Supporting Information

Nickel Boryl Complexes and the Nickel-Catalyzed Alkyne-Borylation

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Content:

1) Additional Figures

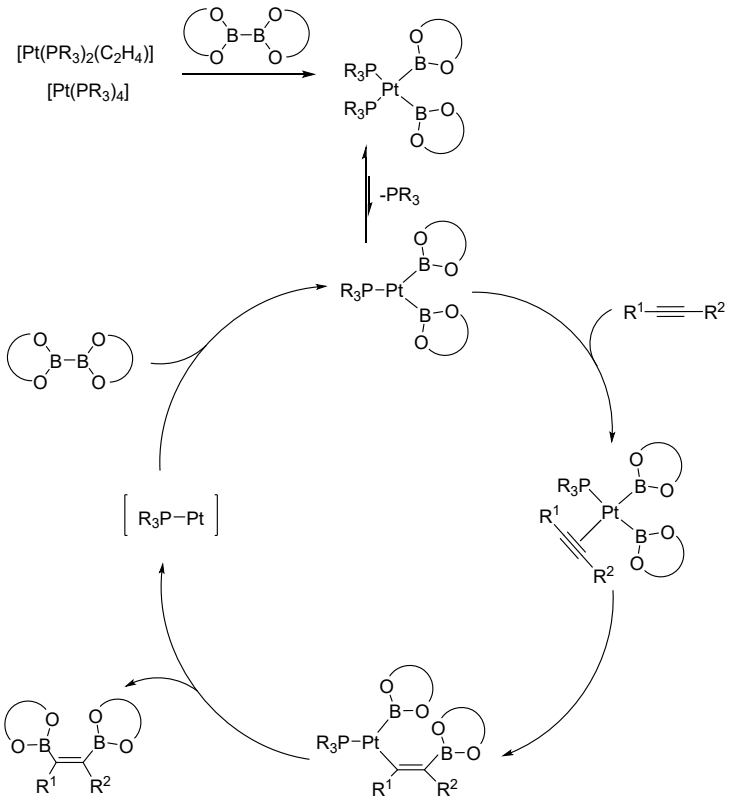


Figure S1. Catalytic cycle for the platinum catalyzed diboration of alkynes.[1]

2) Experimental Section

General

All reactions and subsequent manipulations were performed under an argon atmosphere using standard Schlenk techniques as reported previously[2] or in a glovebox (Innovative Technology Inc. or Braun Uni Lab). All reactions were carried out in oven-dried glassware. Toluene, benzene, hexane and diethylether were purified by distillation from an appropriate drying agent (sodium with benzophenone as indicator). C_6D_6 was purchased from Sigma-Aldrich. B_2eg_2,[3] $^{i}Pr_2Im^{Me}$,[4] [Ni(η^4-COD)$_2$],[5] [Ni$_2$($^{i}Pr_2Im^{Me}$)$_4$(μ-(η^2:η^2)-COD)] **1** and [Ni($^{i}Pr_2Im^{Me}$)$_2$(η^4-COD)] **1a**, [Ni($^{i}Pr_2Im^{Me}$)$_2$(η^2-MeC≡CMe)] **14a**, [Ni($^{i}Pr_2Im^{Me}$)$_2$(η^2-$H_7C_3C{\equiv}CC_3H_7$)] **14b**[6] and [Ni($^{i}Pr_2Im^{Me}$)$_2$(Br)$_2$][7] were prepared according to published procedures. The diboron reagents B_2pin_2 and B_2cat_2 were a generous gift from AllyChem Co. Ltd. All other reagents were purchased from Aldrich or ABCR and used without further purification. NMR spectra were recorded at 298 K using Bruker Avance 400 (^{1}H, 400 MHz; ^{13}C, 100 MHz; ^{11}B, 128 MHz; ^{19}F, 376 MHz; ^{31}P, 162 MHz, ^{29}Si, 79.5 MHz), or Bruker Avance NEO 400 (^{1}H, 400 MHz; ^{13}C, 100 MHz; ^{11}B, 128 MHz; ^{19}F, 376 MHz; ^{31}P, 162 MHz; ^{29}Si, 79.5 MHz), or Bruker Avance 500 (^{1}H, 500 MHz; ^{13}C, 126 MHz; ^{11}B, 160 MHz) spectrometers. ^{1}H NMR chemical shifts are reported relative to TMS and were referenced via residual proton resonances of the corresponding deuterated solvent (C_6D_5H: 7.16 ppm) whereas ^{13}C{^{1}H} NMR spectra are reported relative to TMS using the natural-abundance carbon resonances (C_6D_6: 128.06 ppm). Coupling constants are given in Hertz. Elemental analyses were performed in the microanalytical laboratory of the Institute of Inorganic Chemistry, Universität Würzburg, using an Elementar vario micro cube. GC-MS analyses were performed using a Thermo Fisher Scientific Trace 1310 gas chromatograph (column: TG-SQC 5% phenyl methyl siloxane, 15 m, Ø 0.25 mm, film 0.25 μm; injector: 250 °C; oven: 40 °C (2min), 40 °C to 280 °C; carrier gas: He (1.2 mL min^{-1})). High-resolution mass spectra were obtained using a Thermo Scientific Exactive Plus spectrometer equipped with an Orbitrap Mass Analyzer. Ionizations were accomplished in Liquid Injection Field Desorption Ionization mode using a LIFDI 700 from Linden CMS with 10 kV at the emitter and an accelerating voltage of 5 V.

Synthesis

[Ni(^{i}Pr$_2$Im^{Me})$_2$(η^2-C$_2$H$_4$)] 1b

A 60:40 mixture of [Ni$_2$(^{i}Pr$_2$Im^{Me})$_4$(μ-(η^2:η^2)-COD)] **1** and [Ni(^{i}Pr$_2$Im^{Me})$_2$(η^4-COD)] **1a** (770 mg, 1.58 mmol) was dissolved in 20 mL of toluene. The flask was evacuated and charged with 1 bar of ethylene. After stirring the reaction mixture for 2 h at room temperature, all volatiles were removed *in vacuo* to give a pale-yellow powder (680 mg, 1.52 mmol, 96 %).

Yellow crystals of [Ni(^{i}Pr$_2$Im^{Me})$_2$(η^2-C$_2$H$_4$)] **1b** suitable for single-crystal X-ray diffraction were obtained from storing a saturated solution of the compound in hexane at -30 °C.

Elemental analysis $C_{24}H_{44}N_4Ni$ [447.33 g/mol] calculated (found): C 64.44 (64.49), H 9.91 (10.12), N 12.52 (12.54).

^{1}H-NMR (400.1 MHz, C_6D_6, 298 K): δ = 1.32 (d, 24H, $^3J_{HH}$ = 7.0 Hz, ^{i}Pr-CH_3), 1.86 (s, 12H, NCCH_3CCH_3N), 1.87 (s, 4H, H_2C=CH_2), 5.89 (sept, 4H, $^3J_{HH}$ = 7.0 Hz, ^{i}Pr-CH).

^{13}C{^{1}H}-NMR (100.6 MHz, C_6D_6, 298 K): δ = 10.4 (NCCH$_3$CCH$_3$N), 22.4 (^{i}Pr-CH$_3$), 26.0 (H$_2$$C$=$CH_2$), 51.9 (^{i}Pr-$C$H), 122.8 (N$CCH_3$$CCH_3$N), 205.0 (N$C$N).

IR (ATR [cm^{-1}]): 2968 (m), 2922 (m), 2870 (m), 1686 (vw), 1641 (vw), 1463 (w), 1405 (m), 1364 (m), 1364 (s), 1305 (m), 1281 (m), 1257 (vs), 1208 (m), 1142 (s), 1098 (m), 1061 (m), 1018 (m), 960 (w), 924 (w), 903 (w), 881 (w), 854 (w), 796 (m), 754 (w), 673 (m), 614 (w), 549 (w), 460 (m).

[Ni(^{i}Pr$_2$Im^{Me})$_2$(η^2-COE)] 1c

Cyclooctene (411 μL, 349 mg, 3,17 mmol) and KC_8 (1.46 g, 10.8 mmol) were added successively at -78 °C to a suspension of [Ni(^{i}Pr$_2$Im^{Me})$_2$(Br)$_2$] (1.53 g, 2.64 mmol) in 60 mL of THF. The reaction mixture was allowed to warm to room temperature overnight and was then filtered through a pad of celite. All volatiles were removed *in vacuo* and the remaining residue was suspended in 20 mL of toluene and again filtered through a pad of celite. The solvent was removed *in vacuo* and the product was suspended in 6 mL of hexane, filtered, and dried *in vacuo* to give a pale-yellow powder (850 mg, 1.61 mmol, 61 %).

Yellow crystals of [Ni(^{i}Pr$_2$Im^{Me})$_2$(η^2-COE)] **1c** suitable for single-crystal X-ray diffraction were obtained from storing a saturated solution of the compound in hexane at -30 °C.

Elemental analysis $C_{30}H_{54}N_4Ni$ [529.48 g/mol] calculated (found): C 68.05 (67.62), H 10.28 (10.34), N 10.58 (10.39).

^{1}H-NMR (400.1 MHz, C_6D_6, 298 K): δ = 1.34 (d, 12H, $^3J_{HH}$ = 7.1 Hz, ^{i}Pr-CH_3), 1.36 (d, 12H, $^3J_{HH}$ = 7.1 Hz, ^{i}Pr-CH_3), 1.69 - 2.37 (m, 14H, COE-CH_2 and COE-CH), 1.88 (s, 12H, NCCH_3CCH_3N), 5.92 (sept, 4H, $^3J_{HH}$ = 7.1 Hz, ^{i}Pr-CH).

^{13}C{^{1}H}-NMR (100.6 MHz, C_6D_6, 298 K): δ = 10.6 (NCH_3CH_3N), 22.9 (^{i}Pr-CH$_3$), 27.7 (COE-CH$_2$), 30.8 (COE-CH$_2$), 33.7 (COE-CH$_2$), 47.9 (COE-CH), 51.9 (^{i}Pr-CH), 122.5 (NCCH$_3$$CCH_3$N), 205.9 (N$C$N).

IR (ATR [cm^{-1}]): 2972 (w), 2918 (m), 2899 (m), 2870 (m), 2820 (w), 1461 (w), 1433 (vw), 1419 (vw), 1399 (m), 1381 (m), 1361 (m), 1335 (vs), 1306 (w), 1281 (s), 1253 (vs), 1205 (s), 1195 (m), 1161 (w), 1141 (w), 1127 (m), 1097 (m), 1055 (m), 1017 (w), 962 (vw), 917 (vw), 903 (vw), 890 (vw), 865 (vw), 837 (vw), 806 (vw), 789 (w), 750 (w), 731 (vw), 684 (m), 671 (w), 652 (vw), 594 (vw), 541 (s), 459 (w), 445 (w).

cis-[Ni(^{i}Pr$_2$Im^{Me})$_2$(Bcat)$_2$] 2a

A 60:40 mixture of [Ni$_2$(^{i}Pr$_2$Im^{Me})$_4$(μ-(η^2:η^2)-COD)] **1** and [Ni(^{i}Pr$_2$Im^{Me})$_2$(η^4-COD)] **1a** (461 mg, 946 μmol) and B_2cat_2 (225 mg, 946 μmol) were suspended in 5 mL of diethylether. The mixture was stirred for 2 h at room temperature with a color change of the suspension from bright to pale yellow. The product was collected by filtration, washed with 1 mL of cold diethyl ether and dried *in vacuo* to give a pale-yellow powder (360 mg, 548 μmol, 58 %).

Yellow crystals of *cis*-[Ni(^{i}Pr$_2$Im^{Me})$_2$(Bcat)$_2$] **2a** suitable for single-crystal X-ray diffraction were obtained from storing the mother liquor at -30 °C.

Elemental analysis $C_{34}H_{48}B_2N_4NiO_4$ [657.10 g/mol] calculated (found): C 62.15 (62.09), H 7.36 (7.49), N 8.53 (8.61).

^{1}H-NMR (500.1 MHz, C_6D_6, 298 K): δ = 1.28 (s, br, 12H, ^{i}Pr-CH_3), 1.45 (s, br, 12H, ^{i}Pr-CH_3), 1.63 (s, 12H, NCCH_3CCH_3N), 6.05 (sept, 4H, $^{3}J_{HH}$ = 7.0 Hz, ^{i}Pr-CH), 6.65 (dd, 4H, $^{3}J_{HH}$ = 5.5 Hz, $^{4}J_{HH}$ = 3.4 Hz, BO_2C_6-4,5-H_4), 7.01 (dd, 4H, $^{3}J_{HH}$ = 5.5 Hz, $^{4}J_{HH}$ = 3.4 Hz, BO_2C_6-3,6-H_4).

^{13}C{^{1}H}-NMR (125.8 MHz, C_6D_6, 298 K): δ = 10.2 (NCCH$_3$CCH$_3$N), 22.2 (^{i}Pr-CH$_3$), 22.5 (^{i}Pr-CH$_3$), 52.9 (^{i}Pr-CH), 110.7 (BO_2-3,6-C_6H_4), 120.3 (BO_2-4,5-C_6H_4), 123.7 (NCCH$_3$$CCH_3$N), 151.4 ($BO_2$-1,2-$C_6H_4$), 194.3 (N$C$N).

^{11}B{^{1}H}-NMR (160.5 MHz, C_6D_6, 298 K): δ = 48.69 (s, 2B, *B*cat).

IR (ATR [cm^{-1}]): 2972 (w), 2932 (vw), 2875 (vw), 1471 (m), 1403 (w), 1352 (m), 1282 (m), 1228 (s), 1147 (vw), 1117 (m), 1097 (s),1060 (m), 1014 (vs), 972 (m), 906 (m), 863 (vw), 806 (w), 754 (w), 736 (vs), 696 (vw), 681 (w), 618 (vw), 594 (m), 551 (w), 425 (m).

cis-[Ni(^{i}Pr$_2$Im^{Me})$_2$(Bpin)$_2$] 2b

In a Young's tab NMR tube, a 60:40 mixture of [Ni$_2$(^{i}Pr$_2$Im^{Me})$_4$(μ-(η^2:η^2)-COD)] **1** and [Ni(^{i}Pr$_2$Im^{Me})$_2$(η^4-COD)] **1a** (20.0 mg, 41.1 μmol) and B_2pin_2 (4 eq) were dissolved in 0.6 mL of C_6D_6. The mixture was shaken until all components were completely dissolved. After 16 h at room temperature, the mixture was analyzed by NMR spectroscopy and the partial formation of *cis*-[Ni(^{i}Pr$_2$Im^{Me})$_2$(Bpin)$_2$] **2b** (ca. 30-40 %) was detected. The reaction never proceeded quantitatively and is very sensitive to temperature. Hence, isolation of bulk pure material of the complex *cis*-[Ni(^{i}Pr$_2$Im^{Me})$_2$(Bpin)$_2$] **2b** for further characterization was not possible. However, yellow crystals of *cis*-[Ni(^{i}Pr$_2$Im^{Me})$_2$(Bpin)$_2$] **2b** suitable for single-crystal X-ray diffraction were obtained from an equilibrium mixture of the reaction components in diethyl ether at -30 °C.

^{1}H-NMR (400.1 MHz, C_6D_6, 298 K): δ = 1.21 (s, 24H, CH_{3Bpin}), 1.32 (d, 12H, $^{3}J_{HH}$ = 7.1 Hz, ^{i}Pr-CH_3), 1.69 (d, 12H, $^{3}J_{HH}$ = 7.1 Hz, ^{i}Pr-CH_3), 1.84 (s, 12H, NCCH_3CCH_3N), 5.99 (sept, 4H, $^{3}J_{HH}$ = 7.1 Hz, ^{i}Pr-CH).

^{13}C{^{1}H}-NMR (100.6 MHz, C_6D_6, 298 K): δ = 10.5 (NCCH$_3$CCH$_3$N), 22.3 (^{i}Pr-CH$_3$), 25.7 (Bpin-CH$_3$), 52.3 (^{i}Pr-CH), 79.6 (Bpin-C_q), 122.5 (NCCH$_3$$CCH_3$N), 199.4 (N$C$N).

^{11}B{^{1}H}-NMR (128.5 MHz, C_6D_6, 298 K): δ = 46.08 (s, 2B, *B*pin).

cis-[Ni(^{i}Pr$_2$Im^{Me})$_2$(Beg)$_2$] 2c

In a Young's tab NMR tube, a 60:40 mixture of [Ni$_2$(^{i}Pr$_2$Im^{Me})$_4$(μ-(η^2:η^2)-COD)] **1** and [Ni(^{i}Pr$_2$Im^{Me})$_2$(η^4-COD)] **1a** (15.0 mg, 31.0 μmol) and B$_2$eg$_2$ (4.72 mg, 33.3 μmol) were dissolved in 0.6 mL of C_6D_6. The mixture was shaken and, after 15 min at room temperature, analyzed by NMR spectroscopy. The partial formation of *cis*-[Ni(^{i}Pr$_2$Im^{Me})$_2$(Beg)$_2$] **2c** (ca. 50-60 %) was detected. The reaction never proceeded quantitatively and is very sensitive to temperature. Hence, the isolation of bulk pure material of the complex *cis*-[Ni(^{i}Pr$_2$Im^{Me})$_2$(Beg)$_2$] **2c** for further characterization was not possible. However, yellow crystals of *cis*-[Ni(^{i}Pr$_2$Im^{Me})$_2$(Beg)$_2$] **2c** suitable for single-crystal X-ray diffraction were obtained from an equilibrium mixture of the reaction components in hexane at -30 °C.

^{1}H-NMR (500.1 MHz, C_6D_6, 298 K): δ = 1.28 (d, br, 12H, ^{i}Pr-C*H$_3$*), 1.58 (d, br, 12H ^{i}Pr-C*H$_3$*), 1.78 (s, 12H, NCC*H*$_3$CC*H*$_3$N), 3.83 (s, 8H, C*H*$_{2Beg}$), 6.04 (sept, 4H, $^3J_{HH}$ = 7.0 Hz, ^{i}Pr-C*H*).

^{13}C{^{1}H}-NMR (160.5 MHz, C_6D_6, 298 K): δ = 10.4 (NC*C*H$_3$C*C*H$_3$N), 22.3 (^{i}Pr-*C*H$_3$), 22.5 (^{i}Pr-*C*H$_3$), 52.6 (^{i}Pr-*C*H), 64.0 (Beg-*C*H$_2$), 123.0 (N*C*CH$_3$*C*CH$_3$N), 198.5 (N*C*N).

^{11}B{^{1}H}-NMR (128.5 MHz, C_6D_6, 298 K): δ = 46.46 (s, 2B, *B*eg).

[Ni(^{i}Pr$_2$Im^{Me})$_2$(η^2-*cis*-(Bcat)(Me)C=C(Me)(Bcat))] 15a

[Ni(^{i}Pr$_2$Im^{Me})$_2$(η^2-MeC≡CMe)] **14a** (286 mg, 604 μmol) and B$_2$cat$_2$ (144 mg, 604 μmol) were dissolved in 8 mL of benzene. The orange-colored mixture was stirred for 20 min at room temperature and was then filtered through a pad of celite. All volatiles were removed *in vacuo* and the remaining residue was suspended in 15 mL of hexane. The product was collected by filtration and dried *in vacuo* to give an orange-colored powder (340 mg, 478 μmol, 79 %).

Orange-colored crystals of [Ni(^{i}Pr$_2$Im^{Me})$_2$(η^2-*cis*-(Bcat)(Me)C=C(Me)(Bcat))] **15a** suitable for single-crystal X-ray diffraction were obtained from storing a saturated solution in hexane at -30 °C.

Elemental analysis $C_{38}H_{54}B_2N_4NiO_4$ [657.10 g/mol] calculated (found): C 64.18 (65.00), H 7.65 (7.97), N 7.88 (7.68).

^{1}H-NMR (400.1 MHz, C_6D_6, 298 K): δ = 0.78 (d, 6H, $^{3}J_{HH}$ = 7.2 Hz, ^{i}Pr-CH_3), 0.91 (d, 6H, $^{3}J_{HH}$ = 7.2 Hz, ^{i}Pr-CH_3), 0.93 (d, 6H, $^{3}J_{HH}$ = 7.2 Hz, ^{i}Pr-CH_3), 1.34 (d, 6H, $^{3}J_{HH}$ = 7.2 Hz, ^{i}Pr-CH_3), 1.60 (s, 6H, NCCH_3CCH_3N), 1.63 (s, 6H, NCCH_3CCH_3N), 2.11 (s, 6H, H_3CC=CCH_3), 5.78 (sept, 2H, $^{3}J_{HH}$ = 7.2 Hz, ^{i}Pr-CH), 5.98 (sept, 2H, $^{3}J_{HH}$ = 7.2 Hz, ^{i}Pr-CH), 6.81 (dd, 4H, $^{3}J_{HH}$ = 5.5 Hz, $^{4}J_{HH}$ = 3.3 Hz, BO_2C_6-4,5-H_4), 7.07 (dd, 4H, $^{3}J_{HH}$ = 5.5 Hz, $^{4}J_{HH}$ = 3.3 Hz, BO_2C_6-3,6-H_4).

^{13}C{^{1}H}-NMR (100.6 MHz, C_6D_6, 298 K): δ = 10.2 (NCCH$_3$CCH$_3$N), 10.4 (NCCH$_3$CCH$_3$N), 19.4 (H$_3C$C=CCH$_3$), 20.7 (^{i}Pr-CH$_3$), 21.3 (^{i}Pr-CH$_3$), 22.3 (^{i}Pr-CH$_3$), 23.6 (^{i}Pr-CH$_3$), 40.0 (C=C, assigned *via* HMBC), 52.5 (^{i}Pr-CH), 52.7 (^{i}Pr-CH), 111.4 (BO_2-3,6-C_6H_4), 120.7 (BO_2-4,5-C_6H_4), 124.5 (NCCH$_3$$CCH_3$N), 124.7 (N$CCH_3$$CCH_3$N), 151.5 ($BO_2$-1,2-$C_6H_4$), 196.0 (N$C$N).

^{11}B{^{1}H}-NMR (128.5 MHz, C_6D_6, 298 K): δ = 33.25 (s, 2B, Bcat).

IR (ATR [cm^{-1}]): 2978 (vw), 2933 (vw), 2871 (vw), 2840 (vw), 1479 (m), 1444 (w), 1401 (m), 1377 (m), 1340 (s), 1288 (w), 1261 (m), 1233 (vs), 1215 (s), 1165 (vw), 1147 (vw), 1127 (w), 1113 (w), 1103 (w), 1072 (vs), 1034 (m), 1005 (m), 962 (vw), 923 (w), 905 (w), 868 (vw), 823 (w), 810 (w), 762 (w), 740 (vs), 696 (vw), 670 (w), 613 (w), 596 (m), 550 (vw), 515 (vw), 484 (vw), 451 (vw), 423 (w).

[Ni(^{i}Pr$_2$Im^{Me})$_2$(η^2-*cis*-(Bcat)(H$_7$C$_3$)C=C(C$_3$H$_7$)(Bcat))] 15b

[Ni(^{i}Pr$_2$Im^{Me})$_2$(η^2-H$_7$C$_3$C≡CC$_3$H$_7$)] **14b** (50 mg, 94.4 μmol) and B_2cat_2 (22.5 mg, 94.4 μmol) were dissolved in 3 mL of benzene. The yellow mixture was stirred for 48 h at room temperature and was then filtered through a pad of celite. All volatiles were removed *in vacuo* and the remaining residue was suspended in 3 mL of hexane. The product was collected by filtration and dried *in vacuo* to give an orange powder (25 mg, 32.6 μmol, 35 %).

Orange-colored crystals of [Ni(^{i}Pr$_2$Im^{Me})$_2$(η^2-*cis*-(Bcat)(H$_7$C$_3$)C=C(C$_3$H$_7$)(Bcat))] **15b** suitable for single-crystal X-ray diffraction were obtained from storing a saturated solution in hexane at -30 °C.

Elemental analysis $C_{42}H_{62}B_2N_4NiO_4$ [767.30 g/mol] calculated (found): C 65.75 (64.97), H 8.14 (8.01), N 7.30 (6.79).

^{1}H-NMR (400.1 MHz, C_6D_6, 298 K): δ = 0.76 (d, 6H, $^{3}J_{HH}$ = 7.1 Hz, ^{i}Pr-CH_3), 0.92 (d, 12H, $^{3}J_{HH}$ = 7.1 Hz, ^{i}Pr-CH_3), 1.28 (t, 6H, $^{3}J_{HH}$ = 7.1 Hz, CH$_2$CH$_2$CH_3), 1.39 (d, 6H, $^{3}J_{HH}$ = 7.1 Hz, ^{i}Pr-CH_3), 1.62

(s, 6H, NCCH_3CCH_3N), 1.64 (s, 6H, NCCH_3CCH_3N), 1.97 (m, 2H, $CH_2CH_2CH_3$), 2.13 (m, 2H, $CH_2CH_2CH_3$), 2.40 (m, 2H, $CH_2CH_2CH_3$), 2.81 (m, 2H $CH_2CH_2CH_3$), 5.81 (sept, 2H, $^3J_{HH}$ = 7.1 Hz, ^{i}Pr-C*H*), 5.96 (sept, 2H, $^3J_{HH}$ = 7.1 Hz, ^{i}Pr-C*H*), 6.81 (dd, 4H, $^3J_{HH}$ = 5.6 Hz, $^4J_{HH}$ = 3.3 Hz, BO_2C_6-4,5-H_4), 7.05 (dd, 4H, $^3J_{HH}$ = 5.6 Hz, $^4J_{HH}$ = 3.3 Hz, BO_2C_6-3,6-H_4).

^{13}C{^{1}H}-NMR (100.6 MHz, C_6D_6, 298 K): δ = 10.2 (NCCH_3CCH_3N), 10.4 (NCCH_3CCH_3N), 15.7 ($CH_2CH_2CH_3$), 20.7 (^{i}Pr-CH_3), 21.4 (^{i}Pr-CH_3), 22.2 (^{i}Pr-CH_3), 23.8 (^{i}Pr-CH_3), 26.7 ($CH_2CH_2CH_3$), 38.3 ($CH_2CH_2CH_3$), 47.3 (*C*=*C*, assigned *via* HMBC), 52.4 (^{i}Pr-*C*H), 52.8 (^{i}Pr-*C*H), 111.4 (BO_2-3,6-C_6H_4), 120.7 (BO_2-4,5-C_6H_4), 124.6 (N*C*CH_3*C*CH_3N), 124.7 (N*C*CH_3*C*CH_3N), 151.5 (BO_2-1,2-C_6H_4), 196.2 (N*C*N).

^{11}B{^{1}H}-NMR (128.5 MHz, C_6D_6, 298 K): δ = 31.91 (s, 2B, *B*cat).

IR (ATR [cm^{-1}]): 2952 (w), 2867 (w), 1635 (vw), 1596 (vw), 1484 (vs), 1415 (w), 1372 (m), 1302 (w), 1238 (vs), 1131 (w), 1096 (w), 1055 (s), 1007 (m), 906 (m), 813 (w), 729 (s), 702 (w), 550 (vw), 466 (vw), 432 (vw).

Z-(Bcat)(4-Me-C_6H_4)C=C(4-Me-C_6H_4)(Bcat) • (^{i}Pr$_2$Im^{Me}) **4^{NHC}**

Z-(Bcat)(4-Me-C_6H_4)C=C(4-Me-C_6H_4)(Bcat) **4** (62 mg, 140 μmol) and iPr$_2$Im^{Me} (25.2 mg, 140 μmol) were dissolved in 5 mL of benzene. The mixture was stirred for 48 h at room temperature and was then filtered through a pad of celite. All volatiles were removed *in vacuo* and the remaining residue was suspended in 5 mL of hexane. The product was collected by filtration and dried *in vacuo* to give an off-white powder (45 mg, 72.1 μmol, 52 %).

Colorless crystals of *Z*-(Bcat)(4-Me-C_6H_4)C=C(4-Me-C_6H_4)(Bcat) • (^{i}Pr$_2$Im^{Me}) **4^{NHC}** suitable for single-crystal X-ray diffraction were obtained by slow evaporation of a saturated solution of the compound in C_6D_6.

Elemental analysis $C_{39}H_{42}B_2N_2O_4$ [624.40 g/mol] calculated (found): C 75.02 (73.84), H 6.78 (6.80), N 4.49 (3.88).

^{1}H-NMR (400.1 MHz, C_6D_6, 298 K): δ = 1.12 (d, 12H, $^3J_{HH}$ = 7.0 Hz, ^{i}Pr-CH_3), 1.36 (s, 6H, NCCH_3CCH_3N), 1.94 (s, 3H, C_6H_4-CH_3), 2.04 (s, 3H, C_6H_4-CH_3), 6.03 (sept, 2H, $^3J_{HH}$ = 7.0 Hz, ^{i}Pr-C*H*), 6.60 (dd, 2H, $^3J_{HH}$ = 5.7 Hz, $^4J_{HH}$ = 3.4 Hz, $BO_2C_6H_4$), 6.70 (dd, 2H, $^3J_{HH}$ = 5.7 Hz, $^4J_{HH}$ = 3.4 Hz, $BO_2C_6H_4$), 6.81 (d, 2H, $^3J_{HH}$ = 8.0 Hz, aryl-CH_{meta}), 6.89 (d, 2H, $^3J_{HH}$ = 8.0 Hz, aryl-CH_{meta}),

6.91 (dd, 2H, $^3J_{HH}$ = 5.7 Hz, $^4J_{HH}$ = 3.4 Hz, $BO_2C_6H_4$), 7.14 (dd, 2H, $^3J_{HH}$ = 5.7 Hz, $^4J_{HH}$ = 3.4 Hz, $BO_2C_6H_4$), 7.26 (d, 2H, $^3J_{HH}$ = 8.0 Hz, aryl-CH_{ortho}), 7.50 (d, 2H, $^3J_{HH}$ = 8.0 Hz, aryl-CH_{ortho}). **^{13}C{^{1}H}-NMR** (100.6 MHz, C_6D_6, 298 K): δ = 10.0 (NCCH_3CCH_3N), 21.0 (C_6H_4-CH_3), 21.1 (C_6H_4-CH_3), 21.5 (^{i}Pr-CH_3), 50.3 (^{i}Pr-CH), 111.6 ($BO_2C_6H_4$), 111.9 ($BO_2C_6H_4$), 120.4 ($BO_2C_6H_4$), 121.0 ($BO_2C_6H_4$), 125.7 (NCCH_3CCH_3N), 128.8 (aryl-CH_{meta}), 128.9 (aryl-CH_{ortho}), 129.0 (aryl-CH_{meta}), 129.7 (aryl-CH_{ortho}), 134.2 (aryl-C_{para}), 134.7 (aryl-C_{para}), 139.5 (aryl-C_{ipso}), 140.7 (*C*=*C*, assigned via HMBC), 142.1 (aryl-C_{ipso}), 151.2 ($BO_2C_6H_4$), 151.3 ($BO_2C_6H_4$), 157.5 (*C*=*C*, assigned via HMBC), 157.9 (N*C*N, assigned via HMBC)

^{11}B{^{1}H}-NMR (128.5 MHz, C_6D_6, 298 K): δ = 9.71 (s, br, 1B, sp^3-*B*cat), 28.02 (s, br, 1B, sp^2-*B*cat).

IR (ATR [cm^{-1}]): 3019 (vw), 2981 (vw), 2935 (vw), 1632 (vw), 1605 (vw), 1553 (vw), 1506 (w), 1485 (s), 1403 (w), 1362 (w), 1314 (w), 1300 (w), 1243 (s), 1233 (s), 1186 (w), 1170 (w), 1139 (w), 1097 (m), 1086 (m), 1060 (w), 1022 (w), 1007 (w), 951 (m), 934 (w), 896 (m), 880 (w), 848 (w), 817 (m), 800 (m), 778 (m), 747 (w), 729 (vs), 703 (vw), 654 (vw), 630 (vw), 607 (w), 572 (vw), 544 (vw), 528 (w), 512 (m), 496 (w), 422 (w).

HRMS-LIFDI *m/z* (%) calculated for [$C_{39}H_{42}B_2N_2O_4$]: 624.3331(100) [M]$^+$; found 625.3398(100) [M+H]$^+$, 299.1921 [^{i}Pr$_2$Im^{Me}Bcat]$^+$, 181.1698 [^{i}Pr$_2$Im^{Me}+H]$^+$.

General procedures for the synthesis of organoboronic esters

Method A:

A Young's tap NMR tube was charged with a 60:40 mixture of [Ni$_2$(^{i}Pr$_2$Im^{Me})$_4$(μ-(η^2:η^2)-COD)] **1** and [Ni(^{i}Pr$_2$Im^{Me})$_2$(η^4-COD)] **1a** (4-10 mol% [Ni(^{i}Pr$_2$Im^{Me})$_2$]) and B_2cat_2 (23.8 mg, 100 μmol). In close succession, 1 equiv. of alkyne (0.5 equiv. for tetra-borylation; 4 equiv. for alkyne coupling + borylation) and 0.6 mL C_6D_6 were added. The mixture was shaken, and the reaction progress was monitored by ^{1}H- and ^{11}B{^{1}H}-NMR spectroscopy. If necessary, the reaction mixture was heated to 50 °C until the alkyne (or B_2cat_2 if an excess alkyne was used) was completely consumed. Upon completion, an aliquot was removed and analyzed by GC/MS. From the remaining mixture all volatiles were removed *in vacuo* and the crude product was analyzed by ^{1}H-, ^{11}B{^{1}H}- and ^{13}C{^{1}H}-NMR spectroscopy (C_6D_6).

Method B:

The synthesis of **4**, **7**, **8a** and **13** were scaled-up to a preparative scale. As column chromatography is not suitable for the purification of the compounds, work-up cannot be described in a general method. Scaled-up procedures and purification are therefore reported separately for each case.

***Z*-(Bcat)(Ph)C=C(Ph)(Bcat) 3**

Method A was employed for the preparation of **3**, using diphenylacetylene (17.8 mg, 100 μmol, 1 eq.) as the alkyne and 10 mol% [Ni(^{i}Pr$_2$Im^{Me})$_2$].

^{1}H-NMR (400.1 MHz, C_6D_6, 298 K): δ = 6.74 (dd, 4H, $^3J_{HH}$ = 5.8 Hz, $^4J_{HH}$ = 3.4 Hz, $BO_2C_6\mathit{H}_4$), 6.89 (dd, 4H, $^3J_{HH}$ = 5.8 Hz, $^4J_{HH}$ = 3.4 Hz, $BO_2C_6\mathit{H}_4$), 6.91 (m, 2H, aryl-CH_{para}), 6.99 (m, 4H, aryl-CH_{meta}), 7.24 (m, 4H, aryl-CH_{ortho}).**^{13}C{^{1}H}-NMR** (100.6 MHz, C_6D_6, 298 K): δ = 112.8 ($BO_2\mathit{C}_6H_4$), 123.1 ($BO_2\mathit{C}_6H_4$), 127.4 (aryl-$\mathit{C}H_{para}$), 128.6 (aryl-$\mathit{C}H_{meta}$), 129.8 (aryl-$\mathit{C}H_{ortho}$), 139.9 (aryl-C_{ipso}), 146.4 (*C*=*C*, assigned via HMBC), 148.8 ($BO_2\mathit{C}_6H_4$).

^{11}B{^{1}H}-NMR (128.5 MHz, C_6D_6, 298 K): δ = 32.22 (s, br, 2B, *B*cat).

GC/MS Ret.: 15.42 min, (m/z): 416.0 $[M]^+$.

The spectroscopic data for **3** match those reported in the literature.[1]

***Z*-(Bcat)(4-Me-C$_6$H$_4$)C=C(4-Me-C$_6$H$_4$)(Bcat) 4**

Method A was employed for the preparation of **4**, using bis-(p-tolyl)acetylene (20.7 mg, 100 μmol, 1 eq.) as the alkyne and 10 mol% [Ni(^{i}Pr$_2$Im^{Me})$_2$].

The reaction was also performed on a preparative scale:

A Schlenk-tube was charged with a 60:40 mixture of [Ni$_2$(^{i}Pr$_2$Im^{Me})$_4$(μ-(η^2:η^2)-COD)] **1** and [Ni(^{i}Pr$_2$Im^{Me})$_2$(η^4-COD)] **1a** (20.0 mg, 40.4 μmol, 9.6 mol% [Ni(^{i}Pr$_2$Im^{Me})$_2$]), B_2cat_2 (100 mg, 421 μmol, 1 eq.) and bis-(p-tolyl)acetylene (86.8 mg, 421 μmol, 1 eq.). The mixture was dissolved in 4 mL of benzene, stirred for 20 h at 50 °C and was then filtered through a pad of celite. All volatiles were removed *in vacuo* and the remaining residue was suspended in 30 mL

of hexane. The product was collected by filtration and dried *in vacuo* to give an off-white powder (112 mg, 252 μmol, 60 %). The crude product was re-crystallized by storing a saturated hexane solution at -30 °C.

Elemental analysis $C_{28}H_{22}B_2O_4$ [444.10 g/mol] calculated (found): C 75.73 (75.64), H 4.99 (4.96).

^{1}H-NMR (400.1 MHz, C_6D_6, 298 K): δ = 1.98 (s, 6H, CH_3), 6.74 (dd, 4H, $^3J_{HH}$ = 5.8 Hz, $^4J_{HH}$ = 3.4 Hz, $BO_2C_6H_4$), 6.84 (d, 4H, $^3J_{HH}$ = 8.0 Hz, aryl-CH_{meta}), 6.90 (dd, 4H, $^3J_{HH}$ = 5.8 Hz, $^4J_{HH}$ = 3.4 Hz, $BO_2C_6H_4$), 7.23 (d, 4H, $^3J_{HH}$ = 8.0 Hz, aryl-CH_{ortho}).**^{13}C{^{1}H}-NMR** (100.6 MHz, C_6D_6, 298 K): δ = 21.1 (CH_3), 112.8 ($BO_2C_6H_4$), 123.0 ($BO_2C_6H_4$), 129.4 (aryl-CH_{meta}), 129.9 (aryl-CH_{ortho}), 136.9 (aryl-C_{ipso}), 137.2 (aryl-C_{para}), 146.2 (*C*=*C*, assigned via HMBC), 148.9 ($BO_2C_6H_4$).

^{11}B{^{1}H}-NMR (128.5 MHz, C_6D_6, 298 K): δ = 32.54 (s, br, 2B, *B*cat).

GC/MS Ret.: 16.53 min, (m/z): 444.1 $[M]^+$.

IR (ATR [cm^{-1}]): 2920 (vw), 1603 (vw), 1575 (vw), 1507 (w), 1470 (s), 1412 (w), 1397 (w), 1372 (m), 1350 (w), 1322 (s), 1308 (s), 1281 (w), 1253 (w), 1228 (vs), 1187 (w), 1167 (m), 1131 (m), 1119 (w), 1083 (w), 1036 (w), 1022 (w), 1004 (w), 993 (w), 970 (w), 944 (vw), 923 (w), 891 (w), 865 (w), 841 (vw), 807 (s), 746 (vs), 738 (vs), 703 (m), 654 (m), 578 (w), 550 (m), 522 (w), 505 (w), 490 (m), 473 (m), 426 (m).

The spectroscopic data for **4** match those reported in the literature.[1]

***Z*-(Bcat)(4-CF_3-C_6H_4)C=C(4-CF_3-C_6H_4)(Bcat) 5**

Method A was employed for the preparation of **5**, using 1,2-Bis[*p*-(trifluoromethyl)phenyl]acetylene (31.5 mg, 100 μmol, 1 eq.) as the alkyne and 10 mol% [Ni(^{i}Pr$_2$Im^{Me})$_2$].

^{1}H-NMR (400.1 MHz, C_6D_6, 298 K): δ = 6.78 (dd, 4H, $^3J_{HH}$ = 5.9 Hz, $^4J_{HH}$ = 3.4 Hz, $BO_2C_6H_4$), 6.92 (dd, 4H, $^3J_{HH}$ = 5.9 Hz, $^4J_{HH}$ = 3.4 Hz, $BO_2C_6H_4$), 6.96 (d, 4H, $^3J_{HH}$ = 8.1 Hz, aryl-CH_{meta}), 7.13 (d, 4H, $^3J_{HH}$ = 8.1 Hz, aryl-CH_{ortho}).**^{13}C{^{1}H}-NMR** (100.6 MHz, C_6D_6, 298 K): δ = 113.0 ($BO_2C_6H_4$), 123.6 ($BO_2C_6H_4$), 125.6 (aryl-CH_{meta}), 129.9 (aryl-CH_{ortho}), 142.7 (aryl-C_{ipso}), 148.5 ($BO_2C_6H_4$).

^{11}B{^{1}H}-NMR (128.5 MHz, C_6D_6, 298 K): δ = 31.3(s, br, 2B, *B*cat).

^{19}F{^{1}H}-NMR (376.8 MHz, C_6D_6, 298 K): δ = -62.40(s, 6F, CF_3).

GC/MS Ret.: 14.34 min, (m/z): 552.0 $[M]^+$.

The spectroscopic data for **5** match those reported in the literature.[8]

Z-(Bcat)(C_3H_7)C=C(C_3H_7)(Bcat) 6

Method A was employed for the preparation of **6**, using 4-octyne (14.7μL, 11.0 mg, 100 μmol, 1 eq.) as the alkyne and 4 mol% [Ni(^{i}Pr$_2$Im^{Me})$_2$].

^{1}H-NMR (400.1 MHz, C_6D_6, 298 K): δ = 0.91 (t, 6H, $^3J_{HH}$ = 7.5 Hz, $CH_2CH_2CH_3$), 1.54 (m, 4H, $CH_2CH_2CH_3$), 2.50 (t, 4H, $^3J_{HH}$ = 7.5 Hz, $CH_2CH_2CH_3$), 6.74 (dd, 4H, $^3J_{HH}$ = 5.8 Hz, $^4J_{HH}$ = 3.4 Hz, $BO_2C_6H_4$), 6.91 (dd, 4H, $^3J_{HH}$ = 5.8 Hz, $^4J_{HH}$ = 3.4 Hz, $BO_2C_6H_4$).**^{13}C{^{1}H}-NMR** (100.6 MHz, C_6D_6, 298 K): δ = 14.4 ($CH_2CH_2CH_3$), 23.2 ($CH_2CH_2CH_3$), 33.3 ($CH_2CH_2CH_3$), 112.7 ($BO_2C_6H_4$), 122.9 ($BO_2C_6H_4$), 148.8 ($BO_2C_6H_4$).

^{11}B{^{1}H}-NMR (128.5 MHz, C_6D_6, 298 K): δ = 32.38 (s, br, 2B, *B*cat).

GC/MS Ret.: 12.29 min, (m/z): 348.0 $[M]^+$.

Z-(Bcat)(Me)C=C(Ph)(Bcat) 7

Method A was employed for the preparation of **7**, using 1-phenyl-1-propyne (12.5μL, 11.6 mg, 100 μmol, 1 eq.) as the alkyne and 4 mol% [Ni(^{i}Pr$_2$Im^{Me})$_2$].

The reaction was also performed on a preparative scale:

A Schlenk-tube was charged with a 60:40 mixture of [Ni$_2$(^{i}Pr$_2$Im^{Me})$_4$(μ-(η^2:η^2)-COD)] **1** and [Ni(^{i}Pr$_2$Im^{Me})$_2$(η^4-COD)] **1a** (26.0 mg, 53.5 μmol, 3.6 mol% [Ni(^{i}Pr$_2$Im^{Me})$_2$]) and B_2cat_2 (352 mg, 1.48 mmol, 1 eq.). In close succession, 1-phenylpropyne (184 μL, 172 mg, 1.48 mmol, 1 eq.) and 10 mL benzene were added. The reaction mixture was stirred for 3 h at 50 °C and was then filtered through a pad of celite. All volatiles were removed *in vacuo*, the remaining residue was suspended in 30 mL of hexane and filtered again through a pad of celite. The filtrate was then stored for 24 h at -30 °C. The supernatant solution was removed from the precipitated product via a syringe and the product was dried *in vacuo* to yield light brown crystals of **7** (341 mg, 963 μmol, 65 %).

Elemental analysis $C_{21}H_{16}B_2O_4$ [353.98 g/mol] calculated (found): C 71.26 (71.54), H 4.56 (4.87).

^{1}H-NMR (400.1 MHz, C_6D_6, 298 K): δ = 2.00 (s, 3H, CH_3), 6.74 (m, 4H, $BO_2C_6H_4$), 6.86 (m, 2H, $BO_2C_6H_4$), 6.94 (m, 2H, $BO_2C_6H_4$), 7.07 (m, 1H, aryl-CH_{para}), 7.18 (m, ,2H, aryl-CH_{meta}), 7.29 (m, 2H, aryl-CH_{ortho}).**^{13}C{^{1}H}-NMR** (100.6 MHz, C_6D_6, 298 K): δ = 18.2 (CH$_3$), 112.7 ($BO_2C_6H_4$), 112.8 ($BO_2C_6H_4$), 122.9 ($BO_2C_6H_4$), 123.0 ($BO_2C_6H_4$), 127.4 (aryl-CH$_{para}$), 128.7 (aryl-CH$_{meta}$), 128.8 (aryl-CH$_{ortho}$), 140.1 (aryl-C_{ipso}), 148.7 ($BO_2C_6H_4$), 148.9 ($BO_2C_6H_4$).

^{11}B{^{1}H}-NMR (128.5 MHz, C_6D_6, 298 K): δ = 31.97 (s, br, 2B, *B*cat).

GC/MS Ret.: 13.43 min, (m/z): 354.0 $[M]^+$.

IR (ATR [cm^{-1}]): 3063 (vw), 1590 (vw), 1470 (s), 1441 (w), 1390 (w), 1371 (m), 1350 (w), 1323 (s), 1312 (s), 1274 (w), 1230 (vs), 1198 (m), 1124 (m), 1108 (s), 1006 (w), 914 (w), 866 (w), 812 (m), 779 (w), 762 (w), 737 (vs), 706 (s), 688 (m), 672 (s), 611 (w), 583 (w), 539 (w), 499 (w), 488 (w), 428 (m).

Z-(Bcat)(Me)C=C(Me)(Bcat) 8

Method A was employed for the preparation of **8**, using 2-butyne (7.85 μL, 5.41 mg, 100 μmol, 1 eq.) as the alkyne and 4 mol% [Ni(^{i}Pr$_2$Im^{Me})$_2$].

^{1}H-NMR (400.1 MHz, C_6D_6, 298 K): δ = 1.88 (s, 6H, CH_3), 6.75 (dd, 4H, $^3J_{HH}$ = 5.8 Hz, $^4J_{HH}$ = 3.3 Hz, $BO_2C_6H_4$), 6.92 (dd, 4H, $^3J_{HH}$ = 5.8 Hz, $^4J_{HH}$ = 3.3 Hz, $BO_2C_6H_4$).**^{13}C{^{1}H}-NMR** (100.6 MHz, C_6D_6, 298 K): δ = 16.7 (CH$_3$), 112.7 ($BO_2C_6H_4$), 122.9 ($BO_2C_6H_4$), 148.9 ($BO_2C_6H_4$).

^{11}B{^{1}H}-NMR (128.5 MHz, C_6D_6, 298 K): δ = 31.90 (s, br, 2B, *B*cat).

GC/MS Ret.: 11.28 min, (m/z): 292.0 $[M]^+$.

(Bcat)$_2$(Me)C–C(Me)(Bcat)$_2$ 8a

Method A was employed for the preparation of **8a**, using 2-butyne (3.92 μL, 2.71 mg, 50 μmol, 0.5 eq.) as the alkyne and 4 mol% [Ni(^{i}Pr$_2$Im^{Me})$_2$].

The reaction was also performed on a preparative scale:

A Schlenk-tube was charged with a 60:40 mixture of $[Ni_2(^iPr_2Im^{Me})_4(\mu\text{-}(\eta^2\text{:}\eta^2)\text{-COD})]$ **1** and $[Ni(^iPr_2Im^{Me})_2(\eta^4\text{-COD})]$ **1a** (14.0 mg, 28.7 μmol, 3.9 mol% $[Ni(^iPr_2Im^{Me})_2]$) and B_2cat_2 (352 mg, 1.48 mmol, 2 eq.). In close succession, 2-butyne (58.0 μL, 40.0 mg, 740 μmol, 1 eq.) and 10 mL benzene were added. The reaction mixture was stirred for 20 h at 50 °C and was then filtered through a pad of celite. All volatiles were removed *in vacuo* and the remaining residue was suspended in 25 mL of hexane. The product was collected by filtration and dried *in vacuo* to give an off-white powder of **8a** (150 mg, 283 μmol, 38 %).

Elemental analysis $C_{28}H_{22}B_4O_8$ [529.72 g/mol] calculated (found): C 63.49 (63.82), H 4.19 (4.60).

^{1}H-NMR (400.1 MHz, C_6D_6, 298 K): δ = 2.01 (s, 6H, CH_3), 6.67 (dd, 8H, $^3J_{HH}$ = 5.8 Hz, $^4J_{HH}$ = 3.3 Hz, $BO_2C_6H_4$), 6.86 (dd, 8H, $^3J_{HH}$ = 5.8 Hz, $^4J_{HH}$ = 3.3 Hz, $BO_2C_6H_4$).**^{13}C{^{1}H}-NMR** (100.6 MHz, C_6D_6, 298 K): δ = 16.5 (CH_3), 112.8 ($BO_2C_6H_4$), 122.8 ($BO_2C_6H_4$), 148.8 ($BO_2C_6H_4$).

^{11}B{^{1}H}-NMR (128.5 MHz, C_6D_6, 298 K): δ = 35.90 (s, br, 4B, *B*cat).

GC/MS Ret.: 13.54 min, (m/z): 530.1 $[M]^+$.

IR (ATR [cm^{-1}]): 1470 (s), 1423 (vw), 1390 (vw), 1362 (vw), 1273 (s), 1149 (vw), 1132 (m), 1084 (w), 1053 (m), 1006 (w), 960 (vw), 919 (vw), 865 (w), 853 (vw), 809 (m), 740 (vs), 695 (w), 631 (vw), 613 (w), 557 (vw), 452 (vw), 424 (m).

***E,E*-(Bcat)(Me)C=C(Me)–(Me)C=C(Me)(Bcat) 8b**

Method A was employed for the preparation of **8b**, using 2-butyne (31.2 μL, 21.7 mg, 400 μmol, 4 eq.) as the alkyne and 4 mol% $[Ni(^iPr_2Im^{Me})_2]$.

^{1}H-NMR (400.1 MHz, C_6D_6, 298 K): δ = 1.97 (q, br, 6H, $^5J_{HH}$ = 1 Hz, CH_3), 2.01(q, br, 6H, $^5J_{HH}$ = 1 Hz, CH_3), 6.73 (dd, 4H, $^3J_{HH}$ = 5.9 Hz, $^4J_{HH}$ = 3.3 Hz, $BO_2C_6H_4$), 6.95 (dd, 4H, $^3J_{HH}$ = 5.9 Hz, $^4J_{HH}$ = 3.3 Hz, $BO_2C_6H_4$).**^{13}C{^{1}H}-NMR** (100.6 MHz, C_6D_6, 298 K): δ = 16.4 (CH_3), 19.3 (CH_3), 112.4($BO_2C_6H_4$), 119.8 (C=*C*(Me)(Bcat), assigned via HMBC),122.6 ($BO_2C_6H_4$), 148.9 ($BO_2C_6H_4$), 159.5 ((Me)*C*=C).

^{11}B{^{1}H}-NMR (128.5 MHz, C_6D_6, 298 K): δ = 31.88 (s, br, 4B, *B*cat).

GC/MS Ret.: 12.05 min, (m/z): 346.1 $[M]^+$.

***E*-(Bcat)HC=C(Ph)(Bcat) 9**

Method A was employed for the preparation of **9**, using phenylacetylene (11.0μL, 10.2 mg, 100 μmol, 1 eq.) as the alkyne and 4 mol% [Ni(^{i}Pr$_2$Im^{Me})$_2$].

^{1}H-NMR (400.1 MHz, C_6D_6, 298 K): δ = 6.68 (dd, 2H, $^3J_{HH}$ = 5.8 Hz, $^4J_{HH}$ = 3.4 Hz, $BO_2C_6H_4$), 6.78 (dd, 2H, $^3J_{HH}$ = 5.8 Hz, $^4J_{HH}$ = 3.4 Hz, $BO_2C_6H_4$), 6.85 (dd, 2H, $^3J_{HH}$ = 5.8 Hz, $^4J_{HH}$ = 3.4 Hz, $BO_2C_6H_4$), 6.89 (s, 1H, C=*C*H), 7.05 – 7.10 (m, 2H $BO_2C_6H_4$, 3H aryl-C$H_{para/meta}$), 7.45 (m, 2H, aryl-CH_{ortho}).**^{13}C{^{1}H}-NMR** (100.6 MHz, C_6D_6, 298 K): δ = 112.7 ($BO_2C_6H_4$), 112.9 ($BO_2C_6H_4$), 123.0 ($BO_2C_6H_4$), 123.2 ($BO_2C_6H_4$), 127.4 (aryl-*C*H$_{ortho}$), 129.0 (aryl-*C*H$_{meta}$), 129.1 (aryl-*C*H$_{para}$), 141.1 (aryl-C_{ipso}), 148.6 ($BO_2C_6H_4$), 149.0 ($BO_2C_6H_4$), 154.7 (*C*=CH, assigned via HMBC).

^{11}B{^{1}H}-NMR (128.5 MHz, C_6D_6, 298 K): δ = 30.87 (s, br, 2B, *B*cat).

GC/MS Ret.: 13.58 min, (m/z): 340.0 $[M]^+$.

The spectroscopic data for **9** match those reported in the literature.[1]

***E*-(Bcat)HC=C(4-Me-C_6H_4)(Bcat) 10**

Method A was employed for the preparation of **10**, using *p*-tolylacetylene (12.7μL, 11.6 mg, 100 μmol, 1 eq.) as the alkyne and 4 mol% [Ni(^{i}Pr$_2$Im^{Me})$_2$].

^{1}H-NMR (400.1 MHz, C_6D_6, 298 K): δ = 2.05 (s, 3H, CH_3), 6.67 (dd, 2H, $^3J_{HH}$ = 5.8 Hz, $^4J_{HH}$ = 3.4 Hz, $BO_2C_6H_4$), 6.78 (dd, 2H, $^3J_{HH}$ = 5.8 Hz, $^4J_{HH}$ = 3.4 Hz, $BO_2C_6H_4$), 6.86 (dd, 2H, $^3J_{HH}$ = 5.8 Hz, $^4J_{HH}$ = 3.4 Hz, $BO_2C_6H_4$), 6.92 (d, 2H, $^3J_{HH}$ = 7.8 Hz, aryl-CH_{meta}), 6.93 (s, 1H, C=C*H*), 7.10 (dd, 2H, $^3J_{HH}$ = 5.8 Hz, $^4J_{HH}$ = 3.4 Hz, $BO_2C_6H_4$), 7.42 (d, 2H, $^3J_{HH}$ = 7.8 Hz, aryl-CH_{ortho}).**^{13}C{^{1}H}-NMR** (100.6 MHz, C_6D_6, 298 K): δ = 21.2 (*C*H$_3$), 112.7 ($BO_2C_6H_4$), 113.0 ($BO_2C_6H_4$), 122.9 ($BO_2C_6H_4$), 123.2 ($BO_2C_6H_4$), 127.4 (aryl-*C*H$_{ortho}$), 129.8 (aryl-*C*H$_{meta}$), 138.3 (aryl-C_{ipso}), 139.2 (aryl-*C*CH$_3$), 148.6 ($BO_2C_6H_4$), 149.0 ($BO_2C_6H_4$), 154.8 (*C*=CH, assigned via HMBC).

^{11}B{^{1}H}-NMR (128.5 MHz, C_6D_6, 298 K): δ = 30.84 (s, br, 2B, *B*cat).

GC/MS Ret.: 14.05 min, (m/z): 354.0 $[M]^+$.

***E*-(Bcat)HC=C(4-^{t}Bu-C$_6$H$_4$)(Bcat) 11**

Method A was employed for the preparation of **11**, using 4-(*tert*-butyl)phenylacetylene (17.8 μL, 15.8 mg, 100 μmol, 1 eq.) as the alkyne and 4 mol% [Ni(^{i}Pr$_2$Im^{Me})$_2$].

^{1}H-NMR (400.1 MHz, C_6D_6, 298 K): δ = 1.20 (s, 9H, C(C*H*$_3$)$_3$), 6.67 (dd, 2H, $^3J_{HH}$ = 5.8 Hz, $^4J_{HH}$ = 3.4 Hz, BO$_2$C$_6$*H*$_4$), 6.78 (dd, 2H, $^3J_{HH}$ = 5.8 Hz, $^4J_{HH}$ = 3.4 Hz, BO$_2$C$_6$*H*$_4$), 6.87 (dd, 2H, $^3J_{HH}$ = 5.8 Hz, $^4J_{HH}$ = 3.4 Hz, BO$_2$C$_6$*H*$_4$), 6.97 (s, 1H, C=C*H*), 7.13 (dd, 2H, $^3J_{HH}$ = 5.8 Hz, $^4J_{HH}$ = 3.4 Hz, BO$_2$C$_6$*H*$_4$), 7.18 (d, 2H, $^3J_{HH}$ = 8.6 Hz, aryl-C*H*$_{meta}$), 7.46 (d, 2H, $^3J_{HH}$ = 8.6 Hz, aryl-C*H*$_{ortho}$).**^{13}C{^{1}H}-NMR** (100.6 MHz, C_6D_6, 298 K): δ = 31.3 (C(*C*H$_3$)$_3$), 34.7 (*C*(CH$_3$)$_3$), 112.7 (BO$_2$*C*$_6$H$_4$), 113.0 (BO$_2$*C*$_6$H$_4$), 122.9 (BO$_2$*C*$_6$H$_4$), 123.2 (BO$_2$*C*$_6$H$_4$), 126.1 (aryl-*C*H$_{meta}$), 127.3 (aryl-*C*H$_{ortho}$), 138.2 (aryl-*C*$_{ipso}$), 148.6 (BO$_2$*C*$_6$H$_4$), 149.1 (BO$_2$*C*$_6$H$_4$), 152.3 (aryl-*C*-^{t}Bu), 154.9 (*C*=CH, assigned via HMBC).

^{11}B{^{1}H}-NMR (128.5 MHz, C_6D_6, 298 K): δ = 30.81 (s, br, 2B, *B*cat).

GC/MS Ret.: 15.06 min, (m/z): 396.1 [M]$^+$.

***Z,Z*-(Bcat)HC=C(C$_3$H$_7$)–(C$_3$H$_7$)C=CH(Bcat) 12a**

Method A was employed for the preparation of **12a** and **12b**, using 1-pentyne (39.4 μL, 27.3 mg, 100 μmol, 4 eq.) as the alkyne and 4 mol% [Ni(^{i}Pr$_2$Im^{Me})$_2$].

^{1}H-NMR (400.1 MHz, C_6D_6, 298 K): δ = 0.90 (t, 6H, $^3J_{HH}$ = 7.3 Hz, CH$_2$CH$_2$C*H*$_3$), 1.57 (m, 4H, CH$_2$C*H*$_2$CH$_3$), 2.31 (m, 4H, C*H*$_2$CH$_2$CH$_3$), 5.89 (t, 2H, $^4J_{HH}$ = 1.3 Hz, *H*C=C(C$_3$H$_7$)–(C$_3$H$_7$)C=C*H*), 6.69 (dd, 4H, $^3J_{HH}$ = 5.8 Hz, $^4J_{HH}$ = 3.4 Hz, BO$_2$C$_6$*H*$_4$), 6.96 (dd, 4H, $^3J_{HH}$ = 5.8 Hz, $^4J_{HH}$ = 3.4 Hz, BO$_2$C$_6$*H*$_4$).**^{13}C{^{1}H}-NMR** (100.6 MHz, C_6D_6, 298 K): δ = 14.1 (CH$_2$CH$_2$*C*H$_3$), 21.0 (CH$_2$*C*H$_2$CH$_3$), 41.9 (*C*H$_2$CH$_2$CH$_3$), 112.5 (BO$_2$*C*$_6$H$_4$), 122.7 (BO$_2$*C*$_6$H$_4$), 148.7 (BO$_2$*C*$_6$H$_4$), 169.0 (HC=*C*(C$_3$H$_7$)–(C$_3$H$_7$)*C*=CH).

^{11}B{^{1}H}-NMR (128.5 MHz, C_6D_6, 298 K): δ = 31.33 (s, br, 2B, *B*cat).

GC/MS Ret.: 12.93 min, (m/z): 374.1 [M]$^+$.

***E/Z,E/Z*-(Bcat)HC=C(C$_3$H$_7$)–HC=C(Bcat)(C$_3$H$_7$) 12b**

^{1}H-NMR (400.1 MHz, C_6D_6, 298 K): δ = 0.82 (t, 3H, $^{3}J_{HH}$ = 7.3 Hz, $CH_2CH_2CH_3$), 1.00 (t, 3H, $^{3}J_{HH}$ = 7.3 Hz, $CH_2CH_2CH_3$), 1.51 (m, 2H, $CH_2CH_2CH_3$), 1.67 (m, 2H, $CH_2CH_2CH_3$), 2.28 (m, 2H, $CH_2CH_2CH_3$), 2.52 (m, 2H, $CH_2CH_2CH_3$), 5.81 (dt, 1H, $^{4}J_{HH}$ = 1.2 Hz, $^{4}J_{HH}$ = 1.0 Hz, (Bcat)HC=C(C_3H_7)), 6.71 (dd, 2H, $^{3}J_{HH}$ = 5.8 Hz, $^{4}J_{HH}$ = 3.4 Hz, $BO_2C_6H_4$), 6.75 (dd, 2H, $^{3}J_{HH}$ = 5.8 Hz, $^{4}J_{HH}$ = 3.4 Hz, $BO_2C_6H_4$), 6.98 (dd, 2H, $^{3}J_{HH}$ = 5.8 Hz, $^{4}J_{HH}$ = 3.4 Hz, $BO_2C_6H_4$), 7.01 (dd, 2H, $^{3}J_{HH}$ = 5.8 Hz, $^{4}J_{HH}$ = 3.4 Hz, $BO_2C_6H_4$), 7.17 (br, 1H, HC=C(Bcat)(C_3H_7)).**^{13}C{^{1}H}-NMR** (100.6 MHz, C_6D_6, 298 K): δ = 13.9 ($CH_2CH_2CH_3$), 14.1 ($CH_2CH_2CH_3$), 21.9 ($CH_2CH_2CH_3$), 23.5 ($CH_2CH_2CH_3$), 40.1 ($CH_2CH_2CH_3$), 42.6 ($CH_2CH_2CH_3$), 112.5 ($BO_2C_6H_4$), 112.7 ($BO_2C_6H_4$), 114.0 (Bcat)HC=C(C_3H_7), assigned via HMBC), 122.7 ($BO_2C_6H_4$), 123.0 ($BO_2C_6H_4$), 133.3 (HC=C(Bcat)(C_3H_7), assigned via HMBC), 145.9 (HC=C(Bcat)(C_3H_7)), 148.5 ($BO_2C_6H_4$), 148.7 ($BO_2C_6H_4$), 164.6 (Bcat)HC=C(C_3H_7)).

^{11}B{^{1}H}-NMR (128.5 MHz, C_6D_6, 298 K): δ = 31.33 (s, br, 2B, *B*cat).

GC/MS Ret.: 13.04 min, (m/z): 374.1 $[M]^+$.

(4-NMe_2-C_6H_4)(Bcat)(TMS)C–C(Bcat)$_3$ 13

Method A was employed for the preparation of **13**, using *N*,*N*-dimethyl-4-[(trimethylsilyl)-ethinyl]-aniline (10.9 mg, 50 μmol, 0.5 eq.) as the alkyne and 4 mol% [Ni(^{i}Pr$_2$Im^{Me})$_2$].

The reaction was also performed on a preparative scale:

A Schlenk-tube was charged with a 60:40 mixture of [Ni$_2$(^{i}Pr$_2$Im^{Me})$_4$(μ-(η^2:η^2)-COD)] **1** and [Ni(^{i}Pr$_2$Im^{Me})$_2$(η^4-COD)] **1a** (6.0 mg, 12,3 μmol, 3.9 mol% [Ni(^{i}Pr$_2$Im^{Me})$_2$]), *N*,*N*-dimethyl-4-[(trimethylsilyl)-ethinyl]-aniline (69.0 mg, 317 μmol, 1 eq.) and B_2cat_2 (151 mg, 635 μmol, 2 eq.). The mixture was dissolved in 10 mL of benzene and stirred for 48 h at 50 °C. All volatiles were removed *in vacuo* and the remaining residue was suspended in 5 mL of hexane. The product was collected by filtration and dried *in vacuo* to give an off-white powder (101 mg, 146 μmol, 46 %).

Colorless crystals of (4-NMe_2-C_6H_4)(Bcat)(TMS)C–C(Bcat)$_3$ **13** suitable for single-crystal X-ray diffraction were obtained by slow evaporation of a saturated solution of the compound in C_6D_6.

Elemental analysis $C_{37}H_{35}B_4NO_8Si$ [693.01 g/mol] calculated (found): C 64.13 (64.27), H 5.09 (5.30), N 2.02 (2.13).

^{1}H-NMR (400.1 MHz, C_6D_6, 298 K): δ = 0.49 (s, 9H, Si(CH_3)$_3$), 2.38 (s, 6H, N(CH_3)$_2$), 6.52 (d, 2H, $^3J_{HH}$ = 8.8 Hz, aryl-CH_{meta}), 6.65 (dd, 6H, $^3J_{HH}$ = 5.9 Hz, $^4J_{HH}$ = 3.4 Hz, $BO_2C_6H_4$), 6.67 (dd, 2H, $^3J_{HH}$ = 5.9 Hz, $^4J_{HH}$ = 3.4 Hz, $BO_2C_6H_4$), 6.84 (dd, 2H, $^3J_{HH}$ = 5.9 Hz, $^4J_{HH}$ = 3.4 Hz, $BO_2C_6H_4$), 6.85 (dd, 6H, $^3J_{HH}$ = 5.9 Hz, $^4J_{HH}$ = 3.4 Hz, $BO_2C_6H_4$), 7.85 (d, 2H, $^3J_{HH}$ = 8.8 Hz, aryl-CH_{ortho}).

^{13}C{^{1}H}-NMR (100.6 MHz, C_6D_6, 298 K): δ = 1.43 (Si(CH$_3$)$_3$), 32.2 (C–C(Bcat)$_3$, assigned via HMBC), 40.3 (N(CH$_3$)$_2$), 112.6 ($BO_2C_6H_4$), 112.8 ($BO_2C_6H_4$), 112.9 (aryl-CH$_{meta}$) 122.8 ($BO_2C_6H_4$), 122.9 ($BO_2C_6H_4$), 131.4 (aryl-CH$_{ortho}$), 131.7 (aryl-C_{ipso}), 148.3 (aryl-CNMe$_2$), 148.6 ($BO_2C_6H_4$), 148.7 ($BO_2C_6H_4$).

^{11}B{^{1}H}-NMR (128.5 MHz, C_6D_6, 298 K): δ = 35.94 (s, br, 4B, *B*cat).

^{29}Si-NMR (79.5 MHz, C_6D_6, 298 K): 8.82 (s, 1Si, *Si*(CH$_3$)$_3$).

IR (ATR [cm^{-1}]): 2896 (vw), 1609 (vw), 1519 (w), 1470 (s), 1367 (vw), 1291 (s), 1251 (m), 1226 (vs), 1212 (vs), 1153 (vw), 1127 (w), 1058 (vw), 1004 (vw), 939 (w), 918 (vw), 862 (m), 840 (m), 810 (m), 791 (w), 748 (s), 740 (s), 731 (s), 706 (vw), 679 (vw) 630 (vw), 602 (w), 567 (vw), 531 (vw), 520 (vw), 421 (m).

HRMS-LIFDI *m/z* (%) calculated for [$C_{37}H_{35}B_4NO_8Si$]: 693.2505(100) [M]$^+$; found 693.2489(100) [M]$^+$, 575.2237 [M-Bcat+H]$^+$, 502.1797 [M-Bcat-TMS+H]$^{+\cdot}$.

3) Crystallographic Details

Crystals were immersed in a film of perfluoropolyether oil on a glass fiber MicroMount™ (MiTeGen) and transferred to a Bruker D8 Apex-2 diffractometer with CCD area detector and graphite-monochromated Mo-K_α radiation equipped with an Oxford Cryosystems low-temperature device or a Rigaku XtaLAB Synergy-DW diffractometer with HyPix-6000HE detector and monochromated Cu-K_α equipped with an Oxford Cryo 800 cooling unit. Data were collected at 100 K. The images were processed with the Bruker or Crysalis software packages and equivalent reflections were merged. Corrections for Lorentz-polarization effects and absorption were performed if necessary and the structures were solved by direct methods. Subsequent difference Fourier syntheses revealed the positions of all other non-hydrogen atoms. The structures were solved by using the ShelXTL software package.[9] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were usually assigned to idealized positions and were included in structure factors calculations.

Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no.s CCDC 2202537 (**1b**), CCDC 2202538 (**1c**), CCDC 2202539 (**2b**), CCDC 2202540 (**2a**), CCDC 2202541 (**2c**), CCDC 2202542 (**8**), 2202543 (**7**), 2202544 (**5**), 2202545 (**3**), 2202546 (**8a**), 2202547 (**4NHC**), 2202548 (**4**), 2202549 (**13**), 2202550 (**8b**), CCDC 2202551 (**15b**), and CCDC 2202552 (**15a**). Copies of the data can be obtained free of charge on application to CCDC.

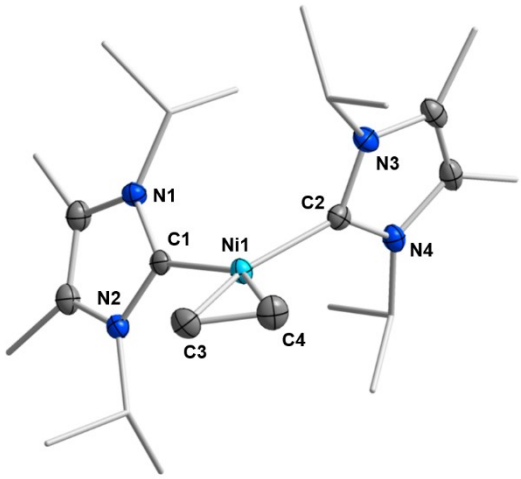


Figure S2. Molecular structure of [Ni(^{i}Pr$_2$Im^{Me})$_2$(η^2-C$_2$H$_4$)] **1b** in the solid state (ellipsoids set at the 50% probability level). Hydrogen atoms have been omitted for clarity. Selected bond lengths [Å] and angles [°] of **1b**: Ni1–C1 1.9191(16), Ni1–C2 1.9265(13), Ni1–C3 1.9596(16), Ni1–C4 1.9659(18), C3–C4 1.428(2); C1–Ni1–C2 105.25(6), C1–Ni1–C3 105.61(7), C2–Ni1–C4 106.79(6), C3–Ni1–C4 42.67(7).

Crystal data for 1b: $C_{24}H_{44}N_4Ni$, M_r = 447.34, yellow block, 0.118 x 0.080 x 0.059 mm, monoclinic space group $P2_1/c$, a = 15.5164(2) Å, b = 9.42990(10) Å, c = 17.7244(3) Å, α = 90°, β = 108.412(2)°, γ = 90°, V = 2460.64(6) Å^3, T = 99.9(3) K, Z = 4, $\rho_{calcd.}$ = 1.208 g cm^{-3}, μ = 1.242 mm^{-1}, F(000) = 976, 26885 reflections in h(–19/19), k(–11/10), l(–22/21) measured in the range 3.002° < θ < 74.500°, 5027 independent reflections, 5027 observed reflections [I >2σ(I)], 274 parameters, 0 restraints; all data: R_1 = 0.0369 and wR_2 = 0.0824, I >2σ(I): R_1 = 0.0318 and wR_2 = 0.0794, *Goof* 1.039, largest difference peak/hole 0.301/–0.365 e Å^{-3}.

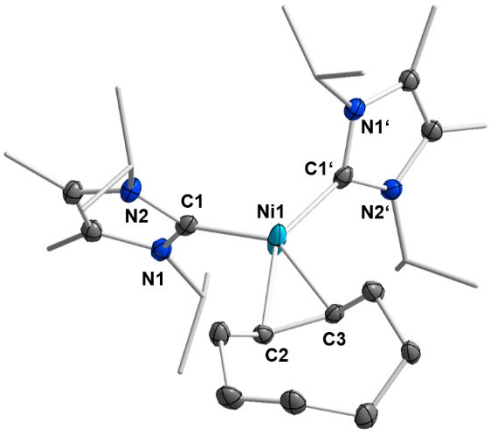


Figure S3. Molecular structure of [Ni(^{i}Pr$_2$Im^{Me})$_2$(η^2-COE)] **1c** in the solid state (ellipsoids set at the 50% probability level). Hydrogen atoms have been omitted for clarity. Selected bond lengths [Å] and angles [°] of **1c**: Ni1–C1/C1' 1.9175(16), Ni1–C2 2.047(3), Ni1–C3 1.992(3), C2–C3 1.439(4); C1–Ni1–C1' 110.88(9), C1–Ni1–C2 100.38(10), C1'–Ni1–C3 104.24(10), C2–Ni1–C3 41.71(12).

Crystal data for 1c: $C_{30}H_{54}N_4Ni$, M_r = 529.48, yellow block, 0.378 x 0.334 x 0.284 mm, monoclinic space group C2/c, a = 15.7119(3) Å, b = 9.6716(2) Å, c = 19.5224(3) Å, α = 90°, β = 94.027(2)°, γ = 90°, V = 2959.28(10) Å^3, T = 100.00(10) K, Z = 4, $\rho_{calcd.}$ = 1.188 g cm^{-3}, μ = 1.106 mm^{-1}, F(000) = 1160, 15596 reflections in h(–19/18), k(–11/12), l(–23/24) measured in the range 4.541° < θ < 74.498°, 3034 independent reflections, 3034 observed reflections [I >2σ(I)], 202 parameters, 96 restraints; all data: R_1 = 0.0453 and wR_2 = 0.1132, I >2σ(I): R_1 = 0.0433 and wR_2 = 0.1115, *Goof* 1.044, largest difference peak/hole 0.469/–0.983 e Å^{-3}.

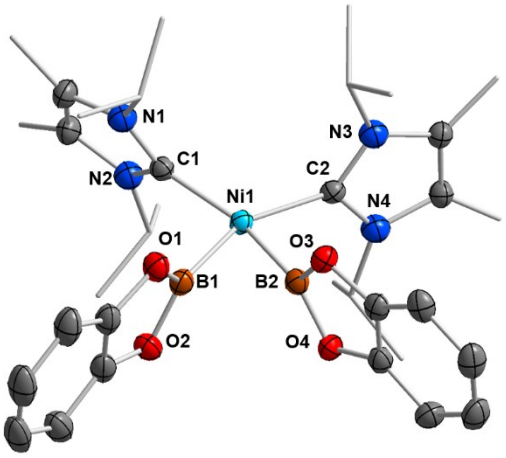


Figure S4. Molecular structure of *cis*-[Ni(^{i}Pr$_2$Im^{Me})$_2$(Bcat)$_2$] **2a** in the solid state (ellipsoids set at the 50% probability level). Hydrogen atoms have been omitted for clarity. Selected bond lengths [Å] and angles [°] of **2a**: Ni1–C1 1.9393(16), Ni1–C2 1.9448(15), Ni1–B1 1.9231(19), Ni1–B2 1.9092(18), B1···B2 2.156(3); C1–Ni1–C2 112.04(6), C1–Ni1–B1 94.21(7), B1–Ni1–B2 68.45(7), C2–Ni1–B2 85.63(7), B1–Ni1–C2 153.68(7), B2–Ni1–C1 161.52(7), plane (C1–Ni1–C2) – plane (B1–Ni1–B2) 7.02(10), plane (O1–B1–O2) – plane (O3–B2–O4) 83.24(16).

Crystal data for 2a: $C_{34}H_{48}B_2N_4NiO_4$, M_r = 657.07, yellow block, 0.151 x 0.131 x 0.052 mm, triclinic space group P-1, a = 10.8305(2) Å, b = 18.8820(3) Å, c = 19.1567(3) Å, α = 62.566(2)°, β = 83.687(2)°, γ = 81.6060(10)°, V = 3435.70(11) Å^3, T = 100.0(3) K, Z = 4, $\rho_{calcd.}$ = 1.270 g cm^{-3}, μ = 1.146 mm^{-1}, F(000) = 1400, 59441 reflections in h(–12/13), k(–23/23), l(–23/23) measured in the range 2.602° < θ < 74.498°, 14025 independent reflections, 14025 observed reflections [I >2σ(I)], 835 parameters, 0 restraints; all data: R_1 = 0.0451 and wR_2 = 0.1076, I >2σ(I): R_1 = 0.0396 and wR_2 = 0.1039, *Goof* 1.074, largest difference peak/hole 0.508/–0.472 e Å^{-3}.

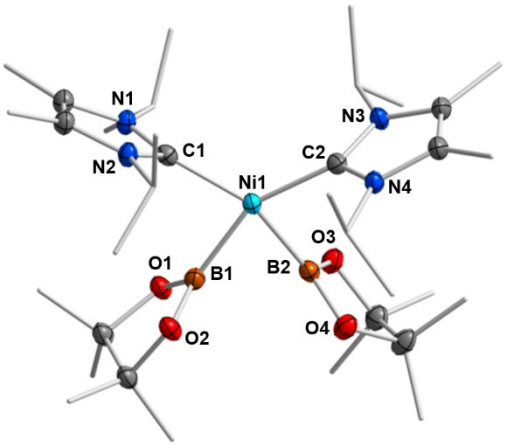


Figure S5. Molecular structure of *cis*-[Ni(^{i}Pr$_2$Im^{Me})$_2$(Bpin)$_2$] **2b** in the solid state (ellipsoids set at the 50% probability level). Hydrogen atoms have been omitted for clarity. Selected bond lengths [Å] and angles [°] of **2b**: Ni1–C1 1.9318(18), Ni1–C2 1.9185(17), Ni1–B1 1.936(2), Ni1–B2 1.942(2), B1···B2 2.247(3); C1–Ni1–C2 118.45(7), C1–Ni1–B1 86.46(8), B1–Ni1–B2 70.82(8), C2–Ni1–B2 85.76(8), B1–Ni1–C2 153.89(8), B2–Ni1–C1 154.92(8), plane (C1–Ni1–C2) – plane (B1–Ni1–B2) 13.14(7), plane (O1–B1–O2) – plane (O3–B2–O4) 89.36(15).

Crystal data for 2b: $C_{34}H_{64}B_2N_4NiO_4$, M_r = 673.20, yellow block, 0.230 x 0.103 x 0.087 mm, monoclinic space group $P2_1/c$, a = 12.04960(10) Å, b = 19.77260(10) Å, c = 16.77860(10) Å, α = 90°, β = 110.8770(10)°, γ = 90°, V = 3735.09(5) Å^3, T = 100.00(10) K, Z = 4, $\rho_{calcd.}$ = 1.197 g cm^{-3}, μ = 1.055 mm^{-1}, F(000) = 1464, 76585 reflections in h(–15/15), k(–20/24), l(–20/20) measured in the range 3.598° < θ < 74.501°, 7608 independent reflections, 7608 observed reflections [I >2σ(I)], 426 parameters, 0 restraints; all data: R_1 = 0.0408 and wR_2 = 0.0949, I >2σ(I): R_1 = 0.0397 and wR_2 = 0.0945, *Goof* 1.201, largest difference peak/hole 0.315/–0.236 e Å^{-3}.

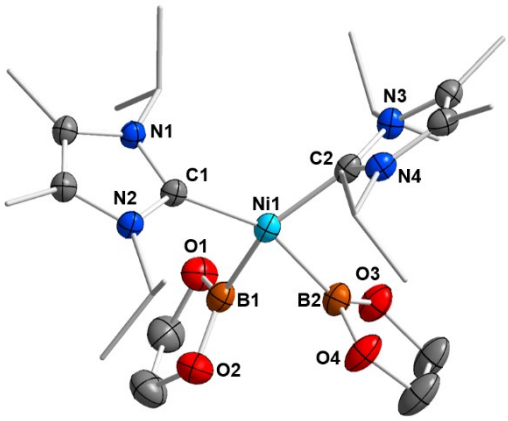
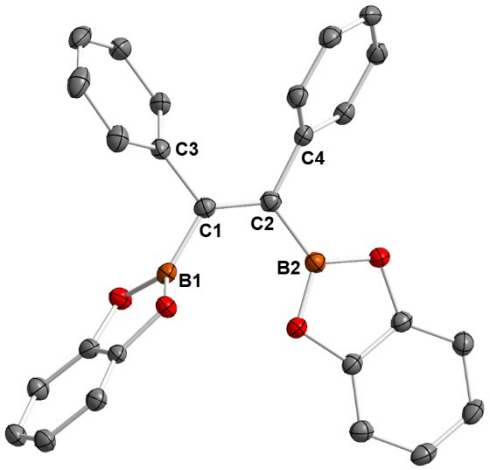


Figure S6. Molecular structure of *cis*-[Ni(^{i}Pr$_2$Im^{Me})$_2$(Beg)$_2$] **2c** in the solid state (ellipsoids set at the 50% probability level). Hydrogen atoms have been omitted for clarity. Selected bond lengths [Å] and angles [°] of **2c**: Ni1–C1 1.9180(15), Ni1–C2 1.9265(17), Ni1–B1 1.939(2), Ni1–B2 1.9353(19), B1···B2 2.189(4); C1–Ni1–C2 112.90(6), C1–Ni1–B1 91.31(7), B1–Ni1–B2 68.79(8), C2–Ni1–B2 89.22(8), B1–Ni1–C2 154.26(7), B2–Ni1–C1 156.06(8), plane (C1–Ni1–C2) – plane (B1–Ni1–B2) 16.48(8), plane (O1–B1–O2) – plane (O3–B2–O4) 78.9(2).

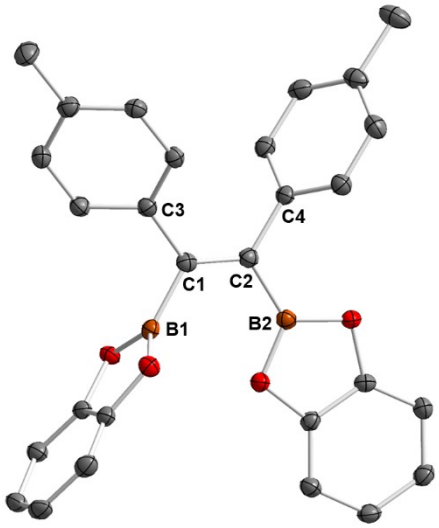
Crystal data for 2c: $C_{26}H_{48}B_2N_4NiO_4$, M_r = 561.01, yellow plate, 0.333 x 0.083 x 0.050 mm, triclinic space group P-1, a = 10.2981(2) Å, b = 17.9201(2) Å, c = 18.0389(3) Å, α = 116.089(2)°, β = 93.6880(10)°, γ = 93.5090(10)°, V = 2968.67(9) Å^3, T = 99.9(7) K, Z = 4, $\rho_{calcd.}$ = 1.255 g cm^{-3}, μ = 1.229 mm^{-1}, F(000) = 1208, 61400 reflections in h(–12/12), k(–22/19), l(–22/22) measured in the range 2.742° < θ < 74.503°, 12093 independent reflections, 12093 observed reflections [I >2σ(I)], 750 parameters, 240 restraints; all data: R_1 = 0.0485 and wR_2 = 0.1246, I >2σ(I): R_1 = 0.0445 and wR_2 = 0.1212, *Goof* 1.017, largest difference peak/hole 0.812/–0.854 e Å^{-3}.



This structure has been reported previously by Marder and Norman et al.[1]

Figure S7. Molecular structure of *Z*-(Bcat)(Ph)C=C(Ph)(Bcat) **3** in the solid state (ellipsoids set at 50% probability level). Hydrogen atoms have been omitted for clarity. Selected bond lengths [Å] and angles [°] of **3**: C1–C2 1.3550(16), B1–C1 1.5641(17), B2–C2 1.5547(17), C1–C3 1.4965(16), C2–C4 1.4964(16); B1–C1–C3 111.97(10), B2–C2–C4 116.84(10).

Crystal data for 3: $C_{26}H_{18}B_2O_4$, M_r = 416.02, colorless block, 0.337 x 0.216 x 0.108 mm, triclinic space group P-1, a = 9.80080(10) Å, b = 11.16390(10) Å, c = 20.6104(3) Å, α = 81.5130(10)°, β = 82.3600(10)°, γ = 66.2130(10)°, V = 2034.20(4) Å^3, T = 100.00(10) K, Z = 4, $\rho_{calcd.}$ = 1.358 g cm^{-3}, μ = 0.717 mm^{-1}, F(000) = 864, 42444 reflections in h(–12/11), k(–13/13), l(–25/25) measured in the range 2.175° < θ < 74.502°, 8287 independent reflections, 8287 observed reflections [I >2σ(I)], 577 parameters, 0 restraints; all data: R_1 = 0.0397 and wR_2 = 0.0973, I >2σ(I): R_1 = 0.0368 and wR_2 = 0.0941, *Goof* 0.647, largest difference peak/hole 0.291/–0.241 e Å^{-3}.



This structure has been reported previously by Marder and Norman et al.[10]

Figure S8. Molecular structure of *Z*-(Bcat)(4-Me-C_6H_4)C=C(4-Me-C_6H_4)(Bcat) **4** in the solid state (ellipsoids set at 50% probability level). Hydrogen atoms have been omitted for clarity. Selected bond lengths [Å] and angles [°] of **4**: C1–C2 1.3523(16), B1–C1 1.5702(16), B2–C2 1.5513(17), C1–C3 1.4927(15), C2–C4 1.4947(15); B1–C1–C3 112.88(9), B2–C2–C4 115.57(10).

Crystal data for 4: $C_{28}H_{22}B_2O_4$, M_r = 444.07, colorless block, 0.190 x 0.150 x 0.070 mm, triclinic space group P-1, a = 10.3698(2) Å, b = 10.8321(2) Å, c = 11.1405(3) Å, α = 94.791(2)°, β = 108.533(2)°, γ = 103.715(2)°, V = 1135.37(5) Å^3, T = 100.00(10) K, Z = 2, $\rho_{calcd.}$ = 1.299 g cm^{-3}, μ = 0.675 mm^{-1}, F(000) = 464, 23004 reflections in h(–12/12), k(–13/12), l(–13/13) measured in the range 4.249° < θ < 72.114°, 4475 independent reflections, 4475 observed reflections [I >2σ(I)], 309 parameters, 0 restraints; all data: R_1 = 0.0399 and wR_2 = 0.0985, I >2σ(I): R_1 = 0.0370 and wR_2 = 0.0959, *Goof* 1.050, largest difference peak/hole 0.240/–0.221 e Å^{-3}.

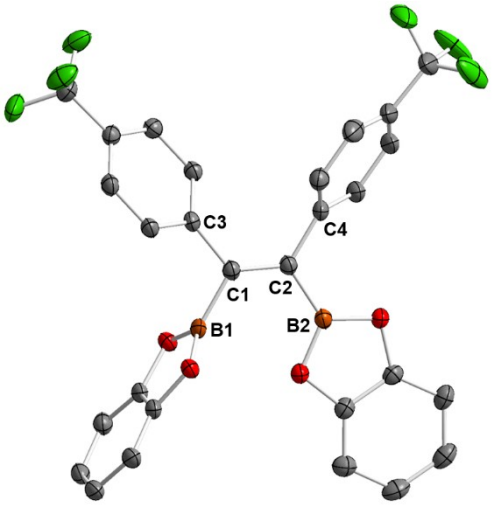


Figure S9. Molecular structure of *Z*-(Bcat)(4-CF_3-C_6H_4)C=C(4-CF_3-C_6H_4)(Bcat) **5** in the solid state (ellipsoids set at 50% probability level). Hydrogen atoms have been omitted for clarity. Selected bond lengths [Å] and angles [°] of **5**: C1–C2 1.3547(18), B1–C1 1.5720(19), B2–C2 1.554(2), C1–C3 1.4949(18), C2–C4 1.4919(18); B1–C1–C3 112.07(10), B2–C2–C4 116.56(11).

Crystal data for 5: $C_{28}H_{16}B_2F_6O_4 + C_6H_6$, M_r = 630.13, colorless block, 0.320 x 0.120 x 0.030 mm, triclinic space group P-1, a = 10.2370(2) Å, b = 11.4631(2) Å, c = 13.6600(3) Å, α = 113.599(2)°, β = 91.470(2)°, γ = 93.724(2)°, V = 1463.47(5) $Å^3$, T = 100.00(10) K, Z = 2, $\rho_{calcd.}$ = 1.430 g cm^{-3}, μ = 1.006 mm^{-1}, F(000) = 644, 29131 reflections in h(–12/12), k(–12/14), l(–16/16) measured in the range 3.537° < θ < 72.106°, 5750 independent reflections, 5750 observed reflections [I >2σ(I)], 445 parameters, 36 restraints; all data: R_1 = 0.0461 and wR_2 = 0.1114, I >2σ(I): R_1 = 0.0405 and wR_2 = 0.1069, *Goof* 1.071, largest difference peak/hole 0.386/–0.284 e $Å^{-3}$.

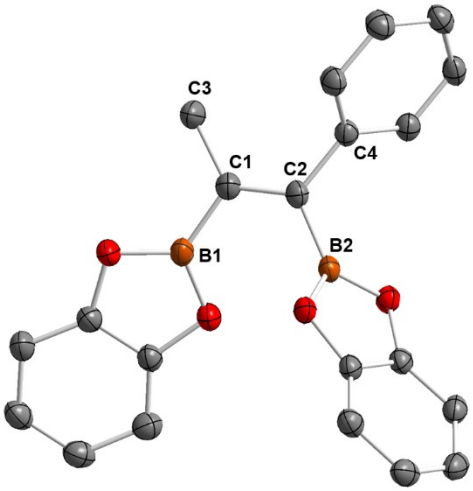


Figure S10. Molecular structure of *Z*-(Bcat)(Me)C=C(Ph)(Bcat) **7** in the solid state (ellipsoids set at the 50% probability level). Hydrogen atoms have been omitted for clarity. Selected bond lengths [Å] and angles [°] of **7**: C1–C2 1.3519(18), B1–C1 1.5502(19), B2–C2 1.5628(18), C1–C3 1.5128(18), C2–C4 1.4975(17); B1–C1–C3 116.42(11), B2–C2–C4 115.01(10).

Crystal data for 7: $C_{21}H_{16}B_2O_4$, M_r = 353.96, colorless block, 0.193 x 0.137 x 0.096 mm, triclinic space group P-1, a = 6.35850(10) Å, b = 8.8436(2) Å, c = 16.0653(4) Å, α = 100.552(2)°, β = 97.420(2)°, γ = 93.988(2)°, V = 876.64(3) Å^3, T = 99.9(6) K, Z = 2, $\rho_{calcd.}$ = 1.341 g cm^{-3}, μ = 0.729 mm^{-1}, F(000) = 368, 18064 reflections in h(–7/7), k(–9/11), l(–19/20) measured in the range 2.828° < θ < 74.490°, 3562 independent reflections, 3562 observed reflections [I >2σ(I)], 245 parameters, 0 restraints; all data: R_1 = 0.0464 and wR_2 = 0.1173, I >2σ(I): R_1 = 0.0419 and wR_2 = 0.1127, *Goof* 1.047, largest difference peak/hole 0.293/–0.290 e Å^{-3}.

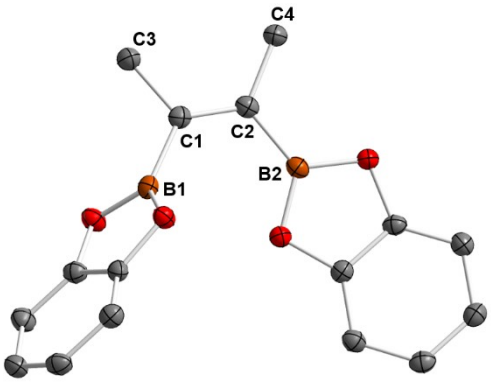


Figure S11. Molecular structure of *Z*-(Bcat)(Me)C=C(Me)(Bcat) **8** in the solid state (ellipsoids set at the 50% probability level). Hydrogen atoms have been omitted for clarity. Selected bond lengths [Å] and angles [°] of **8**: C1–C2 1.352(4), B1–C1 1.564(4), B2–C2 1.543(4), C1–C3 1.514(4), C2–C4 1.518(4); B1–C1–C3 113.0(3), B2–C2–C4 117.6(3).

Crystal data for 8: $C_{16}H_{14}B_2O_4$, M_r = 291.89, colorless block, 0.365 x 0.162 x 0.060 mm, triclinic space group P-1, a = 5.7823(2) Å, b = 8.4295(4) Å, c = 14.2439(5) Å, α = 87.274(3)°, β = 84.401(3)°, γ = 89.585(3)°, V = 690.18(5) Å^3, T = 100.00(10) K, Z = 2, $\rho_{calcd.}$ = 1.405 g cm^{-3}, μ = 0.796 mm^{-1}, F(000) = 304, 2746 reflections in h(–7/7), k(–10/10), l(–3/17) measured in the range 5.253° < θ < 74.502°, 2746 independent reflections, 2746 observed reflections [I >2σ(I)], 202 parameters, 0 restraints; all data: R_1 = 0.0687 and wR_2 = 0.2231, I >2σ(I): R_1 = 0.0668 and wR_2 = 0.2217, *Goof* 1.187, largest difference peak/hole 0.383/–0.329 e Å^{-3}.

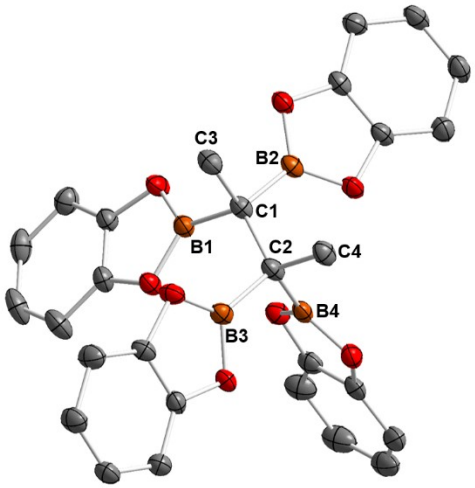


Figure S12. Molecular structure of $(Bcat)_2(Me)C–C(Me)(Bcat)_2$ **8a** in the solid state (ellipsoids set at the 50% probability level). Hydrogen atoms have been omitted for clarity. Selected bond lengths [Å] and angles [°] of **8a**: C1–C2 1.564(3), B1–C1 1.5718(19), B2–C1 1.5758(19), C1–C3 1.5699(19), C2–B3 1.588(2), C2–B4 1.574(2), C2–C4 1.565(2); B1–C1–C3 103.94(11), B1–C1–B2 110.33(11), B2–C1–C3 107.15(11), B3–C2–C4 105.30(16), B3–C2–B4 105.77(16), B4–C2–C4 111.25(15).

Crystal data for 8a: $C_{28}H_{22}B_4O_8 + 0.5(C_6H_6)$, M_r = 568.75, colorless block, 0.313 x 0.213 x 0.127 mm, triclinic space group P-1, a = 10.03360(10) Å, b = 12.4047(2) Å, c = 12.9515(3) Å, α = 62.329(2)°, β = 78.2950(10)°, γ = 83.9380(10)°, V = 1397.82(5) Å^3, T = 100.00(10) K, Z = 2, $\rho_{calcd.}$ = 1.351 g cm^{-3}, μ = 0.773 mm^{-1}, F(000) = 590, 29158 reflections in h(–12/12), k(–15/15), l(–16/16) measured in the range 3.914° < θ < 74.497°, 5723 independent reflections, 5723 observed reflections [I >2σ(I)], 416 parameters, 237 restraints; all data: R_1 = 0.0470 and wR_2 = 0.1144, I >2σ(I): R_1 = 0.0440 and wR_2 = 0.1120, *Goof* 1.020, largest difference peak/hole 0.451/–0.353 e Å^{-3}.

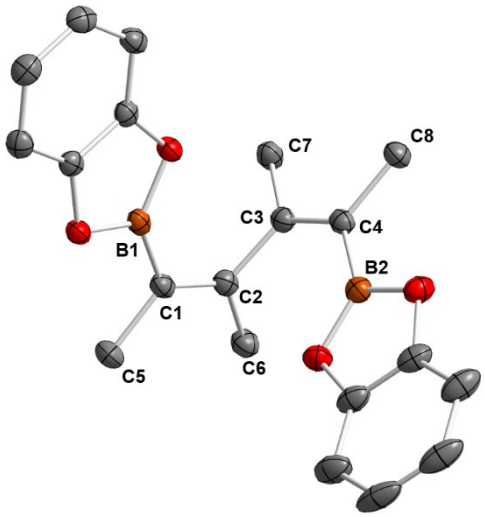


Figure S13. Molecular structure of *E,E*-(Bcat)(Me)C=C(Me)–(Me)C=C(Me)(Bcat) **8b** in the solid state (ellipsoids set at the 50% probability level). Hydrogen atoms have been omitted for clarity. Selected bond lengths [Å] and angles [°] of **8b**: C1–C2 1.3484(18), C3–C4 1.3492(19), B1–C1 1.438(19), C1–C5 1.5186(17), C2–C6 1.5094(18), B2–C4 1.540(2), C3–C7 1.5051(18), C4–C8 1.5224(17); B1–C1–C5 115.49(11), B2–C4–C8 116.43(11), C3–C2–C6 114.51(11), C2–C3–C7 114.20(11).

Crystal data for 8b: $C_{20}H_{20}B_2O_4$, M_r = 345.98, colorless plate, 0.386 x 0.190 x 0.071 mm, monoclinic space group $P2_1/c$, a = 12.9444(2) Å, b = 15.05970(10) Å, c = 9.51950(10) Å, α = 90°, β = 98.5030(10)°, γ = 90°, V = 1835.32(4) Å^3, T = 100.00(10) K, Z = 4, $\rho_{calcd.}$ = 1.252 g cm^{-3}, μ = 0.678 mm^{-1}, F(000) = 728, 36922 reflections in h(–16/16), k(–18/12), l(–11/11) measured in the range 3.452° < θ < 74.479°, 3750 independent reflections, 3750 observed reflections [I >2σ(I)], 239 parameters, 0 restraints; all data: R_1 = 0.0469 and wR_2 = 0.1185, I >2σ(I): R_1 = 0.0436 and wR_2 = 0.1156, *Goof* 1.046, largest difference peak/hole 0.326/–0.311 e Å^{-3}.

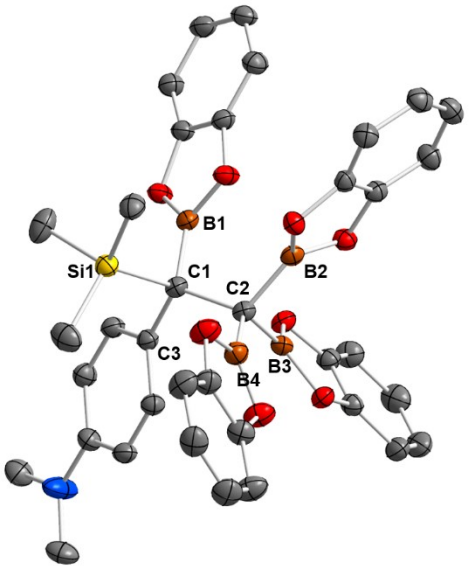


Figure S14. Molecular structure of (4-NMe_2-C_6H_4)(Bcat)(TMS)C–C(Bcat)$_3$ **13** in the solid state (ellipsoids set at the 50% probability level). Hydrogen atoms have been omitted for clarity. Selected bond lengths [Å] and angles [°] of **13**: C1–C2 1.626(2), B1–C1 1.563(2), Si1–C1 1.9626(17), C1–C3 1.534(2), C2–B2 1.594(3), C2–B3 1.574(2), C2–B4 1.581(3); B1–C1–C3 116.71(14), B1–C1–Si1 100.22(11), Si1–C1–C3 103.83(11), B2–C2–B3 101.95(13), B2–C2–B4 104.57(14), B3–C2–B4 114.20(14).

Crystal data for 13: $C_{37}H_{35}B_4NO_8Si$, M_r = 692.99, colorless block, 0.410 x 0.240 x 0.050 mm, triclinic space group P-1, a = 9.7326(2) Å, b = 10.1947(2) Å, c = 19.1912(5) Å, α = 76.146(2)°, β = 86.927(2)°, γ = 64.991(2)°, V = 1672.98(7) Å^3, T = 100(2) K, Z = 2, $\rho_{calcd.}$ = 1.376 g cm^{-3}, μ = 1.087 mm^{-1}, F(000) = 724, 33072 reflections in h(–12/12), k(–11/12), l(–23/23) measured in the range 2.375° < θ < 72.100°, 6524 independent reflections, 6524 observed reflections [I >2σ(I)], 465 parameters, 0 restraints; all data: R_1 = 0.0495 and wR_2 = 0.1210, I >2σ(I): R_1 = 0.0429 and wR_2 = 0.1164, *Goof* 1.040, largest difference peak/hole 0.416/–0.352 e Å^{-3}.

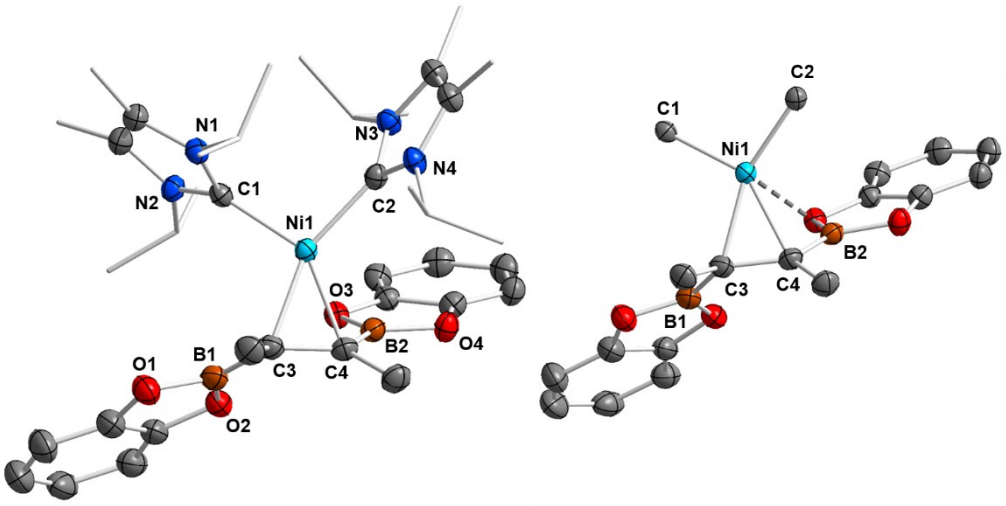


Figure S15. Molecular structure of [Ni(^{i}Pr$_2$Im^{Me})$_2$(η^2-*cis*-(Bcat)(Me)C=C(Me)(Bcat))] **15a** in the solid state (ellipsoids set at the 50% probability level). Hydrogen atoms have been omitted for clarity. Selected bond lengths [Å] and angles [°] of **15a**: Ni1–C1 1.9454(14), Ni1–C2 1.9470(14), Ni1–C3 2.0161(14), Ni1–C4 2.0288(14), Ni1···B1 3.0525(19), Ni1···B2 2.3694(16) C3–C4 1.453(2), C3–B1 1.514(2), C4–B2 1.508(2); C1–Ni1–C2 100.55(6), C1–Ni1–C3 103.18(6), C3–Ni1–C4 42.09(6), C2–Ni1–C4 115.01(6), Ni1–C3–B1 119.02(11), Ni1–C4–B2 82.71(9), B1–C3–C4 124.06(14), B2–C4–C3 123.01(13).

Crystal data for 15a: $C_{38}H_{54}B_2N_4NiO_4$, M_r = 711.18, orange block, 0.211 x 0.099 x 0.086 mm, monoclinic space group $P2_1/c$, a = 12.33620(10) Å, b = 17.5427(2) Å, c = 17.1923(2) Å, α = 90°, β = 97.9660(10)°, γ = 90°, V = 3684.69(7) Å^3, T = 99.9(4) K, Z = 4, $\rho_{calcd.}$ = 1.282 g cm^{-3}, μ = 1.108 mm^{-1}, F(000) = 1520, 39700 reflections in h(–15/15), k(–21/13), l(–21/21) measured in the range 3.618° < θ < 74.488°, 7534 independent reflections, 7534 observed reflections [I >2σ(I)], 456 parameters, 0 restraints; all data: R_1 = 0.0399 and wR_2 = 0.1003, I >2σ(I): R_1 = 0.0362 and wR_2 = 0.0977, *Goof* 1.046, largest difference peak/hole 0.301/–0.256 e Å^{-3}.

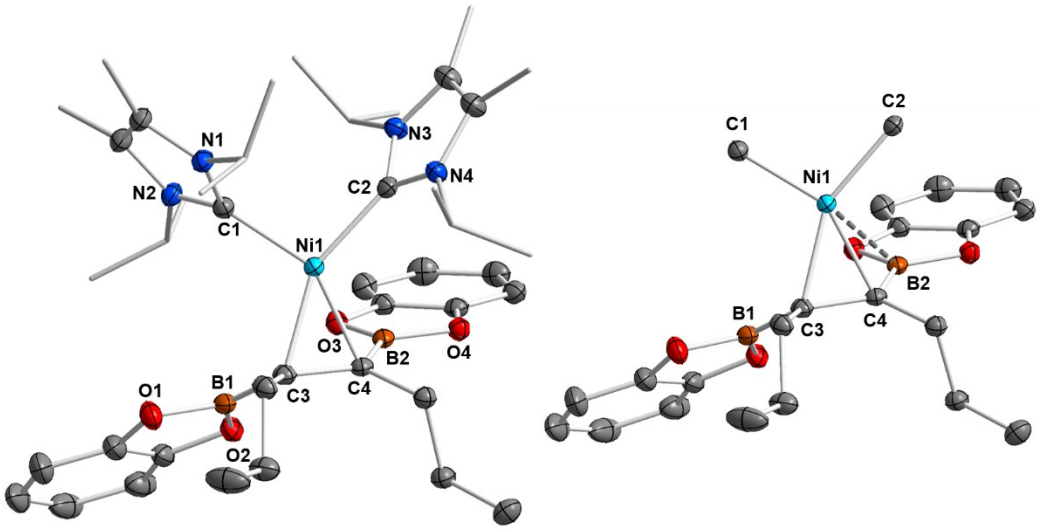


Figure S16. Molecular structure of [Ni(^{i}Pr$_2$Im^{Me})$_2$(η^2-*cis*-(Bcat)(H$_7$C$_3$)C=C(C$_3$H$_7$)(Bcat))] **15b** in the solid state (ellipsoids set at the 50% probability level). Hydrogen atoms have been omitted for clarity. Selected bond lengths [Å] and angles [°] of **15b**: Ni1–C1 1.9517(13), Ni1–C2 1.9560(13), Ni1–C3 2.0373(12), Ni1–C4 2.0070(12), Ni1···B1 3.0262(14), Ni1···B2 2.3376(14), C3–C4 1.4550(17), C3–B1 1.5188(19), C4–B2 1.5122(18); C1–Ni1–C2 99.47(5), C1–Ni1–C3 107.70(5), C3–Ni1–C4 42.16(5), C2–Ni1–C4 111.80(5), Ni1–C3–B1 115.88(9), Ni1–C4–B2 81.94(7), B1–C3–C4 123.63(11), B2–C4–C3 121.28(11).

Crystal data for 15b: $C_{42}H_{62}B_2N_4NiO_4$, M_r = 767.28, orange plate, 0.321 x 0.155 x 0.043 mm, monoclinic space group $P2_1/n$, a = 11.23960(10) Å, b = 19.39160(10) Å, c = 19.42560(10) Å, α = 90°, β = 97.7140(10)°, γ = 90°, V = 4195.57(5) Å^3, T = 99.99(10) K, Z = 4, $\rho_{calcd.}$ = 1.215 g cm^{-3}, μ = 1.007 mm^{-1}, F(000) = 1648, 45015 reflections in h(–14/14), k(–19/24), l(–24/23) measured in the range 3.235° < θ < 74.502°, 8567 independent reflections, 8567observed reflections [I >2σ(I)], 492 parameters, 0 restraints; all data: R_1 = 0.0379 and wR_2 = 0.0910, I >2σ(I): R_1 = 0.0342 and wR_2 = 0.0884, *Goof* 1.063, largest difference peak/hole 0.309/–0.312 e Å^{-3}.

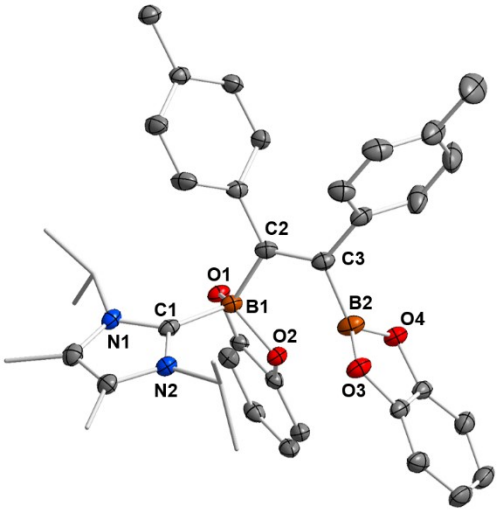


Figure S17. Molecular structure of *Z*-(Bcat)(4-Me-C_6H_4)C=C(4-Me-C_6H_4)(Bcat) • (^{i}Pr$_2$Im^{Me}) **4^{NHC}** in the solid state (ellipsoids set at 50% probability level). Hydrogen atoms have been omitted for clarity. Selected bond lengths [Å] and angles [°] of **4^{NHC}**: C1–B1 1.6604(17), C2–C3 1.3451(17), B1–C2 1.5976(16), B2–C3 1.5816(17), B1–O1 1.4936(14), B1–O2 1.5370(14), B2–O3 1.4257(16), B2–O4 1.4252(17), B2···O2 1.9633(17); C1–B1–C2 116.03(9), C1–B1–O1 108.75(9), C1–B1–O2 108.08(9).

Crystal data for 4^{NHC}: $C_{39}H_{42}B_2N_2O_4$, M_r = 624.36, colorless block, 0.260 x 0.180 x 0.080 mm, monoclinic space group $P2_1/c$, a = 10.35860(10) Å, b = 16.2208(2) Å, c = 20.3367(2) Å, α = 90°, β = 94.8820(10)°, γ = 90°, V = 3404.67(6) Å^3, T = 100(2) K, Z = 4, $\rho_{calcd.}$ = 1.218 g cm^{-3}, μ = 0.608 mm^{-1}, F(000) = 1328, 34811 reflections in h(–12/12), k(–19/20), l(–25/25) measured in the range 3.490° < θ < 72.124°, 6704 independent reflections, 6704 observed reflections [I >2σ(I)], 432 parameters, 0 restraints; all data: R_1 = 0.0422 and wR_2 = 0.0987, I >2σ(I): R_1 = 0.0372 and wR_2 = 0.0953, *Goof* 1.055, largest difference peak/hole 0.292/–0.221 e Å^{-3}.

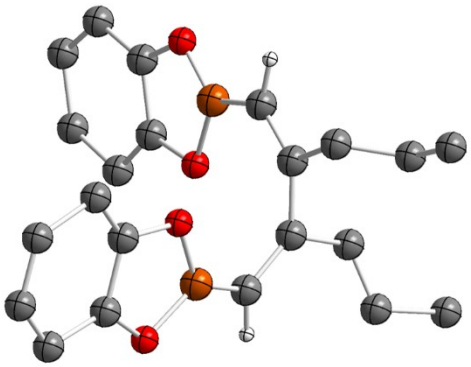


Figure S18: Molecular structure of *Z,Z*-(Bcat)HC=C(C_3H_7)–(C_3H_7)C=CH(Bcat) **12a** in the solid state. Due to poor crystal quality, the structural data is sufficient for proof of connectivity but insufficient for detailed discussion of bond parameters.

4) NMR Spectra and HRMS Data

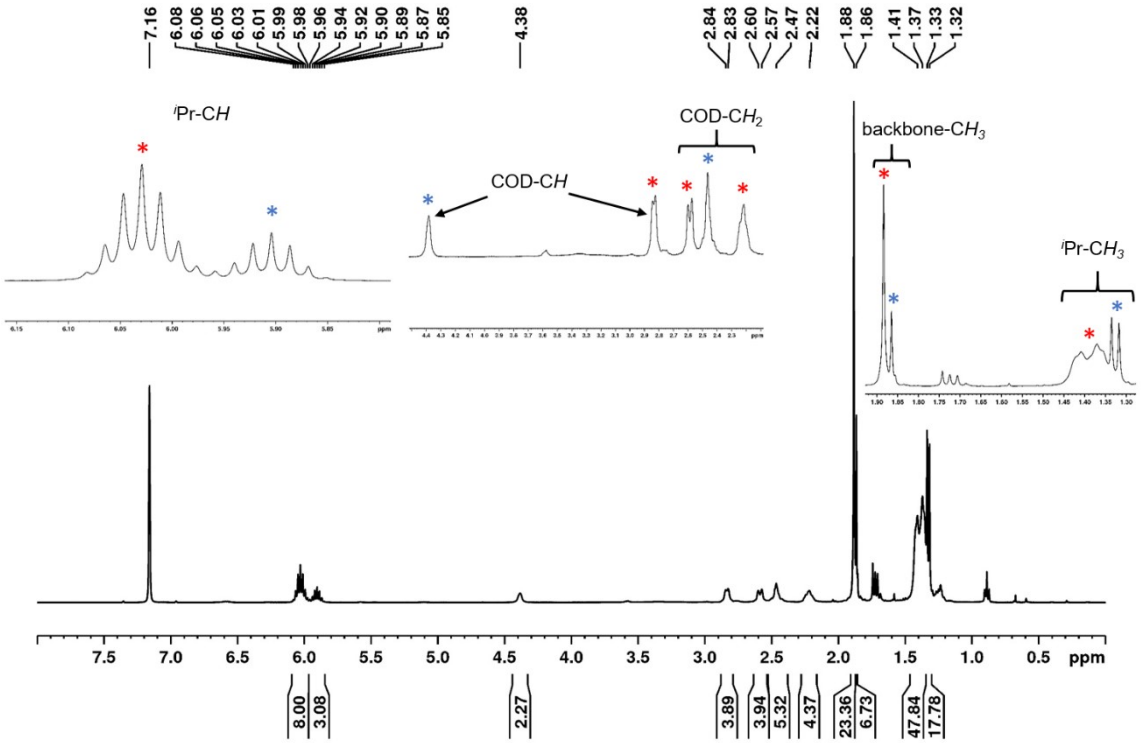


Figure S19. ^{1}H NMR spectrum of the mixture of [Ni_2($^{i}Pr_2Im^{Me}$)$_4$(*μ-(η²:η²)*-COD)] **1** (*) and [Ni($^{i}Pr_2Im^{Me}$)$_2$(COD)] **1a** (*) used (400 MHz, 298 K, C_6D_6).[6]

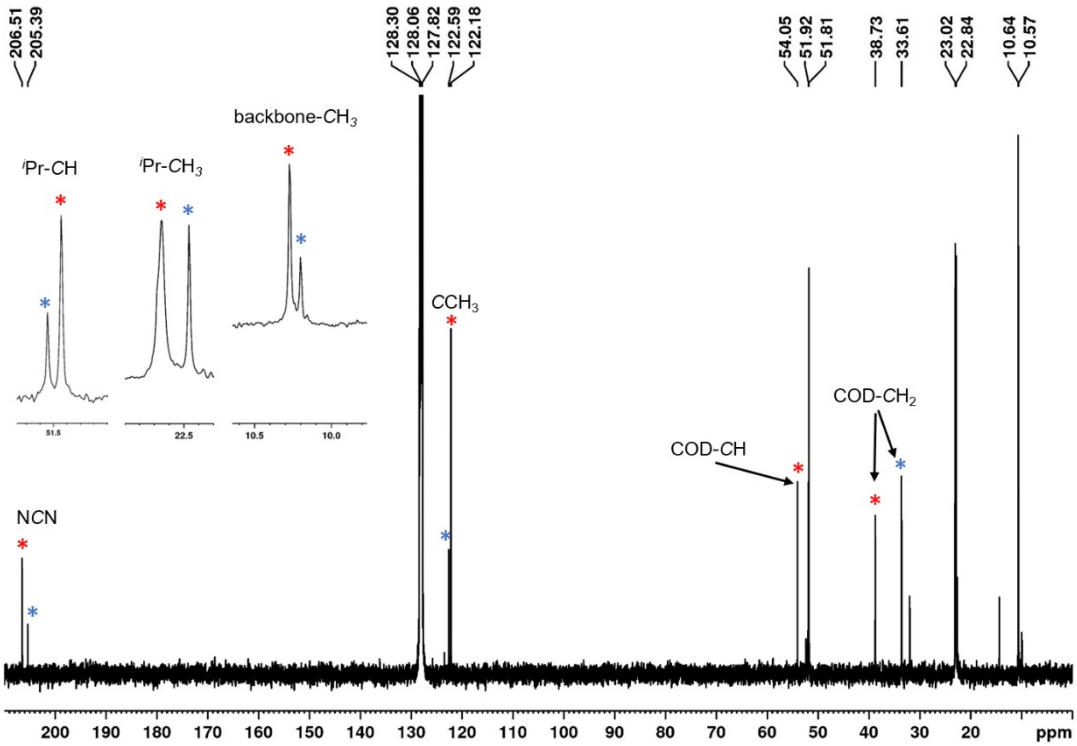


Figure S20. ^{13}C{^{1}H} NMR spectrum of the mixture of [Ni_2($^{i}Pr_2Im^{Me}$)$_4$(*μ-(η²:η²)*-COD)] **1** (*) and [Ni($^{i}Pr_2Im^{Me}$)$_2$(COD)] **1a** (*) used (100 MHz, 298 K, C_6D_6).[6]

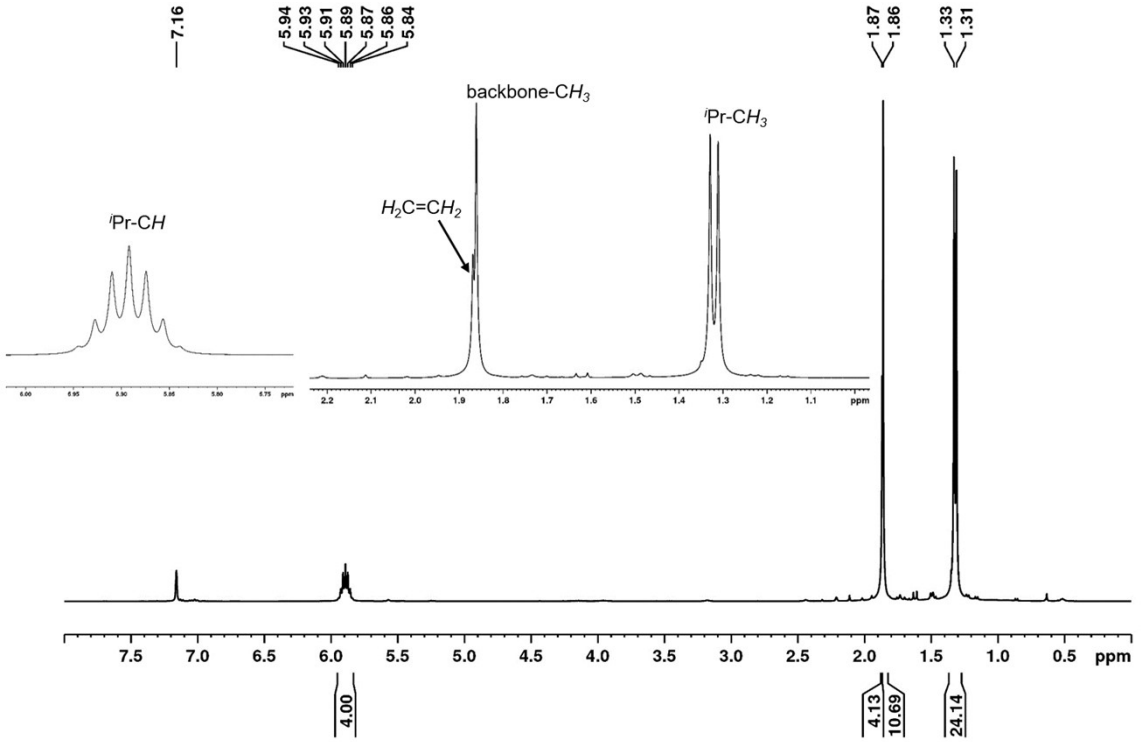


Figure S21. ^{1}H NMR spectrum of [Ni(^{i}Pr$_2$Im^{Me})$_2$(η^2-C$_2$H$_4$)] **1b** (500 MHz, 298 K, C$_6$D$_6$).

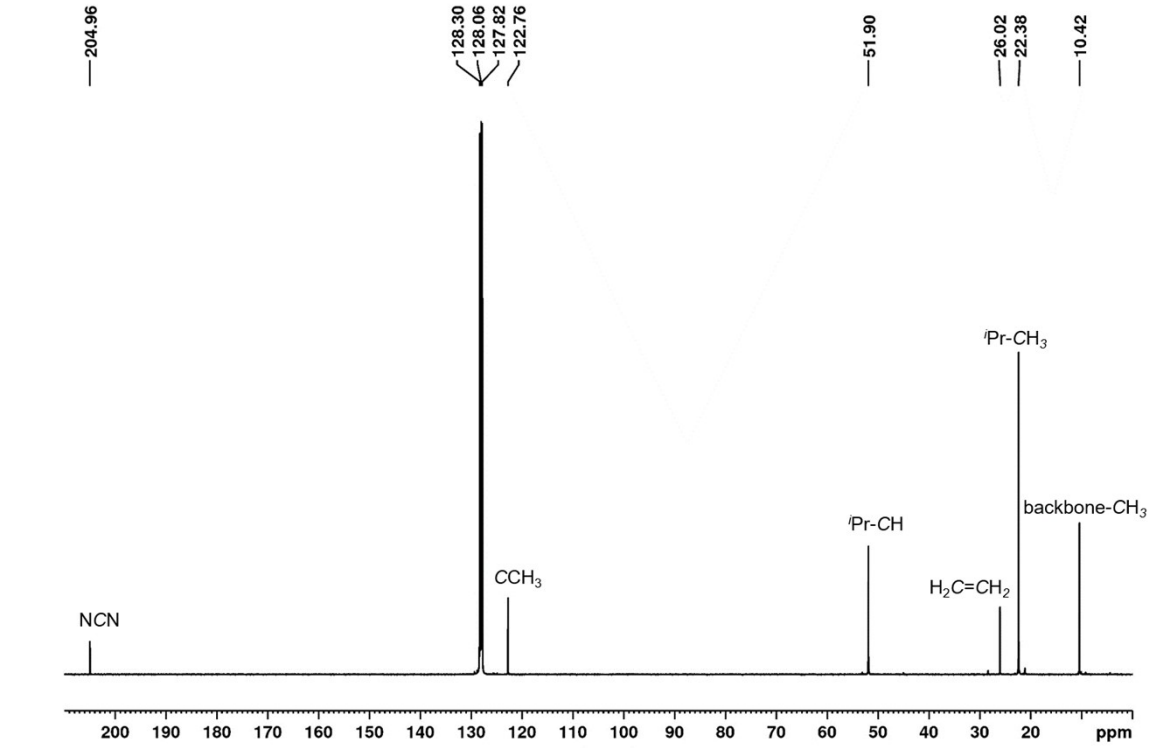


Figure S22. ^{13}C{^{1}H} NMR spectrum of [Ni(^{i}Pr$_2$Im^{Me})$_2$(η^2-C$_2$H$_4$)] **1b** (126 MHz, 298 K, C$_6$D$_6$).

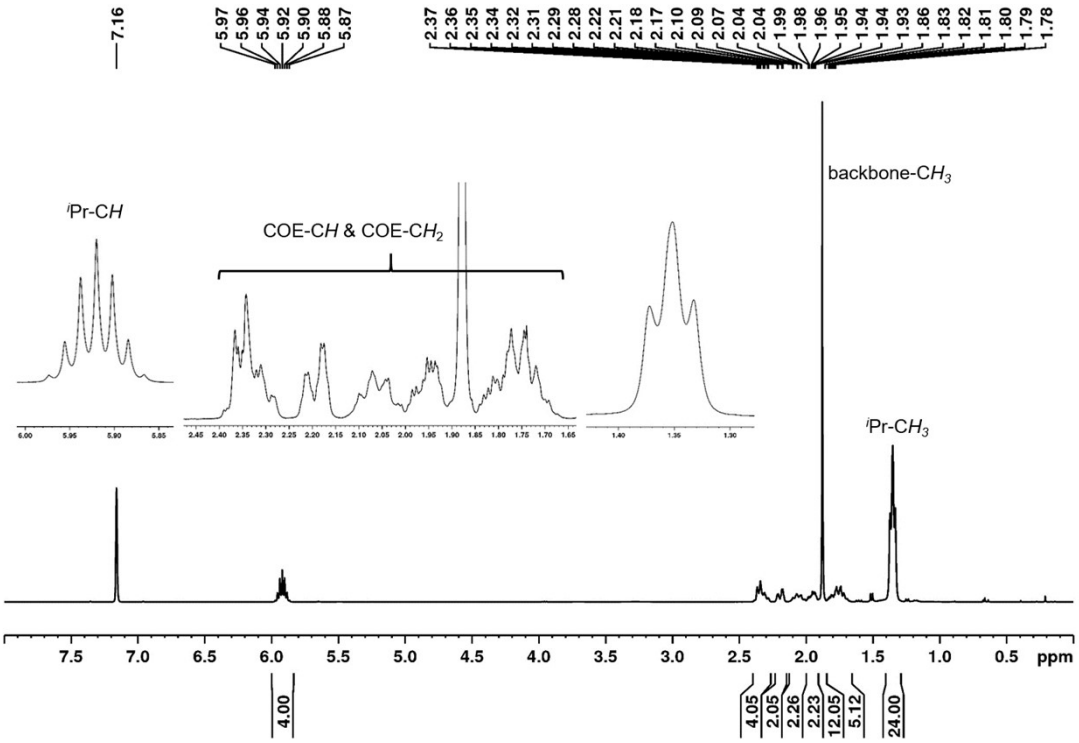


Figure S23. ^{1}H NMR spectrum of [Ni(^{i}Pr$_2$Im^{Me})$_2$(η^2-COE)] **1c** (500 MHz, 298 K, C_6D_6).

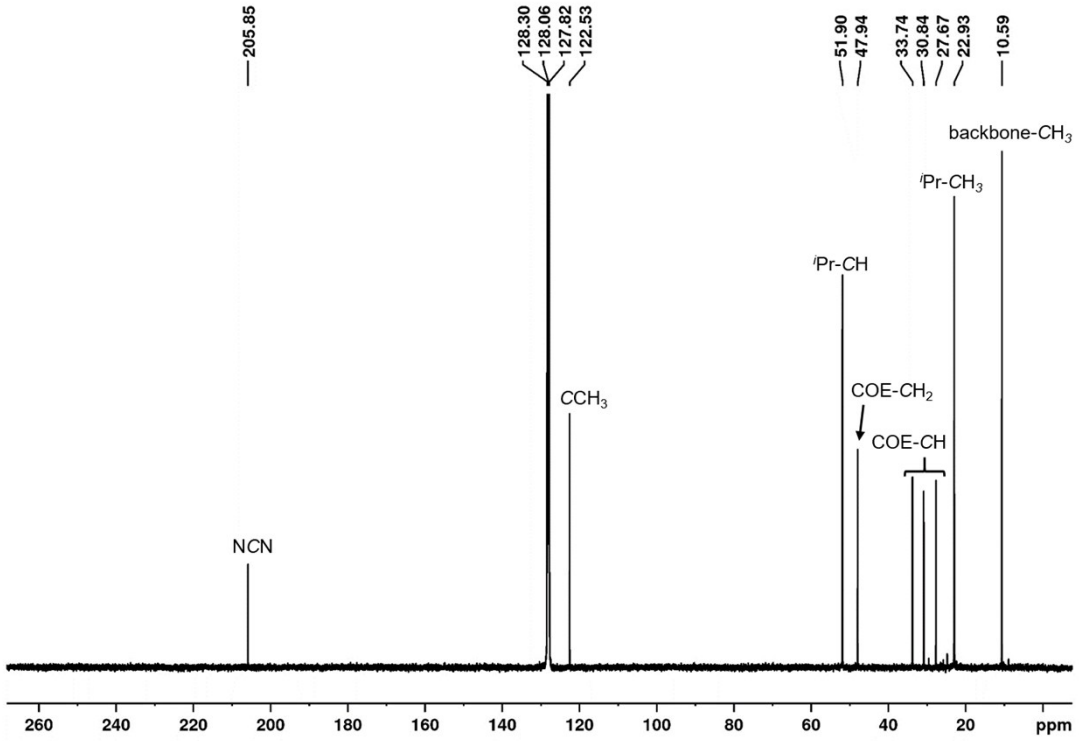


Figure S24. ^{13}C{^{1}H} NMR spectrum of [Ni(^{i}Pr$_2$Im^{Me})$_2$(η^2-COE)] **1c** (126 MHz, 298 K, C_6D_6).

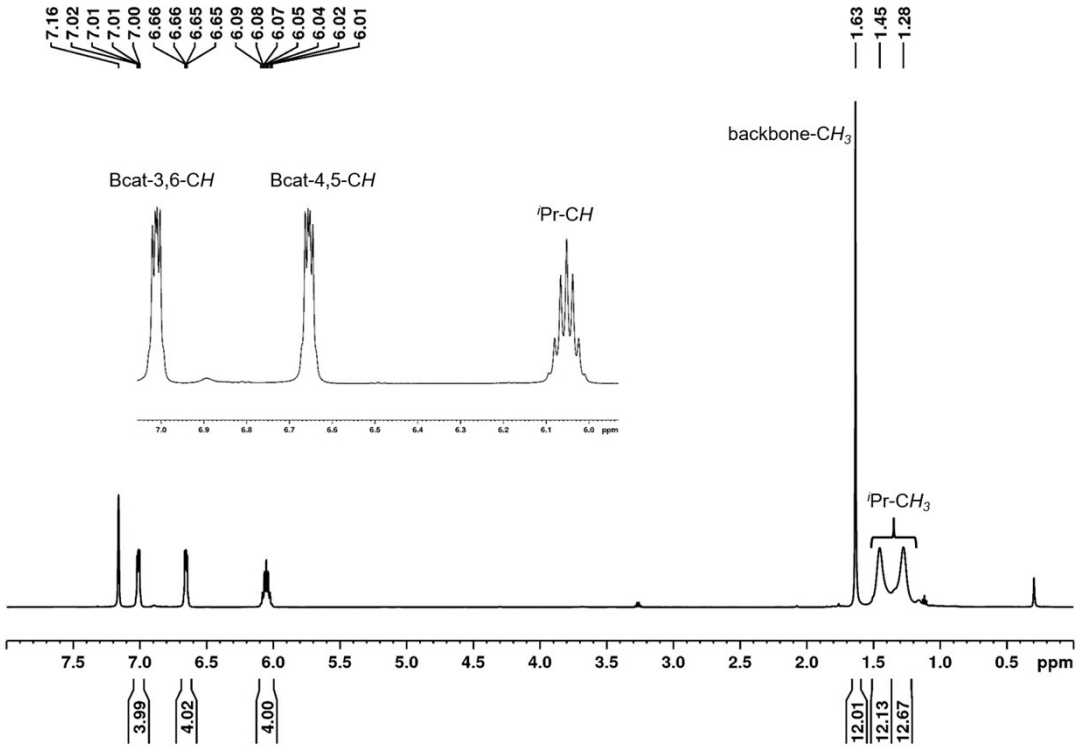


Figure S25. ^{1}H NMR spectrum of *cis*-[Ni(^{i}Pr$_2$Im^{Me})$_2$(Bcat)$_2$] **2a** (500 MHz, 298 K, C_6D_6).

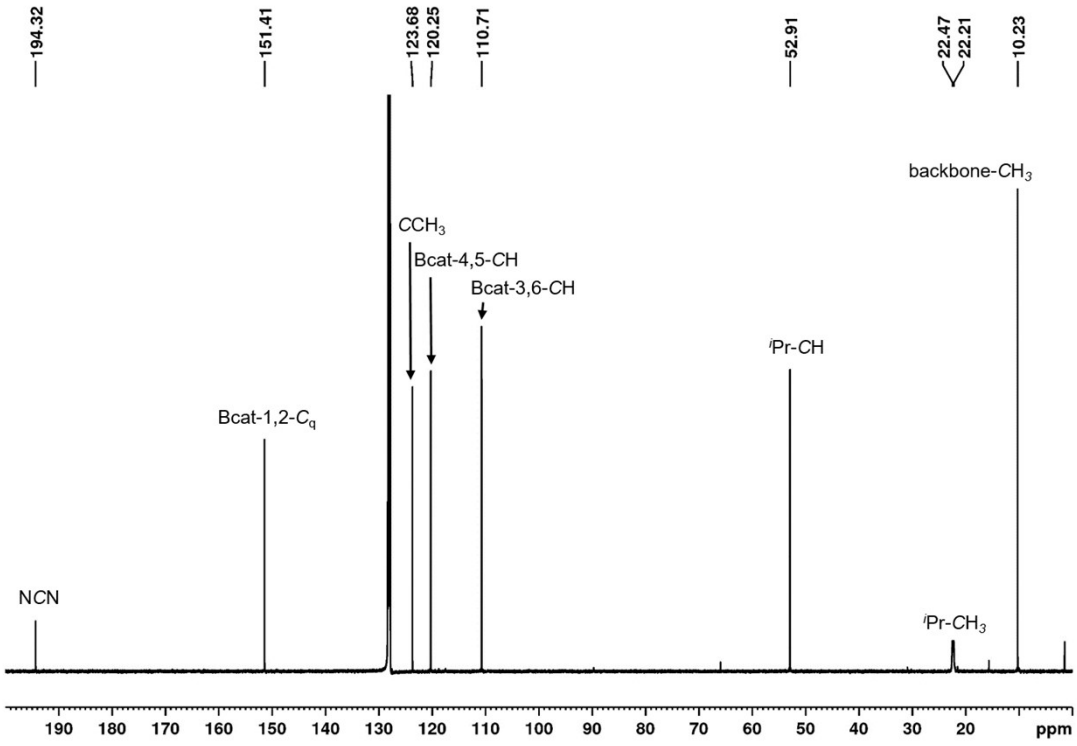


Figure S26. ^{13}C{^{1}H} NMR spectrum of *cis*-[Ni(^{i}Pr$_2$Im^{Me})$_2$(Bcat)$_2$] **2a** (126 MHz, 298 K, C_6D_6).

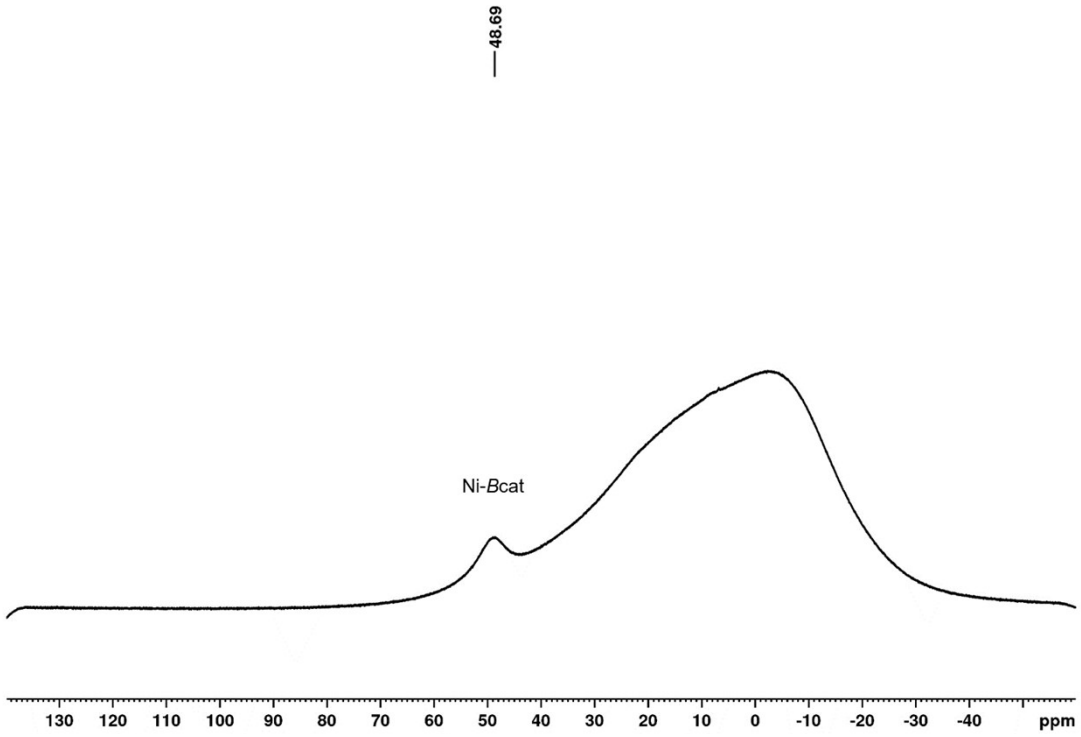


Figure S27. $^{11}B\{^{1}H\}$ NMR spectrum of *cis*-[Ni($^{i}Pr_2Im^{Me}$)$_2$(Bcat)$_2$] **2a** (160 MHz, 298 K, C_6D_6).

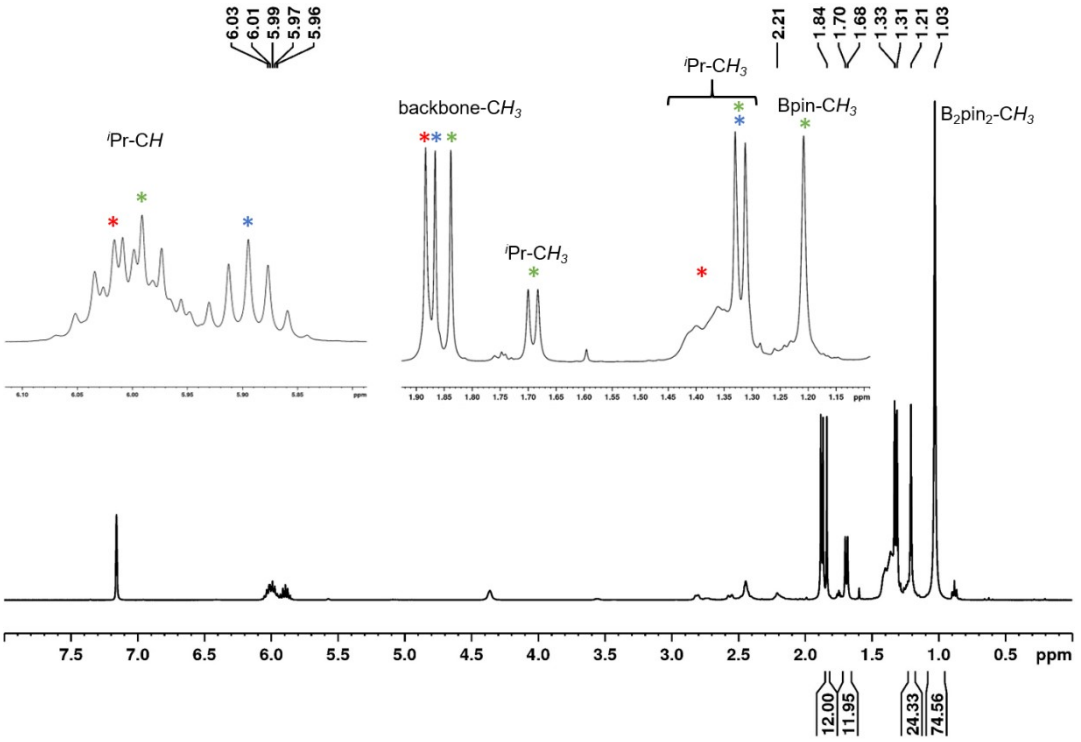


Figure S28. *In situ* ^{1}H NMR spectrum of the equilibrium reaction mixture of *cis*-[Ni($^{i}Pr_2Im^{Me}$)$_2$(Bpin)$_2$] **2b** (*), [Ni$_2$($^{i}Pr_2Im^{Me}$)$_4$(*μ-(η^2:η^2)*-COD)] **1** (*), [Ni($^{i}Pr_2Im^{Me}$)$_2$(COD)] **1a** (*) and B_2pin_2 (400 MHz, 298 K, C_6D_6).

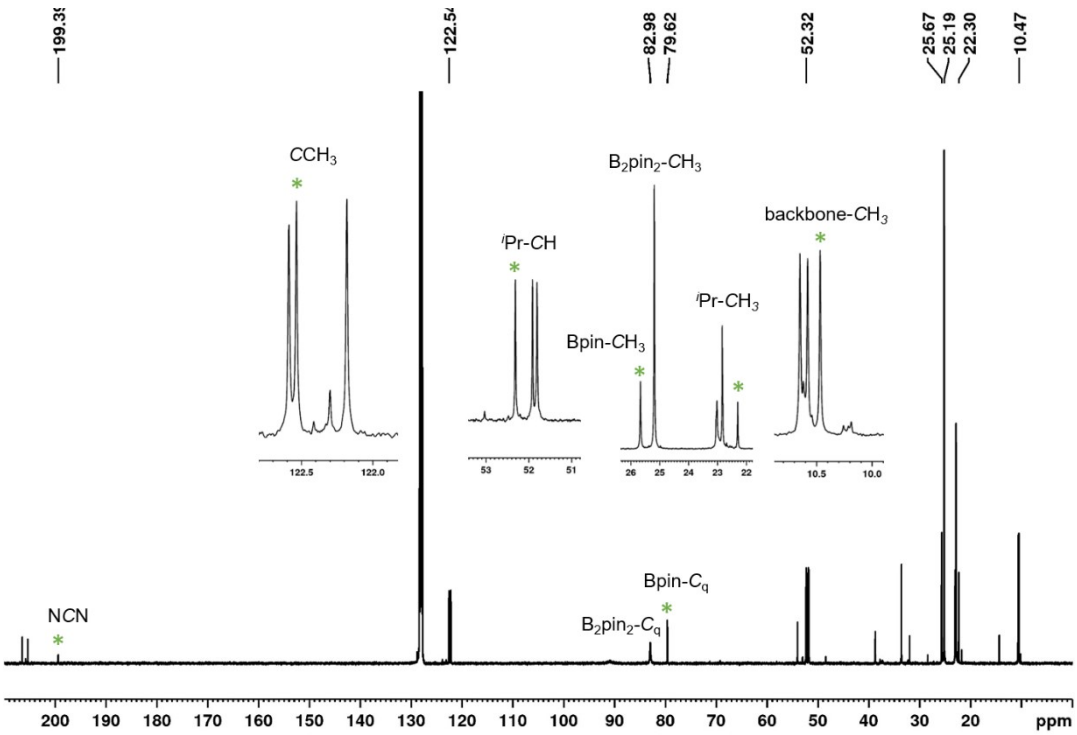


Figure S29. *In situ* $^{13}C\{^1H\}$ NMR spectrum of the equilibrium reaction mixture of *cis*-[Ni(^{i}Pr$_2$Im^{Me})$_2$(Bpin)$_2$] **2b** (*), [Ni$_2$(^{i}Pr$_2$Im^{Me})$_4$(*μ*-*(η^2:η^2)*-COD)] **1** (*), [Ni(^{i}Pr$_2$Im^{Me})$_2$(COD)] **1a** (*) and B_2pin_2 (100 MHz, 298 K, C_6D_6).

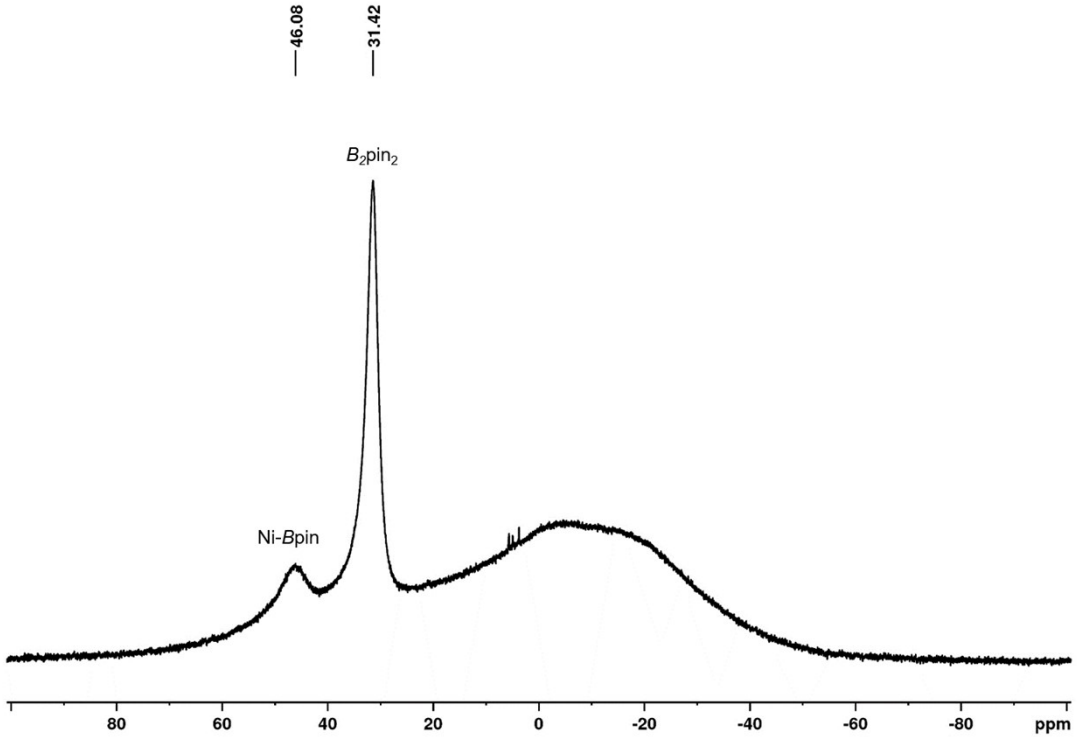


Figure S30. *In situ* $^{11}B\{^1H\}$ NMR spectrum of the equilibrium reaction mixture of *cis*-[Ni(^{i}Pr$_2$Im^{Me})$_2$(Bpin)$_2$] **2b** (*), [Ni$_2$(^{i}Pr$_2$Im^{Me})$_4$(*μ*-*(η^2:η^2)*-COD)] **1** (*), [Ni(^{i}Pr$_2$Im^{Me})$_2$(COD)] **1a** (*) and B_2pin_2 (128 MHz, 298 K, C_6D_6).

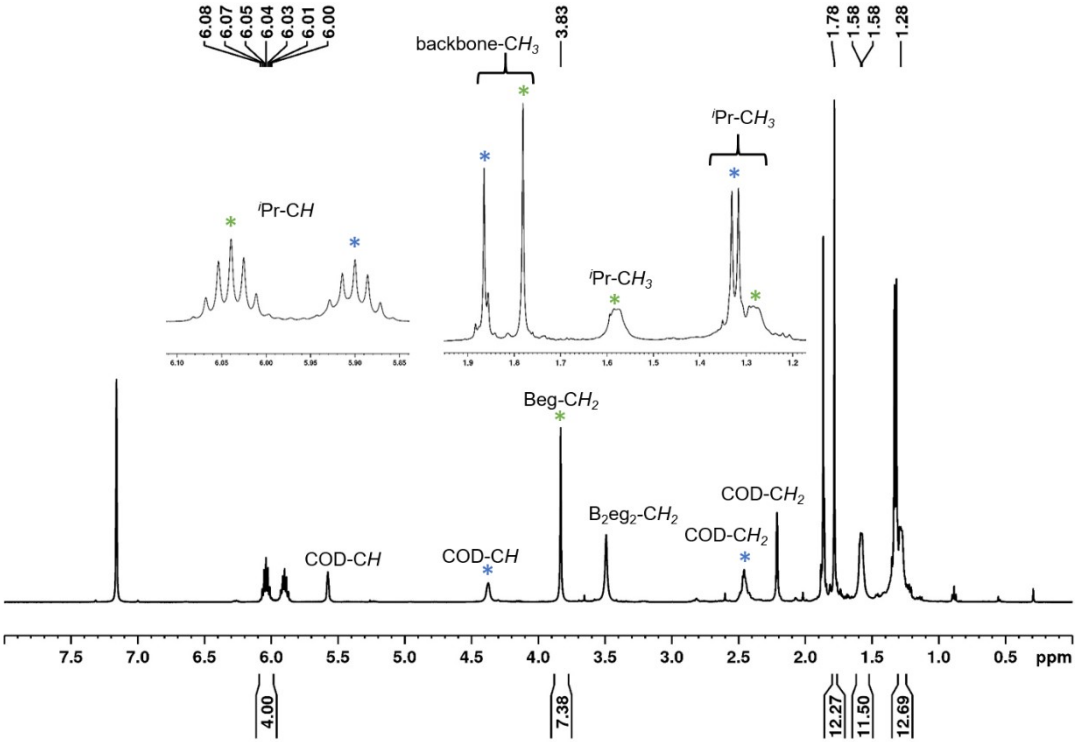


Figure S31. *In situ* ^{1}H NMR spectrum of the equilibrium reaction mixture of *cis*-[Ni(^{i}Pr$_2$Im^{Me})$_2$(Beg)$_2$] **2c** (*), [Ni$_2$(^{i}Pr$_2$Im^{Me})$_4$(*μ*-(*η*^{2}:*η*^{2})-COD)] **1** (*), [Ni(^{i}Pr$_2$Im^{Me})$_2$(COD)] **1a** (*) and B$_2$eg$_2$(500 MHz, 298 K, C$_6$D$_6$).

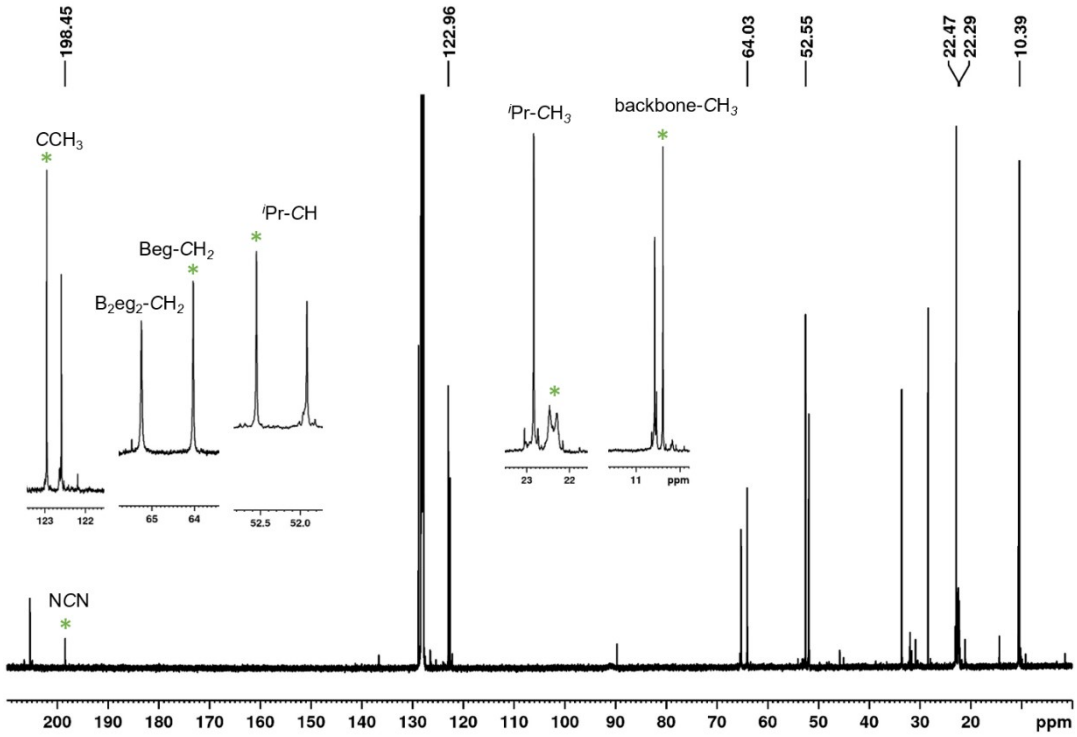


Figure S32. *In situ* ^{13}C{^{1}H} NMR spectrum of the equilibrium reaction mixture of *cis*-[Ni(^{i}Pr$_2$Im^{Me})$_2$(Beg)$_2$] **2c** (*), [Ni$_2$(^{i}Pr$_2$Im^{Me})$_4$(*μ*-(*η*^{2}:*η*^{2})-COD)] **1** (*), [Ni(^{i}Pr$_2$Im^{Me})$_2$(COD)] **1a** (*) and B$_2$eg$_2$ (126 MHz, 298 K, C$_6$D$_6$).

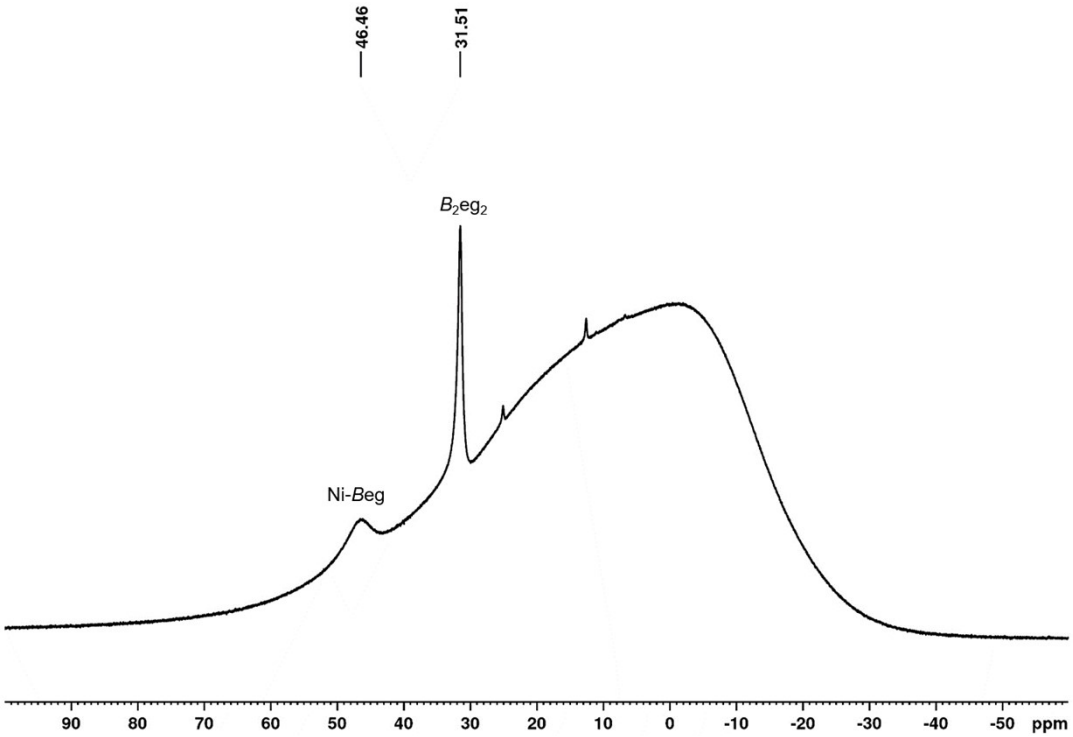


Figure S33. *In situ* $^{11}B\{^1H\}$ NMR spectrum of the equilibrium reaction mixture of *cis*-[Ni(^{i}Pr$_2$Im^{Me})$_2$(Beg)$_2$] **2c** (*), [Ni$_2$(^{i}Pr$_2$Im^{Me})$_4$(*μ*-(*η*^{2}:*η*^{2})-COD)] **1** (*), [Ni(^{i}Pr$_2$Im^{Me})$_2$(COD)] **1a** (*) and B_2eg_2 (160 MHz, 298 K, C_6D_6).

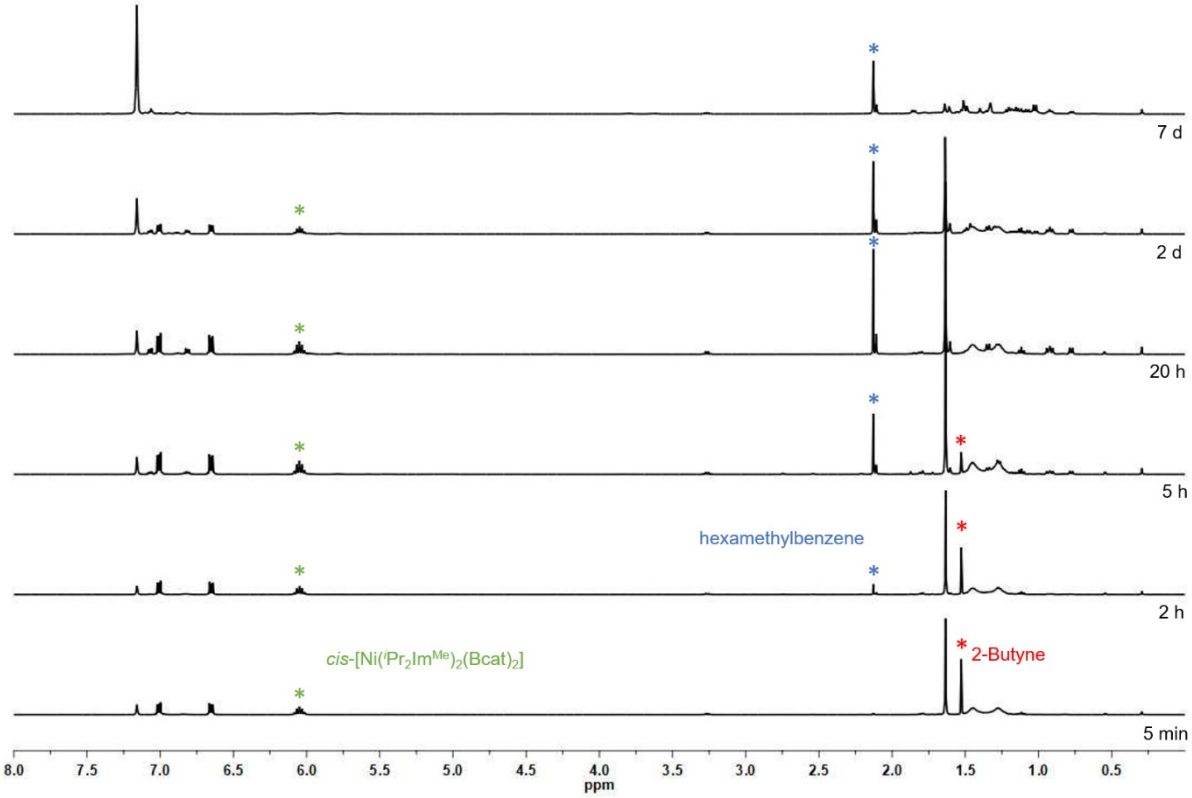


Figure S34. Time resolved *in situ* ^{1}H NMR spectrum of the reaction mixture of *cis*-[Ni(^{i}Pr$_2$Im^{Me})$_2$(Bcat)$_2$] **2a** (*) and 2-butyne (*) (400 MHz, 298 K, C_6D_6) to yield hexamethylbenzene. This reaction indicated that the bis(boryl) complex **2a** serves as a source for [Ni(^{i}Pr$_2$Im^{Me})$_2$], which catalyzes the trimerization of 2-butyne.[6]

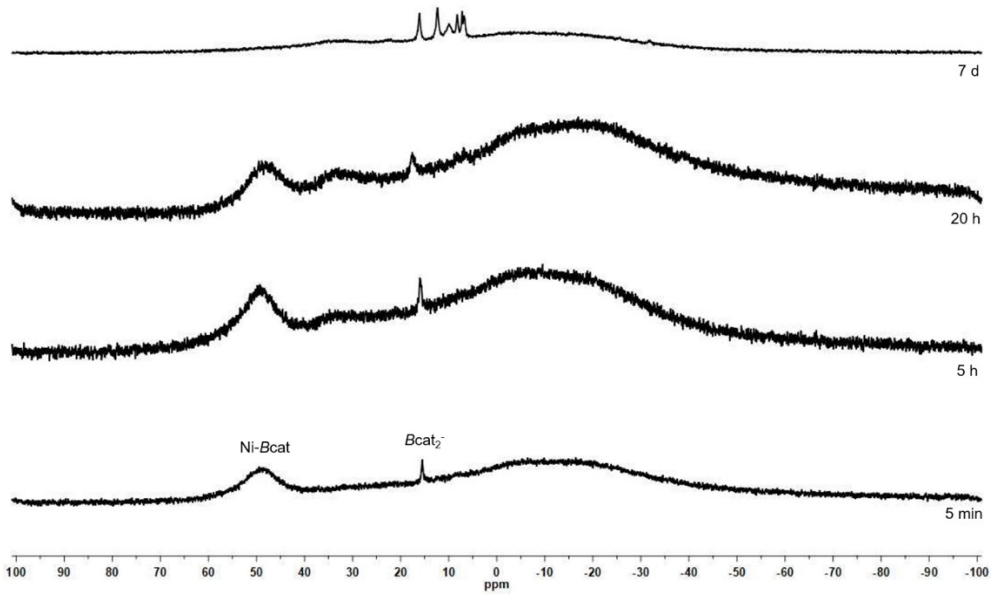


Figure S35. Time resolved *in situ* ^{11}B{^{1}H} NMR spectrum of the reaction mixture of *cis*-[Ni(^{i}Pr$_2$Im^{Me})$_2$(Bcat)$_2$] **2a** (*) and 2-Butyne (*) (128 MHz, 298 K, C_6D_6) to yield

hexamethylbenzene. This reaction indicated that the bis(boryl) complex **2a** serves as a source for [Ni(^{i}Pr$_2$Im^{Me})$_2$], which catalyzes the trimerization of 2-butyne.[6]

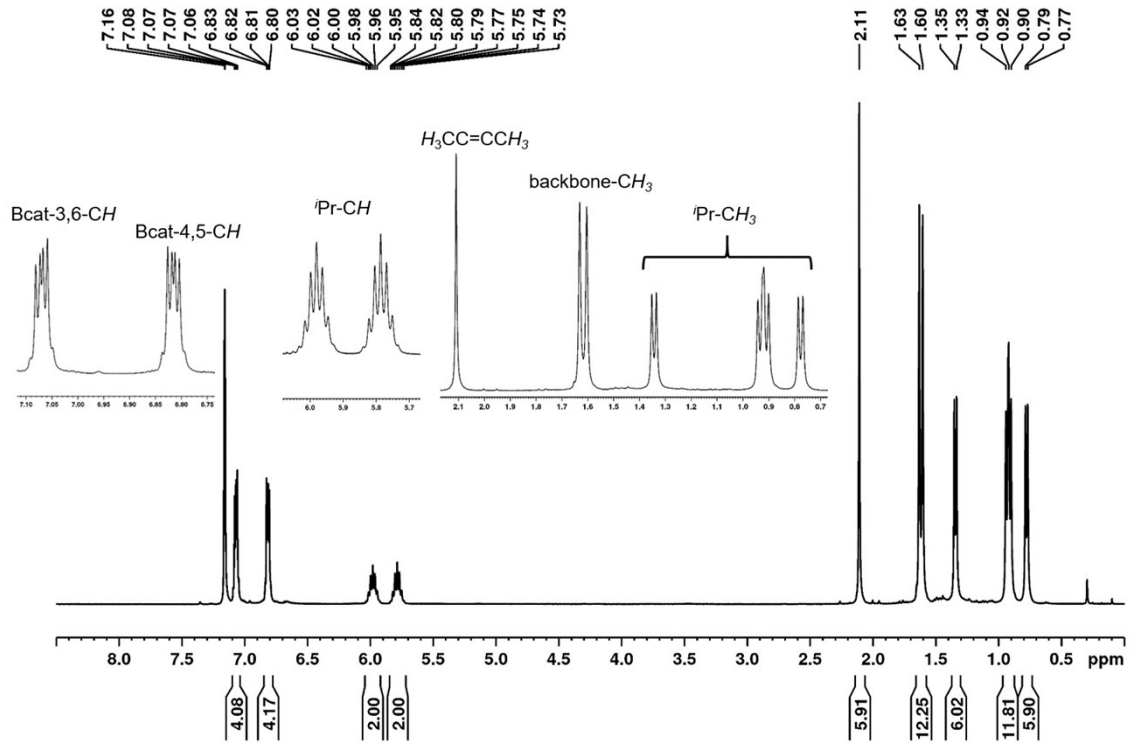


Figure S36. ^{1}H NMR spectrum of [Ni(^{i}Pr$_2$Im^{Me})$_2$(η^2-*cis*-(Bcat)(Me)C=C(Me)(Bcat))] **15a** (400 MHz, 298 K, C_6D_6).

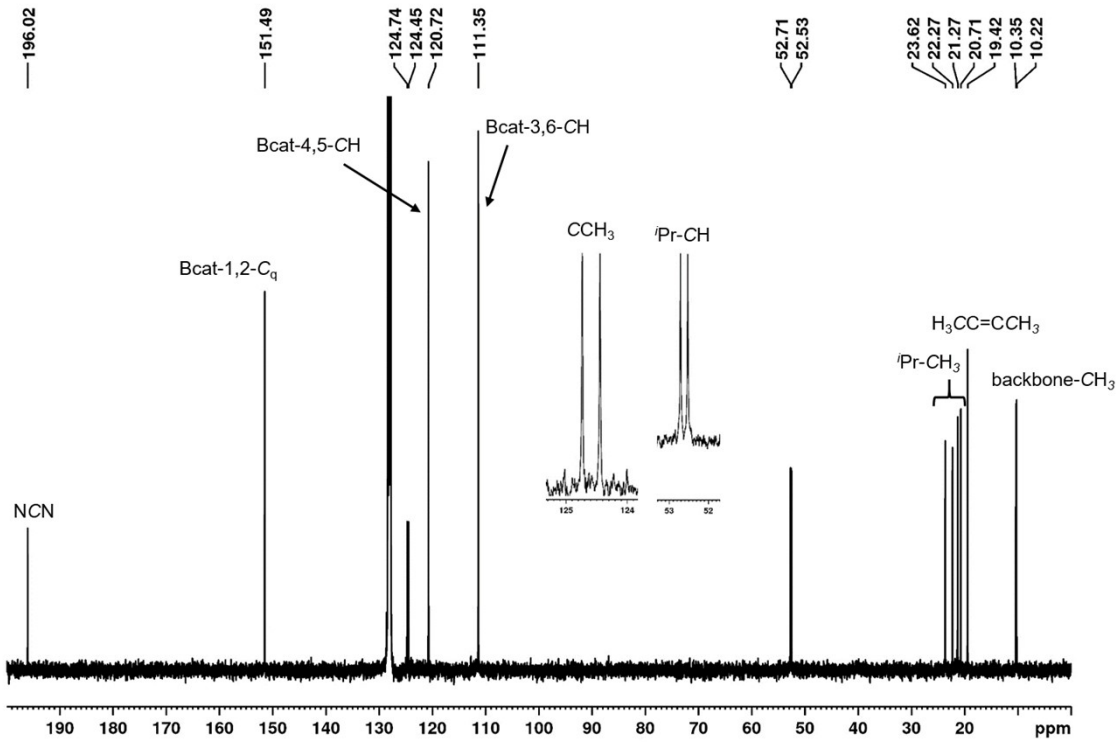


Figure S37. $^{13}C\{^{1}H\}$ NMR spectrum of [Ni($^{i}Pr_2Im^{Me}$)$_2$(η^2-*cis*-(Bcat)(Me)C=C(Me)(Bcat))] **15a** (100 MHz, 298 K, C_6D_6).

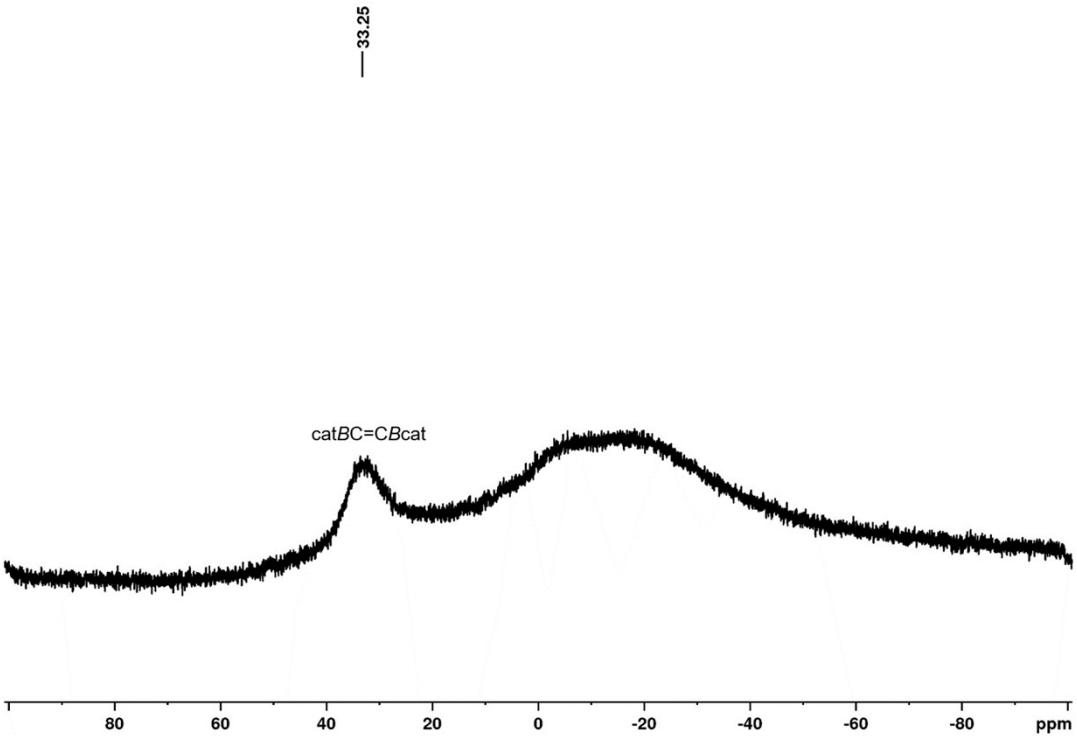


Figure S38. $^{11}B\{^{1}H\}$ NMR spectrum of [Ni($^{i}Pr_2Im^{Me}$)$_2$(η^2-*cis*-(Bcat)(Me)C=C(Me)(Bcat))] **15a** (128 MHz, 298 K, C_6D_6).

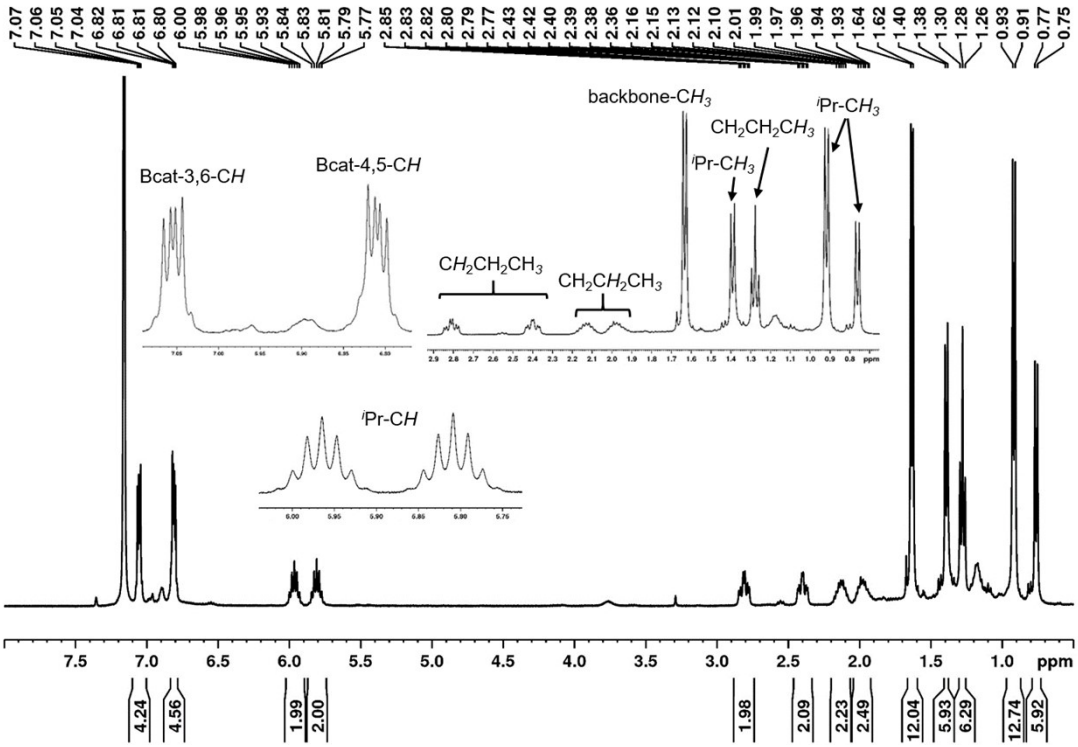


Figure S39. ^{1}H NMR spectrum of [Ni($^{i}Pr_2Im^{Me}$)$_2$(η^2-*cis*-(Bcat)(H_7C_3)C=C(C_3H_7)(Bcat))] **15b** (400 MHz, 298 K, C_6D_6).

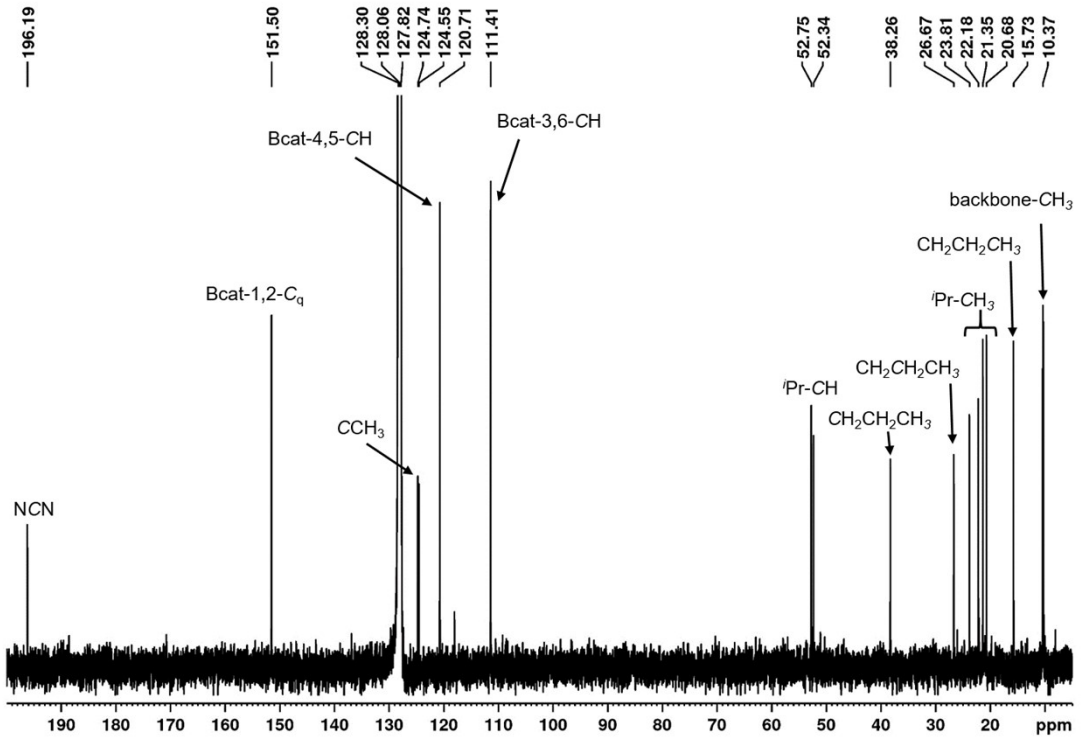


Figure S40. $^{13}C\{^{1}H\}$ NMR spectrum of [Ni($^{i}Pr_2Im^{Me}$)$_2$(η^2-*cis*-(Bcat)(H_7C_3)C=C(C_3H_7)(Bcat))] **15b** (100 MHz, 298 K, C_6D_6).

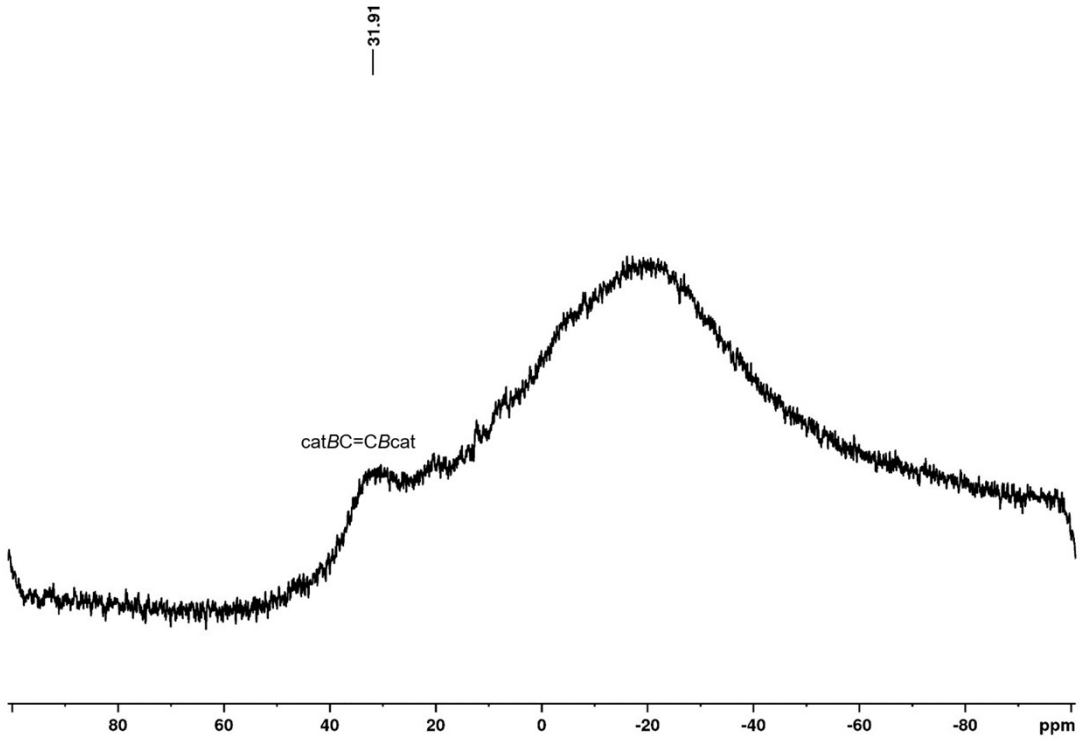


Figure S41. $^{11}B\{^{1}H\}$ NMR spectrum of [Ni($^{i}Pr_2Im^{Me}$)$_2$(η^2-*cis*-(Bcat)(H_7C_3)C=C(C_3H_7)(Bcat))] **15b** (128 MHz, 298 K, C_6D_6).

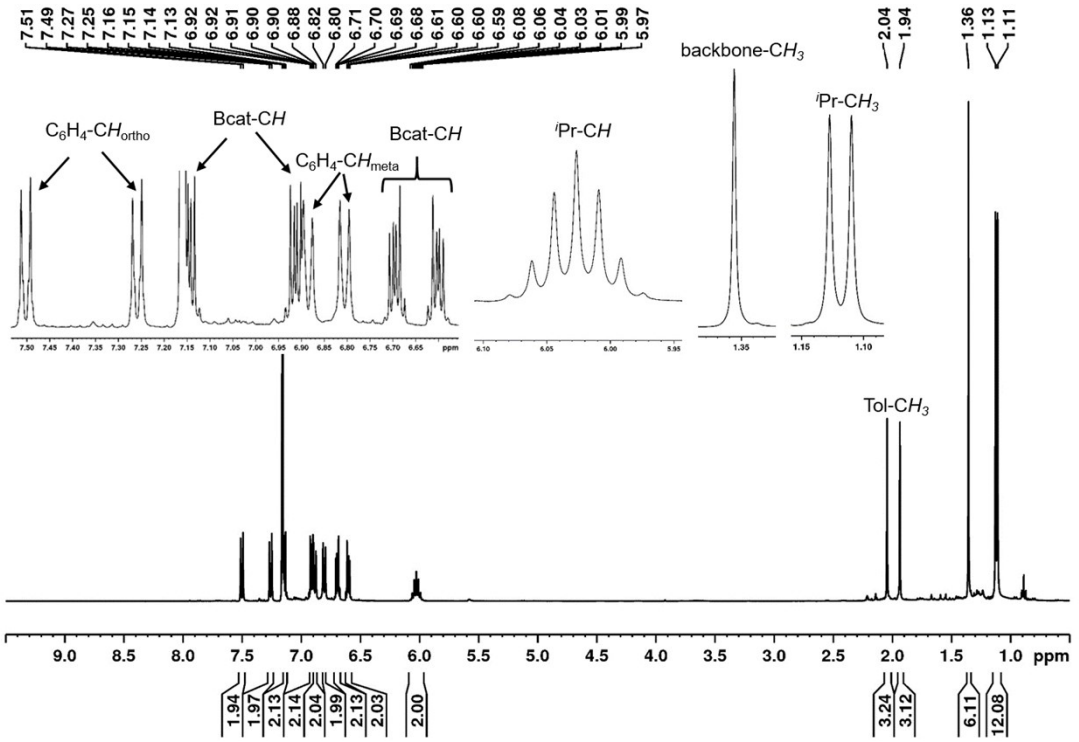


Figure S42. ^{1}H NMR spectrum of *Z*-(Bcat)(4-Me-C_6H_4)C=C(4-Me-C_6H_4)(Bcat) • ($^{i}Pr_2Im^{Me}$) **4^{NHC}** (400 MHz, 298 K, C_6D_6).

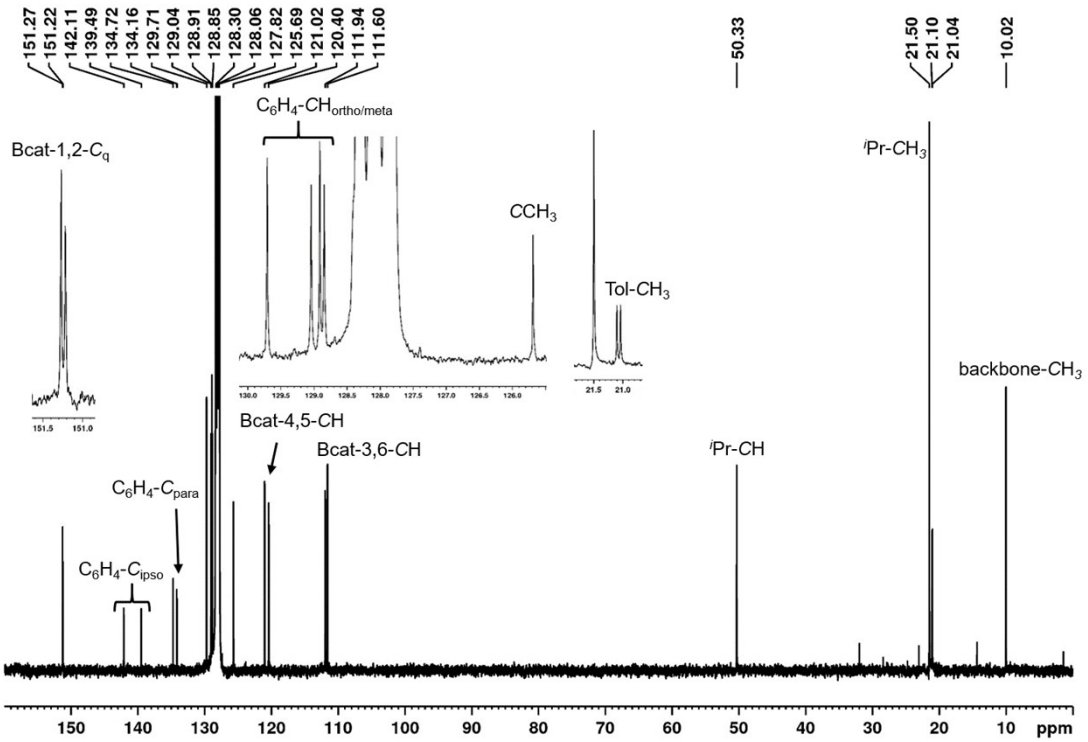


Figure S43. $^{13}C\{^{1}H\}$ NMR spectrum of *Z*-(Bcat)(4-Me-C_6H_4)C=C(4-Me-C_6H_4)(Bcat) • ($^{i}Pr_2Im^{Me}$) **4^{NHC}** (100 MHz, 298 K, C_6D_6).

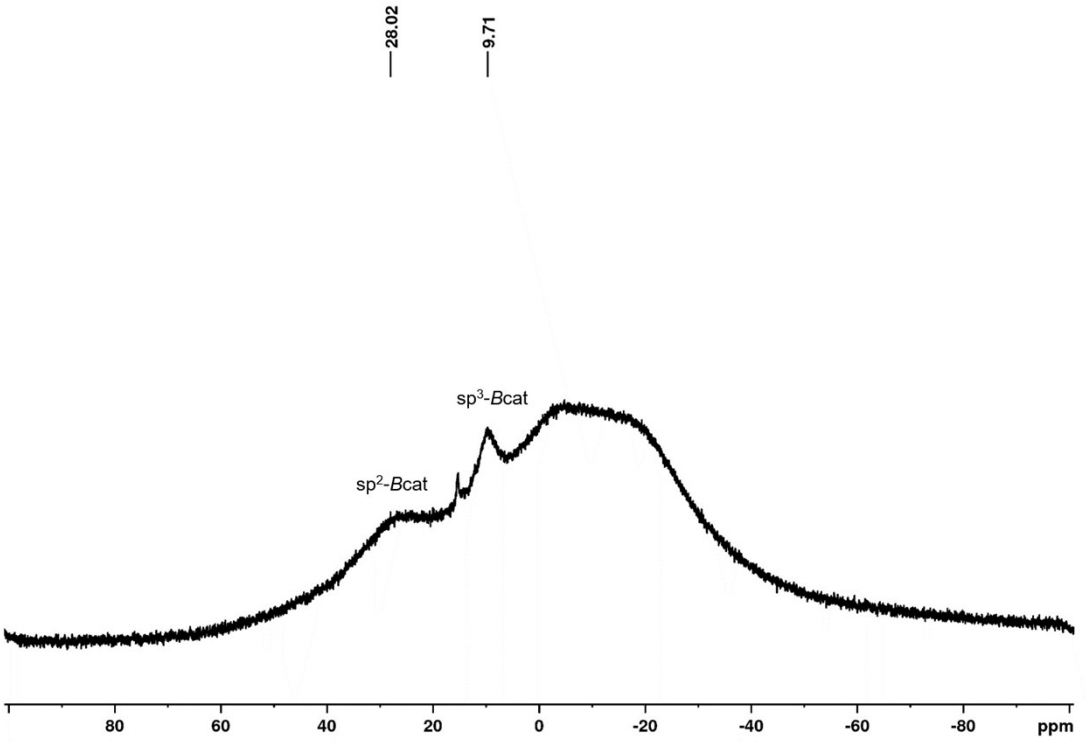


Figure S44. $^{11}B\{^{1}H\}$ NMR spectrum of *Z*-(Bcat)(4-Me-C_6H_4)C=C(4-Me-C_6H_4)(Bcat) • ($^{i}Pr_2Im^{Me}$) **4^{NHC}** (128 MHz, 298 K, C_6D_6).

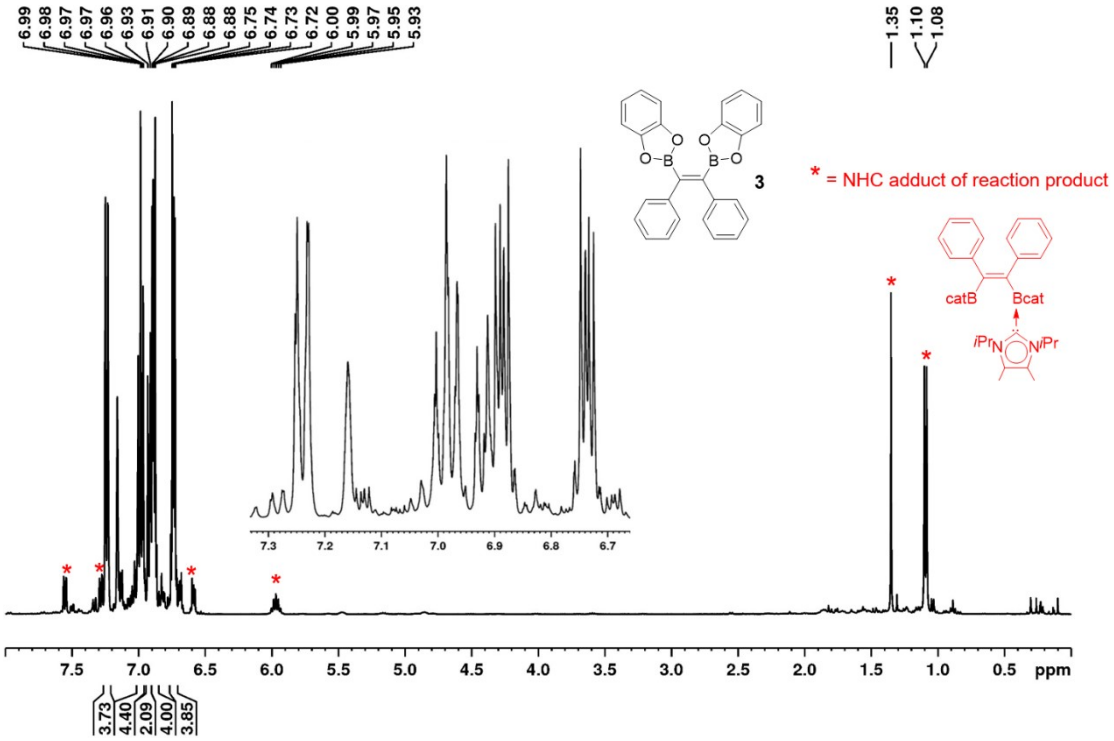


Figure S45. ^{1}H NMR spectrum of **3** from the crude reaction product of the catalysis (400 MHz, 298 K, C_6D_6).

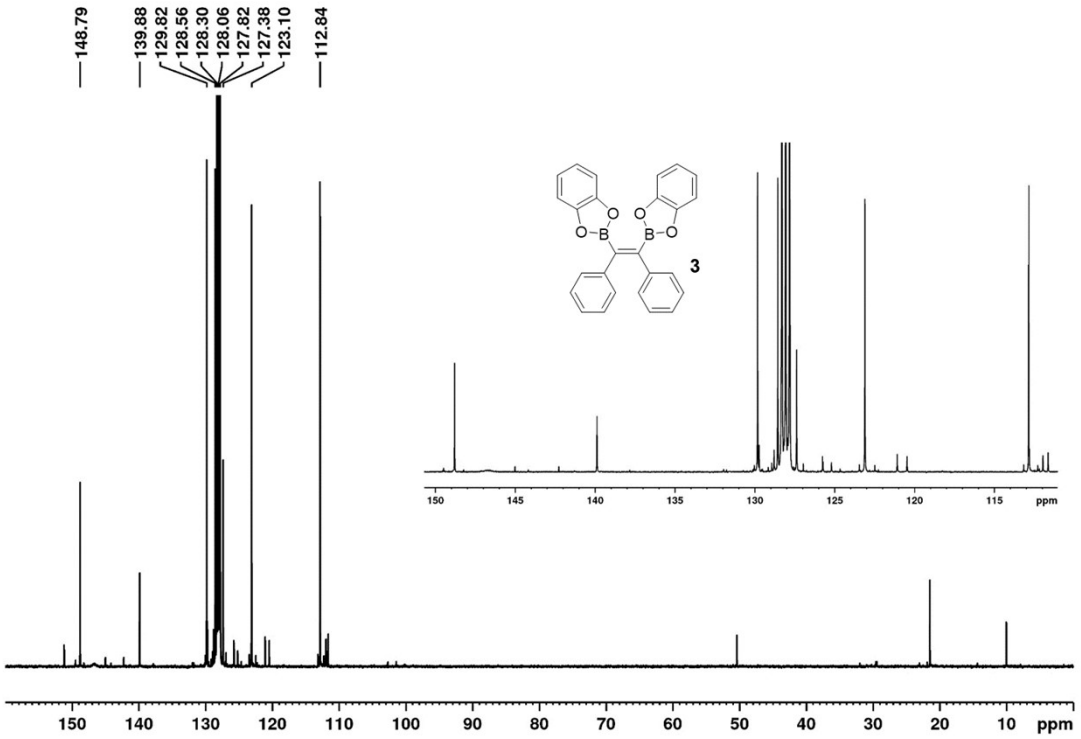


Figure S46. ^{13}C{^{1}H} NMR spectrum of **3** from the crude reaction product of the catalysis (100 MHz, 298 K, C_6D_6).

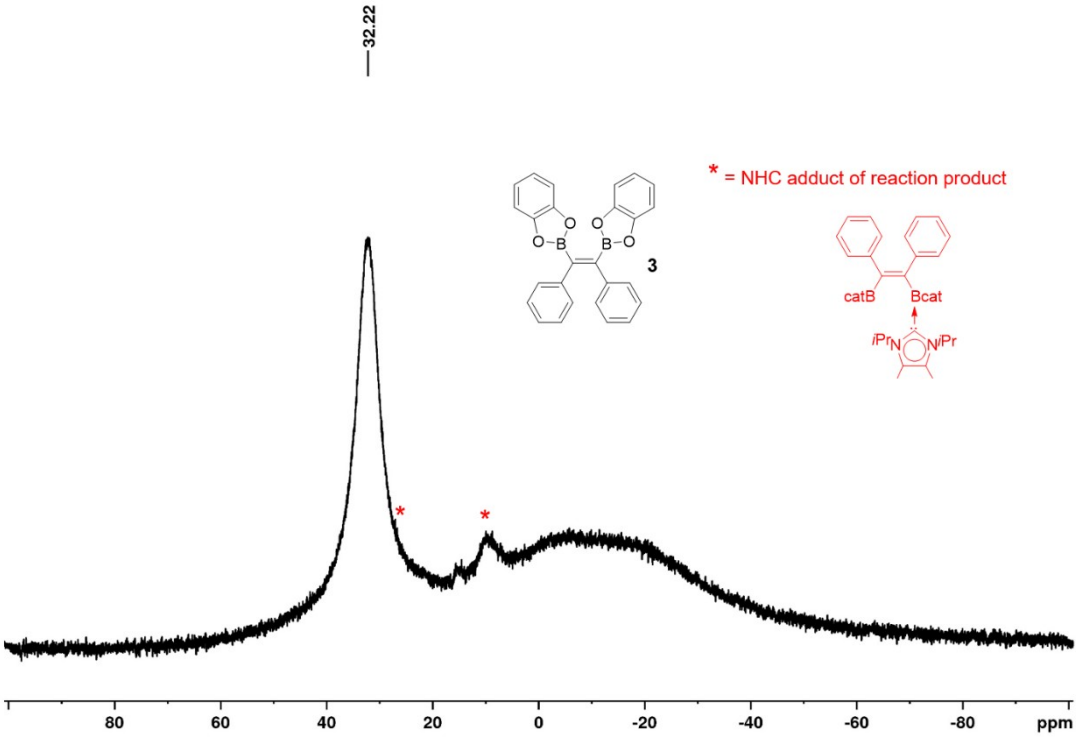


Figure S47. $^{11}B\{^{1}H\}$ NMR spectrum of **3** from the crude reaction product of the catalysis (128 MHz, 298 K, C_6D_6).

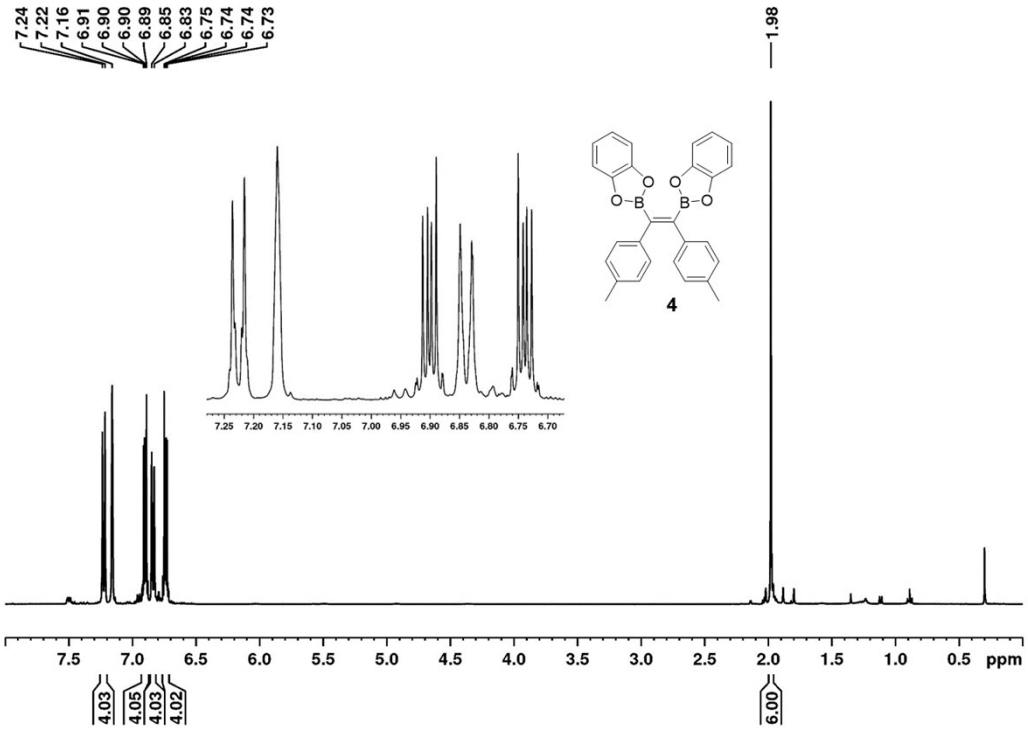


Figure S48. ^{1}H NMR spectrum of isolated **4** (400 MHz, 298 K, C_6D_6).

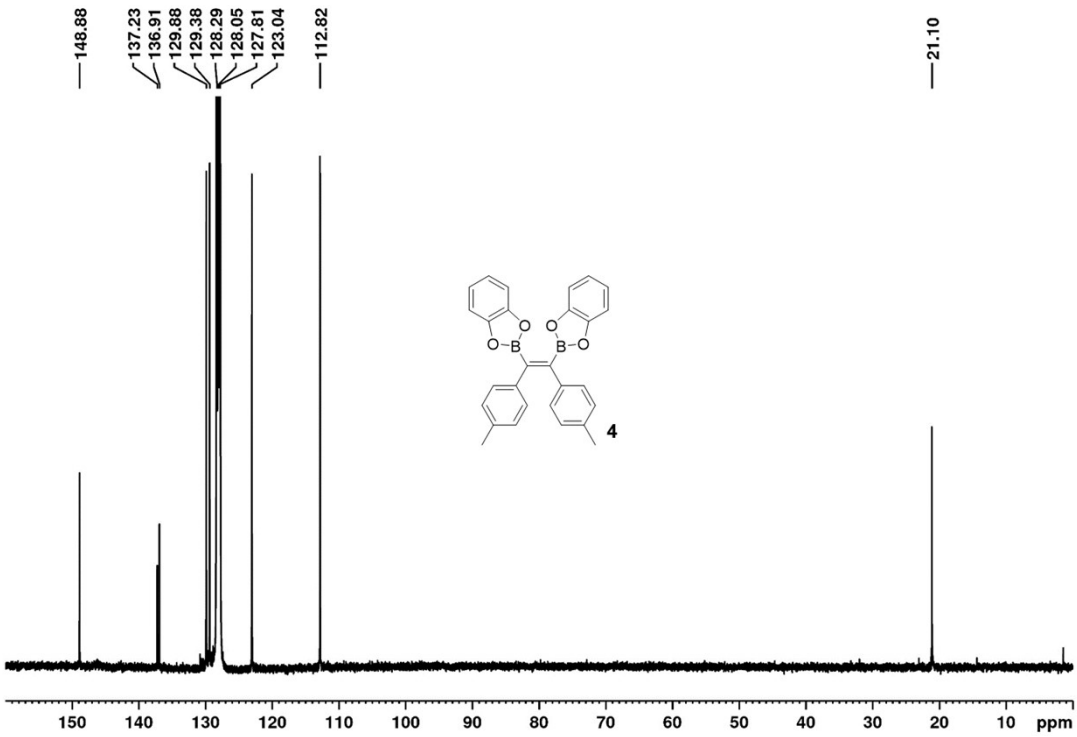


Figure S49. $^{13}C\{^{1}H\}$ NMR spectrum of isolated **4** (100 MHz, 298 K, C_6D_6).

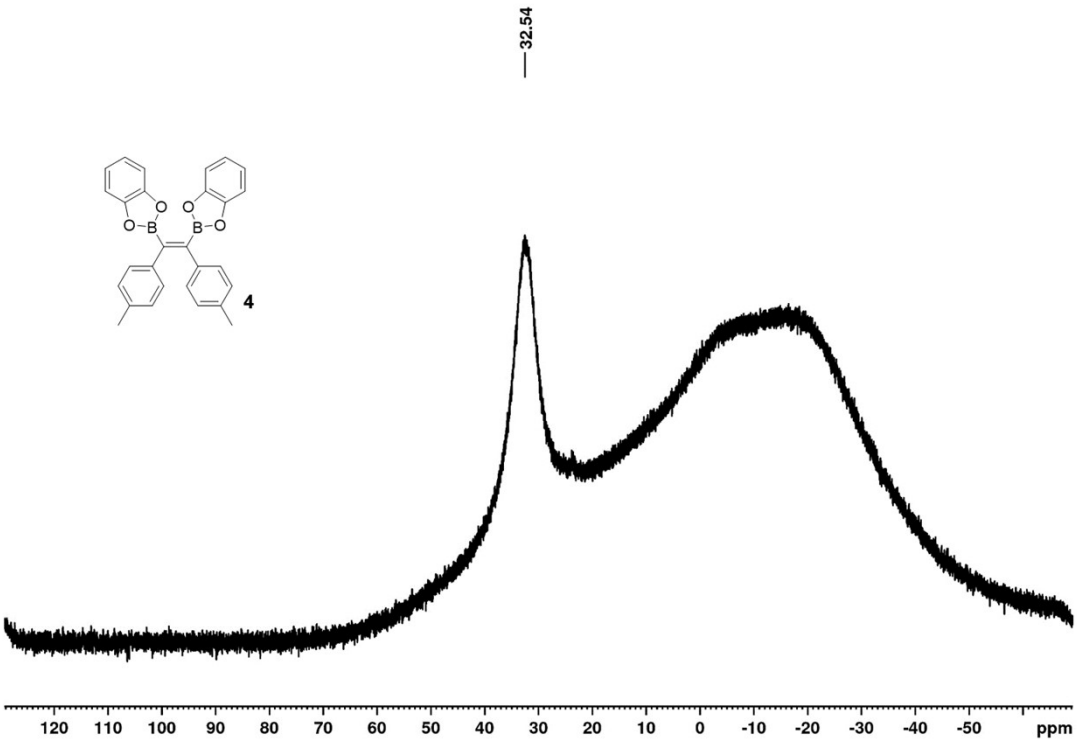


Figure S50. $^{11}B\{^{1}H\}$ NMR spectrum of isolated **4** (128 MHz, 298 K, C_6D_6).

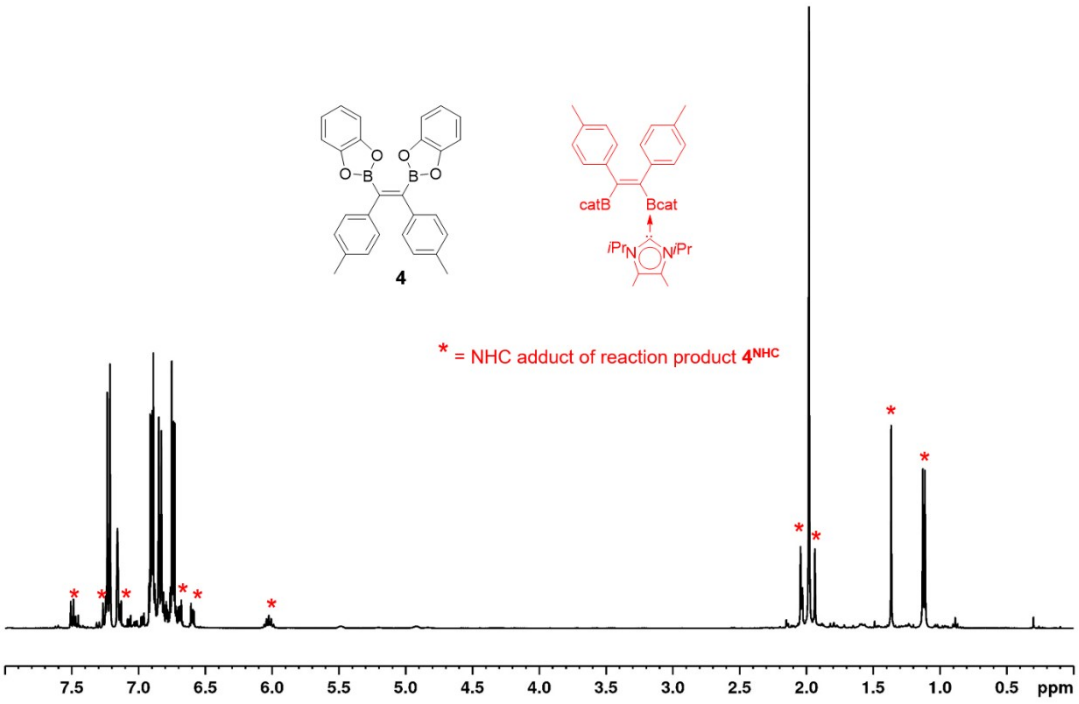


Figure S51. ^{1}H NMR spectrum of **4** from the crude reaction product of the catalysis (400 MHz, 298 K, C_6D_6).

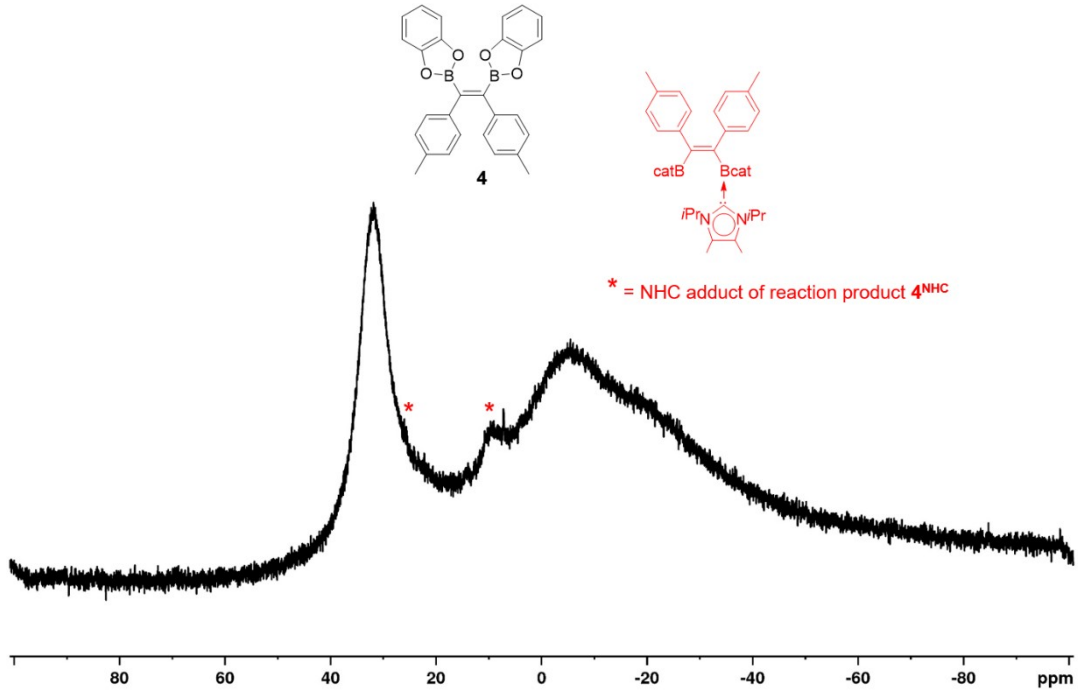


Figure S52. $^{11}B\{^{1}H\}$ NMR spectrum of **4** from the crude reaction product of the catalysis (128 MHz, 298 K, C_6D_6).

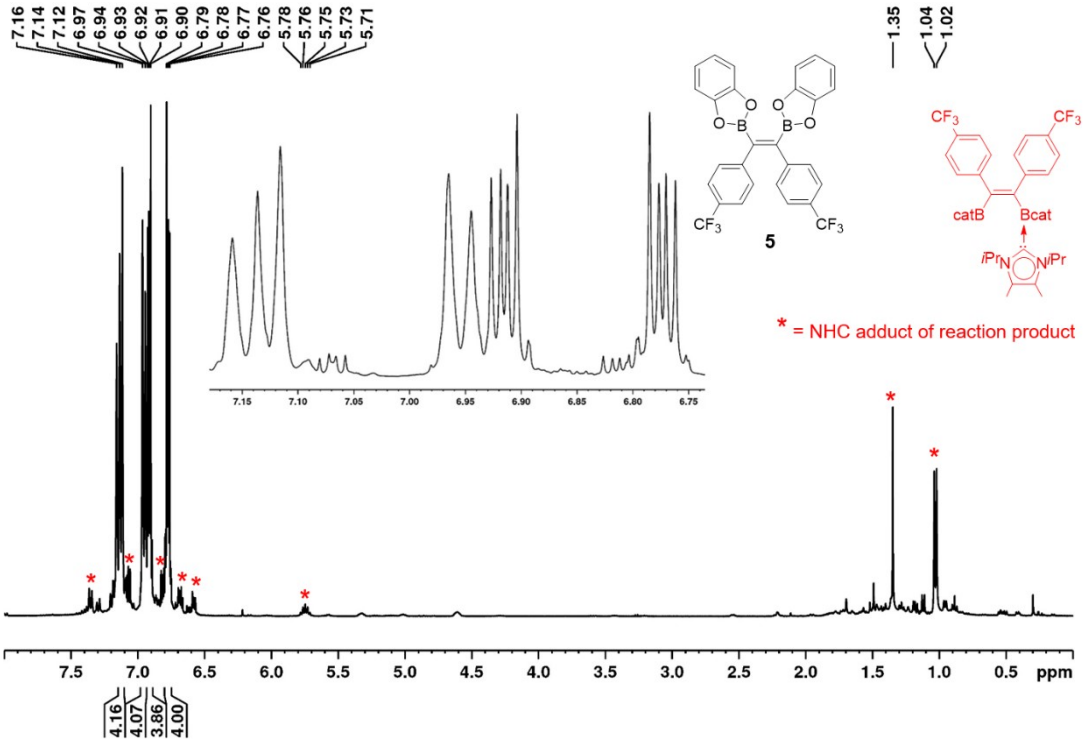


Figure S53. ^{1}H NMR spectrum of **5** from the crude reaction product of the catalysis (400 MHz, 298 K, C_6D_6).

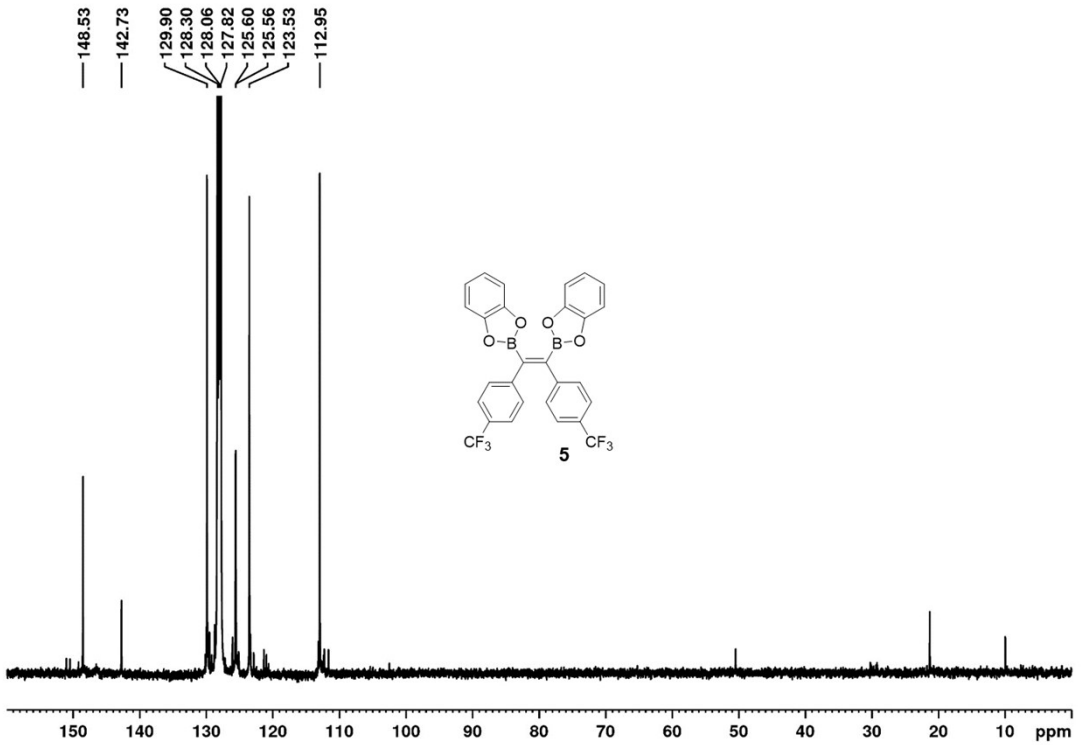


Figure S54. $^{13}C\{^{1}H\}$ NMR spectrum of **5** from the crude reaction product of the catalysis (100 MHz, 298 K, C_6D_6).

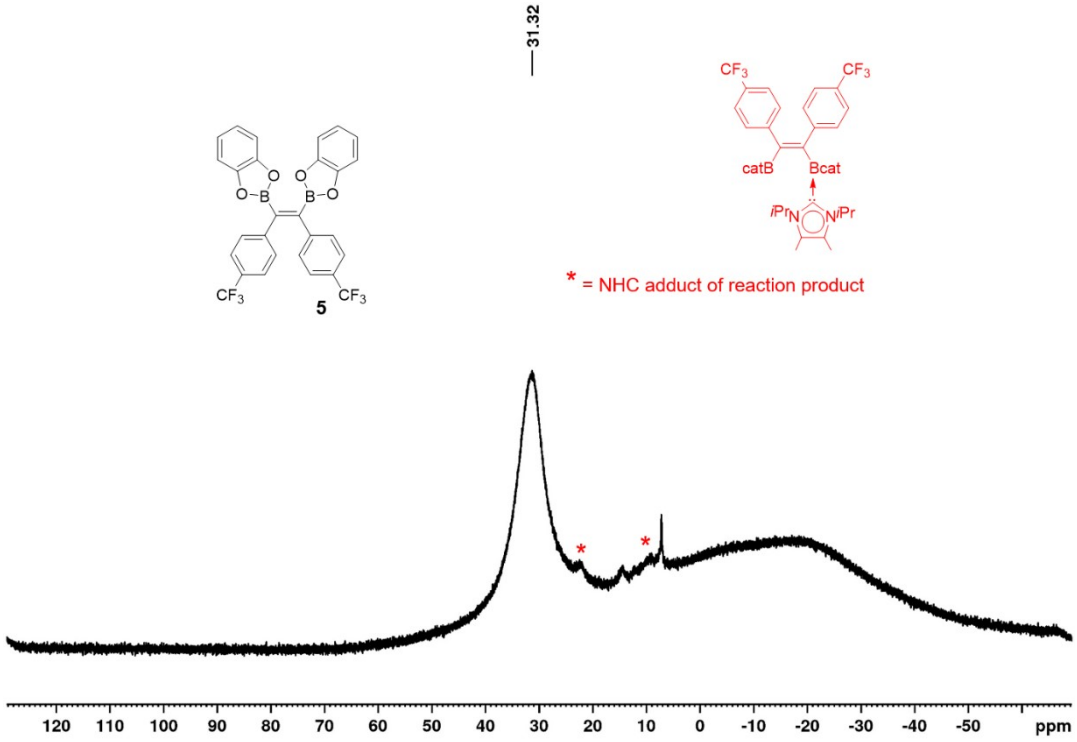


Figure S55. $^{11}B\{^{1}H\}$ NMR spectrum of **5** from the crude reaction product of the catalysis (128 MHz, 298 K, C_6D_6).

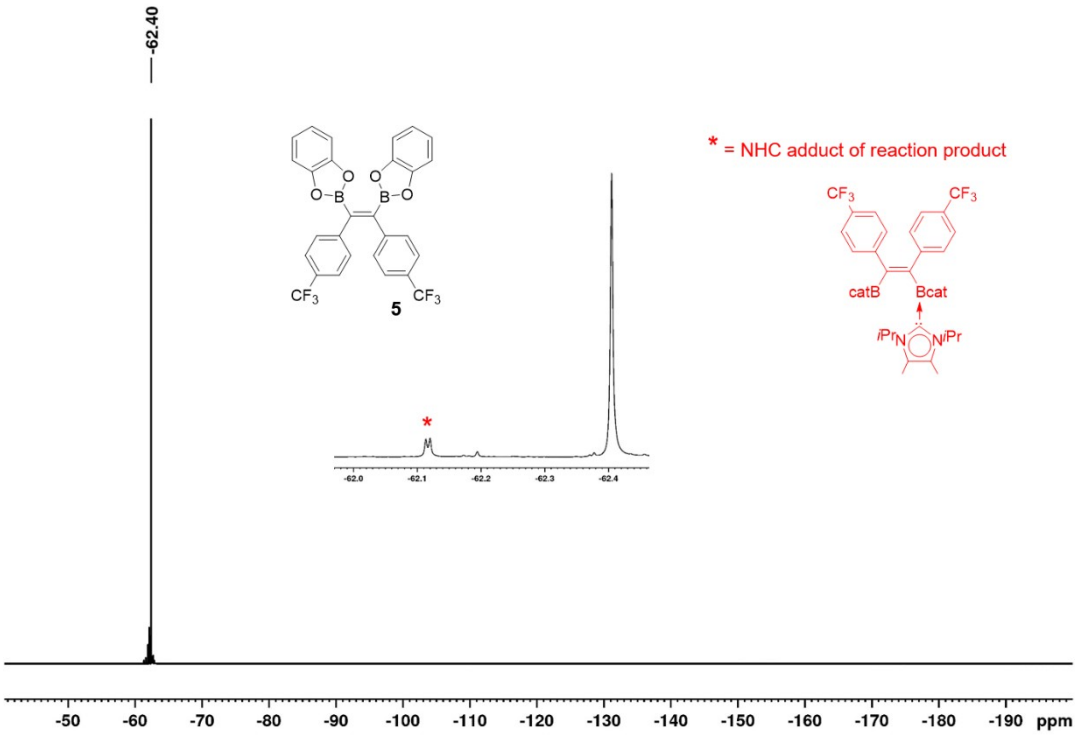


Figure S56. $^{19}F\{^{1}H\}$ NMR spectrum of **5** from the crude reaction product of the catalysis (376 MHz, 298 K, C_6D_6).

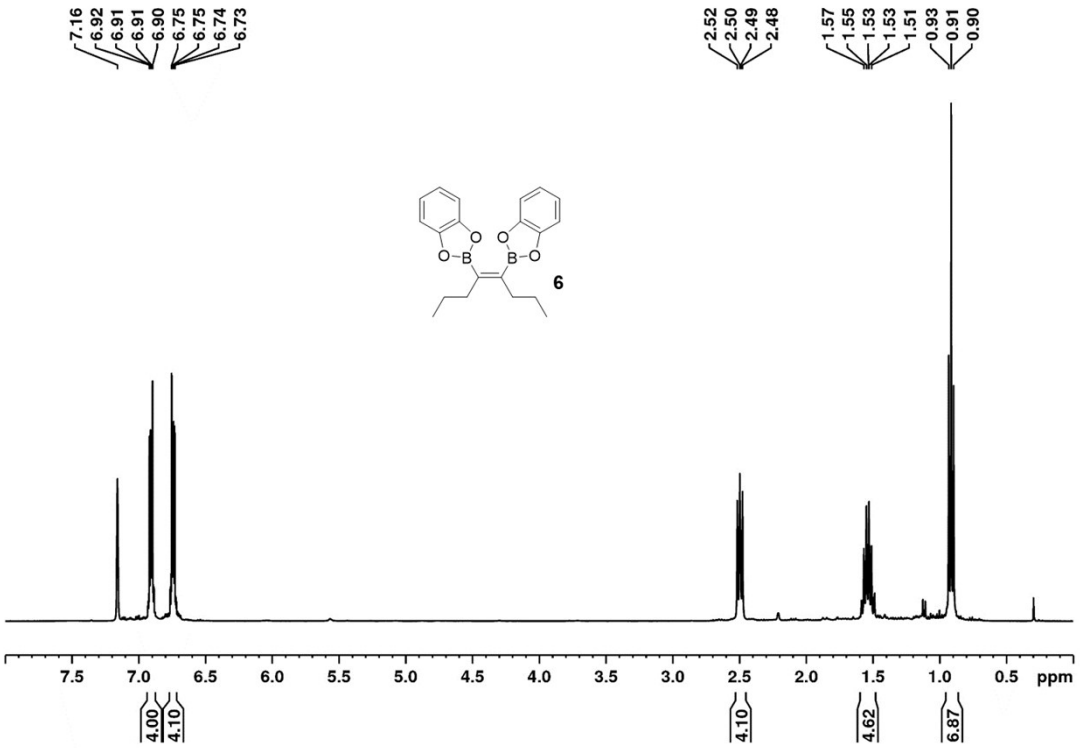


Figure S57. ^{1}H NMR spectrum of **6** from the crude reaction product of the catalysis (400 MHz, 298 K, C_6D_6).

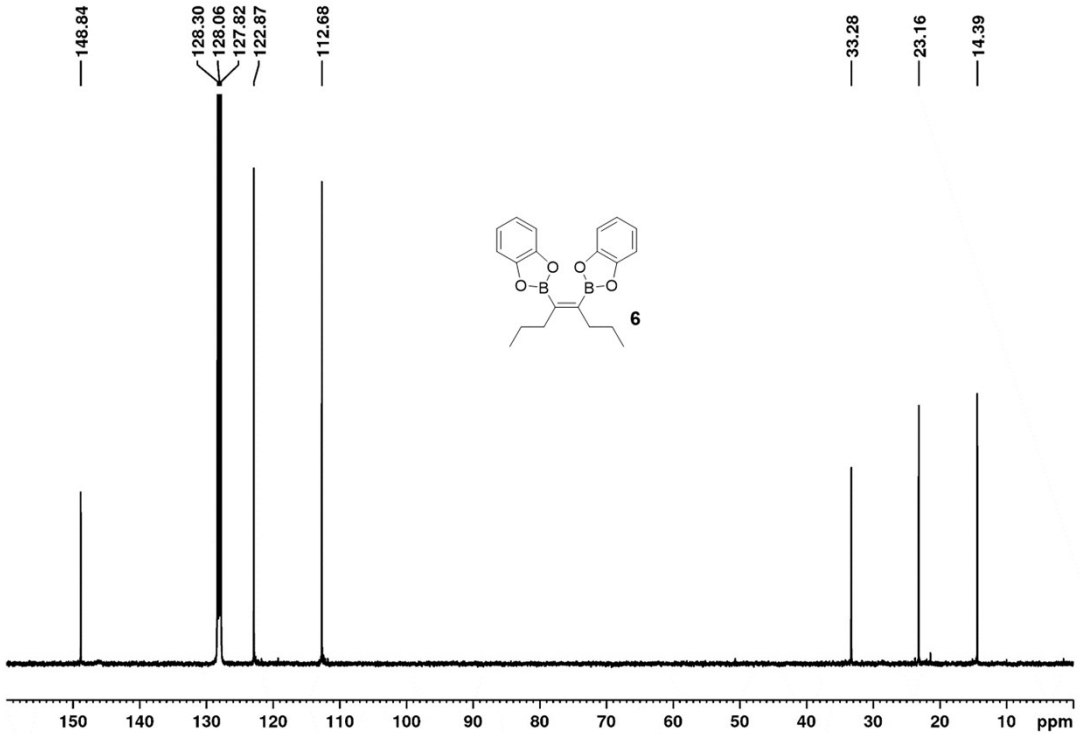


Figure S58. ^{13}C{^{1}H} NMR spectrum of **6** from the crude reaction product of the catalysis (100 MHz, 298 K, C_6D_6).

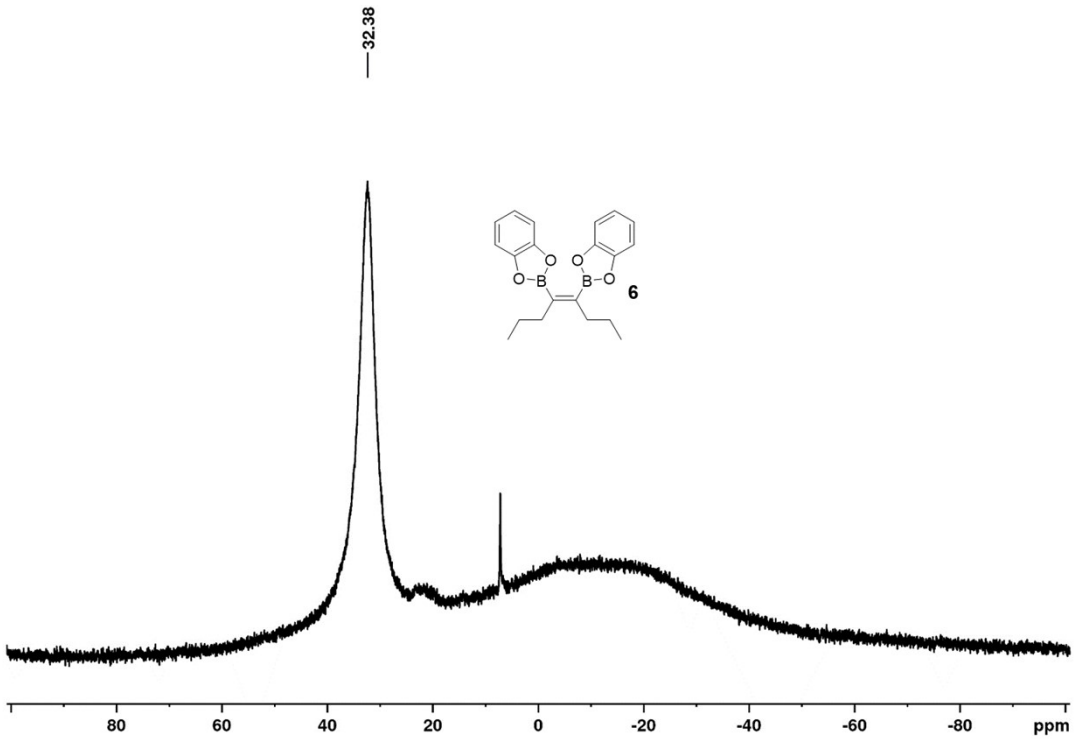


Figure S59. $^{11}B\{^{1}H\}$ NMR spectrum of **6** from the crude reaction product of the catalysis (128 MHz, 298 K, C_6D_6).

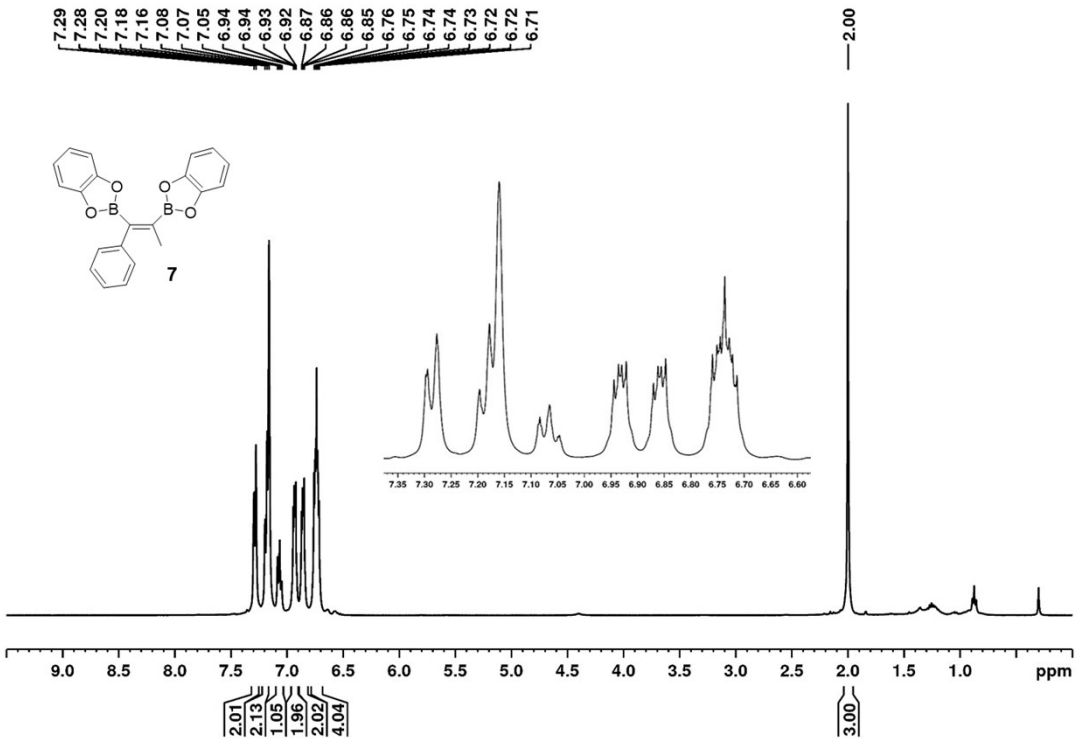


Figure S60. ^{1}H NMR spectrum of isolated **7** (400 MHz, 298 K, C_6D_6).

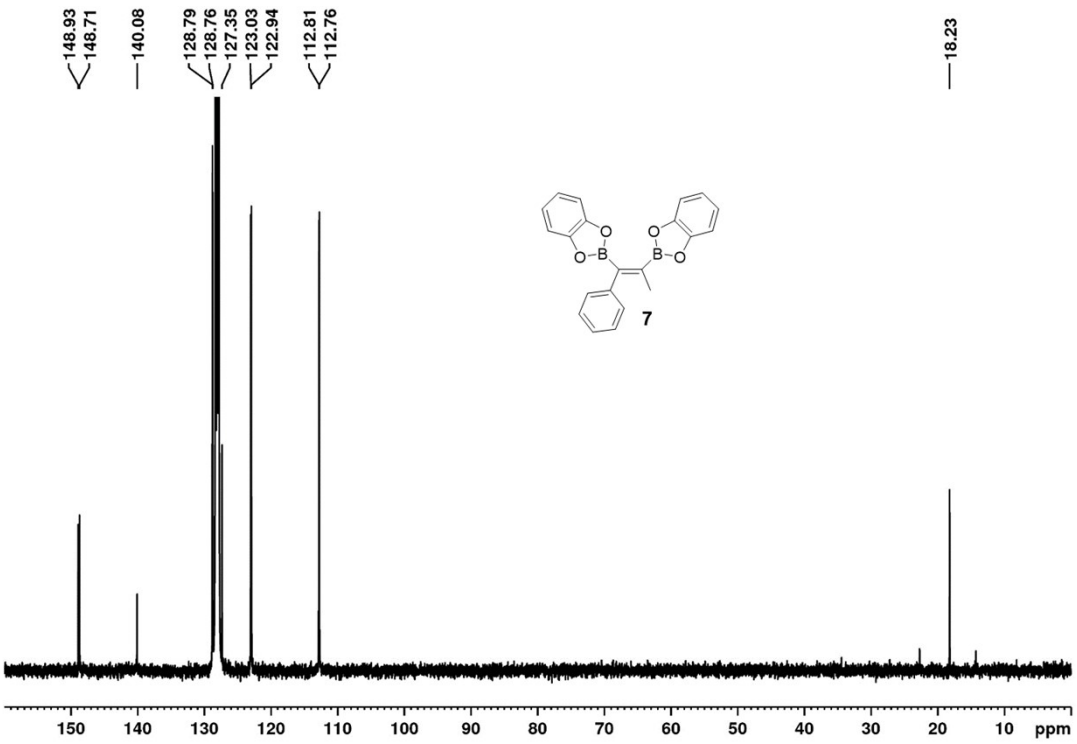


Figure S61. $^{13}C\{^{1}H\}$ NMR spectrum of isolated **7** (100 MHz, 298 K, C_6D_6).

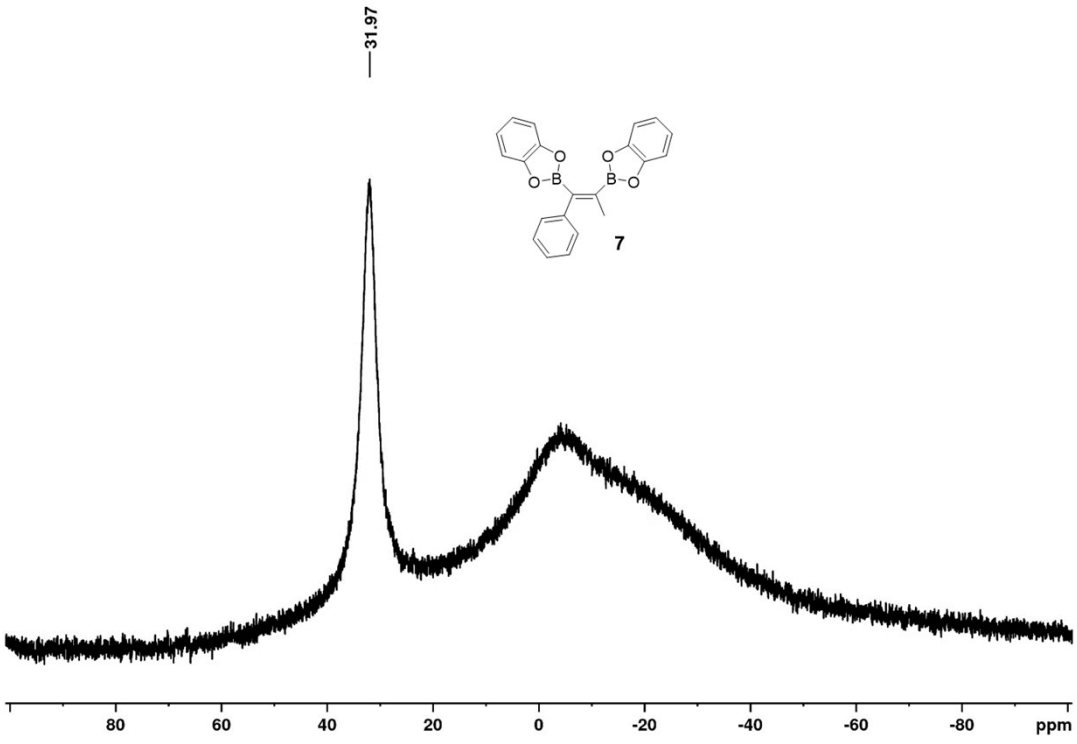


Figure S62. $^{11}B\{^{1}H\}$ NMR spectrum of isolated **7** (128 MHz, 298 K, C_6D_6).

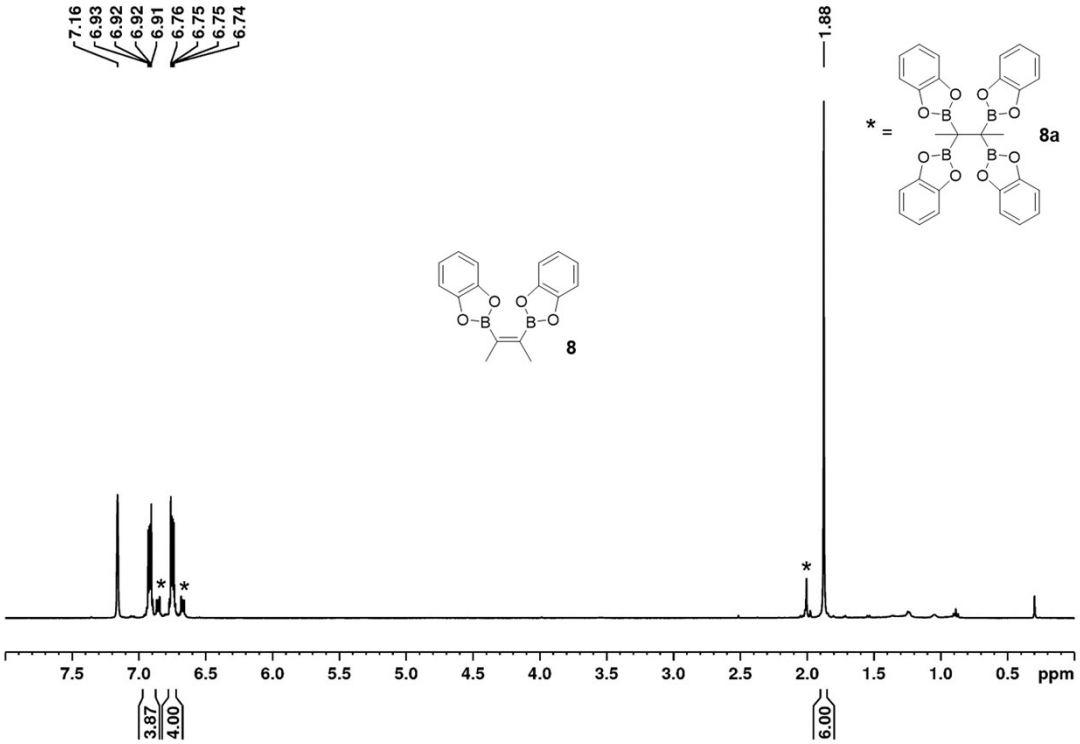


Figure S63. ^{1}H NMR spectrum of **8** from the crude reaction product of the catalysis (400MHz, 25 °C, C_6D_6).

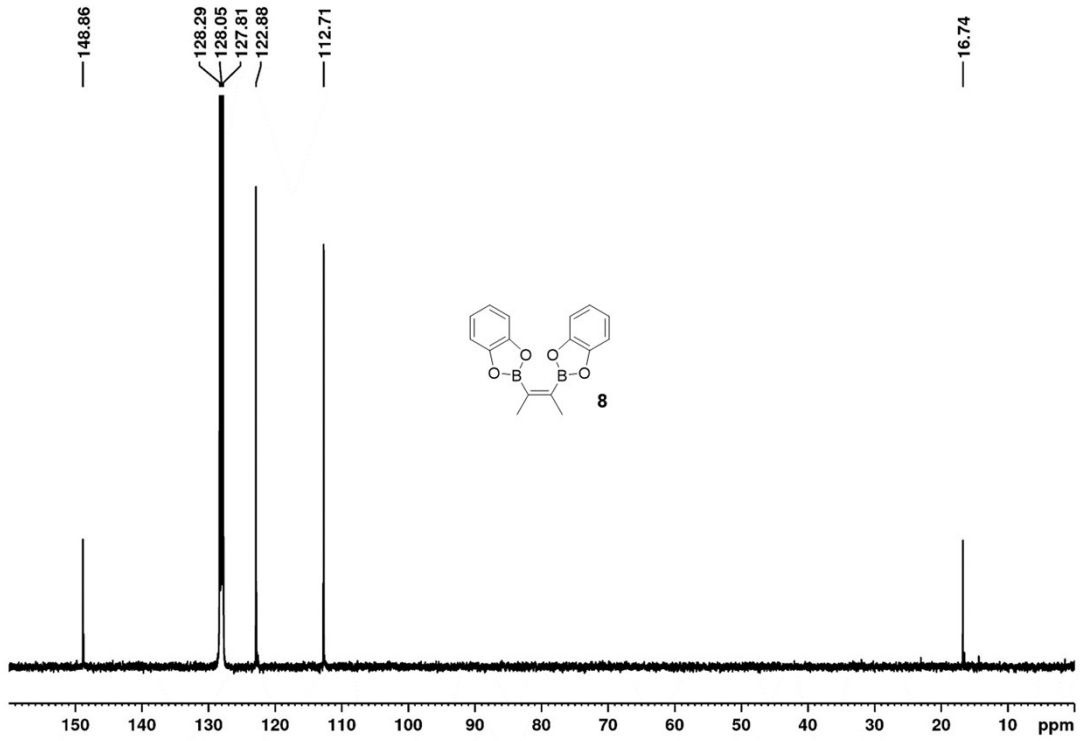


Figure S64. $^{13}C\{^{1}H\}$ NMR spectrum of **8** from the crude reaction product of the catalysis (100 MHz, 298 K, C_6D_6).

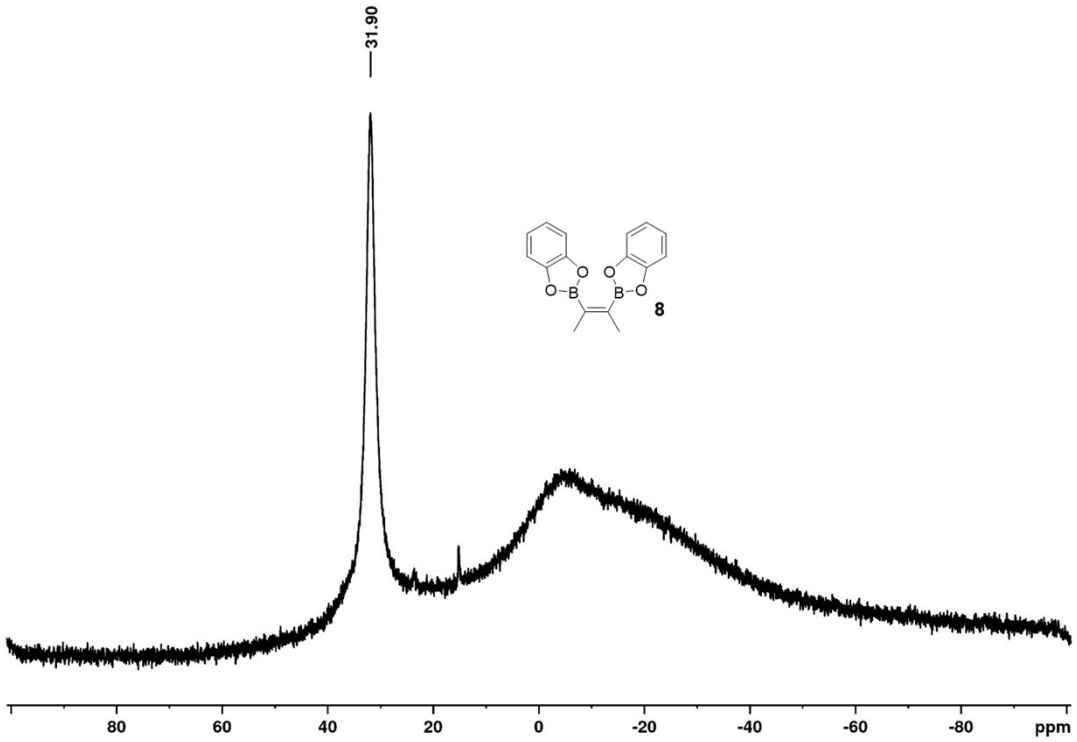


Figure S65. $^{11}B\{^{1}H\}$ NMR spectrum of **8** from the crude reaction product of the catalysis (128 MHz, 298 K, C_6D_6).

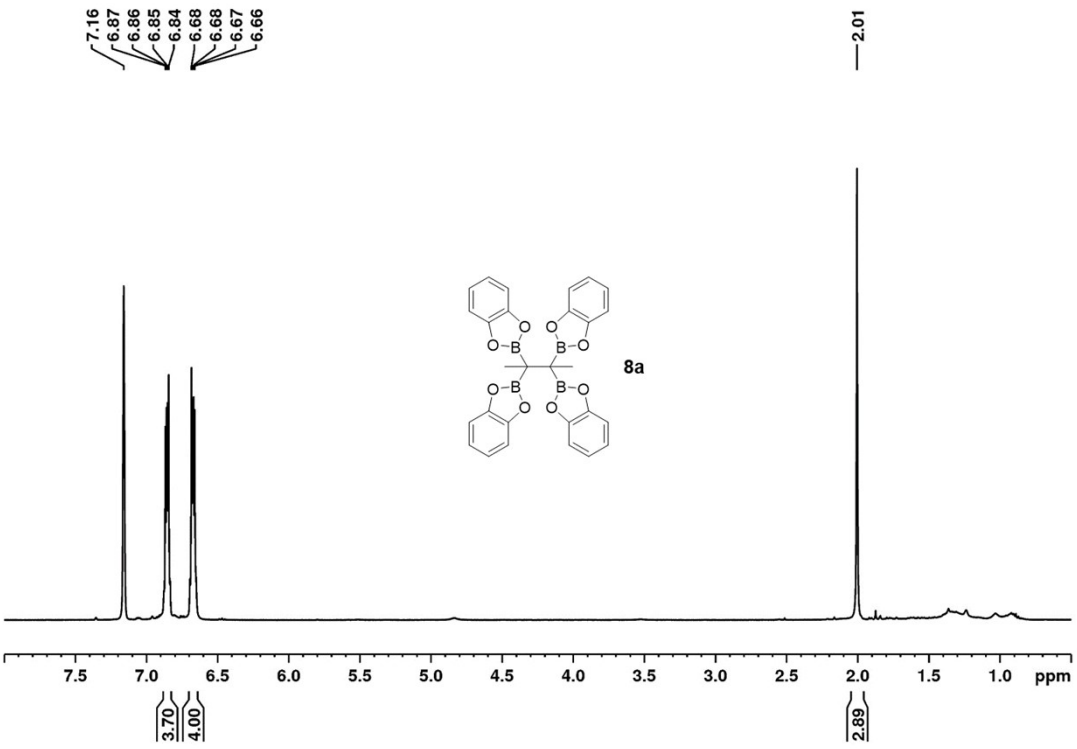


Figure S66. ^{1}H NMR spectrum of isolated **8a** (400 MHz, 298 K, C_6D_6).

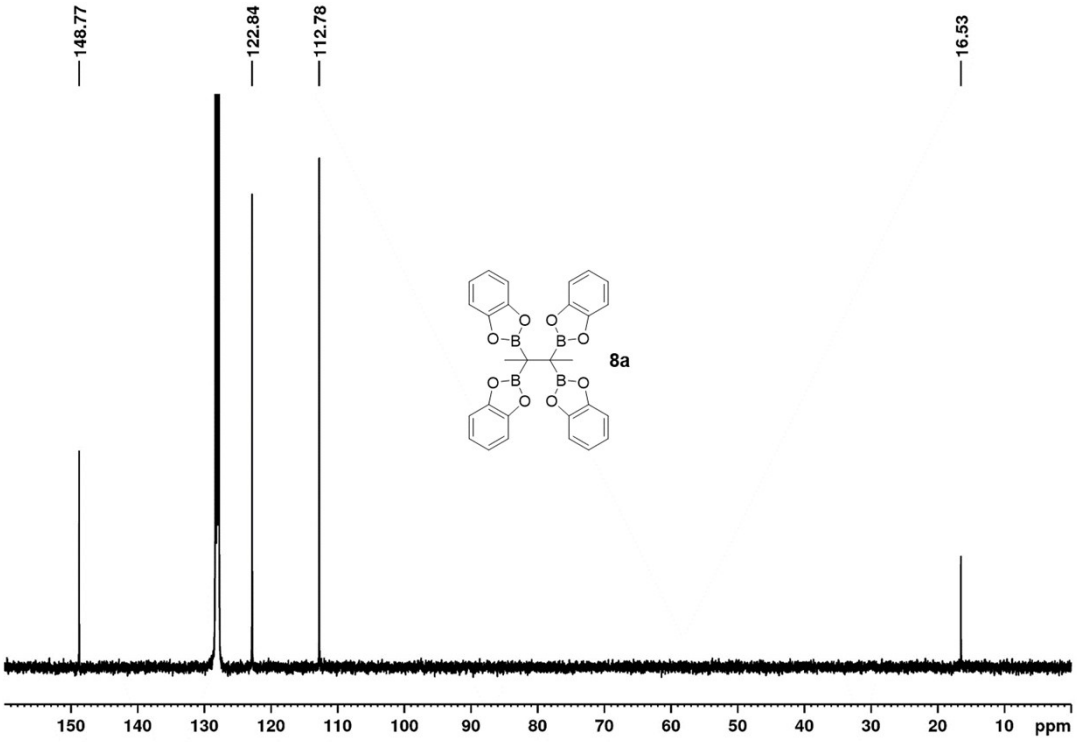


Figure S67. $^{13}C\{^{1}H\}$ NMR spectrum of isolated **8a** (100 MHz, 298 K, C_6D_6).

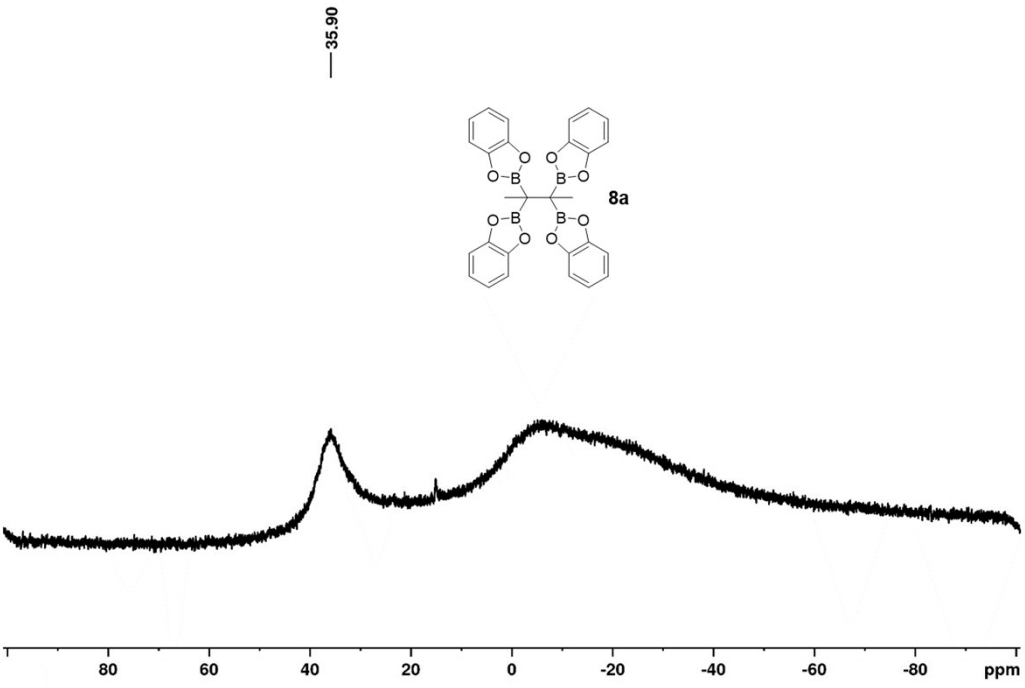


Figure S68. $^{11}B\{^{1}H\}$ NMR spectrum of isolated **8a** (128 MHz, 298 K, C_6D_6).

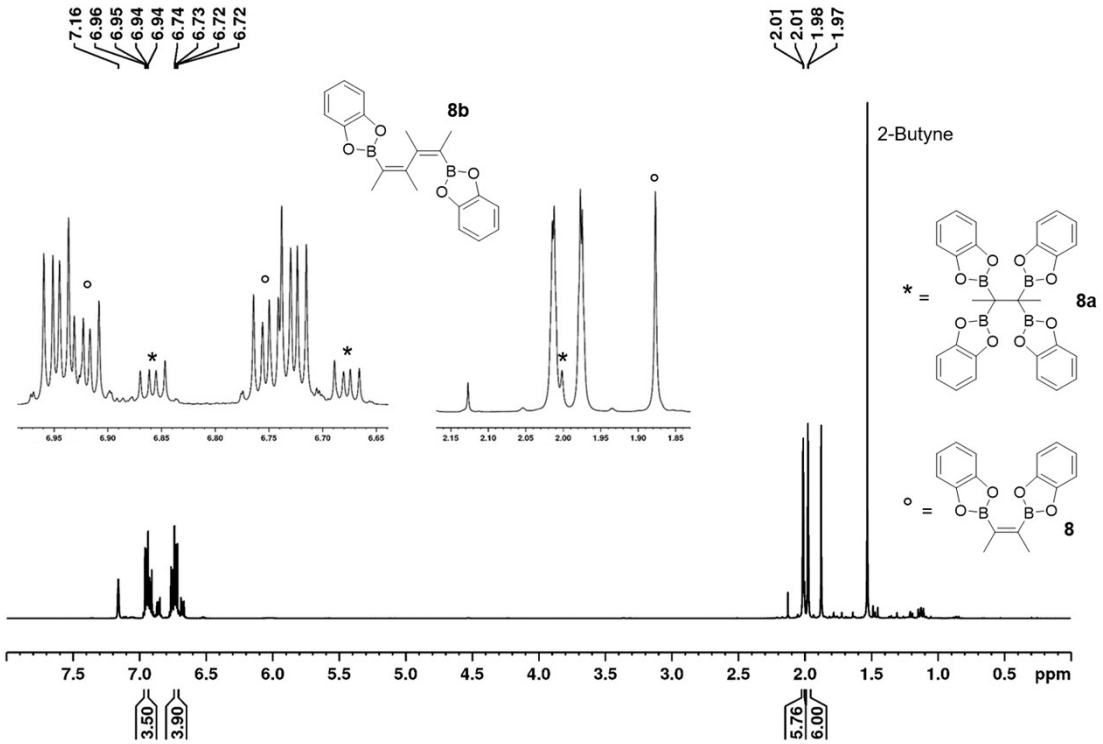


Figure S69. ^{1}H NMR spectrum of **8b** from the crude reaction product of the catalysis (400 MHz, 298 K, C_6D_6).

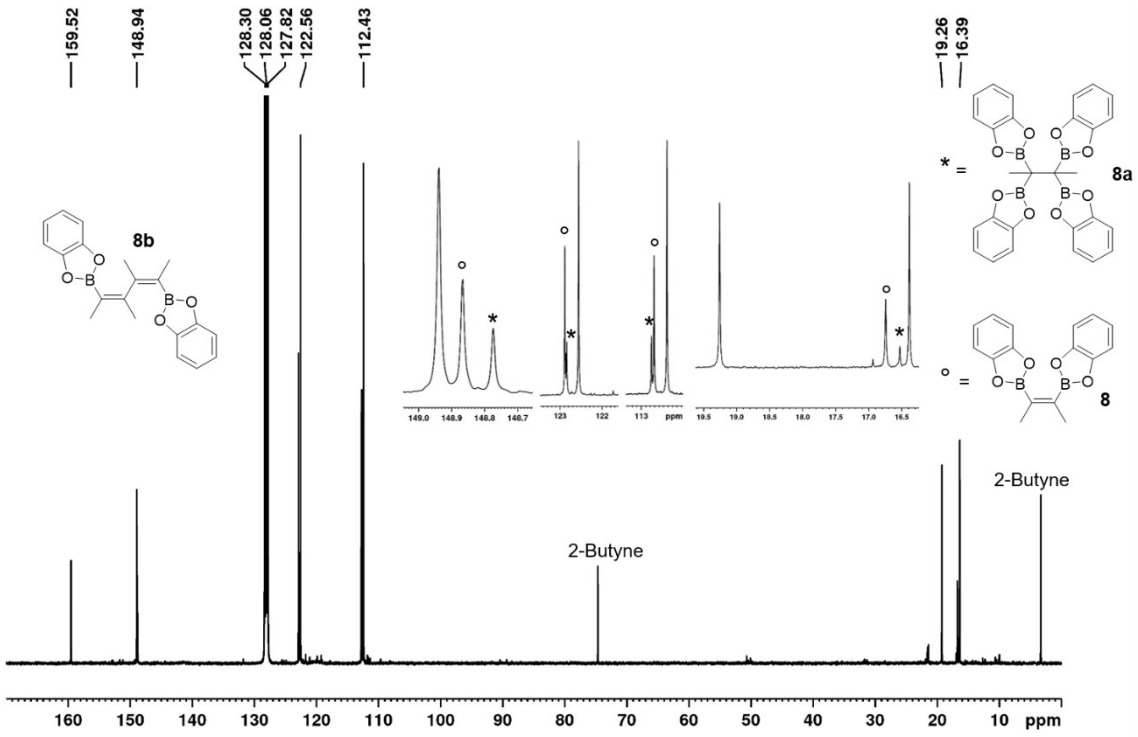


Figure S70. $^{13}C\{^{1}H\}$ NMR spectrum of **8b** from the crude reaction product of the catalysis (100 MHz, 298 K, C_6D_6).

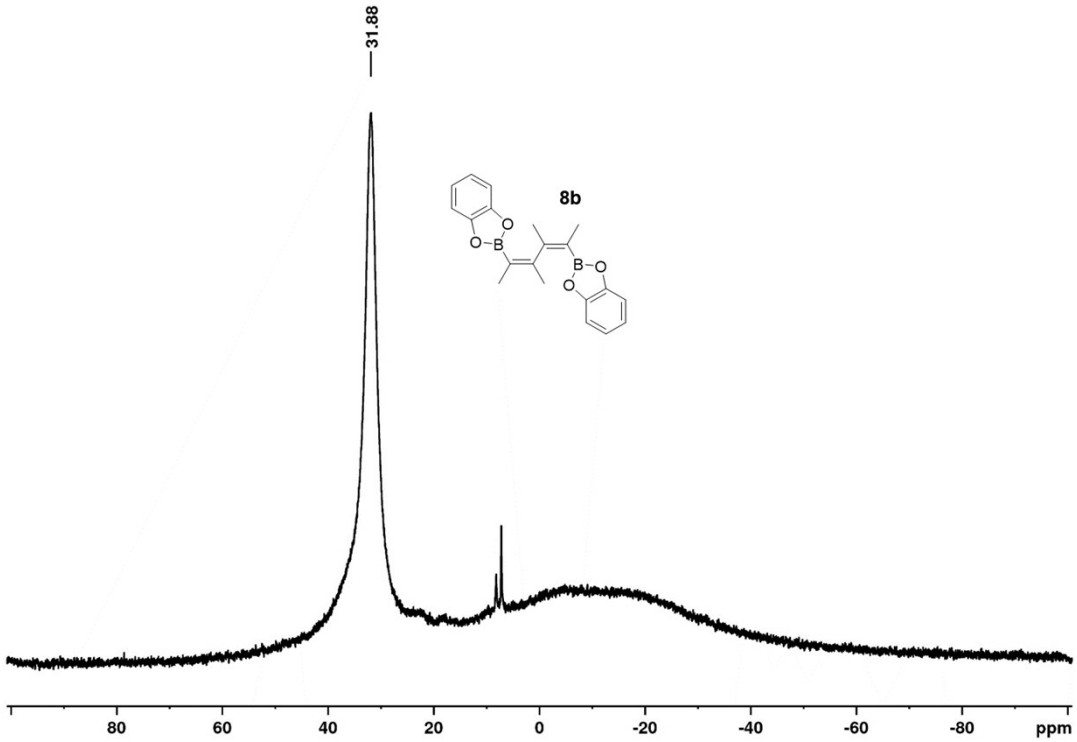


Figure S71. $^{11}B\{^{1}H\}$ NMR spectrum of **8b** from the crude reaction product of the catalysis (128 MHz, 298 K, C_6D_6).

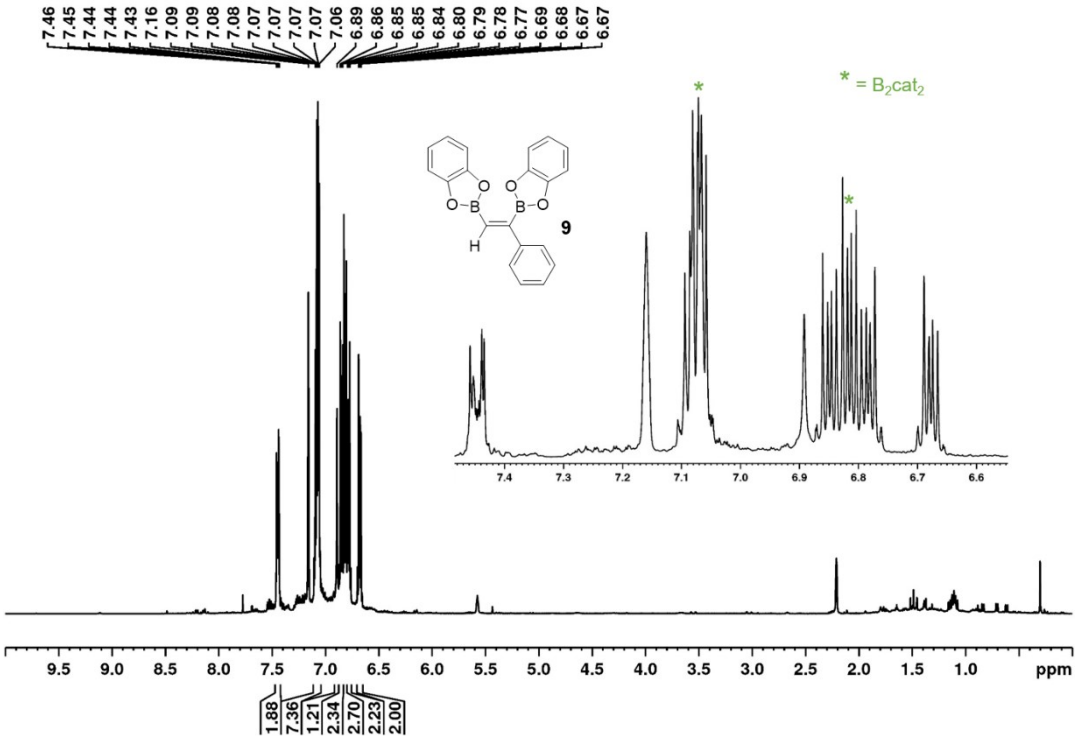


Figure S72. ^{1}H NMR spectrum of **9** from the crude reaction product of the catalysis (400 MHz, 298 K, C_6D_6).

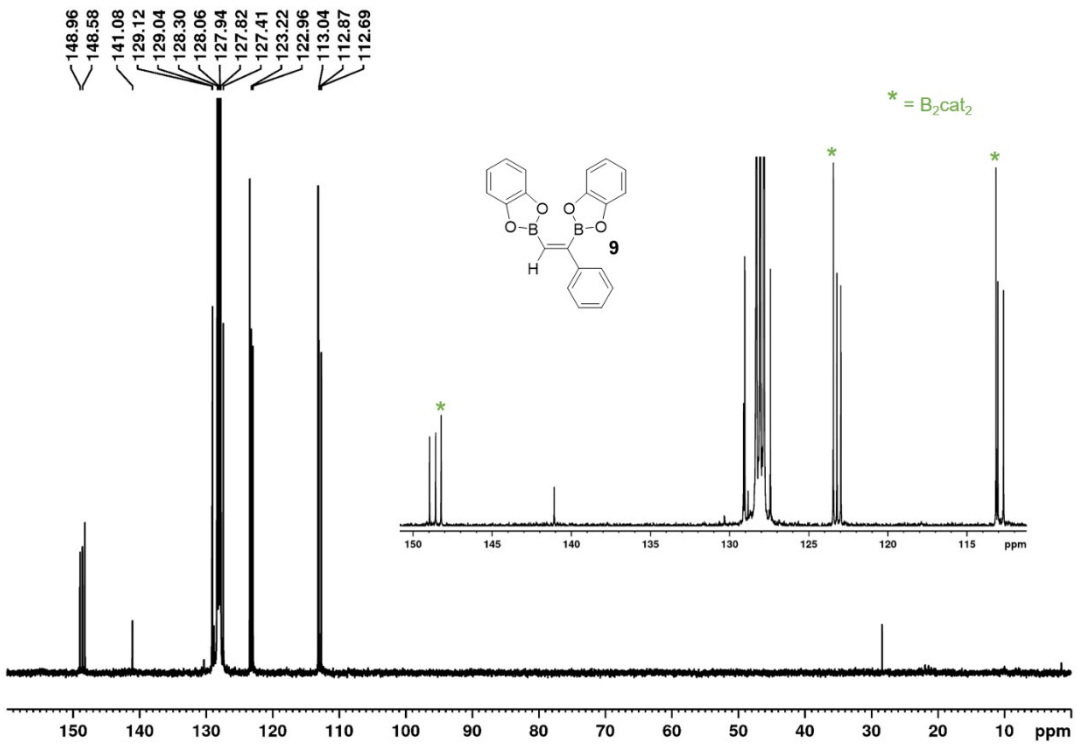


Figure S73. $^{13}C\{^{1}H\}$ NMR spectrum of **9** from the crude reaction product of the catalysis (100 MHz, 298 K, C_6D_6).

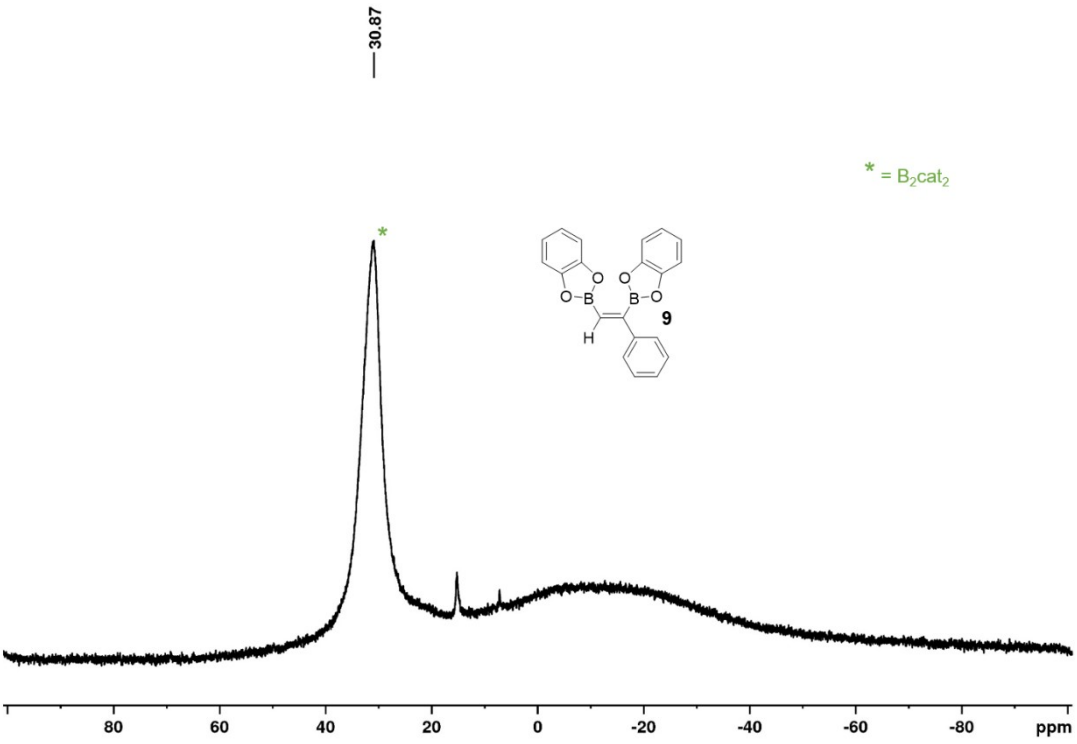


Figure S74. $^{11}B\{^{1}H\}$ NMR spectrum of **9** from the crude reaction product of the catalysis (128 MHz, 298 K, C_6D_6).

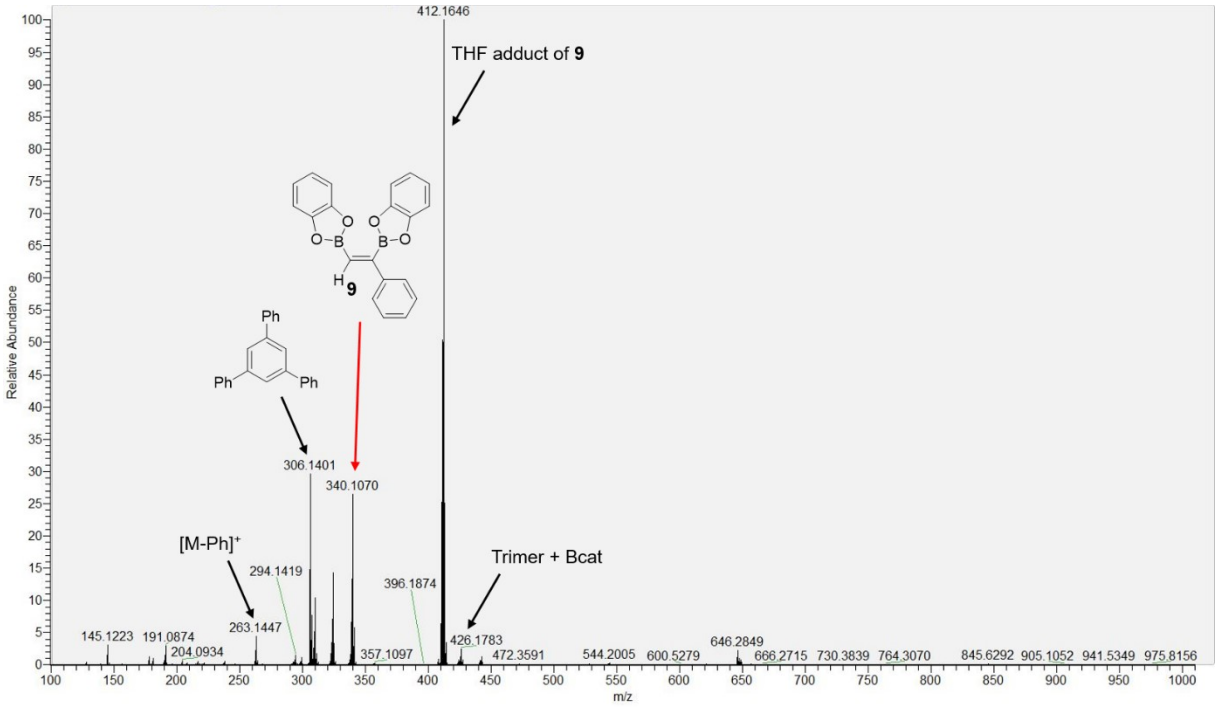


Figure S75. HRMS spectrum of **9** from the crude reaction product of the catalysis (LIFDI, THF).

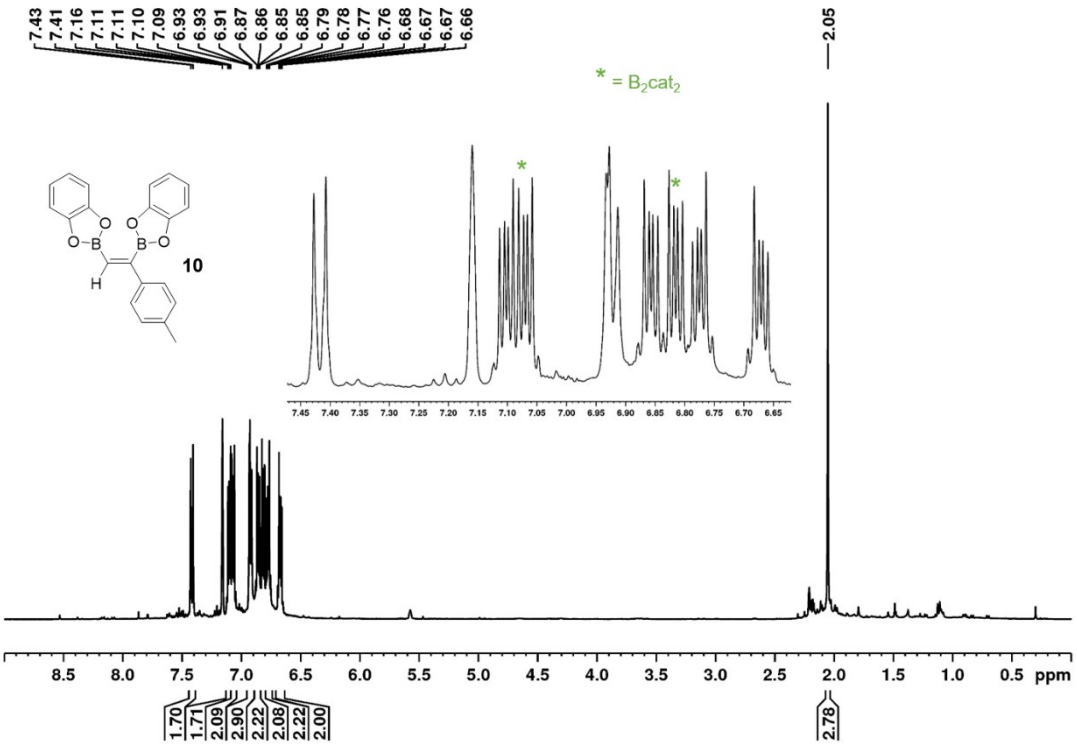


Figure S76. ^{1}H NMR spectrum of **10** from the crude reaction product of the catalysis (400 MHz, 298 K, C_6D_6).

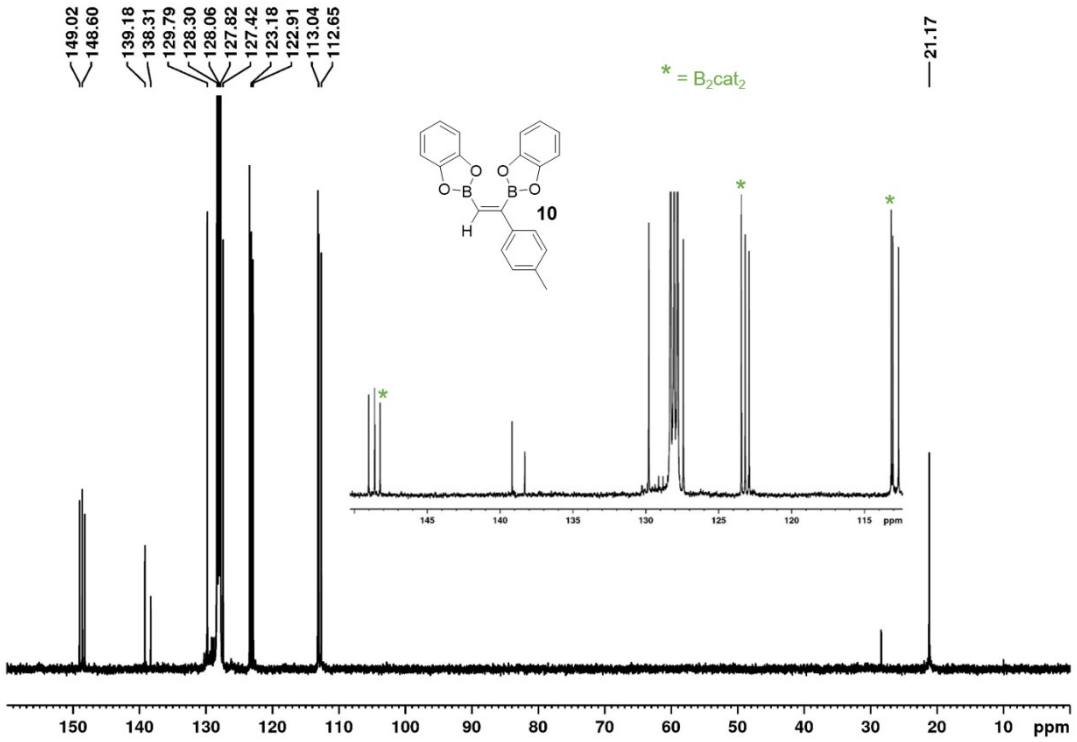


Figure S77. $^{13}C\{^{1}H\}$ NMR spectrum of **10** from the crude reaction product of the catalysis (100 MHz, 298 K, C_6D_6).

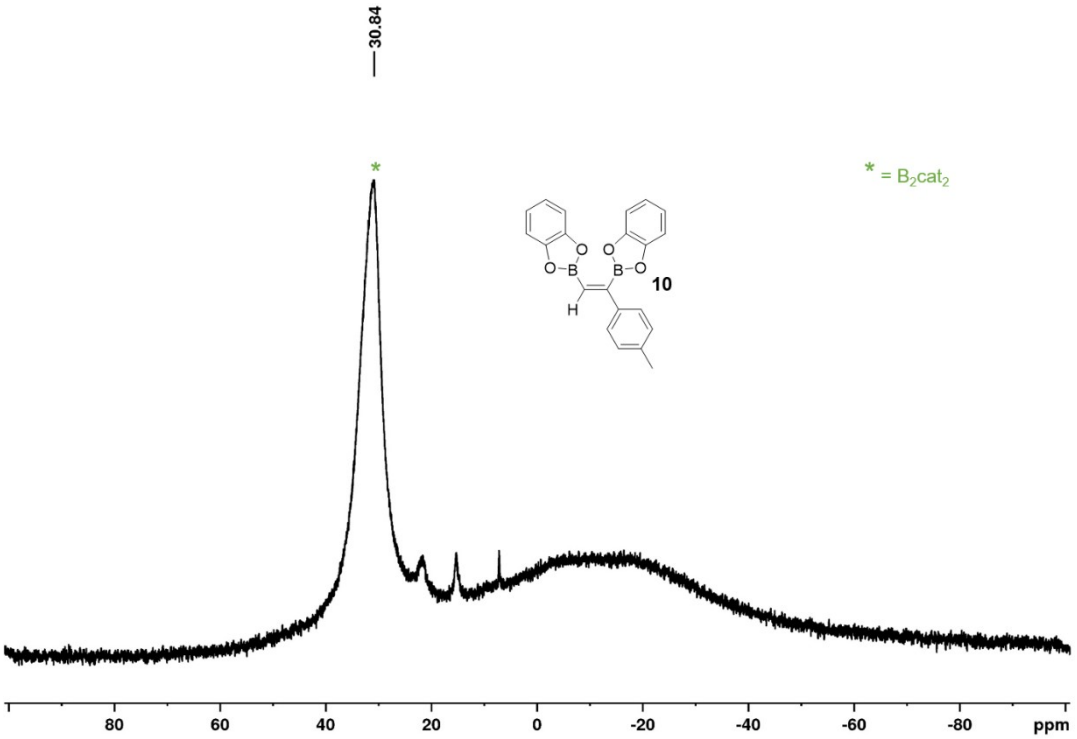


Figure S78. $^{11}B\{^{1}H\}$ NMR spectrum of **10** from the crude reaction product of the catalysis (128 MHz, 298 K, C_6D_6).

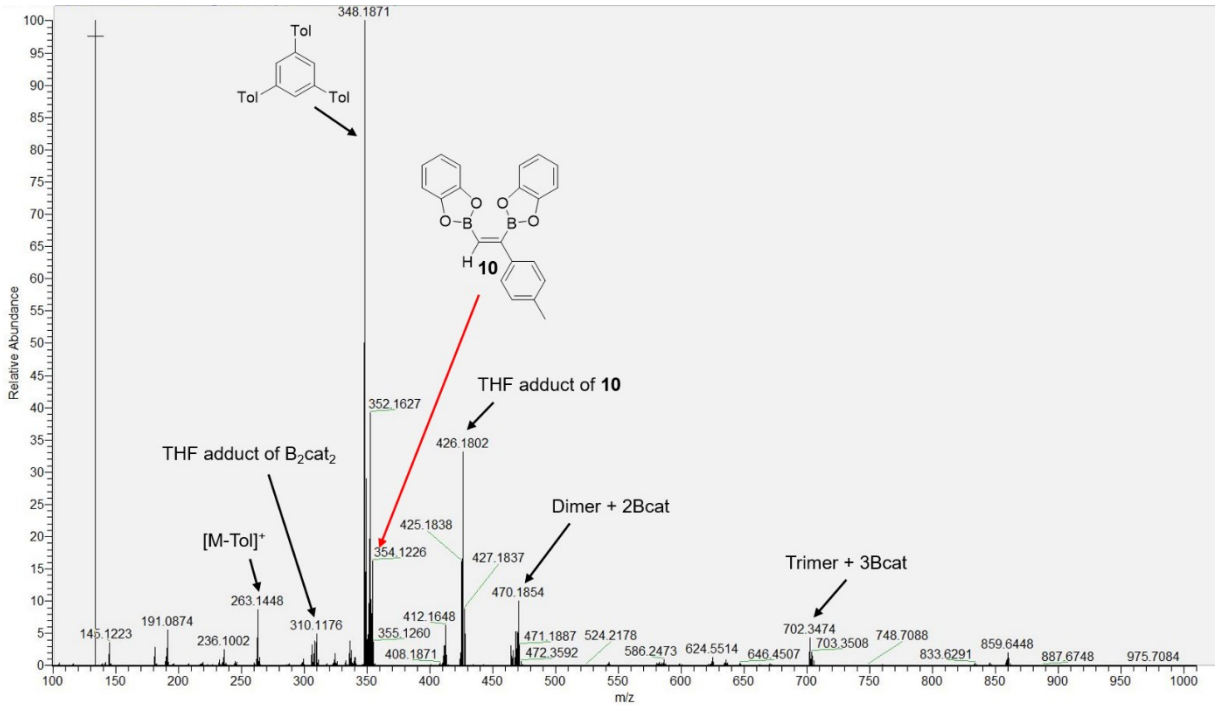


Figure S79. HRMS spectrum of **10** from the crude reaction product of the catalysis (LIFDI, THF).

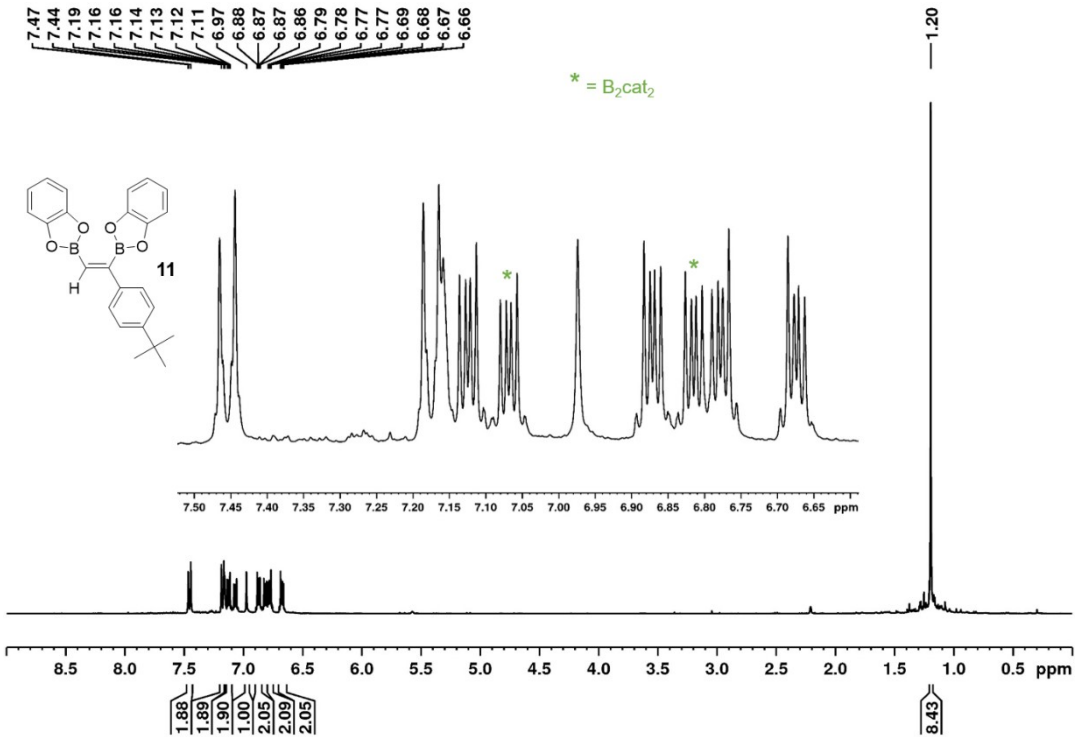


Figure S80. ^{1}H NMR spectrum of **11** from the crude reaction product of the catalysis (400 MHz, 298 K, C_6D_6).

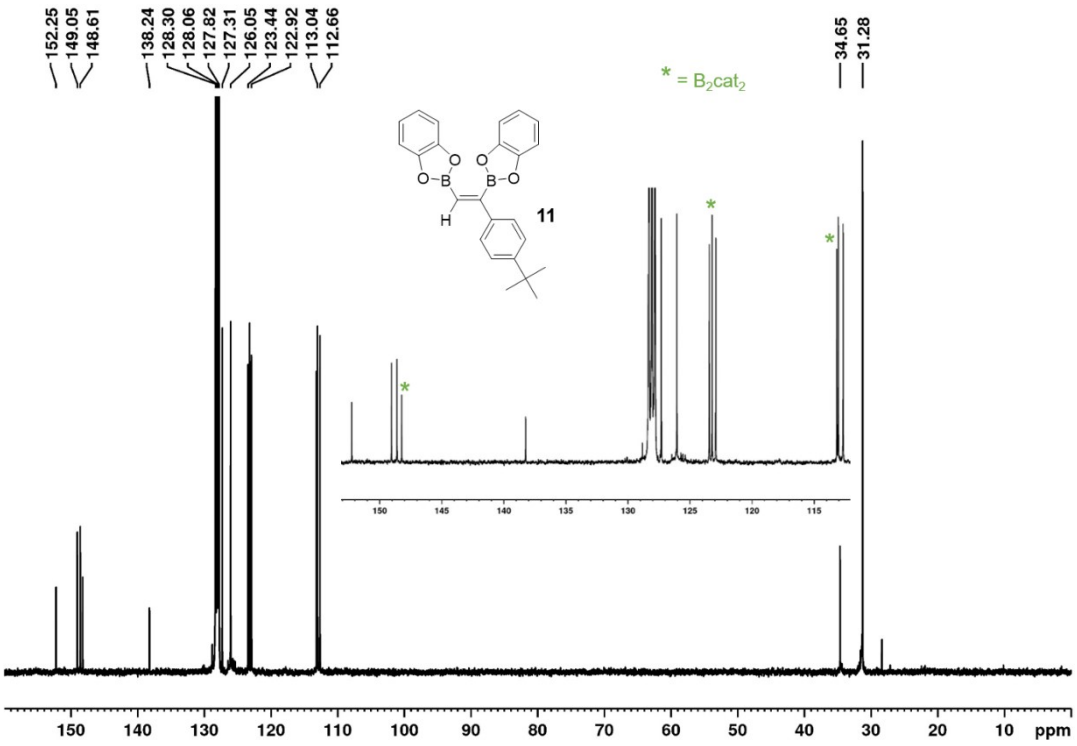


Figure S81. $^{13}C\{^{1}H\}$ NMR spectrum of **11** from the crude reaction product of the catalysis (100 MHz, 298 K, C_6D_6).

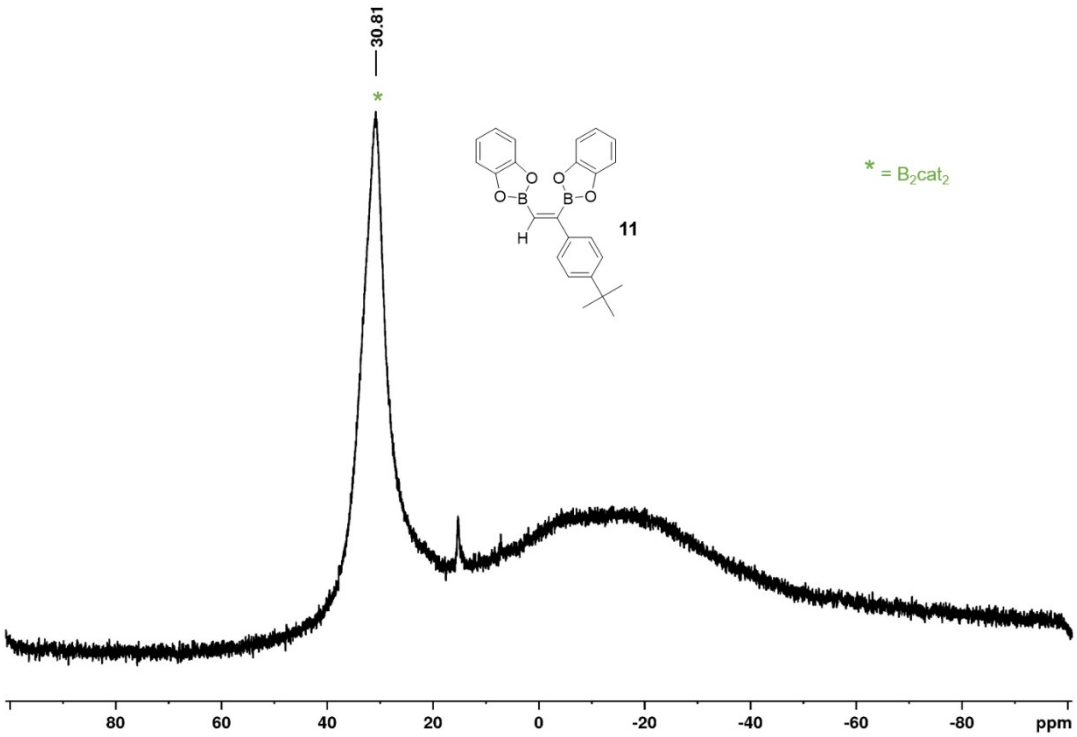


Figure S82. $^{11}B\{^{1}H\}$ NMR spectrum of **11** from the crude reaction product of the catalysis (128 MHz, 298 K, C_6D_6).

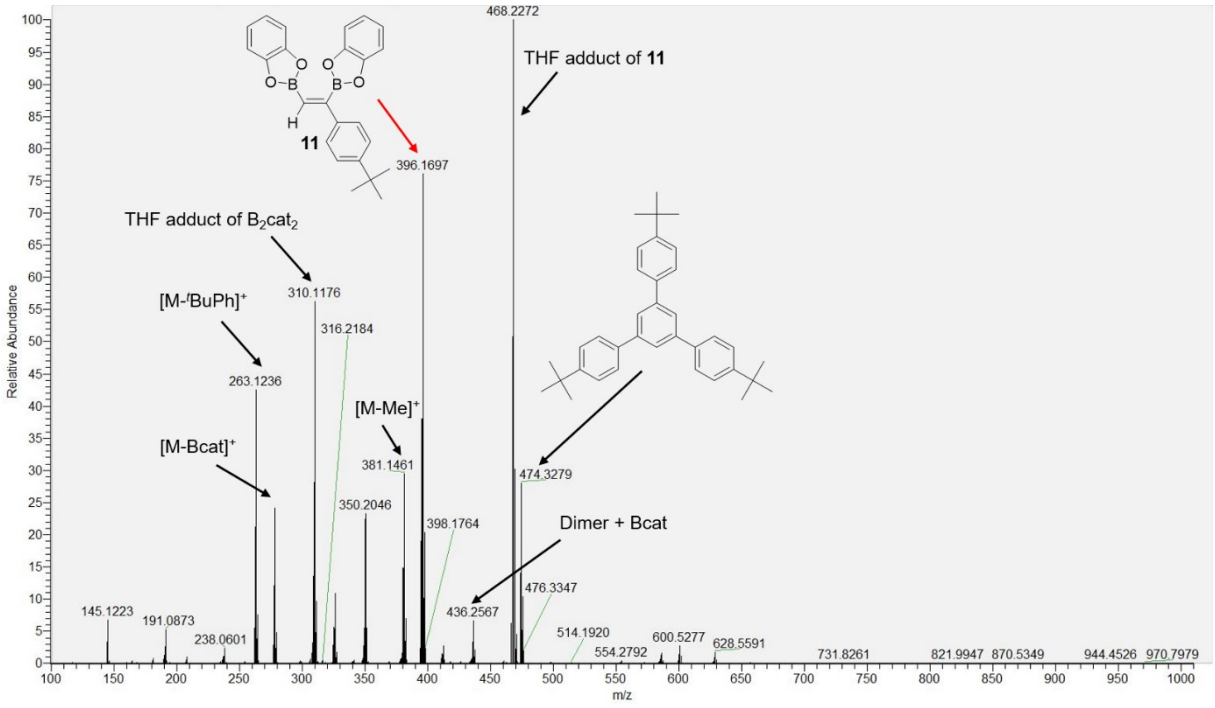


Figure S83. HRMS spectrum of **11** from the crude reaction product of the catalysis (LIFDI, THF).

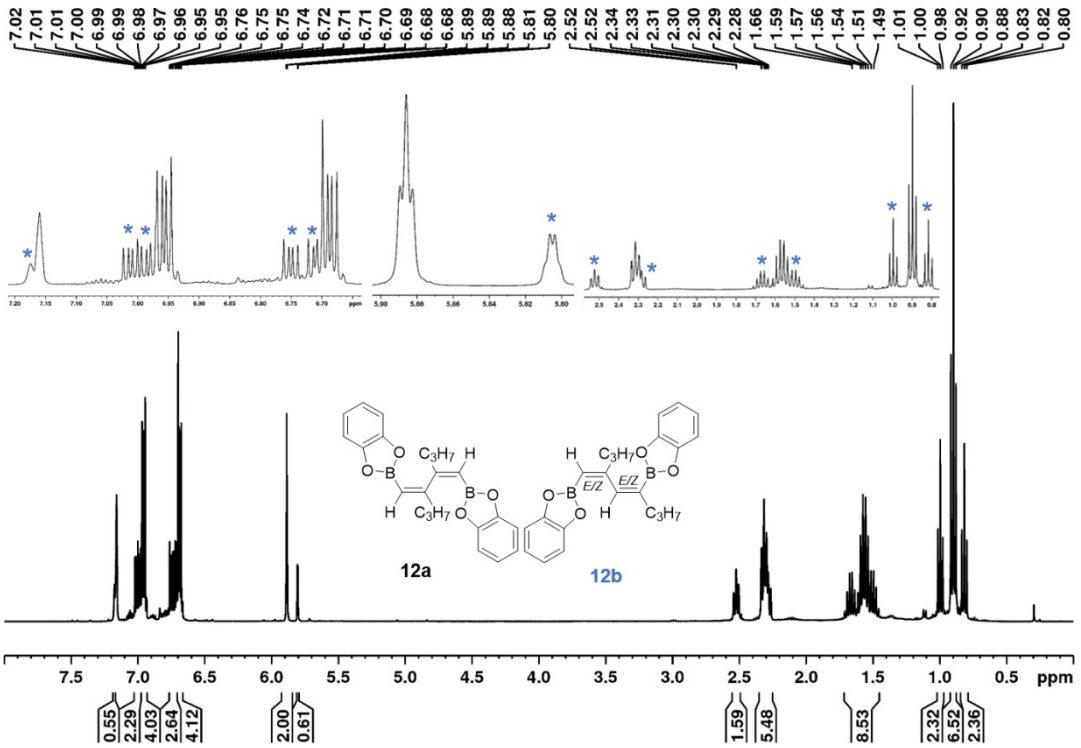


Figure S84. ^{1}H NMR spectrum of **12a** and **12b** from the crude reaction product of the catalysis (400 MHz, 298 K, C_6D_6).

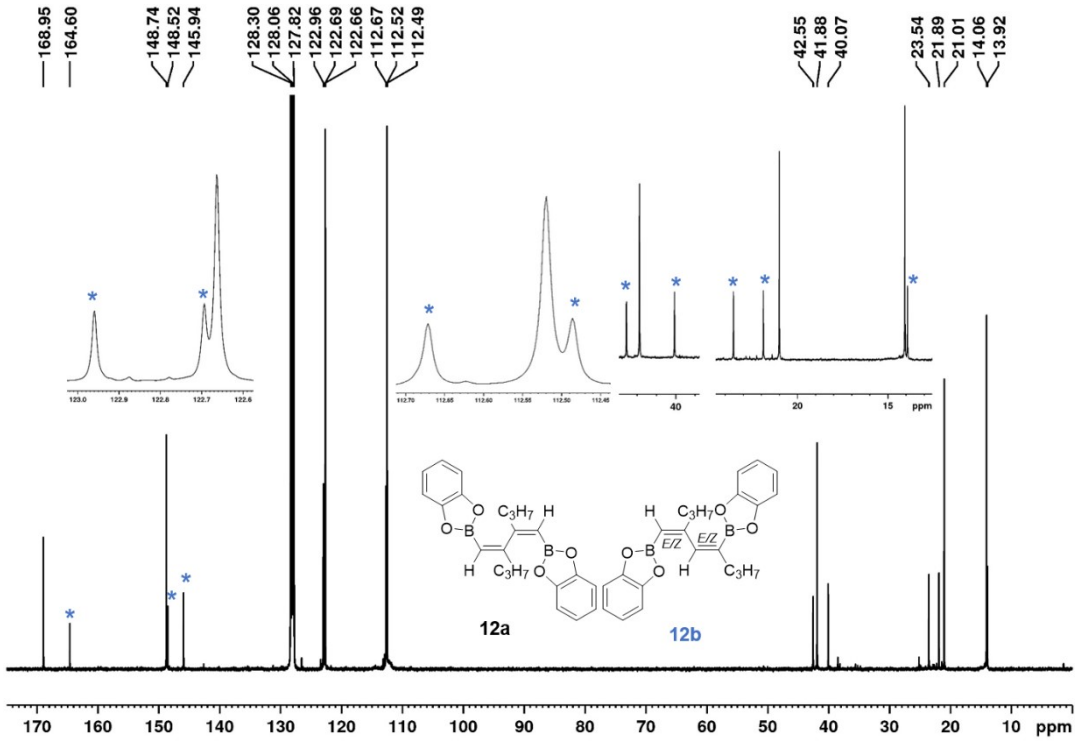


Figure S85. $^{13}C\{^{1}H\}$ NMR spectrum of **12a** and **12b** from the crude reaction product of the catalysis (100 MHz, 298 K, C_6D_6).

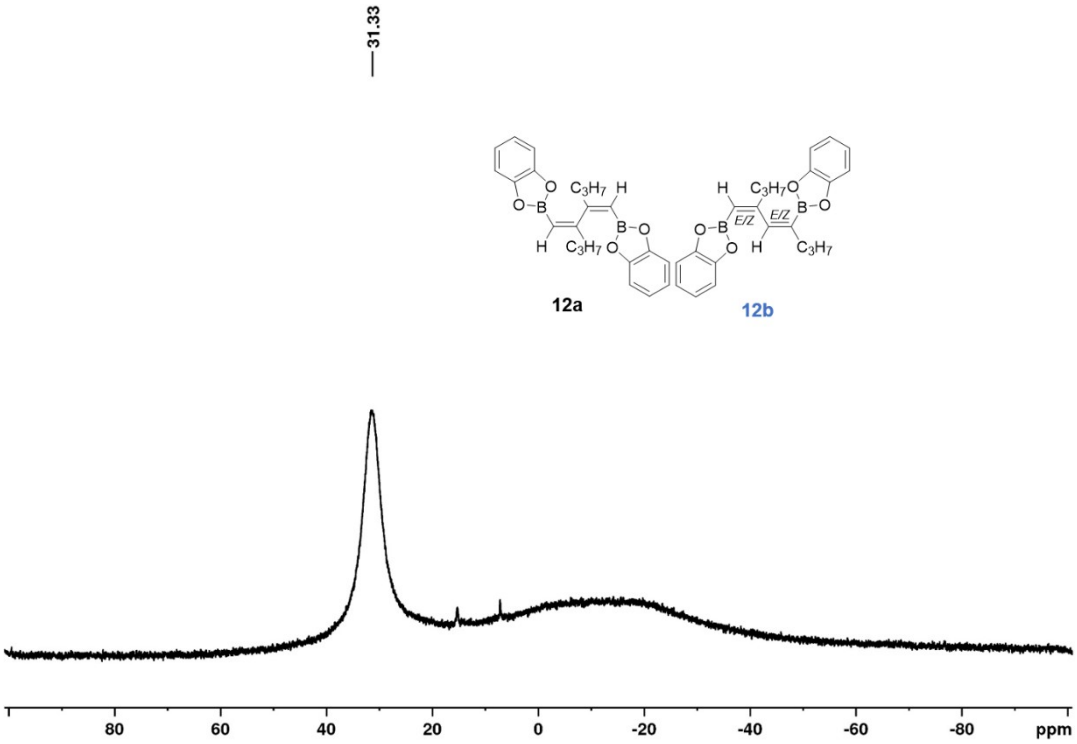


Figure S86. $^{11}B\{^{1}H\}$ NMR spectrum of **12a** and **12b** from the crude reaction product of the catalysis (128 MHz, 298 K, C_6D_6).

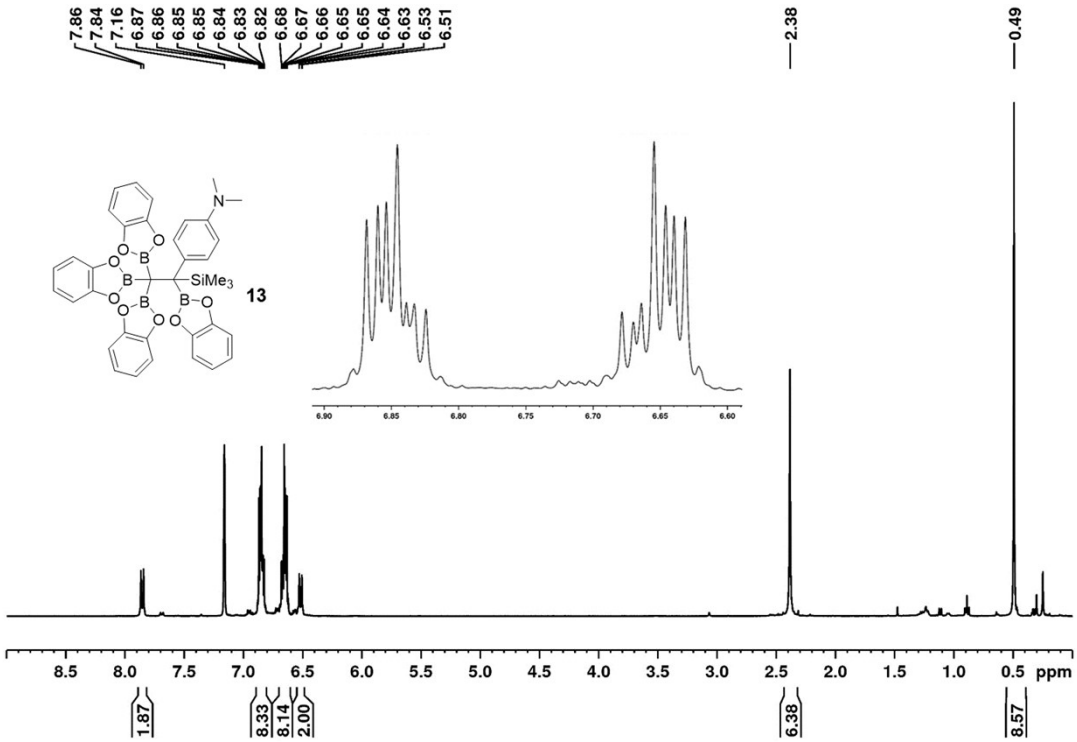


Figure S87. ^{1}H NMR spectrum of isolated **13** (400 MHz, 298 K, C_6D_6).

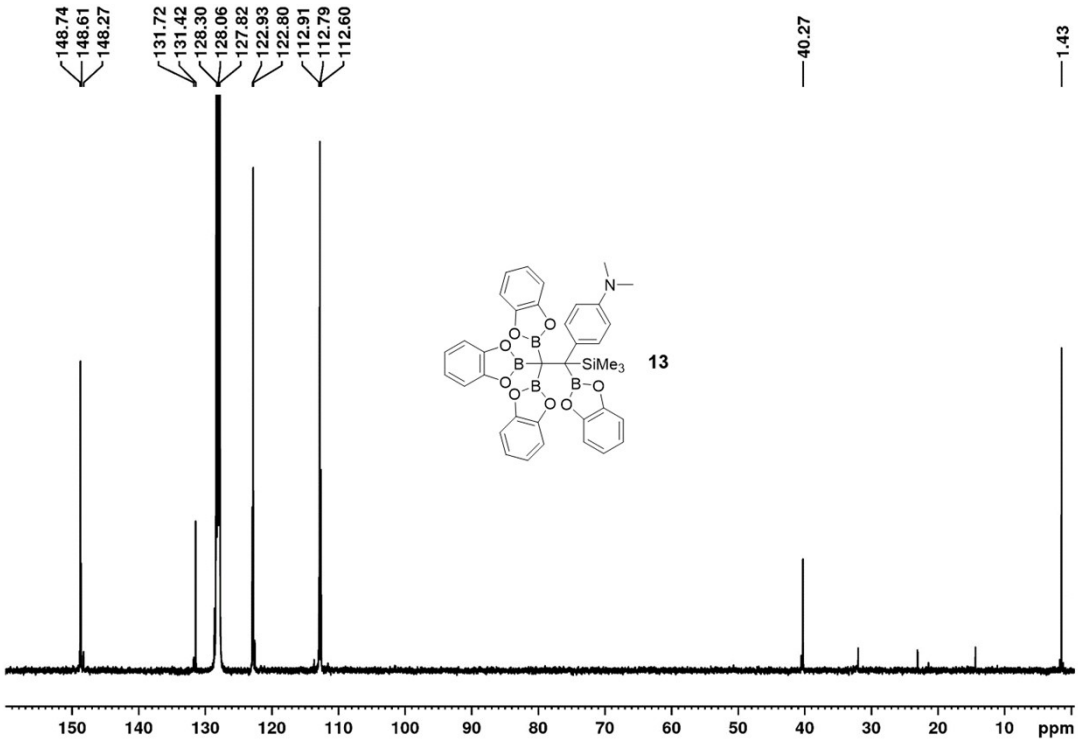


Figure S88. $^{13}C\{^{1}H\}$ NMR spectrum of isolated **13** (100 MHz, 298 K, C_6D_6).

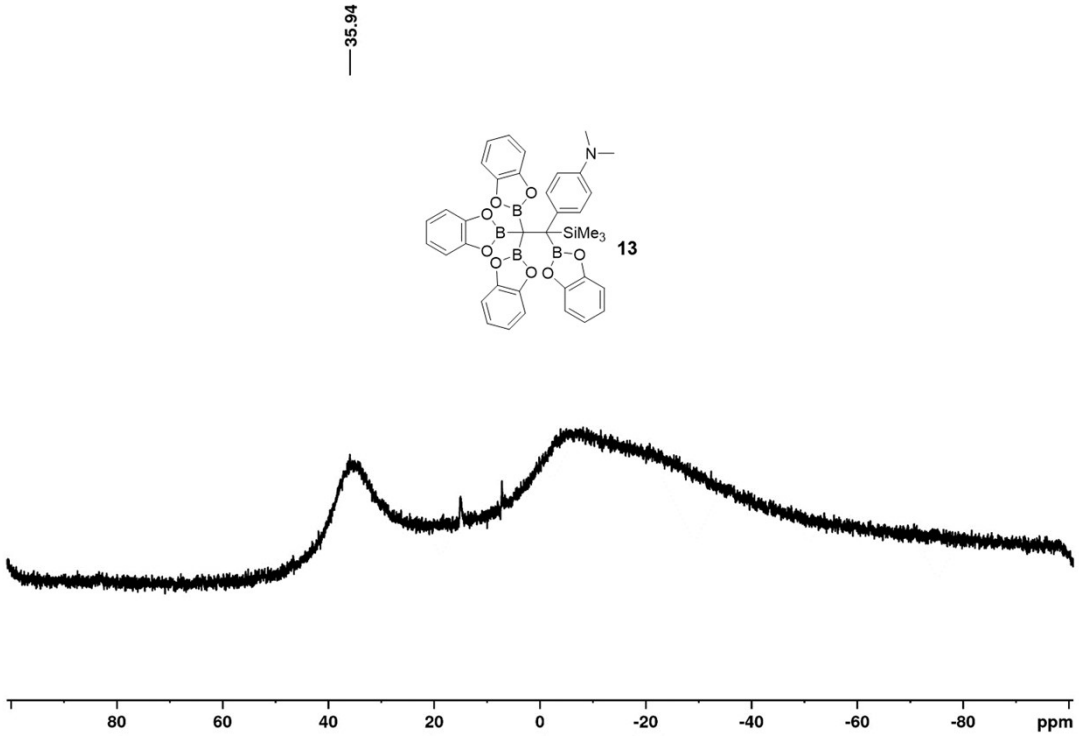


Figure S89. $^{11}B\{^{1}H\}$ NMR spectrum of isolated **13** (128 MHz, 298 K, C_6D_6).

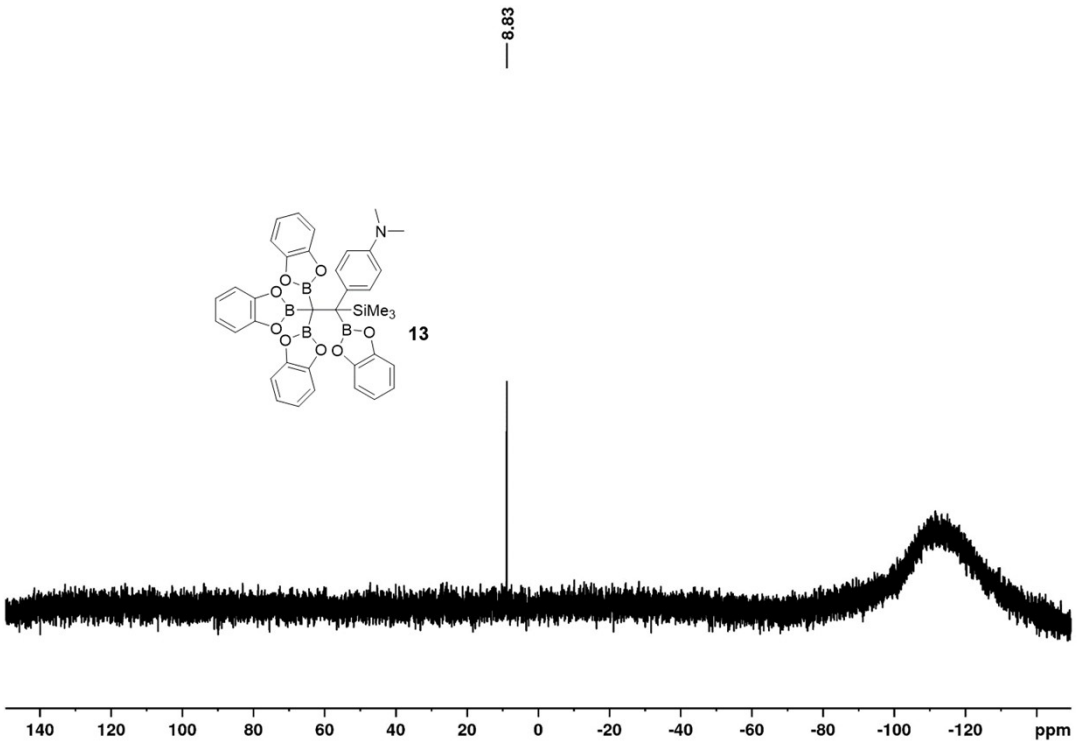


Figure S90. ^{29}Si NMR spectrum of isolated **13** (79.5 MHz, 298 K, C_6D_6).

5) Computational Details

Geometry optimizations were performed using the PBE0[11] functional. Nickel was described with the def2-TZVP[12] basis set while on all other atoms the def2-SVP[12] basis set was used. Dispersion corrections were considered in the geometry optimizations by using Grimme's D3[13] correction together with the Becke-Johnson (BJ) damping function.[14] All stationary points were fully characterized by analytical frequency calculations as either minima (only positive eigenvalues) or transition states (one negative eigenvalue). The connectivity of the transition states was analyzed by geometry optimizations following the imaginary frequency mode and additional intrinsic reaction coordinate (IRC)[15] calculations. Solvation corrections were included from using the solvent model based on density (SMD[16]; solvent=benzene; ε=2.2706) from single-point energy calculations at the PBE0-D3(BJ)/def2-TZVPP level. A concentration correction of $\Delta G^{0\rightarrow *}$ = 1.89 kcal mol^{-1} was included in the free energies of all species to account for the change in standard states in going from the gas phase (1 atm) to the condensed phase (1 M), and to describe properly associative/dissociative steps.[17] Mayer bond orders (MBI)[18] were obtained for selected bonds. The bonding situation of **2a** was investigated by inspection of the canonical Kohn-Sham molecular orbitals and by further calculations based on the intrinsic bond orbital (IBO)[19] approach. WBI calculations were done in Multiwfn 3.8.[20] All geometry optimizations and vibrational frequencies were performed in Gaussian 16, revision C.01.[21] The IBO calculations were done in IboView.

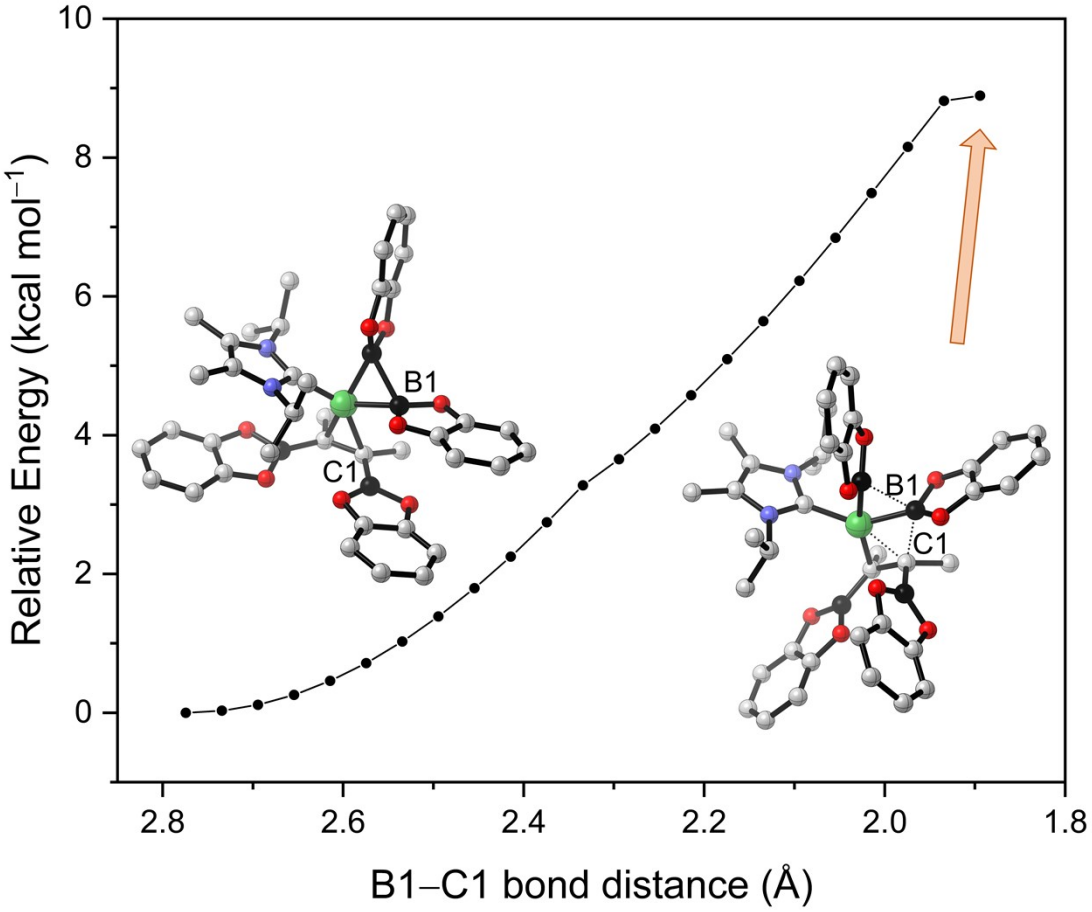


Figure S91. B1–C1 relaxed energy scan at the PBE0-D3(BJ)/def2-SVP/def2-TZVP(Ni) level of theory. The arrow indicates the maximum energy structure in the pathway from **I4** to **I5**.

Table S1. Electronic energy (E) and Gibbs free energy (G) of the systems investigated herein. Values are in Hartree. Level of theory: SMD(benzene)/PBE0-D3(BJ)/def2-TZVPP//PBE0-D3(BJ)/def2-SVP/def2-TZVP(Ni). See text for details regarding the calculation of G.

	E	G
C_2Me_2	-155.763640	-155.790460
[Ni(^{i}Pr$_2$Im^{Me})$_2$] (NHC)	-539.988074	-540.026252
B_2cat_2	-812.109967	-812.148427
8	-967.948536	-967.995335
8a	-1780.109125	-1780.172195
8b	-1123.768043	-1123.821181
NHC-B_2cat_2	-1352.141328	-1352.200756
NHC-prod	-1507.984856	-1508.047195
1	-2588.149720	-2588.215655
2a	-3400.313140	-3400.391908
14a	-2743.960759	-2744.027999
15a	-3556.162611	-3556.242264
I1	-3556.119806	-3556.202950
I2	-3016.119206	-3016.184582
I3	-3171.913737	-3171.982533
I4	-3828.261855	-3828.341587
I5	-3828.249549	-3828.332686
I6	-3171.908729	-3171.979329
I7	-3171.929336	-3172.001838
I8	-3171.919925	-3171.989087
I9	-3016.119201	-3016.184569
I10	-3171.901116	-3171.974517
A	-3556.084797	-3556.167898
B	-3556.094609	-3556.175084
C	-3171.929164	-3171.929164
TS1	-3556.072754	-3556.154577
TS1'	-3556.042921	-3556.125381
TS2	-3556.093591	-3556.174123
TS3	-3556.096861	-3556.179445
TS4	-3171.880315	-3171.949799
TS5	-3171.864472	-3171.935271

6) Cartesian Coordinates of the DFT-Optimized Geometries

Coordinates in angstrom.

C_2Me_2

C	0.606042000	-0.000003000	0.000000000
C	-0.606077000	0.000003000	0.000000000
C	-2.060715000	-0.000002000	0.000000000
H	-2.460464000	0.419997000	-0.936607000
H	-2.460447000	-1.021138000	0.104577000
H	-2.460474000	0.601134000	0.832026000
C	2.060735000	0.000001000	0.000000000
H	2.460477000	1.021126000	-0.104803000
H	2.460493000	-0.419796000	0.936710000
H	2.460503000	-0.601325000	-0.831903000

$[Ni(^iPr_2Im^{Me})_2]$ (NHC)

N	1.064035000	-0.404622000	-0.104670000
N	-1.064047000	-0.404587000	-0.104949000
C	-0.000003000	-1.242257000	-0.212603000
C	0.684218000	0.923585000	0.075369000
C	-0.684242000	0.923613000	0.075160000
C	2.416704000	-0.954624000	-0.130532000
H	2.231078000	-2.010696000	-0.375283000
C	3.079373000	-0.906779000	1.240342000
C	3.279474000	-0.361387000	-1.236135000
H	2.744552000	-0.381898000	-2.196921000
H	3.580357000	0.675497000	-1.027432000
H	4.200491000	-0.953398000	-1.345349000
H	3.304225000	0.121585000	1.561580000
H	4.029472000	-1.461840000	1.220492000
H	2.425745000	-1.368347000	1.994488000
C	-2.416711000	-0.954637000	-0.130523000
H	-2.231062000	-2.010712000	-0.375257000
C	-3.279750000	-0.361431000	-1.235918000
C	-3.079125000	-0.906754000	1.240437000
H	-2.425260000	-1.368107000	1.994500000
H	-3.304193000	0.121589000	1.561569000
H	-4.029055000	-1.462118000	1.220809000
H	-3.580480000	0.675434000	-1.026958000
H	-4.200863000	-0.953338000	-1.344834000
H	-2.745176000	-0.381883000	-2.196900000
C	-1.607032000	2.085078000	0.193532000
H	-2.095446000	2.331611000	-0.763116000
H	-2.402112000	1.915488000	0.934268000
H	-1.049100000	2.975949000	0.512000000
C	1.607081000	2.085047000	0.193594000
H	2.402850000	1.915061000	0.933510000
H	2.094634000	2.332118000	-0.763372000
H	1.049505000	2.975745000	0.513213000

B_2cat_2

B	-0.845966000	0.001048000	-0.000029000
B	0.845960000	0.000983000	-0.000077000
O	-1.636340000	-1.136639000	0.000206000
O	-1.637318000	1.137988000	-0.000328000
O	1.636398000	-1.136653000	-0.000320000
O	1.637267000	1.137962000	0.000209000

C	-2.925903000	-0.697769000	0.000178000
C	-4.100106000	-1.431568000	0.000378000
C	-2.926507000	0.697990000	-0.000148000
C	-5.292687000	-0.700494000	0.000226000
H	-4.085346000	-2.522268000	0.000660000
C	-4.101291000	1.430864000	-0.000328000
C	-5.293278000	0.698841000	-0.000128000
H	-6.244835000	-1.235314000	0.000398000
H	-4.087219000	2.521575000	-0.000633000
H	-6.245891000	1.232840000	-0.000265000
C	2.926482000	0.698039000	0.000164000
C	4.101295000	1.430875000	0.000381000
C	2.925921000	-0.697722000	-0.000170000
C	5.293266000	0.698829000	0.000231000
H	4.087352000	2.521587000	0.000673000
C	4.100109000	-1.431557000	-0.000328000
C	5.292693000	-0.700509000	-0.000121000
H	6.245872000	1.232835000	0.000408000
H	4.085210000	-2.522256000	-0.000627000
H	6.244854000	-1.235317000	-0.000247000

8

C	-1.041492000	2.543320000	-0.000028000
C	0.310293000	2.677582000	-0.000009000
B	-1.615600000	1.113190000	-0.000150000
O	-0.821005000	-0.029663000	-0.000444000
O	-2.957353000	0.761523000	0.000156000
C	-1.677199000	-1.088171000	-0.000298000
C	-2.987153000	-0.602573000	0.000057000
C	-1.391247000	-2.440771000	-0.000439000
C	-4.077731000	-1.453591000	0.000297000
C	-2.489877000	-3.309224000	-0.000210000
H	-0.360365000	-2.798663000	-0.000716000
C	-3.801847000	-2.826811000	0.000145000
H	-5.097259000	-1.065619000	0.000591000
H	-2.316005000	-4.387361000	-0.000316000
H	-4.632536000	-3.535737000	0.000330000
B	1.234052000	1.413373000	-0.000042000
O	1.741410000	0.811385000	1.141288000
O	1.741791000	0.811534000	-1.141255000
C	2.480498000	-0.243049000	0.698791000
C	2.480734000	-0.242965000	-0.698640000
C	3.149686000	-1.208662000	1.429686000
C	3.150167000	-1.208468000	-1.429450000
C	3.829207000	-2.191491000	0.699061000
H	3.139293000	-1.198070000	2.520489000
C	3.829443000	-2.191399000	-0.698732000
H	3.140144000	-1.197714000	-2.520254000
H	4.369446000	-2.975027000	1.234795000
H	4.369872000	-2.974857000	-1.234386000
C	1.017920000	4.000742000	0.000068000
H	1.676180000	4.086349000	0.881589000
H	1.676593000	4.086257000	-0.881149000
H	0.332550000	4.858644000	-0.000150000
C	-1.994633000	3.711501000	0.000045000
H	-1.854533000	4.351717000	0.886131000
H	-1.855613000	4.350875000	-0.886831000
H	-3.039386000	3.372333000	0.000805000

8a

O	1.567454000	-1.198080000	0.656051000
B	0.241389000	-1.470760000	0.345808000
O	-2.574411000	-0.068805000	-0.905607000
B	-1.872201000	-1.263388000	-1.009954000
O	-2.744939000	-2.337401000	-0.982571000
O	-0.447530000	-1.879784000	1.473663000
C	1.676217000	-1.363203000	2.004850000
C	0.442113000	-1.784035000	2.505167000
C	-3.888921000	-0.412123000	-0.781449000
C	-3.992131000	-1.803469000	-0.830746000
C	-5.212532000	-2.446704000	-0.733032000
H	-5.282535000	-3.534560000	-0.772117000
C	-0.314086000	-1.339688000	-1.119322000
C	0.107613000	-2.607394000	-1.893997000
H	-0.270879000	-2.590940000	-2.927427000
H	-0.307743000	-3.507294000	-1.416345000
H	1.200668000	-2.709080000	-1.938194000
C	-6.340569000	-1.630698000	-0.579828000
H	-7.325406000	-2.095337000	-0.497144000
C	-4.993638000	0.404381000	-0.629142000
H	-4.891455000	1.489749000	-0.586898000
C	-6.234001000	-0.238031000	-0.528220000
H	-7.136774000	0.363987000	-0.405202000
C	0.248712000	-2.034051000	3.851422000
H	-0.719608000	-2.362600000	4.231382000
C	1.354378000	-1.841081000	4.689783000
H	1.247644000	-2.024449000	5.761070000
C	2.774640000	-1.169961000	2.821064000
H	3.729487000	-0.836787000	2.411412000
C	2.588117000	-1.418829000	4.186715000
H	3.426061000	-1.277803000	4.872697000
B	1.815200000	0.085862000	-1.596131000
O	2.721111000	-0.835110000	-2.103543000
C	3.954583000	-0.378924000	-1.745900000
C	5.194362000	-0.951998000	-1.963679000
H	5.292589000	-1.902322000	-2.490215000
C	6.304180000	-0.253474000	-1.471668000
H	7.303050000	-0.669777000	-1.618761000
C	6.160688000	0.961723000	-0.796355000
H	7.049556000	1.477049000	-0.426124000
C	4.900503000	1.534771000	-0.583136000
H	4.772722000	2.482331000	-0.057926000
C	3.811545000	0.836331000	-1.072633000
O	2.487821000	1.147839000	-1.005024000
C	-0.149030000	0.203298000	-3.196606000
H	-1.242599000	0.149316000	-3.323645000
H	0.308902000	-0.555883000	-3.847686000
H	0.166821000	1.191307000	-3.563627000
C	0.244807000	0.009209000	-1.722019000
B	-0.286463000	1.186023000	-0.833600000
O	-0.340286000	1.093757000	0.553755000
C	-0.875017000	2.270386000	0.982573000
C	-1.171112000	2.676954000	2.269969000
H	-0.979673000	2.025678000	3.124112000
C	-1.724514000	3.956153000	2.410798000
H	-1.976162000	4.320481000	3.409114000

C	-1.961168000	4.773901000	1.302767000
H	-2.393879000	5.765551000	1.451607000
C	-1.655222000	4.350926000	0.002464000
H	-1.833795000	4.980179000	-0.870597000
C	-1.110307000	3.086458000	-0.126968000
O	-0.727702000	2.426030000	-1.257642000

8b

C	-1.599115000	0.027388000	-0.514542000
C	-0.731958000	-0.771130000	0.157123000
B	-3.125666000	0.041326000	-0.275617000
O	-3.960175000	0.895115000	-0.993142000
O	-3.884365000	-0.718326000	0.612362000
C	-5.222929000	0.659136000	-0.547178000
C	-5.177968000	-0.330073000	0.437159000
C	-6.413503000	1.246082000	-0.938439000
C	-6.318996000	-0.779867000	1.077271000
C	-7.574894000	0.798423000	-0.297136000
H	-6.435508000	2.018124000	-1.708837000
C	-7.528851000	-0.191922000	0.688216000
H	-6.269176000	-1.553517000	1.844782000
H	-8.537438000	1.233719000	-0.574054000
H	-8.455928000	-0.515424000	1.166239000
B	3.125641000	0.041972000	0.275361000
O	3.960041000	0.897363000	0.991105000
O	3.884481000	-0.719709000	-0.610750000
C	5.222859000	0.660389000	0.545864000
C	5.178058000	-0.331039000	-0.436243000
C	6.413372000	1.248228000	0.935974000
C	6.319182000	-0.782273000	-1.075170000
C	7.574860000	0.799133000	0.295853000
H	6.435257000	2.022011000	1.704627000
C	7.528974000	-0.193439000	-0.687264000
H	6.269484000	-1.557660000	-1.840933000
H	8.537360000	1.235062000	0.571927000
H	8.456126000	-0.518011000	-1.164414000
C	-1.099095000	-1.749472000	1.232973000
H	-0.606235000	-1.459519000	2.176322000
H	-2.178410000	-1.818609000	1.402987000
H	-0.712193000	-2.751707000	0.984880000
C	-1.123307000	0.996489000	-1.568189000
H	-1.441454000	2.023467000	-1.327132000
H	-0.029715000	0.998155000	-1.671556000
H	-1.567904000	0.766285000	-2.550224000
C	1.599091000	0.028374000	0.514276000
C	0.731977000	-0.771360000	-0.156008000
C	1.099133000	-1.751491000	-1.230222000
H	0.712789000	-2.753461000	-0.980172000
H	0.605802000	-1.463436000	-2.173895000
H	2.178415000	-1.820529000	-1.400480000
C	1.123180000	0.999286000	1.566203000
H	1.440530000	2.025985000	1.322888000
H	0.029640000	1.000474000	1.670112000
H	1.568414000	0.771399000	2.548488000

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C	3.376208000	-1.100510000	-0.894652000
C	4.515386000	-1.073006000	-1.680430000

O	2.069375000	-1.101582000	-1.271928000
C	3.444489000	-1.129667000	0.499843000
N	-0.822454000	1.536335000	-1.013654000
C	-0.612226000	0.699992000	0.022915000
C	-0.856459000	2.851818000	-0.570233000
C	-0.977202000	1.068321000	-2.403486000
B	1.312820000	-1.139883000	-0.097106000
O	2.179844000	-1.150626000	1.001080000
B	-0.395531000	-0.963432000	-0.009979000
C	-4.490074000	-2.812349000	0.882660000
C	-4.555644000	-2.814081000	-0.507315000
C	-3.328103000	-2.390691000	1.552886000
H	-5.352669000	-3.143924000	1.465541000
C	-3.460817000	-2.394935000	-1.284126000
C	-2.320052000	-1.976027000	-0.620695000
H	-3.495712000	-2.402034000	-2.375558000
N	-0.471208000	1.477464000	1.116674000
C	-0.170964000	0.929825000	2.452777000
C	-1.400913000	0.955761000	3.346103000
C	1.070207000	1.557582000	3.068068000
H	0.056003000	-0.123911000	2.266462000
C	-0.564181000	3.957346000	1.728635000
C	-0.635560000	2.813758000	0.780950000
H	-1.099107000	3.752402000	2.665338000
H	-1.024409000	4.843609000	1.272626000
H	0.473327000	4.221375000	1.985774000
C	-1.070727000	4.047843000	-1.427458000
H	-0.162826000	4.328744000	-1.983639000
H	-1.348713000	4.905487000	-0.801033000
H	-1.876549000	3.897246000	-2.157558000
C	-2.421587000	1.179229000	-2.867640000
H	-3.087996000	0.651941000	-2.169701000
H	-2.523191000	0.701728000	-3.853254000
H	-2.765382000	2.219954000	-2.965925000
C	0.039766000	1.704145000	-3.338303000
H	-0.163254000	2.762156000	-3.554543000
H	0.021715000	1.164809000	-4.296419000
H	1.055096000	1.611950000	-2.925515000
O	-1.048839000	-1.542627000	1.200028000
C	-2.253691000	-1.973168000	0.785491000
C	4.653918000	-1.131617000	1.172810000
C	5.812573000	-1.100977000	0.386562000
H	4.692604000	-1.158990000	2.262913000
O	-1.155692000	-1.550672000	-1.146917000
C	5.744618000	-1.072541000	-1.009197000
H	6.789171000	-1.102180000	0.875646000
H	-3.261341000	-2.394405000	2.642830000
H	1.903284000	1.558458000	2.350310000
H	1.378700000	0.947572000	3.929210000
H	0.909880000	2.581552000	3.432120000
H	-0.753968000	-0.002068000	-2.344728000
H	-1.724941000	1.976922000	3.597991000
H	-1.177715000	0.433969000	4.288141000
H	-2.233243000	0.429693000	2.857780000
H	6.669263000	-1.051933000	-1.590208000
H	4.448674000	-1.055052000	-2.769338000
H	-5.468804000	-3.147340000	-1.006088000

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C	0.334804000	-0.437095000	-2.281888000
C	-0.950568000	-0.850531000	-2.346178000
B	0.642099000	0.382826000	-0.956471000
O	0.857286000	1.846608000	-1.103874000
O	-0.657019000	0.325613000	-0.136369000
C	0.084467000	2.462236000	-0.195121000
C	-0.825045000	1.580436000	0.399159000
C	0.105567000	3.798933000	0.178383000
C	-1.729689000	1.977862000	1.360571000
C	-0.807703000	4.218600000	1.156337000
H	0.806069000	4.493236000	-0.289340000
C	-1.708700000	3.329139000	1.738467000
H	-2.440742000	1.270057000	1.790000000
H	-0.811783000	5.266841000	1.464553000
H	-2.412870000	3.683758000	2.493796000
B	-1.875978000	-0.461519000	-1.119334000
O	-2.381533000	-1.521204000	-0.269598000
O	-2.929877000	0.498687000	-1.263893000
C	-3.546915000	-1.064032000	0.239524000
C	-3.882058000	0.155727000	-0.369970000
C	-4.354348000	-1.631855000	1.209589000
C	-5.035752000	0.839043000	-0.028973000
C	-5.526938000	-0.942888000	1.560344000
H	-4.084665000	-2.581144000	1.676742000
C	-5.860133000	0.266753000	0.952914000
H	-5.278564000	1.789955000	-0.505967000
H	-6.186821000	-1.364473000	2.322125000
H	-6.777706000	0.782184000	1.246055000
C	-1.583118000	-1.633168000	-3.456520000
H	-2.030764000	-2.562699000	-3.065658000
H	-2.414120000	-1.060373000	-3.901742000
H	-0.886246000	-1.901857000	-4.264202000
C	1.405945000	-0.673649000	-3.301407000
H	1.063769000	-1.241581000	-4.178894000
H	1.816272000	0.284507000	-3.664877000
H	2.256923000	-1.225854000	-2.861532000
C	1.857859000	-0.267999000	-0.025172000
N	3.107520000	0.202551000	0.179378000
C	3.801208000	-0.638846000	1.038972000
C	2.948024000	-1.662366000	1.355285000
N	1.765225000	-1.415081000	0.678067000
C	3.657109000	1.387119000	-0.506770000
H	2.797171000	1.792517000	-1.049785000
C	4.098380000	2.464620000	0.471842000
H	3.296039000	2.683994000	1.191421000
H	4.305495000	3.388855000	-0.087093000
H	5.011597000	2.204963000	1.025350000
C	4.712397000	0.996231000	-1.531500000
H	5.639931000	0.614520000	-1.080757000
H	4.977303000	1.880657000	-2.129159000
H	4.320302000	0.232502000	-2.218485000
C	0.582868000	-2.294351000	0.635444000
H	-0.144704000	-1.745405000	0.040444000
C	-0.051779000	-2.487524000	2.001277000
H	0.517167000	-3.159428000	2.659595000
H	-1.051788000	-2.918349000	1.853826000
H	-0.183927000	-1.518454000	2.503748000

C	0.868839000	-3.580304000	-0.123387000
H	1.291255000	-3.354022000	-1.113151000
H	-0.081938000	-4.109312000	-0.281054000
H	1.549988000	-4.263019000	0.405649000
C	3.178401000	-2.795016000	2.290178000
H	2.851584000	-3.755496000	1.871699000
H	4.248996000	-2.878552000	2.516036000
H	2.649144000	-2.649549000	3.244493000
C	5.176757000	-0.405828000	1.553751000
H	5.885115000	-0.135088000	0.760398000
H	5.201640000	0.392922000	2.311281000
H	5.550928000	-1.320745000	2.030376000

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Ni	0.000000000	0.000866000	-0.000002000
N	-2.702500000	0.961632000	-0.481507000
N	-2.701614000	-0.961462000	0.482090000
C	-1.860671000	0.000471000	0.000275000
C	-4.035832000	0.612926000	-0.303789000
C	-4.035263000	-0.613970000	0.304415000
N	2.702498000	0.961636000	0.481501000
N	2.701615000	-0.961459000	-0.482096000
C	1.860671000	0.000472000	-0.000279000
C	4.035831000	0.612928000	0.303789000
C	4.035264000	-0.613967000	-0.304415000
C	-2.139932000	-2.190218000	1.034153000
H	-2.442795000	-1.559847000	3.083568000
C	-2.334459000	-3.375135000	0.099586000
C	-2.580501000	-2.458621000	2.464654000
H	-3.631283000	-2.776359000	2.536822000
H	-3.390683000	-3.671501000	0.004823000
H	-1.965131000	-3.263941000	2.893403000
H	-1.951615000	-3.129027000	-0.901977000
H	-1.777616000	-4.246714000	0.476768000
H	-1.058585000	-1.951472000	1.048585000
C	-2.141963000	2.190851000	-1.033699000
H	-1.060391000	1.953165000	-1.048026000
C	-2.337746000	3.375724000	-0.099336000
C	-2.582685000	2.458591000	-2.464281000
H	-2.443979000	1.559869000	-3.083047000
H	-3.633795000	2.775211000	-2.536583000
H	-1.968125000	3.264495000	-2.893095000
H	-3.394268000	3.671071000	-0.004734000
H	-1.781727000	4.247789000	-0.476604000
H	-1.954765000	3.130161000	0.902306000
C	2.141959000	2.190853000	1.033695000
H	1.060386000	1.953169000	1.048007000
C	2.337757000	3.375733000	0.099346000
C	2.582663000	2.458579000	2.464285000
H	2.443944000	1.559852000	3.083041000
H	3.633775000	2.775192000	2.536603000
H	1.968102000	3.264483000	2.893098000
H	3.394280000	3.671083000	0.004766000
H	1.781730000	4.247795000	0.476612000
H	1.954794000	3.130180000	-0.902306000
C	2.139936000	-2.190217000	-1.034157000
H	1.058590000	-1.951468000	-1.048604000
C	2.334448000	-3.375125000	-0.099576000

C	2.580523000	-2.458633000	-2.464650000
H	2.442830000	-1.559864000	-3.083573000
H	3.631304000	-2.776378000	-2.536802000
H	1.965153000	-3.263954000	-2.893400000
H	3.390671000	-3.671488000	-0.004792000
H	1.777614000	-4.246709000	-0.476760000
H	1.951586000	-3.129008000	0.901978000
C	-5.197692000	-1.438477000	0.729957000
H	-5.138356000	-2.469924000	0.351080000
H	-5.290648000	-1.496308000	1.826296000
H	-6.128416000	-1.002767000	0.343747000
C	-5.199031000	1.436355000	-0.729316000
H	-5.140588000	2.467891000	-0.350546000
H	-5.292128000	1.493996000	-1.825654000
H	-6.129335000	0.999853000	-0.342988000
C	5.197693000	-1.438473000	-0.729960000
H	5.138331000	-2.469934000	-0.351126000
H	5.290677000	-1.496261000	-1.826299000
H	6.128413000	-1.002793000	-0.343706000
C	5.199030000	1.436359000	0.729315000
H	5.140612000	2.467880000	0.350502000
H	5.292099000	1.494041000	1.825652000
H	6.129338000	0.999828000	0.343029000

2a

C	-2.582718000	2.742231000	-0.808611000
C	-3.451211000	3.507131000	-1.568178000
O	-1.673439000	1.824114000	-1.210141000
C	-2.551423000	2.836146000	0.586782000
N	-2.234179000	-1.852900000	-1.158736000
C	-1.661751000	-1.307746000	-0.050348000
C	-3.529929000	-2.292730000	-0.902575000
C	-1.522770000	-1.850963000	-2.434606000
B	-1.062370000	1.288140000	-0.042304000
O	-1.622558000	1.976003000	1.067090000
Ni	0.000138000	-0.321336000	-0.000099000
B	1.062237000	1.288410000	0.042103000
C	1.662022000	-1.307689000	0.050362000
C	4.301322000	4.381648000	0.876402000
C	4.270977000	4.474087000	-0.516503000
C	3.450299000	3.508131000	1.568136000
H	5.000680000	5.003072000	1.440434000
C	3.386956000	3.696726000	-1.278202000
C	2.550956000	2.836776000	-0.586894000
H	3.348999000	3.762078000	-2.366918000
C	1.523010000	-1.850717000	2.434652000
N	2.234416000	-1.852812000	1.158780000
C	2.055227000	-0.788542000	3.386545000
C	1.430966000	-3.235955000	3.057955000
H	0.507717000	-1.545764000	2.132986000
H	3.078257000	-1.011293000	3.726606000
H	1.413844000	-0.737076000	4.279723000
H	2.048226000	0.195869000	2.898071000
N	-2.619844000	-1.425088000	0.912489000
C	-2.365384000	-0.974138000	2.279070000
C	-2.114976000	-2.150897000	3.212978000
C	-3.422117000	-0.015773000	2.810114000
H	-1.429193000	-0.402205000	2.173979000

C	-5.004103000	-2.300667000	1.201806000
C	-3.770269000	-2.031178000	0.416558000
H	-4.792496000	-2.830624000	2.142274000
H	-5.685386000	-2.933611000	0.618759000
H	-5.546158000	-1.376861000	1.457138000
C	-4.435780000	-2.927393000	-1.896980000
H	-4.499387000	-2.347055000	-2.828903000
H	-5.451411000	-2.992729000	-1.485864000
H	-4.120972000	-3.948991000	-2.163263000
C	-1.430612000	-3.236313000	-3.057645000
H	-1.067848000	-3.972462000	-2.324840000
H	-0.722571000	-3.212753000	-3.898519000
H	-2.393077000	-3.585866000	-3.456162000
C	-2.055034000	-0.788995000	-3.386704000
H	-3.077991000	-1.011925000	-3.726862000
H	-1.413552000	-0.737566000	-4.279814000
H	-2.048222000	0.195484000	-2.898365000
O	1.673024000	1.824614000	1.209982000
C	2.582105000	2.742952000	0.808508000
C	-3.387564000	3.695917000	1.278141000
C	-4.271889000	4.472994000	0.516505000
H	-3.349484000	3.761349000	2.366849000
C	3.530179000	-2.292640000	0.902674000
O	1.622380000	1.976358000	-1.067265000
C	3.770550000	-2.031143000	-0.416464000
N	2.620133000	-1.425092000	-0.912454000
C	5.004387000	-2.300688000	-1.201692000
C	-4.302383000	4.380461000	-0.876390000
H	-4.947426000	5.165391000	1.023990000
C	2.365814000	-0.974005000	-2.279014000
C	3.422573000	-0.015506000	-2.809756000
C	2.115631000	-2.150656000	-3.213116000
H	1.429568000	-0.402145000	-2.173986000
H	3.463980000	3.429002000	2.656488000
H	-3.680966000	0.742047000	2.059129000
H	-3.018736000	0.511730000	3.686634000
H	-4.338312000	-0.532548000	3.129254000
C	4.436006000	-2.927255000	1.897129000
H	4.499783000	-2.346745000	2.828937000
H	5.451592000	-2.992831000	1.485941000
H	4.121058000	-3.948749000	2.163638000
H	-0.507503000	-1.545882000	-2.132980000
H	-3.033367000	-2.726633000	3.404229000
H	-1.741622000	-1.790796000	4.183665000
H	-1.368875000	-2.834009000	2.784895000
H	-5.001977000	5.001663000	-1.440374000
H	-3.465007000	3.427935000	-2.656523000
H	1.068380000	-3.972304000	2.325264000
H	0.722823000	-3.212312000	3.898741000
H	2.393430000	-3.585298000	3.456659000
H	4.792731000	-2.830411000	-2.142277000
H	5.685529000	-2.933874000	-0.618742000
H	5.546622000	-1.376925000	-1.456811000
H	3.034102000	-2.726256000	-3.404392000
H	1.742304000	-1.790453000	-4.183775000
H	1.369581000	-2.833922000	-2.785193000
H	3.681113000	0.742335000	-2.058684000
H	3.019373000	0.511959000	-3.686382000

H	4.338925000	-0.532162000	-3.128638000
H	4.946392000	5.166632000	-1.023946000

14a

Ni	0.000061000	1.359163000	-0.000055000
C	1.377375000	0.108279000	0.496254000
N	2.614349000	-0.043456000	-0.063930000
C	3.274817000	-1.160080000	0.441345000
C	2.433067000	-1.723798000	1.358924000
N	1.288306000	-0.932309000	1.374632000
C	3.138936000	0.962900000	-0.986110000
H	2.280671000	1.648637000	-1.092296000
C	4.285207000	1.750676000	-0.365838000
H	3.995822000	2.127751000	0.624521000
H	4.529234000	2.614716000	-1.001716000
H	5.202615000	1.152217000	-0.258336000
C	3.479659000	0.403822000	-2.360080000
H	4.364886000	-0.248880000	-2.347496000
H	3.694269000	1.234696000	-3.048436000
H	2.636278000	-0.165089000	-2.775908000
C	0.120259000	-1.060023000	2.239827000
H	-0.516749000	-0.238631000	1.876078000
C	0.450107000	-0.767184000	3.696671000
H	1.074177000	-1.546150000	4.159978000
H	-0.479439000	-0.699483000	4.282336000
H	0.975138000	0.195421000	3.778360000
C	-0.635358000	-2.363190000	2.026882000
H	-0.870526000	-2.501538000	0.961460000
H	-1.587707000	-2.332246000	2.577214000
H	-0.079615000	-3.242099000	2.385212000
C	-1.377373000	0.108379000	-0.496313000
N	-1.288419000	-0.932243000	-1.374666000
C	-2.433231000	-1.723656000	-1.358882000
C	-3.274892000	-1.159866000	-0.441268000
N	-2.614328000	-0.043272000	0.063941000
C	-0.120437000	-1.060067000	-2.239929000
H	0.516661000	-0.238721000	-1.876234000
C	0.635077000	-2.363297000	-2.027012000
H	0.870300000	-2.501650000	-0.961603000
H	1.587394000	-2.332449000	-2.577405000
H	0.079231000	-3.242162000	-2.385293000
C	-0.450357000	-0.767228000	-3.696757000
H	-1.074523000	-1.546151000	-4.160007000
H	0.479156000	-0.699618000	-4.282486000
H	-0.975312000	0.195419000	-3.778431000
C	-3.138809000	0.963102000	0.986158000
H	-2.280562000	1.648886000	1.092187000
C	-4.285229000	1.750767000	0.366022000
H	-3.996018000	2.127819000	-0.624396000
H	-4.529229000	2.614816000	1.001898000
H	-5.202605000	1.152230000	0.258679000
C	-3.479294000	0.404056000	2.360199000
H	-4.364494000	-0.248685000	2.347778000
H	-3.693832000	1.234945000	3.048560000
H	-2.635820000	-0.164804000	2.775913000
C	0.592798000	3.129380000	0.264654000
C	-0.592484000	3.129455000	-0.264744000
C	-2.628876000	-2.964994000	-2.154250000

H	-1.990404000	-3.791668000	-1.802455000
H	-3.670974000	-3.300843000	-2.073216000
H	-2.414931000	-2.817182000	-3.222497000
C	-4.602879000	-1.651537000	0.013149000
H	-4.567605000	-2.051201000	1.039576000
H	-5.374045000	-0.868367000	-0.008148000
H	-4.943789000	-2.464504000	-0.641208000
C	4.602794000	-1.651858000	-0.012987000
H	4.567550000	-2.051529000	-1.039413000
H	5.374021000	-0.868751000	0.008351000
H	4.943600000	-2.464847000	0.641397000
C	2.628591000	-2.965132000	2.154328000
H	2.414607000	-2.817283000	3.222562000
H	1.990080000	-3.791771000	1.802521000
H	3.670670000	-3.301053000	2.073348000
C	1.659277000	4.040665000	0.745847000
H	2.526258000	4.042620000	0.062960000
H	1.313385000	5.087038000	0.830818000
H	2.047230000	3.734698000	1.731940000
C	-1.658849000	4.040881000	-0.745922000
H	-2.525908000	4.042801000	-0.063137000
H	-1.312875000	5.087242000	-0.830713000
H	-2.046711000	3.735076000	-1.732101000

15a

Ni	0.257387000	-0.191421000	-0.765416000
C	2.100485000	0.096605000	-0.234072000
N	3.189838000	-0.043043000	-1.043290000
C	4.376543000	0.009798000	-0.322075000
C	4.024170000	0.205096000	0.983228000
N	2.634416000	0.257180000	1.007552000
C	3.053747000	-0.052834000	-2.498676000
H	1.962658000	-0.073941000	-2.628039000
C	3.566077000	1.247154000	-3.103360000
H	3.109537000	2.105824000	-2.590990000
H	3.291708000	1.295273000	-4.166843000
H	4.660702000	1.337067000	-3.040044000
C	3.631141000	-1.292197000	-3.165654000
H	4.729784000	-1.320556000	-3.140073000
H	3.328419000	-1.302973000	-4.223092000
H	3.249569000	-2.211697000	-2.700514000
C	1.789158000	0.432237000	2.186170000
H	0.788940000	0.532064000	1.741422000
C	2.096190000	1.713350000	2.947582000
H	3.012632000	1.634856000	3.549162000
H	1.269782000	1.932136000	3.638629000
H	2.185589000	2.570134000	2.265363000
C	1.795821000	-0.803385000	3.076535000
H	1.541651000	-1.705981000	2.505154000
H	1.050806000	-0.689426000	3.877130000
H	2.771964000	-0.959532000	3.559056000
C	-0.175436000	-1.659149000	0.399713000
N	0.440361000	-2.871638000	0.398062000
C	-0.030406000	-3.687783000	1.421550000
C	-0.975375000	-2.957339000	2.086277000
N	-1.052444000	-1.726038000	1.439833000
C	1.460822000	-3.185254000	-0.599517000
H	1.473011000	-2.269736000	-1.211737000

C	2.843320000	-3.344797000	0.017137000
H	3.099380000	-2.468438000	0.629066000
H	3.598011000	-3.431103000	-0.778417000
H	2.925473000	-4.245768000	0.642315000
C	1.055216000	-4.338179000	-1.505068000
H	1.076001000	-5.309853000	-0.990624000
H	1.752649000	-4.401689000	-2.353960000
H	0.045581000	-4.172879000	-1.907404000
C	-2.011386000	-0.649313000	1.715511000
H	-1.843624000	0.056193000	0.888321000
C	-3.448340000	-1.149012000	1.652552000
H	-3.603139000	-1.788981000	0.773985000
H	-4.132205000	-0.293243000	1.570473000
H	-3.735406000	-1.708730000	2.553767000
C	-1.738223000	0.110379000	3.006321000
H	-1.822536000	-0.525152000	3.900333000
H	-2.481803000	0.914962000	3.102055000
H	-0.747592000	0.579338000	3.002924000
C	-0.373483000	1.020496000	-2.232973000
C	-1.269197000	-0.112398000	-2.050507000
B	-0.139234000	2.037170000	-1.143360000
O	-0.828864000	2.200695000	0.098283000
O	0.857777000	3.059804000	-1.222610000
C	-0.225359000	3.219783000	0.741829000
C	0.811431000	3.730791000	-0.055137000
C	-0.517742000	3.754779000	1.984178000
C	1.607880000	4.774854000	0.384019000
C	0.282014000	4.818287000	2.431493000
H	-1.338743000	3.357735000	2.583603000
C	1.326605000	5.312584000	1.651001000
H	2.414056000	5.163032000	-0.240939000
H	0.081449000	5.264350000	3.408300000
H	1.934075000	6.139541000	2.025885000
B	-2.683118000	0.088910000	-1.523608000
O	-3.251018000	1.253998000	-0.988188000
O	-3.694095000	-0.891217000	-1.635492000
C	-4.562997000	0.994044000	-0.789172000
C	-4.838589000	-0.317478000	-1.191916000
C	-5.543848000	1.813921000	-0.259186000
C	-6.105525000	-0.861579000	-1.082932000
C	-6.831906000	1.270834000	-0.145785000
H	-5.312454000	2.833504000	0.053043000
C	-7.106963000	-0.037347000	-0.549234000
H	-6.305912000	-1.887304000	-1.396886000
H	-7.635815000	1.886106000	0.264615000
H	-8.122049000	-0.428061000	-0.448455000
C	0.400702000	-5.087690000	1.677001000
H	1.493431000	-5.190004000	1.738014000
H	-0.014936000	-5.435051000	2.631685000
H	0.045714000	-5.780519000	0.897735000
C	-1.789020000	-3.372566000	3.260351000
H	-1.842236000	-2.587444000	4.026855000
H	-2.821675000	-3.636457000	2.984160000
H	-1.338615000	-4.257430000	3.729156000
C	4.917803000	0.368070000	2.161093000
H	4.627575000	-0.274749000	3.004009000
H	5.945672000	0.099652000	1.885349000
H	4.934902000	1.406372000	2.526482000

C	5.738121000	-0.177111000	-0.890121000
H	5.892375000	-1.202810000	-1.260768000
H	5.949666000	0.509800000	-1.721635000
H	6.492585000	0.008626000	-0.115259000
C	-1.166670000	-1.270853000	-3.037451000
H	-1.692277000	-2.156166000	-2.649949000
H	-1.618327000	-1.035045000	-4.018787000
H	-0.121373000	-1.564932000	-3.229962000
C	0.236349000	1.291914000	-3.589321000
H	1.026345000	2.051801000	-3.539620000
H	0.643514000	0.401020000	-4.095555000
H	-0.543924000	1.691880000	-4.261344000

I1

Ni	-0.410577000	0.245196000	-0.551449000
C	-2.075612000	-0.845525000	-0.332590000
N	-3.064626000	-1.133646000	-1.224033000
C	-4.062210000	-1.918802000	-0.657358000
C	-3.691581000	-2.128888000	0.640126000
N	-2.479256000	-1.467622000	0.809234000
C	-2.961605000	-0.741864000	-2.626156000
H	-2.106941000	-0.056877000	-2.619532000
C	-2.589315000	-1.929836000	-3.501898000
H	-1.653497000	-2.379674000	-3.139815000
H	-2.437722000	-1.600712000	-4.540500000
H	-3.372585000	-2.702493000	-3.510991000
C	-4.169124000	0.033495000	-3.134197000
H	-5.040265000	-0.605986000	-3.333308000
H	-3.905193000	0.528005000	-4.080787000
H	-4.467033000	0.811872000	-2.417013000
C	-1.733105000	-1.326643000	2.057370000
H	-0.802564000	-0.844103000	1.727108000
C	-1.361846000	-2.662044000	2.682474000
H	-2.224962000	-3.196205000	3.101706000
H	-0.658692000	-2.492599000	3.510793000
H	-0.863156000	-3.308476000	1.946821000
C	-2.449190000	-0.379424000	3.011961000
H	-2.632086000	0.587954000	2.522595000
H	-1.832659000	-0.196012000	3.903860000
H	-3.412852000	-0.784121000	3.355509000
C	-0.635815000	1.534130000	0.835273000
N	-1.583101000	2.510540000	0.765369000
C	-1.521133000	3.364281000	1.862111000
C	-0.509642000	2.898403000	2.653136000
N	0.020771000	1.784451000	2.004088000
C	-2.404157000	2.645898000	-0.435987000
H	-2.210054000	1.693622000	-0.958255000
C	-3.893685000	2.710581000	-0.137960000
H	-4.196195000	1.875114000	0.511251000
H	-4.456694000	2.628960000	-1.079385000
H	-4.198003000	3.653233000	0.337477000
C	-1.891497000	3.765039000	-1.331408000
H	-2.018288000	4.758623000	-0.874195000
H	-2.440774000	3.764134000	-2.285252000
H	-0.823997000	3.609655000	-1.547413000
C	1.254337000	1.072575000	2.350795000
H	1.323290000	0.294701000	1.575832000
C	2.474659000	1.973387000	2.203161000

H	2.434966000	2.540098000	1.263655000
H	3.385734000	1.359331000	2.180906000
H	2.570484000	2.688282000	3.034182000
C	1.207474000	0.392406000	3.711160000
H	1.170399000	1.109568000	4.542914000
H	2.118628000	-0.209377000	3.839058000
H	0.342955000	-0.279391000	3.797719000
C	-2.425628000	4.520345000	2.099402000
H	-2.503479000	5.172131000	1.217100000
H	-3.446446000	4.207361000	2.371524000
H	-2.039529000	5.132455000	2.924845000
C	-0.077242000	3.405031000	3.982545000
H	-0.361263000	2.721389000	4.798814000
H	1.009093000	3.559495000	4.042857000
H	-0.557463000	4.371054000	4.185666000
C	-5.289003000	-2.391930000	-1.353317000
H	-5.991225000	-1.570713000	-1.566192000
H	-5.065142000	-2.890219000	-2.307483000
H	-5.815769000	-3.120143000	-0.723464000
C	-4.400662000	-2.929033000	1.675237000
H	-5.414717000	-3.166172000	1.328479000
H	-3.892827000	-3.883560000	1.884393000
H	-4.501206000	-2.392393000	2.629288000
C	1.095440000	-1.574634000	-2.344239000
C	0.353396000	-0.423977000	-2.208452000
B	1.296698000	0.973855000	-0.996806000
B	1.652403000	-2.270910000	-1.107540000
C	2.144429000	-2.828653000	0.973676000
C	2.244682000	-2.952947000	2.348624000
C	2.984785000	-3.544197000	0.113186000
C	3.221718000	-3.828625000	2.842346000
H	1.592314000	-2.389469000	3.014208000
C	3.950321000	-4.413144000	0.590712000
C	4.056111000	-4.544494000	1.981970000
H	3.330837000	-3.950580000	3.922346000
H	4.597488000	-4.962528000	-0.094723000
H	4.807773000	-5.218329000	2.399096000
C	3.499971000	1.381128000	-0.982323000
C	2.872308000	2.400851000	-1.708149000
C	4.872234000	1.355288000	-0.804159000
C	3.593850000	3.433008000	-2.281840000
C	5.611003000	2.397328000	-1.383609000
H	5.347859000	0.551114000	-0.239861000
C	4.985659000	3.414657000	-2.106141000
H	3.092811000	4.221892000	-2.845609000
H	6.697229000	2.409991000	-1.267790000
H	5.589812000	4.211707000	-2.545598000
O	1.298909000	-2.065843000	0.238119000
O	2.679364000	-3.227702000	-1.166135000
O	2.565199000	0.521558000	-0.522975000
O	1.535605000	2.180637000	-1.716437000
C	1.519623000	-2.103444000	-3.695191000
H	2.119467000	-3.019581000	-3.603772000
H	0.655068000	-2.335439000	-4.342380000
H	2.128488000	-1.366949000	-4.249121000
C	0.031541000	0.330496000	-3.485202000
H	-0.490822000	-0.305904000	-4.217836000
H	-0.567571000	1.235961000	-3.309303000

H	0.959563000	0.663481000	-3.981814000

I2

Ni	0.163511000	-1.497159000	0.412511000
C	-0.948201000	-0.159908000	1.190475000
N	-2.258160000	-0.251395000	1.525393000
C	-2.756505000	0.976473000	1.937852000
C	-1.712402000	1.861638000	1.858965000
N	-0.623744000	1.140970000	1.391828000
C	-2.945398000	-1.543833000	1.473797000
H	-2.197266000	-2.188619000	0.982415000
C	-3.193902000	-2.096949000	2.869795000
H	-2.258106000	-2.120744000	3.446984000
H	-3.582508000	-3.123807000	2.800914000
H	-3.929858000	-1.500847000	3.430350000
C	-4.182336000	-1.528433000	0.590608000
H	-5.012623000	-0.957670000	1.029759000
H	-4.533521000	-2.560855000	0.446666000
H	-3.936048000	-1.115829000	-0.396332000
C	0.751256000	1.601980000	1.165759000
H	1.179840000	0.777373000	0.572799000
C	0.839381000	2.859038000	0.316985000
H	0.168666000	2.794942000	-0.550756000
H	1.870029000	2.955800000	-0.053498000
H	0.605430000	3.771624000	0.882871000
C	1.527831000	1.700611000	2.469200000
H	1.129441000	2.490727000	3.124994000
H	2.581650000	1.931917000	2.254698000
H	1.491718000	0.745864000	3.014033000
C	1.365708000	-2.648463000	-0.710295000
C	0.103519000	-2.469564000	-1.331570000
B	2.386713000	-1.515753000	-0.514019000
O	2.691438000	-0.409269000	-1.316894000
O	3.232179000	-1.494683000	0.623415000
C	3.623666000	0.308568000	-0.650510000
C	3.957831000	-0.354945000	0.536165000
C	4.197986000	1.520959000	-0.993198000
C	4.881041000	0.165475000	1.426802000
C	5.130341000	2.057711000	-0.094427000
H	3.927513000	2.025046000	-1.922314000
C	5.464559000	1.394607000	1.089240000
H	5.131384000	-0.361385000	2.348885000
H	5.606963000	3.012598000	-0.327009000
H	6.197311000	1.840511000	1.765436000
B	-0.479003000	-1.104066000	-1.755277000
O	0.142438000	0.071132000	-2.226379000
O	-1.889924000	-0.943208000	-1.890069000
C	-0.847782000	0.944672000	-2.505881000
C	-2.088668000	0.331296000	-2.290462000
C	-0.752654000	2.255314000	-2.942346000
C	-3.278438000	1.012989000	-2.483011000
C	-1.953634000	2.953473000	-3.137356000
H	0.220375000	2.713946000	-3.125598000
C	-3.189413000	2.346711000	-2.908765000
H	-4.241417000	0.526454000	-2.318263000
H	-1.918702000	3.990367000	-3.479162000
H	-4.106804000	2.916605000	-3.072468000
C	-4.166997000	1.245612000	2.322502000

H	-4.560486000	0.496858000	3.024456000
H	-4.239602000	2.225973000	2.811169000
H	-4.834173000	1.265678000	1.446088000
C	-1.707713000	3.315994000	2.165272000
H	-0.849879000	3.603172000	2.790464000
H	-1.676648000	3.929317000	1.251399000
H	-2.620588000	3.584731000	2.712660000
C	-0.821358000	-3.650783000	-1.521815000
H	-1.857097000	-3.324616000	-1.685761000
H	-0.512645000	-4.219157000	-2.417017000
H	-0.808095000	-4.358003000	-0.679155000
C	1.785238000	-4.008073000	-0.190064000
H	2.647190000	-3.921114000	0.485881000
H	0.983437000	-4.528089000	0.357759000
H	2.084821000	-4.671036000	-1.020608000

I3

Ni	-0.477536000	-1.498834000	-0.112092000
C	1.082869000	-0.706153000	0.682298000
N	2.372209000	-1.120560000	0.632163000
C	3.202817000	-0.264124000	1.348256000
C	2.397143000	0.710166000	1.867491000
N	1.099436000	0.406880000	1.462395000
C	2.733536000	-2.374082000	-0.034167000
H	1.813775000	-2.626373000	-0.581981000
C	3.863145000	-2.233572000	-1.044309000
H	3.698397000	-1.362286000	-1.690391000
H	3.884987000	-3.132076000	-1.678557000
H	4.849102000	-2.150461000	-0.566169000
C	2.988476000	-3.482316000	0.978553000
H	3.871798000	-3.274397000	1.601651000
H	3.167071000	-4.432521000	0.453772000
H	2.122043000	-3.614012000	1.639235000
C	-0.144917000	1.015543000	1.954349000
H	-0.922852000	0.452378000	1.417799000
C	-0.307700000	2.481216000	1.592341000
H	0.508911000	3.109165000	1.972895000
H	-1.243199000	2.846314000	2.039664000
H	-0.383420000	2.596649000	0.506436000
C	-0.330174000	0.762193000	3.445698000
H	-0.181747000	-0.296475000	3.690337000
H	-1.354832000	1.037882000	3.735008000
H	0.358647000	1.359127000	4.061926000
C	-0.142373000	-0.972026000	-2.071522000
C	-1.528446000	-1.192692000	-1.840769000
B	0.670249000	0.303783000	-1.835716000
O	0.286998000	1.615208000	-1.522395000
O	2.074115000	0.286724000	-2.019740000
C	1.427236000	2.341429000	-1.418034000
C	2.522678000	1.523443000	-1.708698000
C	1.589687000	3.672949000	-1.075643000
C	3.823132000	1.992799000	-1.651514000
C	2.903883000	4.158427000	-1.011378000
H	0.730783000	4.311915000	-0.866637000
C	3.997466000	3.335653000	-1.288265000
H	4.668631000	1.343314000	-1.884717000
H	3.072424000	5.203893000	-0.743667000
H	5.007771000	3.746778000	-1.230872000

B	-2.495253000	-0.214557000	-1.155561000
O	-2.277921000	1.071503000	-0.643918000
O	-3.857840000	-0.538409000	-0.991561000
C	-3.467898000	1.504028000	-0.157262000
C	-4.433869000	0.514646000	-0.362610000
C	-3.781648000	2.710756000	0.444323000
C	-5.747400000	0.680309000	0.038962000
C	-5.109962000	2.888357000	0.855134000
H	-3.027789000	3.486662000	0.579843000
C	-6.070949000	1.894266000	0.660021000
H	-6.490184000	-0.101218000	-0.128290000
H	-5.398024000	3.826710000	1.334207000
H	-7.096954000	2.066418000	0.992560000
C	2.799829000	1.943067000	2.593730000
H	2.176564000	2.142686000	3.475859000
H	3.838596000	1.850948000	2.936385000
H	2.748161000	2.824309000	1.933607000
C	4.682013000	-0.377853000	1.430959000
H	5.010086000	-1.392523000	1.698499000
H	5.167924000	-0.107165000	0.480237000
H	5.063844000	0.305308000	2.200568000
C	-2.206309000	-2.340618000	-2.564187000
H	-3.248254000	-2.460207000	-2.247033000
H	-2.220200000	-2.137854000	-3.649402000
H	-1.695435000	-3.303264000	-2.424741000
C	0.600437000	-2.026391000	-2.875913000
H	1.680610000	-1.839992000	-2.895913000
H	0.433065000	-3.045987000	-2.494987000
H	0.252073000	-2.022186000	-3.923726000
C	-0.847345000	-2.493133000	1.477177000
C	-1.809679000	-2.682476000	0.666059000
C	-3.100636000	-3.343320000	0.398813000
H	-3.472781000	-3.849627000	1.304431000
H	-3.859431000	-2.622802000	0.062234000
H	-3.003301000	-4.099612000	-0.394737000
C	-0.235030000	-2.795240000	2.787149000
H	-0.006045000	-3.871299000	2.862789000
H	0.699789000	-2.244384000	2.962781000
H	-0.928976000	-2.558474000	3.610812000

I4

Ni	0.049197000	-0.372685000	-0.826320000
C	1.630427000	-0.333694000	0.263516000
N	2.894109000	-0.784528000	0.088377000
C	3.729210000	-0.323686000	1.100757000
C	2.947215000	0.424843000	1.936836000
N	1.662259000	0.392534000	1.410327000
C	3.232218000	-1.723691000	-0.985127000
H	2.308594000	-1.761280000	-1.580048000
C	4.357017000	-1.234184000	-1.886151000
H	4.194543000	-0.189116000	-2.178390000
H	4.380086000	-1.851266000	-2.796344000
H	5.342394000	-1.323604000	-1.407623000
C	3.491450000	-3.119562000	-0.432516000
H	4.450331000	-3.178718000	0.103507000
H	3.527381000	-3.845151000	-1.257949000
H	2.695679000	-3.434518000	0.255092000
C	0.421787000	0.849843000	2.057566000

H	-0.348722000	0.666523000	1.295630000
C	0.383708000	2.335639000	2.366048000
H	1.142434000	2.647303000	3.096252000
H	-0.602418000	2.565819000	2.794262000
H	0.493358000	2.920718000	1.446974000
C	0.090615000	-0.021907000	3.260963000
H	0.096161000	-1.083200000	2.980911000
H	-0.918709000	0.228175000	3.618362000
H	0.792259000	0.134763000	4.094766000
C	0.540324000	0.799270000	-2.389880000
C	-0.883793000	0.662144000	-2.300954000
B	1.453420000	1.792931000	-1.666399000
O	1.170408000	2.881713000	-0.833615000
O	2.857252000	1.686155000	-1.797472000
C	2.362631000	3.360107000	-0.397840000
C	3.395443000	2.620264000	-0.979806000
C	2.619982000	4.392378000	0.487714000
C	4.726019000	2.870087000	-0.694168000
C	3.965126000	4.650984000	0.788204000
H	1.809617000	4.975366000	0.927380000
C	4.995571000	3.904220000	0.213143000
H	5.522560000	2.287946000	-1.160660000
H	4.209710000	5.457454000	1.483012000
H	6.032498000	4.134852000	0.467227000
B	-1.816760000	1.549678000	-1.452961000
O	-1.511942000	2.426435000	-0.411705000
O	-3.206585000	1.498963000	-1.623308000
C	-2.699417000	2.874224000	0.071233000
C	-3.738060000	2.311079000	-0.673930000
C	-2.946352000	3.740318000	1.122407000
C	-5.066407000	2.583586000	-0.404994000
C	-4.289770000	4.020961000	1.406560000
H	-2.129524000	4.182999000	1.693446000
C	-5.326570000	3.455390000	0.659631000
H	-5.863811000	2.118919000	-0.986122000
H	-4.529202000	4.699877000	2.228066000
H	-6.361897000	3.695102000	0.911595000
C	3.365255000	1.229411000	3.113982000
H	2.700937000	1.088659000	3.977582000
H	4.377788000	0.939525000	3.422648000
H	3.388502000	2.303875000	2.870709000
C	5.196573000	-0.546528000	1.168600000
H	5.469190000	-1.602948000	1.037985000
H	5.733390000	0.038033000	0.404906000
H	5.573502000	-0.227677000	2.148751000
C	-1.609473000	-0.108736000	-3.391445000
H	-2.663647000	-0.263720000	-3.135888000
H	-1.575722000	0.457614000	-4.338286000
H	-1.170036000	-1.096398000	-3.583234000
C	1.241536000	0.005778000	-3.481127000
H	2.331921000	0.069415000	-3.394362000
H	0.957418000	-1.057979000	-3.486043000
H	0.969603000	0.405870000	-4.473313000
B	-0.225249000	-2.128914000	-0.058114000
B	-1.768103000	-1.051060000	-0.305878000
O	-0.177690000	-2.670959000	1.241455000
O	0.043424000	-3.163567000	-0.981172000
O	-2.356820000	-0.359390000	0.770441000

O	-2.768003000	-1.760988000	-0.978980000
C	0.139507000	-3.984060000	1.105555000
C	0.336183000	-4.939049000	2.087628000
C	0.271702000	-4.284515000	-0.253236000
C	0.674062000	-6.228216000	1.655651000
H	0.231120000	-4.690281000	3.144690000
C	0.603067000	-5.555618000	-0.689152000
C	0.803268000	-6.529667000	0.297370000
H	0.837399000	-7.013127000	2.397248000
H	0.702282000	-5.777202000	-1.752790000
H	1.064515000	-7.546663000	-0.003217000
C	-3.940302000	-1.477033000	-0.353116000
C	-5.220213000	-1.905742000	-0.659014000
C	-3.689515000	-0.619429000	0.719213000
C	-6.252659000	-1.435887000	0.162220000
H	-5.405058000	-2.572579000	-1.502227000
C	-4.701120000	-0.145932000	1.534614000
C	-5.998732000	-0.576214000	1.235458000
H	-7.279194000	-1.747886000	-0.042515000
H	-4.490543000	0.545641000	2.351473000
H	-6.830725000	-0.225123000	1.849692000

I5

Ni	0.785375000	-0.757191000	-0.794738000
C	2.558188000	-1.030005000	-0.251719000
N	3.597374000	-1.416437000	-1.025783000
C	4.764315000	-1.511888000	-0.276763000
C	4.428183000	-1.161722000	1.005216000
N	3.070343000	-0.865799000	0.988893000
C	3.389602000	-1.680600000	-2.451750000
H	2.347581000	-1.352416000	-2.605246000
C	4.268819000	-0.815065000	-3.339649000
H	4.168521000	0.241919000	-3.055717000
H	3.938984000	-0.916792000	-4.383857000
H	5.328816000	-1.103792000	-3.299414000
C	3.456318000	-3.167900000	-2.764761000
H	4.467771000	-3.580255000	-2.631607000
H	3.161428000	-3.341851000	-3.810006000
H	2.764122000	-3.726543000	-2.117950000
C	2.212539000	-0.414922000	2.092417000
H	1.263292000	-0.178894000	1.582952000
C	1.936101000	-1.531234000	3.088047000
H	1.533103000	-2.419570000	2.580893000
H	1.187132000	-1.193588000	3.818872000
H	2.835341000	-1.826579000	3.649636000
C	2.720070000	0.871087000	2.725617000
H	3.611624000	0.714343000	3.349664000
H	1.932521000	1.293817000	3.364949000
H	2.950084000	1.618100000	1.952751000
C	-1.896294000	0.921012000	-1.143080000
C	-1.090038000	-0.375253000	-1.457916000
B	-1.592986000	1.516263000	0.271250000
O	-1.792731000	2.861331000	0.588471000
O	-1.206036000	0.815544000	1.411060000
C	-1.475144000	2.987209000	1.901290000
C	-1.126233000	1.731032000	2.406516000
C	-1.465204000	4.120515000	2.694921000
C	-0.776501000	1.551263000	3.732801000

C	-1.094115000	3.951041000	4.036294000
H	-1.740505000	5.094650000	2.287466000
C	-0.761800000	2.693549000	4.545450000
H	-0.533810000	0.560426000	4.120247000
H	-1.073516000	4.819989000	4.697637000
H	-0.489649000	2.595953000	5.598739000
B	-1.200278000	-1.557303000	-0.521540000
O	-1.899897000	-1.808221000	0.665254000
O	-0.202780000	-2.603560000	-0.680614000
C	-1.304884000	-2.864593000	1.262376000
C	-0.275911000	-3.359822000	0.455110000
C	-1.588526000	-3.437131000	2.491065000
C	0.505927000	-4.435690000	0.828762000
C	-0.800859000	-4.527489000	2.884331000
H	-2.389984000	-3.042682000	3.117284000
C	0.224384000	-5.018129000	2.072845000
H	1.307605000	-4.801364000	0.185198000
H	-0.994520000	-5.003202000	3.848288000
H	0.818958000	-5.869219000	2.411422000
C	6.097187000	-1.892063000	-0.814350000
H	6.547524000	-1.086487000	-1.415657000
H	6.785840000	-2.106211000	0.013295000
H	6.050615000	-2.790778000	-1.445618000
C	5.307884000	-1.072605000	2.200233000
H	5.534321000	-0.029589000	2.471537000
H	4.859614000	-1.554436000	3.080347000
H	6.263252000	-1.574534000	1.998905000
C	-0.976402000	-0.716244000	-2.942904000
H	-0.478232000	-1.687473000	-3.090682000
H	-1.971749000	-0.794172000	-3.415514000
H	-0.401026000	0.034085000	-3.506815000
C	-1.716068000	2.020261000	-2.204478000
H	-2.236222000	2.941968000	-1.907075000
H	-0.653741000	2.276962000	-2.342653000
H	-2.109734000	1.714522000	-3.183941000
B	-3.380961000	0.425247000	-1.119515000
O	-4.157295000	0.260756000	0.022744000
O	-4.100977000	0.023703000	-2.243736000
C	-5.336131000	-0.276364000	-0.392580000
C	-5.302051000	-0.421130000	-1.781801000
C	-6.439924000	-0.646593000	0.353954000
C	-6.371022000	-0.942726000	-2.487938000
C	-7.527740000	-1.176725000	-0.351652000
H	-6.451055000	-0.528200000	1.438323000
C	-7.494017000	-1.321573000	-1.741002000
H	-6.331339000	-1.050480000	-3.572835000
H	-8.420537000	-1.483589000	0.197570000
H	-8.360962000	-1.739305000	-2.257533000
B	1.234333000	1.036721000	-1.008441000
O	1.944794000	1.613373000	-2.080688000
O	0.957558000	2.052540000	-0.069751000
C	2.058958000	2.942055000	-1.808485000
C	1.455029000	3.211805000	-0.578349000
C	2.651250000	3.942214000	-2.559557000
C	1.413218000	4.485796000	-0.042327000
C	2.617325000	5.238055000	-2.026609000
H	3.116368000	3.724475000	-3.522377000
C	2.012197000	5.504073000	-0.795797000

H	0.930703000	4.674334000	0.918192000
H	3.071808000	6.056971000	-2.588698000
H	2.001726000	6.527142000	-0.413427000

I6

Ni	0.395697000	-1.798654000	0.538568000
C	1.782342000	-0.429996000	0.771252000
N	3.063024000	-0.420484000	0.333662000
C	3.726722000	0.723151000	0.749091000
C	2.823598000	1.446324000	1.486436000
N	1.643206000	0.719313000	1.475679000
C	3.604794000	-1.572532000	-0.391529000
H	2.703272000	-2.177355000	-0.579284000
C	4.209765000	-1.212992000	-1.738745000
H	3.497560000	-0.619703000	-2.326529000
H	4.418280000	-2.139103000	-2.294395000
H	5.158473000	-0.665744000	-1.647453000
C	4.531922000	-2.390988000	0.496448000
H	5.458116000	-1.850579000	0.744189000
H	4.816713000	-3.320345000	-0.018456000
H	4.027998000	-2.659893000	1.436353000
C	0.392794000	0.980035000	2.203195000
H	-0.344671000	0.365678000	1.659325000
C	-0.065225000	2.428007000	2.144434000
H	0.453586000	3.067505000	2.871840000
H	-1.138690000	2.469911000	2.372280000
H	0.072235000	2.847646000	1.140114000
C	0.488941000	0.454217000	3.628162000
H	0.747295000	-0.615129000	3.633896000
H	-0.478714000	0.573718000	4.137621000
H	1.249637000	0.998023000	4.210688000
C	-0.473085000	-1.794682000	-1.226527000
C	-1.999057000	-2.082369000	-1.026408000
B	-0.010932000	-0.362590000	-1.449630000
O	-0.724163000	0.800417000	-1.071714000
O	1.166630000	0.044180000	-2.122200000
C	0.026565000	1.860355000	-1.450699000
C	1.195619000	1.396290000	-2.066441000
C	-0.236030000	3.210868000	-1.303212000
C	2.169661000	2.269765000	-2.518969000
C	0.746499000	4.101487000	-1.760725000
H	-1.170021000	3.553047000	-0.853453000
C	1.926644000	3.640571000	-2.347395000
H	3.079124000	1.902484000	-2.997526000
H	0.580044000	5.176359000	-1.660764000
H	2.670449000	4.361093000	-2.694886000
B	-2.724442000	-0.781506000	-0.518568000
O	-2.721529000	-0.309116000	0.794491000
O	-3.512285000	0.048335000	-1.314811000
C	-3.429762000	0.847425000	0.777619000
C	-3.902969000	1.074277000	-0.518509000
C	-3.704175000	1.719793000	1.816378000
C	-4.645973000	2.197445000	-0.836834000
C	-4.454907000	2.861303000	1.504050000
H	-3.355212000	1.515791000	2.830134000
C	-4.910771000	3.097285000	0.204518000
H	-5.004084000	2.364926000	-1.853675000
H	-4.690641000	3.577910000	2.293944000

H	-5.492583000	3.997773000	-0.004255000
C	3.020449000	2.762594000	2.147483000
H	2.701034000	2.749387000	3.199832000
H	4.084778000	3.030123000	2.128867000
H	2.467517000	3.565237000	1.636606000
C	5.121896000	1.084904000	0.386084000
H	5.823692000	0.252184000	0.534475000
H	5.198402000	1.404721000	-0.665336000
H	5.465452000	1.921148000	1.008517000
C	-2.682450000	-2.543533000	-2.321824000
H	-3.767920000	-2.664954000	-2.183425000
H	-2.541864000	-1.802239000	-3.123562000
H	-2.281935000	-3.506948000	-2.671178000
C	0.229787000	-2.836461000	-2.087023000
H	1.321119000	-2.697214000	-2.082705000
H	0.020224000	-3.859087000	-1.740243000
H	-0.082510000	-2.765001000	-3.144721000
C	-0.901966000	-3.076543000	0.827982000
C	-2.032559000	-3.097212000	0.098766000
C	-3.252869000	-3.929410000	0.342310000
H	-3.167369000	-4.522440000	1.263932000
H	-4.157899000	-3.301251000	0.430738000
H	-3.443038000	-4.631480000	-0.487841000
C	-0.563436000	-3.895086000	2.039096000
H	-0.143526000	-4.879907000	1.769872000
H	0.204359000	-3.395053000	2.663776000
H	-1.430743000	-4.066541000	2.701479000

I7

Ni	0.237349000	-1.413195000	-0.452092000
C	-1.339705000	-0.363223000	-1.017101000
N	-2.609378000	-0.783198000	-1.235068000
C	-3.460528000	0.284816000	-1.477136000
C	-2.683439000	1.412248000	-1.428570000
N	-1.393835000	0.985571000	-1.155056000
C	-2.931438000	-2.208587000	-1.311931000
H	-2.019295000	-2.685304000	-0.924885000
C	-4.091102000	-2.609665000	-0.411143000
H	-4.006696000	-2.125758000	0.572455000
H	-4.072345000	-3.698331000	-0.257533000
H	-5.068976000	-2.356579000	-0.843611000
C	-3.104791000	-2.656081000	-2.756892000
H	-3.983644000	-2.195269000	-3.232599000
H	-3.237466000	-3.747447000	-2.796558000
H	-2.215991000	-2.395684000	-3.349794000
C	-0.163145000	1.782903000	-1.246067000
H	0.589867000	1.127322000	-0.780432000
C	-0.186449000	3.089808000	-0.469570000
H	-0.692928000	3.896243000	-1.017308000
H	0.853186000	3.407866000	-0.304032000
H	-0.661770000	2.976550000	0.512068000
C	0.200242000	1.985686000	-2.709971000
H	0.368405000	1.019660000	-3.207765000
H	1.121097000	2.578330000	-2.788201000
H	-0.599615000	2.520553000	-3.245602000
C	0.065628000	-1.939175000	1.430906000
C	1.364180000	-2.462511000	1.988599000
B	-0.405307000	-0.556641000	1.883899000

O	0.406867000	0.469962000	2.391735000
O	-1.748065000	-0.117138000	1.885263000
C	-0.411084000	1.517851000	2.643660000
C	-1.726654000	1.165659000	2.314243000
C	-0.093067000	2.775868000	3.124848000
C	-2.769327000	2.069874000	2.420274000
C	-1.144953000	3.694991000	3.243718000
H	0.936119000	3.034656000	3.377824000
C	-2.453251000	3.351920000	2.893696000
H	-3.787139000	1.786961000	2.146555000
H	-0.934969000	4.701082000	3.613126000
H	-3.248059000	4.094220000	2.995797000
B	2.499953000	-0.940826000	-0.599235000
O	2.688442000	-0.391487000	-1.895104000
O	2.941309000	-0.001339000	0.354855000
C	3.227249000	0.838917000	-1.708715000
C	3.357333000	1.080406000	-0.334828000
C	3.616751000	1.773762000	-2.652228000
C	3.845524000	2.284244000	0.146453000
C	4.119588000	2.991643000	-2.173009000
H	3.525200000	1.565276000	-3.719443000
C	4.223676000	3.243760000	-0.802856000
H	3.930923000	2.461220000	1.219655000
H	4.436395000	3.756167000	-2.885864000
H	4.617274000	4.204302000	-0.462775000
C	-3.101829000	2.830428000	-1.575309000
H	-2.513682000	3.363406000	-2.336434000
H	-4.155673000	2.878297000	-1.878004000
H	-2.999834000	3.379843000	-0.626836000
C	-4.926834000	0.183778000	-1.701576000
H	-5.181821000	-0.557637000	-2.472487000
H	-5.469013000	-0.091059000	-0.783447000
H	-5.318235000	1.152524000	-2.037567000
C	1.490908000	-2.582364000	3.474588000
H	2.426032000	-3.071054000	3.781350000
H	1.467825000	-1.581187000	3.937988000
H	0.653682000	-3.153537000	3.911753000
C	-1.004006000	-3.027090000	1.451537000
H	-2.001519000	-2.644140000	1.205543000
H	-0.757612000	-3.866614000	0.780107000
H	-1.079426000	-3.457940000	2.467218000
C	1.941774000	-2.330159000	-0.314237000
C	2.275988000	-2.801402000	1.063578000
C	3.597824000	-3.462842000	1.298267000
H	4.428212000	-2.786808000	1.029640000
H	3.738227000	-3.772850000	2.343110000
H	3.707073000	-4.360945000	0.667309000
C	1.931560000	-3.341926000	-1.446677000
H	1.323337000	-4.227391000	-1.196807000
H	1.533037000	-2.905540000	-2.379788000
H	2.945162000	-3.704436000	-1.700899000

I8

Ni	0.243302000	-1.251936000	0.031244000
C	-0.300158000	0.487725000	-0.402170000
N	-0.911141000	1.042022000	-1.473837000
C	-1.383905000	2.315915000	-1.170899000
C	-1.055647000	2.551801000	0.136343000

N	-0.368802000	1.425328000	0.575998000
C	-0.855801000	0.370965000	-2.772990000
H	-0.594151000	-0.659230000	-2.495015000
C	-2.185273000	0.316561000	-3.507419000
H	-2.975981000	-0.053885000	-2.842308000
H	-2.093636000	-0.389139000	-4.346387000
H	-2.482837000	1.285685000	-3.930205000
C	0.286170000	0.929548000	-3.610992000
H	0.115751000	1.983957000	-3.879438000
H	0.384618000	0.356072000	-4.544906000
H	1.235854000	0.856505000	-3.060597000
C	0.370291000	1.234932000	1.828385000
H	0.852611000	0.250241000	1.678654000
C	-0.526828000	1.126818000	3.048878000
H	-1.086789000	2.054137000	3.237418000
H	0.090721000	0.923436000	3.936322000
H	-1.238877000	0.300869000	2.927223000
C	1.488478000	2.256919000	1.976485000
H	2.089715000	2.318887000	1.058555000
H	2.159077000	1.953062000	2.792536000
H	1.109270000	3.260818000	2.216766000
C	-1.452689000	3.694676000	0.999173000
H	-0.609531000	4.120854000	1.559926000
H	-1.879527000	4.496586000	0.383430000
H	-2.226303000	3.391017000	1.723012000
C	-2.146749000	3.184090000	-2.104054000
H	-1.635618000	3.304720000	-3.070669000
H	-3.155187000	2.788137000	-2.301279000
H	-2.264475000	4.184002000	-1.667225000
C	-1.161398000	-2.744010000	-0.259302000
C	-0.094285000	-3.125713000	0.638648000
B	-2.240276000	-1.795556000	0.230965000
O	-3.142025000	-1.179477000	-0.675481000
O	-2.519351000	-1.308306000	1.535733000
C	-3.812223000	-0.241976000	0.033129000
C	-3.442058000	-0.325983000	1.380950000
C	-4.724128000	0.698840000	-0.412303000
C	-3.981092000	0.520646000	2.333794000
C	-5.262868000	1.571772000	0.544850000
H	-5.011373000	0.750921000	-1.463879000
C	-4.901338000	1.482449000	1.889102000
H	-3.699517000	0.439631000	3.384676000
H	-5.984746000	2.328869000	0.230520000
H	-5.345929000	2.169066000	2.613063000
B	2.890692000	-1.082160000	-0.369623000
O	3.443935000	-0.733672000	0.884294000
O	3.371979000	-0.174342000	-1.342295000
C	4.186351000	0.381393000	0.676458000
C	4.130132000	0.729700000	-0.678048000
C	4.907338000	1.127560000	1.591174000
C	4.779332000	1.850307000	-1.165751000
C	5.569064000	2.264519000	1.105033000
H	4.947911000	0.839385000	2.642942000
C	5.503715000	2.619580000	-0.243126000
H	4.726057000	2.113868000	-2.223295000
H	6.146035000	2.882628000	1.796417000
H	6.029827000	3.511756000	-0.589865000
C	-0.483815000	-3.486833000	2.058835000

H	-0.012579000	-2.853780000	2.824462000
H	-1.569372000	-3.427093000	2.185732000
H	-0.180333000	-4.525671000	2.269366000
C	-1.318777000	-3.304530000	-1.655310000
H	-1.641708000	-2.554162000	-2.391629000
H	-0.412188000	-3.797772000	-2.021851000
H	-2.113639000	-4.071072000	-1.634109000
C	1.904742000	-2.187188000	-0.709529000
C	1.316532000	-2.923759000	0.396111000
C	2.223568000	-3.220697000	1.577589000
H	2.072800000	-2.542108000	2.429872000
H	2.034373000	-4.242736000	1.938375000
H	3.276074000	-3.154306000	1.286638000
C	1.693689000	-2.440463000	-2.189975000
H	1.777508000	-3.517598000	-2.407693000
H	0.728497000	-2.108135000	-2.592681000
H	2.474110000	-1.924099000	-2.765975000

I9

Ni	-0.140420000	0.932048000	0.000488000
C	0.093808000	-0.945361000	0.000297000
N	0.162606000	-1.763142000	1.076593000
C	0.253629000	-3.094147000	0.685684000
C	0.253878000	-3.094035000	-0.685351000
N	0.163030000	-1.762979000	-1.076102000
C	0.121107000	-1.197881000	2.429429000
H	0.174114000	-0.113411000	2.233192000
C	-1.202525000	-1.482292000	3.123670000
H	-2.047947000	-1.155683000	2.501335000
H	-1.246658000	-0.930541000	4.074120000
H	-1.334829000	-2.550257000	3.354524000
C	1.342823000	-1.571128000	3.253381000
H	1.340581000	-2.625971000	3.563646000
H	1.360974000	-0.958962000	4.166714000
H	2.262947000	-1.360010000	2.691065000
C	0.121657000	-1.197606000	-2.428888000
H	0.175199000	-0.113178000	-2.232599000
C	1.343062000	-1.571323000	-3.253099000
H	2.263386000	-1.361355000	-2.690685000
H	1.361681000	-0.958521000	-4.165994000
H	1.339951000	-2.625939000	-3.564134000
C	-1.202207000	-1.481395000	-3.122946000
H	-1.335198000	-2.549373000	-3.353341000
H	-1.246065000	-0.929989000	-4.073608000
H	-2.047370000	-1.154035000	-2.500652000
C	0.368287000	-4.251260000	1.612012000
H	1.366862000	-4.315732000	2.072324000
H	-0.369576000	-4.206697000	2.425381000
H	0.199262000	-5.187070000	1.063469000
C	0.368875000	-4.251030000	-1.611789000
H	-0.369030000	-4.206630000	-2.425130000
H	1.367456000	-4.315134000	-2.072138000
H	0.200180000	-5.186937000	-1.063311000
C	-1.512642000	3.387553000	0.000557000
C	-0.238906000	2.861286000	0.000503000
B	1.720763000	0.929817000	0.000283000
B	-2.587540000	2.326857000	0.000412000
C	-3.330956000	0.211382000	0.000069000

C	-3.483678000	-1.162720000	-0.000082000
C	-4.421920000	1.088337000	-0.000589000
C	-4.800773000	-1.645285000	-0.000924000
H	-2.621411000	-1.831270000	0.000384000
C	-5.721575000	0.615422000	-0.001394000
C	-5.892852000	-0.776349000	-0.001560000
H	-4.971685000	-2.723867000	-0.001088000
H	-6.568089000	1.303487000	-0.001900000
H	-6.904722000	-1.187086000	-0.002203000
C	3.833886000	0.827541000	0.698634000
C	3.833518000	0.827329000	-0.699200000
C	5.009318000	0.765665000	1.426203000
C	5.008575000	0.765227000	-1.427360000
C	6.205217000	0.701551000	0.697273000
H	4.996213000	0.770518000	2.517456000
C	6.204852000	0.701335000	-0.699033000
H	4.994910000	0.769748000	-2.518608000
H	7.155348000	0.653326000	1.234012000
H	7.154704000	0.652943000	-1.236252000
O	-2.196365000	0.960092000	0.000826000
O	-3.980803000	2.375260000	-0.000310000
O	2.551797000	0.888537000	1.142235000
O	2.551207000	0.888188000	-1.142141000
C	-1.852307000	4.860739000	0.000474000
H	-2.941046000	5.019367000	0.000773000
H	-1.448550000	5.380123000	0.885697000
H	-1.449085000	5.379921000	-0.885114000
C	0.946739000	3.779738000	0.000197000
H	0.707946000	4.855692000	0.000392000
H	1.583227000	3.570052000	0.876764000
H	1.582485000	3.570218000	-0.876954000

I10

Ni	0.439557000	-0.807430000	-1.007746000
C	1.731655000	-0.478111000	0.407038000
N	3.065328000	-0.438658000	0.167460000
C	3.770379000	-0.063723000	1.306182000
C	2.833631000	0.122608000	2.289149000
N	1.599016000	-0.138848000	1.708612000
C	3.583113000	-0.712043000	-1.177364000
H	2.683480000	-1.074038000	-1.706748000
C	4.044382000	0.555663000	-1.880819000
H	3.231424000	1.293428000	-1.922611000
H	4.336416000	0.317978000	-2.914270000
H	4.913104000	1.017429000	-1.387720000
C	4.616769000	-1.827476000	-1.193672000
H	5.588605000	-1.511575000	-0.788353000
H	4.784826000	-2.150253000	-2.231463000
H	4.262563000	-2.697325000	-0.622386000
C	0.274925000	-0.113434000	2.338971000
H	-0.391533000	-0.263711000	1.481662000
C	0.081260000	-1.286862000	3.287005000
H	0.325938000	-2.230573000	2.780145000
H	-0.973477000	-1.337580000	3.595790000
H	0.691313000	-1.198780000	4.199126000
C	-0.077692000	1.233186000	2.952135000
H	0.451678000	1.426176000	3.896599000
H	-1.155711000	1.250267000	3.170065000

H	0.135145000	2.053349000	2.251896000
C	5.249414000	0.063007000	1.396972000
H	5.753198000	-0.915718000	1.363850000
H	5.665787000	0.677225000	0.585667000
H	5.524666000	0.543542000	2.344521000
C	3.040515000	0.539872000	3.701167000
H	2.669363000	1.558982000	3.889741000
H	2.534593000	-0.132353000	4.408815000
H	4.110886000	0.525507000	3.943077000
C	-1.205578000	0.078520000	-3.093686000
C	-0.657707000	-1.071358000	-2.580410000
B	-2.128078000	-1.836832000	0.526452000
B	-0.749678000	1.293140000	-2.324139000
C	0.563675000	2.389807000	-0.874425000
C	1.534848000	2.808730000	0.016658000
C	-0.510457000	3.207457000	-1.240846000
C	1.382387000	4.094624000	0.554671000
H	2.372399000	2.169276000	0.296255000
C	-0.666191000	4.476336000	-0.711754000
C	0.304652000	4.908244000	0.201856000
H	2.124572000	4.462820000	1.266173000
H	-1.510277000	5.103867000	-1.001421000
H	0.215746000	5.903425000	0.642654000
C	-4.002793000	-0.924635000	1.274489000
C	-3.270311000	0.061787000	0.606837000
C	-5.226530000	-0.647777000	1.858584000
C	-3.725527000	1.362794000	0.487516000
C	-5.696323000	0.668378000	1.748782000
H	-5.791972000	-1.424058000	2.376374000
C	-4.963418000	1.650723000	1.078342000
H	-3.147642000	2.115301000	-0.051461000
H	-6.658548000	0.928796000	2.195271000
H	-5.363969000	2.664387000	1.007989000
O	0.455047000	1.214156000	-1.559414000
O	-1.303817000	2.558807000	-2.133658000
O	-3.314665000	-2.094202000	1.231823000
O	-2.117640000	-0.484077000	0.144963000
C	-2.207860000	0.146440000	-4.220965000
H	-2.536794000	1.179807000	-4.406373000
H	-1.792301000	-0.237272000	-5.168400000
H	-3.110273000	-0.449381000	-4.004575000
C	-1.022460000	-2.398461000	-3.170350000
H	-1.421185000	-2.336143000	-4.196171000
H	-0.167128000	-3.091734000	-3.169835000
H	-1.790484000	-2.879960000	-2.541070000
C	-1.031544000	-2.864847000	0.279163000
C	0.096213000	-2.526277000	-0.417647000
C	1.173122000	-3.541851000	-0.673708000
H	1.735621000	-3.326228000	-1.594540000
H	1.903176000	-3.517702000	0.156459000
H	0.793083000	-4.574585000	-0.737305000
C	-1.248299000	-4.262579000	0.828021000
H	-1.290803000	-5.022260000	0.027960000
H	-0.442105000	-4.572871000	1.515201000
H	-2.193510000	-4.328348000	1.385170000

A

Ni	-0.428866000	0.316464000	0.704649000

C	-1.256922000	1.877495000	-0.031080000
N	-1.906710000	2.117954000	-1.204540000
C	-2.413978000	3.413408000	-1.250214000
C	-2.059509000	4.010950000	-0.073453000
N	-1.360085000	3.051051000	0.654585000
C	-2.125478000	1.037754000	-2.168228000
H	-1.448553000	0.254041000	-1.795271000
C	-3.544372000	0.499311000	-2.088904000
H	-3.785328000	0.209264000	-1.059075000
H	-3.636937000	-0.390537000	-2.727783000
H	-4.281188000	1.244120000	-2.428209000
C	-1.740173000	1.397469000	-3.597782000
H	-2.524638000	1.972416000	-4.110102000
H	-1.584728000	0.472843000	-4.172459000
H	-0.810336000	1.979818000	-3.638306000
C	-0.826608000	3.166135000	2.011462000
H	-0.533231000	2.124675000	2.234962000
C	-1.885844000	3.569204000	3.027532000
H	-2.152857000	4.634581000	2.965211000
H	-1.507235000	3.385434000	4.044119000
H	-2.797228000	2.969216000	2.895659000
C	0.424734000	4.027774000	2.068824000
H	1.223996000	3.594613000	1.449709000
H	0.793313000	4.076247000	3.104549000
H	0.241482000	5.060313000	1.736256000
C	1.493461000	0.573671000	0.395522000
N	2.183765000	1.092207000	-0.659000000
C	3.543972000	1.193872000	-0.388094000
C	3.718569000	0.713417000	0.877677000
N	2.462446000	0.344628000	1.337416000
C	1.491086000	1.645516000	-1.820615000
H	0.500417000	1.184804000	-1.738778000
C	1.331872000	3.152500000	-1.695119000
H	0.800987000	3.415393000	-0.770871000
H	0.746008000	3.542260000	-2.541849000
H	2.308151000	3.662754000	-1.701034000
C	2.083262000	1.236413000	-3.160451000
H	2.927490000	1.869572000	-3.464576000
H	1.315192000	1.324083000	-3.942277000
H	2.422476000	0.196006000	-3.130030000
C	2.117963000	-0.120919000	2.681789000
H	1.059398000	-0.387152000	2.543247000
C	2.858095000	-1.366509000	3.139595000
H	2.824966000	-2.143842000	2.367445000
H	2.345515000	-1.767144000	4.026406000
H	3.903767000	-1.181097000	3.425011000
C	2.178413000	1.003219000	3.705769000
H	3.205871000	1.360339000	3.881623000
H	1.772984000	0.648436000	4.665261000
H	1.571428000	1.857229000	3.378253000
C	4.582757000	1.639205000	-1.352638000
H	4.720771000	0.909893000	-2.166031000
H	4.351687000	2.614908000	-1.807718000
H	5.544623000	1.741458000	-0.834008000
C	4.987336000	0.531859000	1.630014000
H	4.948871000	0.983713000	2.632563000
H	5.237043000	-0.533040000	1.749140000
H	5.815488000	1.004498000	1.086823000

C	-3.154843000	3.997015000	-2.399148000
H	-2.523911000	4.087827000	-3.296963000
H	-4.036933000	3.399606000	-2.676733000
H	-3.509905000	5.002997000	-2.141283000
C	-2.334567000	5.398183000	0.385437000
H	-2.734227000	5.993744000	-0.445517000
H	-3.073110000	5.434539000	1.201405000
H	-1.425591000	5.904615000	0.742445000
C	-0.900007000	-1.117485000	1.910512000
C	-1.936639000	-0.425543000	1.531548000
B	0.601379000	-2.281649000	-0.686104000
B	-1.023983000	-2.630470000	-0.416130000
C	-2.724690000	-3.826834000	0.307929000
C	-3.576346000	-4.690956000	0.973576000
C	-3.195370000	-2.911377000	-0.635638000
C	-4.939211000	-4.600778000	0.662029000
H	-3.195051000	-5.402866000	1.706977000
C	-4.539036000	-2.818579000	-0.955247000
C	-5.410102000	-3.685153000	-0.281743000
H	-5.646345000	-5.262114000	1.167546000
H	-4.898133000	-2.100293000	-1.692652000
H	-6.479475000	-3.640854000	-0.499640000
C	2.781135000	-2.581510000	-0.501844000
C	2.497743000	-2.199076000	-1.814961000
C	4.072786000	-2.860035000	-0.085477000
C	3.494581000	-2.132051000	-2.777290000
C	5.089296000	-2.755619000	-1.042933000
H	4.280224000	-3.173240000	0.938565000
C	4.804244000	-2.409952000	-2.365488000
H	3.258263000	-1.896176000	-3.816189000
H	6.119651000	-2.971809000	-0.752646000
H	5.613554000	-2.364754000	-3.097641000
O	-1.379132000	-3.707173000	0.409795000
O	-2.144879000	-2.198618000	-1.121925000
O	1.623977000	-2.656557000	0.192556000
O	1.167255000	-1.977855000	-1.949017000
C	-0.604002000	-2.223273000	2.861403000
H	0.136163000	-2.931380000	2.460006000
H	-0.173883000	-1.823744000	3.798204000
H	-1.508831000	-2.793168000	3.129730000
C	-3.388123000	-0.210617000	1.724643000
H	-3.963309000	-0.613155000	0.875382000
H	-3.773915000	-0.710680000	2.630349000
H	-3.630232000	0.862532000	1.787796000

B

Ni	0.520918000	0.823030000	0.024739000
C	2.343763000	0.633761000	-0.366311000
N	2.833825000	0.452386000	-1.617994000
C	4.224543000	0.404001000	-1.599200000
C	4.603850000	0.551039000	-0.293205000
N	3.427566000	0.694147000	0.439965000
C	1.945680000	0.404335000	-2.790225000
H	0.943725000	0.314085000	-2.346906000
C	1.963956000	1.700880000	-3.584765000
H	1.617763000	2.537357000	-2.965252000
H	1.272065000	1.609450000	-4.434645000
H	2.961765000	1.936179000	-3.986064000

C	2.171468000	-0.820220000	-3.666799000
H	3.048734000	-0.724053000	-4.322100000
H	1.291960000	-0.952031000	-4.313376000
H	2.284523000	-1.734968000	-3.069113000
C	3.272292000	0.860517000	1.885256000
H	2.207757000	1.125604000	1.973888000
C	4.085155000	2.016352000	2.449659000
H	5.151401000	1.772967000	2.556765000
H	3.705881000	2.266178000	3.451520000
H	3.988227000	2.911325000	1.819386000
C	3.496525000	-0.446652000	2.632629000
H	2.821447000	-1.231368000	2.264470000
H	3.295442000	-0.303093000	3.704579000
H	4.533237000	-0.803058000	2.534477000
C	0.340271000	-0.832216000	1.044488000
N	0.700456000	-2.115528000	0.790208000
C	0.488006000	-2.925822000	1.901265000
C	-0.029337000	-2.115360000	2.873607000
N	-0.110961000	-0.842914000	2.323984000
C	1.241859000	-2.530110000	-0.505137000
H	1.064488000	-1.649835000	-1.135894000
C	2.742710000	-2.780024000	-0.430906000
H	3.279243000	-1.890676000	-0.075130000
H	3.130377000	-3.033929000	-1.428557000
H	2.984304000	-3.620551000	0.236552000
C	0.482434000	-3.697971000	-1.122115000
H	0.778277000	-4.666018000	-0.694782000
H	0.697564000	-3.736158000	-2.199764000
H	-0.603387000	-3.574171000	-1.010708000
C	-0.693484000	0.353694000	2.946753000
H	-0.695212000	1.094887000	2.133360000
C	-2.144927000	0.142801000	3.343066000
H	-2.707757000	-0.291528000	2.506418000
H	-2.590014000	1.121708000	3.564091000
H	-2.252720000	-0.490216000	4.235880000
C	0.158354000	0.903981000	4.081680000
H	0.165478000	0.249159000	4.965674000
H	-0.250280000	1.875571000	4.394749000
H	1.197779000	1.064424000	3.766034000
C	0.738381000	-4.390071000	1.964047000
H	-0.022281000	-4.963615000	1.411890000
H	1.722219000	-4.667638000	1.560494000
H	0.705800000	-4.724950000	3.009048000
C	-0.466303000	-2.494684000	4.243266000
H	-0.123187000	-1.780220000	5.003316000
H	-1.562213000	-2.562967000	4.322812000
H	-0.055680000	-3.478610000	4.505228000
C	5.084782000	0.201502000	-2.794577000
H	5.011231000	-0.823035000	-3.190931000
H	4.826315000	0.891592000	-3.610345000
H	6.135150000	0.382131000	-2.532996000
C	5.975360000	0.569430000	0.280356000
H	6.699584000	0.248750000	-0.479309000
H	6.273579000	1.573790000	0.618754000
H	6.077309000	-0.113437000	1.136641000
C	-0.582655000	3.133380000	-0.362197000
C	0.682028000	2.664197000	-0.429824000
B	-1.323569000	0.137197000	-0.609338000

B	-1.645990000	1.982683000	-0.235333000
C	-3.757391000	1.834471000	0.627219000
C	-4.879838000	1.720843000	1.431670000
C	-3.858038000	1.719396000	-0.771028000
C	-6.114859000	1.478271000	0.805895000
H	-4.801756000	1.819684000	2.515970000
C	-5.068985000	1.467886000	-1.391460000
C	-6.208292000	1.351435000	-0.577453000
H	-7.014934000	1.387454000	1.419066000
H	-5.122119000	1.366308000	-2.476926000
H	-7.179468000	1.158950000	-1.039659000
C	-2.675270000	-1.612780000	-0.884287000
C	-1.944002000	-1.439119000	-2.064695000
C	-3.598704000	-2.634008000	-0.745839000
C	-2.112385000	-2.275032000	-3.154731000
C	-3.770520000	-3.490628000	-1.842882000
H	-4.169695000	-2.749973000	0.176560000
C	-3.044721000	-3.314010000	-3.022847000
H	-1.540112000	-2.124858000	-4.071984000
H	-4.494507000	-4.305738000	-1.774952000
H	-3.209492000	-3.993869000	-3.861830000
O	-2.484435000	2.047707000	0.989467000
O	-2.649911000	1.867648000	-1.342592000
O	-2.304831000	-0.673206000	0.012905000
O	-1.095359000	-0.397226000	-1.912746000
C	-1.027470000	4.568074000	-0.328431000
H	-1.533457000	4.783789000	0.627742000
H	-0.210046000	5.294793000	-0.451126000
H	-1.776792000	4.752691000	-1.116521000
C	1.912886000	3.525608000	-0.500657000
H	2.704515000	3.102928000	-1.138889000
H	1.696136000	4.539595000	-0.875452000
H	2.361273000	3.646068000	0.501381000

C

Ni	1.151050000	-0.841180000	-0.718290000
C	2.737314000	0.083764000	-0.163796000
N	4.017033000	-0.361474000	-0.242104000
C	4.900007000	0.533743000	0.344436000
C	4.137204000	1.577399000	0.803831000
N	2.823669000	1.273384000	0.480809000
C	4.314089000	-1.626142000	-0.916824000
H	3.303651000	-2.016618000	-1.133469000
C	5.016486000	-1.407609000	-2.248497000
H	4.445515000	-0.703435000	-2.870672000
H	5.091970000	-2.361868000	-2.790560000
H	6.036946000	-1.014624000	-2.126218000
C	5.014933000	-2.626137000	-0.010247000
H	6.061676000	-2.355574000	0.189358000
H	5.017846000	-3.615708000	-0.490344000
H	4.488236000	-2.715767000	0.951091000
C	1.617572000	2.072738000	0.722431000
H	0.821177000	1.394314000	0.380648000
C	1.370143000	2.338685000	2.197977000
H	1.438841000	1.406456000	2.777742000
H	0.352442000	2.737142000	2.319262000
H	2.067915000	3.073647000	2.625141000
C	1.574795000	3.321157000	-0.144386000

H	2.335576000	4.062247000	0.144584000
H	0.587941000	3.798140000	-0.054478000
H	1.725192000	3.059151000	-1.201421000
C	6.369281000	0.338988000	0.465925000
H	6.627161000	-0.427366000	1.214093000
H	6.831323000	0.041813000	-0.486224000
H	6.844530000	1.276488000	0.782510000
C	4.578533000	2.789980000	1.542498000
H	4.148131000	3.709954000	1.123076000
H	4.300652000	2.749497000	2.607507000
H	5.671142000	2.883017000	1.491897000
C	-0.602070000	-1.536018000	-1.231589000
C	-0.055135000	-2.331242000	-0.194596000
B	-2.603724000	-1.320772000	1.282562000
B	-0.923806000	-0.052927000	-1.038561000
C	-1.732409000	1.890959000	-0.307614000
C	-2.241217000	2.938857000	0.438544000
C	-1.368363000	2.041259000	-1.651274000
C	-2.370066000	4.174611000	-0.212730000
H	-2.531249000	2.792630000	1.480312000
C	-1.493825000	3.258179000	-2.299477000
C	-2.002544000	4.329879000	-1.551188000
H	-2.770968000	5.029116000	0.336946000
H	-1.205555000	3.368638000	-3.345987000
H	-2.117400000	5.305396000	-2.028964000
C	-4.633840000	-0.490720000	1.062221000
C	-4.385189000	-1.354873000	-0.008928000
C	-5.819859000	0.213365000	1.170213000
C	-5.311888000	-1.552046000	-1.017163000
C	-6.764432000	0.020986000	0.153137000
H	-6.000441000	0.886769000	2.009480000
C	-6.515983000	-0.842442000	-0.916412000
H	-5.102800000	-2.226088000	-1.849268000
H	-7.712994000	0.560646000	0.197576000
H	-7.273750000	-0.965622000	-1.693336000
O	-1.485379000	0.619387000	0.079047000
O	-0.901445000	0.865129000	-2.124679000
O	-3.557430000	-0.491375000	1.888029000
O	-3.152261000	-1.900912000	0.138372000
C	-0.819629000	-2.097505000	-2.616877000
H	-0.919113000	-1.291005000	-3.356055000
H	-0.016443000	-2.767977000	-2.958693000
H	-1.758192000	-2.679715000	-2.635423000
C	0.342224000	-3.762180000	-0.489176000
H	-0.560696000	-4.398189000	-0.492828000
H	0.829228000	-3.880033000	-1.466876000
H	1.017226000	-4.166069000	0.277807000
C	-1.229248000	-1.575357000	1.927373000
C	-0.127474000	-2.023099000	1.260655000
C	1.138169000	-2.281253000	2.047219000
H	1.966534000	-2.603014000	1.403139000
H	1.467729000	-1.364184000	2.560879000
H	0.981754000	-3.043292000	2.829909000
C	-1.124977000	-1.226202000	3.392556000
H	-0.814860000	-2.090657000	4.004507000
H	-0.374420000	-0.435078000	3.568414000
H	-2.081606000	-0.863178000	3.790521000

TS1 (Im. Freq.: –110.9 cm^{-1})

Ni	0.339328000	-0.479568000	0.625706000
C	-0.156189000	-2.061698000	-0.272932000
N	0.064864000	-2.449928000	-1.551809000
C	-0.395390000	-3.745667000	-1.770054000
C	-0.917212000	-4.178258000	-0.582086000
N	-0.745427000	-3.132551000	0.323445000
C	0.840060000	-1.596497000	-2.459653000
H	0.934918000	-0.655931000	-1.899238000
C	2.248795000	-2.133056000	-2.655254000
H	2.726700000	-2.296945000	-1.680600000
H	2.848631000	-1.387624000	-3.195720000
H	2.266667000	-3.072810000	-3.228772000
C	0.126728000	-1.290808000	-3.767788000
H	0.129991000	-2.139046000	-4.467606000
H	0.639523000	-0.450879000	-4.257721000
H	-0.915487000	-0.986585000	-3.594942000
C	-1.123014000	-3.078412000	1.738391000
H	-0.586110000	-2.180069000	2.086245000
C	-0.609716000	-4.264079000	2.542722000
H	-1.197407000	-5.178306000	2.378537000
H	-0.673967000	-4.024261000	3.614269000
H	0.443326000	-4.475537000	2.309984000
C	-2.612308000	-2.831507000	1.934454000
H	-2.920658000	-1.893003000	1.454541000
H	-2.834764000	-2.749520000	3.008993000
H	-3.226077000	-3.650572000	1.528418000
C	-1.412204000	0.427070000	0.793642000
N	-2.551956000	0.372402000	0.041647000
C	-3.646291000	0.876752000	0.736165000
C	-3.176332000	1.278853000	1.954397000
N	-1.818041000	1.003052000	1.959844000
C	-2.574049000	-0.114058000	-1.340493000
H	-1.508382000	-0.174498000	-1.594249000
C	-3.182681000	-1.503833000	-1.468522000
H	-2.664392000	-2.237063000	-0.842757000
H	-3.109415000	-1.839228000	-2.513958000
H	-4.249062000	-1.506372000	-1.196334000
C	-3.245666000	0.862731000	-2.300746000
H	-4.334583000	0.721364000	-2.340486000
H	-2.859819000	0.694858000	-3.316311000
H	-3.035199000	1.906511000	-2.038398000
C	-0.874668000	1.291869000	3.039644000
H	0.085651000	1.023528000	2.579276000
C	-0.816261000	2.769877000	3.391327000
H	-0.686414000	3.365645000	2.476873000
H	0.057513000	2.948216000	4.035375000
H	-1.702718000	3.125425000	3.936419000
C	-1.069933000	0.368876000	4.232737000
H	-2.017855000	0.541348000	4.764653000
H	-0.253010000	0.523359000	4.953052000
H	-1.040352000	-0.682384000	3.910260000
C	-5.036804000	0.979719000	0.218156000
H	-5.157692000	1.812406000	-0.491799000
H	-5.365545000	0.060847000	-0.286946000
H	-5.726602000	1.158720000	1.053610000
C	-3.931471000	1.928891000	3.058636000
H	-3.676758000	1.512062000	4.042278000

H	-3.749041000	3.014239000	3.102243000
H	-5.009550000	1.785032000	2.907846000
C	-0.347035000	-4.454281000	-3.075784000
H	-1.012339000	-3.991502000	-3.821644000
H	0.666170000	-4.469806000	-3.502933000
H	-0.664913000	-5.497026000	-2.948486000
C	-1.562874000	-5.480811000	-0.270022000
H	-1.760725000	-6.030072000	-1.199564000
H	-0.931568000	-6.122235000	0.364517000
H	-2.526579000	-5.351788000	0.244855000
C	1.888310000	0.020173000	1.767182000
C	1.883354000	-1.216486000	1.323796000
B	0.685404000	1.923757000	-0.585966000
B	2.066264000	1.213080000	0.091003000
C	4.224221000	1.693913000	0.437375000
C	5.438722000	2.130216000	0.939130000
C	4.151778000	0.640176000	-0.490896000
C	6.599544000	1.479233000	0.489537000
H	5.479747000	2.951075000	1.657531000
C	5.293915000	-0.005412000	-0.935133000
C	6.528348000	0.432874000	-0.427870000
H	7.572904000	1.799716000	0.868487000
H	5.227894000	-0.822199000	-1.656654000
H	7.446898000	-0.057021000	-0.759845000
C	-0.852876000	3.454049000	-1.037895000
C	-0.530493000	2.791245000	-2.227145000
C	-1.806297000	4.457830000	-1.003865000
C	-1.099736000	3.143651000	-3.438030000
C	-2.409180000	4.803113000	-2.221940000
H	-2.060393000	4.961032000	-0.069564000
C	-2.054772000	4.168706000	-3.415481000
H	-0.820900000	2.631172000	-4.360225000
H	-3.160957000	5.595400000	-2.238700000
H	-2.532714000	4.475093000	-4.348549000
O	2.988563000	2.155190000	0.709516000
O	2.871248000	0.420919000	-0.835454000
O	-0.100363000	2.953121000	-0.031961000
O	0.388145000	1.832236000	-1.961373000
C	2.505053000	0.671398000	2.967117000
H	2.274239000	1.743647000	3.027178000
H	2.151044000	0.180498000	3.889316000
H	3.604115000	0.584478000	2.946581000
C	2.658230000	-2.467596000	1.417312000
H	3.492085000	-2.427156000	0.695117000
H	3.112357000	-2.595462000	2.415489000
H	2.063583000	-3.362150000	1.176606000

TS1' (Im. Freq.: –334.0 cm^{-1})

Ni	-0.107485000	0.554890000	-0.776486000
C	1.196229000	1.983787000	-0.474035000
N	2.518561000	1.988637000	-0.155672000
C	3.051888000	3.272611000	-0.189326000
C	2.025267000	4.105655000	-0.535180000
N	0.907811000	3.296025000	-0.703042000
C	3.243233000	0.743789000	0.097226000
H	2.437591000	0.000819000	0.139282000
C	4.151556000	0.370267000	-1.065644000
H	3.591383000	0.398362000	-2.009969000

H	4.534909000	-0.650921000	-0.921061000
H	5.018812000	1.041849000	-1.154487000
C	3.962038000	0.734760000	1.437610000
H	4.840008000	1.394704000	1.454024000
H	4.314778000	-0.284190000	1.646107000
H	3.285269000	1.035377000	2.249771000
C	-0.448504000	3.730159000	-1.034019000
H	-0.976761000	2.773005000	-1.163626000
C	-0.528588000	4.482558000	-2.353936000
H	-0.134623000	5.506711000	-2.291262000
H	-1.581054000	4.556967000	-2.666043000
H	0.019024000	3.943276000	-3.140617000
C	-1.099206000	4.458565000	0.133631000
H	-1.119134000	3.811360000	1.022227000
H	-2.137355000	4.723547000	-0.114035000
H	-0.575818000	5.390723000	0.392308000
C	-1.528486000	0.971669000	0.462087000
N	-1.328889000	0.917409000	1.805304000
C	-2.523038000	1.053272000	2.502625000
C	-3.502437000	1.205079000	1.562124000
N	-2.868646000	1.153112000	0.324651000
C	-0.002992000	0.663617000	2.373963000
H	0.610201000	0.470851000	1.481472000
C	0.552769000	1.902041000	3.062490000
H	0.611808000	2.744419000	2.357414000
H	1.567489000	1.700065000	3.435736000
H	-0.054994000	2.214600000	3.924611000
C	0.044986000	-0.600404000	3.216941000
H	-0.473243000	-0.496290000	4.180693000
H	1.096118000	-0.843046000	3.431243000
H	-0.379828000	-1.437394000	2.646264000
C	-3.512140000	1.171936000	-0.988412000
H	-2.673436000	0.954697000	-1.663110000
C	-4.536994000	0.056150000	-1.142522000
H	-4.132537000	-0.902391000	-0.785984000
H	-4.799849000	-0.052473000	-2.204672000
H	-5.468538000	0.264934000	-0.598158000
C	-4.073688000	2.539276000	-1.354858000
H	-4.927764000	2.827900000	-0.724622000
H	-4.425922000	2.522674000	-2.396980000
H	-3.307767000	3.321085000	-1.267799000
C	-2.678231000	0.983815000	3.980368000
H	-1.913183000	1.565174000	4.512889000
H	-3.658124000	1.386285000	4.269657000
H	-2.626412000	-0.051213000	4.353465000
C	-4.967302000	1.336747000	1.782131000
H	-5.422289000	2.107611000	1.145240000
H	-5.498522000	0.390455000	1.592738000
H	-5.161509000	1.617286000	2.825928000
C	4.463671000	3.633058000	0.111308000
H	4.698527000	3.546413000	1.183609000
H	5.180619000	3.004955000	-0.435962000
H	4.651673000	4.673353000	-0.183725000
C	2.065757000	5.578562000	-0.741609000
H	1.988134000	5.852633000	-1.805442000
H	1.260485000	6.101698000	-0.206635000
H	3.016486000	5.979481000	-0.367716000
C	-0.848764000	-0.811338000	-1.885915000

C	0.525559000	-0.855671000	-1.955019000
B	1.268001000	-2.293685000	-0.604767000
B	-0.447128000	-2.125964000	-0.976767000
C	-2.196794000	-2.771206000	0.260384000
C	-3.288307000	-2.805369000	1.114267000
C	-2.169599000	-3.544084000	-0.922738000
C	-4.370265000	-3.636415000	0.771645000
H	-3.295723000	-2.193537000	2.019348000
C	-3.234599000	-4.364650000	-1.257009000
C	-4.342499000	-4.401102000	-0.390727000
H	-5.242576000	-3.679754000	1.428659000
H	-3.204145000	-4.957670000	-2.173212000
H	-5.193430000	-5.040062000	-0.639200000
C	2.892286000	-2.686686000	0.849950000
C	3.251217000	-3.250766000	-0.377534000
C	3.704416000	-2.794621000	1.966248000
C	4.449403000	-3.921755000	-0.551011000
C	4.918680000	-3.474302000	1.801817000
H	3.403136000	-2.371476000	2.925813000
C	5.285302000	-4.020905000	0.569068000
H	4.716410000	-4.356096000	-1.515504000
H	5.589086000	-3.582737000	2.657189000
H	6.238675000	-4.545850000	0.477855000
O	-1.070359000	-2.059690000	0.398336000
O	-1.026554000	-3.348328000	-1.602968000
O	1.689098000	-2.076397000	0.719683000
O	2.261724000	-3.016861000	-1.274448000
C	-1.824434000	-0.956897000	-3.015653000
H	-1.920334000	-0.021478000	-3.593284000
H	-1.493257000	-1.744931000	-3.711814000
H	-2.825359000	-1.246340000	-2.670766000
C	1.356518000	-1.178188000	-3.160012000
H	1.061725000	-2.127897000	-3.633022000
H	1.142310000	-0.366577000	-3.875747000
H	2.437451000	-1.203754000	-2.977667000

TS2 (Im. Freq.: –63.5 cm^{-1})

Ni	0.597632000	-0.682727000	-0.353395000
C	2.448203000	-0.694439000	0.112289000
N	2.877279000	-1.090395000	1.337909000
C	4.264114000	-1.017257000	1.425625000
C	4.707142000	-0.549768000	0.218558000
N	3.570455000	-0.364563000	-0.565769000
C	1.931726000	-1.579760000	2.353760000
H	0.950065000	-1.305947000	1.937093000
C	1.949934000	-3.094847000	2.483427000
H	1.657112000	-3.566920000	1.537675000
H	1.217813000	-3.398095000	3.246026000
H	2.935208000	-3.478860000	2.790132000
C	2.077040000	-0.880803000	3.699034000
H	2.913158000	-1.271423000	4.296500000
H	1.155597000	-1.041844000	4.276831000
H	2.212153000	0.203217000	3.583762000
C	3.480752000	0.132654000	-1.937407000
H	2.430426000	-0.078933000	-2.187919000
C	4.354632000	-0.638693000	-2.915282000
H	5.417300000	-0.368914000	-2.839080000
H	4.033528000	-0.411375000	-3.942616000

H	4.253153000	-1.722281000	-2.761107000
C	3.684070000	1.639530000	-2.009743000
H	2.968558000	2.161880000	-1.359436000
H	3.523091000	1.989701000	-3.040246000
H	4.703361000	1.932293000	-1.714691000
C	0.432297000	1.215613000	-0.533791000
N	0.738161000	2.261229000	0.274772000
C	0.518897000	3.475159000	-0.371138000
C	0.056921000	3.166708000	-1.620917000
N	0.009386000	1.780568000	-1.694962000
C	1.218273000	2.053689000	1.640206000
H	1.091088000	0.972381000	1.776974000
C	2.699552000	2.381031000	1.774139000
H	3.299282000	1.790401000	1.068127000
H	3.045122000	2.145365000	2.791588000
H	2.905125000	3.447364000	1.598710000
C	0.351153000	2.745538000	2.682792000
H	0.531134000	3.828508000	2.733977000
H	0.578488000	2.327873000	3.674632000
H	-0.716365000	2.570434000	2.488636000
C	-0.521538000	0.958423000	-2.790645000
H	-0.527155000	-0.057490000	-2.360245000
C	-1.962676000	1.304696000	-3.128046000
H	-2.564401000	1.355862000	-2.211376000
H	-2.376024000	0.499788000	-3.750687000
H	-2.052470000	2.247170000	-3.687804000
C	0.383324000	0.949962000	-4.014250000
H	0.408231000	1.922741000	-4.528186000
H	0.008795000	0.206345000	-4.732539000
H	1.413437000	0.673647000	-3.753531000
C	0.713885000	4.819357000	0.233301000
H	-0.079443000	5.067283000	0.955947000
H	1.677689000	4.912266000	0.753435000
H	0.689743000	5.585263000	-0.552931000
C	-0.353486000	4.098855000	-2.703892000
H	0.045058000	3.798794000	-3.682632000
H	-1.448335000	4.166844000	-2.798284000
H	0.021728000	5.108106000	-2.489214000
C	5.060985000	-1.368591000	2.630627000
H	4.927426000	-0.639931000	3.445186000
H	4.794585000	-2.359229000	3.026241000
H	6.128824000	-1.392935000	2.378252000
C	6.102372000	-0.284568000	-0.221695000
H	6.779289000	-0.328059000	0.641197000
H	6.456952000	-1.023003000	-0.957599000
H	6.213271000	0.712580000	-0.672944000
C	-0.556598000	-3.057485000	-1.159771000
C	0.651289000	-2.555166000	-0.802760000
B	-1.190832000	-0.301344000	0.415041000
B	-1.761287000	-2.129693000	-0.844571000
C	-3.782544000	-1.347717000	-1.418515000
C	-4.868855000	-0.736479000	-2.021058000
C	-3.861892000	-1.847560000	-0.110982000
C	-6.049557000	-0.636154000	-1.268806000
H	-4.803072000	-0.348611000	-3.038901000
C	-5.018509000	-1.744173000	0.640707000
C	-6.122804000	-1.128052000	0.034755000
H	-6.927372000	-0.162792000	-1.715268000

H	-5.052307000	-2.115960000	1.665888000
H	-7.053931000	-1.028223000	0.597142000
C	-2.880740000	0.910777000	1.248354000
C	-2.215844000	0.302108000	2.317102000
C	-3.993663000	1.709372000	1.439778000
C	-2.635515000	0.475346000	3.625069000
C	-4.425090000	1.890618000	2.761035000
H	-4.516722000	2.153181000	0.591506000
C	-3.759818000	1.287635000	3.830920000
H	-2.112490000	-0.008372000	4.451991000
H	-5.304443000	2.508830000	2.955460000
H	-4.125491000	1.445174000	4.848246000
O	-2.540406000	-1.550089000	-1.904031000
O	-2.668880000	-2.370654000	0.245058000
O	-2.262405000	0.572115000	0.093621000
O	-1.172497000	-0.415447000	1.839991000
C	-0.838808000	-4.355691000	-1.872677000
H	-1.267272000	-4.163082000	-2.871796000
H	0.048447000	-4.990712000	-2.010656000
H	-1.595005000	-4.945264000	-1.326189000
C	1.932366000	-3.297439000	-1.105498000
H	2.688853000	-3.195910000	-0.312468000
H	1.785814000	-4.376507000	-1.278649000
H	2.400870000	-2.890929000	-2.019855000

TS3 (Im. Freq.: –156.2 cm^{-1})

Ni	0.589049000	-0.165065000	-0.685433000
C	2.003438000	1.048134000	-0.213658000
N	2.958566000	1.651624000	-0.979016000
C	3.845260000	2.395475000	-0.207277000
C	3.439461000	2.251934000	1.088353000
N	2.315337000	1.430734000	1.057185000
C	2.890322000	1.613496000	-2.435781000
H	2.142865000	0.833020000	-2.618623000
C	2.335881000	2.920102000	-2.986842000
H	1.358487000	3.133272000	-2.529852000
H	2.202313000	2.847704000	-4.076501000
H	3.007561000	3.769594000	-2.790814000
C	4.184059000	1.174949000	-3.107416000
H	4.955715000	1.957034000	-3.111692000
H	3.973179000	0.920323000	-4.156605000
H	4.599580000	0.280660000	-2.621313000
C	1.548606000	0.953818000	2.206983000
H	0.698420000	0.439972000	1.733531000
C	0.985567000	2.089044000	3.046935000
H	1.760156000	2.639315000	3.598175000
H	0.290568000	1.679375000	3.793330000
H	0.423147000	2.791586000	2.416879000
C	2.338077000	-0.066662000	3.016687000
H	2.674509000	-0.893526000	2.375980000
H	1.705317000	-0.490345000	3.810257000
H	3.218631000	0.377332000	3.504198000
C	1.096633000	-1.741265000	0.303754000
N	2.278484000	-2.406512000	0.172932000
C	2.379238000	-3.458603000	1.077423000
C	1.219137000	-3.450367000	1.801540000
N	0.456964000	-2.395108000	1.312986000
C	3.236206000	-2.015434000	-0.857828000

H	2.765604000	-1.110539000	-1.274474000
C	4.582109000	-1.608445000	-0.277538000
H	4.451266000	-0.832251000	0.491130000
H	5.217250000	-1.190305000	-1.072280000
H	5.129447000	-2.453559000	0.163707000
C	3.324588000	-3.039360000	-1.980089000
H	3.804850000	-3.978214000	-1.666084000
H	3.916207000	-2.628400000	-2.812179000
H	2.318966000	-3.273321000	-2.358484000
C	-0.927870000	-2.065672000	1.658610000
H	-1.104555000	-1.127437000	1.113342000
C	-1.887729000	-3.104136000	1.097525000
H	-1.721282000	-3.231153000	0.018086000
H	-2.925933000	-2.774274000	1.241716000
H	-1.772570000	-4.085673000	1.582410000
C	-1.148127000	-1.789380000	3.137987000
H	-1.107201000	-2.695100000	3.759226000
H	-2.146283000	-1.346769000	3.267078000
H	-0.409927000	-1.071459000	3.522968000
C	3.554072000	-4.358481000	1.224921000
H	3.901693000	-4.753587000	0.260055000
H	4.409883000	-3.856174000	1.704314000
H	3.288184000	-5.218519000	1.853397000
C	0.832116000	-4.339702000	2.928602000
H	0.863311000	-3.817888000	3.898324000
H	-0.179837000	-4.751769000	2.807668000
H	1.527355000	-5.187100000	2.990553000
C	5.008780000	3.159926000	-0.730875000
H	5.804457000	2.500848000	-1.112579000
H	4.728935000	3.844761000	-1.544730000
H	5.443451000	3.770627000	0.070727000
C	4.035645000	2.867445000	2.305015000
H	5.019468000	3.288894000	2.061483000
H	3.416865000	3.686308000	2.704171000
H	4.185397000	2.141523000	3.116501000
C	-1.351036000	1.851555000	-1.879257000
C	-0.466680000	0.772671000	-1.991571000
B	-1.645960000	-0.651975000	-1.420911000
B	-1.952412000	2.182517000	-0.525875000
C	-2.490246000	2.084639000	1.613747000
C	-2.607796000	1.792227000	2.961858000
C	-3.444416000	2.867521000	0.951713000
C	-3.713585000	2.325045000	3.639675000
H	-1.874682000	1.164638000	3.467998000
C	-4.536943000	3.401151000	1.613188000
C	-4.656371000	3.115529000	2.980305000
H	-3.839089000	2.113057000	4.703891000
H	-5.271198000	4.008134000	1.081240000
H	-5.507254000	3.514745000	3.536888000
C	-3.769251000	-1.153685000	-1.008044000
C	-3.405291000	-1.738828000	-2.225132000
C	-5.044572000	-1.282463000	-0.487378000
C	-4.303346000	-2.481469000	-2.970499000
C	-5.961514000	-2.033654000	-1.237132000
H	-5.313796000	-0.809249000	0.458660000
C	-5.598828000	-2.620957000	-2.450482000
H	-4.008425000	-2.933200000	-3.919009000
H	-6.980763000	-2.157419000	-0.864187000

H	-6.338087000	-3.199067000	-3.009479000
O	-1.535434000	1.704368000	0.732020000
O	-3.108972000	2.964999000	-0.354471000
O	-2.699867000	-0.509038000	-0.487181000
O	-2.102482000	-1.454621000	-2.483229000
C	-1.826244000	2.625839000	-3.083689000
H	-2.571448000	3.384529000	-2.805977000
H	-1.001119000	3.147597000	-3.601979000
H	-2.293448000	1.968455000	-3.838768000
C	-0.037136000	0.394147000	-3.401073000
H	0.457741000	1.238341000	-3.904154000
H	0.641903000	-0.473274000	-3.410527000
H	-0.902001000	0.119685000	-4.026791000

TS4 (Im. Freq.: –210.5 cm^{-1})

Ni	-0.036034000	-1.533729000	-0.409628000
C	-1.750368000	-0.667202000	-0.721231000
N	-2.985415000	-1.152368000	-0.450008000
C	-3.974260000	-0.291399000	-0.899143000
C	-3.324935000	0.763663000	-1.487443000
N	-1.969189000	0.509674000	-1.358099000
C	-3.156786000	-2.447826000	0.208461000
H	-2.122613000	-2.720389000	0.468305000
C	-3.951601000	-2.340362000	1.501351000
H	-3.590363000	-1.493306000	2.102441000
H	-3.819897000	-3.259937000	2.089895000
H	-5.029403000	-2.214422000	1.325801000
C	-3.680115000	-3.507663000	-0.750206000
H	-4.714883000	-3.314540000	-1.069712000
H	-3.663613000	-4.491586000	-0.258546000
H	-3.046837000	-3.562945000	-1.647679000
C	-0.845358000	1.287299000	-1.901390000
H	0.020398000	0.929002000	-1.323987000
C	-0.970854000	2.787124000	-1.681037000
H	-1.623780000	3.275166000	-2.417541000
H	0.025679000	3.238370000	-1.785684000
H	-1.333280000	3.023612000	-0.671815000
C	-0.598808000	0.927394000	-3.358999000
H	-0.443637000	-0.155959000	-3.471399000
H	0.308064000	1.436546000	-3.716747000
H	-1.438842000	1.227002000	-4.006132000
C	0.471081000	-1.228015000	1.470079000
C	1.950568000	-1.502420000	1.492988000
B	-0.015579000	0.218887000	1.636438000
O	0.751944000	1.382704000	1.547896000
O	-1.348916000	0.571531000	1.928121000
C	-0.102170000	2.422187000	1.695811000
C	-1.392832000	1.925764000	1.914511000
C	0.157947000	3.779201000	1.625666000
C	-2.482349000	2.768653000	2.049655000
C	-0.939129000	4.639904000	1.767447000
H	1.170764000	4.145381000	1.450529000
C	-2.230709000	4.146194000	1.970430000
H	-3.486083000	2.370748000	2.207780000
H	-0.780575000	5.719161000	1.713606000
H	-3.062304000	4.846842000	2.073496000
B	2.409079000	-1.125943000	-0.262352000
O	3.876648000	-1.065655000	-0.441000000

O	1.937237000	0.189889000	-0.740715000
C	4.190330000	0.214989000	-0.692817000
C	3.022266000	0.979230000	-0.858135000
C	5.442927000	0.795295000	-0.797049000
C	3.078289000	2.337181000	-1.114654000
C	5.506615000	2.173659000	-1.065579000
H	6.344612000	0.193377000	-0.668988000
C	4.348778000	2.930616000	-1.219599000
H	2.163804000	2.923050000	-1.223216000
H	6.483132000	2.656538000	-1.149572000
H	4.424286000	4.001776000	-1.421270000
C	-3.919649000	1.963473000	-2.132255000
H	-3.497616000	2.146259000	-3.131038000
H	-5.001610000	1.822115000	-2.251413000
H	-3.766075000	2.872671000	-1.531617000
C	-5.437021000	-0.491698000	-0.722128000
H	-5.759502000	-1.503040000	-1.006597000
H	-5.754967000	-0.321545000	0.318567000
H	-5.988642000	0.217848000	-1.352210000
C	2.798524000	-1.013662000	2.631733000
H	3.868093000	-1.182900000	2.437028000
H	2.657128000	0.068474000	2.771773000
H	2.543168000	-1.506555000	3.588013000
C	-0.309525000	-2.241756000	2.306260000
H	-1.382999000	-2.015109000	2.350448000
H	-0.182231000	-3.273785000	1.943605000
H	0.056477000	-2.221160000	3.350335000
C	1.637552000	-2.520878000	-0.524538000
C	2.249746000	-2.684700000	0.750227000
C	3.336176000	-3.651694000	1.069674000
H	4.295844000	-3.214404000	0.748468000
H	3.396724000	-3.852856000	2.148712000
H	3.199986000	-4.596580000	0.524549000
C	1.742810000	-3.510426000	-1.647192000
H	1.454326000	-4.531309000	-1.344379000
H	1.093681000	-3.227212000	-2.494004000
H	2.769145000	-3.556359000	-2.053717000

TS5 (Im. Freq.: –179.5 cm^{-1})

Ni	1.026143000	-0.732386000	-0.833280000
C	2.120610000	0.290926000	0.328154000
N	3.460000000	0.488438000	0.210331000
C	3.954064000	1.254415000	1.260870000
C	2.881405000	1.539508000	2.062873000
N	1.775798000	0.946006000	1.465716000
C	4.176272000	-0.040383000	-0.948918000
H	3.397038000	-0.653801000	-1.437504000
C	4.574051000	1.060011000	-1.921952000
H	3.697913000	1.667808000	-2.191298000
H	4.979738000	0.617086000	-2.843701000
H	5.344768000	1.727279000	-1.507434000
C	5.323480000	-0.962966000	-0.566776000
H	6.185225000	-0.419577000	-0.153223000
H	5.674110000	-1.500681000	-1.460075000
H	4.991801000	-1.708256000	0.170595000
C	0.395097000	0.895339000	1.952837000
H	-0.132072000	0.416802000	1.115950000
C	0.255291000	-0.021088000	3.158979000

H	0.677695000	-1.010570000	2.935695000
H	-0.810066000	-0.156892000	3.397938000
H	0.747088000	0.384817000	4.056491000
C	-0.225545000	2.268219000	2.159880000
H	0.158161000	2.782219000	3.053214000
H	-1.311902000	2.150512000	2.287466000
H	-0.063504000	2.910851000	1.282711000
C	5.378273000	1.641818000	1.443505000
H	6.016071000	0.780678000	1.698205000
H	5.802296000	2.112319000	0.544151000
H	5.465018000	2.367929000	2.261939000
C	2.846483000	2.338814000	3.316343000
H	2.325347000	3.299527000	3.181969000
H	2.344206000	1.803332000	4.134927000
H	3.868880000	2.560134000	3.648585000
C	-0.989431000	-1.664003000	-2.316510000
C	0.084817000	-2.317045000	-1.736211000
B	-1.604517000	-1.901592000	0.947615000
B	-1.314446000	-0.189684000	-2.076704000
C	-0.912250000	1.982394000	-1.809936000
C	-0.379263000	3.228277000	-1.537015000
C	-2.247066000	1.808038000	-2.190813000
C	-1.246730000	4.322946000	-1.657110000
H	0.665974000	3.340814000	-1.244666000
C	-3.106731000	2.885630000	-2.317591000
C	-2.579519000	4.154561000	-2.039122000
H	-0.870754000	5.327021000	-1.449366000
H	-4.146749000	2.741454000	-2.614075000
H	-3.227155000	5.029748000	-2.124233000
C	-3.507942000	-1.223785000	1.865905000
C	-3.114301000	-0.261586000	0.929875000
C	-4.648674000	-1.064210000	2.635107000
C	-3.829798000	0.907521000	0.740321000
C	-5.386639000	0.110798000	2.442144000
H	-4.945626000	-1.824135000	3.359486000
C	-4.983212000	1.077122000	1.518592000
H	-3.507245000	1.662257000	0.023345000
H	-6.292439000	0.274405000	3.030282000
H	-5.575704000	1.986567000	1.397122000
O	-0.311927000	0.763903000	-1.787666000
O	-2.498905000	0.487392000	-2.378064000
O	-2.610718000	-2.233357000	1.878376000
O	-1.960021000	-0.671604000	0.335631000
C	-1.836568000	-2.330083000	-3.381416000
H	-2.749134000	-1.745847000	-3.568117000
H	-1.314457000	-2.424535000	-4.350653000
H	-2.143254000	-3.344997000	-3.080228000
C	0.527370000	-3.602656000	-2.400360000
H	0.210269000	-3.644064000	-3.450305000
H	1.619500000	-3.709738000	-2.382485000
H	0.110255000	-4.487075000	-1.889514000
C	-0.332033000	-2.688441000	0.792955000
C	0.682300000	-2.389653000	-0.145871000
C	1.964421000	-3.189353000	-0.002710000
H	2.710007000	-2.933645000	-0.766616000
H	2.400691000	-2.941309000	0.977126000
H	1.815804000	-4.282734000	-0.019781000
C	-0.117762000	-3.795110000	1.799132000

H	0.080295000	-4.769334000	1.317276000
H	0.744318000	-3.606852000	2.466756000
H	-1.000438000	-3.923970000	2.439832000

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