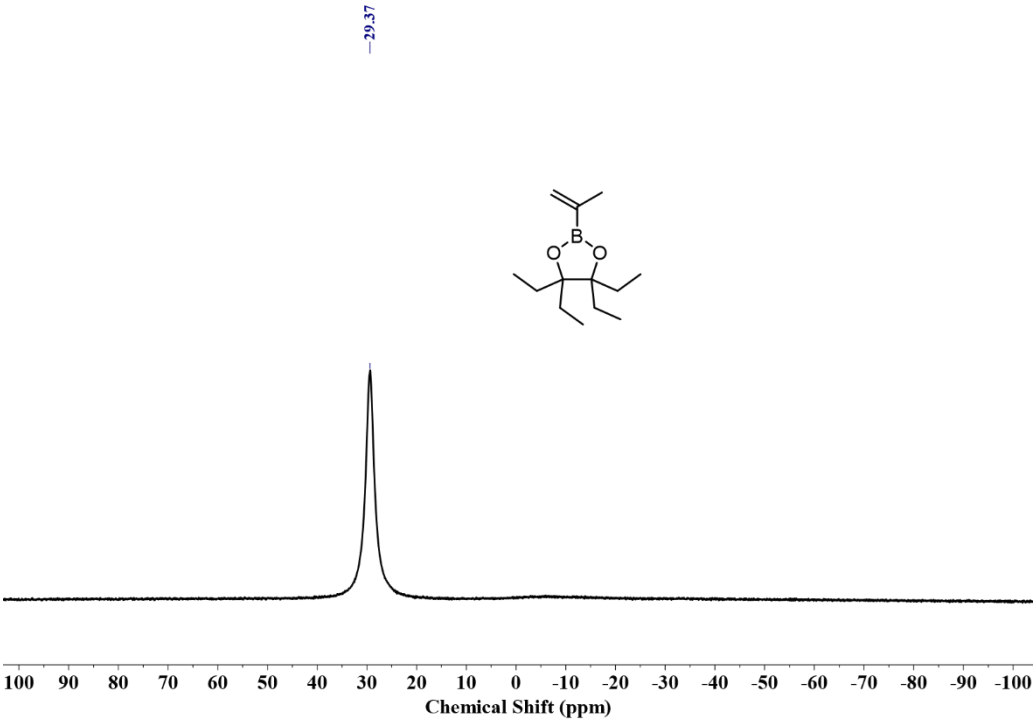


Figure S50. ^{11}B NMR Spectrum of IB_{epin} in $CDCl_3$.

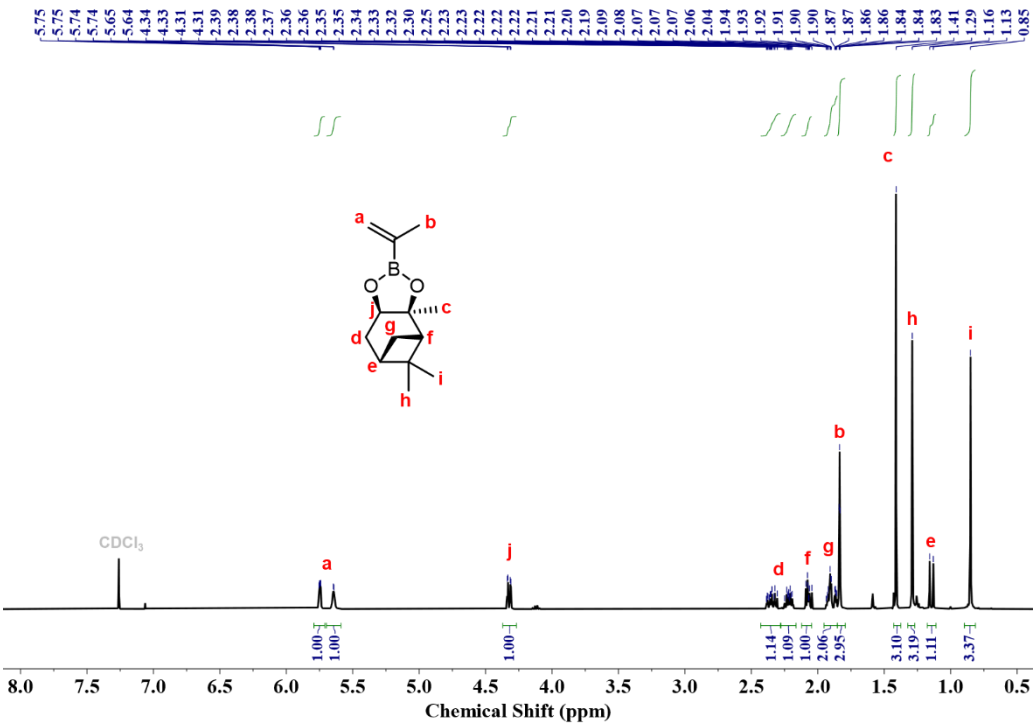


Figure S51. ^{1}H NMR Spectrum of IB_{pnd} in $CDCl_3$.

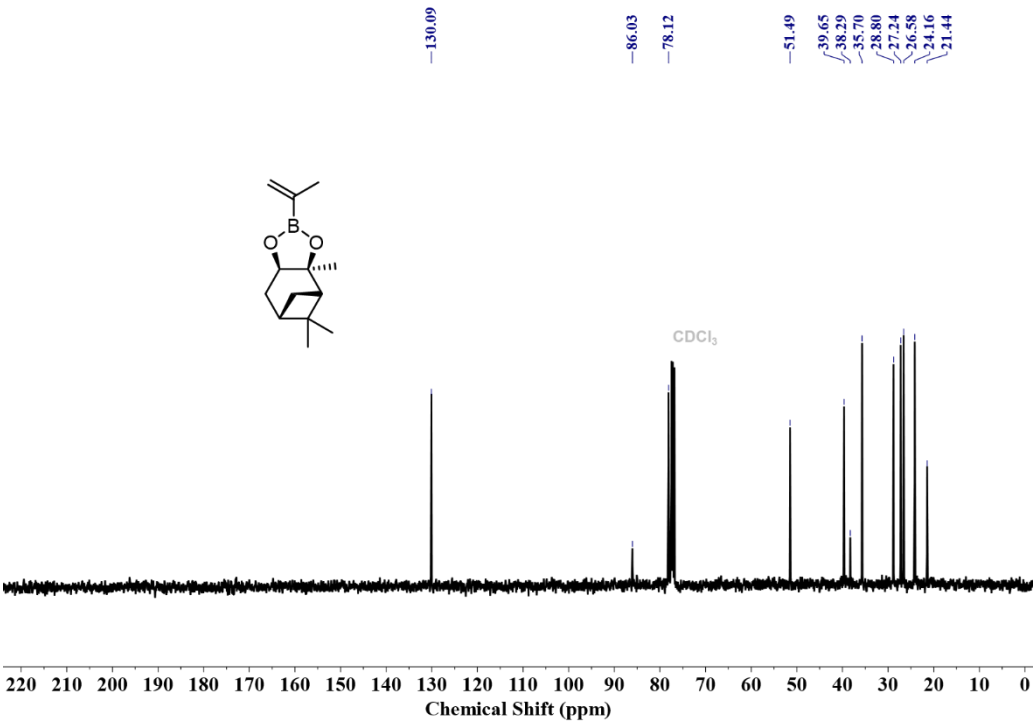


Figure S52. ^{13}C NMR Spectrum of IB_{pnd} in $CDCl_3$.

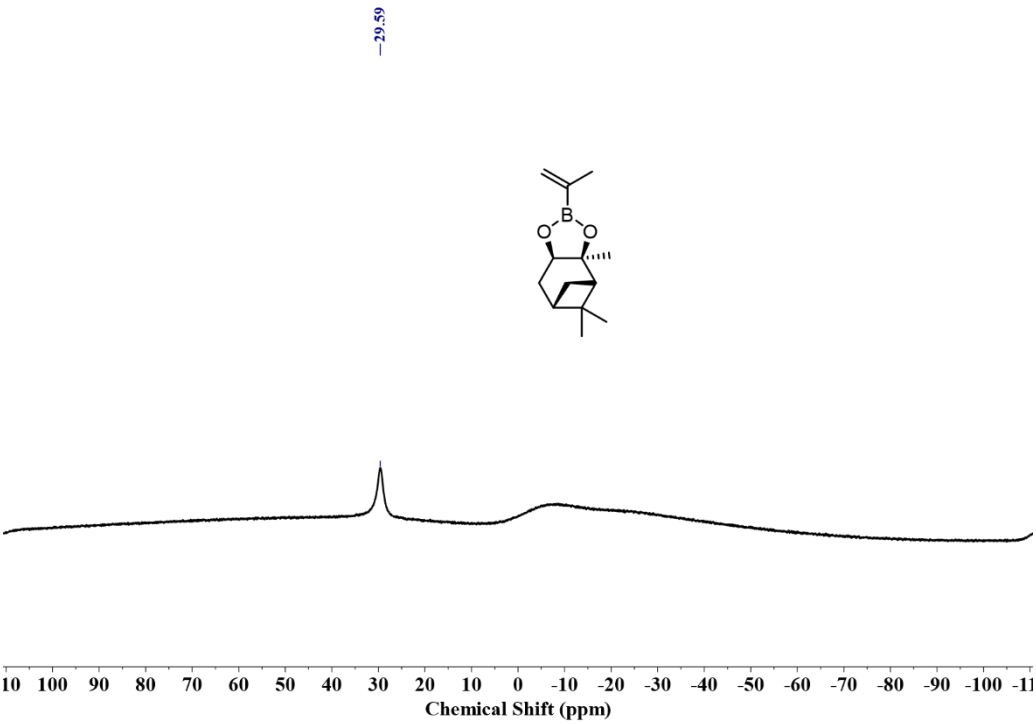


Figure S53. ^{11}B NMR Spectrum of IB_{pnd} in $CDCl_3$.

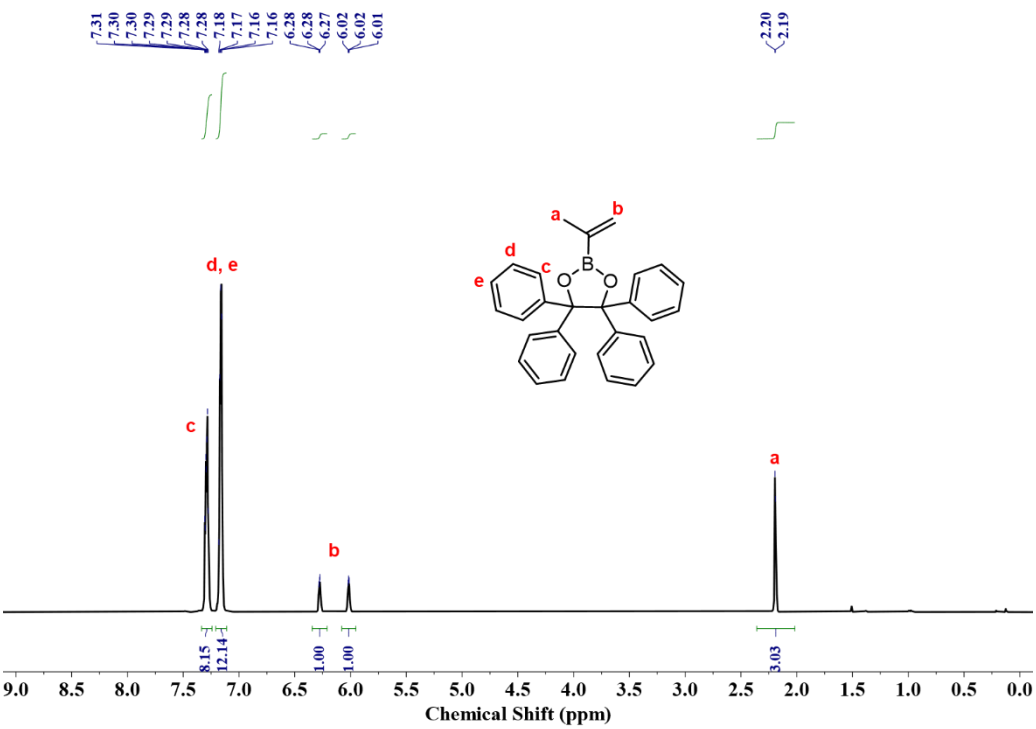


Figure S54. ^{1}H NMR Spectrum of IB_{Phpin} in $CDCl_3$.

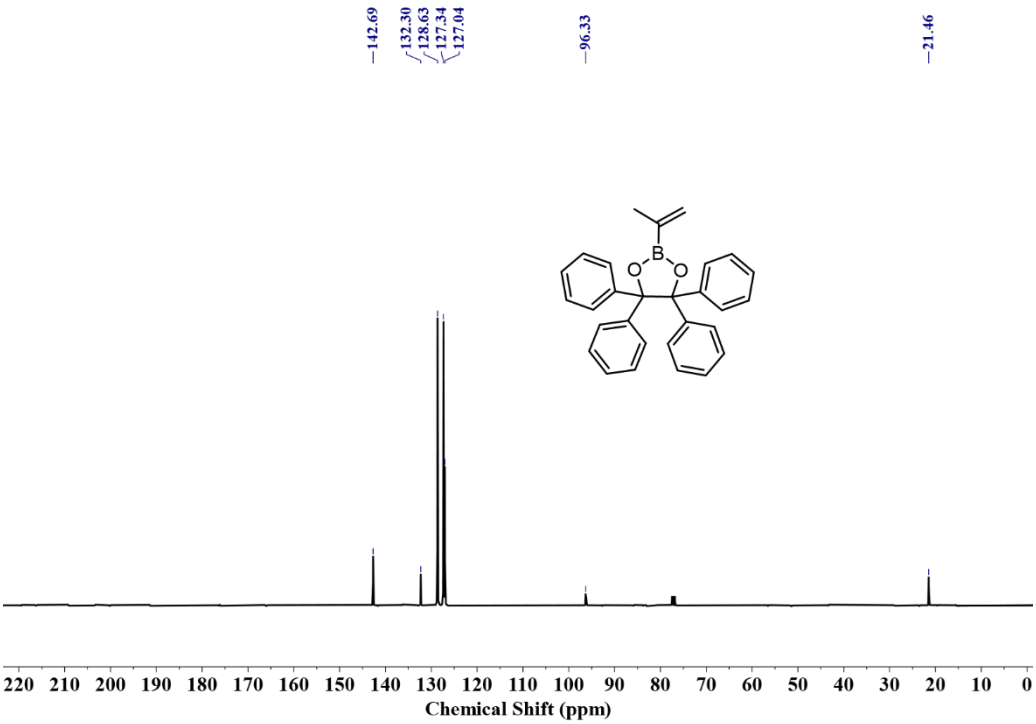


Figure S55. ^{13}C NMR Spectrum of IB_{Phpin} in $CDCl_3$.

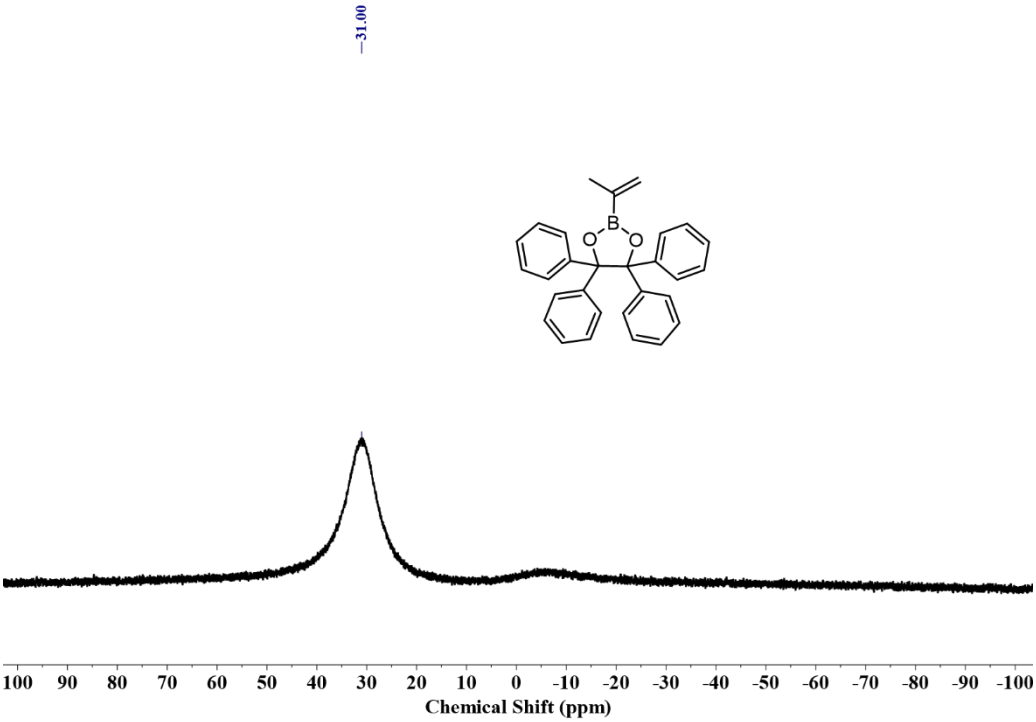


Figure S56. ^{11}B NMR Spectrum of IB_{Phpin} in $CDCl_3$.

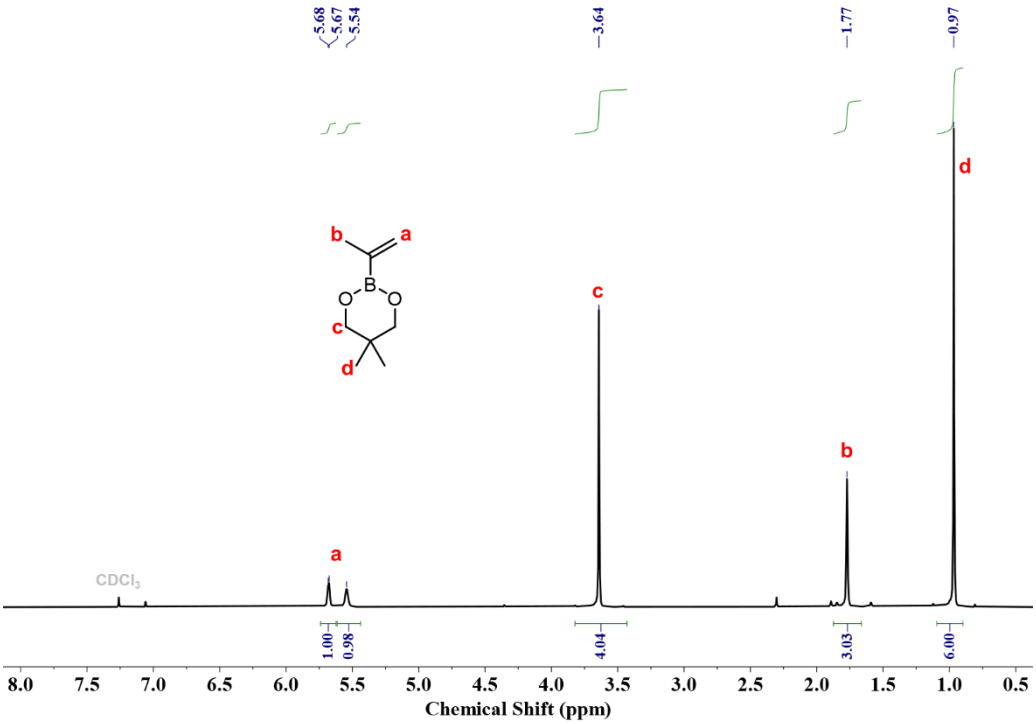


Figure S57. ^{1}H NMR Spectrum of $IB_{6\text{-}1}$ in $CDCl_3$.

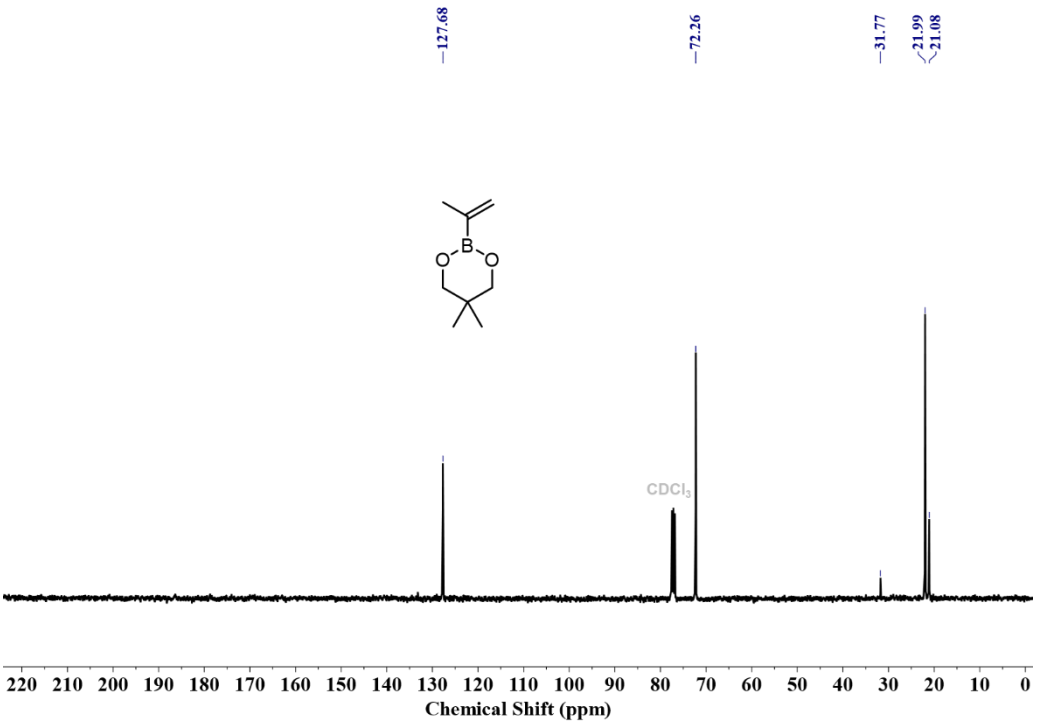


Figure S58. ^{13}C NMR Spectrum of $IB_{6\text{-}1}$ in $CDCl_3$.

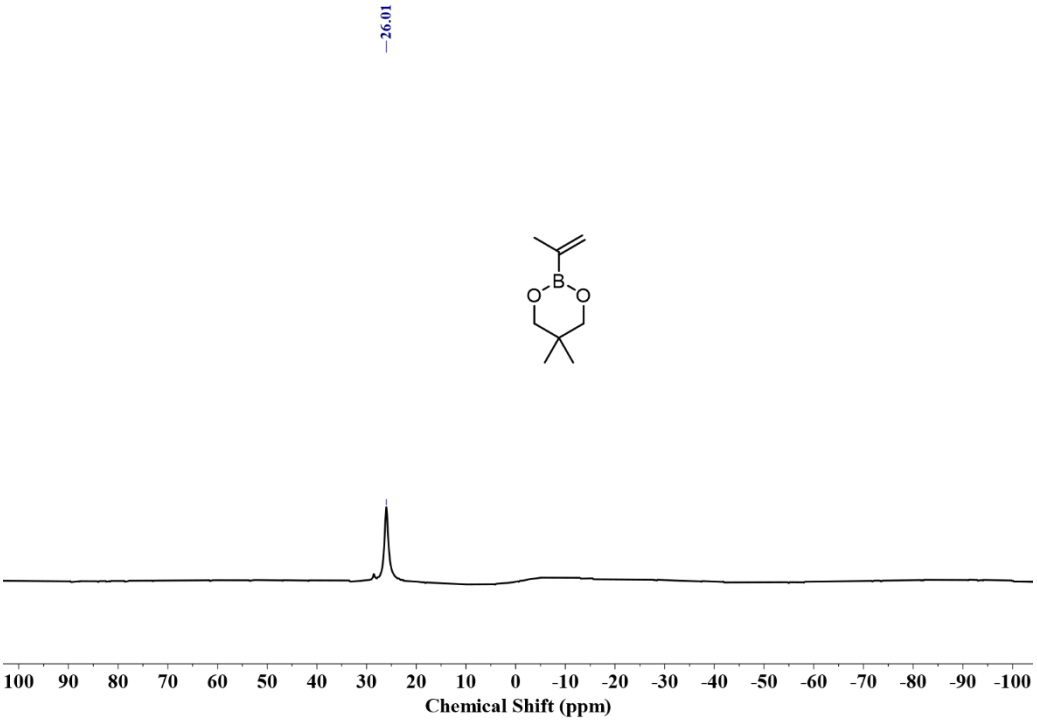


Figure S59. ^{11}B NMR Spectrum of $IB_{6\text{-}1}$ in $CDCl_3$.

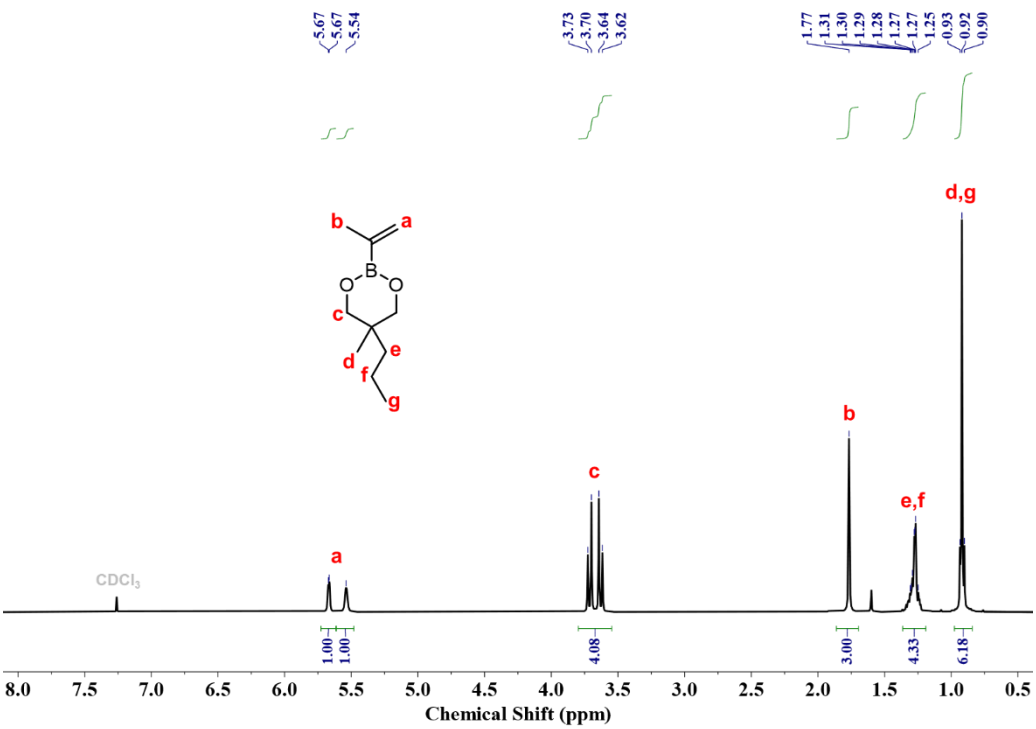


Figure S60. ^{1}H NMR Spectrum of $IB_{6\text{-}2}$ in $CDCl_3$.

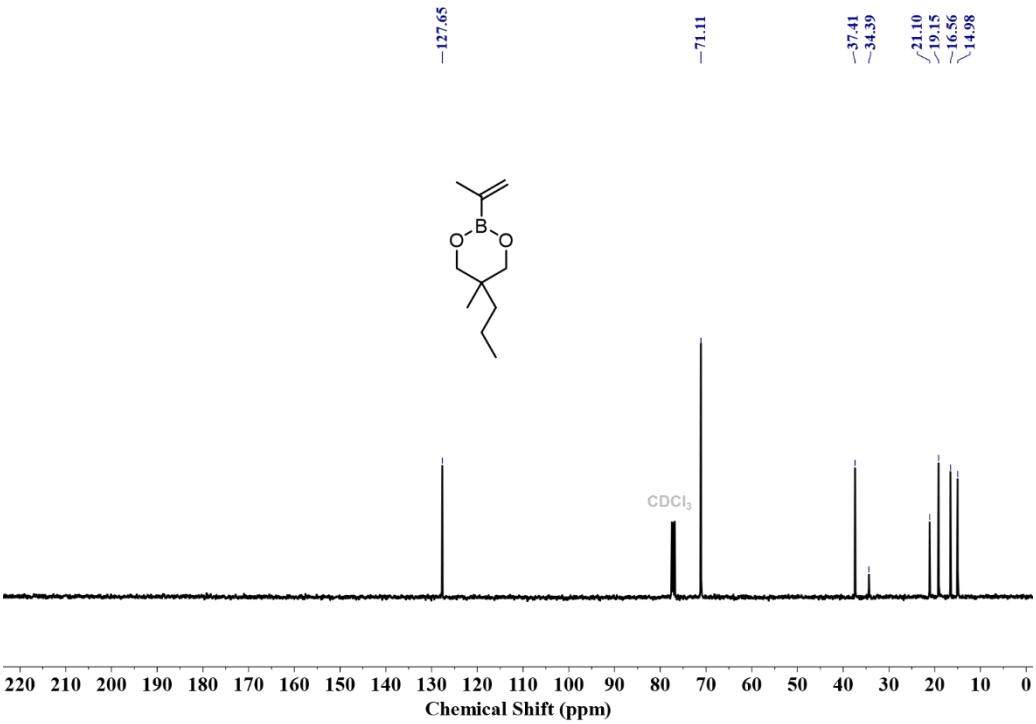


Figure S61. ^{13}C NMR Spectrum of $IB_{6\text{-}2}$ in $CDCl_3$.

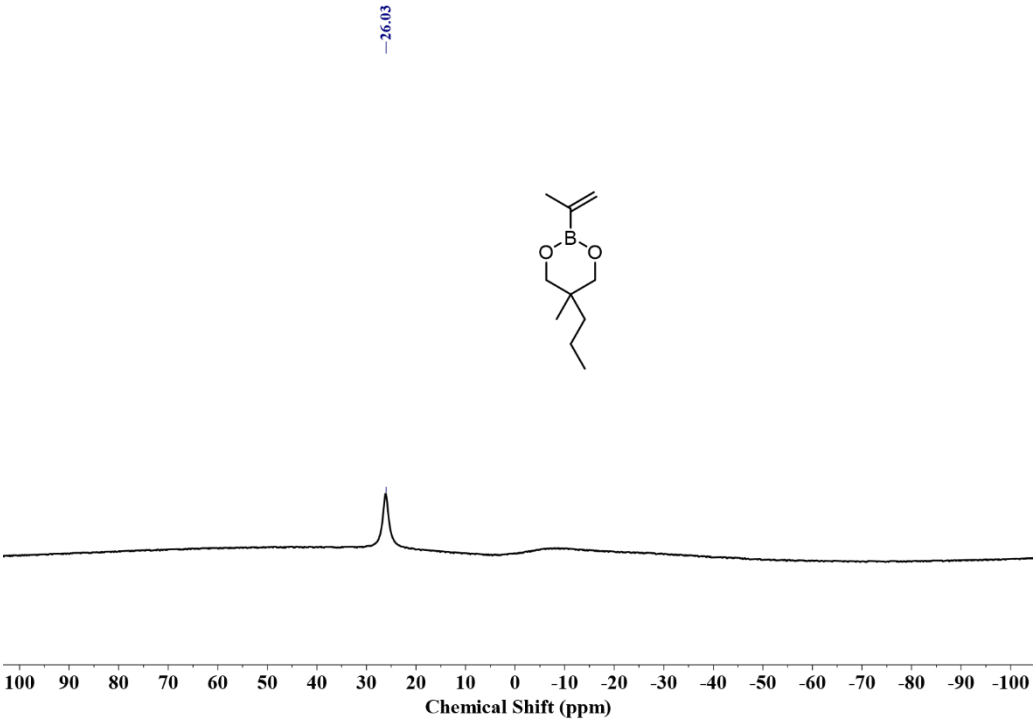


Figure S62. ^{11}B NMR Spectrum of $IB_{6\text{-}2}$ in $CDCl_3$.

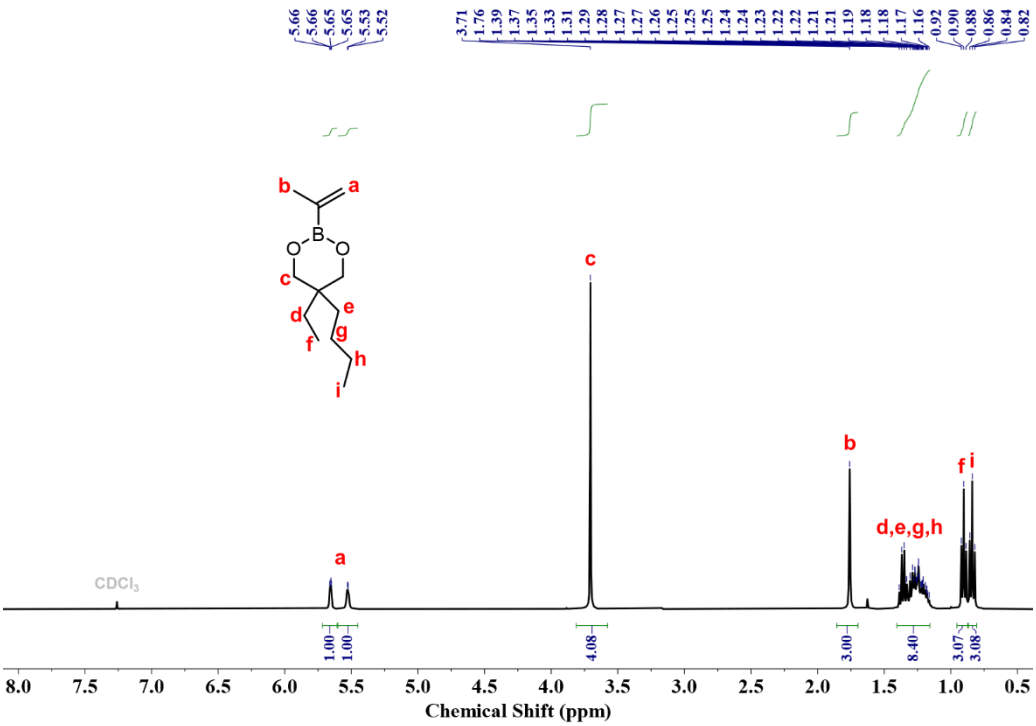


Figure S63. ^{1}H NMR Spectrum of $IB_{6\text{-}3}$ in $CDCl_3$.

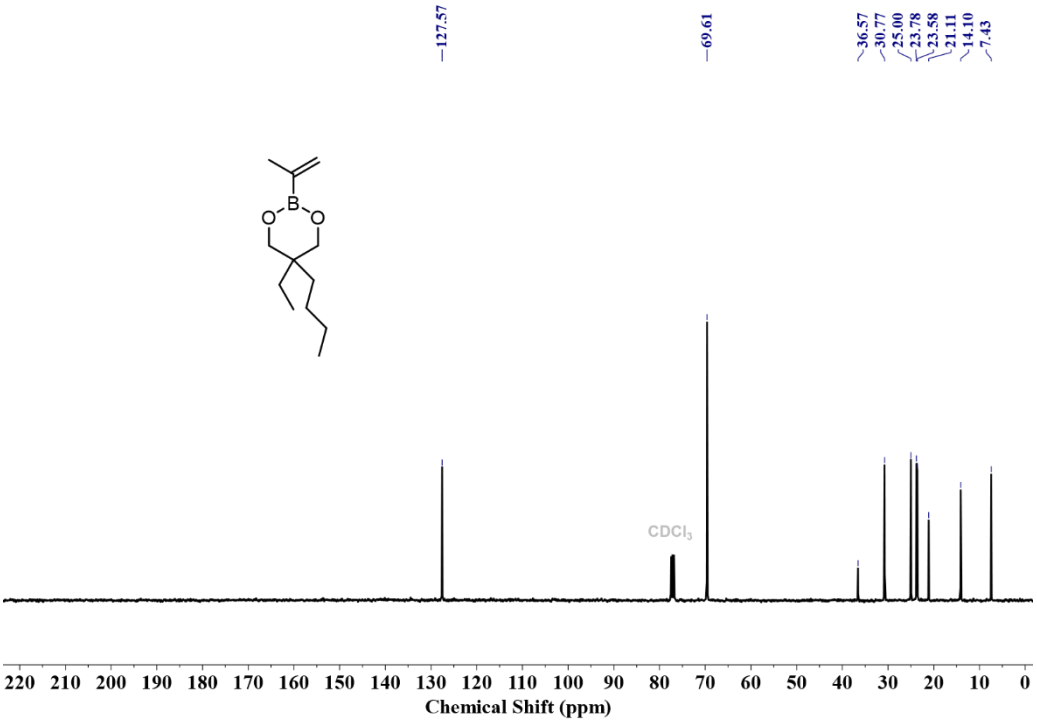


Figure S64. ^{13}C NMR Spectrum of $IB_{6\text{-}3}$ in $CDCl_3$.

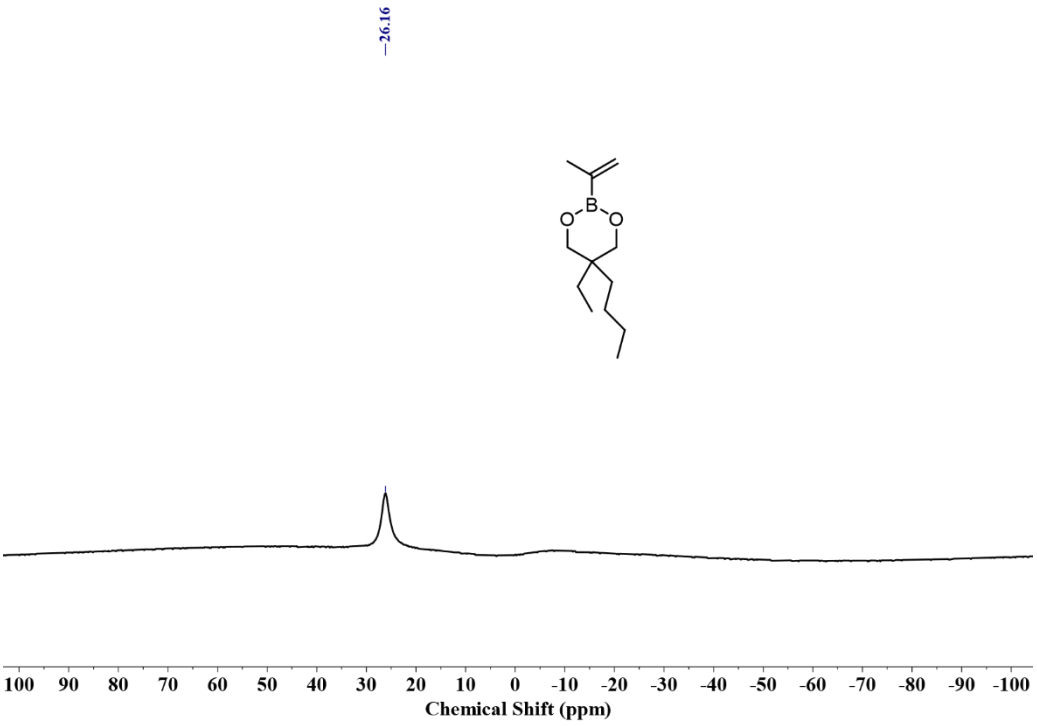


Figure S65. ^{11}B NMR Spectrum of $IB_{6\text{-}3}$ in $CDCl_3$.

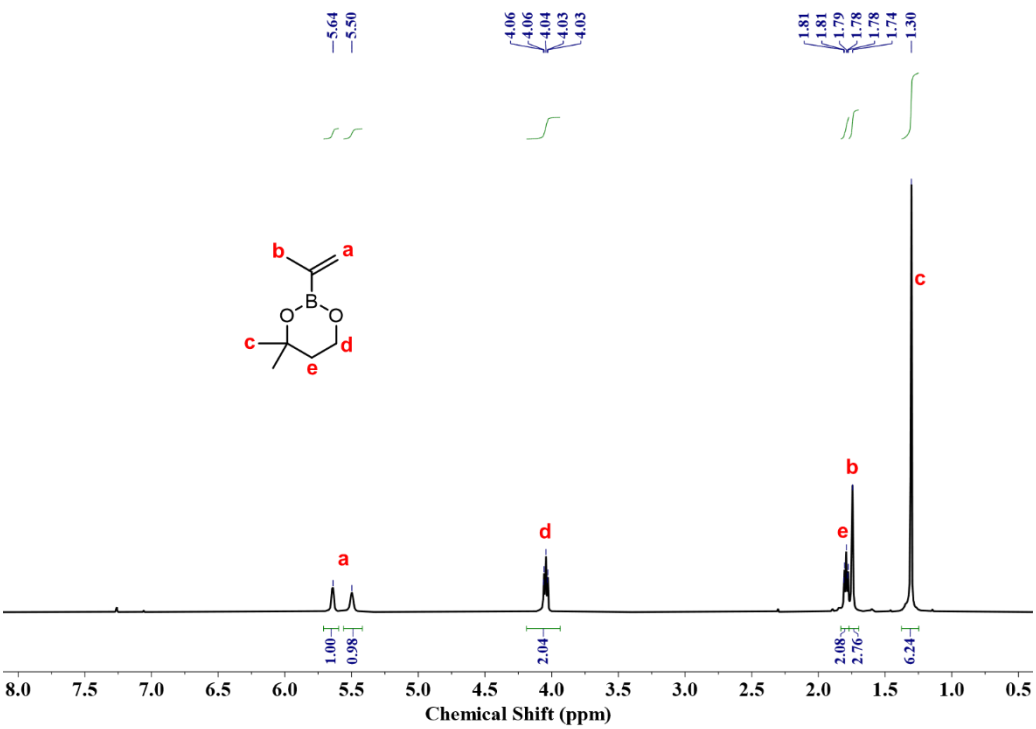


Figure S66. ^{1}H NMR Spectrum of $IB_{6\text{-}4}$ in $CDCl_3$.

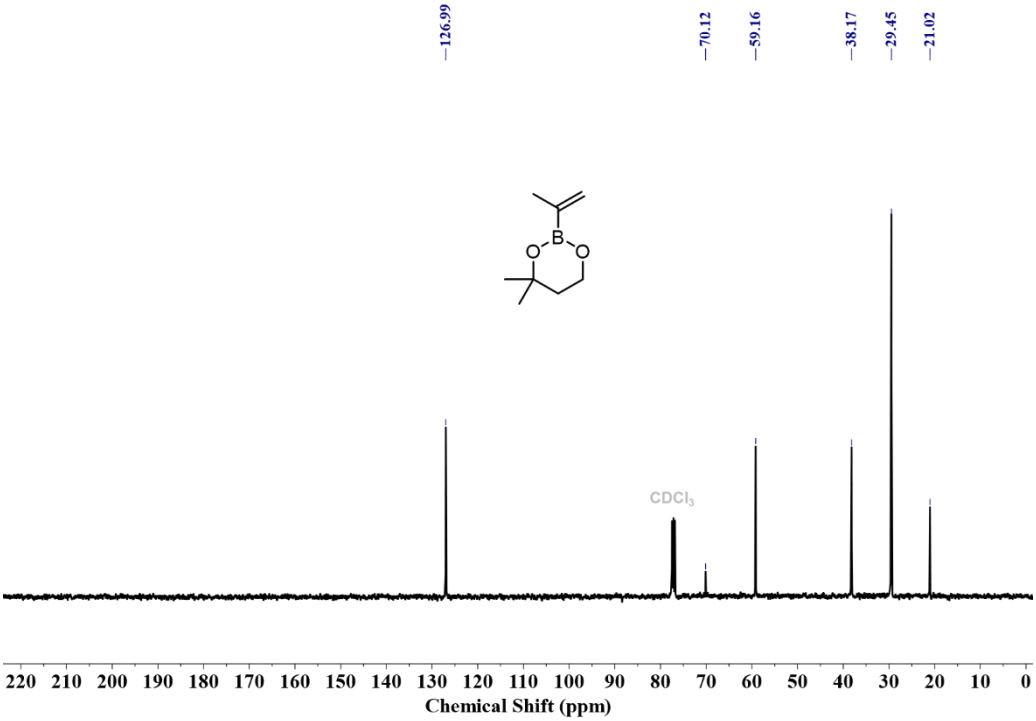


Figure S67. ^{13}C NMR Spectrum of $IB_{6\text{-}4}$ in $CDCl_3$.

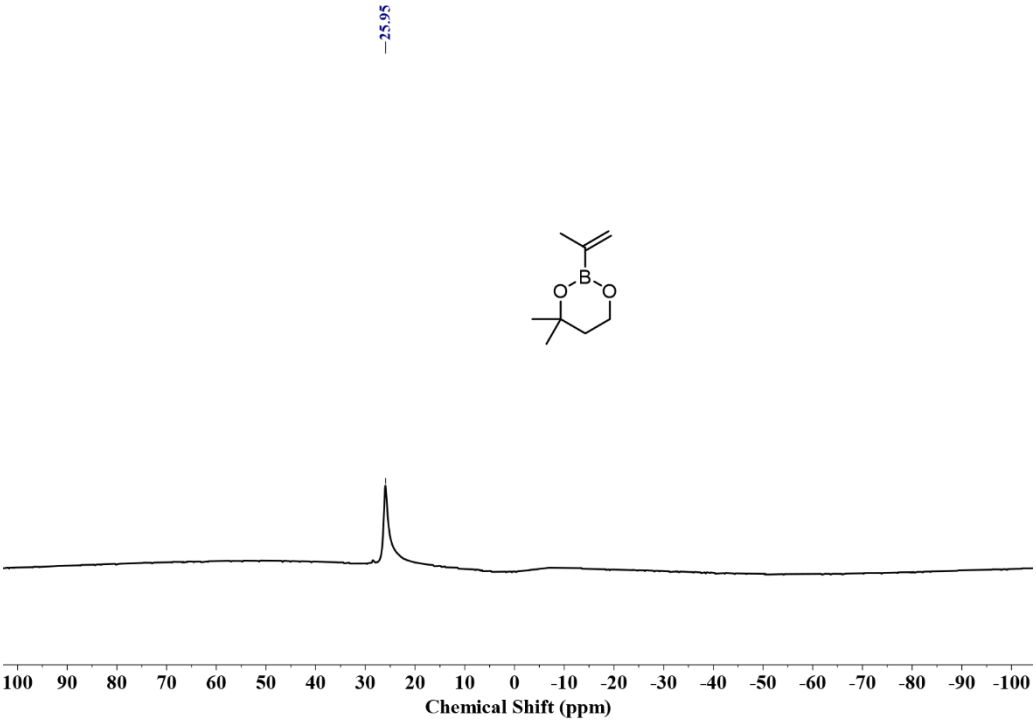


Figure S68. ^{11}B NMR Spectrum of $IB_{6\text{-}4}$ in $CDCl_3$.

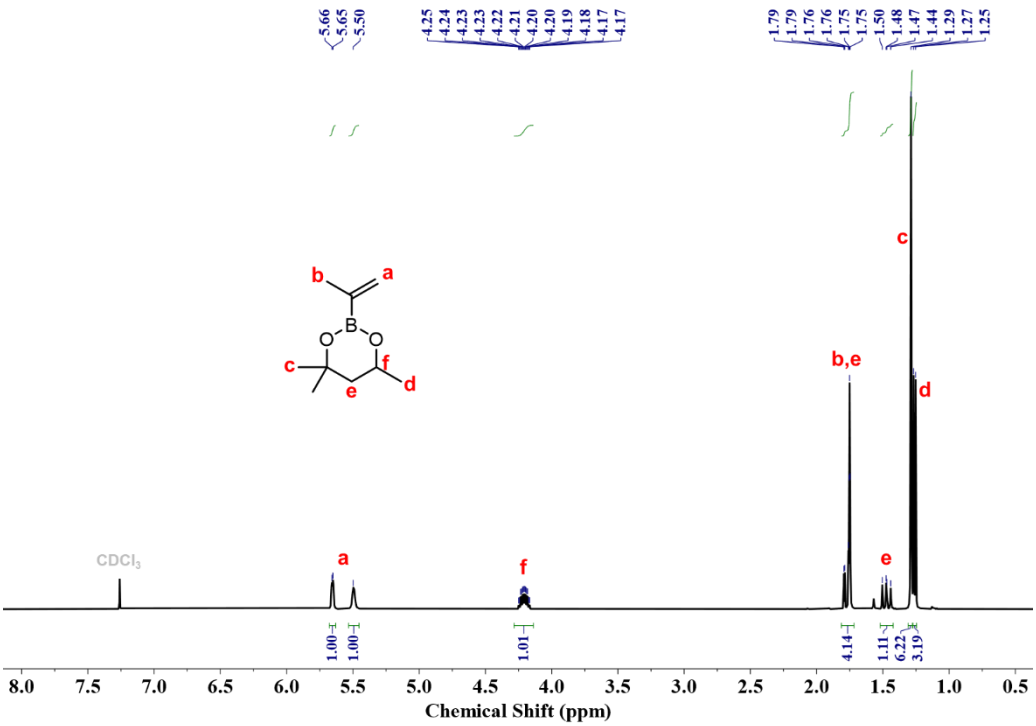


Figure S69. ^{1}H NMR Spectrum of $IB_{6\text{-}5}$ in $CDCl_3$.

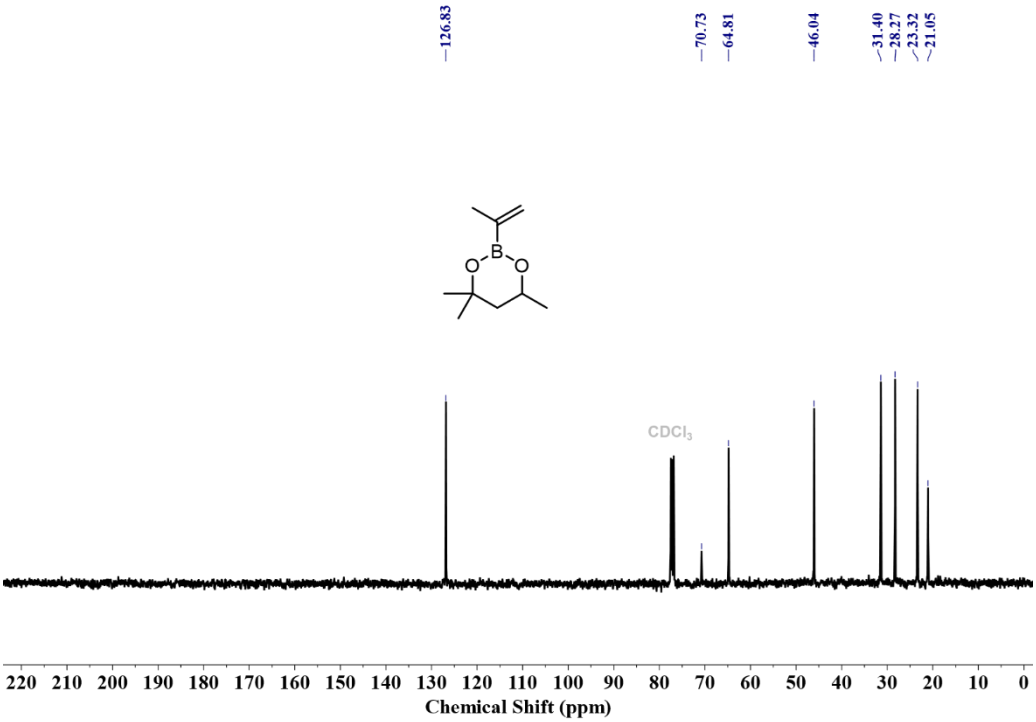


Figure S70. ^{13}C NMR Spectrum of $IB_{6\text{-}5}$ in $CDCl_3$.

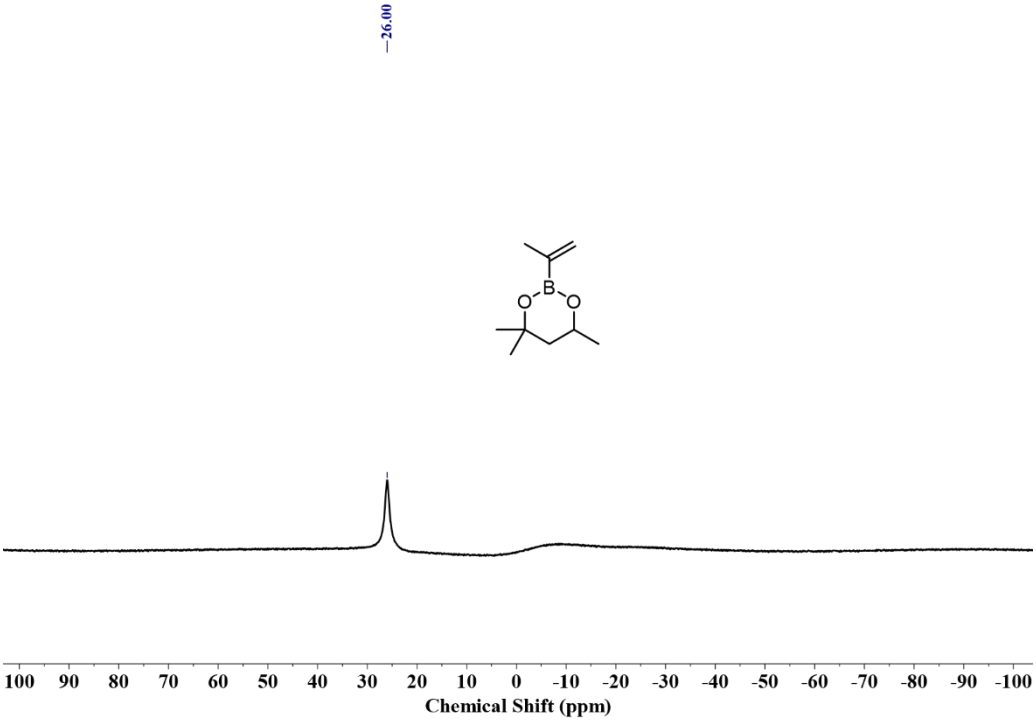


Figure S71. ^{11}B NMR Spectrum of $IB_{6\text{-}5}$ in $CDCl_3$.

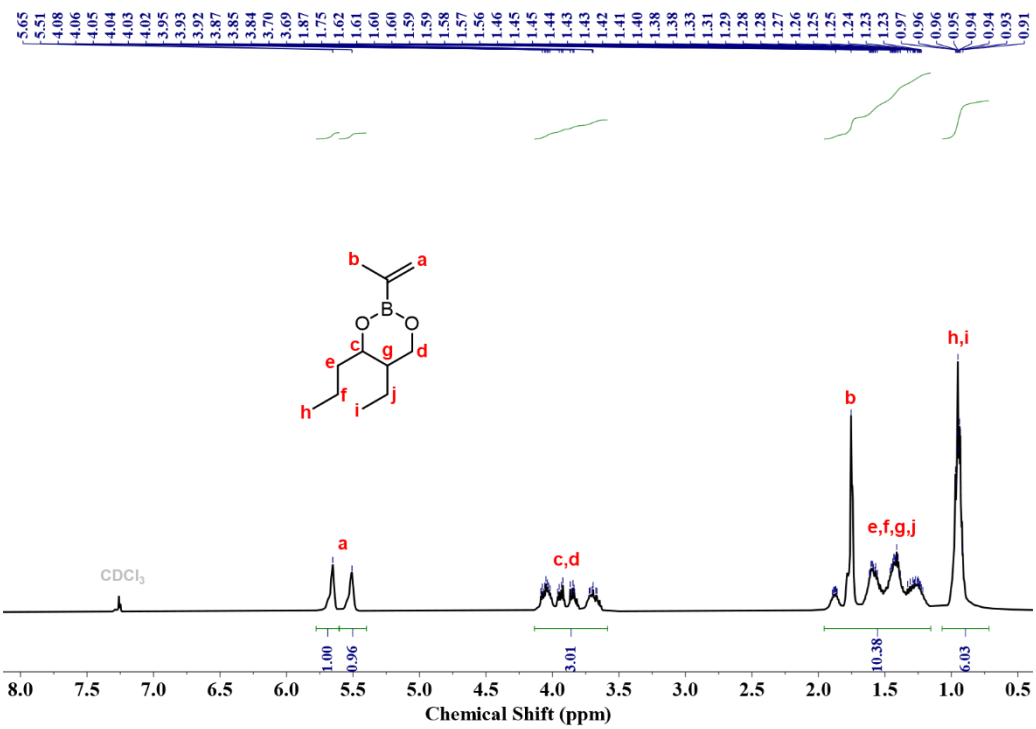


Figure S72. ^{1}H NMR Spectrum of $IB_{6\text{-}6}$ in $CDCl_3$.

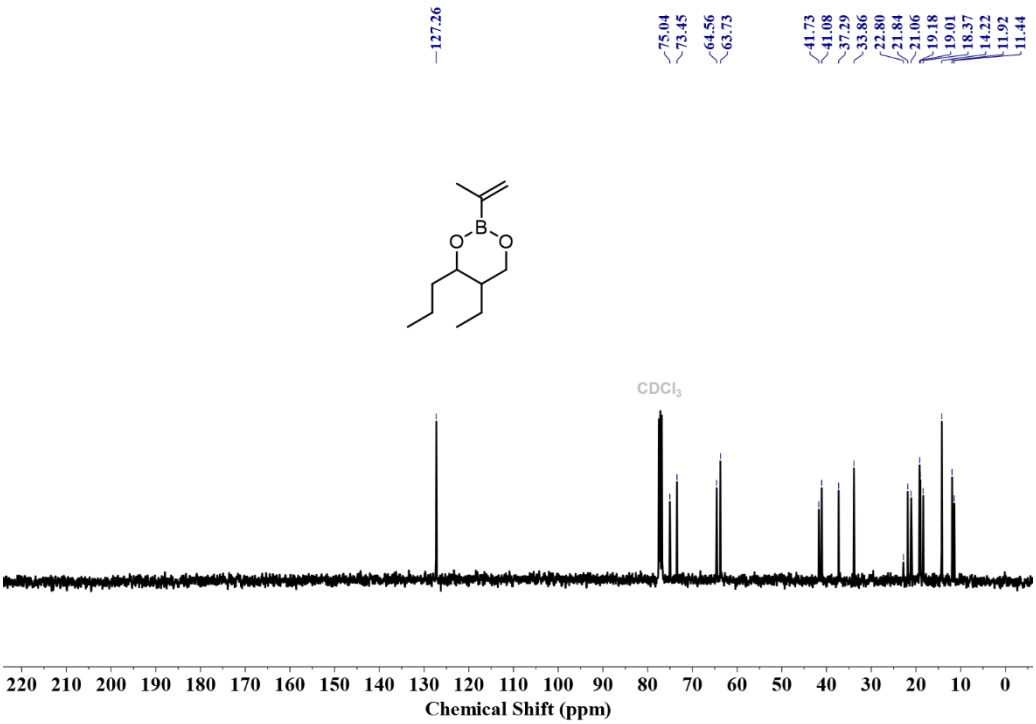


Figure S73. ^{13}C NMR Spectrum of $IB_{6\text{-}6}$ in $CDCl_3$.

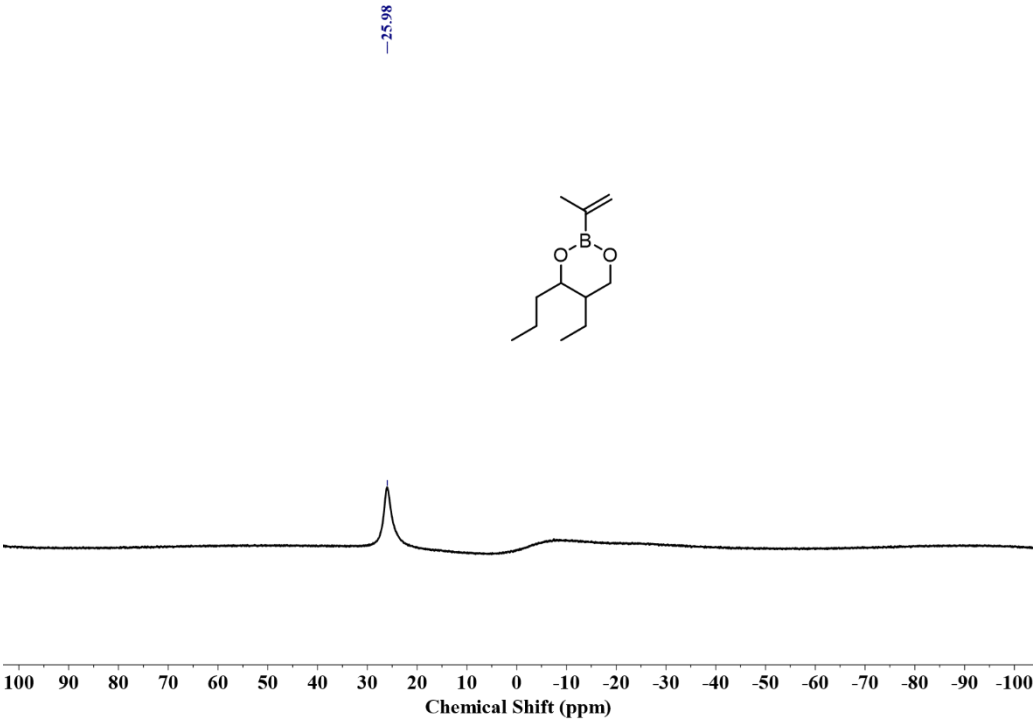


Figure S74. ^{11}B NMR Spectrum of $IB_{6\text{-}6}$ in $CDCl_3$.

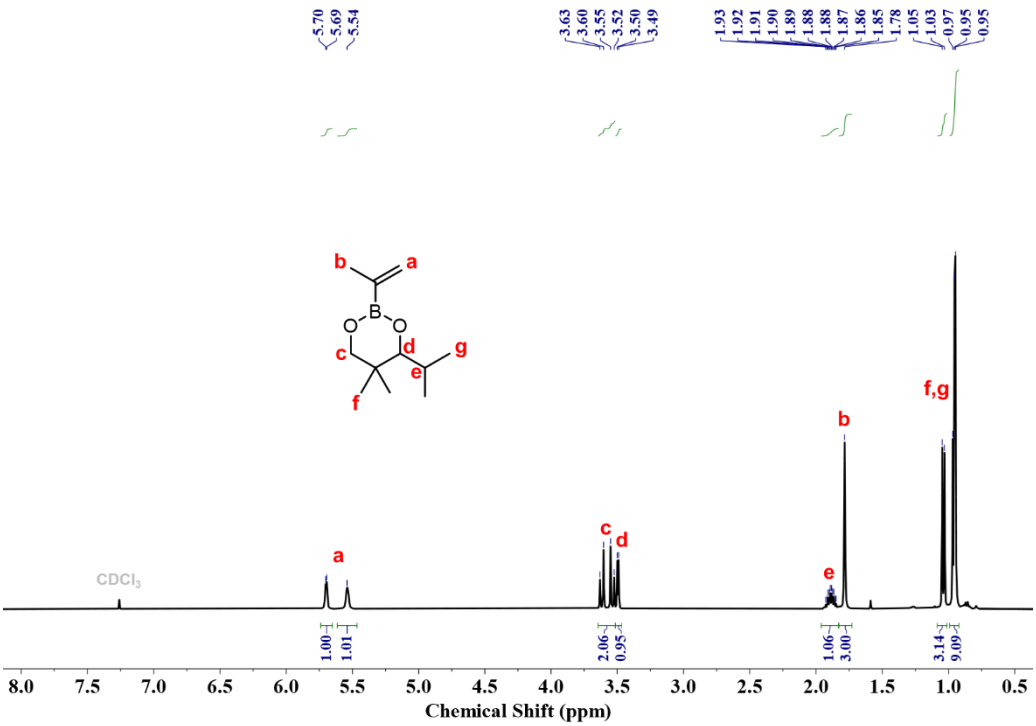


Figure S75. ^{1}H NMR Spectrum of $IB_{6\text{-}7}$ in $CDCl_3$.

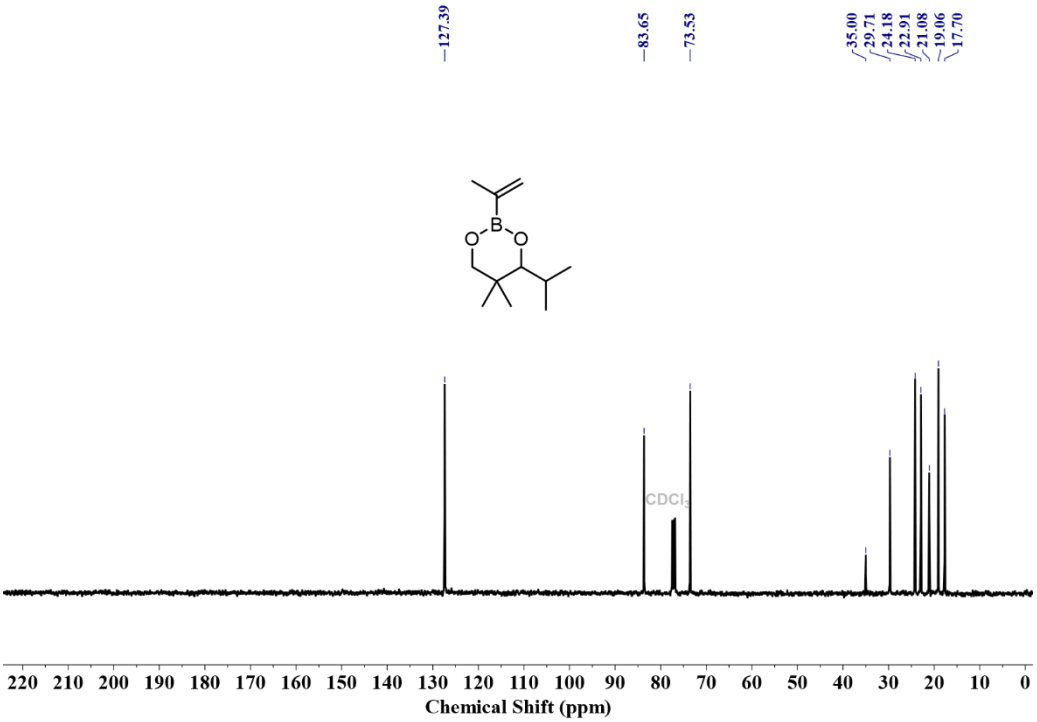


Figure S76. ^{13}C NMR Spectrum of $IB_{6\text{-}7}$ in $CDCl_3$.

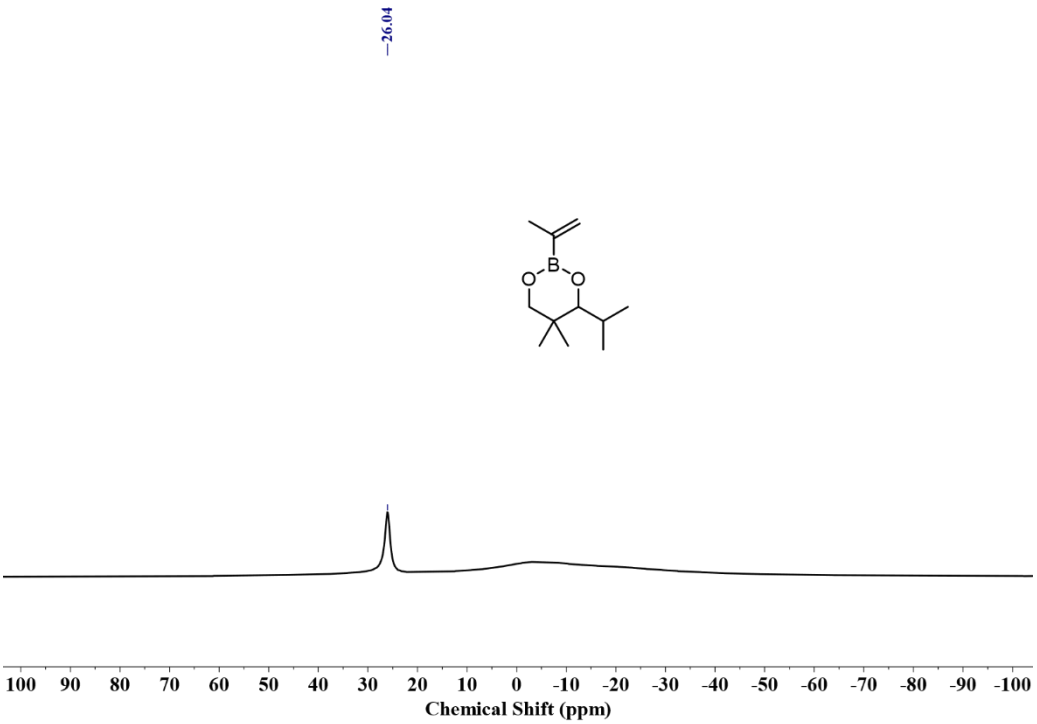


Figure S77. ^{11}B NMR Spectrum of $IB_{6\text{-}7}$ in $CDCl_3$.

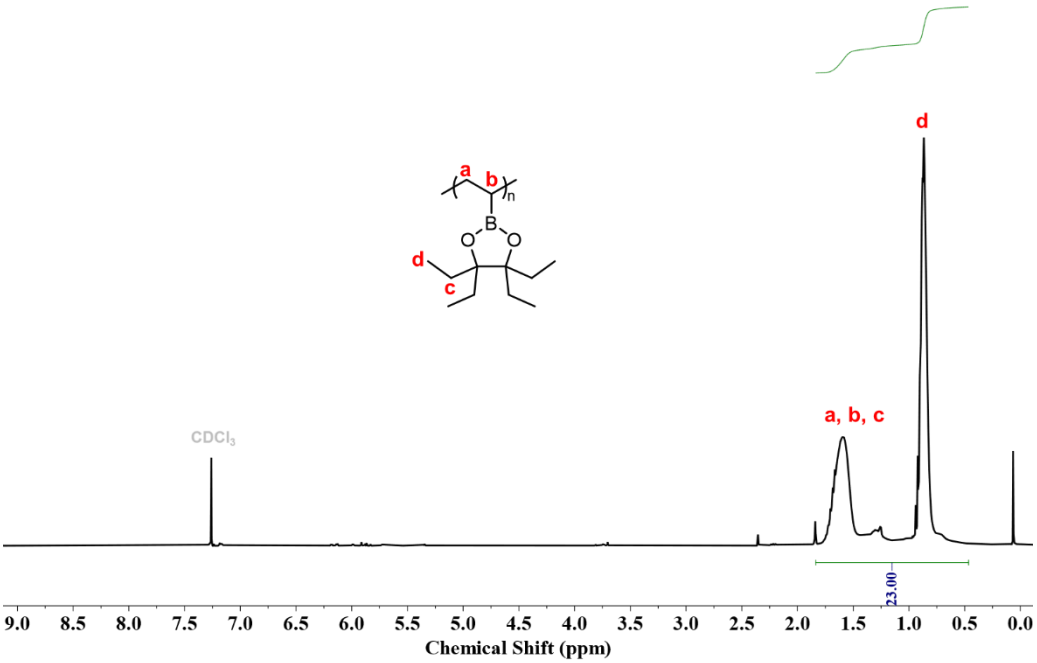


Figure S78. ^{1}H NMR Spectrum of PVB_{epin} in $CDCl_3$.

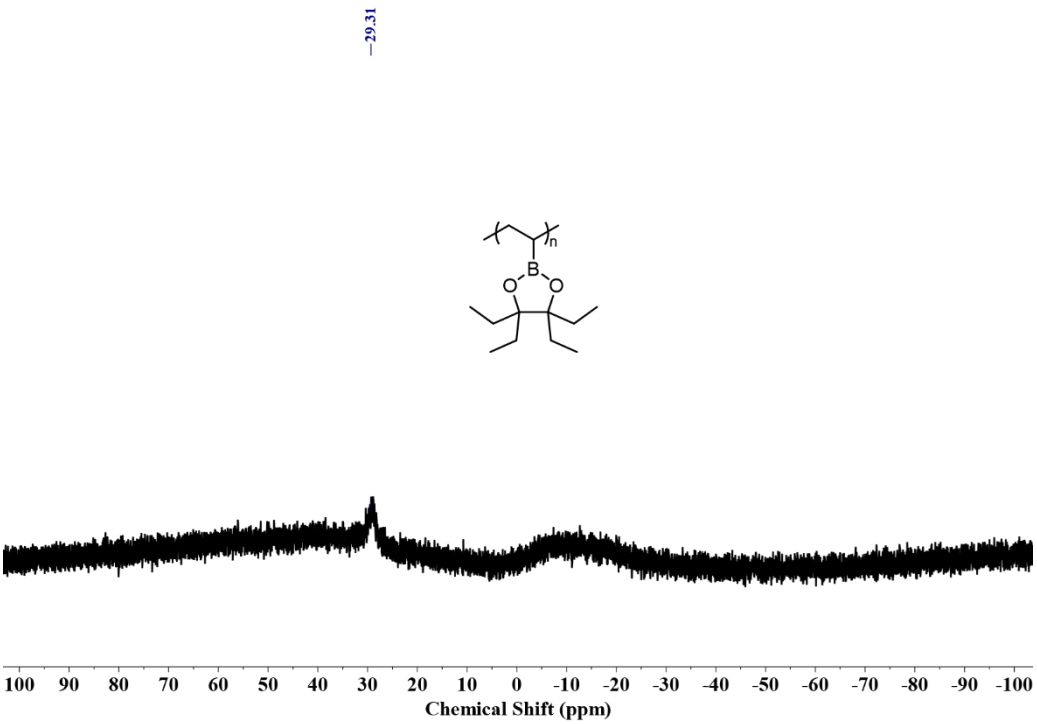


Figure S79. ^{11}B NMR Spectrum of PVB_{epin} in $CDCl_3$.

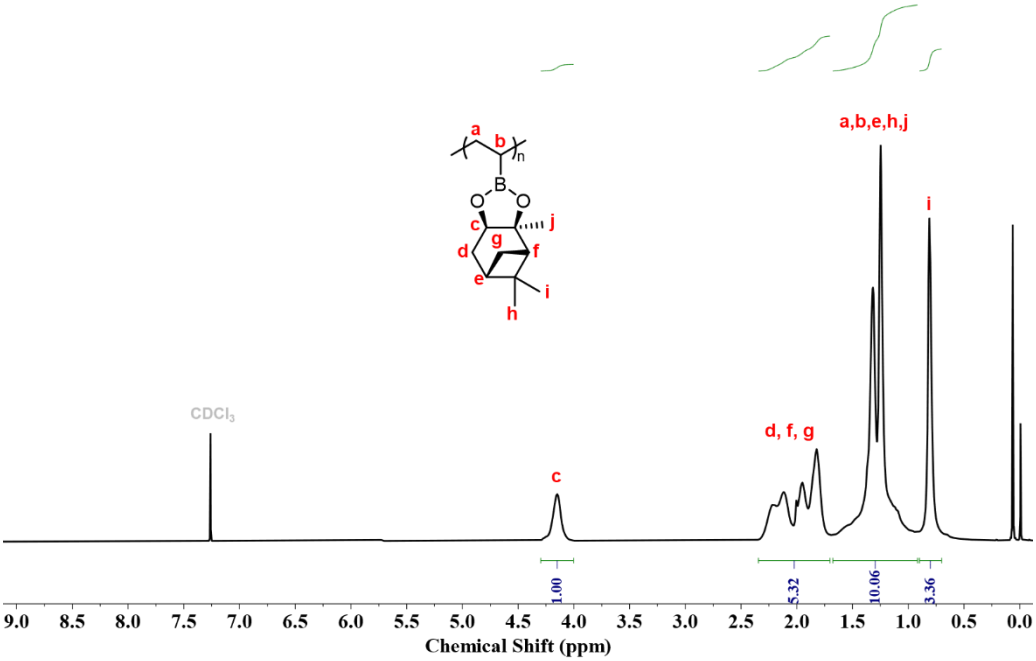


Figure S80. ^{1}H NMR Spectrum of PVB_{pnd} in $CDCl_3$.

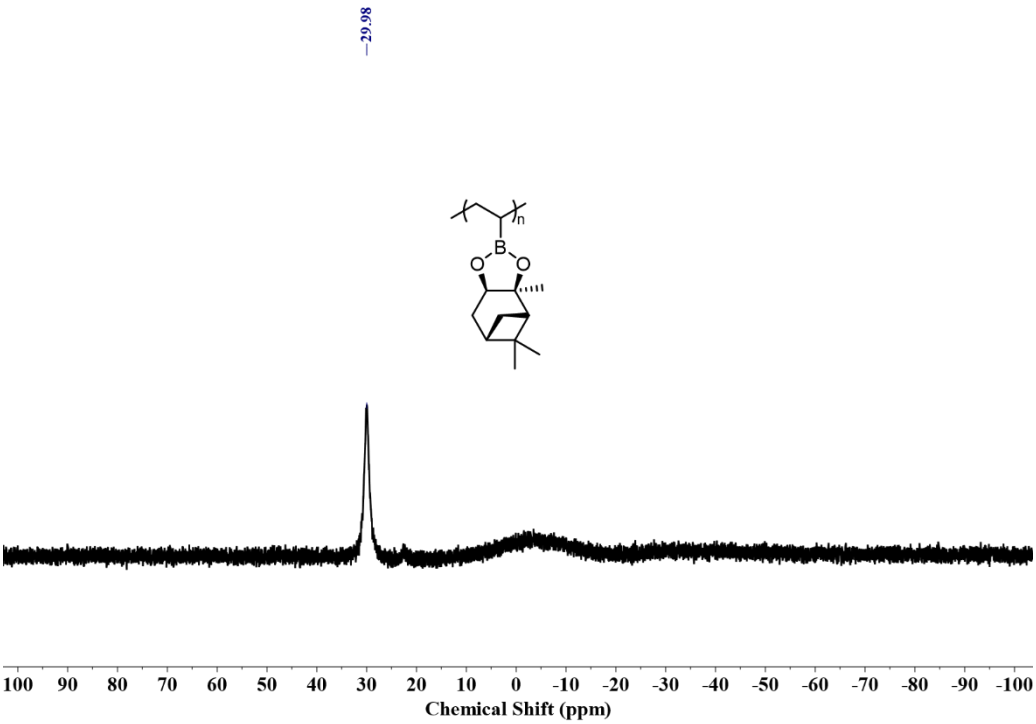


Figure S81. ^{11}B NMR Spectrum of PVB_{pnd} in $CDCl_3$.

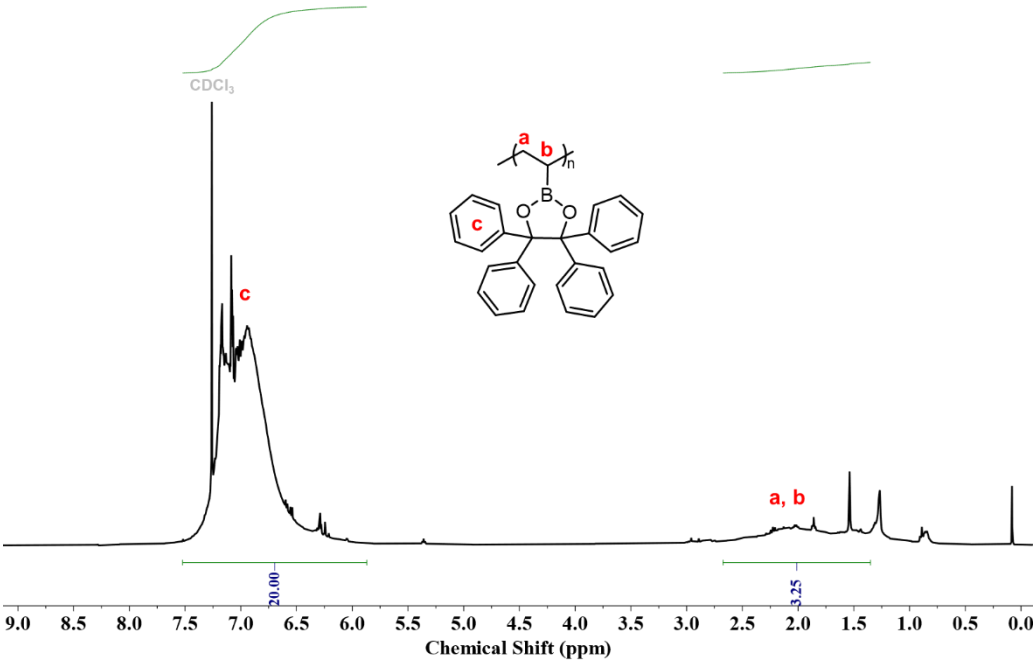


Figure S82. ^{1}H NMR Spectrum of PVB_{Phpin} in $CDCl_3$.

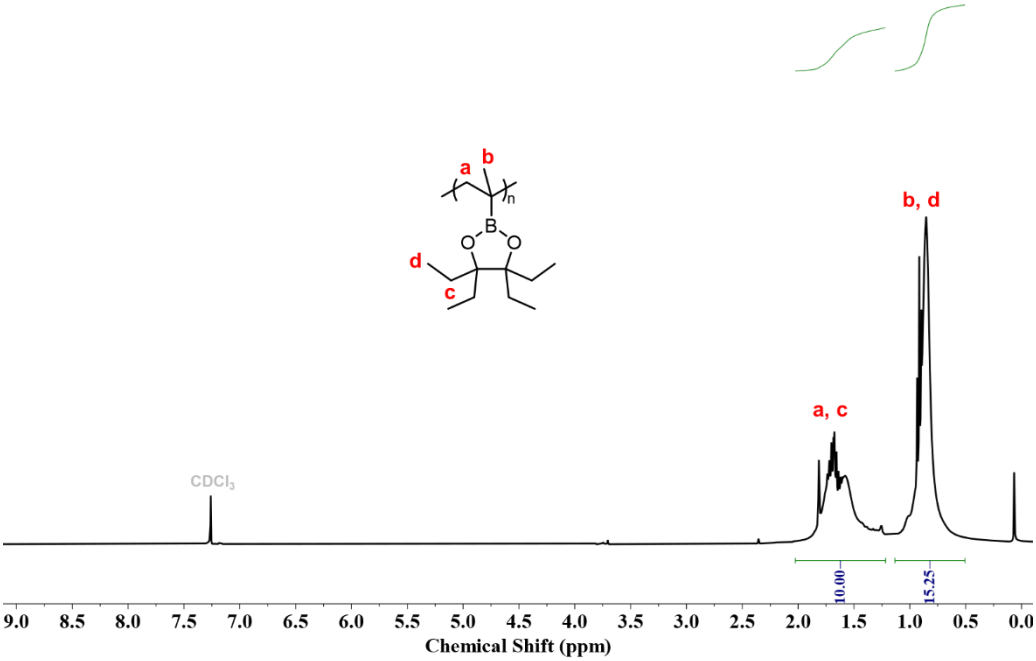


Figure S83. ^{1}H NMR Spectrum of PIB_{epin} in $CDCl_3$.

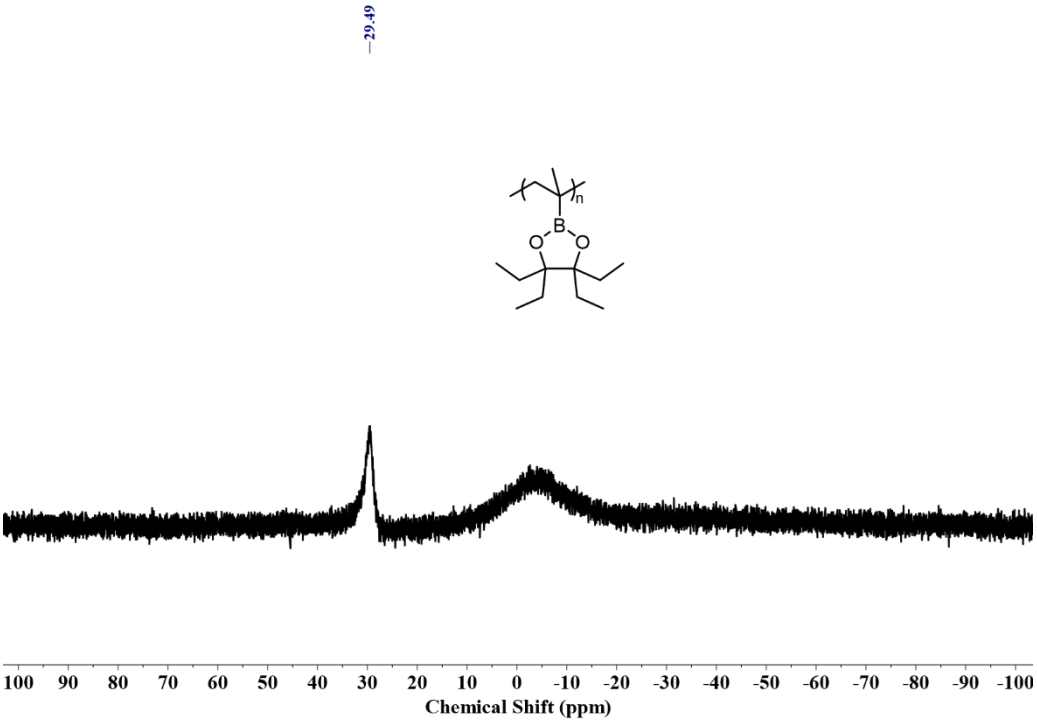


Figure S84. ^{11}B NMR Spectrum of PIB_{epin} in $CDCl_3$.

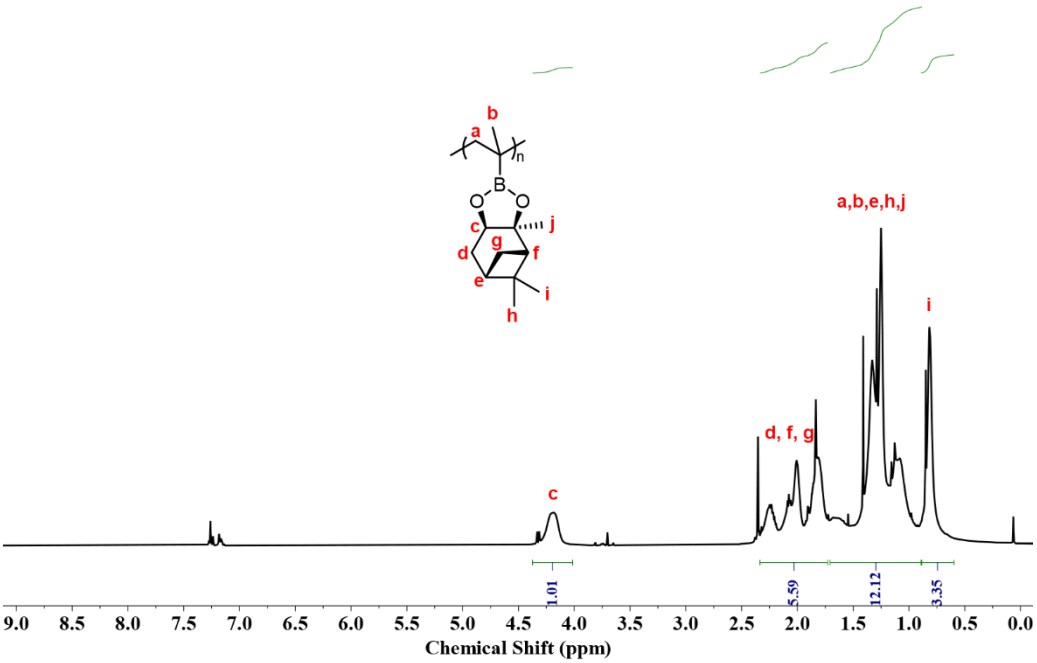


Figure S85. ^{1}H NMR Spectrum of PIB_{pnd} in $CDCl_3$.

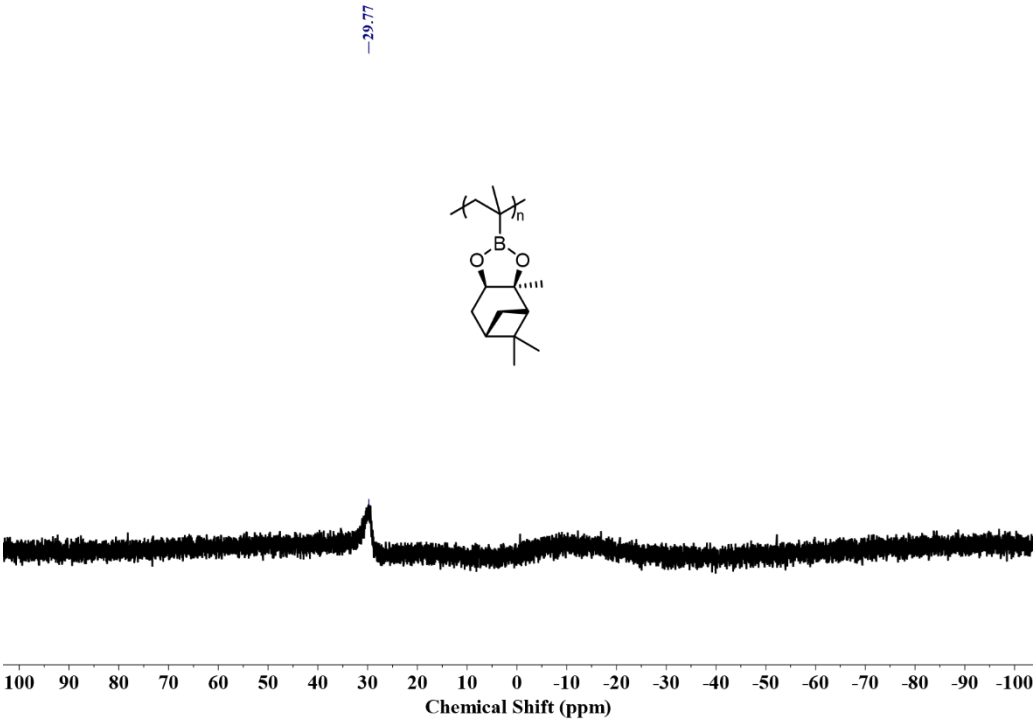


Figure S86. ^{11}B NMR Spectrum of PIB_{pnd} in $CDCl_3$.

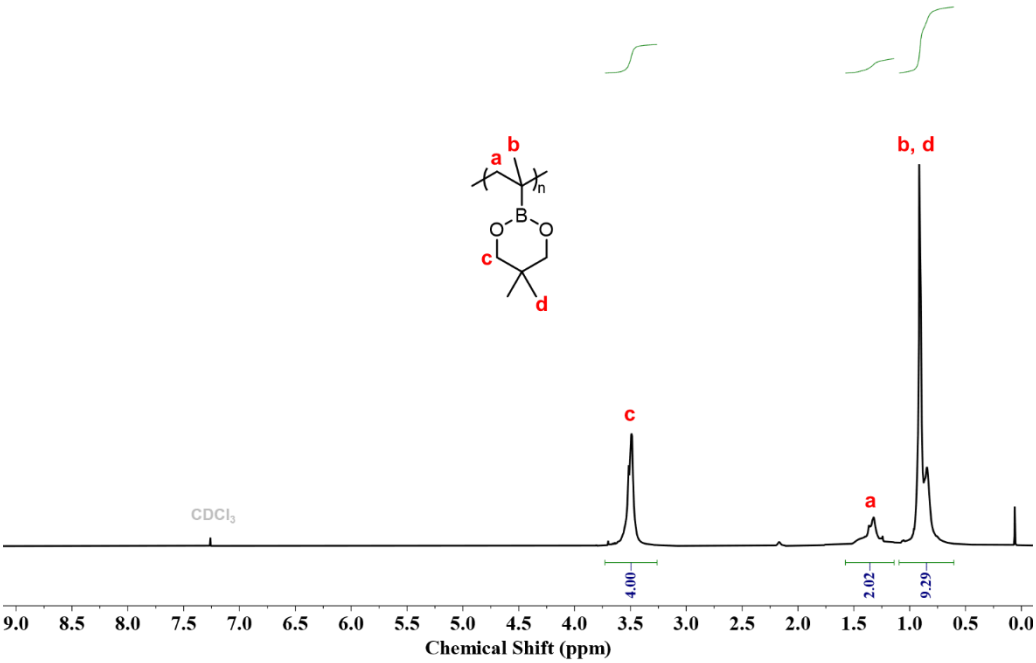


Figure S87. ^{1}H NMR Spectrum of $PIB_{6\text{-}1}$ in $CDCl_3$.

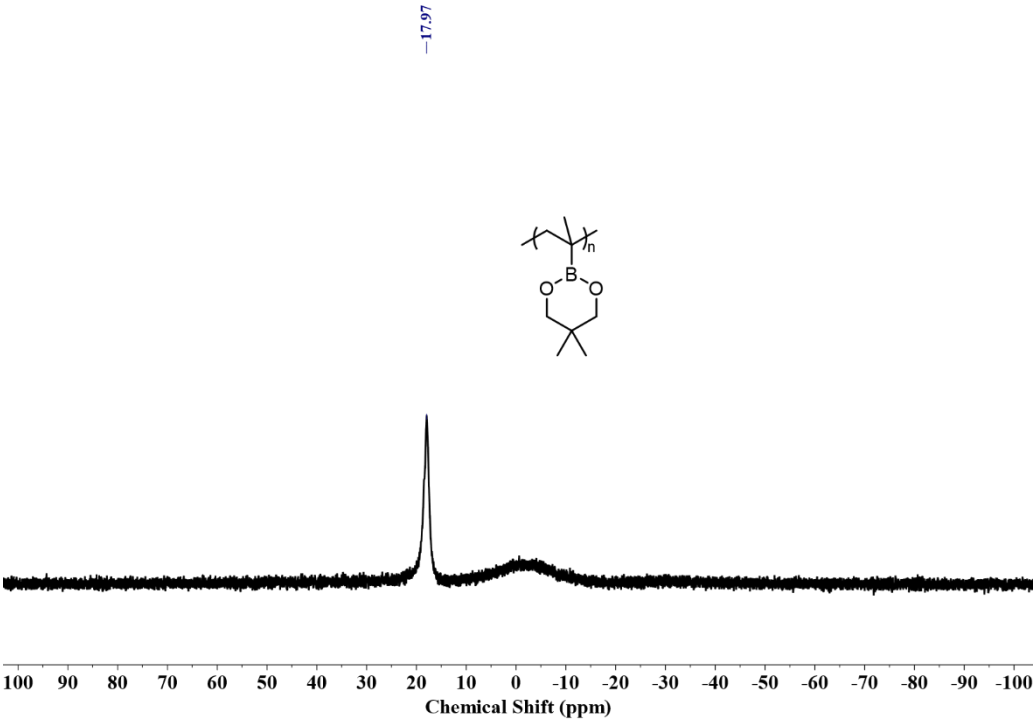


Figure S88. ^{11}B NMR Spectrum of $PIB_{6\text{-}1}$ in $CDCl_3$.

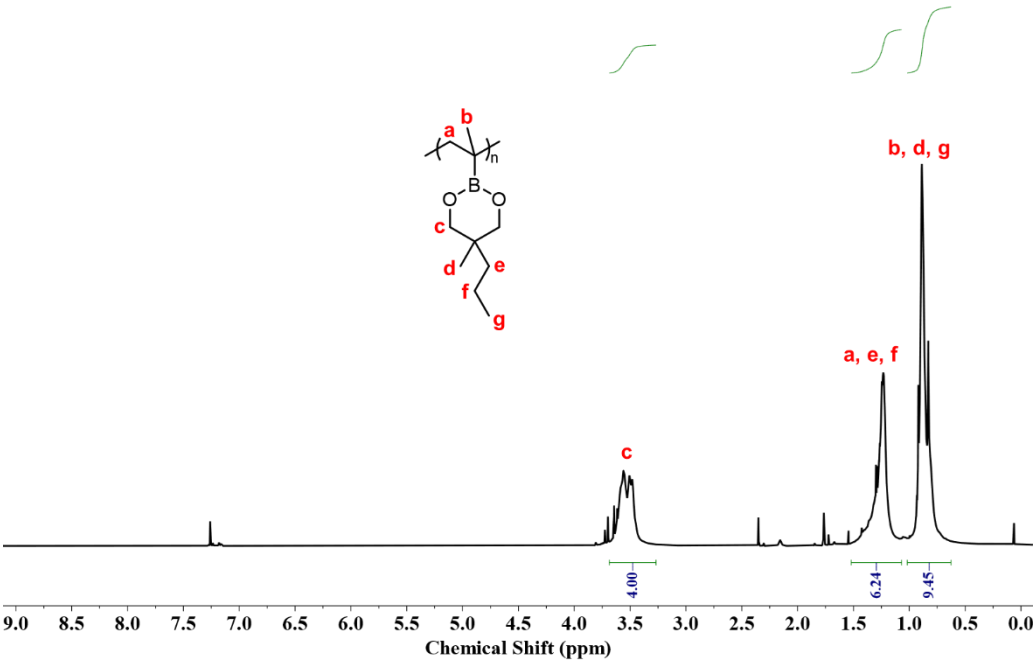


Figure S89. ^{1}H NMR Spectrum of $PIB_{6\text{-}2}$ in $CDCl_3$.

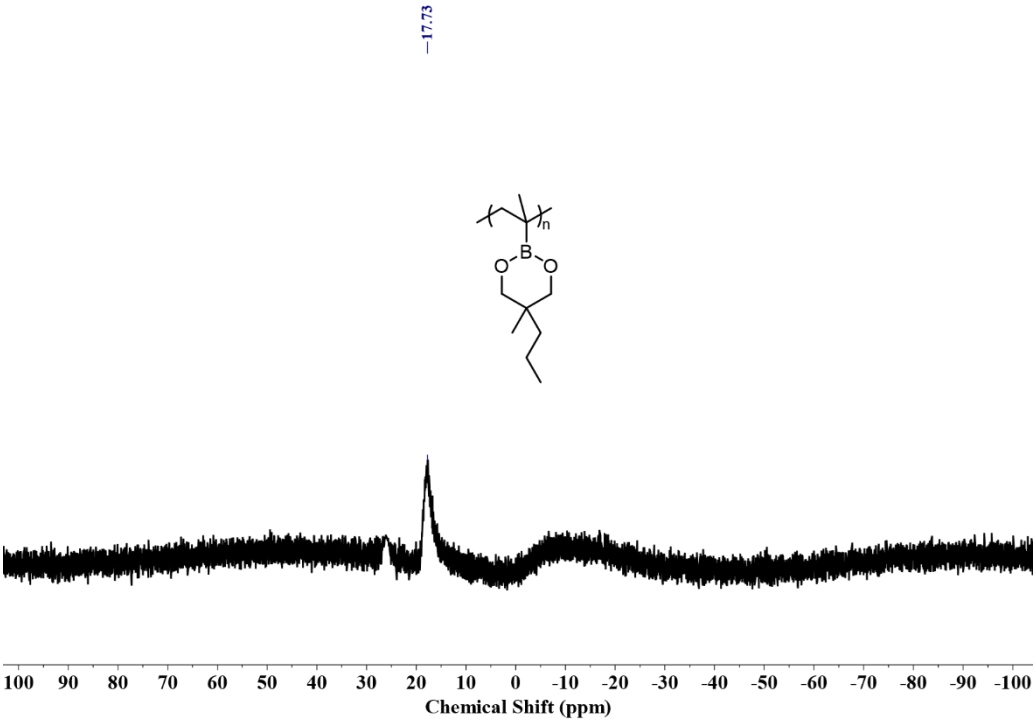


Figure S90. ^{11}B NMR Spectrum of $PIB_{6\text{-}2}$ in $CDCl_3$.

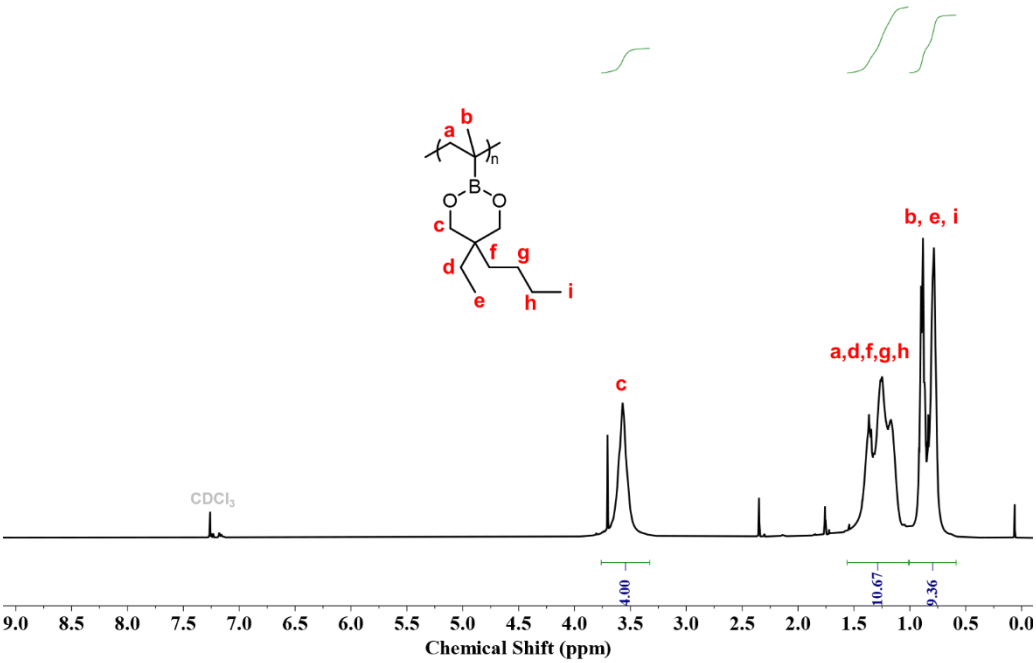


Figure S91. ^{1}H NMR Spectrum of $PIB_{6\text{-}3}$ in $CDCl_3$.

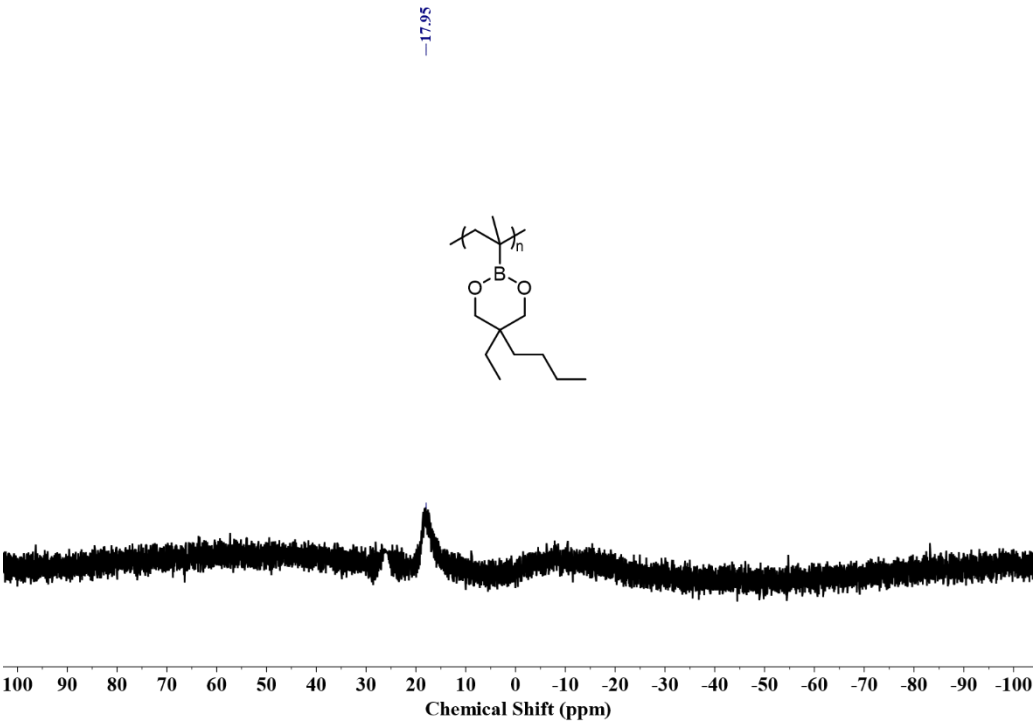


Figure S92. ^{11}B NMR Spectrum of $PIB_{6\text{-}3}$ in $CDCl_3$.

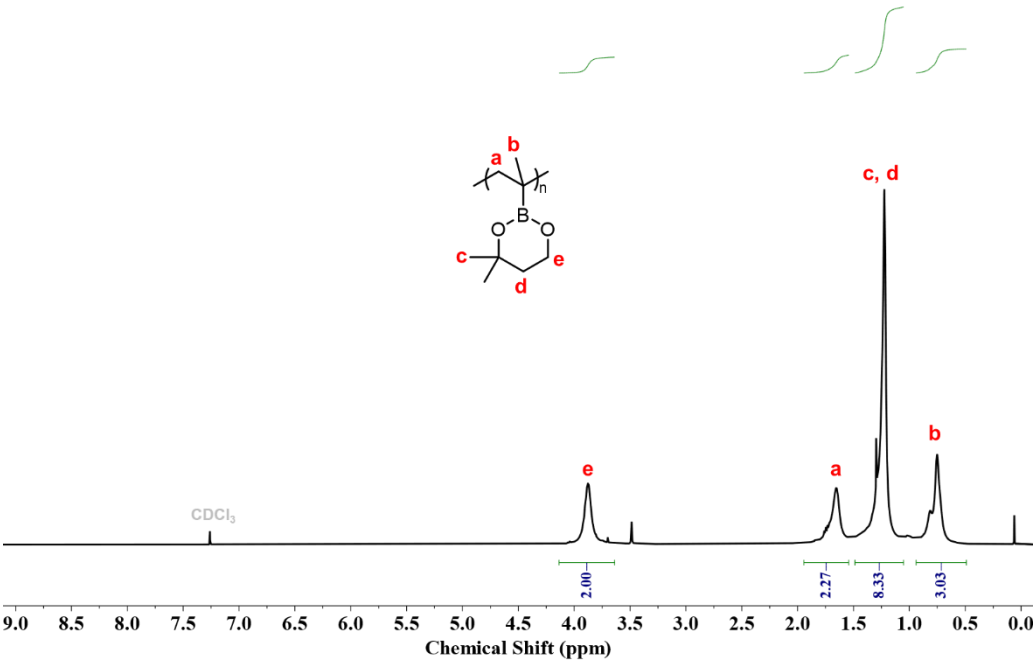


Figure S93. ^{1}H NMR Spectrum of $PIB_{6\text{-}4}$ in $CDCl_3$.

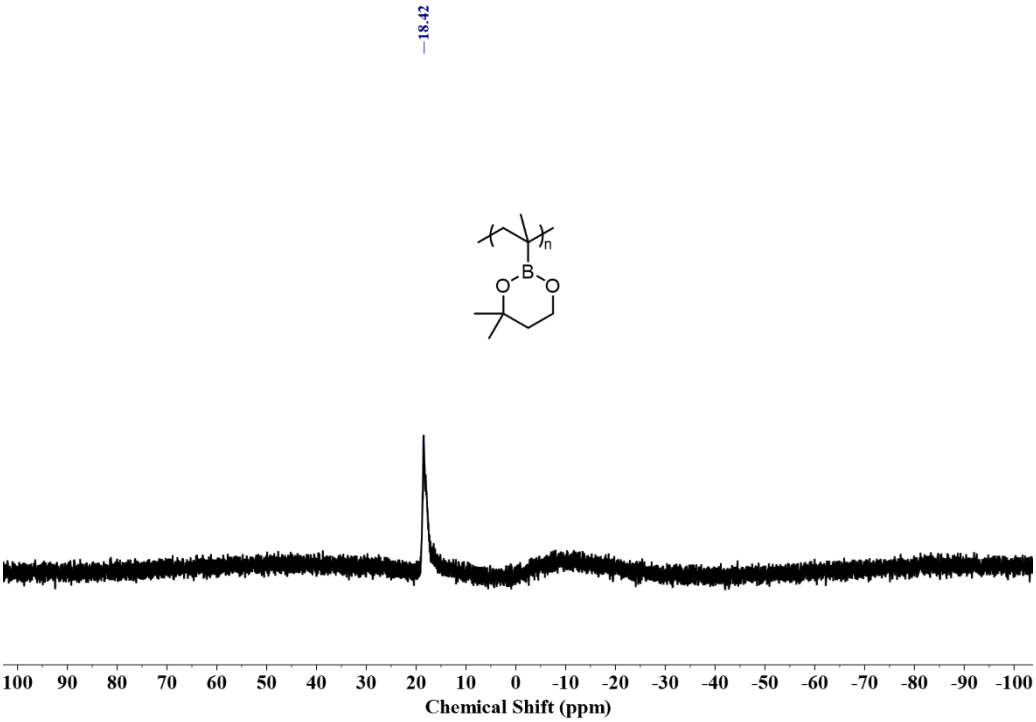


Figure S94. ^{11}B NMR Spectrum of $PIB_{6\text{-}4}$ in $CDCl_3$.

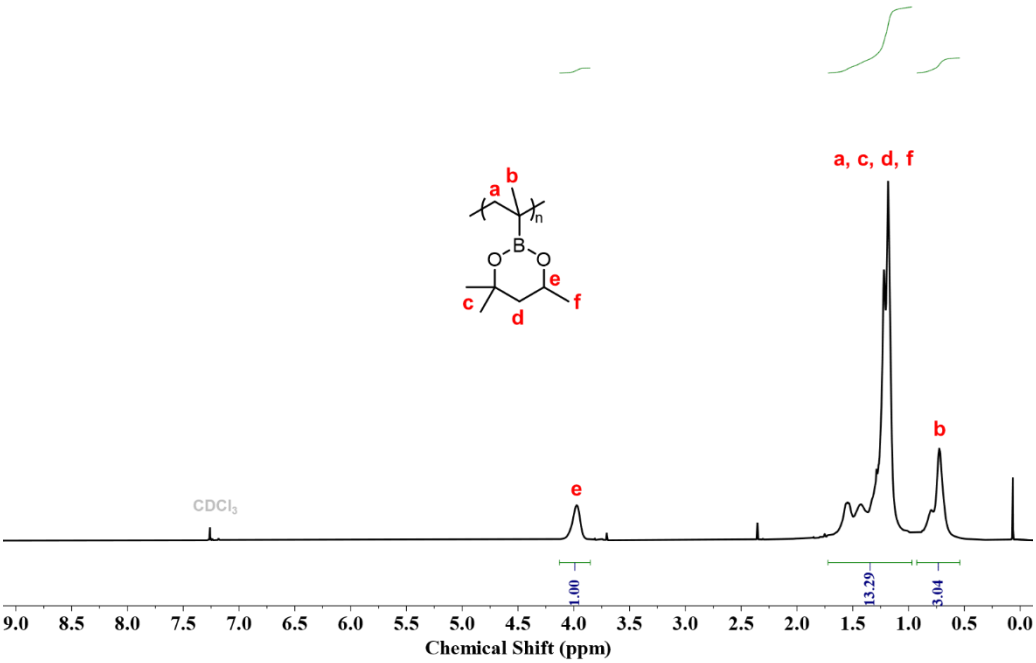


Figure S95. ^{1}H NMR Spectrum of $PIB_{6\text{-}5}$ in $CDCl_3$.

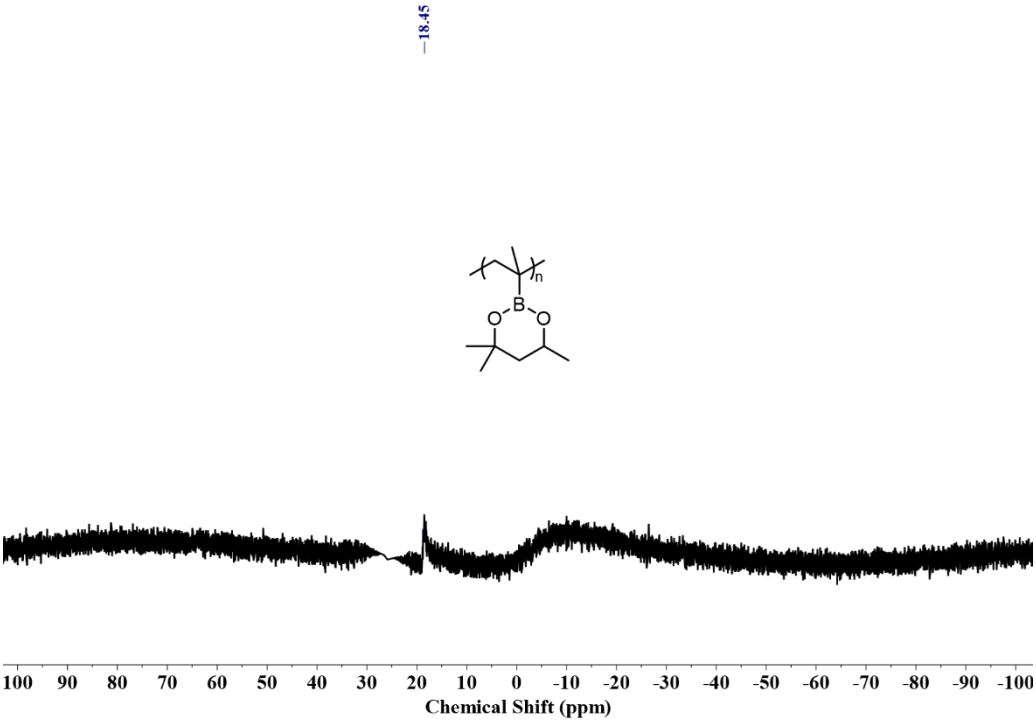


Figure S96. ^{11}B NMR Spectrum of $PIB_{6\text{-}5}$ in $CDCl_3$.

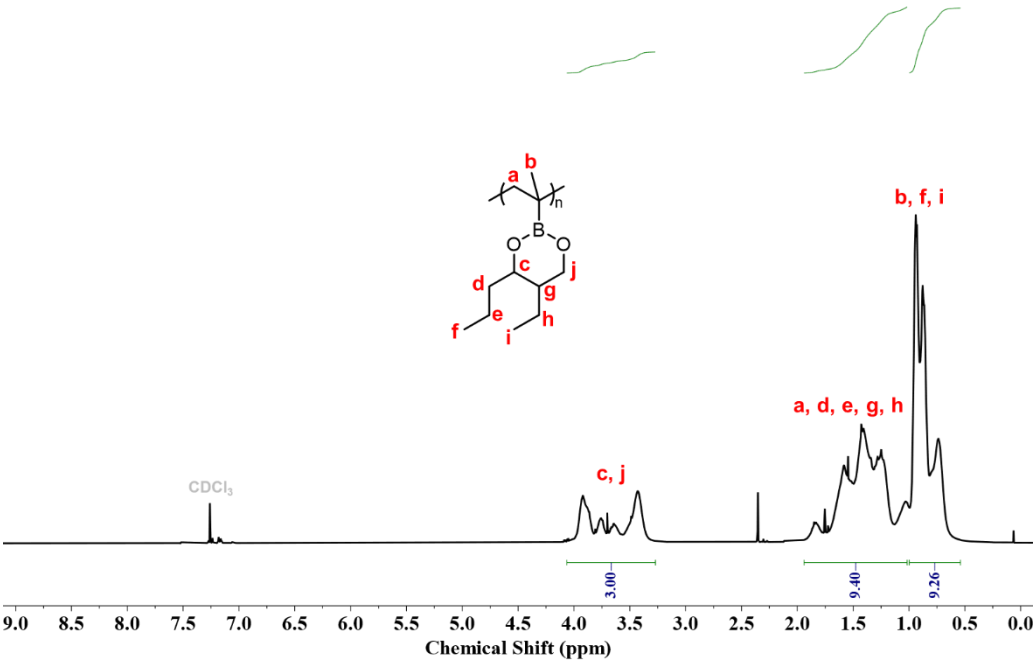


Figure S97. ^{1}H NMR Spectrum of $PIB_{6\text{-}6}$ in $CDCl_3$.

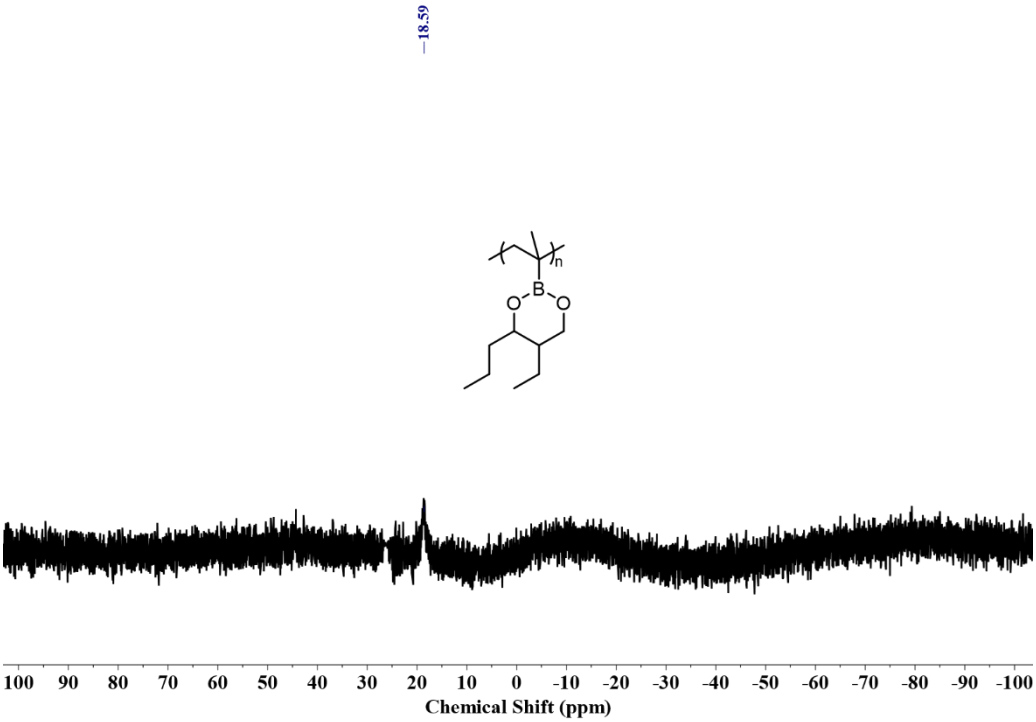


Figure S98. ^{11}B NMR Spectrum of $PIB_{6\text{-}6}$ in $CDCl_3$.

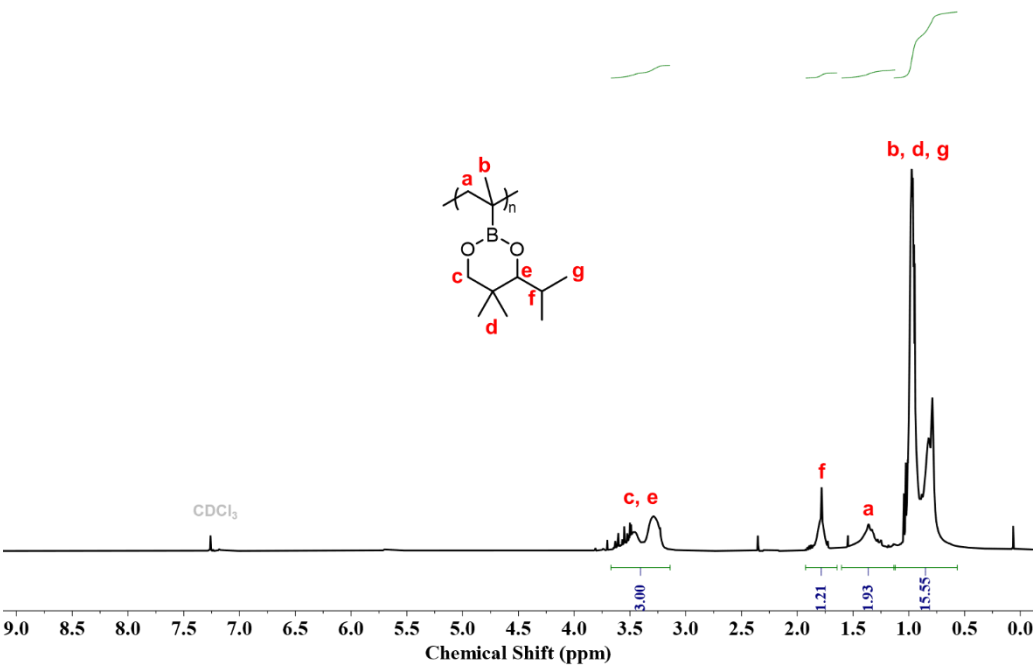


Figure S99. ^{1}H NMR Spectrum of $PIB_{6\text{-}7}$ in $CDCl_3$.

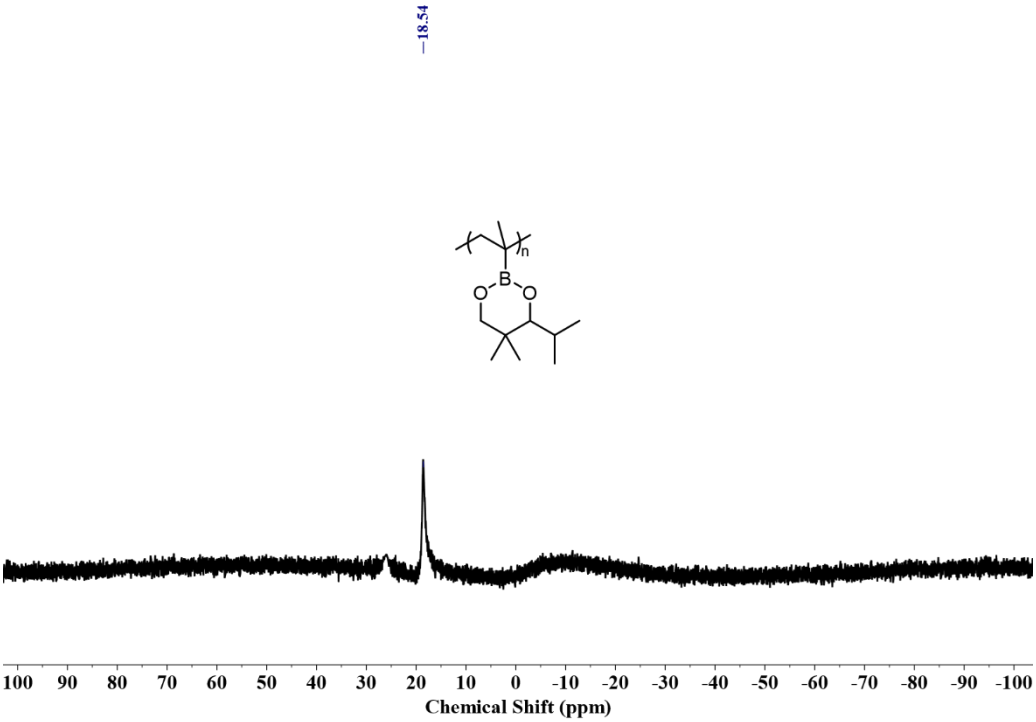


Figure S100. ^{11}B NMR Spectrum of $PIB_{6\text{-}7}$ in $CDCl_3$.

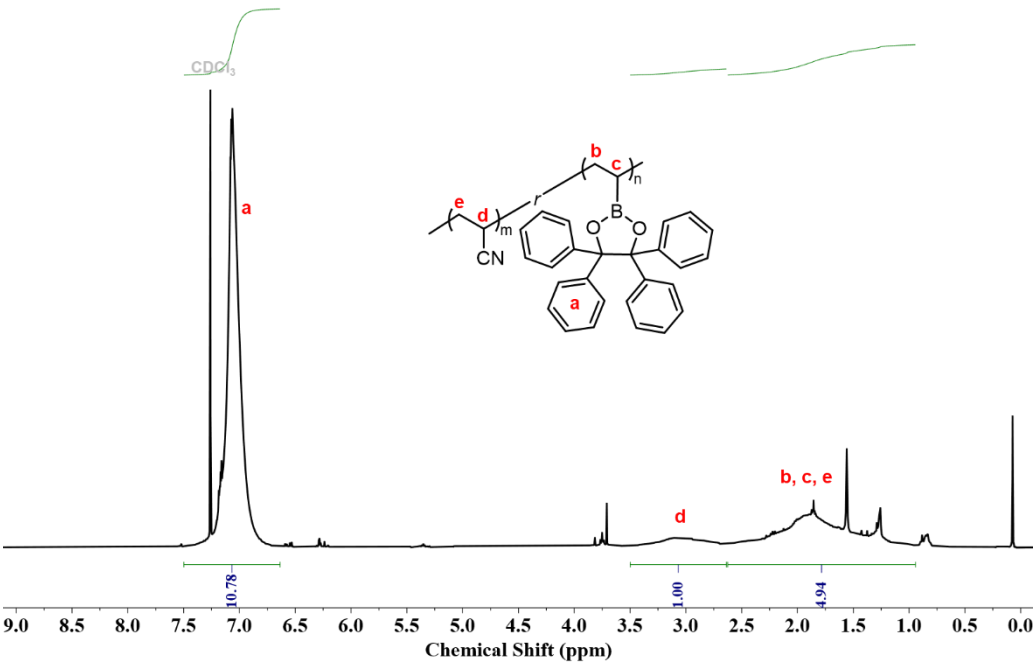


Figure S101. ^{1}H NMR Spectrum of Poly(AN-*co*-VB_{Phpin}) in $CDCl_3$.

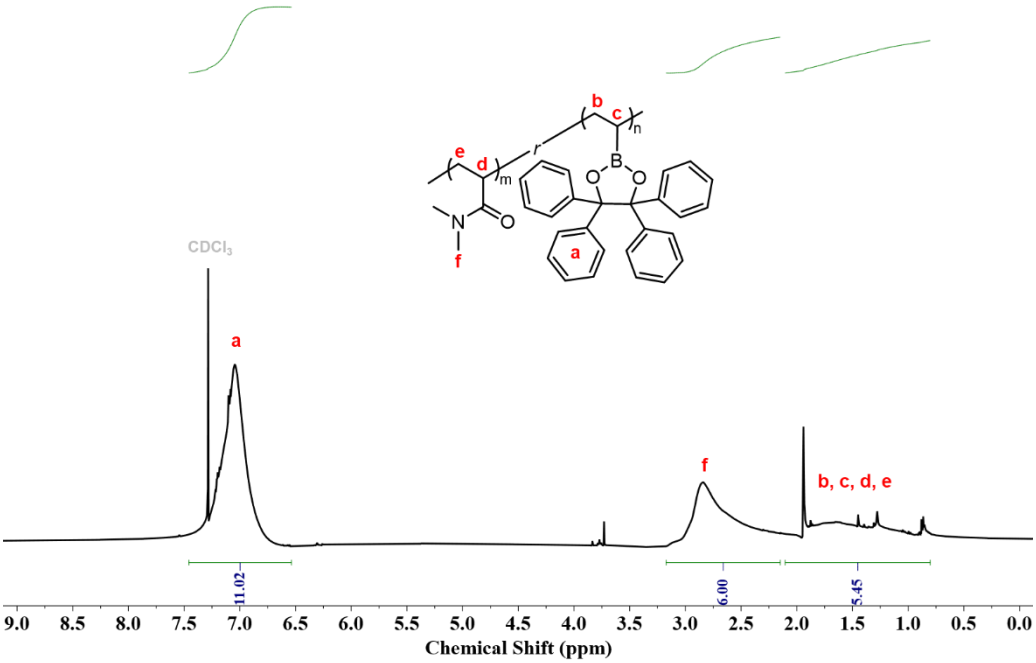


Figure S102. ^{1}H NMR Spectrum of Poly(DMAA-*co*-VB$_{Phpin}$) in $CDCl_3$.

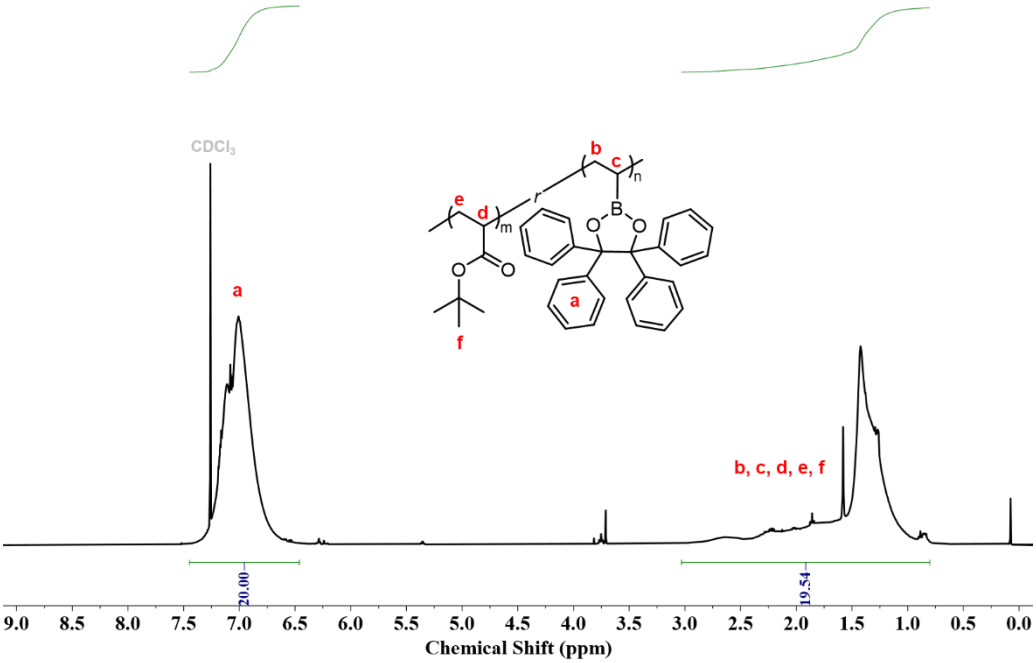


Figure S103. ^{1}H NMR Spectrum of Poly(*t*BA-*co*-VB$_{Phpin}$) in $CDCl_3$.

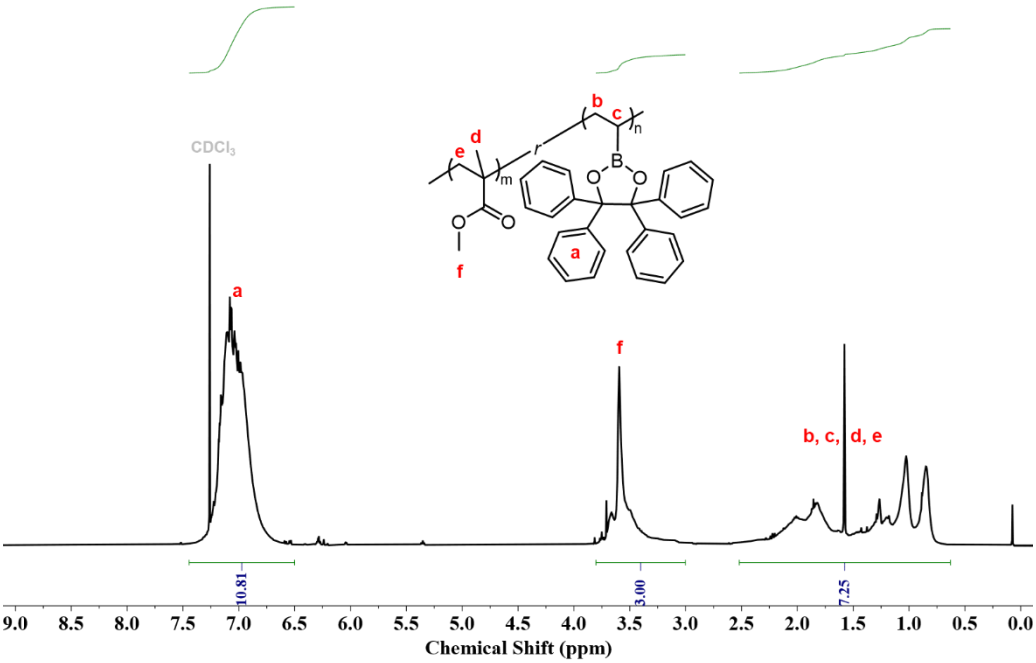


Figure S104. ^{1}H NMR Spectrum of Poly(MMA-*co*-VB$_{Phpin}$) in $CDCl_3$.

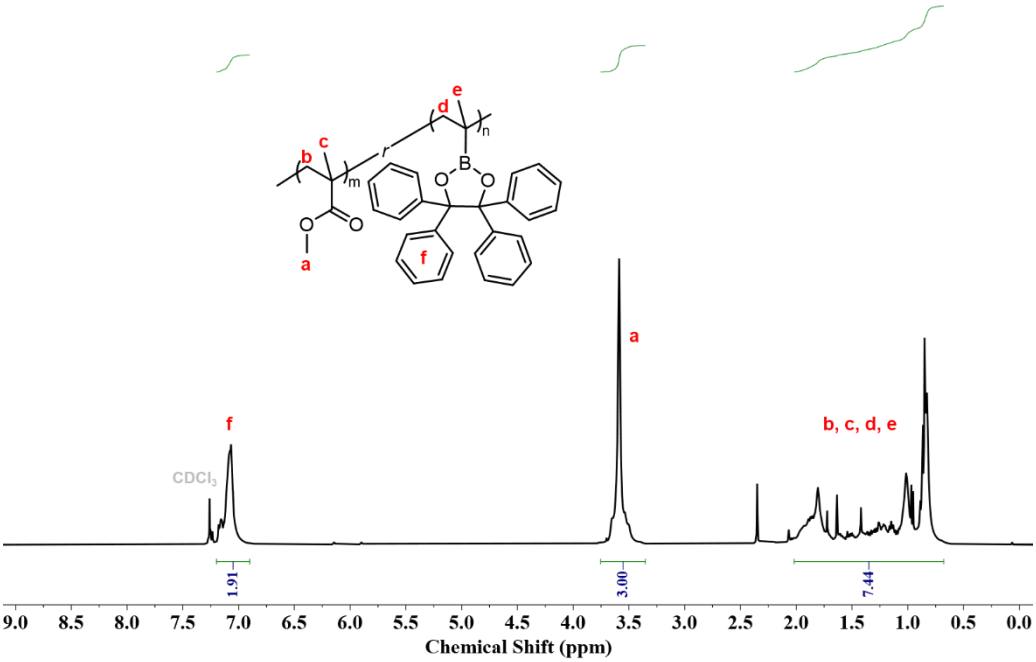


Figure S105. ^{1}H NMR Spectrum of Poly(MMA-*co*-IB$_{Phpin}$) in $CDCl_3$.

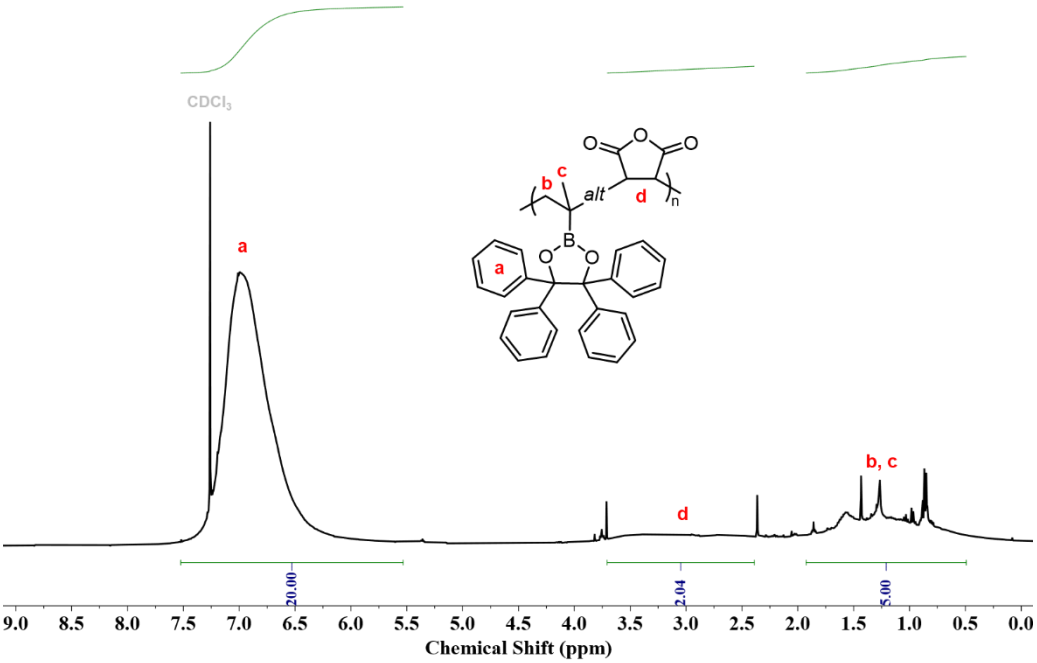


Figure S106. ^{1}H NMR Spectrum of Poly(IB$_{Phpin}$-*alt*-MAH) in $CDCl_3$.

VIII. DSC Data of the Polymers

Poly(DMAA-*co*-IB$_{Phpin}$)

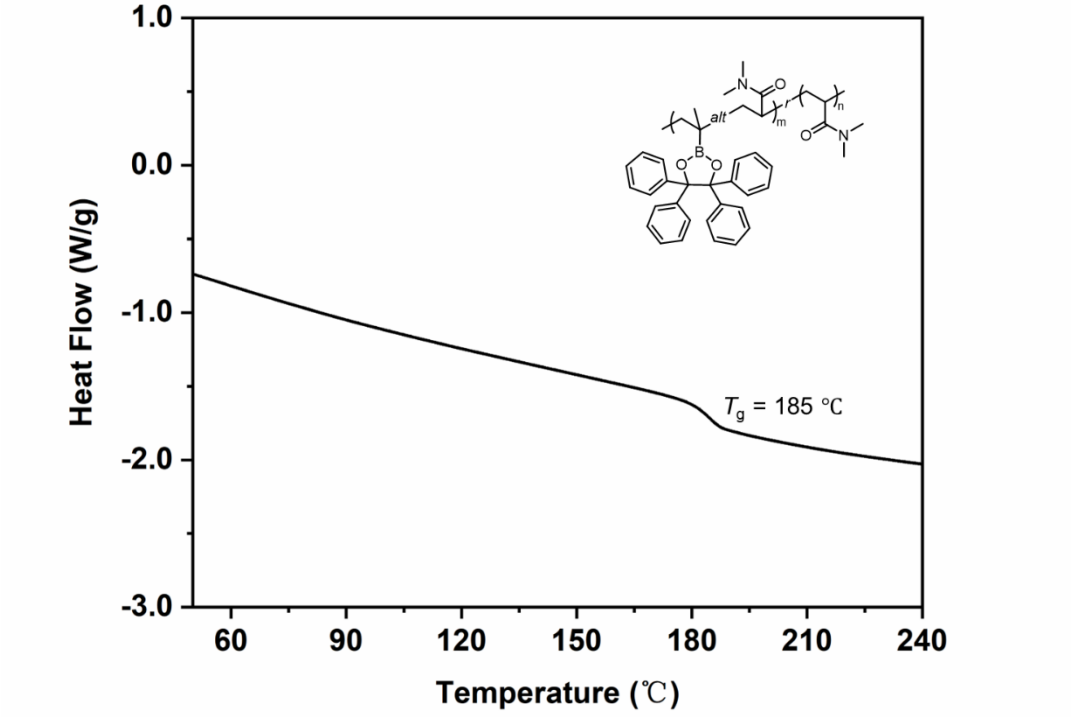


Figure S107. DSC Curves for Poly(DMAA-*co*-IB$_{Phpin}$).

Poly(*t*BA-*co*-IB$_{Phpin}$)

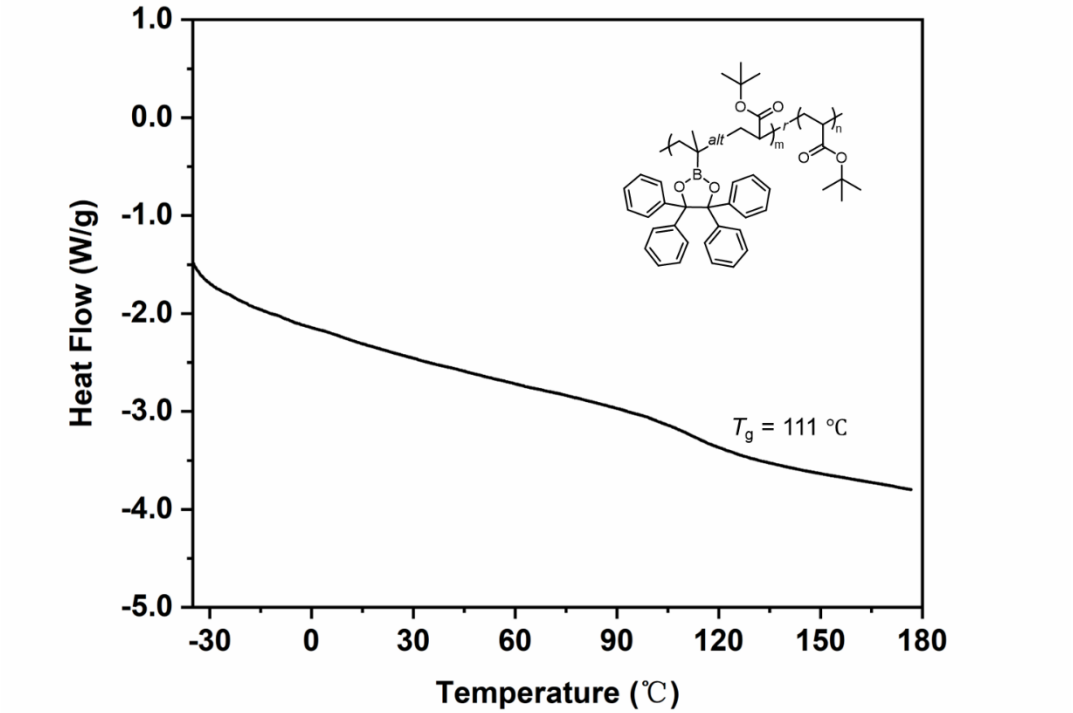


Figure S108. DSC Curves for Poly(*t*BA-*co*-IB$_{Phpin}$).

Poly(Diene-*co*-IB$_{Phpin}$)

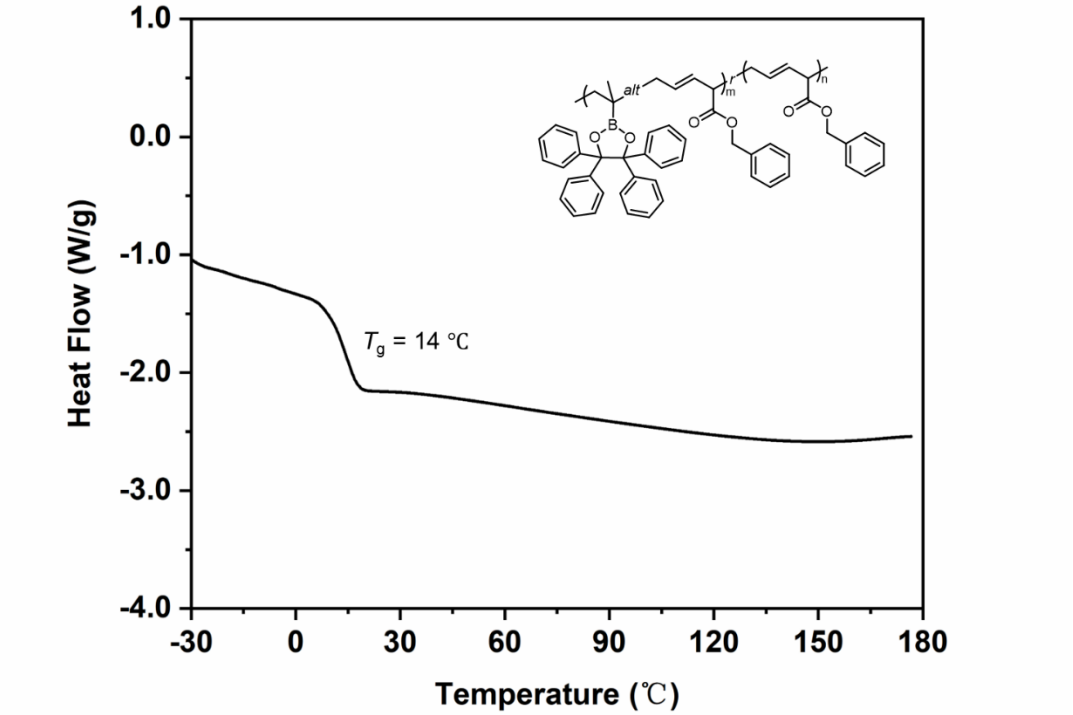


Figure S109. DSC Curves for Poly(Diene-*co*-IB$_{Phpin}$).

Poly(NPMI-*co*-IB$_{Phpin}$)

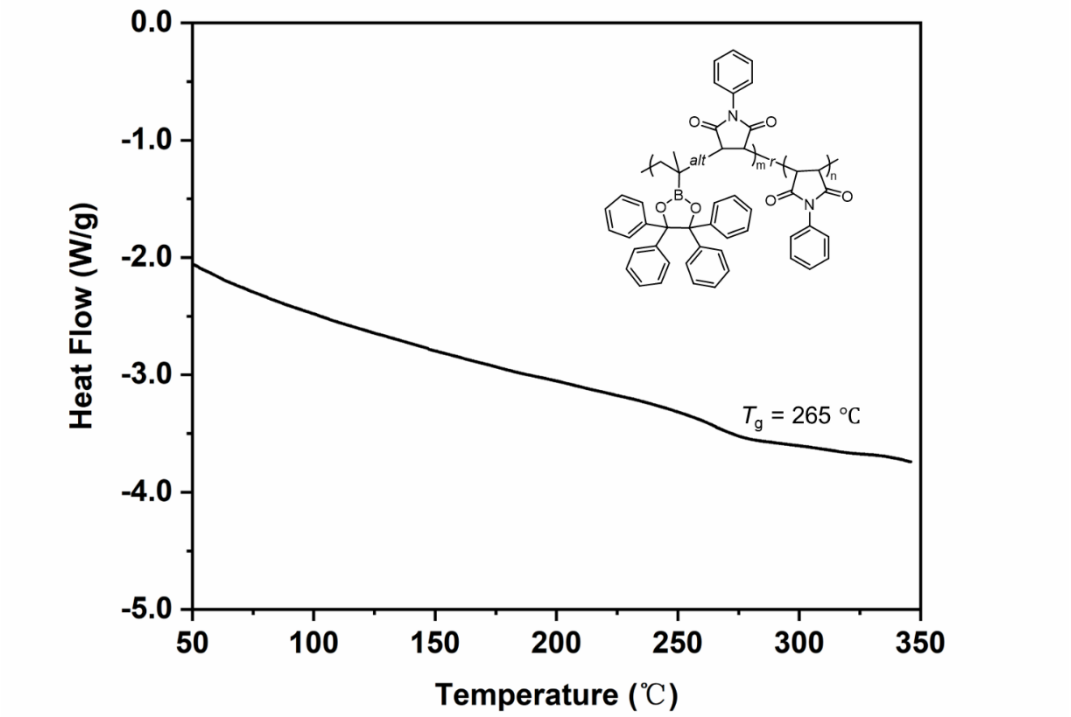


Figure S110. DSC Curves for Poly(NPMI-*co*-IB$_{Phpin}$).

Poly(AN-*co*-IB$_{Phpin}$)

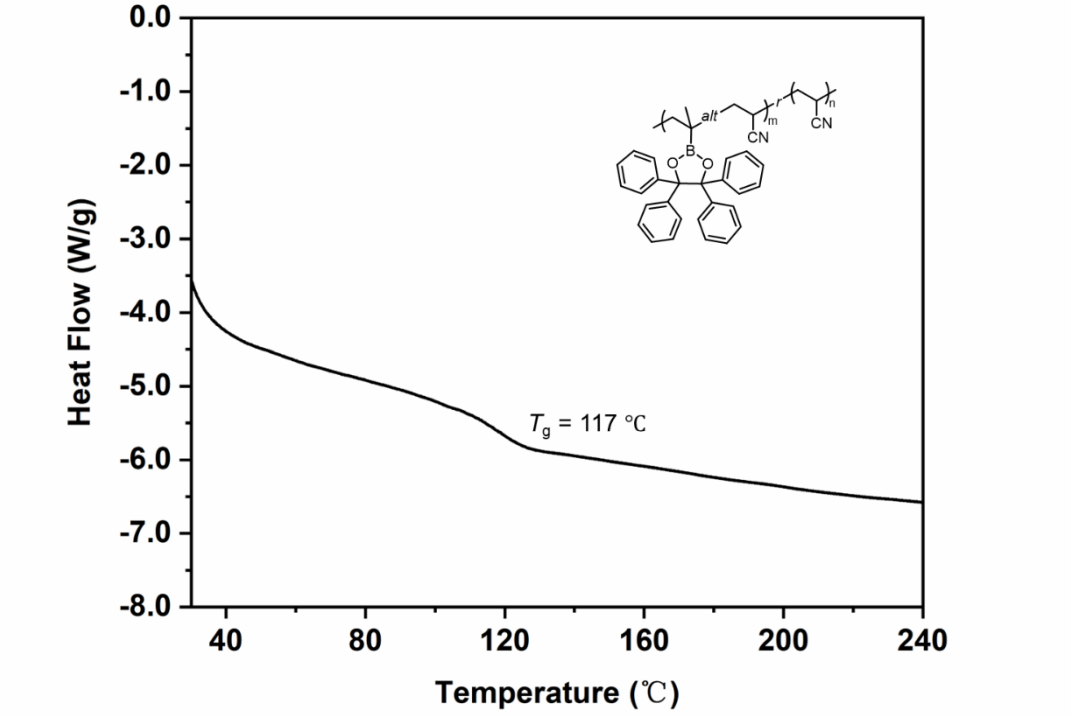


Figure S111. DSC Curves for Poly(AN-*co*-IB$_{Phpin}$).

Poly(VAc-*co*-IB$_{Phpin}$)

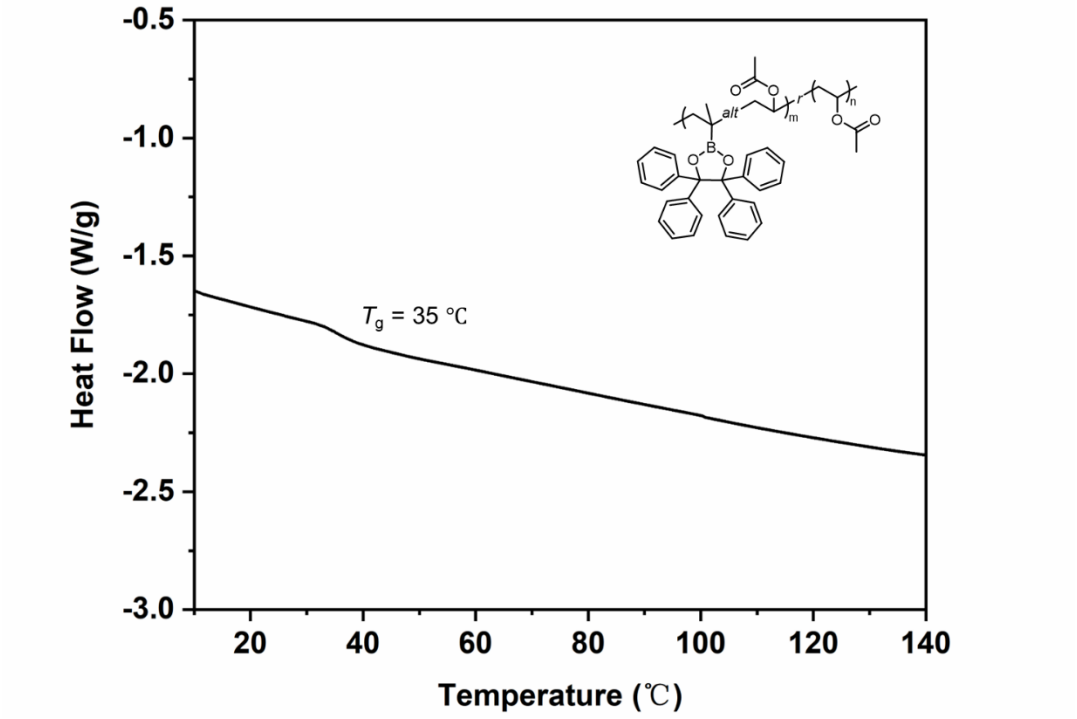


Figure S112. DSC Curves for Poly(VAc-*co*-IB$_{Phpin}$).

Poly(St-*co*-IB$_{Phpin}$)

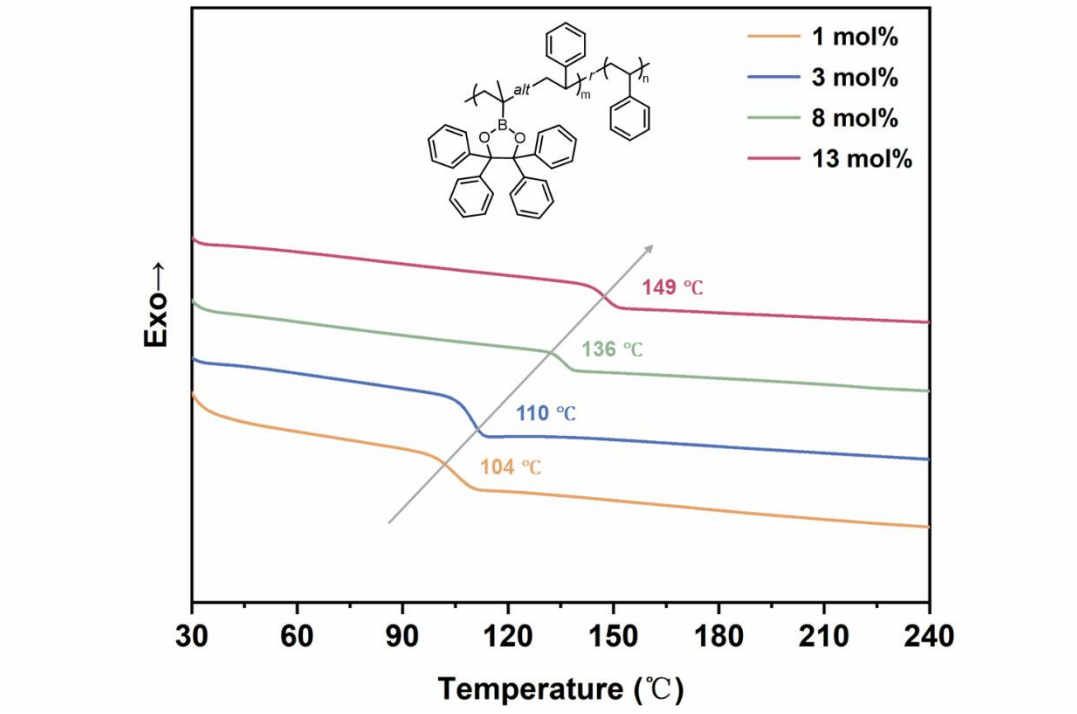


Figure S113. DSC Curves for Poly(St-*co*-IB$_{Phpin}$) with Different Proportions.

IX. TGA Data of the Polymers

PVB_{epin}

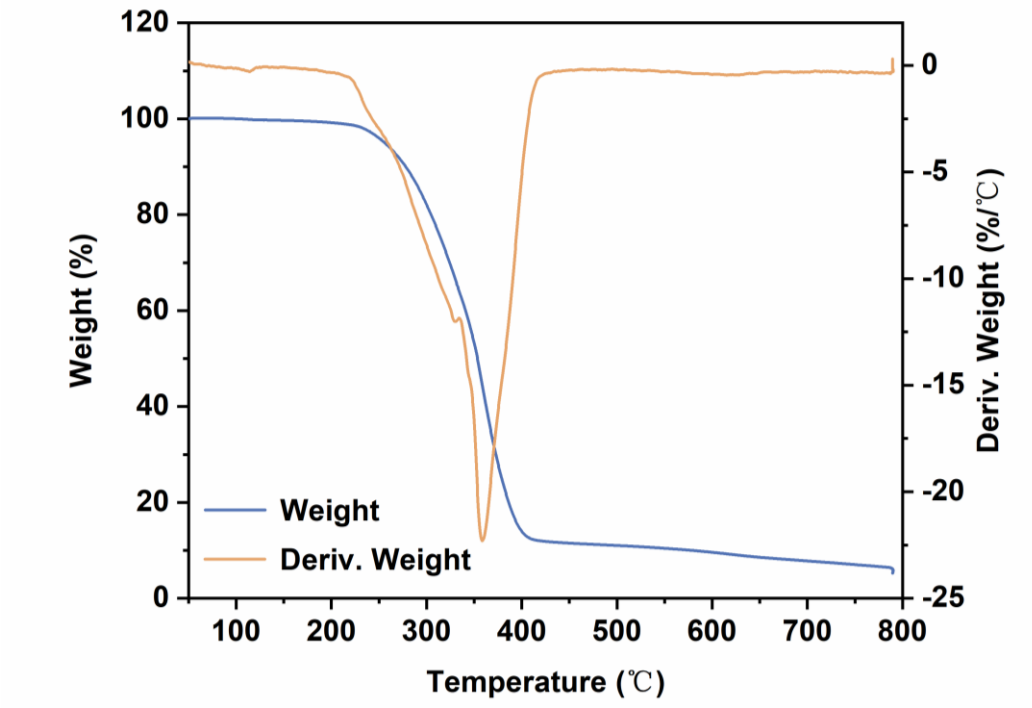


Figure S114. TGA Curves for PVB_{epin}.

PVB_{pnd}

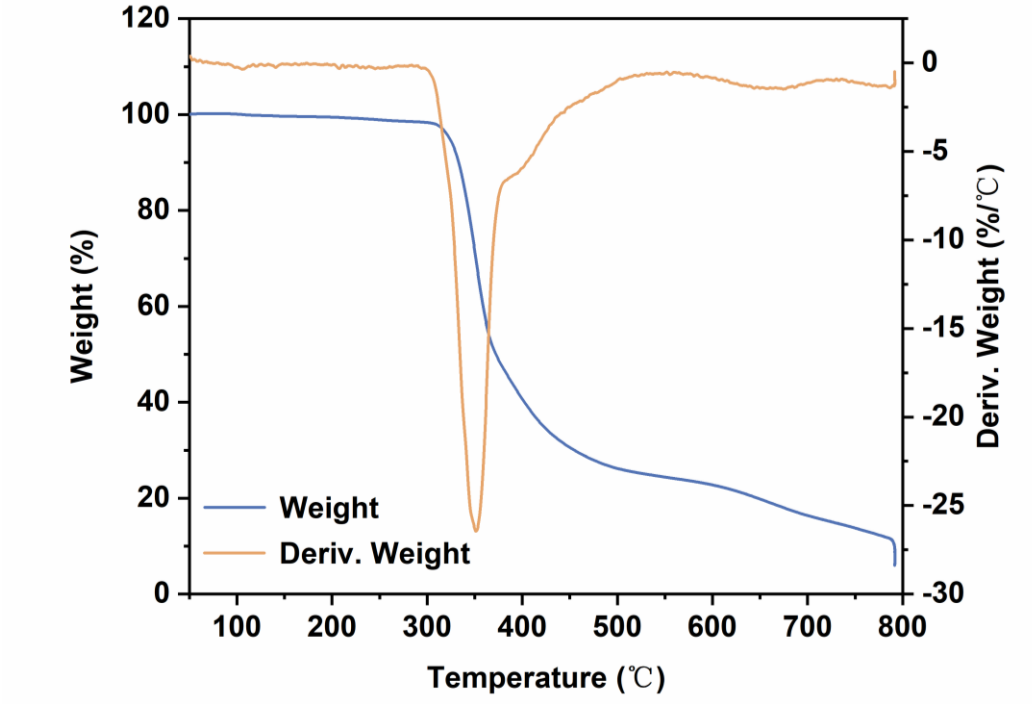


Figure S115. TGA Curves for PVB_{pnd}.

PVB_{Phpin}

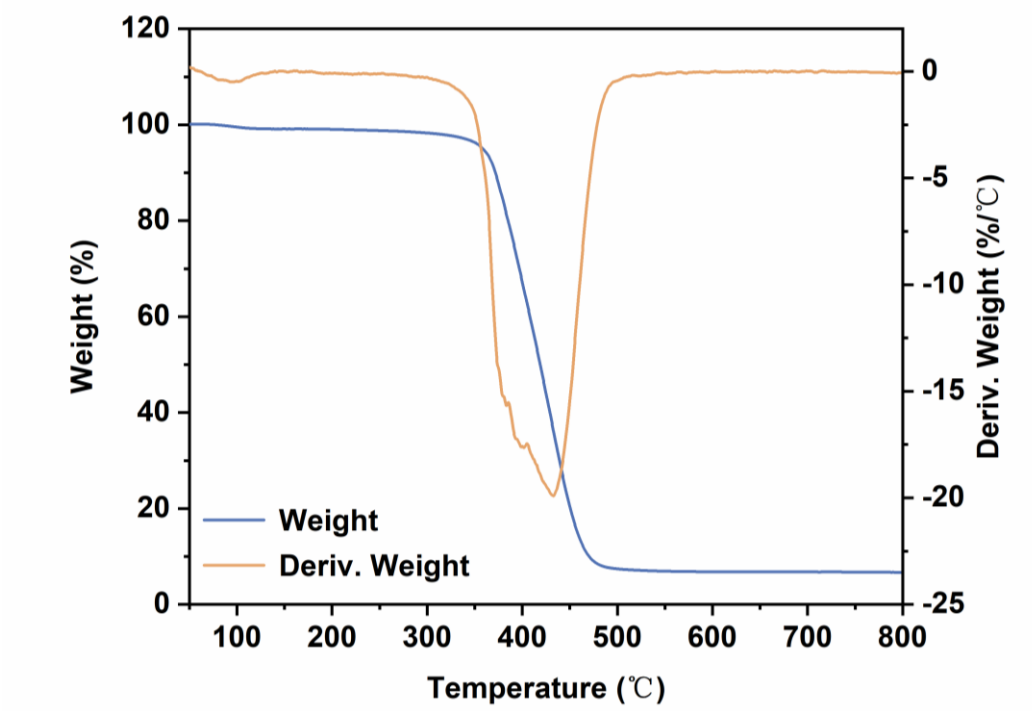


Figure S116. TGA Curves for PVB_{Phpin}.

PIB_{epin}

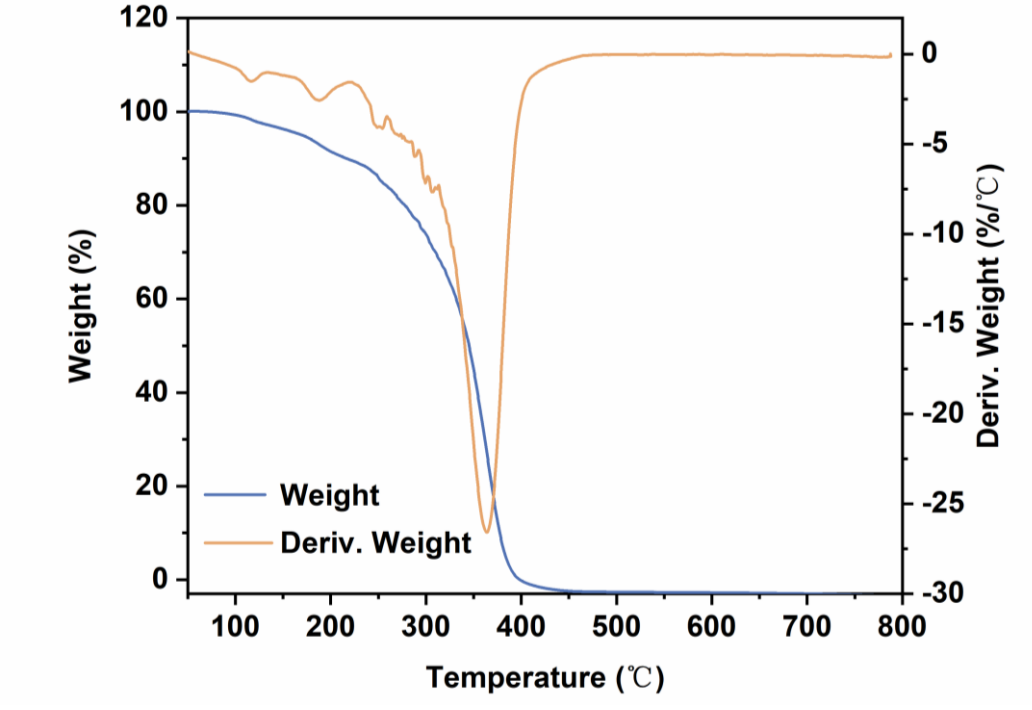


Figure S117. TGA Curves for PIB_{epin}.

PIB_{pnd}

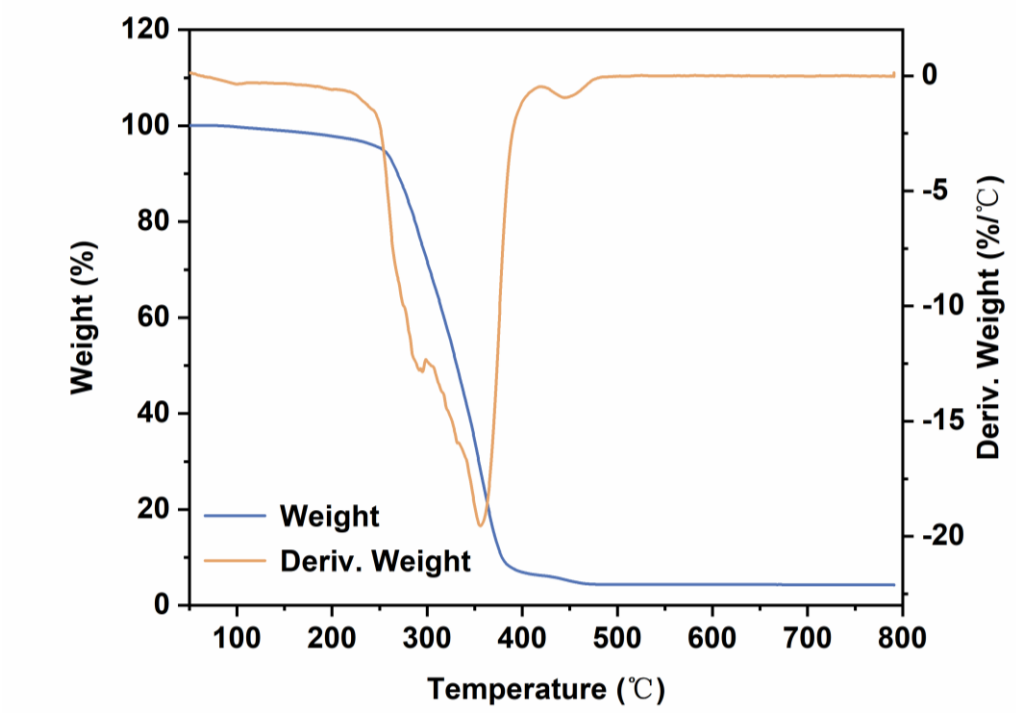


Figure S118. TGA Curves for PIB_{pnd}.

$PIB_{6\text{-}1}$

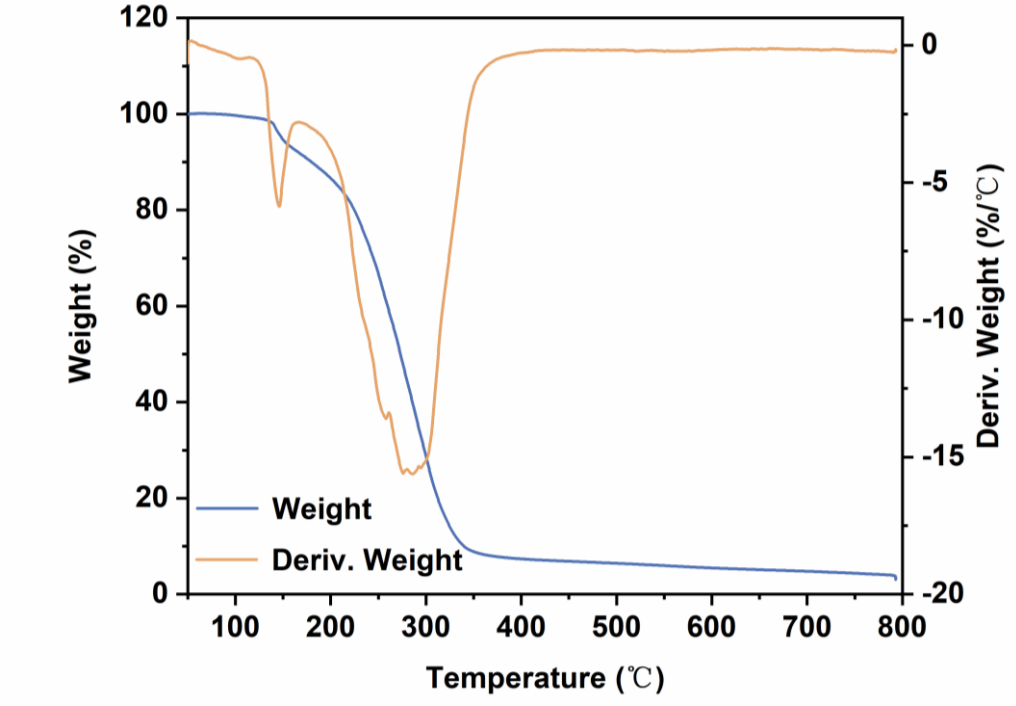


Figure S119. TGA Curves for $PIB_{6\text{-}1}$.

PIB$_{6\text{-}2}$

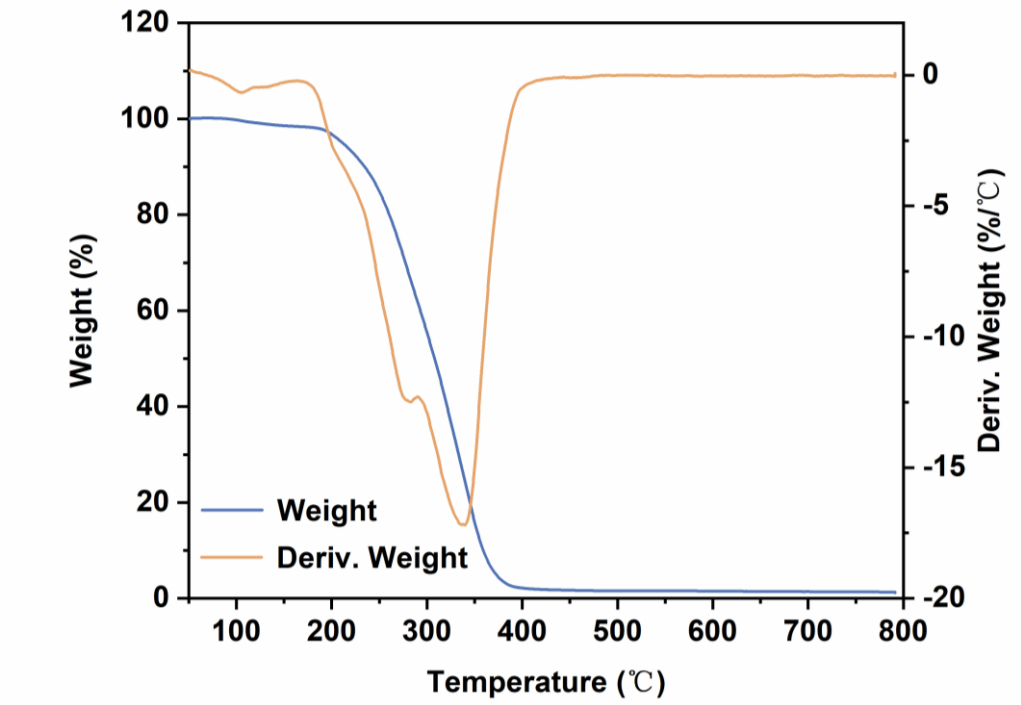


Figure S120. TGA Curves for PIB$_{6\text{-}2}$.

PIB$_{6\text{-}3}$

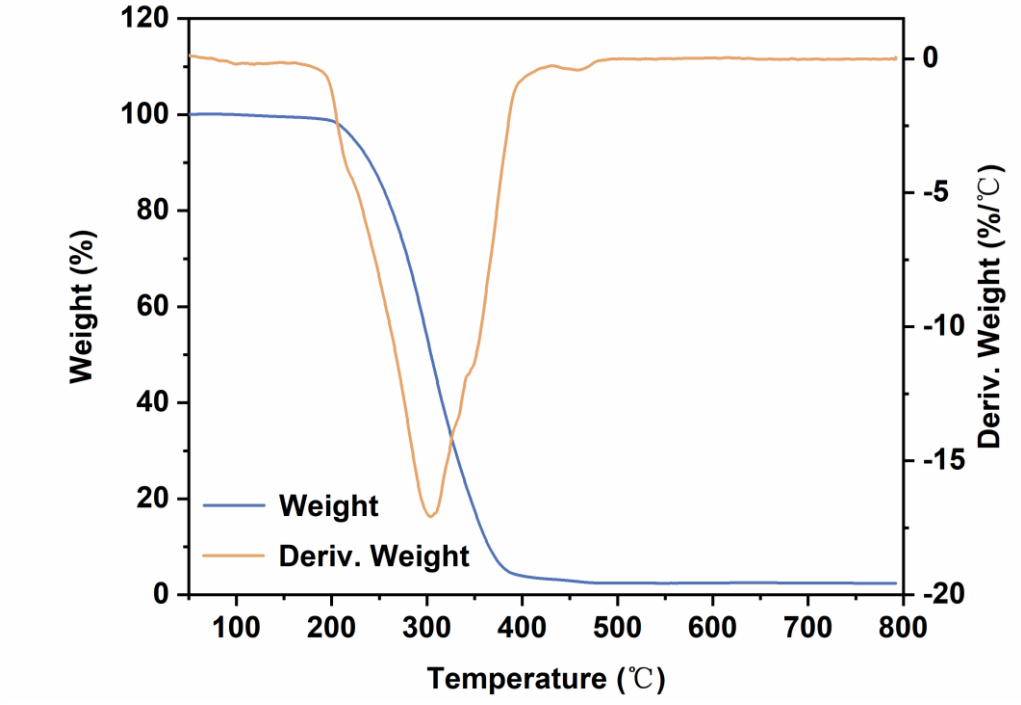


Figure S121. TGA Curves for PIB$_{6\text{-}3}$.

PIB$_{6\text{-}4}$

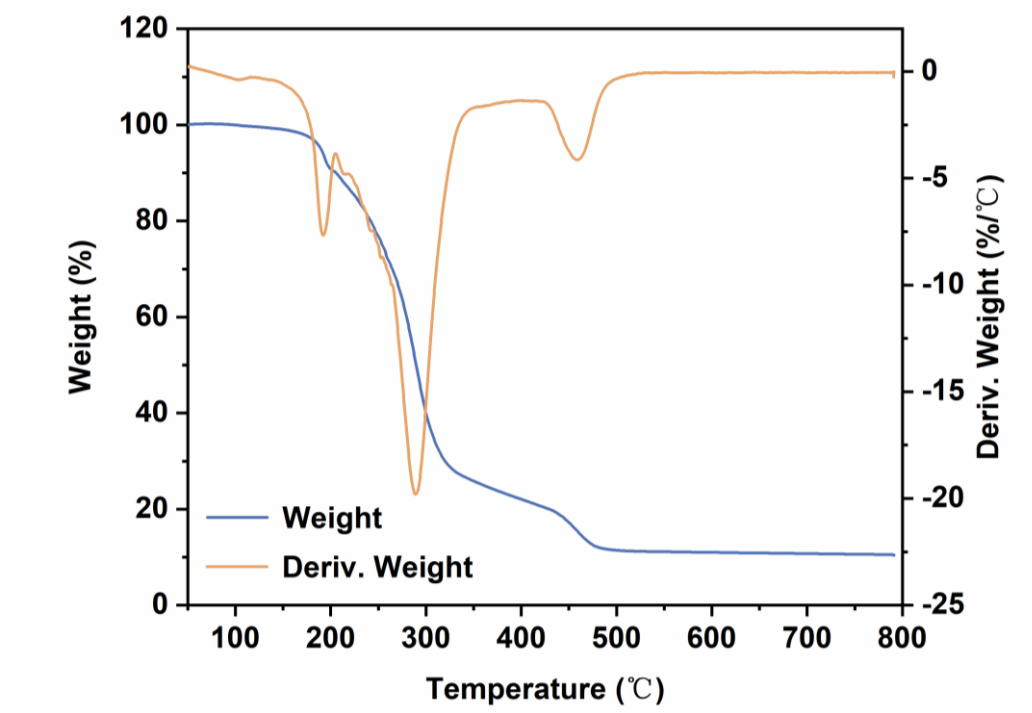


Figure S122. TGA Curves for PIB$_{6\text{-}4}$.

PIB$_{6\text{-}5}$

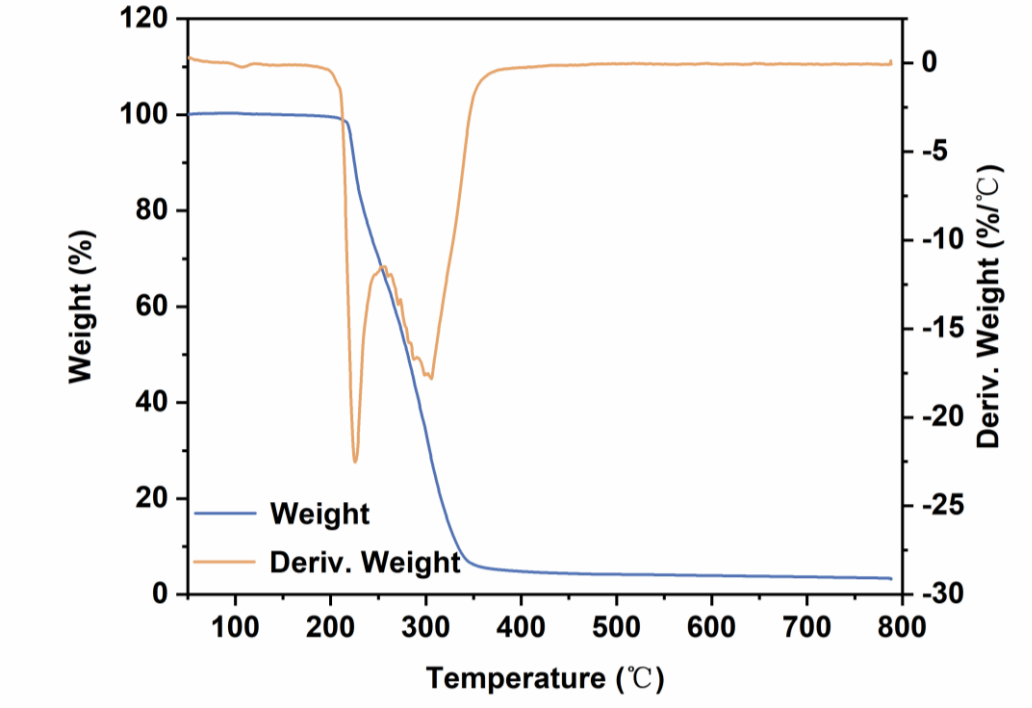


Figure S123. TGA Curves for PIB$_{6\text{-}5}$.

PIB$_{6\text{-}6}$

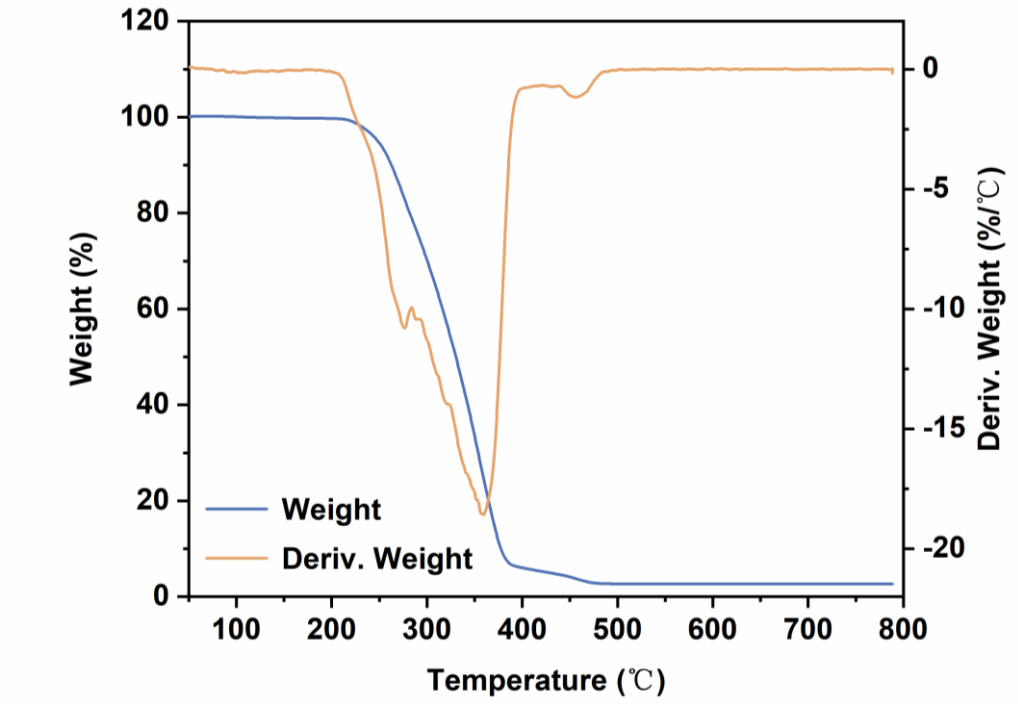


Figure S124. TGA Curves for PIB$_{6\text{-}6}$.

PIB$_{6\text{-}7}$

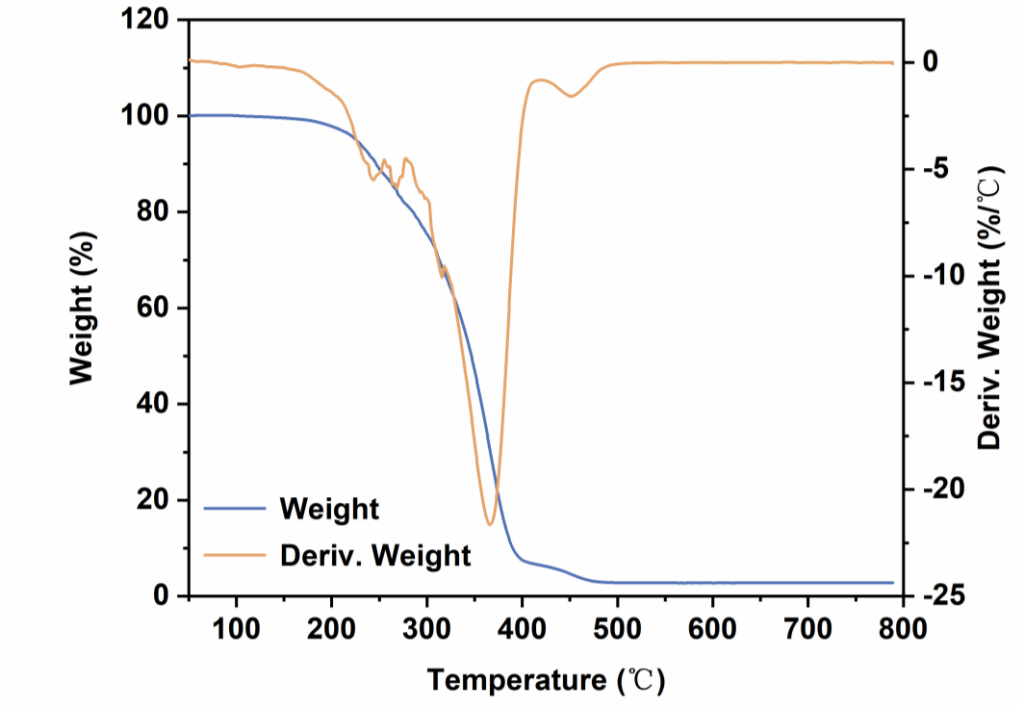


Figure S125. TGA Curves for PIB$_{6\text{-}7}$.

Poly(DMAA-*co*-IB$_{Phpin}$)

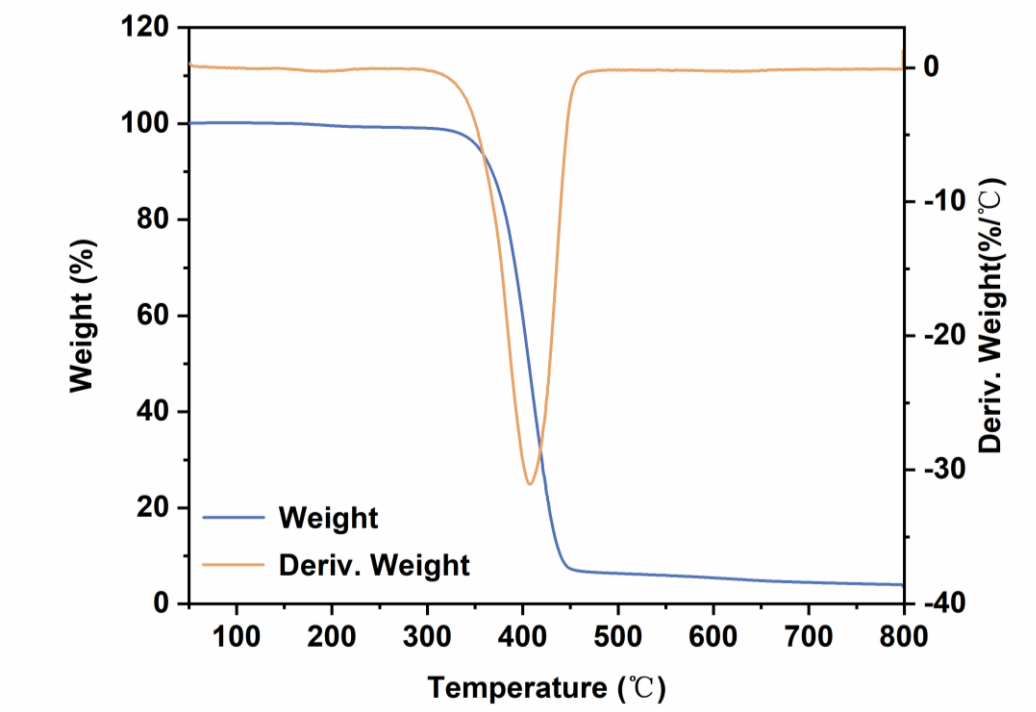


Figure S126. TGA Curves for Poly(DMAA-*co*-IB$_{Phpin}$).

Poly(*t*BA-*co*-IB$_{Phpin}$)

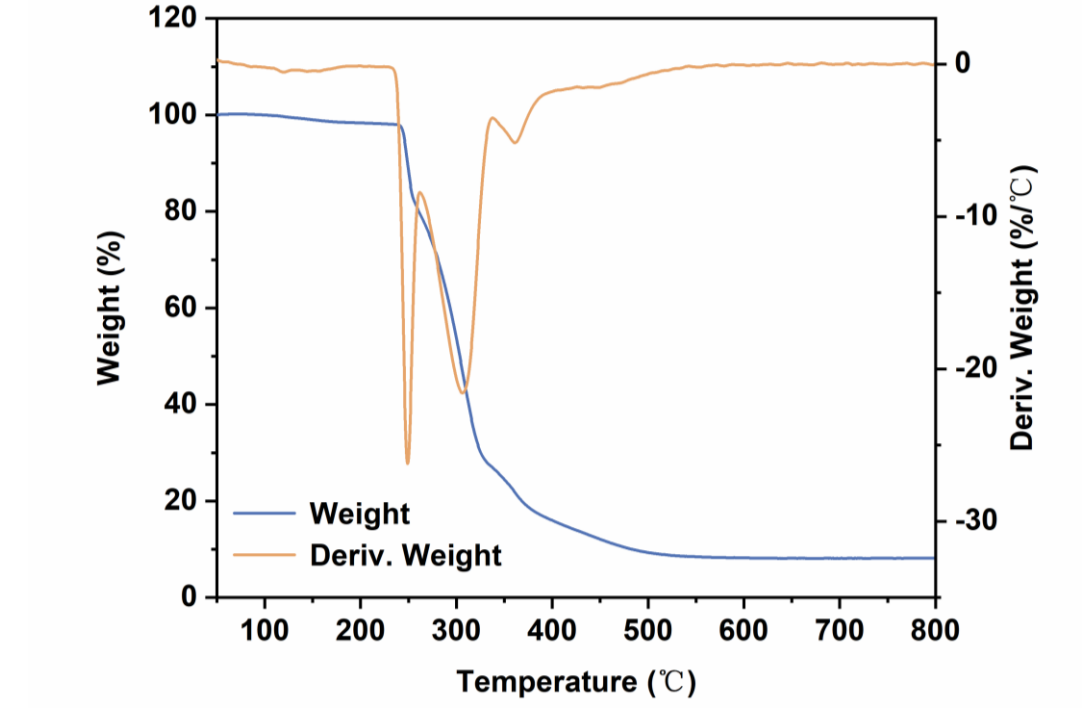


Figure S127. TGA Curves for Poly(*t*BA-*co*-IB$_{Phpin}$).

Poly(Diene-*co*-IB$_{Phpin}$)

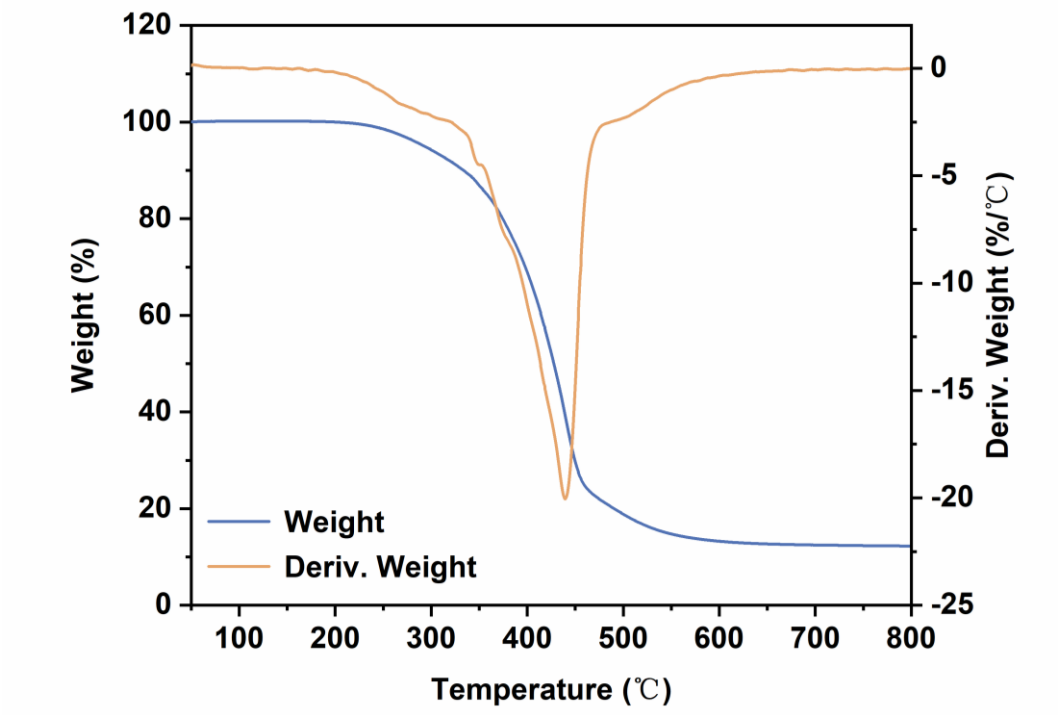


Figure S128. TGA Curves for Poly(Diene-*co*-IB$_{Phpin}$).

Poly(NPMI-*co*-IB$_{Phpin}$)

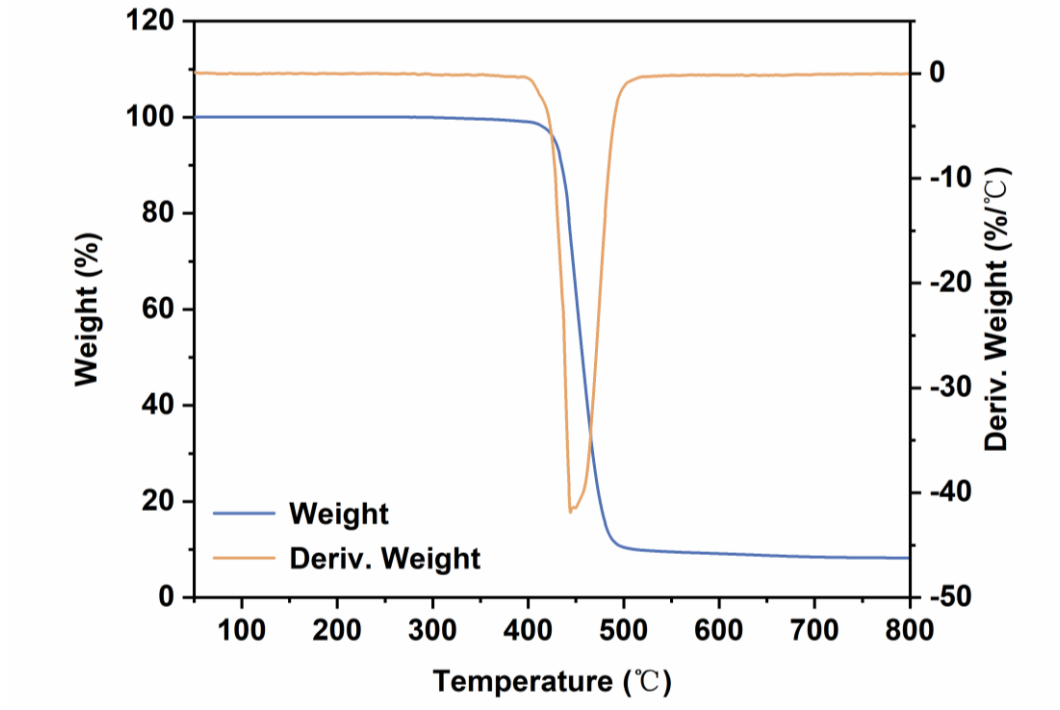


Figure S129. TGA Curves for Poly(NPMI-*co*-IB$_{Phpin}$).

Poly(AN-*co*-IB$_{Phpin}$)

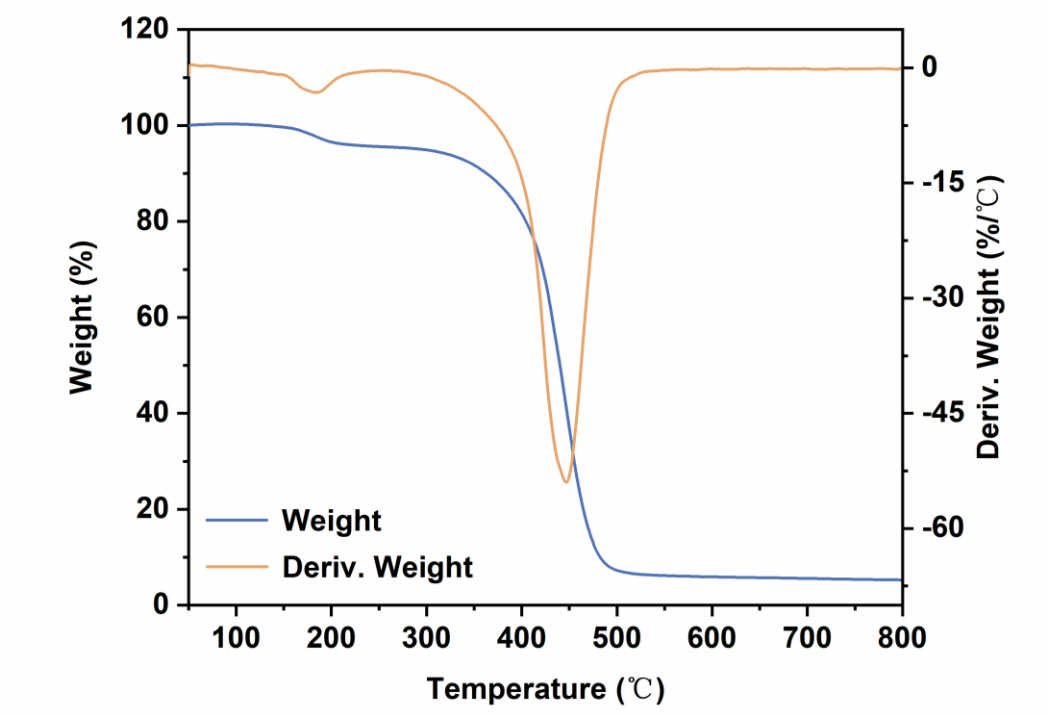


Figure S130. TGA Curves for Poly(AN-*co*-IB$_{Phpin}$).

Poly(VAc-*co*-IB$_{Phpin}$)

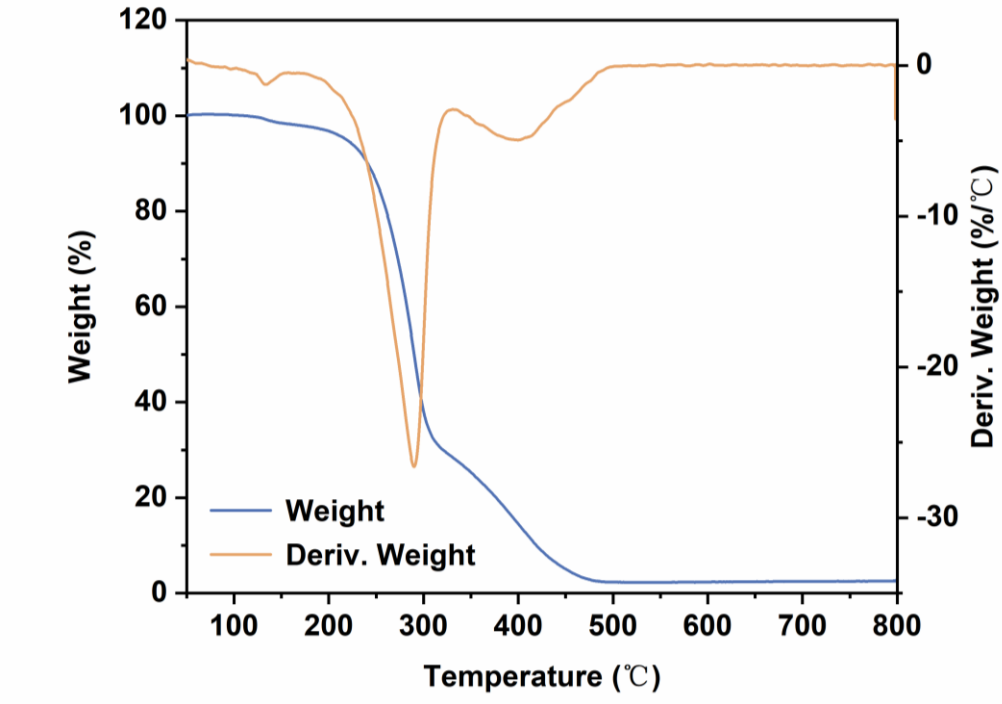


Figure S131. TGA Curves for Poly(VAc-*co*-IB$_{Phpin}$).

Poly(MAH-*co*-IB$_{Phpin}$)

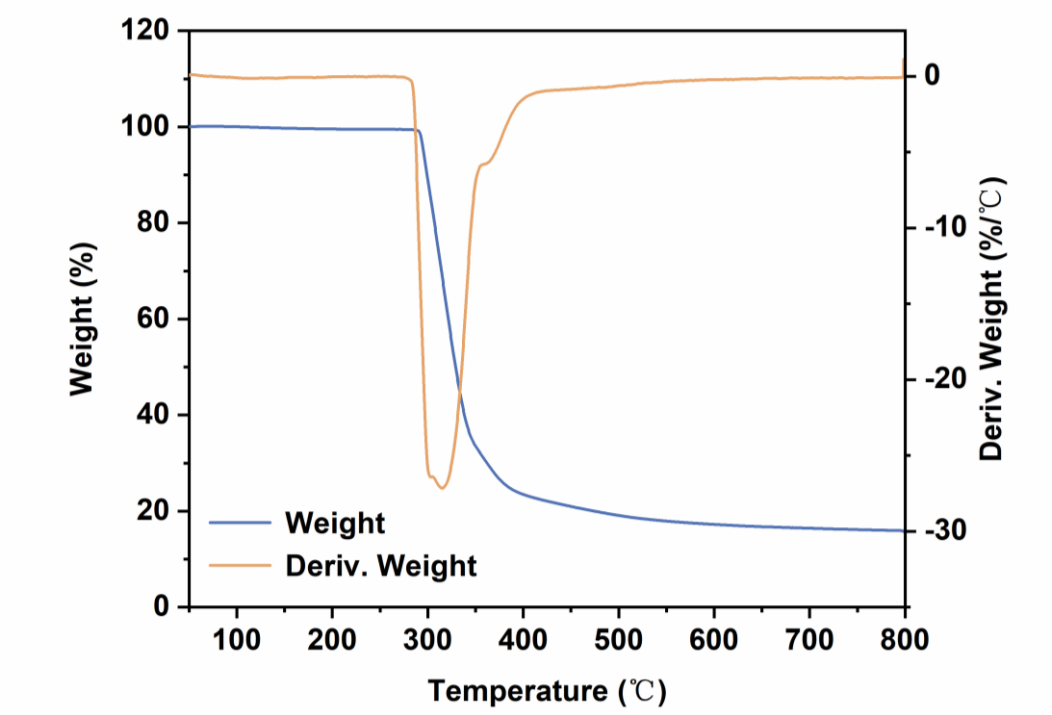


Figure S132. TGA Curves for Poly(MAH-*co*-IB$_{Phpin}$).

Poly(MMA-*co*-IB$_{Phpin}$)

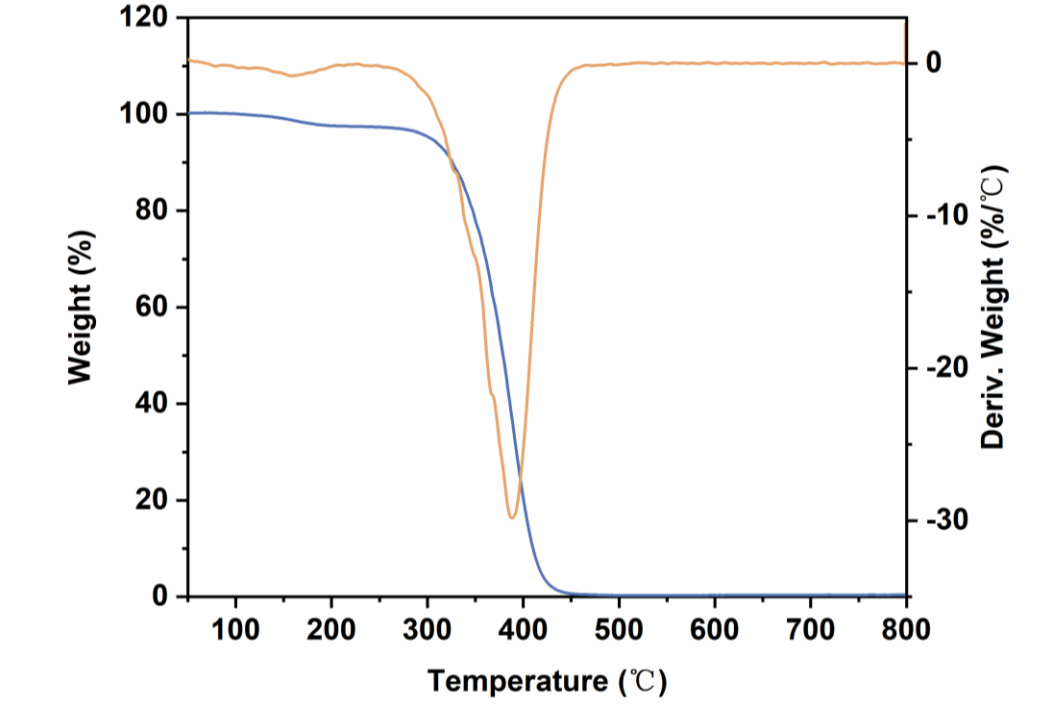


Figure S133. TGA Curves for Poly(MMA-*co*-IB$_{Phpin}$).

Poly(St-*co*-IB$_{Phpin}$)

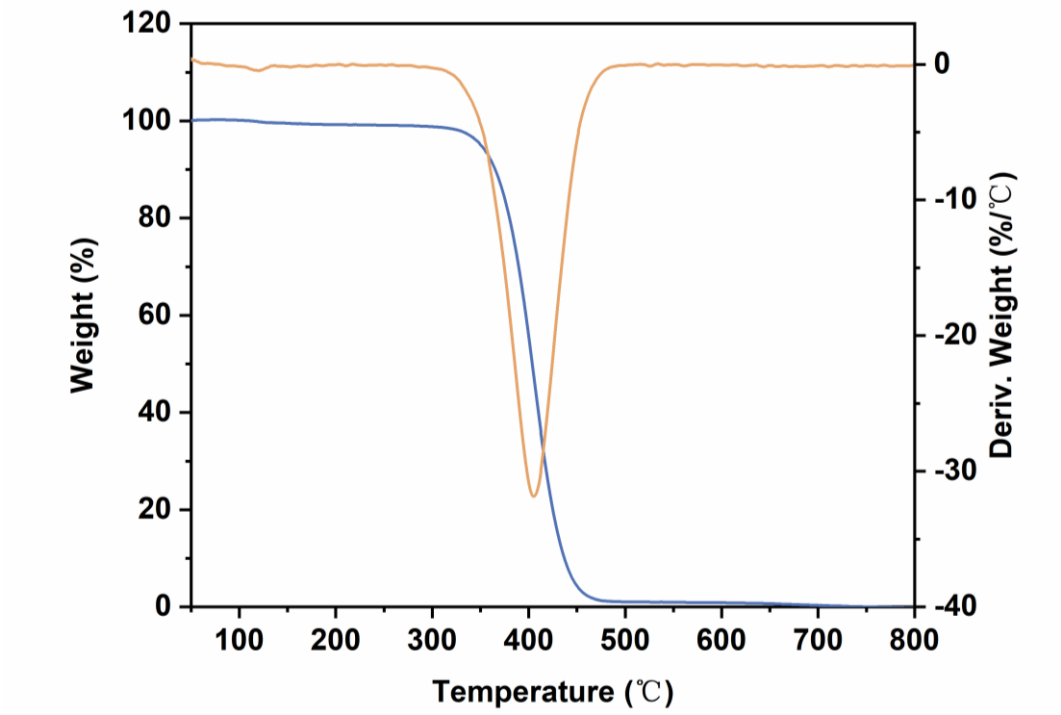


Figure S134. TGA Curves for Poly(St-*co*-IB$_{Phpin}$).

X. DFT Calculations Study for the Radical Polymerization Behavior

The calculations were carried out with DFT in the Gaussian 16A.03 program package.[4] The optimization of the structures was performed at density functional theory (DFT) (U)B3LYP with 6-31G(d) basis set. The Cartesian coordinates of the optimized structures and the corresponding electronic energies are presented for each species.

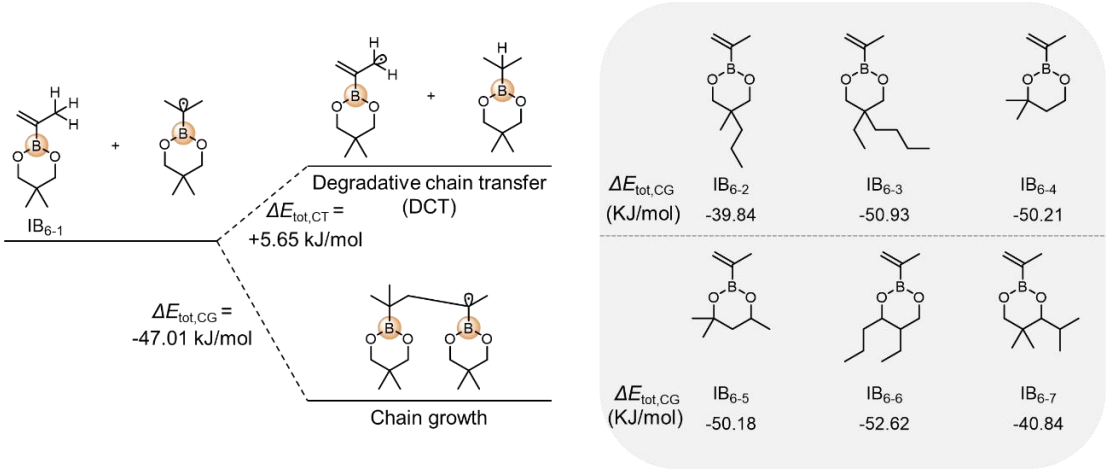
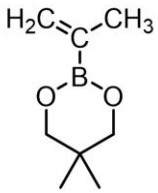
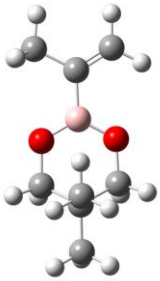


Figure S135. Calculated Energies for the Chain Growth Reactions of Monomers.

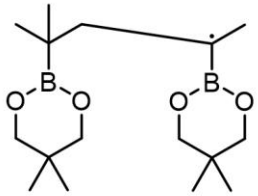
Cartesian Coordinates of the Structures Reported in the Manuscript:

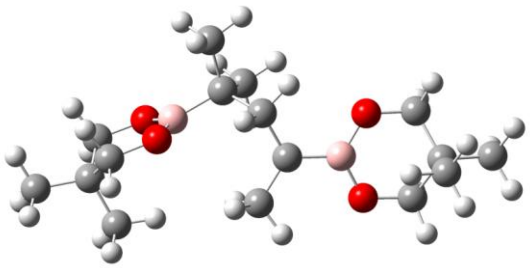




Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.195719	1.242357	0.471473
2	6	0	-1.112942	-1.227091	0.510350
3	6	0	-1.874857	-0.025584	-0.075934
4	1	0	-1.384278	1.333086	1.550952
5	1	0	-1.604099	2.137461	-0.012424
6	1	0	-1.456021	-2.162638	0.053081
7	1	0	-1.297754	-1.298448	1.591713
8	6	0	-1.818999	-0.047994	-1.614866
9	1	0	-2.291724	-0.956980	-2.005266
10	1	0	-2.351236	0.814450	-2.033153
11	1	0	-0.791377	-0.018906	-1.989066
12	6	0	-3.335769	-0.067410	0.397072
13	1	0	-3.896652	0.791911	0.010665
14	1	0	-3.836696	-0.975235	0.040278
15	1	0	-3.407547	-0.051490	1.491386
16	8	0	0.296601	-1.146599	0.297120
17	8	0	0.214225	1.252685	0.254145
18	5	0	0.914499	0.074436	0.192925
19	6	0	2.467505	0.102901	-0.021014
20	6	0	3.105531	1.279607	-0.116036
21	1	0	4.183931	1.345894	-0.262015
22	1	0	2.568170	2.222092	-0.050404
23	6	0	3.215410	-1.209004	-0.111088
24	1	0	3.071473	-1.810441	0.795557
25	1	0	2.842419	-1.822086	-0.941557
26	1	0	4.291327	-1.056226	-0.254235

Electronic Energy = -489.274958 Hartree

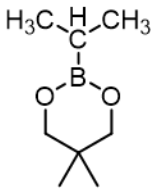


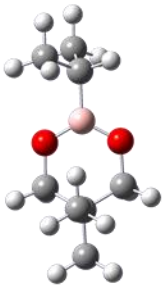


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.470220	0.233960	-1.111132
2	6	0	-4.678986	-0.869668	-0.059547
3	6	0	-4.138790	-0.327961	1.276155
4	1	0	-5.153623	1.072770	-0.916150
5	1	0	-4.690989	-0.145599	-2.115628
6	1	0	-4.802335	0.462296	1.655379
7	1	0	-4.109181	-1.124104	2.029201
8	6	0	-3.936427	-2.154330	-0.468957
9	1	0	-4.071486	-2.937118	0.286906
10	1	0	-4.323108	-2.536362	-1.421266
11	1	0	-2.862726	-1.986862	-0.587097
12	6	0	-6.181467	-1.159779	0.082039
13	1	0	-6.599266	-1.527028	-0.862948
14	1	0	-6.361007	-1.929247	0.842414
15	1	0	-6.742117	-0.262830	0.371948
16	8	0	-3.134811	0.740828	-1.136945
17	8	0	-2.817972	0.207182	1.176386
18	5	0	-2.372183	0.765189	0.003485
19	6	0	-0.992245	1.562046	-0.000599
20	6	0	0.099189	0.931927	0.934612
21	1	0	0.846820	1.709060	1.135484
22	1	0	-0.387158	0.697678	1.895027
23	6	0	-1.348145	2.954404	0.591014
24	1	0	-0.463981	3.606581	0.595459
25	1	0	-2.124821	3.456578	-0.000348
26	1	0	-1.708998	2.872868	1.623341
27	6	0	-0.433047	1.763137	-1.422099
28	1	0	0.488267	2.360219	-1.393118
29	1	0	-0.192259	0.809009	-1.904587
30	1	0	-1.156661	2.279618	-2.061862
31	6	0	0.802568	-0.294818	0.422246
32	6	0	0.011380	-1.560692	0.269326

33	1	0	-0.659514	-1.727545	1.123303
34	1	0	-0.636625	-1.519793	-0.623929
35	1	0	0.658840	-2.433831	0.145972
36	6	0	4.367893	0.994693	-0.209714
37	6	0	4.277098	-1.406457	-0.780876
38	6	0	5.103054	-0.345660	-0.031747
39	1	0	4.833551	1.773418	0.406832
40	1	0	4.435024	1.319805	-1.258677
41	1	0	4.676374	-2.410155	-0.589486
42	1	0	4.337743	-1.228094	-1.864954
43	5	0	2.294672	-0.256412	0.039334
44	8	0	2.906378	-1.415763	-0.395116
45	8	0	2.994583	0.927182	0.160519
46	6	0	5.218703	-0.705166	1.461078
47	1	0	5.729853	-1.666905	1.588630
48	1	0	5.795960	0.056685	1.998451
49	1	0	4.238459	-0.781431	1.940647
50	6	0	6.501804	-0.249350	-0.658938
51	1	0	7.103443	0.518585	-0.158027
52	1	0	7.038824	-1.201027	-0.566425
53	1	0	6.450669	0.005722	-1.724496

Electronic Energy = -979.148108 Hartree

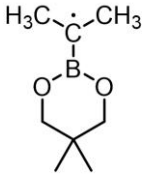


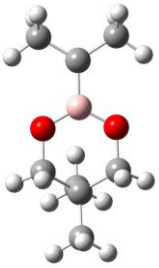


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.932973	-0.063197	0.025465
2	6	0	-1.062590	-0.317828	1.268633
3	6	0	-1.311718	1.134160	-0.715085
4	1	0	-1.187099	0.502896	1.989404
5	1	0	-1.364939	-1.245920	1.768007
6	1	0	-1.448665	2.052470	-0.126503
7	1	0	-1.802294	1.285250	-1.683840
8	6	0	-1.957571	-1.307377	-0.881891

9	1	0	-2.390688	-2.163670	-0.351542
10	1	0	-2.565361	-1.122177	-1.775412
11	1	0	-0.955133	-1.593387	-1.213957
12	6	0	-3.361076	0.293024	0.465270
13	1	0	-3.997408	0.501243	-0.403130
14	1	0	-3.818626	-0.536268	1.017845
15	1	0	-3.376133	1.177843	1.113190
16	8	0	0.325600	-0.440043	0.956618
17	8	0	0.083539	0.964732	-0.972459
18	5	0	0.857439	0.208695	-0.129170
19	6	0	2.414464	0.091746	-0.402970
20	1	0	2.600847	0.452469	-1.424368
21	6	0	3.188988	1.012327	0.567675
22	1	0	4.269776	0.964823	0.379421
23	1	0	2.881704	2.060601	0.466675
24	1	0	3.021575	0.714342	1.610197
25	6	0	2.923296	-1.358169	-0.293996
26	1	0	2.438335	-2.016146	-1.025931
27	1	0	4.006226	-1.413035	-0.467727
28	1	0	2.722659	-1.770455	0.701640

Electronic Energy = -490.501058 Hartree

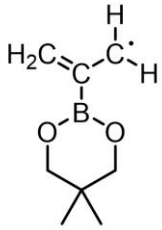


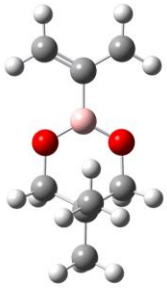


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.926986	-0.000011	-0.076532
2	6	0	-1.206727	-1.235223	0.492985
3	6	0	-1.206797	1.235560	0.492302
4	1	0	-1.394854	-1.310867	1.574333
5	1	0	-1.588340	-2.151936	0.027056
6	1	0	-1.395511	1.312239	1.573470
7	1	0	-1.588011	2.151914	0.025323
8	6	0	-3.389728	0.000122	0.392289
9	1	0	-3.920250	0.884386	0.019279

10	1	0	-3.920363	-0.884142	0.019445
11	1	0	-3.463886	0.000233	1.486606
12	6	0	-1.867126	-0.000481	-1.615275
13	1	0	-2.368664	-0.887039	-2.021230
14	1	0	-2.368830	0.885724	-2.021790
15	1	0	-0.837552	-0.000519	-1.985094
16	8	0	0.200922	-1.205210	0.275755
17	8	0	0.200993	1.205197	0.276002
18	5	0	0.867650	-0.000009	0.196783
19	6	0	2.394239	-0.000015	-0.006730
20	6	0	3.175242	-1.275979	-0.110293
21	1	0	3.715337	-1.337587	-1.069642
22	1	0	3.951779	-1.334246	0.670252
23	1	0	2.537769	-2.159653	-0.022166
24	6	0	3.175114	1.276017	-0.110592
25	1	0	3.715112	1.337472	-1.070011
26	1	0	2.537589	2.159666	-0.022603
27	1	0	3.951720	1.334557	0.669865

Electronic Energy = -489.855244 Hartree

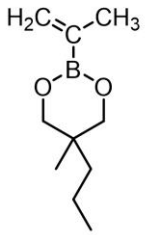


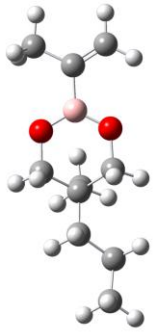


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.834293	0.000060	-0.076661
2	6	0	1.112927	1.234738	0.491511
3	6	0	1.113367	-1.236760	0.487559
4	1	0	1.296933	1.314776	1.572311
5	1	0	1.488613	2.151319	0.021994
6	1	0	1.300341	-1.322550	1.567369
7	1	0	1.486932	-2.151251	0.012254
8	6	0	3.295368	-0.000548	0.398103
9	1	0	3.826857	-0.884621	0.026330
10	1	0	3.827269	0.883711	0.027394
11	1	0	3.365415	-0.001259	1.492613
12	6	0	1.780693	0.002615	-1.615998

13	1	0	2.283346	0.890022	-2.018308
14	1	0	2.284960	-0.882525	-2.021263
15	1	0	0.753096	0.002368	-1.991551
16	8	0	-0.298125	-1.199317	0.275226
17	8	0	-0.297900	1.199300	0.274479
18	5	0	-0.955286	-0.000042	0.192166
19	6	0	-2.515311	-0.000032	-0.024066
20	6	0	-3.187822	1.217514	-0.115830
21	1	0	-2.657690	2.160782	-0.041199
22	1	0	-4.265157	1.261502	-0.264394
23	6	0	-3.187552	-1.217516	-0.116816
24	1	0	-4.264912	-1.261576	-0.265196
25	1	0	-2.657157	-2.160770	-0.043633

Electronic Energy = -488.626993 Hartree

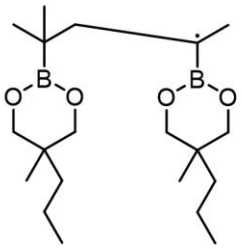


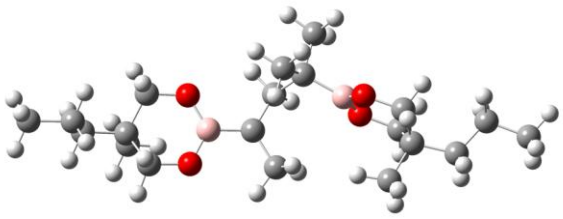


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.172043	-1.386673	-0.476359
2	6	0	-0.485986	1.063524	-0.393955
3	6	0	-1.031310	-0.270529	0.150326
4	1	0	-0.379175	-1.460716	-1.553401
5	1	0	-0.414971	-2.355904	-0.025046
6	1	0	-0.943967	1.914573	0.120751
7	1	0	-0.722291	1.155794	-1.464159
8	6	0	-2.492936	-0.486293	-0.310814
9	1	0	-2.803496	-1.494988	0.000852
10	1	0	-2.515723	-0.491453	-1.410947
11	6	0	-0.911584	-0.322720	1.685725
12	1	0	-1.430777	0.517954	2.157411
13	1	0	-1.347623	-1.250967	2.074447
14	1	0	0.132799	-0.286611	2.009366
15	6	0	-3.537639	0.522732	0.192134
16	1	0	-3.258884	1.539298	-0.115359

17	1	0	-3.556928	0.527624	1.288933
18	6	0	-4.942889	0.208559	-0.333685
19	1	0	-5.676504	0.934282	0.034609
20	1	0	-4.971949	0.231812	-1.429950
21	1	0	-5.271150	-0.788557	-0.015455
22	8	0	0.925665	1.196552	-0.228416
23	8	0	1.229535	-1.182129	-0.300147
24	5	0	1.734534	0.089857	-0.201827
25	6	0	3.284218	0.261569	-0.035002
26	6	0	3.812403	1.491584	0.058512
27	1	0	4.883988	1.656902	0.172831
28	1	0	3.187689	2.380323	0.023379
29	6	0	4.153762	-0.975441	0.012680
30	1	0	3.865026	-1.631497	0.843882
31	1	0	4.039087	-1.576044	-0.898710
32	1	0	5.214607	-0.724369	0.126839

Electronic Energy = -567.899128 Hartree



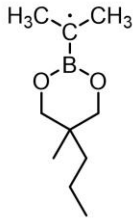


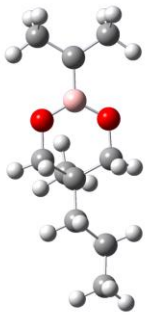
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.347310	0.405457	1.317771
2	6	0	4.658234	-0.739003	0.336387
3	6	0	4.210655	-0.274105	-1.062081
4	1	0	5.009709	1.261605	1.140447
5	1	0	4.501561	0.075249	2.351900
6	1	0	4.873108	0.514120	-1.440308
7	1	0	4.250056	-1.108890	-1.771875
8	6	0	3.875363	-2.002759	0.745405
9	1	0	4.073417	-2.823399	0.045603
10	1	0	4.175854	-2.334957	1.746272
11	1	0	2.796356	-1.831759	0.760472
12	6	0	6.169382	-1.090939	0.346410

13	1	0	6.411467	-1.488897	1.342967
14	1	0	6.318373	-1.931689	-0.347459
15	8	0	2.998319	0.870222	1.221587
16	8	0	2.873898	0.233760	-1.083699
17	5	0	2.326489	0.827712	0.026191
18	6	0	0.933691	1.591038	-0.107369
19	6	0	-0.058334	0.920311	-1.121775
20	1	0	-0.798914	1.678627	-1.404361
21	1	0	0.515837	0.676734	-2.029783
22	6	0	1.311546	2.980144	-0.693238
23	1	0	0.418149	3.612699	-0.787406
24	1	0	2.023666	3.509334	-0.046839
25	1	0	1.762321	2.888031	-1.688788
26	6	0	0.248046	1.805837	1.255635
27	1	0	-0.680210	2.380027	1.134146
28	1	0	-0.013152	0.855422	1.734950
29	1	0	0.901689	2.351078	1.944903
30	6	0	-0.783495	-0.309287	-0.647795
31	6	0	0.008596	-1.562521	-0.415589
32	1	0	0.758058	-1.723324	-1.202472
33	1	0	0.570209	-1.508867	0.533744
34	1	0	-0.635231	-2.444433	-0.346706
35	6	0	-4.403378	0.943062	-0.306828
36	6	0	-4.327431	-1.453409	0.301317
37	6	0	-5.103406	-0.411201	-0.525308
38	1	0	-4.829332	1.705462	-0.971037
39	1	0	-4.543372	1.288504	0.725752
40	1	0	-4.697961	-2.463881	0.087729
41	1	0	-4.461848	-1.272255	1.375752
42	5	0	-2.301191	-0.285549	-0.380411
43	8	0	-2.929953	-1.447443	0.020382
44	8	0	-3.003793	0.886898	-0.571071
45	6	0	-5.052464	-0.788618	-2.020230
46	1	0	-5.528072	-1.762254	-2.188666
47	1	0	-5.586227	-0.044851	-2.623881
48	1	0	-4.027271	-0.848714	-2.395434
49	6	0	-6.592159	-0.349624	-0.096649
50	1	0	-7.098556	0.372331	-0.754567
51	1	0	-7.046148	-1.324612	-0.328675
52	6	0	7.191459	0.006783	0.004055
53	1	0	6.992053	0.421080	-0.992323
54	1	0	7.103889	0.844613	0.707252
55	6	0	8.629563	-0.524401	0.042256
56	1	0	9.350923	0.264041	-0.199475

57	1	0	8.881928	-0.914844	1.035744
58	1	0	8.770864	-1.339006	-0.678557
59	6	0	-6.929674	0.005832	1.361623
60	1	0	-6.516058	0.988185	1.622424
61	1	0	-6.466282	-0.713562	2.048543
62	6	0	-8.443297	0.023000	1.607078
63	1	0	-8.674621	0.276577	2.647641
64	1	0	-8.940898	0.760224	0.965092
65	1	0	-8.890834	-0.955636	1.394336

Electronic Energy = -1136.393682 Hartree

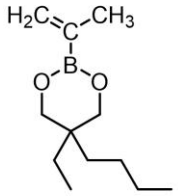


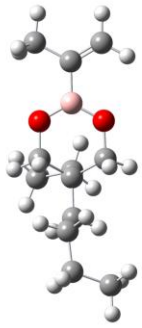


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.250613	-1.421822	-0.468666
2	6	0	-1.085739	-0.282993	0.150773
3	6	0	-0.512116	1.034562	-0.404841
4	1	0	-0.458496	-1.492315	-1.546657
5	1	0	-0.523160	-2.383532	-0.017035
6	1	0	-0.748510	1.120273	-1.476207
7	1	0	-0.954935	1.899640	0.100531
8	6	0	-2.552227	-0.470836	-0.306623
9	1	0	-2.884558	-1.469606	0.014579
10	1	0	-2.576633	-0.485591	-1.406666
11	6	0	-0.964582	-0.326008	1.686179
12	1	0	-1.465143	0.528963	2.152562
13	1	0	-1.419321	-1.241973	2.082786
14	1	0	0.081209	-0.309869	2.006680
15	6	0	-3.574128	0.565280	0.187989
16	1	0	-3.274158	1.572528	-0.130002
17	1	0	-3.591110	0.581512	1.284757
18	6	0	-4.986962	0.276475	-0.332037
19	1	0	-5.704163	1.021508	0.030147

20	1	0	-5.017663	0.289269	-1.428455
21	1	0	-5.336063	-0.710127	-0.003297
22	8	0	0.899927	1.141034	-0.240396
23	8	0	1.151674	-1.253604	-0.285753
24	5	0	1.691481	0.012979	-0.204016
25	6	0	3.215466	0.170149	-0.045815
26	6	0	3.861815	1.519066	0.060865
27	1	0	4.423554	1.620018	1.004347
28	1	0	4.602160	1.672685	-0.741626
29	1	0	3.132916	2.332234	0.010933
30	6	0	4.128388	-1.018329	0.008336
31	1	0	4.701926	-1.039596	0.949884
32	1	0	3.584296	-1.962446	-0.079152
33	1	0	4.881836	-0.981173	-0.795790

Electronic Energy = -568.479381 Hartree

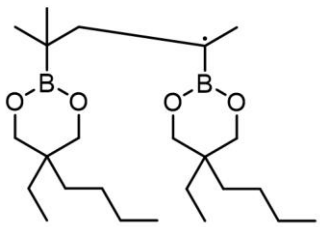


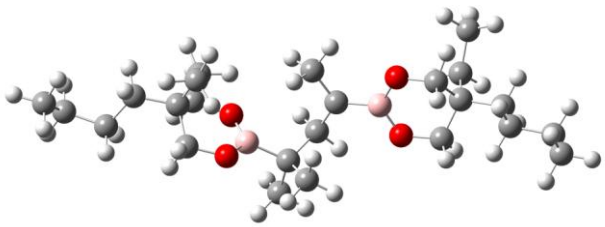


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.136618	-0.954938	-0.873832
2	6	0	-0.603453	0.377638	-0.254175
3	6	0	0.066243	0.471388	1.126888
4	1	0	-0.160763	1.422448	1.618814
5	1	0	-0.595674	-1.808035	-0.358599
6	1	0	-0.432403	-1.006946	-1.928987
7	1	0	-0.293991	-0.331539	1.781323
8	5	0	2.046261	-0.455836	0.095016
9	8	0	1.490132	0.369342	1.040437
10	8	0	1.281685	-1.122309	-0.828547
11	6	0	-0.147256	1.535006	-1.191750
12	1	0	-0.786585	1.499361	-2.084991
13	1	0	0.868931	1.331775	-1.547979
14	6	0	-0.178092	2.950276	-0.602323

15	1	0	0.564593	3.069114	0.193636
16	1	0	0.056579	3.685886	-1.379724
17	1	0	-1.160076	3.213527	-0.191914
18	6	0	-2.151808	0.398275	-0.143686
19	1	0	-2.546899	0.168859	-1.142973
20	1	0	-2.471050	1.427368	0.069640
21	6	0	-2.818952	-0.525501	0.891359
22	1	0	-2.478116	-1.562416	0.763321
23	1	0	-2.513887	-0.225944	1.901979
24	6	0	-4.357734	-0.501510	0.829644
25	1	0	-4.746879	-1.029031	1.710468
26	1	0	-4.706467	0.537259	0.920145
27	6	0	-4.958981	-1.136379	-0.430147
28	1	0	-6.053886	-1.132789	-0.384901
29	1	0	-4.669098	-0.602018	-1.341771
30	1	0	-4.634876	-2.179037	-0.538870
31	6	0	3.606245	-0.616116	0.074046
32	6	0	4.183895	-1.404228	-0.845659
33	1	0	3.593063	-1.938082	-1.585440
34	1	0	5.263843	-1.545989	-0.893947
35	6	0	4.428641	0.126611	1.103915
36	1	0	4.267666	1.210072	1.033477
37	1	0	4.136360	-0.155422	2.123472
38	1	0	5.500992	-0.068640	0.987942

Electronic Energy = -646.520528 Hartree



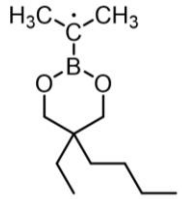


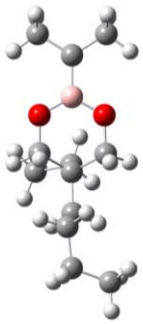
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.384793	-0.983270	0.857906
2	6	0	-4.694950	0.415507	0.301519
3	6	0	-4.224809	0.420634	-1.167461
4	1	0	-4.990621	-1.739878	0.344718

5	1	0	-4.616054	-1.048409	1.925582
6	1	0	-4.900918	-0.171610	-1.796672
7	1	0	-4.222449	1.445314	-1.558724
8	6	0	-3.915394	1.524233	1.066703
9	1	0	-4.315901	2.491774	0.732561
10	1	0	-2.868367	1.511637	0.747634
11	6	0	-6.214377	0.730979	0.368619
12	1	0	-6.464476	0.986472	1.405190
13	1	0	-6.382051	1.652115	-0.210774
14	8	0	-3.007819	-1.339080	0.701236
15	8	0	-2.902562	-0.097373	-1.342980
16	5	0	-2.338466	-0.958772	-0.435423
17	6	0	-0.932488	-1.631383	-0.769133
18	6	0	0.047008	-0.695149	-1.561502
19	1	0	0.796648	-1.337876	-2.039382
20	1	0	-0.533095	-0.220586	-2.368627
21	6	0	-1.288529	-2.816024	-1.710299
22	1	0	-0.385220	-3.386008	-1.967764
23	1	0	-1.992285	-3.510930	-1.234034
24	1	0	-1.740639	-2.465162	-2.645849
25	6	0	-0.241548	-2.196589	0.486907
26	1	0	0.696629	-2.699809	0.217658
27	1	0	0.003269	-1.407659	1.207314
28	1	0	-0.885100	-2.919546	0.999493
29	6	0	0.758414	0.366443	-0.768306
30	6	0	-0.044183	1.512703	-0.226605
31	1	0	-0.766905	1.887841	-0.964588
32	1	0	-0.638401	1.204611	0.651487
33	1	0	0.593878	2.338624	0.101537
34	6	0	4.390708	-0.916369	-0.772259
35	6	0	4.270161	1.160056	0.549699
36	6	0	5.073051	0.448799	-0.552653
37	1	0	4.802625	-1.406505	-1.663809
38	1	0	4.570255	-1.581846	0.082328
39	1	0	4.656920	2.167192	0.737975
40	1	0	4.343346	0.600376	1.491148
41	5	0	2.271468	0.274274	-0.490324
42	8	0	2.891337	1.291218	0.209353
43	8	0	2.981471	-0.810581	-0.963923
44	6	0	5.025414	1.236738	-1.894954
45	1	0	5.749076	0.764867	-2.574586
46	1	0	4.044129	1.093195	-2.360799
47	6	0	6.554059	0.242733	-0.138722
48	1	0	7.017064	-0.411843	-0.892736

49	1	0	7.076942	1.204604	-0.225802
50	6	0	-7.199507	-0.344386	-0.124629
51	1	0	-6.887072	-0.722095	-1.107089
52	1	0	-7.184786	-1.208451	0.553790
53	6	0	-8.648565	0.161509	-0.242466
54	1	0	-9.254592	-0.627992	-0.706412
55	1	0	-8.677213	1.014120	-0.936028
56	6	0	6.848730	-0.333364	1.257168
57	1	0	6.283637	-1.261242	1.421610
58	1	0	6.516772	0.367826	2.034738
59	6	0	8.342844	-0.622037	1.462895
60	1	0	8.681172	-1.336898	0.699443
61	1	0	8.916494	0.299832	1.290586
62	6	0	8.664434	-1.171220	2.856363
63	1	0	8.130568	-2.110669	3.045488
64	1	0	9.736312	-1.369007	2.970043
65	1	0	8.371824	-0.461623	3.640059
66	6	0	5.307958	2.741952	-1.818423
67	1	0	6.262749	2.966227	-1.328160
68	1	0	5.353045	3.167975	-2.827033
69	1	0	4.516356	3.269607	-1.276136
70	6	0	-9.293758	0.564516	1.089004
71	1	0	-8.781356	1.414456	1.553378
72	1	0	-10.341111	0.852998	0.945051
73	1	0	-9.274036	-0.267170	1.804698
74	6	0	-3.953246	1.462082	2.598492
75	1	0	-3.469007	2.349167	3.021756
76	1	0	-4.975482	1.430447	2.993780
77	1	0	-3.416806	0.585994	2.978032

Electronic Energy = -1293.640707 Hartree

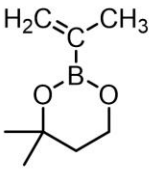


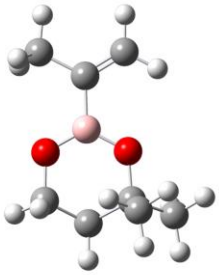


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.155094	-0.952121	-0.835508
2	6	0	-0.653291	0.385561	-0.251983
3	6	0	-0.000283	0.522449	1.133926
4	1	0	-0.260823	1.475596	1.605784
5	1	0	-0.607107	-1.800174	-0.304751
6	1	0	-0.440537	-1.034485	-1.892039
7	1	0	-0.349879	-0.278095	1.798307
8	5	0	2.011679	-0.390117	0.148914
9	8	0	1.423558	0.458791	1.064085
10	8	0	1.263343	-1.094087	-0.771449
11	6	0	3.544516	-0.541592	0.141098
12	6	0	4.244326	-1.431049	-0.842714
13	1	0	4.837600	-2.206170	-0.329914
14	1	0	3.545423	-1.930221	-1.519012
15	1	0	4.965549	-0.862864	-1.453389
16	6	0	4.412722	0.192713	1.118807
17	1	0	3.829918	0.812688	1.805113
18	1	0	5.019283	-0.505747	1.718787
19	1	0	5.136965	0.843200	0.600879
20	6	0	-0.206455	1.529298	-1.210098
21	1	0	-0.835106	1.463752	-2.109349
22	1	0	0.817046	1.334782	-1.549669
23	6	0	-0.266703	2.956192	-0.651848
24	1	0	0.464712	3.102716	0.149823
25	1	0	-0.034672	3.679155	-1.441935
26	1	0	-1.257512	3.212196	-0.258271
27	6	0	-2.202804	0.381120	-0.159564
28	1	0	-2.582628	0.120685	-1.157263
29	1	0	-2.542666	1.409201	0.025348
30	6	0	-2.865629	-0.529019	0.890226
31	1	0	-2.506441	-1.562781	0.790065
32	1	0	-2.575752	-0.200886	1.896407
33	6	0	-4.403874	-0.532108	0.812819
34	1	0	-4.793578	-1.045662	1.701678
35	1	0	-4.770584	0.502530	0.875682
36	6	0	-4.981695	-1.205582	-0.437876
37	1	0	-6.076968	-1.219111	-0.403832
38	1	0	-4.690858	-0.687580	-1.358582
39	1	0	-4.639414	-2.244936	-0.519225

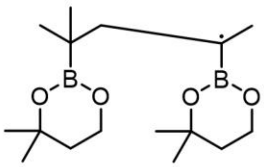
Electronic Energy = -647.100780 Hartree

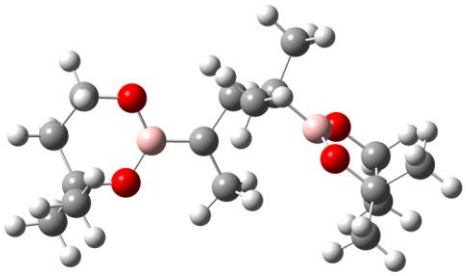




Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.721523	1.025493	-0.637149
2	6	0	-1.631543	-0.378155	-0.007486
3	6	0	-0.720133	1.993000	-0.011916
4	1	0	-1.510127	0.941271	-1.711018
5	1	0	-2.738699	1.423169	-0.535594
6	1	0	-0.999633	2.241490	1.020482
7	1	0	-0.687039	2.932075	-0.575057
8	6	0	-2.141866	-0.403698	1.439931
9	1	0	-3.209417	-0.158723	1.482365
10	1	0	-1.998444	-1.402191	1.864683
11	1	0	-1.599675	0.308008	2.071134
12	6	0	-2.383476	-1.404558	-0.858255
13	1	0	-2.272205	-2.405352	-0.428405
14	1	0	-3.451446	-1.164034	-0.908412
15	1	0	-1.982275	-1.423986	-1.876827
16	8	0	-0.250167	-0.799799	0.003649
17	8	0	0.600104	1.453174	-0.008817
18	5	0	0.790411	0.093396	0.001511
19	6	0	2.266736	-0.439088	0.003420
20	6	0	2.500061	-1.760348	0.017173
21	1	0	1.684634	-2.478925	0.026132
22	1	0	3.509351	-2.172685	0.019956
23	6	0	3.402131	0.560616	-0.008823
24	1	0	3.350701	1.208238	-0.893481
25	1	0	3.349631	1.231179	0.858426
26	1	0	4.380780	0.066907	-0.001965

Electronic Energy = -489.282297 Hartree

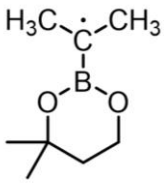


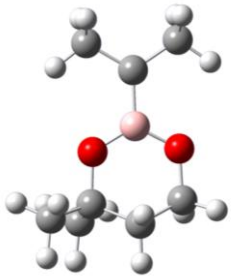


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.959169	-1.107351	0.578349
2	6	0	3.971080	-0.126092	-1.763615
3	1	0	4.888959	0.467213	-1.657208
4	1	0	3.860097	-0.365172	-2.826972
5	8	0	2.829194	-0.238739	0.826758
6	8	0	2.858993	0.685856	-1.391677
7	5	0	2.330686	0.613289	-0.125248
8	6	0	1.134181	1.600679	0.243422
9	6	0	-0.025462	1.526654	-0.816804
10	1	0	-0.681790	2.388309	-0.642145
11	1	0	0.431370	1.664610	-1.809851
12	6	0	1.709950	3.039134	0.188998
13	1	0	0.934019	3.775540	0.440044
14	1	0	2.530783	3.171157	0.906534
15	1	0	2.094647	3.280298	-0.808296
16	6	0	0.577006	1.340241	1.655347
17	1	0	-0.245562	2.032270	1.879933
18	1	0	0.190824	0.320334	1.758387
19	1	0	1.352884	1.472830	2.418005
20	6	0	-0.853776	0.271120	-0.819304
21	6	0	-0.213015	-1.000982	-1.294953
22	1	0	0.353022	-0.845779	-2.225339
23	1	0	0.513048	-1.385495	-0.558040
24	1	0	-0.950763	-1.792022	-1.457279
25	6	0	-4.215509	1.497702	0.570763
26	6	0	-4.413845	-0.979863	0.049301
27	1	0	-4.615973	2.490764	0.336698
28	1	0	-4.220252	1.396127	1.664899
29	5	0	-2.317972	0.277440	-0.335018
30	8	0	-3.038698	-0.899293	-0.374843
31	8	0	-2.869535	1.461611	0.111668

32	6	0	-5.064738	0.410630	-0.083153
33	1	0	-6.069210	0.404200	0.357897
34	1	0	-5.178083	0.643395	-1.149974
35	6	0	-4.431717	-1.496517	1.495486
36	1	0	-5.459746	-1.642009	1.847340
37	1	0	-3.907568	-2.455897	1.551051
38	1	0	-3.929114	-0.802320	2.176821
39	6	0	-5.091310	-1.986893	-0.884288
40	1	0	-4.590692	-2.958546	-0.818386
41	1	0	-6.146284	-2.120212	-0.618856
42	1	0	-5.033910	-1.643166	-1.922360
43	6	0	4.040967	-1.403561	-0.931051
44	1	0	4.964039	-1.949492	-1.161770
45	1	0	3.200832	-2.053804	-1.206052
46	6	0	5.215681	-0.401228	1.105606
47	1	0	5.084656	-0.154745	2.163979
48	1	0	6.096766	-1.045681	1.006284
49	1	0	5.409726	0.532107	0.566862
50	6	0	3.693006	-2.388609	1.371800
51	1	0	4.517358	-3.100744	1.252172
52	1	0	3.583966	-2.157696	2.436433
53	1	0	2.768747	-2.865873	1.029852

Electronic Energy = -979.163837 Hartree

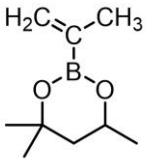


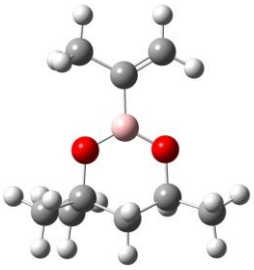


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.811612	0.979922	-0.636153
2	6	0	-1.646065	-0.417080	-0.006884
3	6	0	-0.862239	1.999489	-0.011710
4	1	0	-1.596731	0.907179	-1.710224
5	1	0	-2.848572	1.322781	-0.533567
6	1	0	-1.155159	2.229142	1.022175
7	1	0	-0.887450	2.941281	-0.571662

8	6	0	-2.154129	-0.468234	1.441421
9	1	0	-3.232659	-0.277111	1.485320
10	1	0	-1.960386	-1.458452	1.865792
11	1	0	-1.647528	0.269728	2.072020
12	6	0	-2.347464	-1.481058	-0.855526
13	1	0	-2.182793	-2.474923	-0.426489
14	1	0	-3.426757	-1.296646	-0.902337
15	1	0	-1.949086	-1.479399	-1.875463
16	8	0	-0.247208	-0.766866	0.002247
17	8	0	0.483775	1.537108	-0.015693
18	5	0	0.752079	0.183550	-0.000825
19	6	0	2.221784	-0.281121	0.003281
20	6	0	2.588832	-1.735061	0.012573
21	1	0	1.708672	-2.383310	0.022414
22	1	0	3.198873	-1.999545	-0.867185
23	1	0	3.209652	-1.986106	0.888560
24	6	0	3.358393	0.697176	-0.003700
25	1	0	4.006293	0.551562	-0.884083
26	1	0	3.011996	1.733993	-0.005156
27	1	0	4.013708	0.555947	0.871764

Electronic Energy = -489.862416 Hartree

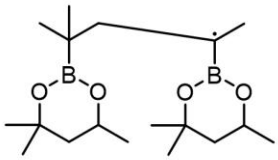


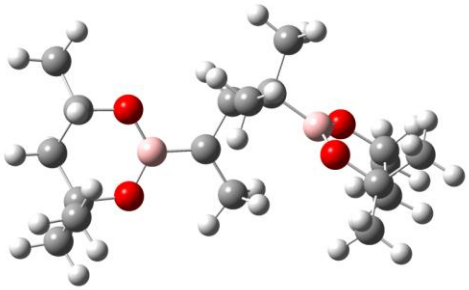


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.303597	-1.037790	-0.001096
2	6	0	-1.811330	0.341050	-0.464789
3	6	0	-1.116619	1.497044	0.258461
4	1	0	-1.622650	0.441516	-1.542436
5	1	0	-2.896169	0.408870	-0.318010
6	1	0	-1.396588	1.487297	1.321628
7	5	0	0.879860	0.104330	0.054842
8	8	0	0.307078	1.343739	0.189879
9	8	0	0.140585	-1.047122	-0.034772

10	6	0	-1.759093	-2.135033	-0.966786
11	1	0	-1.354816	-3.103750	-0.655465
12	1	0	-2.852395	-2.205601	-0.991047
13	1	0	-1.401191	-1.925262	-1.980115
14	6	0	-1.739547	-1.371990	1.432392
15	1	0	-2.830977	-1.445454	1.501545
16	1	0	-1.308166	-2.331082	1.736011
17	1	0	-1.399767	-0.612382	2.143927
18	6	0	-1.469026	2.860135	-0.325055
19	1	0	-2.542660	3.058060	-0.228970
20	1	0	-0.921345	3.648505	0.200678
21	1	0	-1.198948	2.904654	-1.385999
22	6	0	2.443508	-0.019152	-0.006370
23	6	0	3.205077	1.081023	0.093653
24	1	0	2.762870	2.066354	0.215796
25	1	0	4.294019	1.039838	0.057697
26	6	0	3.059997	-1.390250	-0.175280
27	1	0	4.155000	-1.345818	-0.198213
28	1	0	2.760497	-2.062520	0.638921
29	1	0	2.716467	-1.868032	-1.101796

Electronic Energy = -528.602007 Hartree



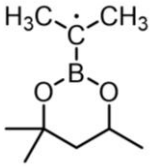


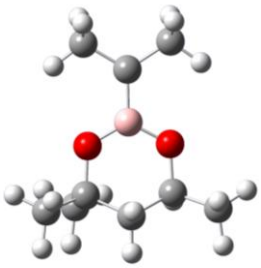
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.999448	-0.905211	1.012858
2	6	0	4.156984	0.001862	-1.368928
3	1	0	4.999811	0.671437	-1.145415
4	8	0	2.799472	-0.108357	1.138943
5	8	0	2.951317	0.733570	-1.106066
6	5	0	2.325744	0.670555	0.115291
7	6	0	1.038152	1.583952	0.343875
8	6	0	-0.039143	1.356143	-0.780361

9	1	0	-0.763650	2.176791	-0.706958
10	1	0	0.473532	1.463121	-1.749630
11	6	0	1.508073	3.056896	0.231507
12	1	0	0.664727	3.744443	0.384731
13	1	0	2.266701	3.295879	0.988795
14	1	0	1.940645	3.266256	-0.753181
15	6	0	0.407703	1.366736	1.732080
16	1	0	-0.479386	2.001759	1.857590
17	1	0	0.095903	0.327084	1.879188
18	1	0	1.117354	1.609453	2.531397
19	6	0	-0.777645	0.046306	-0.747222
20	6	0	-0.025166	-1.201976	-1.107954
21	1	0	0.574757	-1.063141	-2.019782
22	1	0	0.688450	-1.484597	-0.315123
23	1	0	-0.695552	-2.054042	-1.252542
24	6	0	-4.295266	1.130319	0.393845
25	6	0	-4.285727	-1.395770	0.017264
26	1	0	-4.327169	1.043891	1.490007
27	5	0	-2.263793	-0.024024	-0.339599
28	8	0	-2.898138	-1.249269	-0.340814
29	8	0	-2.919144	1.141287	0.003022
30	6	0	-5.019256	-0.063781	-0.232287
31	1	0	-6.044282	-0.122284	0.154085
32	1	0	-5.089311	0.101178	-1.316279
33	6	0	-4.349163	-1.831149	1.489002
34	1	0	-5.383798	-2.020985	1.797734
35	1	0	-3.772323	-2.751258	1.626825
36	1	0	-3.925955	-1.069542	2.151898
37	6	0	-4.846888	-2.497544	-0.886681
38	1	0	-4.290227	-3.428516	-0.736490
39	1	0	-5.904165	-2.685053	-0.667200
40	1	0	-4.755076	-2.211038	-1.939553
41	6	0	4.235084	-1.236073	-0.473112
42	1	0	5.209694	-1.723850	-0.597430
43	1	0	3.469857	-1.952732	-0.800346
44	6	0	5.156652	-0.104765	1.626490
45	1	0	4.918002	0.154925	2.662721
46	1	0	6.083226	-0.690368	1.620516
47	1	0	5.335665	0.827485	1.080834
48	6	0	3.748856	-2.182173	1.819109
49	1	0	4.624945	-2.839976	1.791641
50	1	0	3.533089	-1.933081	2.863193
51	1	0	2.890826	-2.728980	1.414400
52	6	0	-4.906423	2.469254	-0.003880

53	1	0	-5.944062	2.541971	0.341653
54	1	0	-4.333685	3.290689	0.437972
55	1	0	-4.891406	2.588943	-1.093000
56	6	0	4.186826	-0.336232	-2.854692
57	1	0	4.090111	0.576297	-3.451207
58	1	0	5.128543	-0.829202	-3.121869
59	1	0	3.357782	-1.004220	-3.113785

Electronic Energy = -1057.803237 Hartree

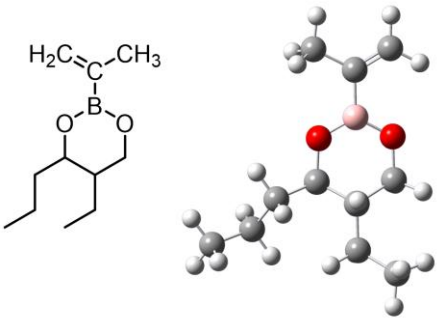




Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.424379	-0.974298	-0.003531
2	6	0	-1.834724	0.438229	-0.463167
3	6	0	-1.059274	1.540571	0.261945
4	1	0	-1.640463	0.527775	-1.540828
5	1	0	-2.912019	0.581824	-0.314702
6	1	0	-1.338656	1.545721	1.325870
7	5	0	0.838200	0.009933	0.049326
8	8	0	0.348444	1.292093	0.188483
9	8	0	0.011680	-1.089258	-0.043224
10	6	0	2.364489	-0.199176	-0.011847
11	6	0	2.967773	-1.563425	-0.165865
12	1	0	3.642898	-1.800160	0.673230
13	1	0	2.207790	-2.347175	-0.222117
14	1	0	3.591461	-1.625501	-1.073169
15	6	0	3.322320	0.951153	0.078967
16	1	0	2.808160	1.909293	0.191182
17	1	0	4.013017	0.831214	0.930142
18	1	0	3.963953	1.009601	-0.815963
19	6	0	-1.965010	-2.033569	-0.968558
20	1	0	-1.630991	-3.029895	-0.660705
21	1	0	-3.060731	-2.024342	-0.987556
22	1	0	-1.597382	-1.848785	-1.983293

23	6	0	-1.881229	-1.278076	1.431093
24	1	0	-2.974984	-1.270550	1.504050
25	1	0	-1.521021	-2.267104	1.731620
26	1	0	-1.483571	-0.547350	2.142871
27	6	0	-1.321395	2.927386	-0.314377
28	1	0	-2.378659	3.197783	-0.212939
29	1	0	-0.719009	3.674455	0.212017
30	1	0	-1.053215	2.958084	-1.376372

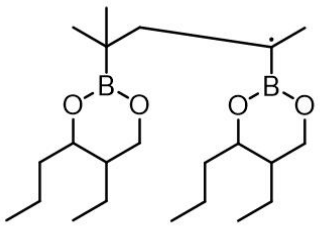
Electronic Energy = -529.182116 Hartree

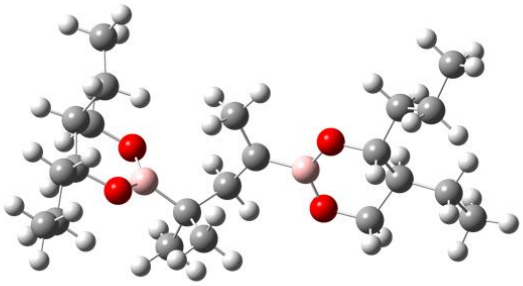


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.599337	-0.324424	-0.332384
2	6	0	0.722132	1.118400	0.197285
3	6	0	-0.384537	1.971742	-0.435026
4	1	0	-0.424432	2.962843	0.026861
5	1	0	0.535959	1.078427	1.282050
6	1	0	0.771205	-0.315115	-1.420551
7	1	0	-0.182188	2.114956	-1.507435
8	5	0	-1.819476	0.045949	-0.117500
9	8	0	-1.680851	1.398908	-0.285191
10	8	0	-0.743254	-0.802639	-0.123446
11	6	0	1.552704	-1.348970	0.312191
12	1	0	0.974962	-2.271157	0.443256
13	1	0	1.834118	-1.015932	1.321633
14	6	0	2.811545	-1.671909	-0.507138
15	1	0	3.395433	-0.761485	-0.692872
16	1	0	2.505493	-2.041975	-1.495708
17	6	0	3.703831	-2.714739	0.173775
18	1	0	3.159422	-3.651946	0.341513
19	1	0	4.584920	-2.944492	-0.435838
20	1	0	4.057135	-2.359192	1.149570

21	6	0	2.115723	1.731102	-0.034380
22	1	0	2.865048	1.082278	0.432962
23	1	0	2.339496	1.730786	-1.111094
24	6	0	2.291893	3.150524	0.523643
25	1	0	1.668688	3.884492	0.001897
26	1	0	2.035036	3.191961	1.589226
27	1	0	3.332845	3.476088	0.420599
28	6	0	-3.247043	-0.568737	0.095426
29	6	0	-4.323321	0.232531	0.105423
30	1	0	-5.333442	-0.152291	0.248133
31	1	0	-4.230627	1.306966	-0.030121
32	6	0	-3.376654	-2.064084	0.283693
33	1	0	-4.420587	-2.369729	0.419067
34	1	0	-2.968293	-2.608954	-0.577143
35	1	0	-2.803621	-2.405049	1.155537

Electronic Energy = -607.214757 Hartree



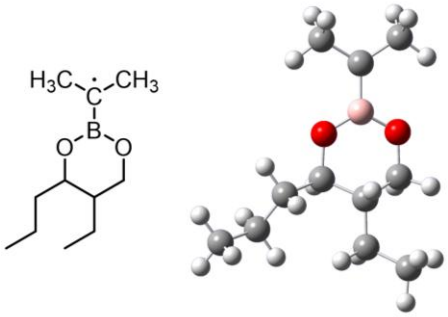


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.767194	0.071637	0.179748
2	6	0	-4.203924	-0.047882	-2.224840
3	1	0	-5.507205	-0.727425	0.014185
4	1	0	-4.964767	-0.817568	-2.415139
5	1	0	-4.033654	0.480802	-3.167011
6	6	0	-3.852935	2.189666	-0.996541
7	1	0	-4.252463	2.783750	-0.166512
8	1	0	-2.822080	1.938747	-0.722505
9	8	0	-3.507942	-0.575489	0.447742
10	8	0	-2.977820	-0.701362	-1.884140
11	5	0	-2.685249	-0.982845	-0.572275
12	6	0	-1.428158	-1.905856	-0.242568
13	6	0	-0.197965	-1.646650	-1.182426

14	1	0	0.452722	-2.527645	-1.120957
15	1	0	-0.578605	-1.599199	-2.215190
16	6	0	-1.922074	-3.351027	-0.529673
17	1	0	-1.134723	-4.079807	-0.292729
18	1	0	-2.799815	-3.605056	0.078898
19	1	0	-2.193063	-3.481317	-1.584137
20	6	0	-1.003149	-1.818936	1.235629
21	1	0	-0.163954	-2.498281	1.436388
22	1	0	-0.681090	-0.807724	1.509098
23	1	0	-1.829870	-2.090403	1.901185
24	6	0	0.622542	-0.418637	-0.897891
25	6	0	-0.002332	0.925503	-1.130759
26	1	0	-0.571116	0.952850	-2.070716
27	1	0	-0.722927	1.173950	-0.331719
28	1	0	0.743347	1.725943	-1.140358
29	6	0	3.939286	-1.905117	0.340572
30	6	0	4.120645	0.585866	0.396497
31	1	0	4.329747	-2.834733	-0.085682
32	1	0	3.934334	-2.022588	1.435672
33	1	0	4.030973	0.574196	1.495415
34	5	0	2.062338	-0.529616	-0.357713
35	8	0	2.788531	0.622181	-0.139157
36	8	0	2.597954	-1.776416	-0.115052
37	6	0	6.249819	-0.855686	0.512155
38	1	0	6.834678	0.020217	0.209080
39	1	0	6.213541	-0.833961	1.611141
40	6	0	4.822872	-0.713073	-0.048676
41	1	0	4.882540	-0.683602	-1.148041
42	6	0	-4.692208	0.901216	-1.120878
43	1	0	-5.721775	1.192299	-1.379276
44	6	0	6.996134	-2.115775	0.051142
45	1	0	8.035359	-2.094476	0.397571
46	1	0	6.542903	-3.034306	0.438671
47	1	0	7.012361	-2.188093	-1.043278
48	6	0	-3.846698	3.063903	-2.256901
49	1	0	-4.867194	3.307046	-2.579652
50	1	0	-3.326585	4.008960	-2.065397
51	1	0	-3.337115	2.579536	-3.096715
52	6	0	4.818927	1.892630	-0.028173
53	1	0	5.418686	1.720606	-0.933716
54	1	0	4.023377	2.589909	-0.315293
55	6	0	5.680934	2.553877	1.057882
56	1	0	6.465185	1.866727	1.399865
57	1	0	5.051378	2.755014	1.936040

58	6	0	6.325441	3.860182	0.582863
59	1	0	6.919212	4.324673	1.378251
60	1	0	6.990870	3.687075	-0.271974
61	1	0	5.564681	4.584405	0.266985
62	6	0	-5.179256	0.839585	1.435790
63	1	0	-6.075631	1.433210	1.203523
64	1	0	-4.385482	1.549771	1.698495
65	6	0	-5.460445	-0.073422	2.636617
66	1	0	-4.572465	-0.686627	2.828214
67	1	0	-6.270109	-0.771472	2.378965
68	6	0	-5.839364	0.704919	3.900146
69	1	0	-6.740567	1.310670	3.741746
70	1	0	-6.036675	0.028729	4.739670
71	1	0	-5.033590	1.384660	4.203448

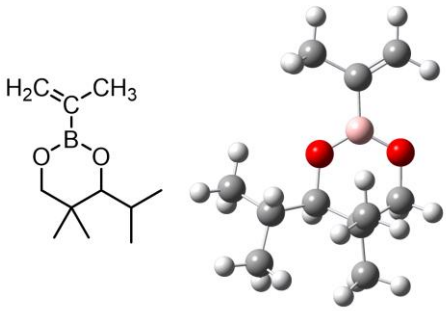
Electronic Energy = -1215.029694 Hartree



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.660344	-0.334453	-0.325496
2	6	0	0.763377	1.112728	0.198015
3	6	0	-0.353717	1.947389	-0.441387
4	1	0	-0.405836	2.941724	0.013228
5	1	0	0.575485	1.074775	1.282574
6	1	0	0.829912	-0.324061	-1.414842
7	1	0	-0.147336	2.086904	-1.514173
8	5	0	-1.766209	-0.000033	-0.116348
9	8	0	-1.641767	1.360697	-0.292794
10	8	0	-0.669384	-0.833527	-0.107342
11	6	0	-3.169700	-0.603784	0.084345
12	6	0	-3.374929	-2.076244	0.280053
13	1	0	-4.039218	-2.494572	-0.494266

14	1	0	-2.433679	-2.631692	0.256240
15	1	0	-3.872449	-2.286878	1.241341
16	6	0	-4.400805	0.252531	0.094473
17	1	0	-4.170163	1.310097	-0.058425
18	1	0	-5.112308	-0.059650	-0.687887
19	1	0	-4.947863	0.155714	1.047049
20	6	0	1.635725	-1.339957	0.317107
21	1	0	1.075331	-2.272270	0.452200
22	1	0	1.914694	-1.000167	1.325049
23	6	0	2.897144	-1.642253	-0.505950
24	1	0	3.464341	-0.722196	-0.695676
25	1	0	2.594188	-2.019573	-1.492756
26	6	0	3.810307	-2.667866	0.173542
27	1	0	3.283114	-3.614194	0.345247
28	1	0	4.693194	-2.883441	-0.438752
29	1	0	4.160819	-2.304230	1.147393
30	6	0	2.148561	1.744078	-0.033626
31	1	0	2.906248	1.108500	0.438469
32	1	0	2.374832	1.741823	-1.109859
33	6	0	2.303864	3.168639	0.517595
34	1	0	1.672122	3.891328	-0.009587
35	1	0	2.043200	3.211957	1.582218
36	1	0	3.340601	3.508058	0.416023

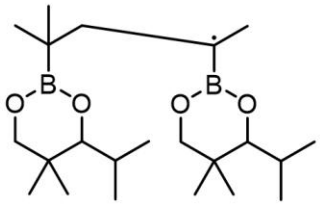
Electronic Energy = -607.794897 Hartree

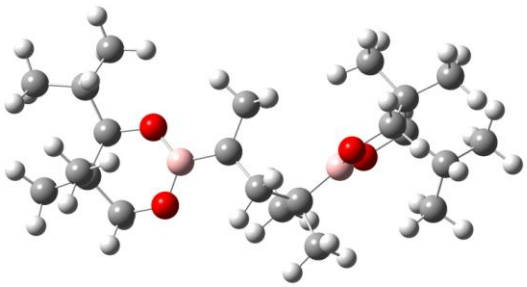


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.130080	-1.214833	0.046098
2	6	0	-0.922054	0.258136	-0.423774
3	6	0	-0.001509	-2.051411	-0.600912
4	1	0	-1.140599	0.289597	-1.503311
5	1	0	-0.132397	-2.066816	-1.693026

6	1	0	-0.067672	-3.086459	-0.246291
7	5	0	1.503688	-0.241353	-0.186349
8	8	0	1.310489	-1.592184	-0.303044
9	8	0	0.461078	0.640650	-0.265861
10	6	0	-1.728131	1.394210	0.254518
11	1	0	-1.400852	1.430207	1.302487
12	6	0	-1.365039	2.742094	-0.395551
13	1	0	-1.859178	3.564795	0.133845
14	1	0	-0.287803	2.916938	-0.379007
15	1	0	-1.700511	2.772615	-1.441077
16	6	0	-3.254100	1.214140	0.227771
17	1	0	-3.600121	0.405356	0.876810
18	1	0	-3.737745	2.134388	0.574672
19	1	0	-3.620667	1.016881	-0.787418
20	6	0	-2.442428	-1.823614	-0.489050
21	1	0	-3.324653	-1.451630	0.033653
22	1	0	-2.573046	-1.621368	-1.559033
23	1	0	-2.425853	-2.913135	-0.358935
24	6	0	-1.063410	-1.350943	1.578559
25	1	0	-1.887857	-0.818753	2.063999
26	1	0	-1.133384	-2.406018	1.868751
27	1	0	-0.125713	-0.958434	1.984059
28	6	0	2.946226	0.324230	0.057767
29	6	0	3.988587	-0.519137	0.112389
30	1	0	3.856469	-1.591234	-0.008182
31	1	0	5.008830	-0.172600	0.278908
32	6	0	3.131553	1.816267	0.223224
33	1	0	4.182458	2.081678	0.386507
34	1	0	2.774907	2.360455	-0.660852
35	1	0	2.546710	2.197745	1.070193

Electronic Energy = -607.212640 Hartree



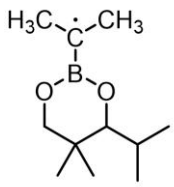


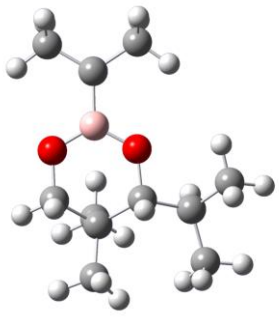
Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	4.371564	0.502706	-0.724333
2	6	0	4.359959	1.489643	0.486705
3	6	0	3.971902	0.699364	1.751215
4	1	0	4.339872	1.096375	-1.648011
5	1	0	4.778923	0.006418	2.028918
6	1	0	3.832240	1.390304	2.590867
7	6	0	3.322857	2.598787	0.213123
8	1	0	3.238482	3.269804	1.076294
9	1	0	3.627797	3.201459	-0.650665
10	1	0	2.329549	2.196322	0.004728
11	6	0	5.715356	2.164830	0.759510
12	1	0	6.037301	2.773961	-0.091879
13	1	0	5.622255	2.837447	1.621135
14	1	0	6.508731	1.446229	0.987539
15	8	0	3.142856	-0.250178	-0.736947
16	8	0	2.765438	-0.047111	1.615626
17	5	0	2.415268	-0.544380	0.385714
18	6	0	1.197476	-1.572511	0.291882
19	6	0	-0.011958	-1.191761	1.221907
20	1	0	-0.610070	-2.100631	1.361561
21	1	0	0.402797	-0.924172	2.206438
22	6	0	1.762088	-2.916324	0.829919
23	1	0	0.994336	-3.700767	0.781914
24	1	0	2.619652	-3.263454	0.238833
25	1	0	2.086109	-2.827176	1.873469
26	6	0	0.715403	-1.785701	-1.155434
27	1	0	-0.098607	-2.522054	-1.187130
28	1	0	0.338976	-0.857639	-1.600329
29	1	0	1.528988	-2.146334	-1.794188
30	6	0	-0.916165	-0.089148	0.744440
31	6	0	-0.385790	1.314213	0.730178
32	1	0	0.267031	1.514150	1.590295
33	1	0	0.224666	1.499981	-0.171083
34	1	0	-1.191083	2.055495	0.713522
35	6	0	-4.095538	-1.948862	-0.262697
36	6	0	-4.514460	0.481673	-0.605522
37	6	0	-5.123138	-0.822292	-0.002915
38	1	0	-4.453665	-2.878852	0.194986
39	1	0	-4.011604	-2.125744	-1.345822
40	1	0	-4.503619	0.355597	-1.700979
41	5	0	-2.343863	-0.395405	0.249255
42	8	0	-3.146740	0.635489	-0.183165

43	8	0	-2.803016	-1.694254	0.264230
44	6	0	-5.384253	-0.696421	1.509295
45	1	0	-6.151958	0.054793	1.721982
46	1	0	-5.735069	-1.653065	1.914697
47	1	0	-4.479471	-0.416607	2.057596
48	6	0	-6.406351	-1.268264	-0.733209
49	1	0	-6.646937	-2.303859	-0.460934
50	1	0	-7.273630	-0.659133	-0.474817
51	1	0	-6.281969	-1.234541	-1.822408
52	6	0	5.593645	-0.459064	-0.837058
53	1	0	5.962464	-0.680437	0.175464
54	6	0	5.229051	-1.799260	-1.497902
55	1	0	4.500526	-2.364714	-0.913484
56	1	0	4.804042	-1.645204	-2.496537
57	1	0	6.130341	-2.414138	-1.605933
58	6	0	6.737382	0.188010	-1.641148
59	1	0	7.063491	1.148734	-1.236197
60	1	0	7.609767	-0.474965	-1.662939
61	1	0	6.423811	0.353729	-2.679900
62	6	0	-5.181441	1.846497	-0.296699
63	1	0	-5.058954	2.018088	0.781368
64	6	0	-6.677432	1.937446	-0.636317
65	1	0	-6.878097	1.623970	-1.668480
66	1	0	-7.303508	1.336630	0.028687
67	1	0	-7.012335	2.976856	-0.541710
68	6	0	-4.426378	2.965181	-1.037991
69	1	0	-3.357877	2.941328	-0.816251
70	1	0	-4.551436	2.863817	-2.124660
71	1	0	-4.820266	3.946893	-0.750461

Electronic Energy = -1215.020835 Hartree





Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-1.150974	-1.223664	0.043442
2	6	0	-0.983645	0.256552	-0.421099
3	6	0	-0.004792	-2.026226	-0.615934
4	1	0	-1.207244	0.282941	-1.500490
5	1	0	-0.143423	-2.034576	-1.707793
6	1	0	-0.045649	-3.066530	-0.271795
7	5	0	1.458206	-0.177806	-0.193179
8	8	0	1.295296	-1.539090	-0.320592
9	8	0	0.384479	0.678232	-0.262564
10	6	0	2.870587	0.390032	0.046823
11	6	0	3.121412	1.858019	0.219816
12	1	0	3.811395	2.239740	-0.550927
13	1	0	2.201062	2.445929	0.170442
14	1	0	3.610526	2.069558	1.185059
15	6	0	4.071526	-0.505997	0.115834
16	1	0	3.811016	-1.558577	-0.022512
17	1	0	4.817859	-0.234382	-0.649027
18	1	0	4.590259	-0.405939	1.083684
19	6	0	-1.823909	1.366814	0.260034
20	1	0	-1.489183	1.417038	1.305056
21	6	0	-1.511856	2.723690	-0.397583
22	1	0	-2.024037	3.532605	0.136033
23	1	0	-0.440461	2.932347	-0.396729
24	1	0	-1.861738	2.740528	-1.438719
25	6	0	-3.343567	1.138439	0.246830
26	1	0	-3.658286	0.321139	0.901091
27	1	0	-3.853339	2.044012	0.595269
28	1	0	-3.712363	0.926591	-0.764591
29	6	0	-2.450163	-1.865097	-0.485507
30	1	0	-3.338397	-1.522271	0.046844
31	1	0	-2.595201	-1.658856	-1.552907
32	1	0	-2.401890	-2.954733	-0.363918
33	6	0	-1.069299	-1.364716	1.574598
34	1	0	-1.903507	-0.856093	2.068787
35	1	0	-1.109591	-2.422524	1.860880
36	1	0	-0.138961	-0.949127	1.973880

Electronic Energy = -607.792641 Hartree

XI. Reference

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