Supporting Information

Unsymmetrical β-Diketiminate Magnesium(I) Complexes: Syntheses and Application in Catalytic Hydroboration of Alkyne, Nitrile and Carbonyl Compounds

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Syntheses

General Methods: All air-sensitive compounds were carried out using standard Schlenk-line or glovebox techniques under high-purity argon. Diethyl ether, toluene, THF and hexane were dried and distilled from molten sodium. ^{1}H, ^{13}C{^{1}H} and ^{11}B NMR spectra were recorded at 25 ℃ with a Bruker Avance III 600 MHz spectrometer and were referenced to the resonances of the solvent used. Elemental analysis was performed by the Elemental Analysis Laboratory of the Advanced Analysis and Testing Center at Nanjing Forestry University. Melting points were determined with an INESA-WRR apparatus and are uncorrected. Ligands **2b**, **2d** and 2-diphenylmethyl-4,6-dimethylaniline were prepared according to literature procedures.[S1-3] Other reagents were used as received.

Synthesis of ligand (^{DipMes}NacnacH) (2a)

2,6-Diisopropylaniline (7.39 mL, 39.17 mmol) was mixed with acetylacetone (4.02 mL, 39.17 mmol) and a catalytic amount of *p*-toluenesulfonic acid monohydrate (0.32 g, 1.7 mmol) in 120 mL of toluene. The solution was refluxed (160 ℃) for 8 h with a Dean-Stark apparatus under argon. Without separation of **1**, subsequently 2,4,6-trimethylaniline (5.5 mL, 39.17 mmol) and *p*-toluenesulfonic acid monohydrate (7.45 g, 39.17 mmol) were added into the above mixture and refluxed for 24 h. The solvent was removed under reduced pressure to give a yellow solid. The obtained solid was treated with diethyl ether (100 mL), water (100 mL) and sodium carbonate (8.6 g). After complete dissolution, the aqueous phase was separated and extracted with diethyl ether (2 x 50 mL). The combined organic phases were dried over $MgSO_4$, filtered and dried under vacuum to afford a yellow solid. Yellow crystals of **2a** (Yield 9.30 g, 63%) were obtained after recrystallization from methanol. M.p. 104-106 ℃. ^{1}H NMR ($CDCl_3$, 600 MHz): δ 12.27 (s, 1 H, N*H*), 7.13 (s, 3 H, Ar-*H*), 6.89 (s, 2 H, Ar-*H*), 4.89 (s, 1 H, =C*H*), 3.08 (sept, $^{3}J_{HH}$ = 6.6 Hz, 2 H, C*H*(CH_3)$_2$), 2.28 (s, 3 H, C*H*$_3$), 2.16 (s, 6 H, C*H*$_3$), 1.73 (s, 3 H, NCC*H*$_3$), 1.72 (s, 3 H, NCC*H*$_3$), 1.24 (d, $^{3}J_{HH}$ = 6.6 Hz, 6 H, CH(C*H*$_3$)$_2$), 1.14 (d, $^{3}J_{HH}$ = 6.6 Hz, 6H, CH(C*H*$_3$)$_2$). ^{13}C{^{1}H} NMR ($CDCl_3$, 151 MHz): δ 161.7 (N*C*CH$_3$), 160.4 (N*C*CH$_3$), 141.7, 141.6, 140.4, 134.0,

132.5, 128.5, 124.7, 122.9 (Ar-*C*), 93.2 (=*C*H), 28.3 (*C*H(CH_3)$_2$), 24.2, 22.8, 20.9, 20.8, 20.2, 18.1 (*C*H_3). HRMS (ESI): m/z Calcd. for $C_{26}H_{37}N_2$ [M^++H]: 377.2957; Found: 377.2962.

Synthesis of ligand ($^{DipXyl'}$NacnacH) 2c

The ligand **2c** was synthesized by using a similar procedure to that employed for the preparation of **2a**, but by using 2,4-dimethylaniline (5.03 g, 41.48 mmoL). The yellow ligand was solidified from methanol (Yield 7.50 g, 50%). M.p. 88-90 ℃. ^{1}H NMR ($CDCl_3$, 600 MHz): δ 12.41 (s, 1 H, N*H*), 7.12–6.83 (m, 6 H, Ar-*H*), 4.86 (s, 1 H, =C*H*), 3.03 (sept, $^3J_{HH}$ = 6.6 Hz, 2 H, C*H*(CH_3)$_2$), 2.28 (s, 3 H, CH_3), 2.15 (s, 6 H, CH_3), 1.90 (s, 3 H, NCCH_3), 1.69 (s, 3 H, NCCH_3), 1.20 (d, $^3J_{HH}$ = 6.6 Hz, 6 H, CH(CH_3)$_2$), 1.10 (d, $^3J_{HH}$ = 6.6 Hz, 6H, CH(CH_3)$_2$). ^{13}C{^{1}H} NMR ($CDCl_3$, 151 MHz): δ 162.6 (N*C*CH_3), 158.2 (N*C*CH_3), 142.4, 141.2, 140.7, 133.5, 131.4, 131.0, 126.7, 124.4, 123.8, 122.9 (Ar-*C*), 94.8 (=*C*H), 28.2 (*C*H(CH_3)$_2$), 24.2, 22.9, 21.0, 20.8, 20.6, 18.1 (*C*H_3). HRMS (ESI): m/z Calcd. for $C_{25}H_{35}N_2$ [M^++H]: 363.2800; Found: 363.2821.

Synthesis of (^{DipMes}Nacnac)MgI(Et_2O) (3a)

MeMgI (2.23 mL, 3 M in Et_2O, 6.69 mmol) was added dropwise to a solution of ligand **2a** (2.50 g, 6.65 mmol) in diethyl ether (30 mL) at –70 ℃. The mixture was warmed to room temperature and stirred for overnight to yield a colorless precipitate. The precipitate of **3a** was collected by filtration. The supernatant solution was concentrated to ca. 10 mL and cooled to –30 ℃ to afford a second crop. (Yield 3.10 g, 80%). M.p. 204-206 ℃. ^{1}H NMR (C_6D_6, 600 MHz): δ 7.13 (s, 3 H, Ar-*H*), 6.83 (s, 2 H, Ar-*H*), 4.90 (s, 1 H, =C*H*), 3.31 (m, 6 H, C*H*(CH_3)$_2$ + OC$H_2$$CH_3$ overlap), 2.54 (br s, 3 H, Ar-CH_3), 2.19 (s, 6 H, Ar-CH_3), 1.68 (s, 3 H, NCCH_3), 1.59 (s, 3 H, NCCH_3), 1.19 (br, 12 H, CH(CH_3)$_2$), 0.62 (br, 6 H, OCH$_2$CH_3). ^{13}C{^{1}H} NMR (C_6D_6, 151 MHz): δ 169.4 (N*C*CH_3), 168.6 (N*C*CH_3), 144.6, 143.5, 141.8, 133.2, 129.8, 128.7, 125.4, 124.4, 123.4 (Ar-*C*), 95.0 (=*C*H), 65.7 (O*C*$H_2$$CH_3$), 28.0 (*C*H($CH_3$)$_2$), 27.7, 26.1, 24.4, 24.1, 23.2, 20.6, 18.5 (*C*H_3), 12.8 (OCH$_2$*C*H_3). Anal. Calc. for

$C_{30}H_{45}IMgN_2O$: C, 59.96; H, 7.55; N, 4.66. Found: C, 60.31; H, 7.84; N, 4.37.

Synthesis of (^{DipMes}Nacnac)MgBr(Et_2O) (3a')

MeMgBr (2.23 mL, 3 M in Et_2O, 6.69 mmol) was added dropwise to a solution of ligand **2a** (2.50 g, 6.65 mmol) in diethyl ether (30 mL) at room temperature. Gas bubbles were noticed and an amount of precipitate was formed. The mixture was stirred for overnight. The precipitate of **3a'** was collected by filtration. The supernatant solution was concentrated to ca. 10 mL and cooled to –30 ℃ to afford a second crop (Yield 3.11 g, 84%). M.p. 253-255 ℃. ^{1}H NMR (C_6D_6, 600 MHz): δ 7.07 (m, 3 H, Ar-*H*), 6.78 (s, 2 H, Ar-*H*), 4.79 (s, 1 H, =C*H*), 3.22 (m, 6 H, C*H*$(CH_3)_2$ + OC*H*$_2$CH$_3$ overlap), 2.35 (s, 3 H, Ar-C*H*$_3$), 2.04 (s, 6 H, Ar-C*H*$_3$), 1.58 (s, 3 H, NCC*H*$_3$), 1.46 (s, 3 H, NCC*H*$_3$), 1.11–1.07 (m, 18 H, CH(C*H*$_3$)$_2$ + OCH$_2$C*H*$_3$ overlap). ^{13}C{^{1}H} NMR (C_6D_6, 151 MHz): δ 170.0 (N*C*CH$_3$), 168.8 (N*C*CH$_3$), 146.4, 143.2, 142.3, 131.6, 128.8, 125.7, 124.4, 123.9 (Ar-*C*), 95.0 (=*C*H), 28.1 (*C*H(CH$_3$)$_2$), 27.9, 24.7, 24.6, 23.7, 23.1, 18.3 (*C*H$_3$). Anal. Calc. for $C_{30}H_{45}BrMgN_2O$: C, 65.05; H, 8.19; N, 5.06. Found: C, 65.41; H, 8.52; N, 4.73.

Synthesis of (^{DipXyl}Nacnac)MgI(Et_2O) (3b)

The complex was synthesized by using a similar procedure to that employed for the preparation of **3a**, but by using ligand **2b** (3.01 g, 8.29 mmol). After work-up complex **3b** was obtained as a colorless crystalline solid (Yield 4.12 g, 84%). M.p. 150-152 ℃. ^{1}H NMR (C_6D_6, 600 MHz): δ 7.13–6.94 (m, 6 H, Ar-*H*), 4.89 (s, 1 H, =C*H*), 3.26 (m, 6 H, C*H*$(CH_3)_2$ + OC*H*$_2$CH$_3$ overlap), 2.60 (br s, 3 H, Ar-C*H*$_3$), 2.13 (br s, 3 H, Ar-C*H*$_3$), 1.67 (s, 3 H, NCC*H*$_3$), 1.56 (s, 3 H, NCC*H*$_3$), 1.19 (br, 12 H, CH(C*H*$_3$)$_2$), 0.59 (br, 6H, OCH$_2$C*H*$_3$). ^{13}C{^{1}H} NMR (C_6D_6, 151 MHz): δ 169.9, 168.6 (N*C*CH$_3$), 147.7, 145.1, 144.8, 143.9, 142.2, 133.6, 131.5, 129.4, 125.8, 124.8, 123.8 (Ar-*C*), 95.4 (=*C*H), 66.1 (O*C*H$_2$CH$_3$), 28.4 (*C*H(CH$_3$)$_2$), 27.8, 24.5, 24.2, 24.1, 23.2 (*C*H$_3$), 12.8 (OCH$_2$*C*H$_3$). Anal. Calc. for $C_{29}H_{43}IMgN_2O$: C, 59.35; H, 7.39; N, 4.77. Found: C, 59.73; H, 7.75; N, 4.39.

Synthesis of (^{DipXyl}Nacnac)MgBr(Et_2O) (3b')

The complex was synthesized by using a similar procedure to that employed for the preparation of **3a'**, but by using ligand **2b** (4.00 g, 11.04 mmol). After work-up complex **3b'** was obtained as a colorless crystalline solid. (Yield 4.97 g, 83%). M.p. 246-248 ℃. ^{1}H NMR (C_6D_6, 600 MHz): δ 7.14–6.91 (m, 6 H, Ar-*H*), 4.78 (s, 1 H, =C*H*), 3.26 (br, 4 H, OCH_2CH$_3$), 3.18 (br sept, $^3J_{HH}$ = 6.6 Hz, 2 H, C*H*(CH$_3$)$_2$), 2.07 (s, 6 H, Ar-CH_3), 1.57 (s, 3 H, NCCH_3), 1.43 (s, 3 H, NCCH_3), 1.09 (m, 18 H, CH(CH_3)$_2$ + OCH$_2$CH_3 overlap). ^{13}C{^{1}H} NMR (C_6D_6, 151 MHz): δ 170.4 (N*C*CH$_3$), 169.1 (N*C*CH$_3$), 146.8, 143.5, 142.7, 132.0, 129.1, 126.1, 124.8, 124.3 (Ar-*C*), 95.4 (=*C*H), 65.9 (O*C*H$_2$CH$_3$), 28.5 (*C*H(CH$_3$)$_2$), 25.0, 24.9, 24.1, 23.4, 18.6 (*C*H$_3$), 15.6 (OCH$_2$*C*H$_3$). Anal. Calc. for $C_{29}H_{43}BrMgN_2O$: C, 64.52; H, 8.03; N, 5.19. Found: C, 64.85; H, 8.41; N, 4.97.

Synthesis of ($^{DipXyl'}$Nacnac)MgI(Et_2O) (3c)

MeMgI (1.90 mL, 3 M in Et_2O, 5.70 mmol) was added dropwise to a solution of ligand **2c** (2.01 g, 5.54 mmol) in diethyl ether (20 mL) at –60 ℃. The mixture was stirred for overnight to give a yellow solution and only little precipitate was formed. The yellow solution was filtered. The solvent was removed in vacuo, the residue was washed with n-hexane (ca. 20 mL) to afford pale-yellow solid power (Yield 2.84 g, 87%). M.p. 129-131 ℃. ^{1}H NMR (C_6D_6, 600 MHz): δ 7.15–6.90 (m, 6 H, Ar-*H*), 4.84 (s, 1 H, =C*H*), 3.21-3.47 (m, 6 H, C*H*(CH$_3$)$_2$ + OCH_2CH$_3$ overlap), 2.18 (s, 3 H, Ar-CH_3), 1.67 (s, 3 H, NCCH_3), 1.65 (s, 3 H, NCCH_3), 1.53 (br s, 3 H, Ar-CH_3), 1.22 (br, 12 H, CH(CH_3)$_2$), 0.85 (br, 6 H, OCH$_2$CH_3). ^{13}C{^{1}H} NMR (C_6D_6, 151 MHz): δ 169.8, 168.9 (N*C*CH$_3$), 145.8, 144.5, 143.1, 134.0, 132.4, 131.4, 126.4, 125.8, 124.5, 123.7 (Ar-*C*), 95.0 (=*C*H), 66.0 (O*C*H$_2$CH$_3$), 32.0, 28.2, 24.5, 24.3, 23.5, 21.0, 14.3 (*C*H$_3$), 13.8 (OCH$_2$*C*H$_3$). Anal. Calc. for $C_{29}H_{43}IMgN_2O$: C, 59.35; H, 7.39; N, 4.77. Found: C, 59.62; H, 7.64; N, 4.46.

Synthesis of (^{DipPh}Nacnac)MgBr(Et_2O) (3d)

MeMgBr (2.01 mL, 3 M in Et_2O, 6.03 mmol) was added dropwise to a solution of

ligand **2d** (2.00 g, 5.98 mmol) in diethyl ether (20 mL) at room temperature, gas bubble was noticed, but no precipitate was formed. The mixture was stirred for overnight and filtered. The filtrate was concentrated to ca. 8 mL to afford colorless crystals. (Yield 2.21 g, 72%). M.p. 287-289 ℃. ^{1}H NMR (C_6D_6, 600 MHz): δ 7.15–6.91 (m, 8 H, Ar-*H*), 4.84 (s, 1 H, =C*H*), 3.29 (m, 6 H, C*H*$(CH_3)_2$ + OCH_2CH$_3$ overlap), 1.76 (s, 3 H, NCCH_3), 1.68 (s, 3 H, NCCH_3), 1.18 (d, $^{3}J_{HH}$ = 6.6 Hz, 12 H, CH(CH_3)$_2$), 0.85 (br, 6 H, OCH$_2$CH_3). ^{13}C{^{1}H} NMR (C_6D_6, 151 MHz): δ 169.6 (N*C*CH$_3$), 167.2 (N*C*CH$_3$), 149.6, 144.4, 142.4, 128.8, 128.7, 125.4, 125.2, 123.8 (Ar-*C*), 95.4 (=*C*H), 65.7 (O*C*H$_2$CH$_3$), 27.9 (*C*H$(CH_3)_2$), 24.7, 24.3, 23.9, 23.4 (*C*H$_3$), 14.0 (OCH$_2$*C*H$_3$). Anal. Calc. for $C_{27}H_{39}BrMgN_2O$: C, 63.36; H, 7.68; N, 5.47. Found: C, 63.71; H, 7.95; N, 5.13.

Synthesis of [(^{DipMes}Nacnac)]$_2$ (4a)

A solution of **3a** or **3a**' (2.52 mmol) in toluene (30 mL) was stirred vigorously for 4 days over a sodium mirror (0.56 g, 24.3 mmol) at room temperature. The yellow-green suspension was filtered and the solvent was removed in vacuo. The residue was extracted with n-hexane (30 mL), filtered and concentrated to ca. 10 mL to give yellow crystals of **4a**. A second crop of **4a** was isolated after further concentration and cooled to –30 ℃. (Yield 0.41 g, 41%). M.p. 218-220 ℃. ^{1}H NMR (C_6D_6, 600 MHz): δ 7.10–7.04 (m, 6 H, Ar-*H*), 6.88 (s, 4 H, Ar-*H*), 4.85 (s, 2 H, =C*H*), 2.98 (sept, $^{3}J_{HH}$ = 6.6 Hz, 4 H, C*H*$(CH_3)_2$), 2.31 (s, 6 H, CH_3), 1.93 (s, 12 H, CH_3), 1.57 (s, 6 H, NCCH_3), 1.52 (s, 6 H, NCCH_3), 1.10 (d, $^{3}J_{HH}$ = 6.6 Hz, 12 H, CH(CH_3)$_2$), 0.94 (d, $^{3}J_{HH}$ = 6.6 Hz, 12 H, CH(CH_3)$_2$). ^{13}C{^{1}H} NMR (C_6D_6, 151 MHz): δ 167.1 (N*C*CH$_3$), 166.4 (N*C*CH$_3$), 145.4, 144.9, 141.8, 132.4, 131.1, 129.1, 125.0, 123.3 (Ar-*C*), 95.3 (=*C*H), 27.8 (*C*H$(CH_3)_2$), 25.0, 23.7, 23.3, 22.9, 20.8, 19.0 (*C*H$_3$). Anal. Calc. for $C_{52}H_{70}Mg_2N_4$: C, 78.09; H, 8.82; N, 7.01. Found: C, 78.32; H, 9.07; N, 6.82.

Synthesis of [(^{DipXyl}Nacnac)Mg]$_2$ (4b)

n-Hexane (30 mL) was added to **3b** or **3b**' (2.48 mmol). The resultant solution was

rapidly stirred over a sodium mirror (0.60 g, 26.09 mmol) for 4 days to yield a yellow-green suspension. This was filtered, the yellow filtrate was concentrated to ca. 10 mL to give yellow crystals of **4b**. A second crop of **4b** was isolated after further concentration (Yield 0.57 g, 60%). M.p. 205-207 ℃. ^{1}H NMR (C_6D_6, 600 MHz): δ 7.10–7.00 (m, 12 H, Ar-*H*), 4.84 (s, 2 H, =C*H*), 2.96 (sept, $^{3}J_{HH}$ = 6.6 Hz, 4 H, C*H*(CH_3)$_2$), 1.96 (s, 12 H, Ar-CH_3), 1.57 (s, 6 H, NCCH_3), 1.48 (s, 6 H, NCCH_3), 1.10 (d, $^{3}J_{HH}$ = 6.6 Hz, 12 H, CH(CH_3)$_2$), 0.92 (d, $^{3}J_{HH}$ = 6.6 Hz, 12 H, CH(CH_3)$_2$). ^{13}C{^{1}H} NMR (C_6D_6, 151 MHz): δ 167.6 (N*C*CH$_3$), 166.4 (N*C*CH$_3$), 148.5, 145.1, 142.1, 132.0, 128.7, 125.4, 124.2, 123.7 (Ar-*C*), 95.7 (=*C*H), 28.1 (*C*H(CH_3)$_2$), 25.5, 24.1, 23.7, 23.3, 19.6 (*C*H$_3$). Anal. Calc. for $C_{50}H_{66}Mg_2N_4$: C, 77.82; H, 8.62; N, 7.26. Found: C, 78.10; H, 8.86; N, 6.97.

Synthesis of [($^{DipXyl'}$Nacnac)Mg]$_2$ (4c)

The complex was synthesized by using a similar procedure to that employed for the preparation of **4b**, but by using complex **3c** (2.05 g, 3.49 mmol). After work-up the yellow filtrate was concentrated to ca. 2 mL to yield yellow crystals of **4c**. Due to **4c** is too soluble in hexane, it couldn't be purified completely *via* recrystallization to get pure NMR data.

Synthesis of (^{DipPh}Nacnac)$_2$Mg (4d)

The complex was synthesized by using a similar procedure to that employed for the preparation of **4a**, but by using complex **3d** (1.01 g, 1.98 mmol). After work-up complex **4d** was obtained as yellow crystals (Yield 0.20 g, 29%). M.p. 210-212 ℃. ^{1}H NMR (C_6D_6, 600 MHz): δ 7.11–6.78 (m, 16 H, Ar-*H*), 4.76 (s, 2 H, =C*H*), 3.18 (sept, $^{3}J_{HH}$ = 6.6 Hz, 2 H, C*H*(CH_3)$_2$), 2.87 (sept, $^{3}J_{HH}$ = 6.6 Hz, 2 H, C*H*(CH_3)$_2$), 1.73 (s, 6 H, NCCH_3), 1.56 (s, 6 H, NCCH_3), 1.18 (d, $^{3}J_{HH}$ = 6.6 Hz, 6 H, CH(CH_3)$_2$), 1.03 (d, $^{3}J_{HH}$ = 6.6 Hz, 12 H, CH(CH_3)$_2$), 0.83 (d, $^{3}J_{HH}$ = 6.6 Hz, 6 H, CH(CH_3)$_2$). ^{13}C{^{1}H} NMR (C_6D_6, 151 MHz): δ 169.9 (N*C*CH$_3$), 166.4 (N*C*CH$_3$), 150.1, 146.0, 142.3, 142.1, 128.2, 125.0, 124.9, 124.1, 123.2, 122.8 (Ar-*C*), 97.1 (=*C*H), 28.8 (*C*H(CH_3)$_2$), 27.2 (*C*H(CH_3)$_2$), 24.7, 24.6, 24.4, 24.1, 23.7, 23.6 (*C*H$_3$). Anal. Calc. for

$C_{46}H_{58}MgN_4$: C, 79.92; H, 8.46; N, 8.10. Found: C, 80.27; H, 8.71; N, 7.84.

Synthesis of ligand (^{Ar}NacnacH) (5)

To a mixture of 2-(diphenylmethyl)-4,6-dimethylaniline (5.15 g, 17.92 mmol) and acetylacetone (0.89 g, 8.93 mmol) in toluene (120 mL) was added p-toluenesulfonic acid monohydrate (3.42 g, 17.98 mmol). The solution was refluxed (160 ℃) for 3 days with a Dean-stark apparatus and cooled to room temperature. All the volatiles were removed under reduced pressure to give a yellow solid. The solid was treated with CH_2Cl_2 (50 mL) and excess saturate $NaHCO_3$ solution. The aqueous phase was extracted with CH_2Cl_2 (2 x 20 mL) and the combined organic phase was dried over $MgSO_4$. The solvent was concentrated to ca. 30 mL and n-hexane (60 mL) was added to afford white solids of **5** (Yield 5.20 g, 92%). M.p. 130-132 ℃. ^{1}H NMR ($CDCl_3$, 600 MHz): δ 12.06, 11.98 (s, 1 H, N*H*), 7.25–6.66 (m, 24 H, Ar-*H*), 5.86, 5.69 (s, 1 H, C*H*Ph_2), 4.54, 4.52 (s, 1 H, =C*H*), 2.219, 2.215 (s, 6 H, Ar-CH_3), 2.09, 2.07 (s, 6 H, Ar-CH_3), 1.15 (s, 3 H, NCCH_3), 1.01 (s, 3 H, NCCH_3). ^{13}C{^{1}H} NMR ($CDCl_3$, 151 MHz): δ 162.3, 161.8 (N*C*CH_3), 144.2, 143.3, 143.0, 141.1, 141.0, 139.0, 138.4, 133.5, 133.4, 132.1, 132.0, 130.1, 130.0, 129.5, 129.4, 129.22, 129.18, 128.2, 128.1, 128.0, 126.04, 125.96, 125.90, 125.8 (Ar-*C*), 94.3, 94.0 (=*C*H), 52.2, 52.0 (*C*HPh_2), 21.2, 20.0, 19.8, 18.5, 18.2 (*C*H_3) (two isomers of this ligand in solution were determined by ^{1}H NMR spectroscopy). HRMS (ESI): m/z Calcd. for $C_{47}H_{47}N_2$ [M^++H]: 639.3739; Found: 639.3740.

Synthesis of (^{Ar}Nacnac)MgI(Et_2O) (6)

The complex was synthesized by using a similar procedure to that employed for the preparation of **3a**, but by using ligand **5** (1.00 g, 1.57 mmol). After work-up complex **6** was obtained as a colorless crystalline solid (Yield 1.21 g, 89%). M.p. 219-221 ℃. ^{1}H NMR (C_6D_6, 600 MHz): δ 7.59–7.02 (m, 24 H, Ar-*H*), 6.79 (s, 2 H, C*H*Ph_2) 4.66 (s, 1 H, =C*H*), 3.41 (br, 4 H, OC$H_2$$CH_3$), 2.01 (s, 6 H, Ar-C$H_3$), 0.98 (br, 6 H, NCC$H_3$), 0.72 (br, 6 H, OCH_2CH_3). ^{13}C{^{1}H} NMR (C_6D_6, 151 MHz): δ 170.6 (N*C*CH_3), 145.0, 142.9, 133.5, 133.3, 130.6, 130.3, 129.6, 127.2, 126.3, 126.1, 125.98,

125.91 (Ar-*C*), 95.4 (=*C*H), 66.4 (O*C*H_2CH$_3$), 51.2 (*C*HPh$_2$), 22.8, 20.72, 20.67 (*C*H$_3$), 13.3 (OCH$_2$*C*H$_3$). Anal. Calc. for $C_{51}H_{55}IMgN_2O$: C, 70.96; H, 6.42; N, 3.25. Found: C, 80.26; H, 6.73; N, 2.95.

Synthesis of [(^{Ar}Nacnac)Mg]$_2$ (7)

Toluene (30 mL) was added to **6** (1.00 g, 1.18 mmol). The resultant solution was rapidly stirred over a sodium mirror (0.60 g, 26.1 mmol) for 7 days. The yellow-green suspension was filtered and concentrated to ca. 5 mL to give yellow crystals of complex **7**. A second crop of **7** was isolated after further concentration and cooled to –30 ℃ (Yield 0.20 g, 25%). M.p. 250-252 ℃. ^{1}H NMR (C_6D_6, 600 MHz): δ 7.34–6.77 (m, 48 H, Ar-*H*), 5.93 (s, 4 H, C*H*Ph$_2$) 4.57 (s, 2 H, =C*H*), 2.15 (s, 12 H, Ar-C*H*$_3$), 2.06 (s, 12 H, Ar-C*H*$_3$), 1.14 (s, 12 H, NCC*H*$_3$). ^{13}C{^{1}H} NMR (C_6D_6, 151 MHz): δ 168.6 (N*C*CH$_3$), 146.0, 145.3, 143.6, 138.2, 133.2, 132.1, 130.9, 130.3, 129.9, 129.0, 128.7, 126.5, 126.2 (Ar-*C*), 96.1 (=*C*H), 52.4 (*C*HPh$_2$), 23.2, 21.4, 21.3, 20.2 (*C*H$_3$). Anal. Calc. for $C_{94}H_{90}Mg_2N_4$: C, 85.25; H, 6.85; N, 4.23. Found: C, 85.63; H, 7.06; N, 3.97.

Synthesis of [(^{DipMes}Nacnac)MgCl]$_2$ (8)

Ph$_2$PCl (24 μL, 0.13 mmol) was added dropwise to a benzene solution (10 mL) of **4a** (0.10 g, 0.13 mmol) at room temperature, and the solution color was turned to colorless immediately. The mixture was stirred for 1h to afford white precipitate, then filtered. Colorless crystals **8** were obtained from the filtrate (Yield: 46%). ^{1}H NMR (C_6D_6, 600 MHz): δ 7.05 (s, 6 H, Ar-*H*), 6.72 (s, 4 H, Ar-*H*), 4.81 (s, 2 H, =C*H*), 3.18 (br s, 4 H, C*H*(CH$_3$)$_2$), 2.33 (s, 6 H, Ar-C*H*$_3$), 2.00 (s, 12 H, Ar-C*H*$_3$), 1.58 (s, 6 H, NCC*H*$_3$), 1.44 (s, 6 H, NCC*H*$_3$), 1.11 (br s, 24 H, CH(C*H*$_3$)$_2$). ^{13}C{^{1}H} NMR (C_6D_6, 151 MHz): δ 170.2, 169.6 (N*C*CH$_3$), 144.5, 143.6, 142.6, 132.8, 131.6, 129.9, 125.9, 124.1 (Ar-*C*), 95.3 (=*C*H), 28.2, 25.0, 24.5, 23.9, 23.4, 21.3, 18.3 (*C*H$_3$). Anal. Calc. for $C_{52}H_{70}Cl_2Mg_2N_4$: C, 71.73; H, 8.10; N, 6.44. Found: C, 72.04; H, 8.36; N, 6.15. The white precipitate was tetraphenyldiphosphine that was determined by ^{31}P NMR spectroscopy (δ = -14.92 ppm) and was in accordance with literature.[S4]

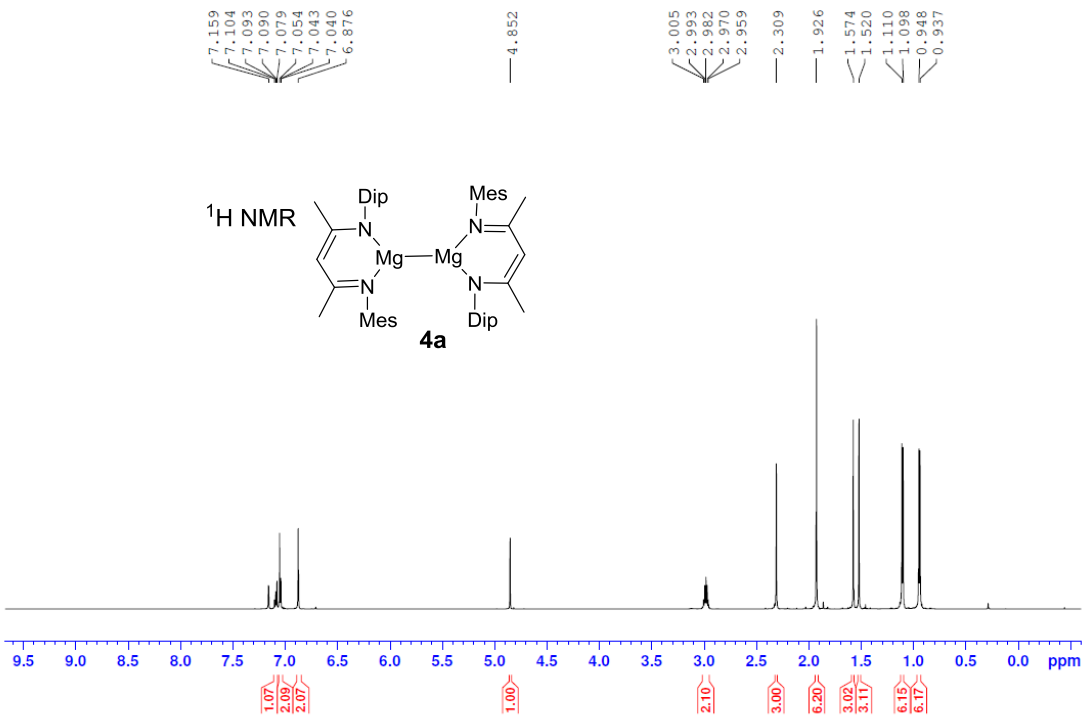
Synthesis of compound 9

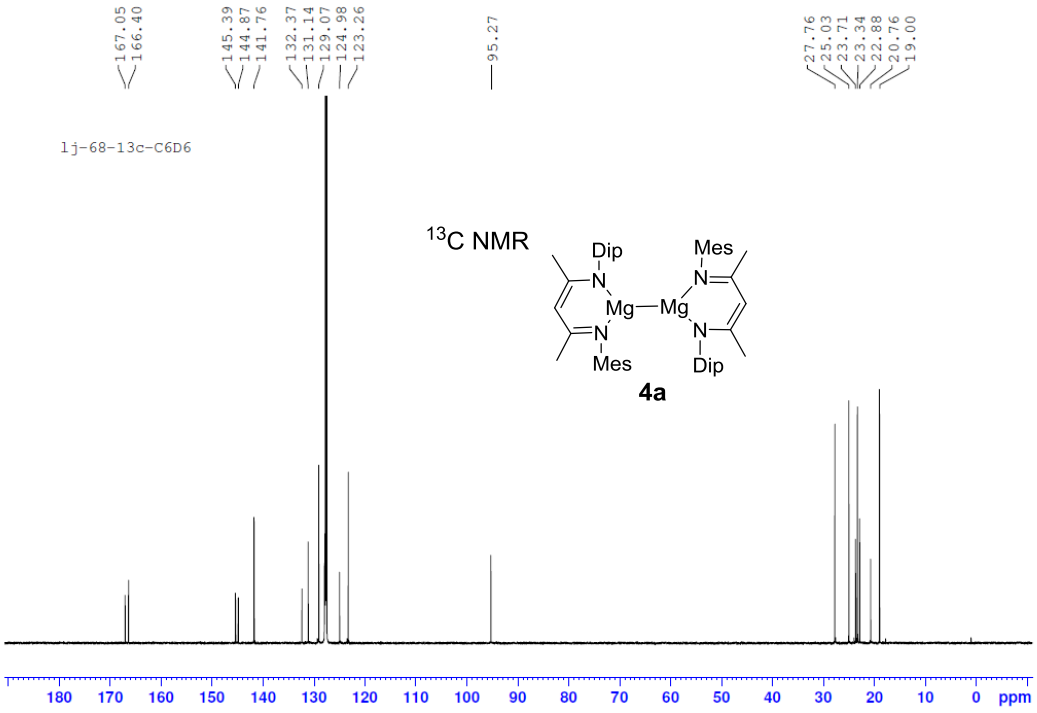
In a glove box, a special sample of PhCCH (27.4 μL, 0.25 mmol), HBpin (54.4 μL, 0.375 mmol) and complex **4b** (30 mg, 0.039 mmol) were added to a J. Young NMR tube equipped with a Teflon screw cap, which was charged with C_6D_6 (0.5 mL), then the mixture was heated at 90 ℃ for 12h before it was cooled to room temperature. Colorless crystals **9** were obtained (15 mg, 36% yield). ^{1}H NMR (C_6D_6, 500 MHz): δ 7.10-7.04 (m, 6 H, Ar-H), 4.87 (s, 1 H, =C*H*), 3.50 (sept, $^3J_{HH}$ = 6.8 Hz, 1 H, C*H*(CH_3)$_2$), 3.15 (sept, $^3J_{HH}$ = 6.8 Hz, 1 H, C*H*(CH_3)$_2$), 2.40 (s, 3 H, Ar-C*H*$_3$), 1.68 (s, 3 H, Ar-C*H*$_3$), 1.54 (s, 3 H, Ar-C*H*$_3$), 1.46 (d, $^3J_{HH}$ = 8.4 Hz, 6 H, CH(C*H*$_3$)$_2$), 1.18 (t, $^3J_{HH}$ = 7.4 Hz, 6 H, CH(C*H*$_3$)$_2$), 1.04 (s, 6 H, C(C*H*$_3$)$_2$), 1.02 (s, 6 H, C(C*H*$_3$)$_2$) 0.32 (d, $^3J_{HH}$ = 6.8 Hz, 3 H, Ar-C*H*$_3$). ^{13}C{^{1}H} NMR (C_6D_6, 126 MHz): δ 169.0, 167.7 (N*C*CH$_3$), 149.6, 146.5, 143.5, 142.6, 132.9, 125.3, 124.1, 123.8 (Ar-*C*), 95.8 (=*C*H), 81.2 (O*C*(CH_3)$_2$), 28.6, 26.7, 26.2, 24.7 (O*C*(CH_3)$_2$), 24.3, 24.0, 23.4, 19.2, 19.0 (*C*H$_3$)). ^{11}B{^{1}H} NMR (160 MHz, C_6D_6): δ 21.79 (O*B*pin).

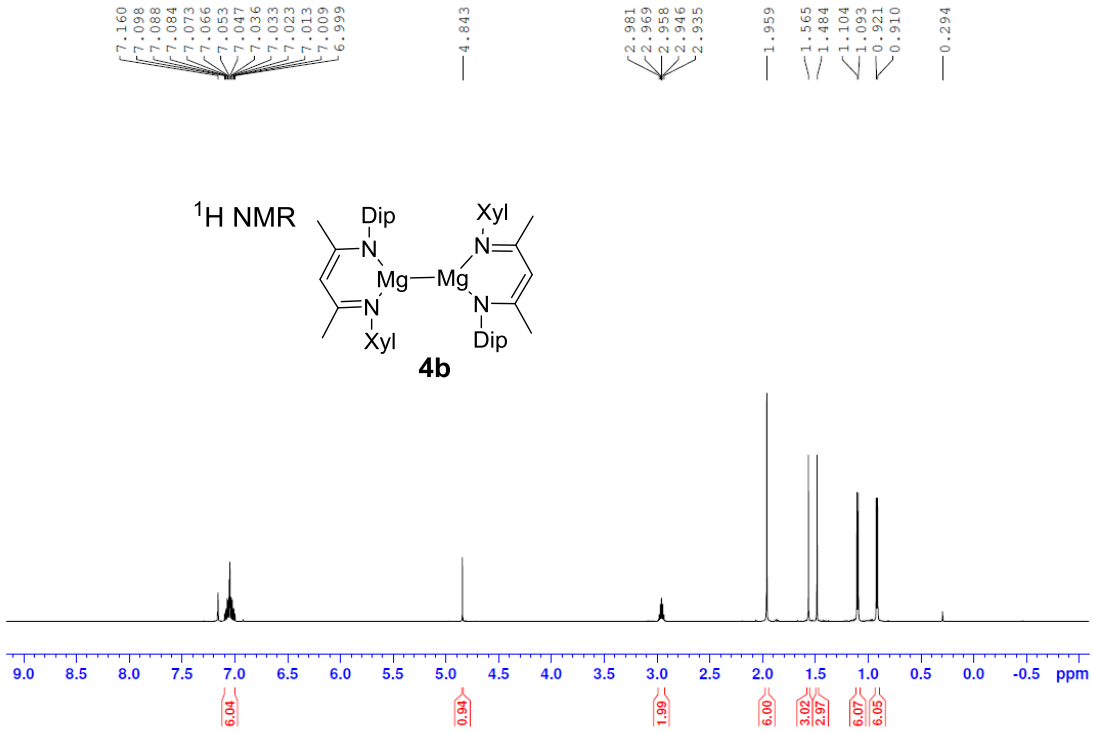
Synthesis of compound 10

In a glove box, complex **4b** (70 mg, 0.091 mmol) and HBpin (100 μL, 0.689 mmol) were added to a J. Young NMR tube equipped with a Teflon screw cap, which was charged with C_6D_6 (0.5 mL), then the mixture was heated at 90 ℃ for 12h before it was cooled to room temperature. Colorless crystals **10** were obtained after several days (ca. 6 mg). ^{1}H NMR (C_6D_6, 600 MHz): δ 1.06 (s, 24 H, C*H*$_3$(Bpin)), 1.64 (s, 12 H, C*H*$_3$). ^{13}C{^{1}H} NMR (C_6D_6, 151 MHz): δ 81.8, 79.8 (*C*(CH_3)$_2$), 24.7, 23.2 (C(*C*H$_3$)$_2$). ^{11}B{^{1}H} NMR (193 MHz, C_6D_6): δ 21.76.

^{1}H and ^{13}C NMR Spectra of Mg(I) Complexes **4a**, **4b** and **7**.



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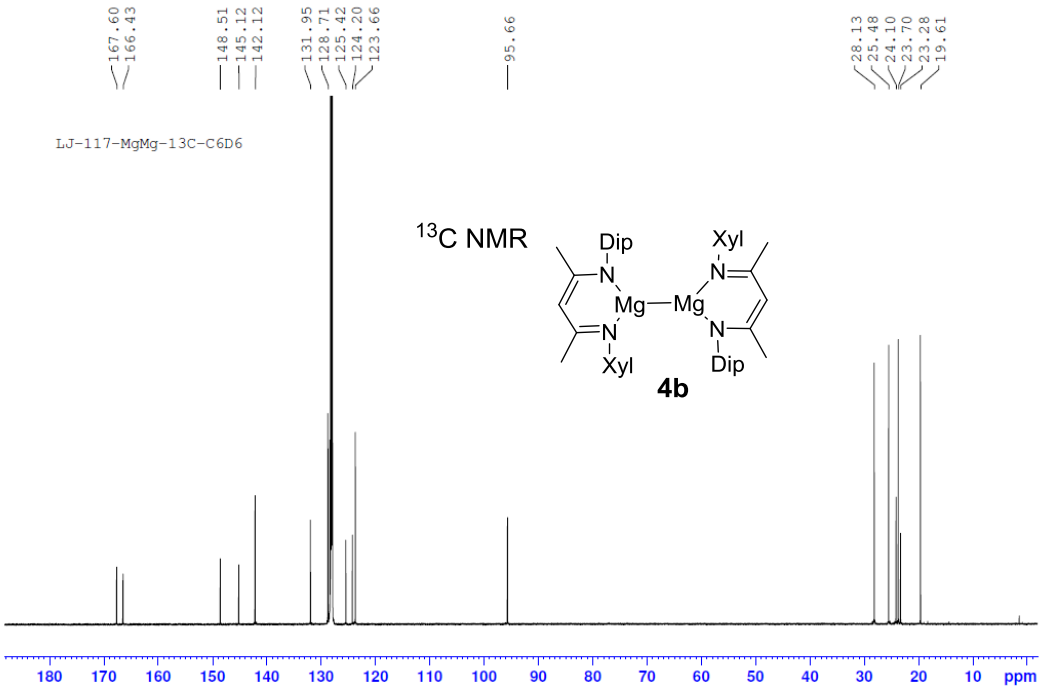
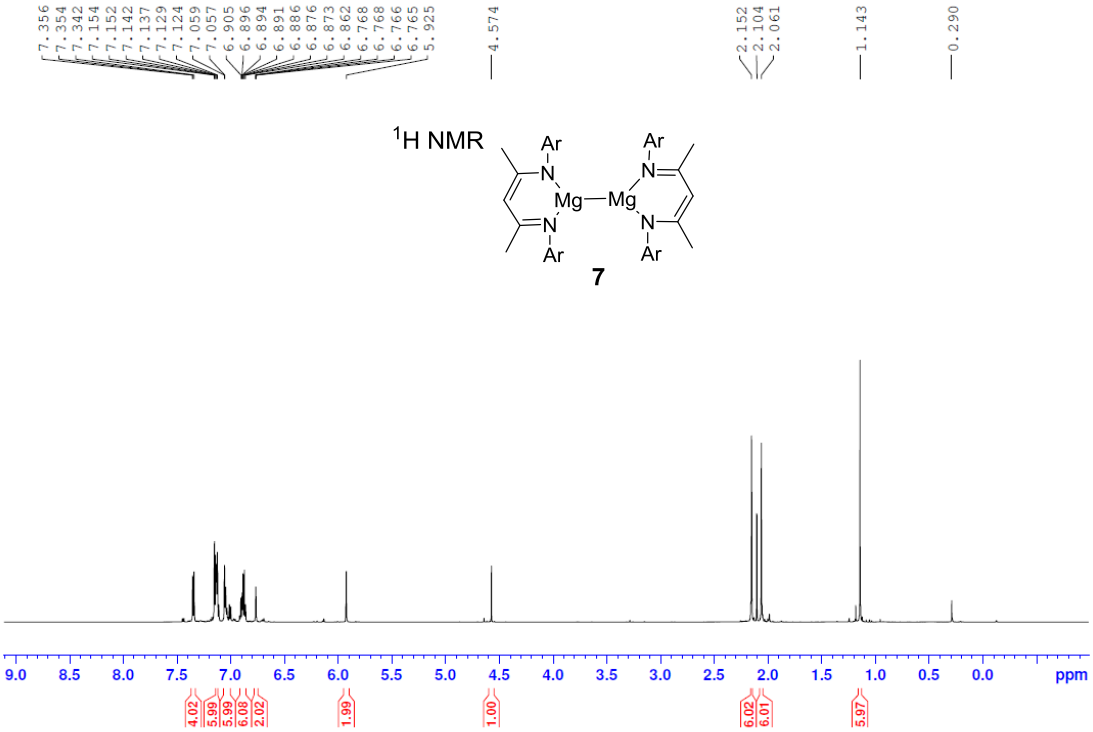
7.098
7.088
7.084
7.073
7.066
7.053
7.047
7.036
7.033
7.023
7.013
7.009
6.999
4.843
2.981
2.969
2.958
2.946
2.935
1.959
1.565
1.484
1.104
1.093
0.921
0.910
0.294
1H NMR
Dip
Xyl
N
Mg
Mg
N
N
Xyl
Dip
4b
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
ppm
6.04
0.94
1.99
6.00
3.02
2.97
6.07
6.05


167.60
166.43
148.51
145.12
142.12
131.95
128.71
125.42
124.20
123.66
95.66
28.13
25.48
24.10
23.70
23.28
19.61
LJ-117-MgMg-13C-C6D6
13C NMR
Dip
Xyl
N
Mg
Mg
N
N
Xyl
Dip
4b
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.129
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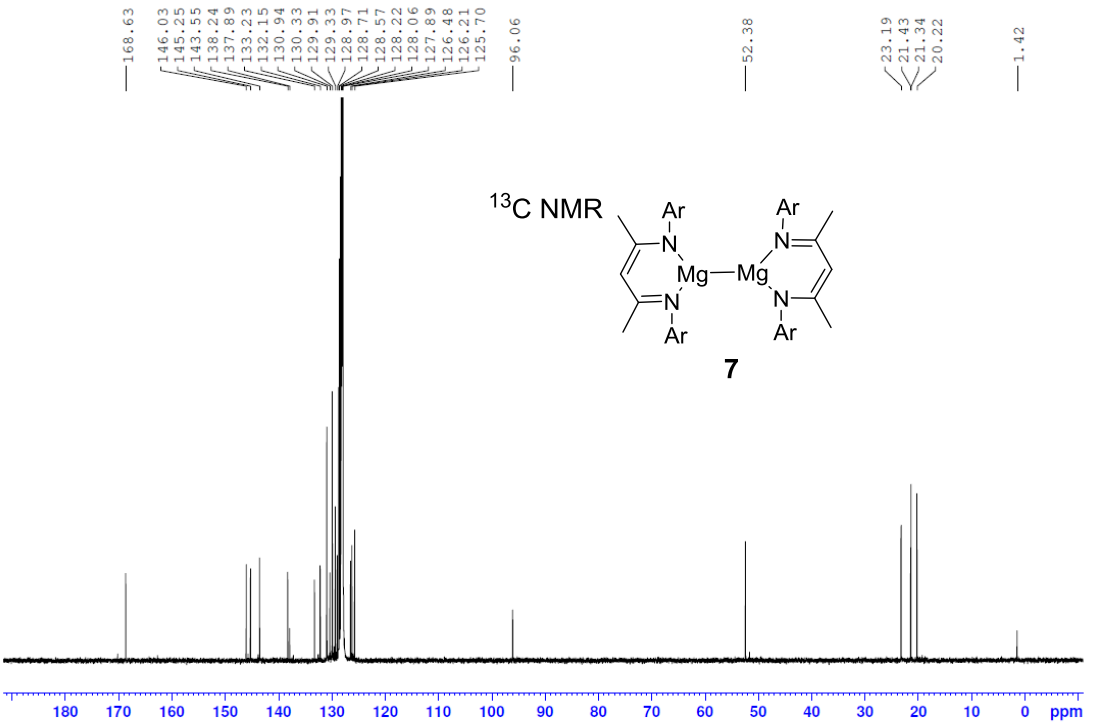
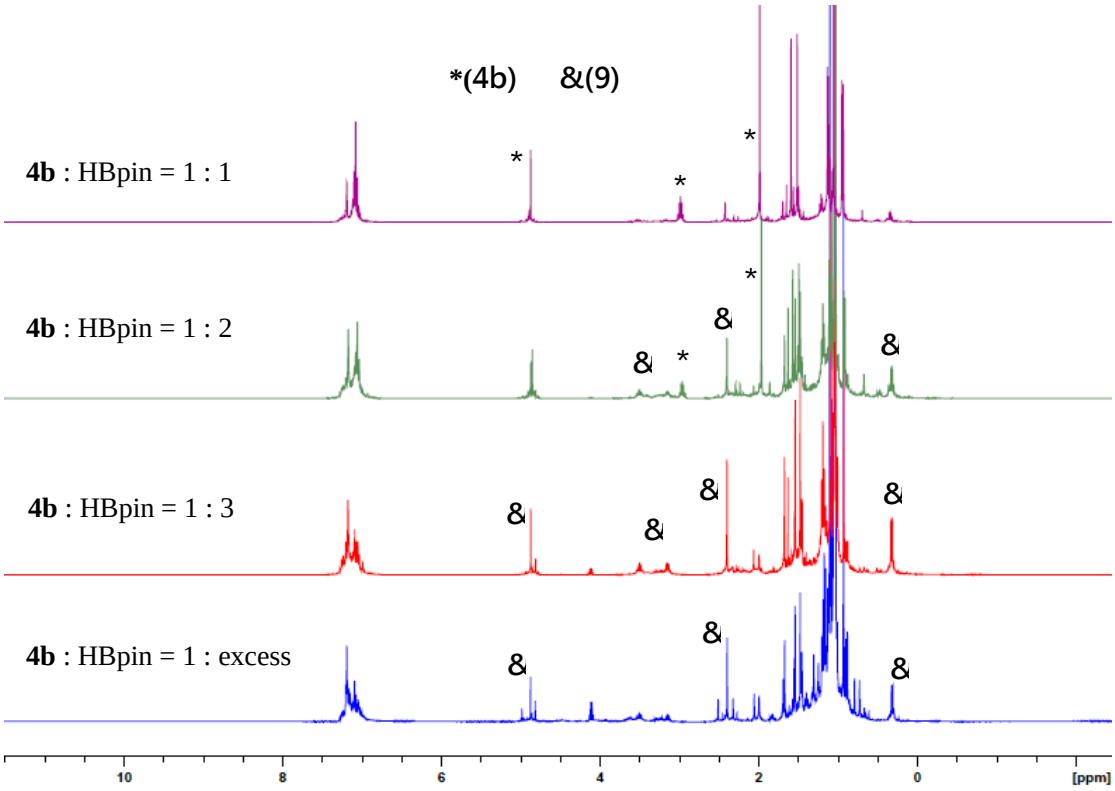
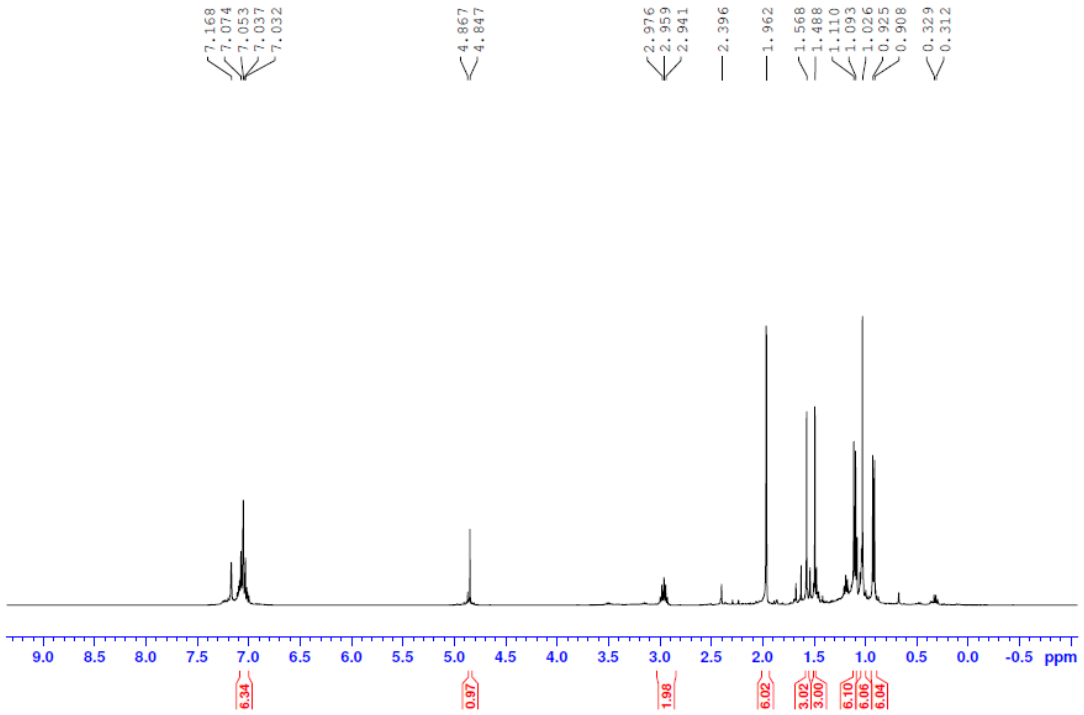
6.894
6.891
6.886
6.876
6.873
6.862
6.768
6.768
6.766
6.765
5.925
4.574
2.152
2.104
2.061
1.143
0.290
1H NMR
Ar
N
Mg
Mg
N
Ar
7
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
4.02
5.99
5.99
6.08
2.02
1.99
1.00
6.02
6.01
5.97


168.63
146.03
145.25
143.55
138.24
137.89
133.23
132.15
130.94
130.33
129.91
129.33
128.97
128.71
128.57
128.22
128.06
127.89
126.48
126.21
125.70
96.06
52.38
23.19
21.43
21.34
20.22
1.42
13C NMR
Ar
N
Mg
Mg
N
Ar
7
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

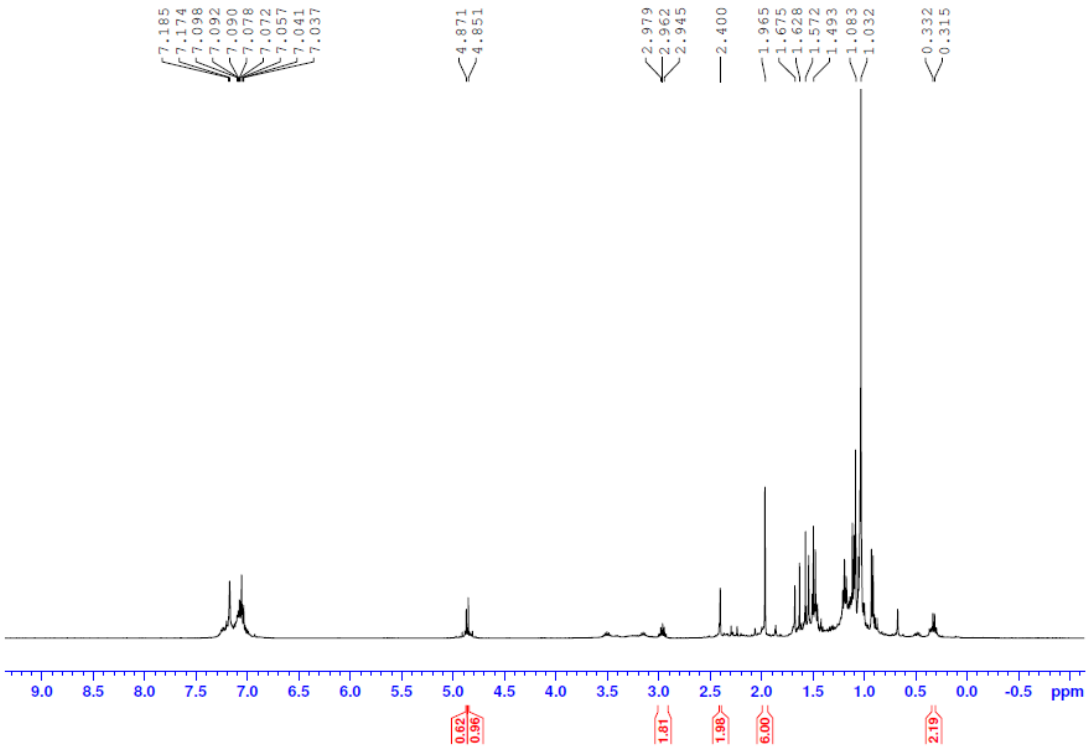
The crude ^{1}H NMR spectra of the reaction mixture between **4b** and HBpin:



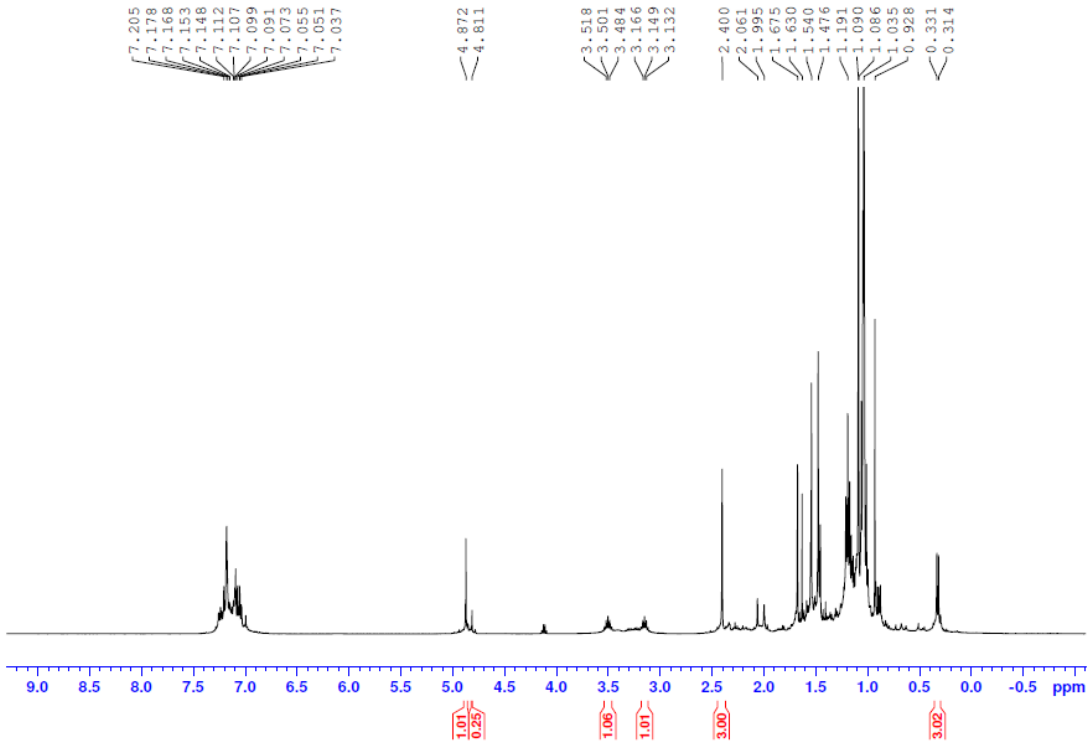
4b + 1HBpin, 90 ℃, 4 h



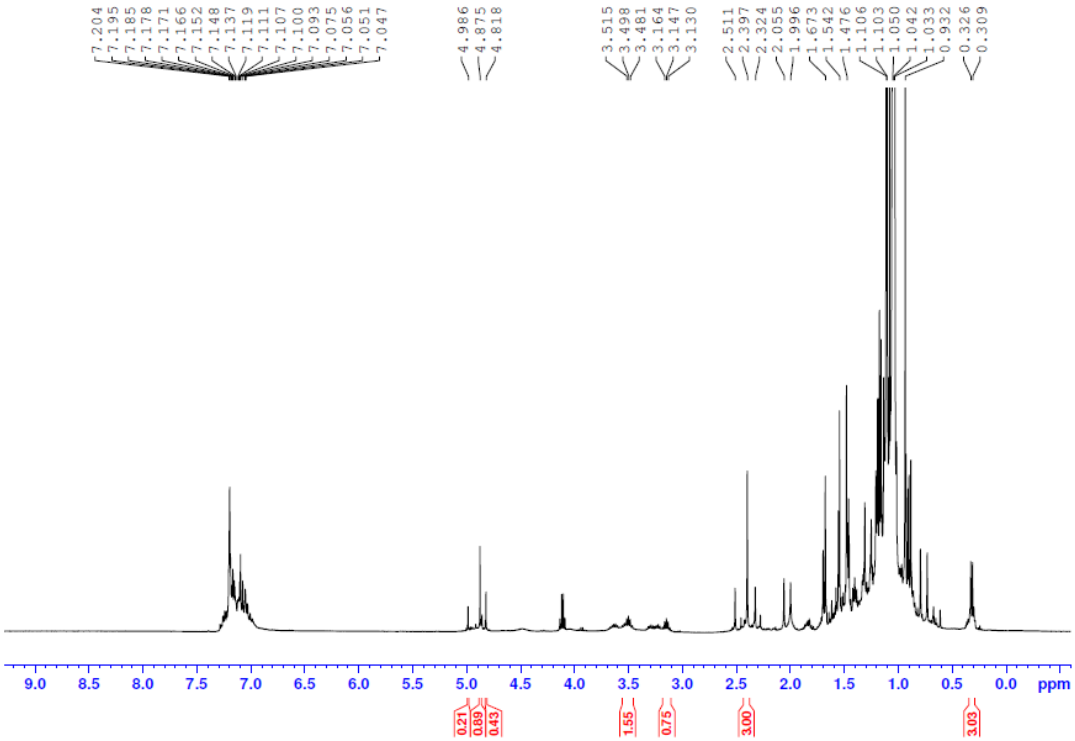
4b + 2HBpin, 90 ℃, 4 h



4b + 3HBpin, 90 ℃, 4 h



4b + excess HBpin, 90 ℃, 4 h



X-ray Crystal Structure Determination

Crystallographic data for complexes **3b**, **4a-4d** and **5-10** is given in Table S1. Diffraction data were collected on a Bruker D8 VENTURE PHOTON 100 diffractometer using a graphite-monochromated MoKα radiation (0.71073Å) in the ω-2θ scan mode. In all cases, an empirical absorption correction by SADABS was applied to the intensity data. The structures were solved by direct methods and refined on F2 by full-matrix least-squares methods using the SHELXTL crystallographic software package. All non-hydrogen atoms were refined anisotropically with hydrogen atoms included in calculated positions (riding model). CCDC 1814209-1814214, 1814216-1814220 contain the supplementary crystallographic data for complexes **3b**, **4a-4d** and **5-10**. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

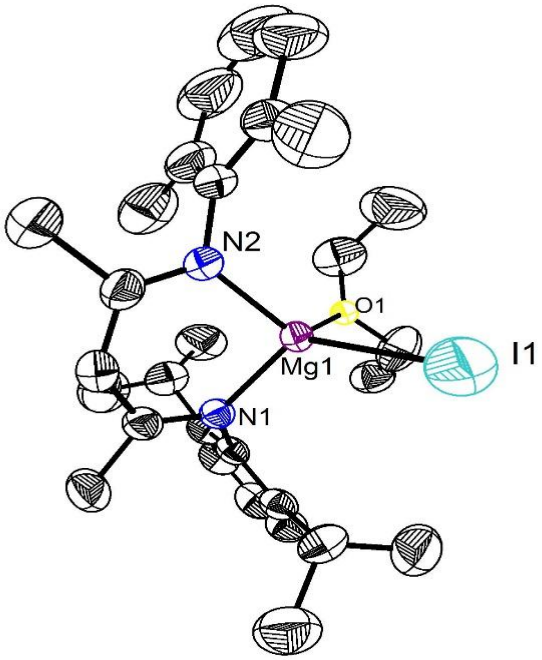


Figure S1. Molecular structure of **3b** (50% thermal ellipsoids; hydrogen atoms omitted). Selected bond lengths (Å) and angles (°): Mg(1)−I(1) 2.7001(11), Mg(1)−N(1) 2.049(3), Mg(1)−N(2) 2.046(3), Mg(1)−O(1) 2.034(3), N(1)−Mg(1)−N(2) 94.06(11), N(1)−Mg(1)−O(1) 111.44(12), N(2)−Mg(1)−O(1) 117.35(13), N(1)−Mg(1)−I(1) 118.26(8), N(2)−Mg(1)−I(1) 115.23(10), O(1)−Mg(1)−I(1) 101.43(9).

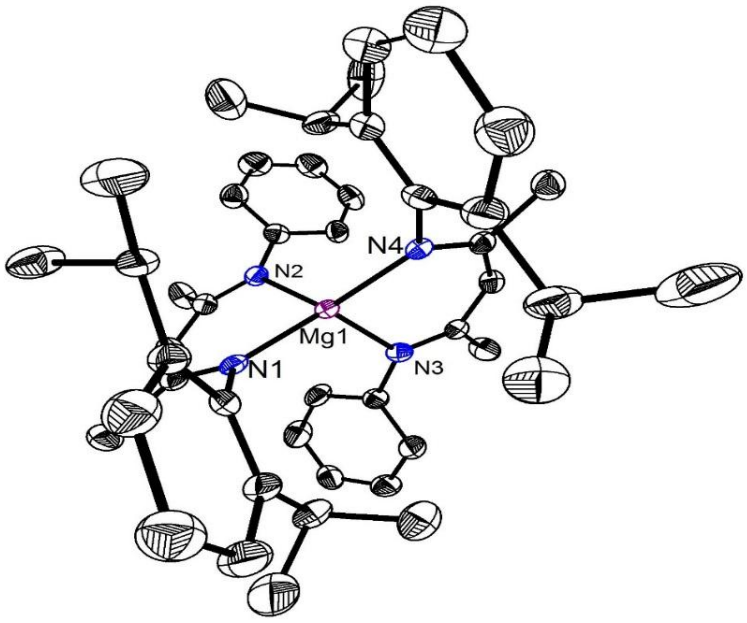


Figure S2. Molecular structure of **4d** (50% thermal ellipsoids; hydrogen atoms omitted). Selected bond lengths (Å) and angles (°): Mg(1)−N(1) 2.067(3), Mg(1)−N(2) 2.078(3), Mg(1)−N(3) 2.062(3), Mg(1)−N(4) 2.076(3), N(1)−Mg(1)−N(2) 92.69(10), N(3)−Mg(1)−N(2) 107.55(11), N(1)−Mg(1)−N(4) 126.24(11), N(3)−Mg(1)−N(1) 118.01(11), N(3)−Mg(1)−N(4) 92.56(11), N(4)−Mg(1)−N(2) 120.44(11).

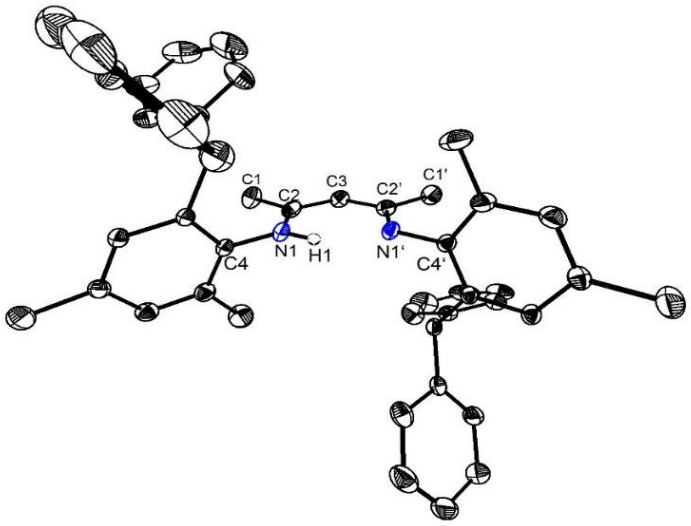


Figure S3. Molecular structure of **5** (50% thermal ellipsoids; hydrogen atoms omitted). Selected bond lengths (Å) and angles (°): C(2)−N(1) 1.3289(16), C(2)−C(3) 1.4044(15), C(2)−C(1) 1.5012(17), N(1)−C(4) 1.4180(15), N(1)−H(1) 0.93(3), N(1)−C(2)−C(3) 120.74(11), N(1)−C(2)−C(1) 120.70(12), C(3)−C(2)−C(1) 118.57(12), C(2)−N(1)−C(4) 124.27(10), C(2)−N(1)−H(1) 112.(2), C(4)−N(1)−H(1) 124.(2).

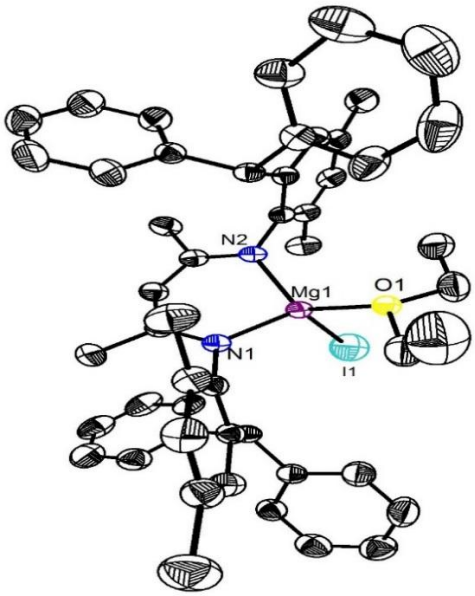


Figure S4. Molecular structure of **6** (50% thermal ellipsoids; hydrogen atoms omitted). Selected bond lengths (Å) and angles (°): Mg(1)−I(1) 2.6948(8), Mg(1)−N(1) 2.053(2), Mg(1)−N(2) 2.035(2), Mg(1)−O(1) 2.056(2), N(1)−Mg(1)−N(2) 95.77(8), N(1)−Mg(1)−O(1) 111.78(8), N(2)−Mg(1)−O(1) 117.76(9), N(1)−Mg(1)−I(1) 116.10(6), N(2)−Mg(1)−I(1) 117.07(6), O(1)−Mg(1)−I(1) 99.39(6).

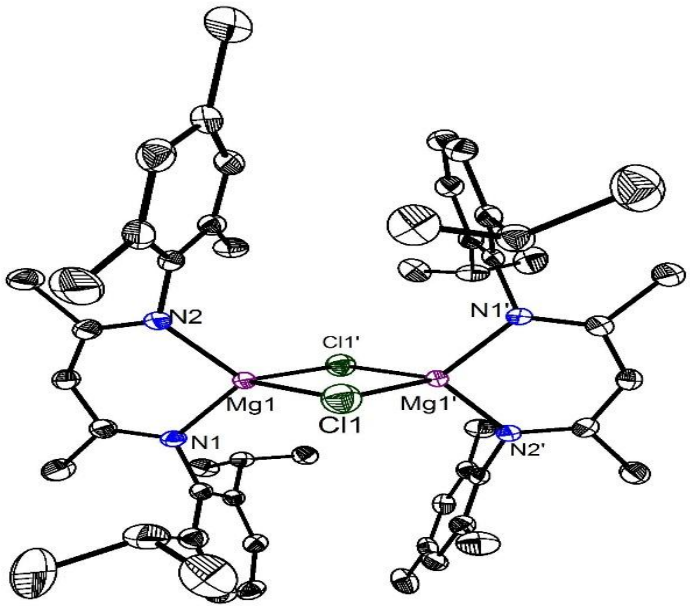


Figure S5. Molecular structure of [(^{DipMes}Nacnac)MgCl]$_2$ (**8**) (50% thermal ellipsoids; hydrogen atoms omitted). Selected bond lengths (Å) and angles (°): Mg(1)−N(1) 2.0164(16), Mg(1)−N(2) 2.0097(16), Mg(1)−Cl(1) 2.3949(8), Mg(1)−Cl(1′) 2.3701(7), N(1)−Mg(1)−N(2) 95.62(6), N(2)−Mg(1)−Cl(1) 116.25(5), N(2)−Mg(1)−Cl(1′) 120.64(5), N(1)−Mg(1)−Cl(1) 118.23(5), N(1)−Mg(1)−Cl(1′) 117.91(5), Mg(1)−Cl(1)−Mg(1′) 89.68(3), Cl(1)−Mg(1)−Cl(1′) 90.32(3).

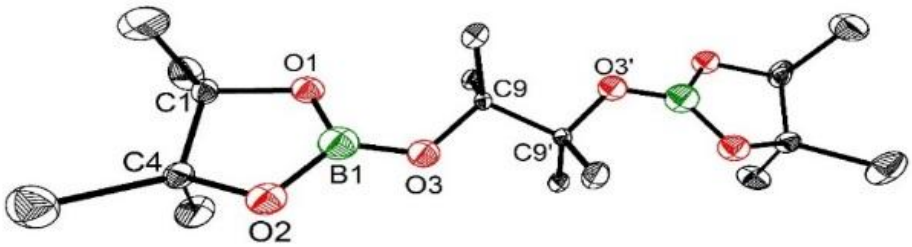


Figure S6. Molecular structure of **10** (50% thermal ellipsoids; hydrogen atoms omitted). Selected bond lengths (Å) and angles (°): B(1)−O(3) 1.348(2), B(1)−O(2) 1.371(2), B(1)−O(1) 1.371(3), C(9)−O(3) 1.450(2), C(9)−C(9)′ 1.566(4), C(1)−C(4) 1.555(3), B(1)−O(3)−C(9) 123.90(15), O(3)−C(9)−C(9)′ 103.88(17), O(3)−B(1)−O(2) 119.79(18), O(3)−B(1)−O(1) 126.73(18), O(2)−B(1)−O(1) 113.48(17).

Table S1. Summary of Crystallographic Data for Compounds **3b**, **4a-4d** and **5-10**.

	3b	**4a**	**4b**	**4c**
Formula	$C_{29}H_{43}IMgN_2O$	$C_{52}H_{70}Mg_2N_4$	$C_{50}H_{66}Mg_2N_4$	$C_{50}H_{66}Mg_2N_4$
Mr	586.86	799.74	771.68	771.68
Crystal system	triclinic	orthorhombic	orthorhombic	monoclinic
Space group	*P*-1	*Pccn*	$Pna2_1$	$P2_1/c$
a (Å)	8.4477(15)	17.7085(9)	21.9804(13)	12.5799(11)
b (Å)	11.883(2)	33.2898(16)	19.3508(11)	19.2069(16)
c (Å)	15.889(3)	17.0054(9)	11.2830(7)	20.3357(17)
α (°)	97.790(4)	90	90	90
β (°)	90.120(4)	90	90	102.473(2)
γ (°)	96.968(4)	90	90	90
V (A^3)	1568.3(5)	10024.9(9)	4799.1(5)	4797.6(7)
Z	2	16	8	8
ρ_{calc} (g cm^{-3})	1.243	1.060	1.068	1.068
μ/mm^{-1}	1.062	0.084	0.085	0.085
Temp (K)	298(2)	135(2)	140(2)	140(2)
F (000)	608	3472	1672	1672
R (obs data)	0.0511	0.1024	0.0662	0.0641
wR (obs data)	0.1217	0.1999	0.0993	0.1810
largest peak and hole (e A^{-3})	1.052, -0.653	0.342, -0.276	0.438, -0.383	1.923, -0.590

Table S1 (contd.). Summary of Crystallographic Data for Compounds **3b**, **4a-4d** and **5-10**.

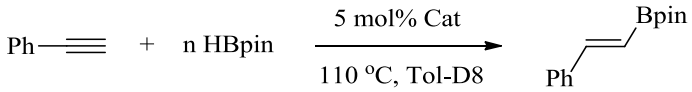
	4d	**5** $\cdot CH_2Cl_2$	**6**	**7** $\cdot (toluene)_2$
Formula	$C_{46}H_{58}MgN_4$	$C_{48}H_{49}Cl_2N_2$	$C_{51}H_{55}IMgN_2O$	$C_{108}H_{106}Mg_2N_4$
Mr	691.27	724.79	863.18	1508.58
Crystal system	triclinic	orthorhombic	monoclinic	monoclinic
Space group	*P*-1	*Pccn*	*C*2/*c*	$P2_1/c$
a (Å)	11.0139(12)	21.607(2)	25.689(3)	11.4271(14)
b (Å)	11.3202(12)	13.2782(12)	11.0511(14)	17.954(2)
c (Å)	18.565(2)	14.0261(13)	32.698(4)	20.908(3)
α (°)	75.316(3)	90	90	90
β (°)	83.401(3)	90	105.996(3)	93.495(3)
γ (°)	62.905(3)	90	90	90
V (A^3)	1993.4(4)	4024.1(6)	8923.3(19)	4281.6(9)
Z	2	4	8	4
ρ_{calc} (g cm^{-3})	1.152	1.196	1.285	1.170
μ/mm^{-1}	0.081	0.197	0.770	0.080
Temp (K)	140(2)	130(2)	298(2)	130(2)
F(000)	748	1540	3584	1612
R (obs data)	0.0747	0.0641	0.0517	0.0559
wR (obs data)	0.1632	0.1752	0.1234	0.1467
largest peak and hole (e A^{-3})	0.563, -0.337	1.088, -1.386	1.045, -1.294	2.047, -0.256

Table S1 (contd.). Summary of Crystallographic Data for Compounds **3b**, **4a-4d** and **5-10**.

	8	**9**	**10**
Formula	$C_{58}H_{76}Cl_2Mg_2N_4$	$C_{68}H_{96}B_2Mg_2N_4O_6$	$C_{18}H_{36}B_2O_6$
Mr	948.75	1135.73	370.09
Crystal system	monoclinic	tetragonal	monoclinic
Space group	$P2_1/c$	P-4	$P2_1/c$
a (Å)	11.9804(6)	13.2295(8)	10.5800(7)
b (Å)	15.2444(7)	13.2295(8)	10.4047(7)
c (Å)	15.0882(7)	19.2267(13)	10.7850(7)
α (°)	90	90	90
β (°)	95.2980(10)	90	118.687(2)
γ (°)	90	90	90
V (A^3)	2743.8(2)	3365.1(5)	1041.5(12)
Z	2	2	2
ρ_{calc} (g cm^{-3})	1.148	1.121	1.180
μ/mm^{-1}	0.181	0.087	0.084
Temp (K)	135(2)	140(2)	140(2)
F(000)	1020	1228	404
R (obs data)	0.0406	0.0647	0.0677
wR (obs data)	0.0939	0.1293	0.1435
largest peak and hole (e A^{-3})	0.306, -0.234	0.430, -0.215	0.397, -0.287

Catalysis and NMR Spectra

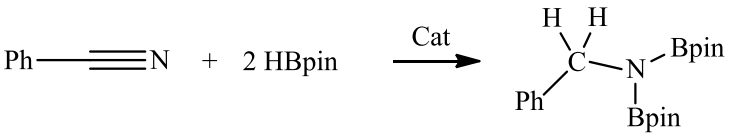
Table S2 Optimization of reaction conditions of alkyne hydroboration



Entry	Cat	n	Time (h)	Yield (%)[a]
1	**4a**	1.5	6	97
2	**4b**	1.5	6	99
3	**7**	1.5	6	77
4	**4b**	1.5	3	75
5	**4b**	1.2	6	89
6	[(^{Dipp}Nacnac)Mg]$_2$	1.5	6	88

[a] Yields were determined by ^{1}H NMR spectroscopy.

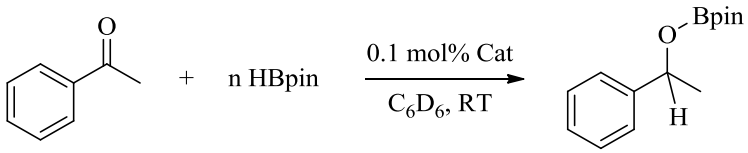
Table S3 Optimization of the reaction conditions of nitrile hydroboration



Entry	Cat	Cat loading (mol %)	Temp. (℃)	Time (h)	Yield (%) [a]
1	**4a**	10	25	2	0
2	**4a**	10	60	8	97
3	**4a**	5	60	10	86
4	**4a**	2	60	30	87
5	**4a**	10	40	24	84
6	**4a**	10	80	4	91
7	**4b**	10	60	8	95

[a] Yields were determined by ^{1}H NMR spectroscopy.

Table S4 Optimization of the reaction conditions of ketone hydroboration



Entry	Cat	n	Time (h)	Yield (%) [a]
1	**4a**	1	1	99
2	**4a**	1.5	0.5	99
3	**4b**	1.5	0.5	99
4	**4c**	1.5	0.5	99
5	**7**	1.5	0.5	99

[a] Yields were determined by ^{1}H NMR spectroscopy.

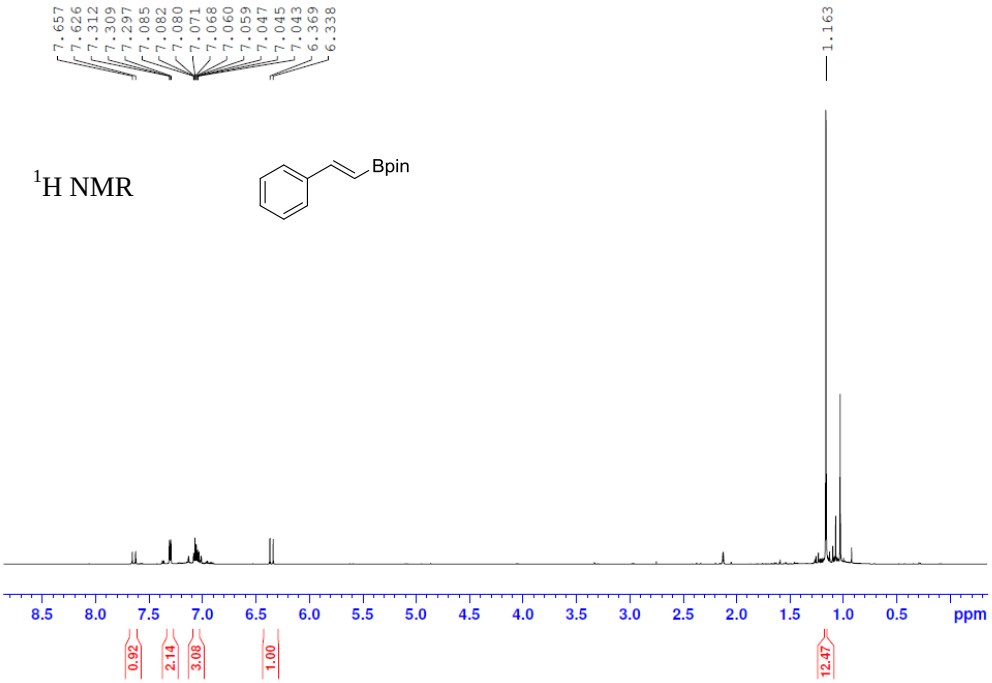
General procedure for catalytic hydroboration of alkynes.

In a glovebox, alkynes (0.12 mmol) was added to a solution of catalyst (5%) and HBpin (0.18 mmol) in toluene-d_8 (0.60 mL) at room temperature, then heated at 110 ℃ for required time. The progress of the reaction was monitored by ^{1}H NMR spectroscopy.

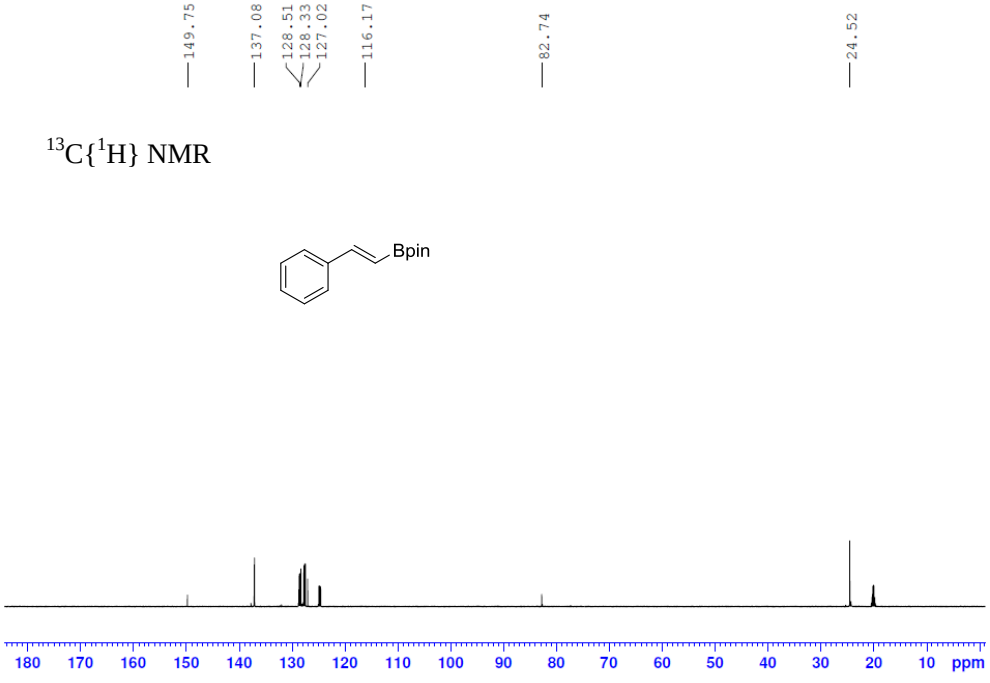
NMR data of the reaction crude. General: The hydroborated products are shown along with the spectra. Resonances are denoted as follows: excess HBpin (*), **9** (#), pinBOBpin (&).

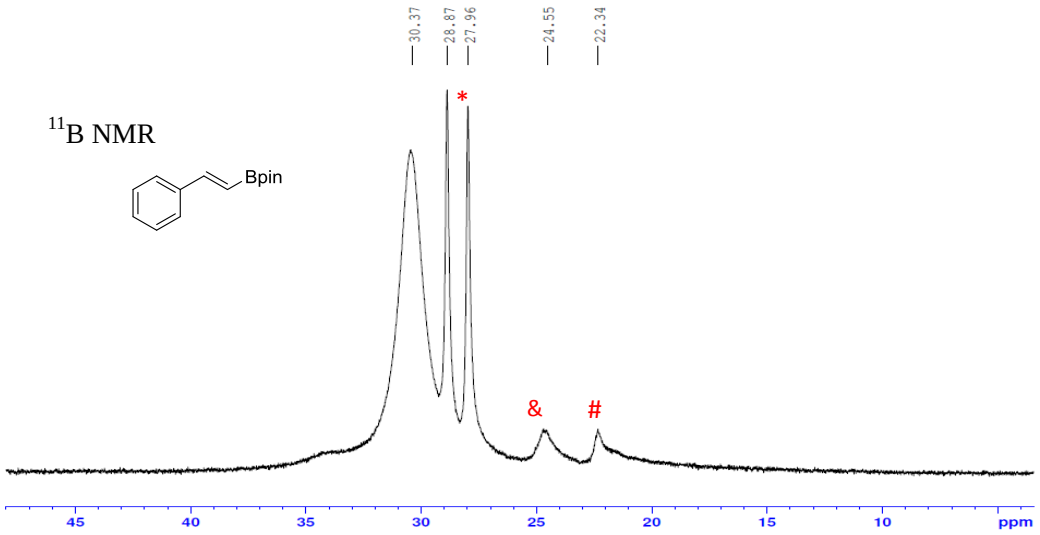
^{1}H NMR (600 MHz, tol-d_8): δ 7.63 (d, *J* = 18.6 Hz, 1H, C*H*), 7.30 (m, 2H, Ar-*H*), 7.06 (m, 3H, Ar-*H*), 6.35 (d, *J* = 18.6 Hz, 1H, C*H*), 1.16 (s, 12H, C(CH_3)$_2$). ^{13}C{^{1}H} NMR (151 MHz, tol-d_8): δ 24.5, 82.7, 116.2, 127.0, 128.3, 137.1, 149.7. ^{11}B NMR (193 MHz, tol-d_8): δ 30.37.

^{1}H NMR

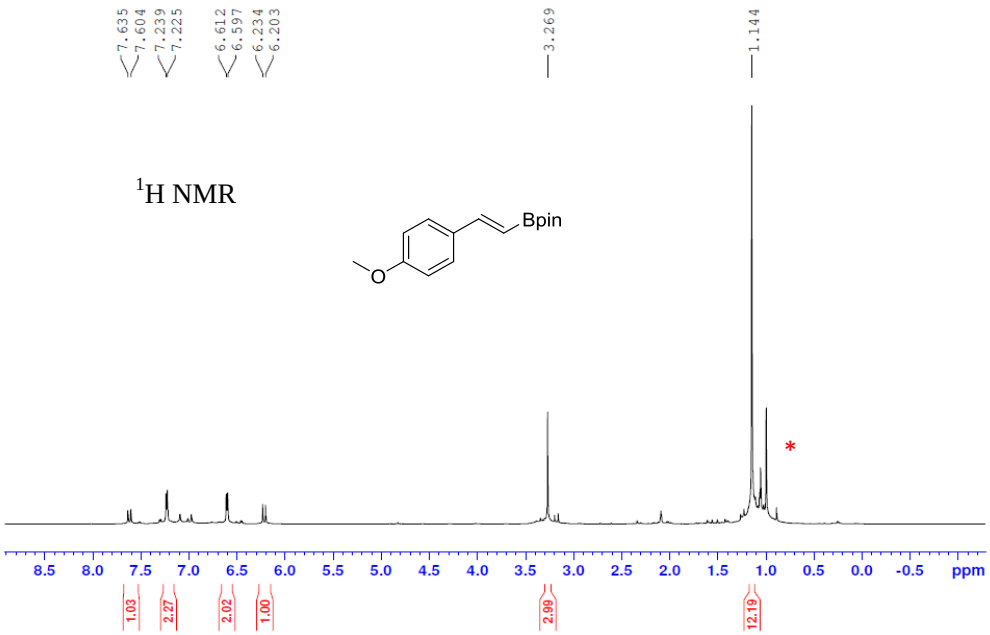


^{13}C{^{1}H} NMR

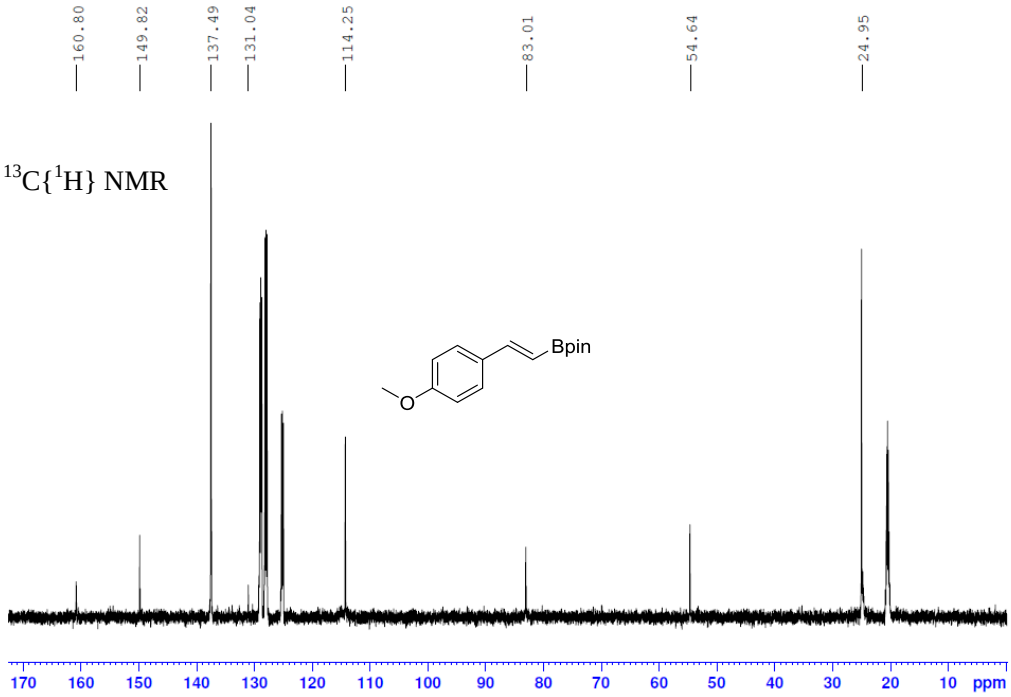




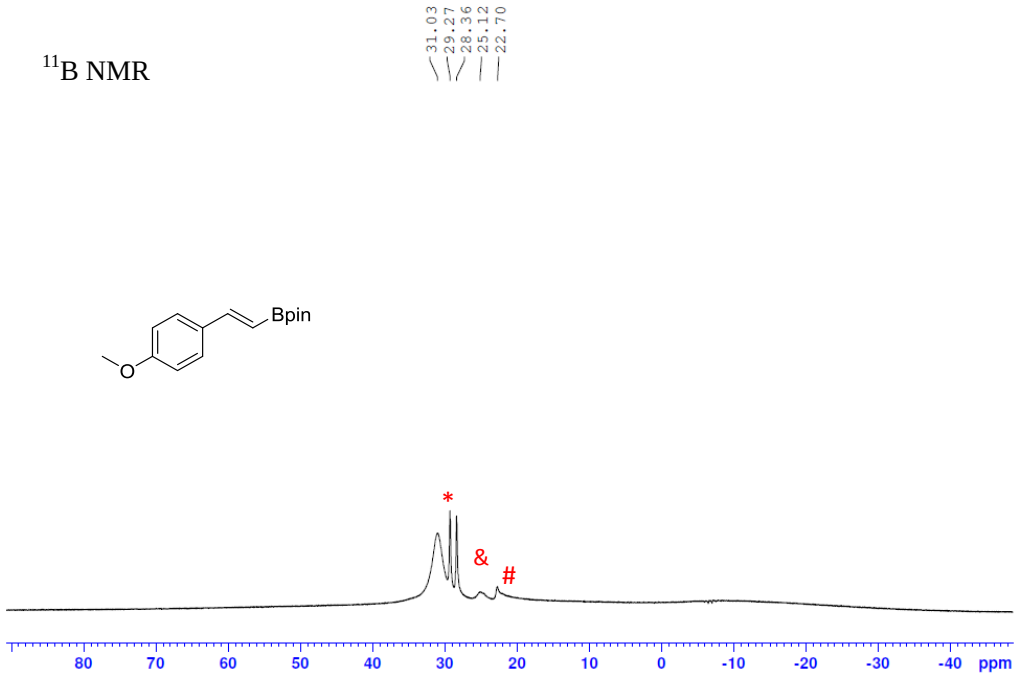
^{1}H NMR (600 MHz, tol-d_8): δ 7.62 (d, *J* = 18.6 Hz, 1H, C*H*), 7.23 (d, *J* = 8.4 Hz, 2H, Ar-*H*), 6.60 (d, *J* = 8.4 Hz, 2H, Ar-*H*), 6.22 (d, *J* = 18.6 Hz, 1H, C*H*), 3.26 (s, 3H, OCH_3). 1.16 (s, 12H, C(CH_3)$_2$). ^{13}C{^{1}H} NMR (151 MHz, tol-d_8): δ 25.0, 83.0, 114.25, 131.0, 137.5, 149.8, 169.8. ^{11}B NMR (193 MHz, tol-d_8): δ 31.0.



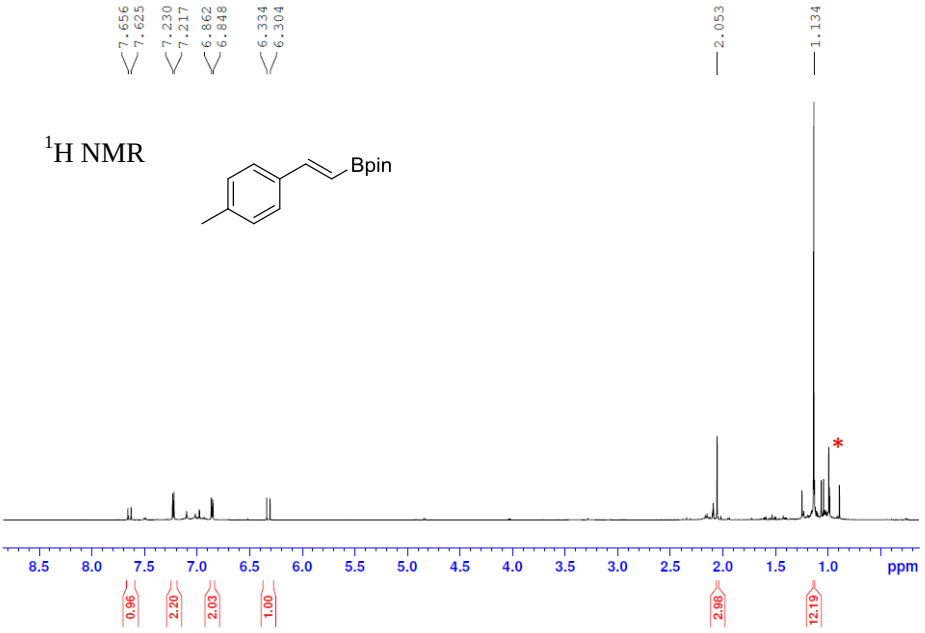
$^{13}C\{^{1}H\}$ NMR

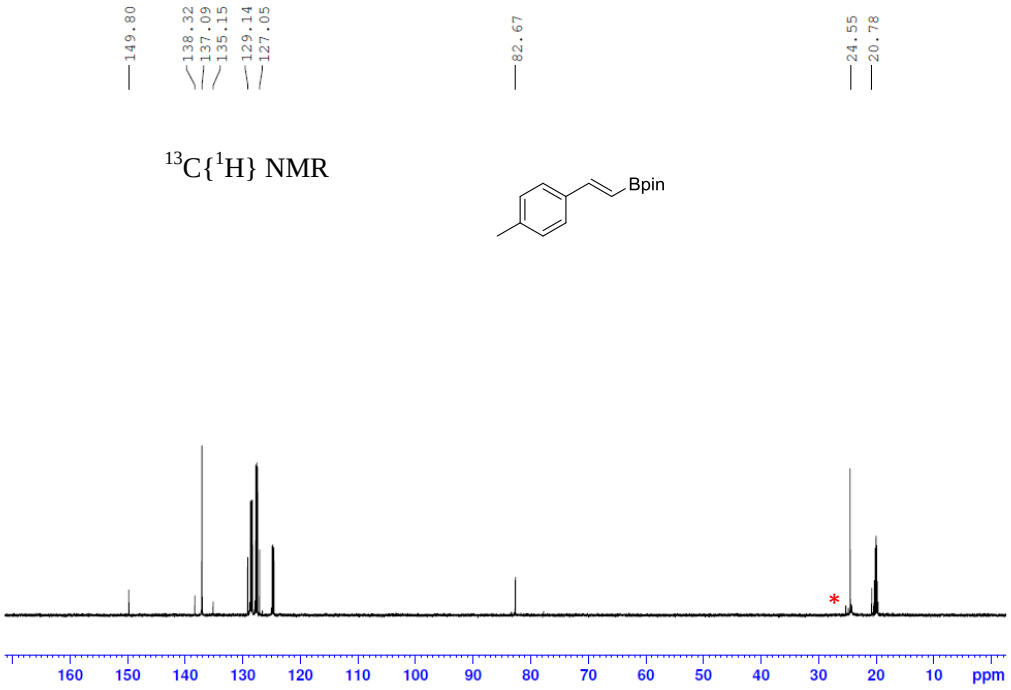


^{11}B NMR

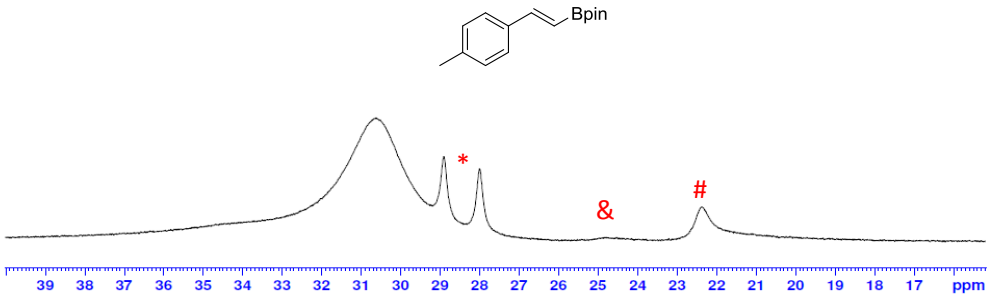


^{1}H NMR (600 MHz, tol-d_8): δ 7.63 (d, *J* = 18 Hz, 1H, C*H*), 7.22 (d, *J* = 8.4 Hz, 2H, Ar-*H*), 6.85 (d, *J* = 8.4 Hz, 2H, Ar-*H*), 6.32 (d, *J* = 18 Hz, 1H, C*H*), 2.05 (s, 3H, Ar-CH_3). 1.13 (s, 12H, C(CH_3)$_2$). ^{13}C{^{1}H} NMR (151 MHz, tol-d_8): δ 20.8, 24.5, 82.7, 127.0, 129.1, 135.2, 137.1, 138.3, 149.8. ^{11}B NMR (193 MHz, tol-d_8): δ 30.6.

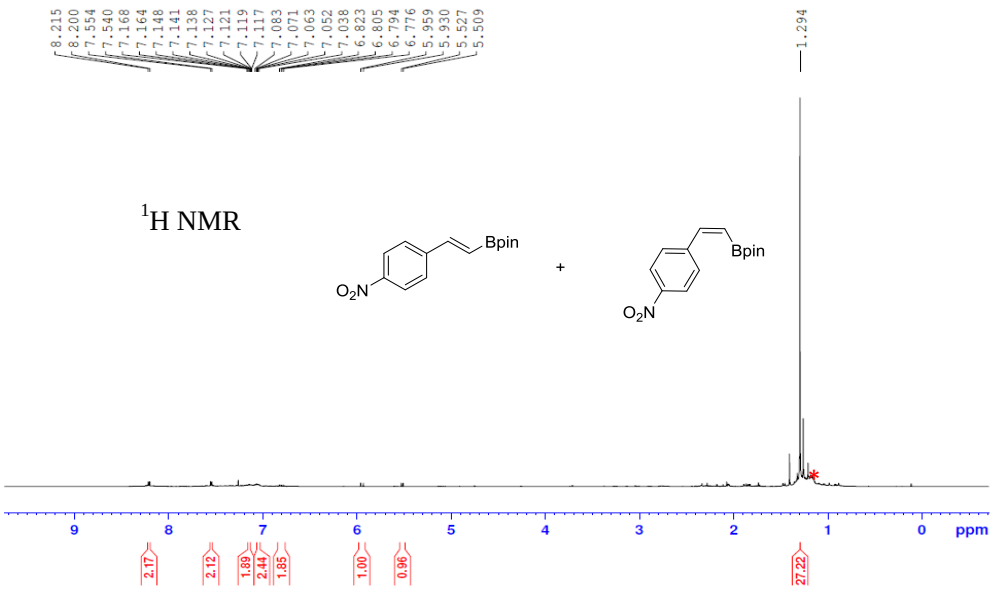




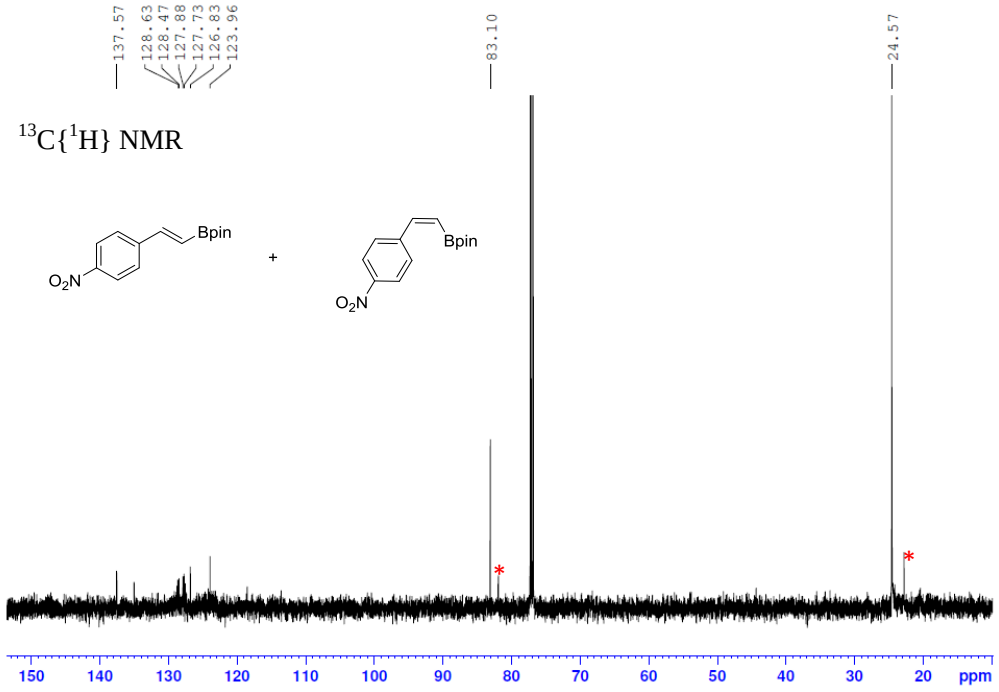
^{11}B NMR



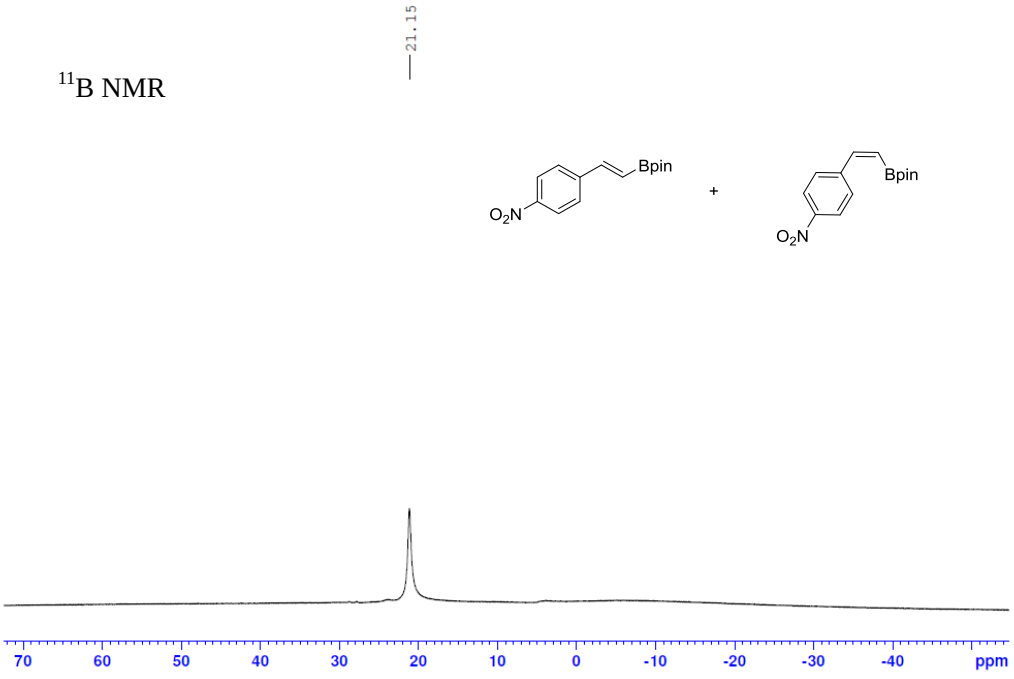
^{1}H NMR (600 MHz, $CDCl_3$): Z isomer δ 8.20 (d, *J* = 9 Hz, 2H, Ar-*H*), 7.55 (d, *J* = 9 Hz, 2H, Ar-*H*), 6.80 (d, *J* = 17.6 Hz, 1H, C*H*), 5.95 (d, *J* = 17.6 Hz, 1H, C*H*), 1.29 (s, 12H, C(CH_3)$_2$). E isomer δ 7.10 (m, 4H, Ar-*H*), 6.80 (d, *J* = 10.8 Hz, 1H, C*H*), 5.52 (d, *J* = 10.8 Hz, 1H, C*H*), 1.29 (s, 12H, C(CH_3)$_2$).^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ 24.6, 83.1, 124.0, 126.9, 127.7, 127.9, 128.5, 128.6, 137.6. ^{11}B NMR (193 MHz, $CDCl_3$): δ 21.2.



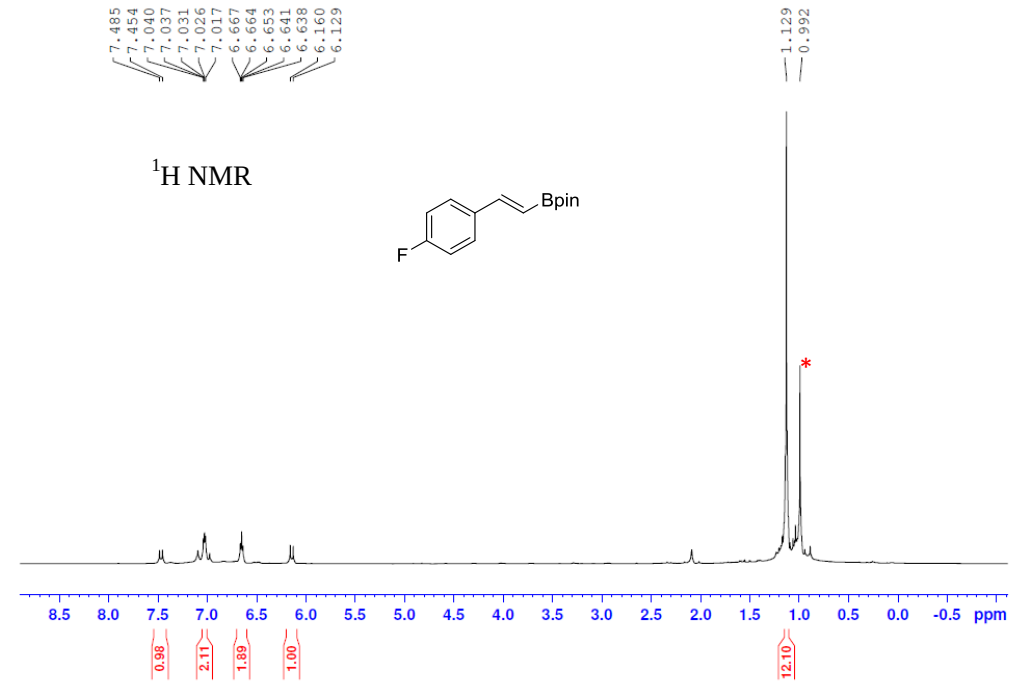
$^{13}C\{^{1}H\}$ NMR

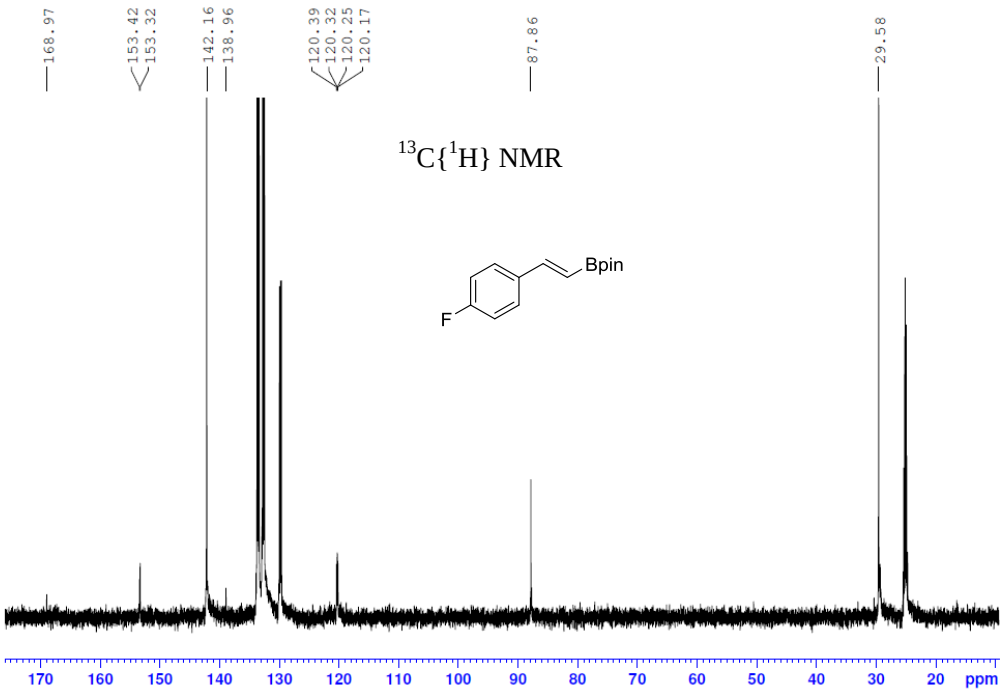


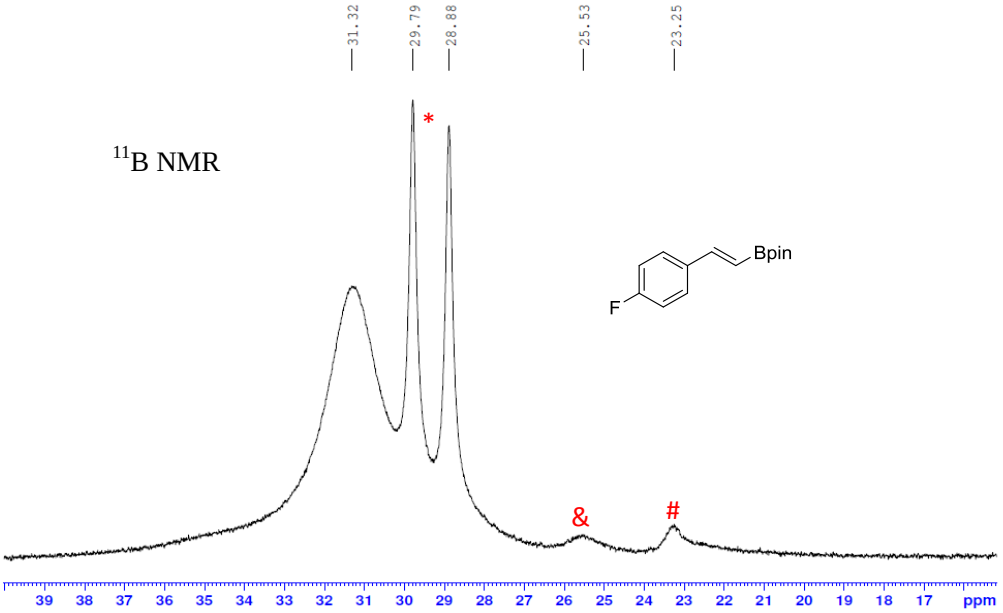
^{11}B NMR



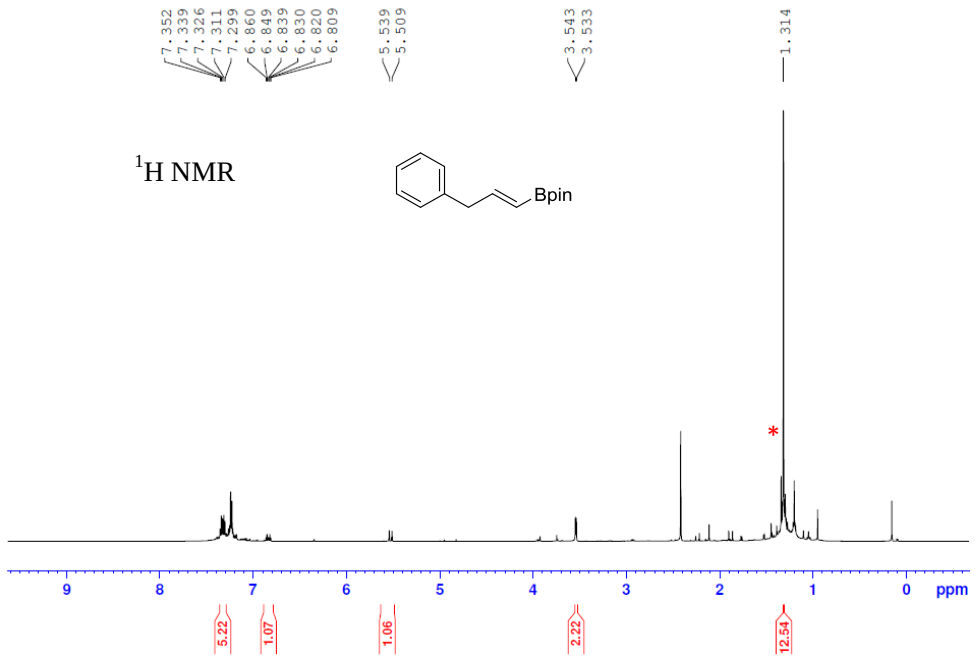
^{1}H NMR (600 MHz, tol-d_8): δ 7.47 (d, *J* = 18.6 Hz, 1H, C*H*), 7.03 (m, 2H, Ar-*H*), 6.66 (m, 2H, Ar-*H*), 6.14 (d, *J* = 18.6 Hz, 1H, C*H*), 1.12 (s, 12H, C(CH_3)$_2$). ^{13}C{^{1}H} NMR (151 MHz, tol-d_8): δ 29.6 , 87.9, 120.3, 139.0, 142.2, 153.4, 168.9. ^{11}B NMR (193 MHz, tol-d_8): δ 31.3.



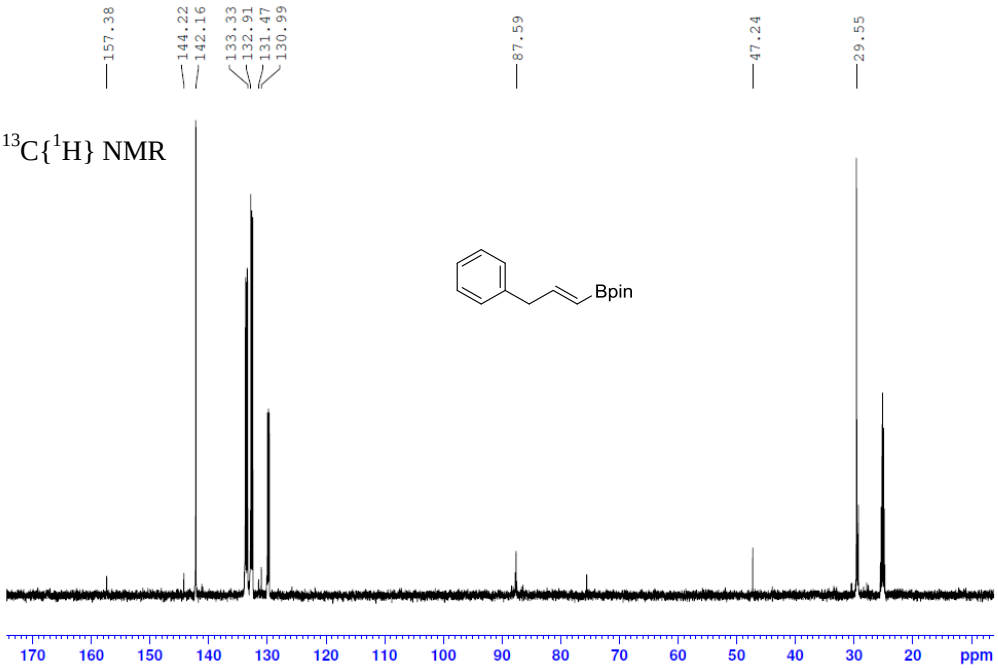




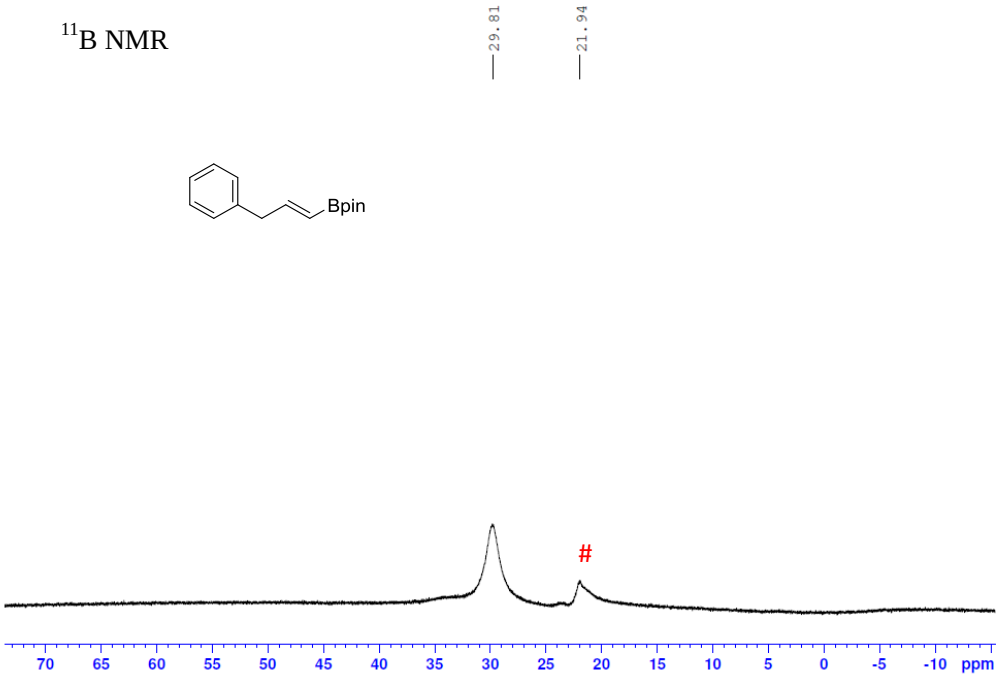
^{1}H NMR (600 MHz, $CDCl_3$): δ 7.39 (m, 5H, Ar-*H*), 6.84 (dt, *J* = 18, 6 Hz, 1H, C*H*), 5.63 (d, *J* = 18, 1H, C*H*), 3.54 (d, *J* = 6 Hz, 2H, Ar-CH_2), 1.31 (s, 12H, C(CH_3)$_2$). ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ 29.6, 47.2, 87.6, 130.1, 131.5, 132.9, 133.3,142.2, 144.2, 157.4. ^{11}B NMR (193 MHz, $CDCl_3$): δ 29.8.



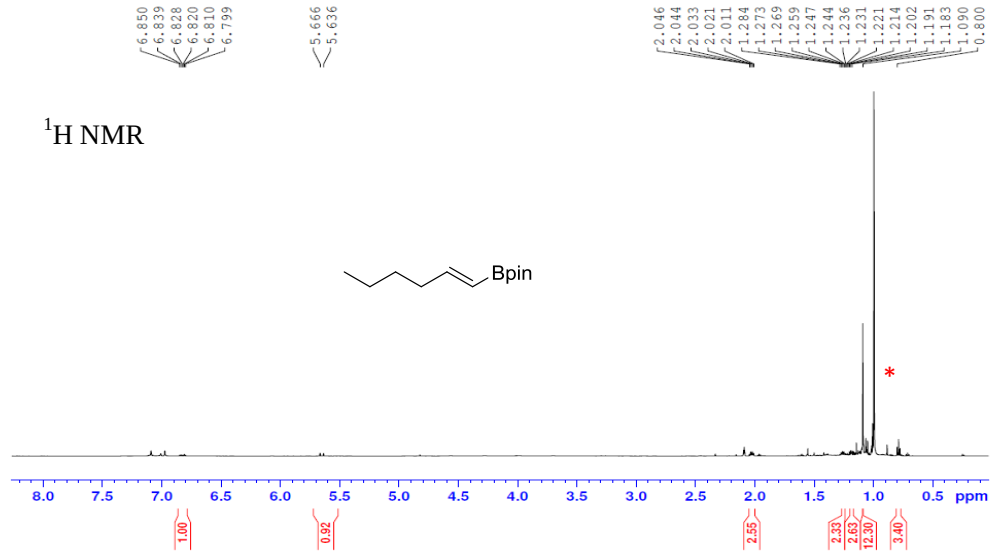
$^{13}C\{^{1}H\}$ NMR

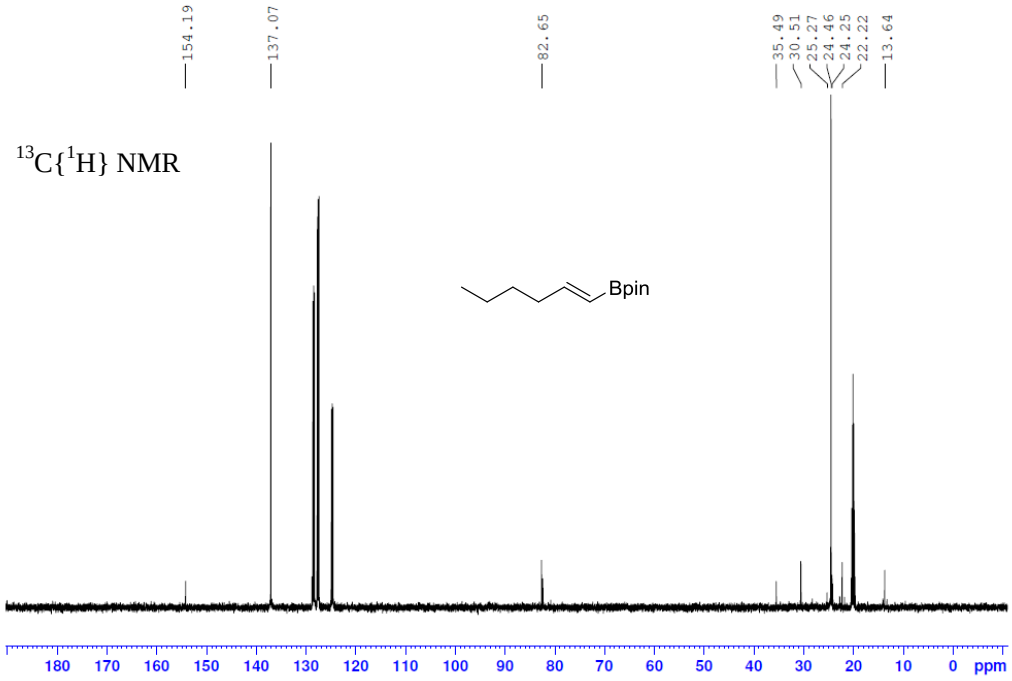


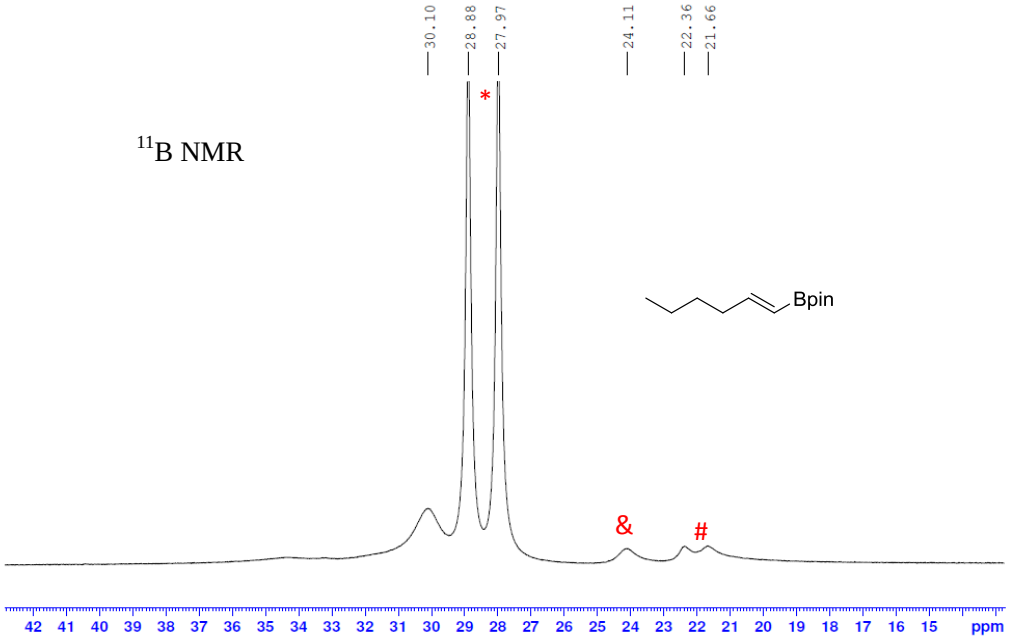
^{11}B NMR



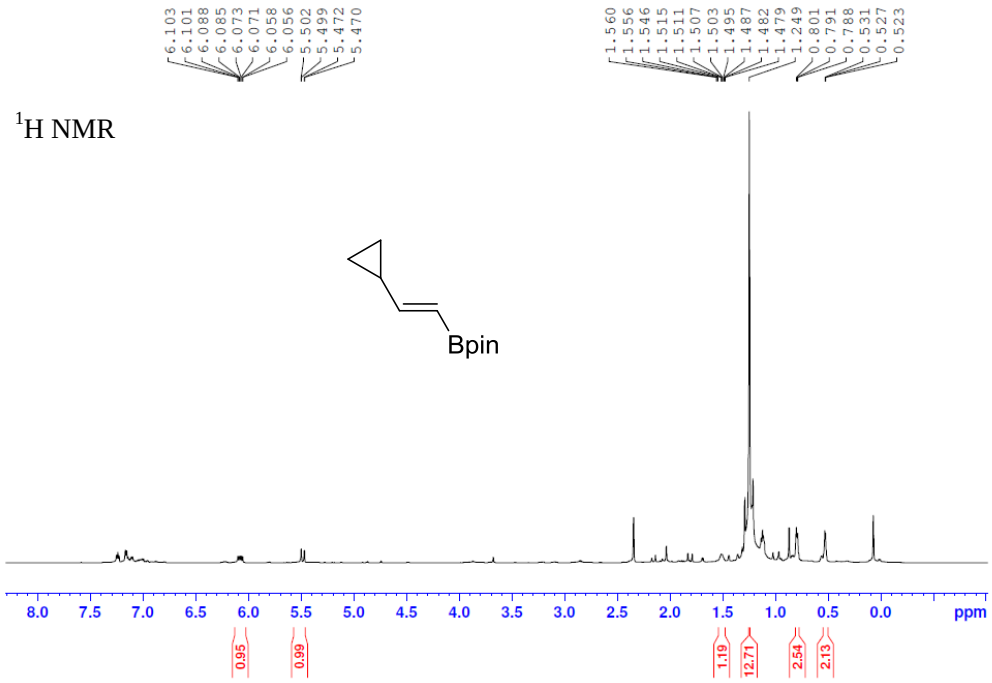
^{1}H NMR (600 MHz, tol-d_8): δ 6.82 (dt, *J* = 18, 6.6 Hz, 1H, C*H*), 5.64 (d, *J* = 18 Hz, 1H, C*H*), 2.03 (m, 2H, CH_2), 1.27 (m, 2H, CH_2), 1.23 (m, 2H, CH_2), 1.09 (s, 12H, C(CH_3)$_2$), 0.79 (t, *J* = 6.6 Hz, 3H, CH_3). ^{13}C{^{1}H} NMR (151 MHz, tol-d_8): δ 13.6, 22.2, 24.5, 30.5, 35.5, 85.7, 137.1, 154.2. ^{11}B NMR (193 MHz, tol-d_8): δ 30.1.

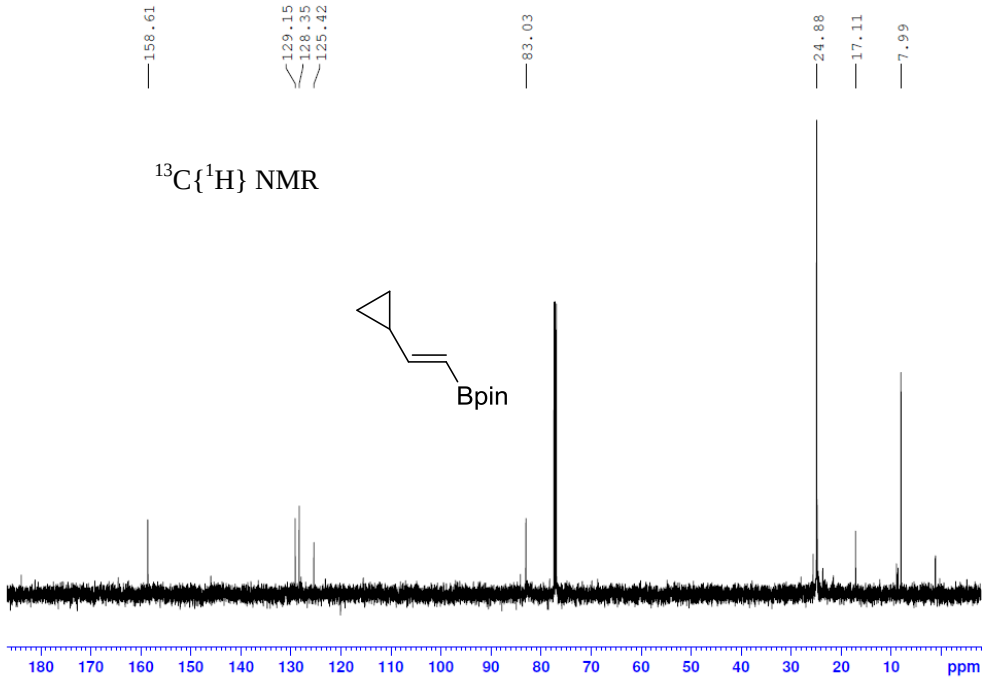




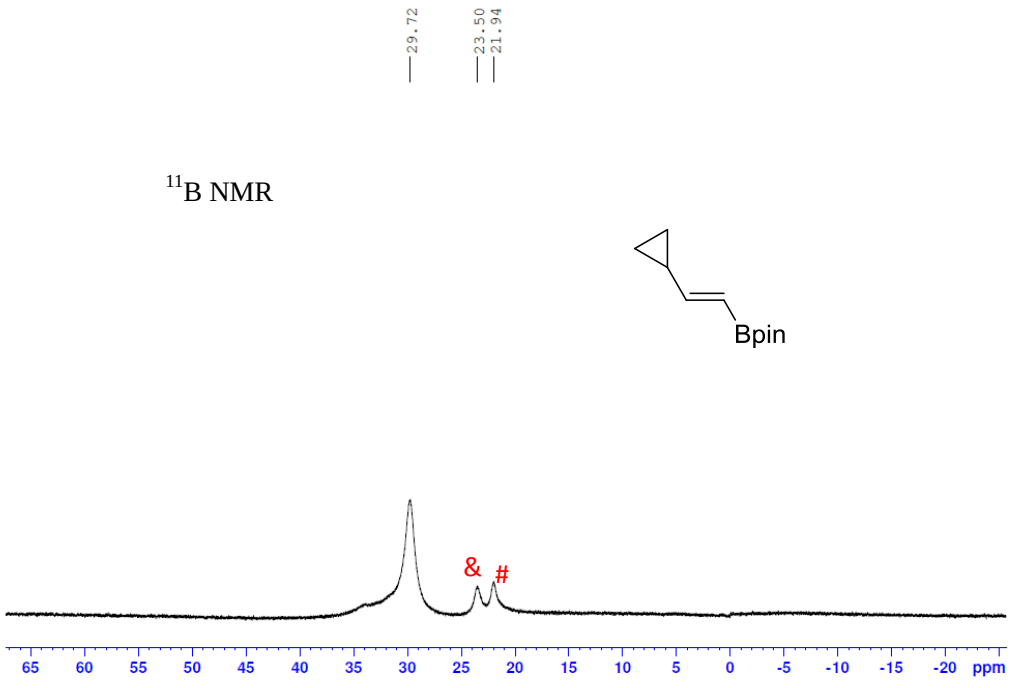


^{1}H NMR (600 MHz, $CDCl_3$): δ 6.67 (ddd, *J* = 17.8, 9.2, 1.5 Hz, 1H, C*H*), 5.49 (dd, *J* = 17.8, 1.5Hz, 1H, C*H*), 1.51 (m, 1H, C_3H_5), 1.25 (s, 12H, $C(CH_3)_2$), 0.79 (m, 2H, C_3H_5), 0.53 (m, 2H, C_3H_5). ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ 8.0, 17.1, 24.9, 83.0, 158.6. ^{11}B NMR (193 MHz, $CDCl_3$): δ 29.7.



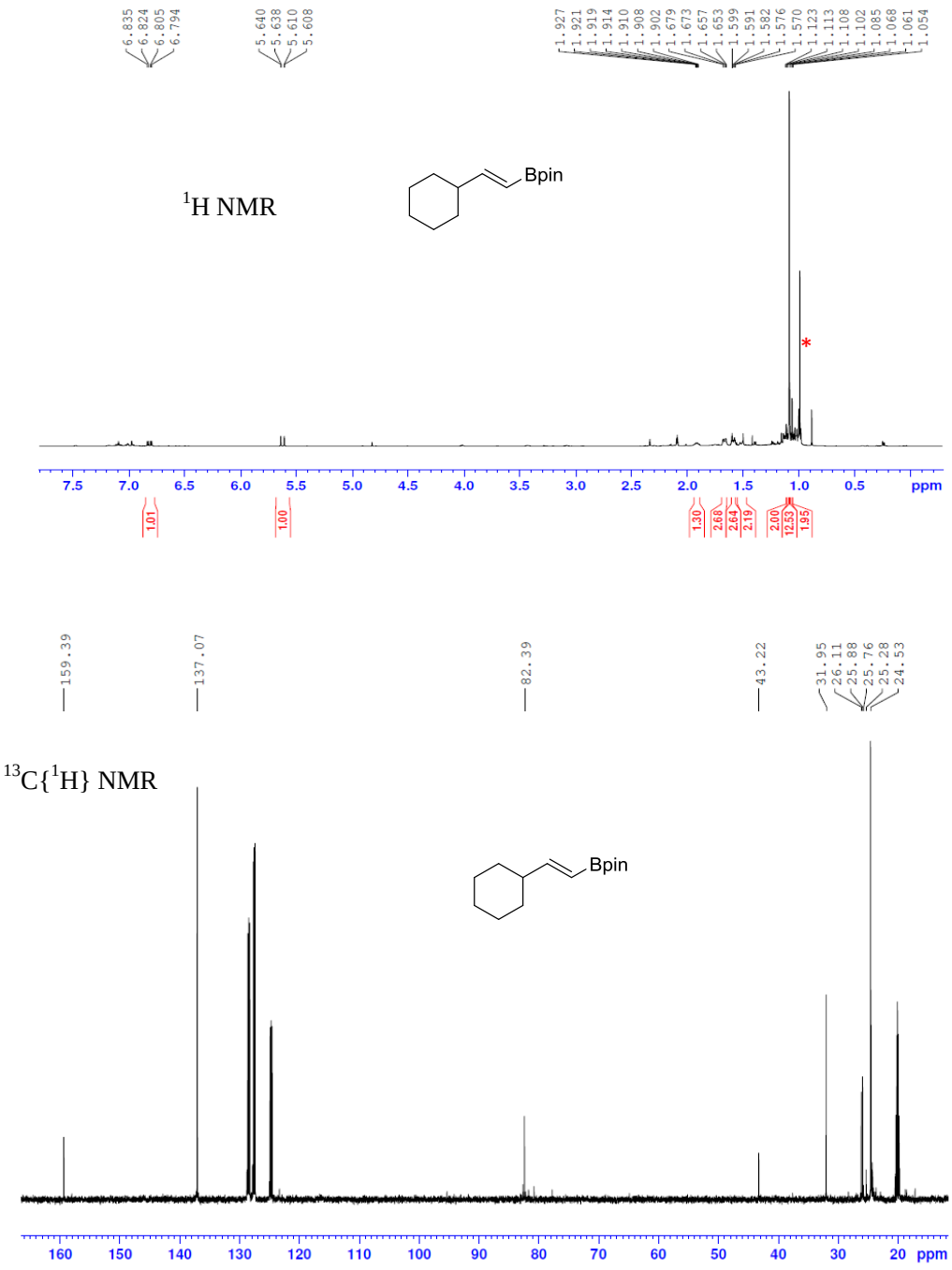


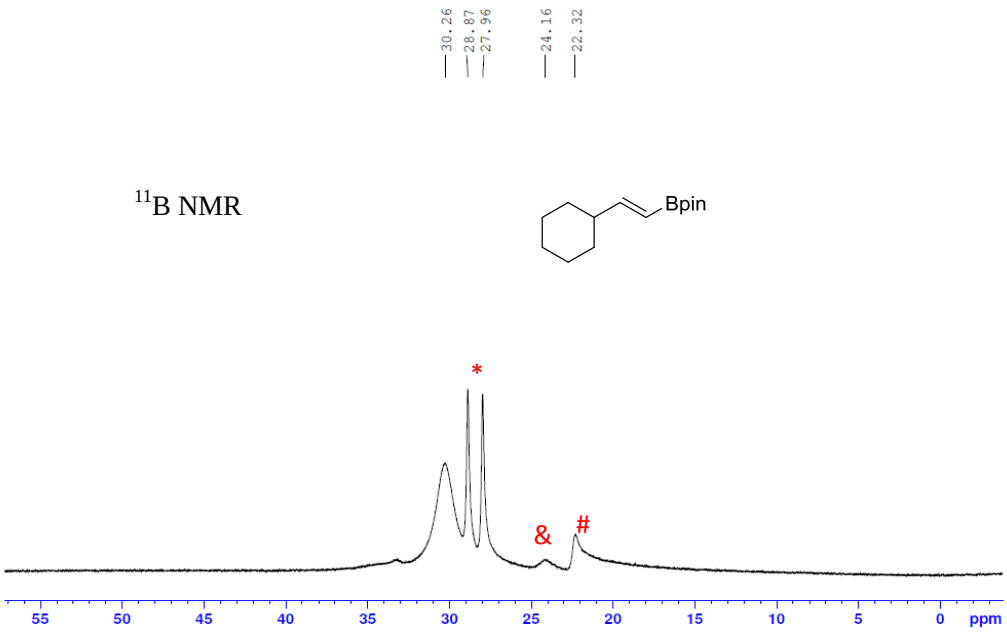
$^{13}C\{^{1}H\}$ NMR



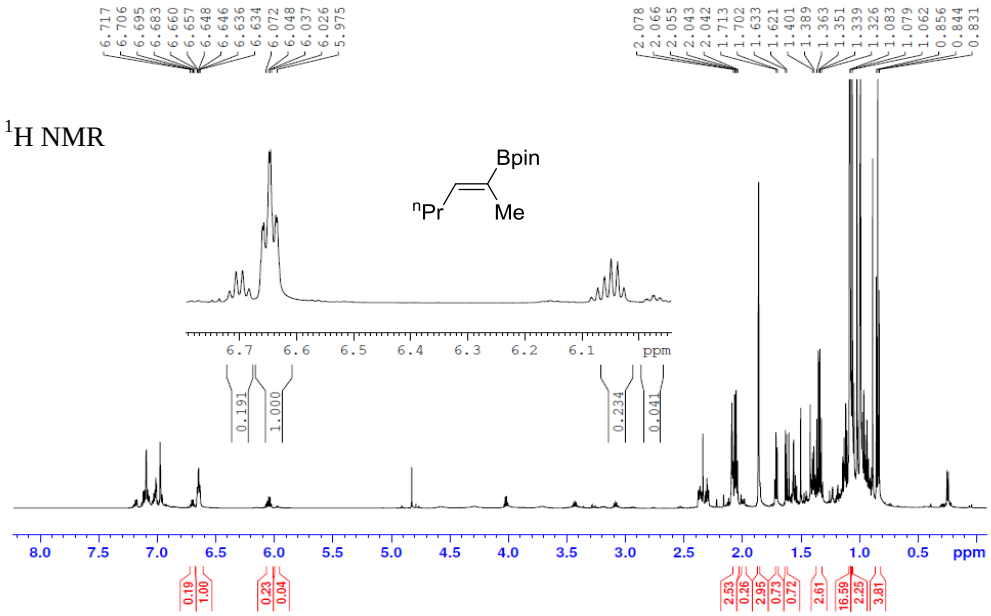
^{11}B NMR

^{1}H NMR (600 MHz, tol-d_8): δ 6.82 (dd, *J* = 18, 6.6 Hz, 1H, C*H*), 5.63 (dd, *J* = 18, 6.6 Hz, 1H), 1.91 (m, 1H, C_6H_{11}), 1.67 (m, 2H, C_6H_{11}), 1.59 (m, 4H, C_6H_{11}), 1.12 (m, 2H, C_6H_{11}), 1.09 (s, 12H, $C(CH_3)_2$), 1.06 (m, 2H, C_6H_{11}). ^{13}C{^{1}H} NMR (151 MHz, tol-d_8): δ 24.3, 25.3, 25.8, 25.9, 26.1, 31.9, 43.2, 82.4, 137.1, 159.4. ^{11}B NMR (193 MHz, tol-d_8): δ 30.3.

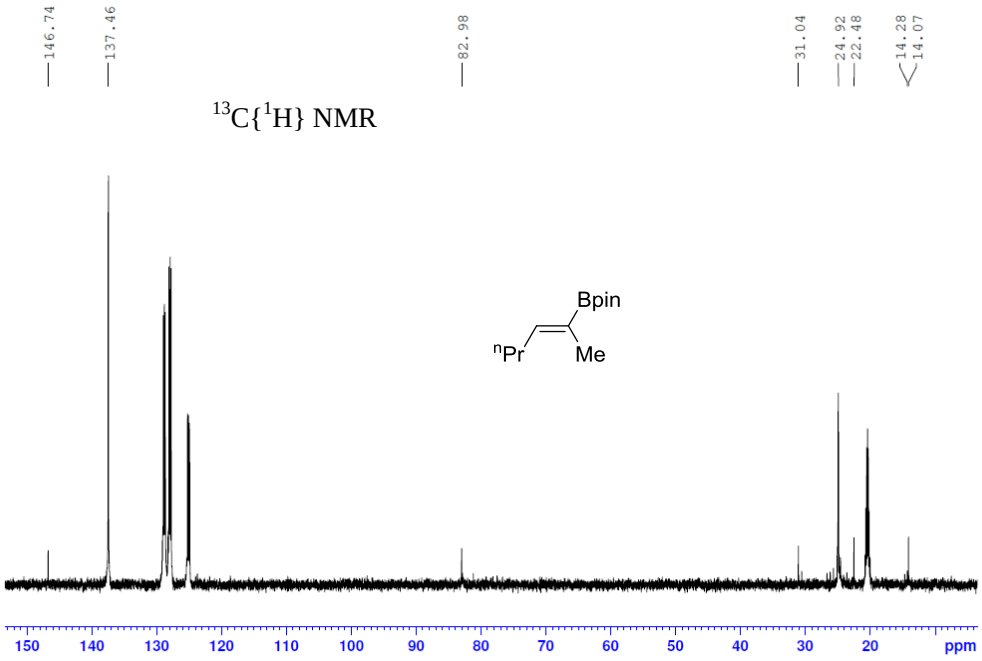


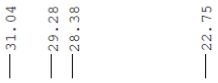


^{1}H NMR Za isomer (600 MHz, tol-d_8): δ 6.04 (td, *J* = 18, 6.6 Hz, 1H, C*H*), 2.05 (t, *J* = 6.6 Hz, 2H, CH_2), 1.72 (s, 3H, CH_3), 1.09 (s, 12H, C(CH_3)$_2$), 1.06 (m, 2H, CH_2), 0.85 (t, *J* = 7.2 Hz, 3H, CH_3). ^{13}C{^{1}H} NMR (151 MHz, tol-d_8): δ 14.1, 14.3, 22.5, 24.9, 31.0, 83.0, 137.4, 146.7. ^{11}B NMR (193 MHz, tol-d_8): δ 31.0.

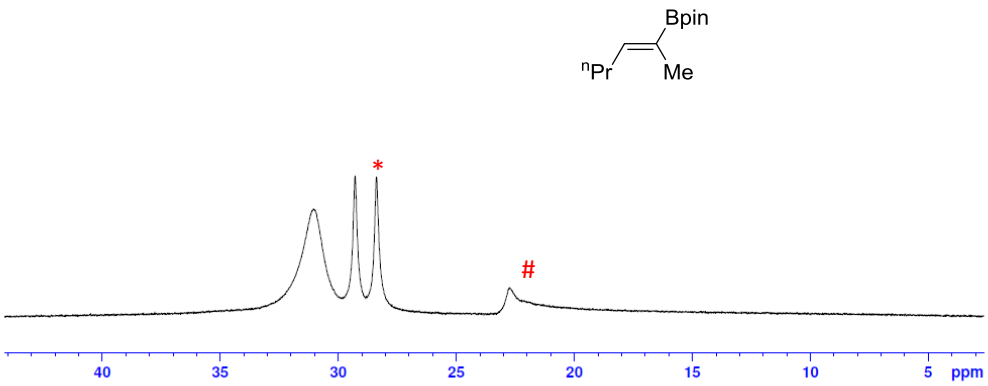


$^{13}C\{^{1}H\}$ NMR

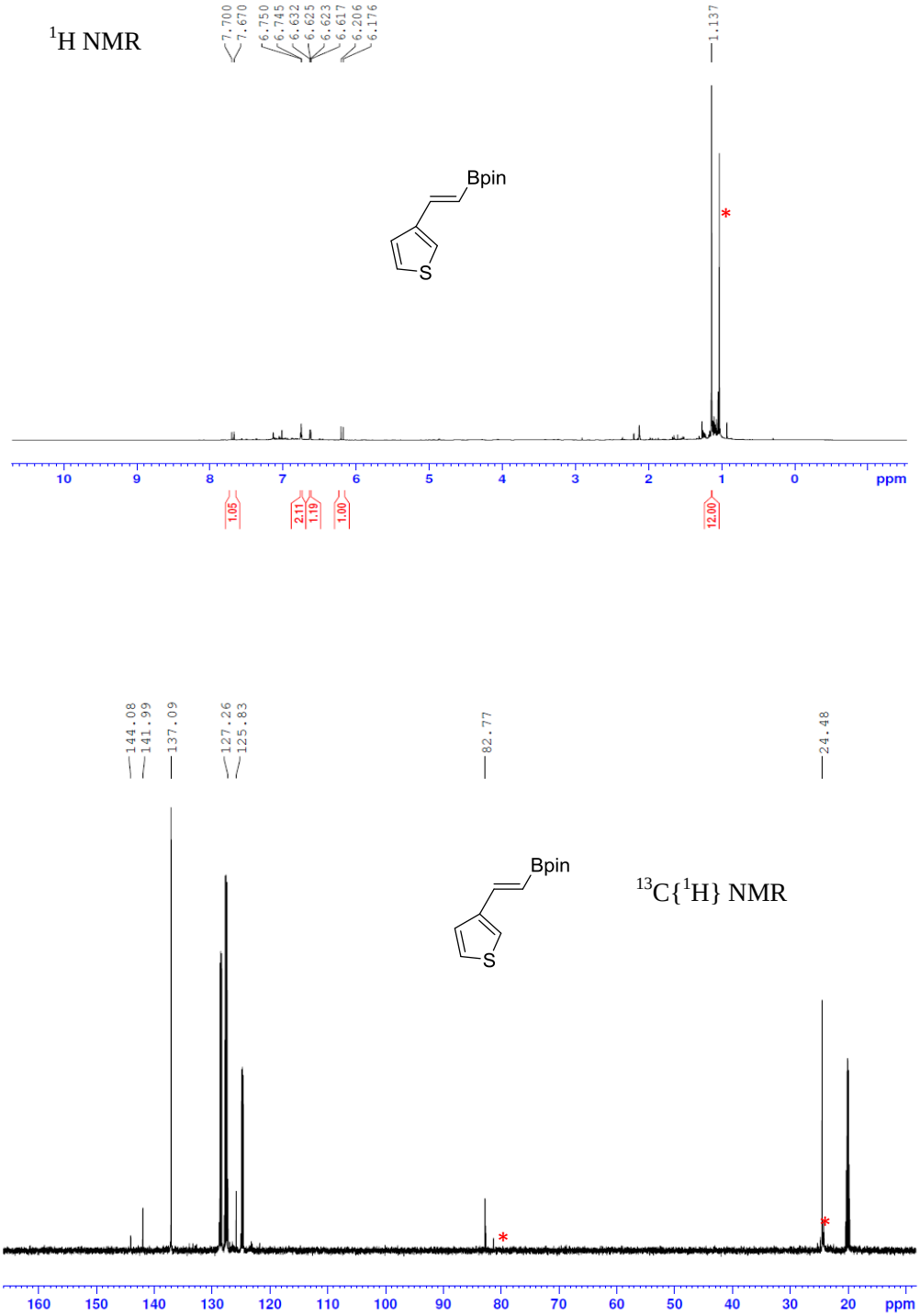


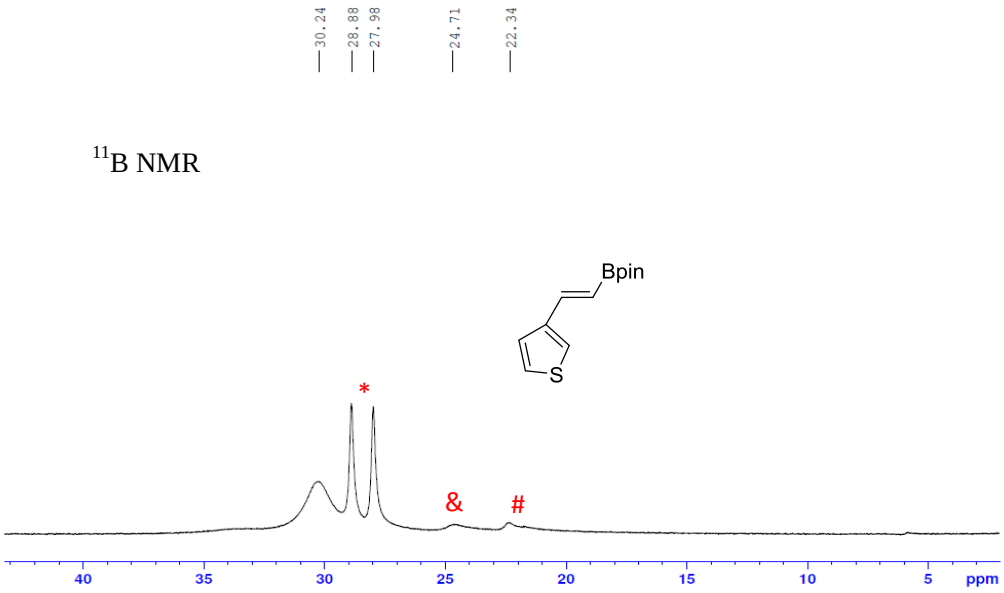


^{11}B NMR



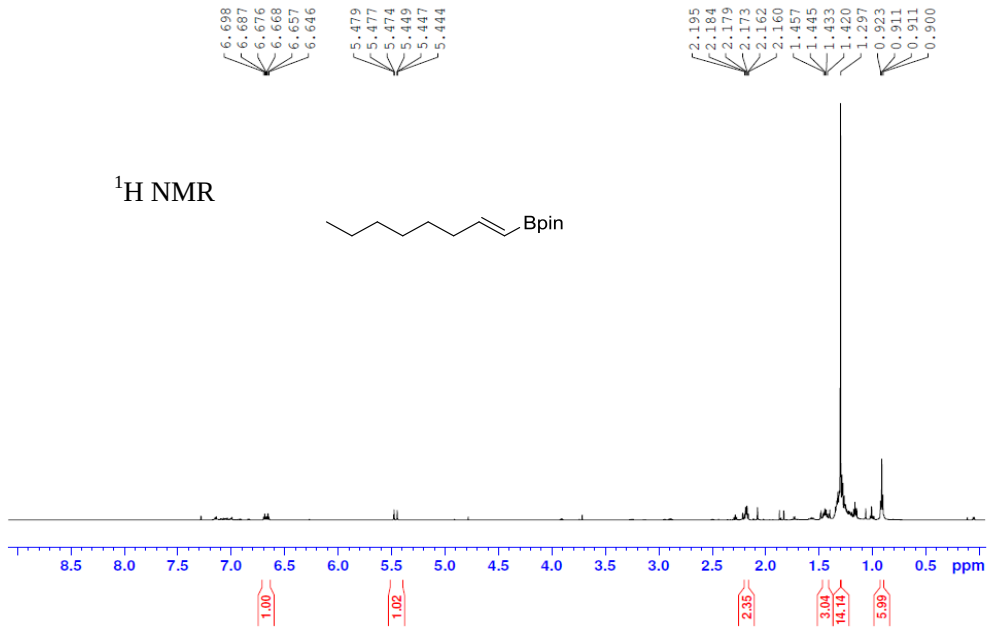
^{1}H NMR (600 MHz, tol-d_8): δ 7.69 (d, *J* = 18 Hz, 1H, C*H*), 6.75 (d, *J* = 9 Hz, 2H, Ar-*H*), 6.63 (m, 1H, Ar-*H*), 6.19 (d, *J* = 18 Hz, 1H, C*H*), 1.13 (s, 12H, C(CH_3)$_2$). ^{13}C{^{1}H} NMR (151 MHz, tol-d_8): δ 24.5, 82.8, 125.8, 127.3, 137.1, 142.0, 144.1. ^{11}B NMR (193 MHz, tol-d_8): δ 30.2.





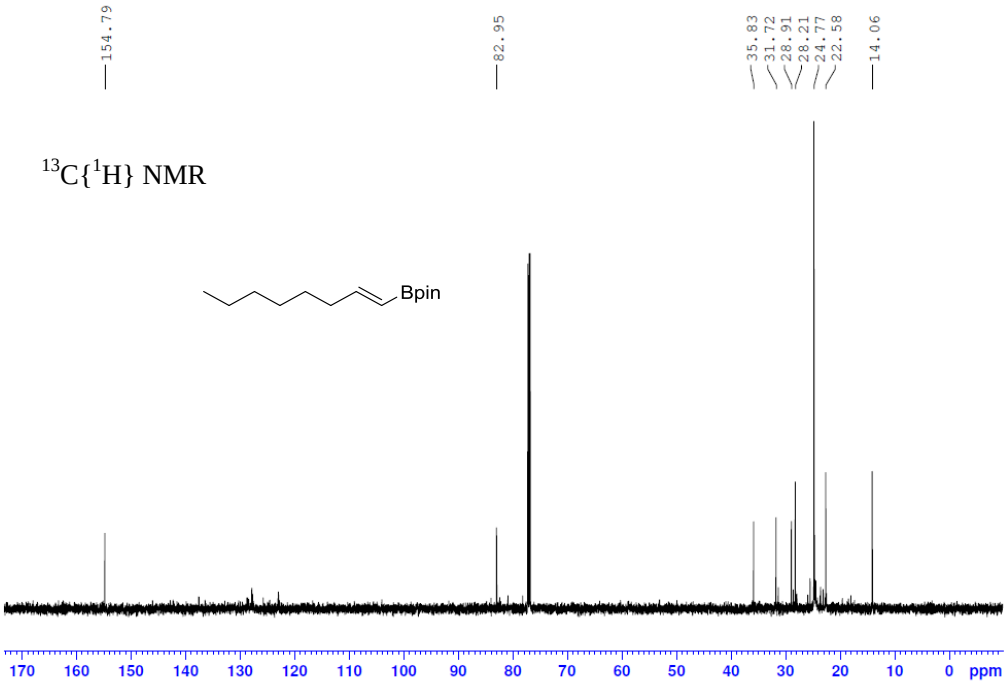
^{11}B NMR

^{1}H NMR (600 MHz, $CDCl_3$): δ 6.67 (dt, *J* = 18, 6.6 Hz, 1H, C*H*), 5.47 (dt, *J* = 18, 6.6 Hz, 1H, C*H*), 2.17 (td, *J* = 19.8, 6.6 Hz, 1H, CH_2), 1.44 (m, 3H, CH_3), 1.29 (s, 14H, C(CH_3)$_2$ + CH_2), 0.91 (m, 6H, CH_2). ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ 14.1, 22.6, 24.7, 28.2, 28.9, 31.7, 35.8, 83.0, 154.8. ^{11}B NMR (193 MHz, $CDCl_3$): δ 29.7.

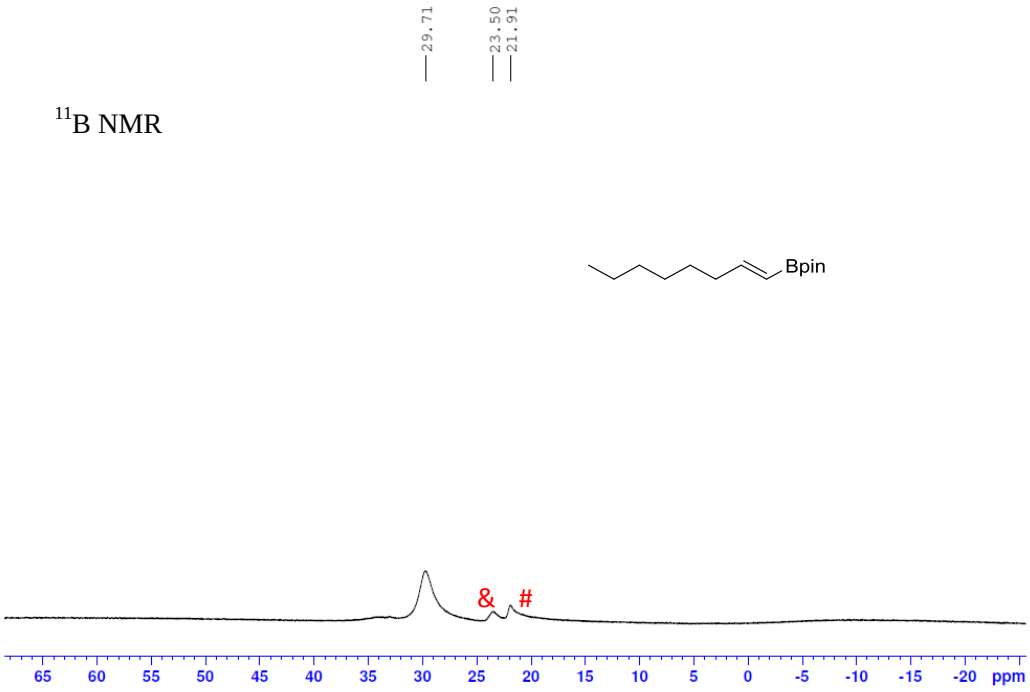


^{1}H NMR

$^{13}C\{^{1}H\}$ NMR



^{11}B NMR

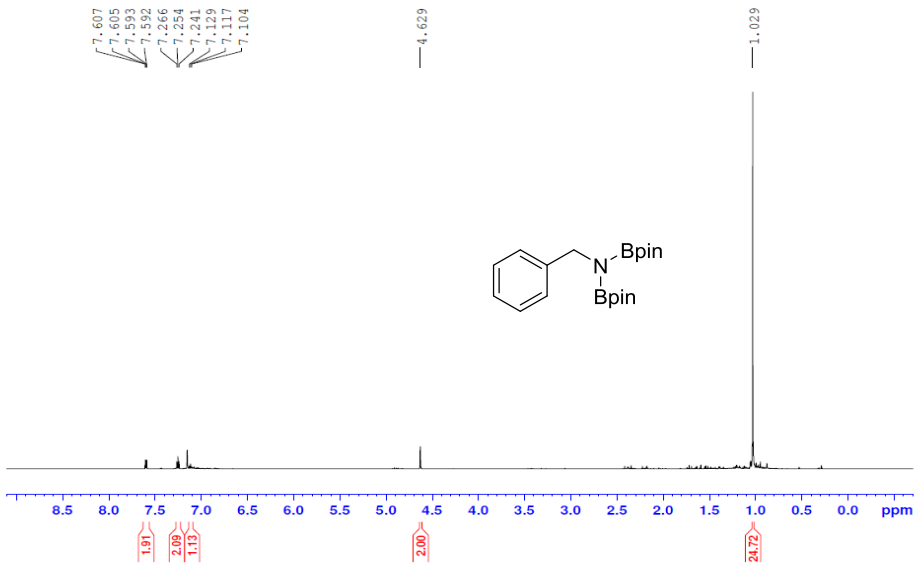


General procedure for catalytic hydroboration of nitriles.

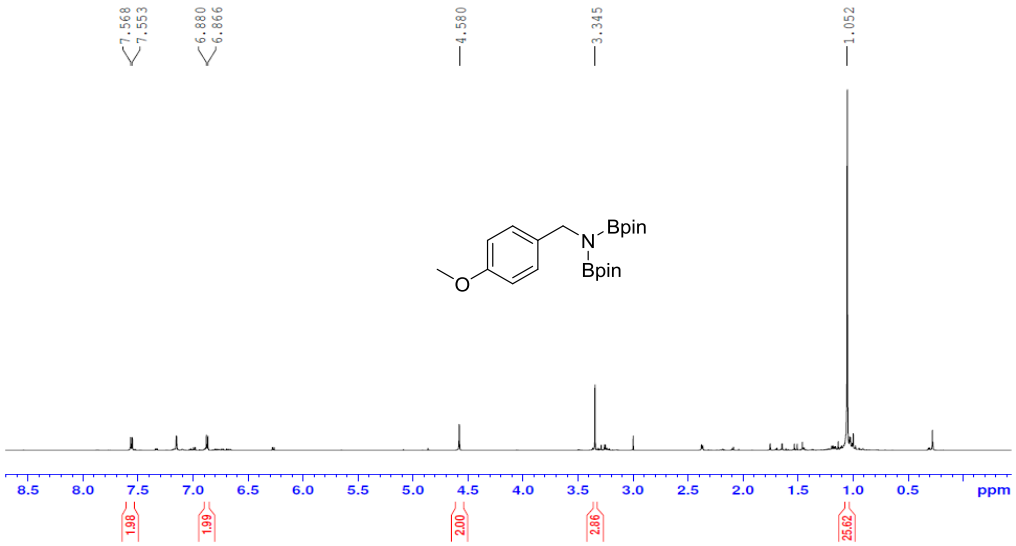
In a glovebox, nitriles (0.12 mmol) was added to a solution of catalyst (10%) and HBpin (0.25 mmol) in C_6D_6 (0.50 mL) at room temperature, then heated at 60 ℃ for required time. The progress of the reaction was monitored by ^{1}H NMR spectroscopy.

NMR data of the crude reaction.

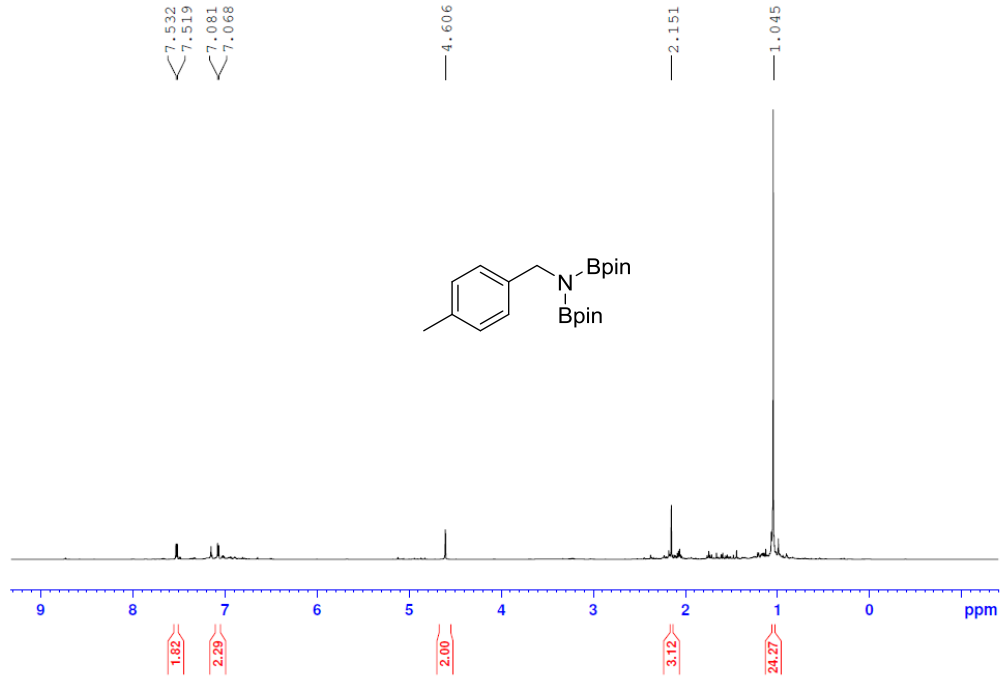
^{1}H NMR (C_6D_6, 600 MHz): δ 7.58 (m, 2H, Ar-*H*), 7.25 (m, 2H, Ar-*H*), 7.11 (m, 1H, Ar-*H*), 4.61 (s, 2H, Ar-CH_2), 1.03 (s, 24H, C(CH_3)$_2$)。



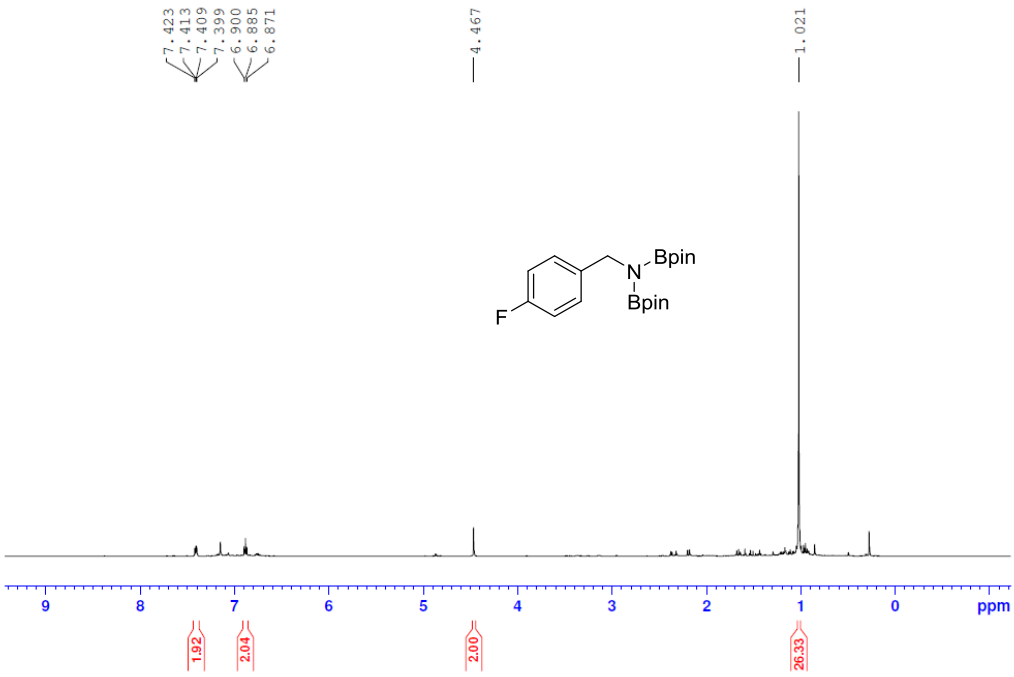
^{1}H NMR (C_6D_6, 600 MHz): δ 7.56 (d, *J* = 8.4 Hz, 2 H, Ar-*H*), 6.87 (d, *J* = 8.4 Hz, 2H, Ar-*H*), 4.58 (s, 2H, Ar-CH_2), 3.34 (s, 3H, OCH_3), 1.05 (s, 24H, C(CH_3)$_2$)。



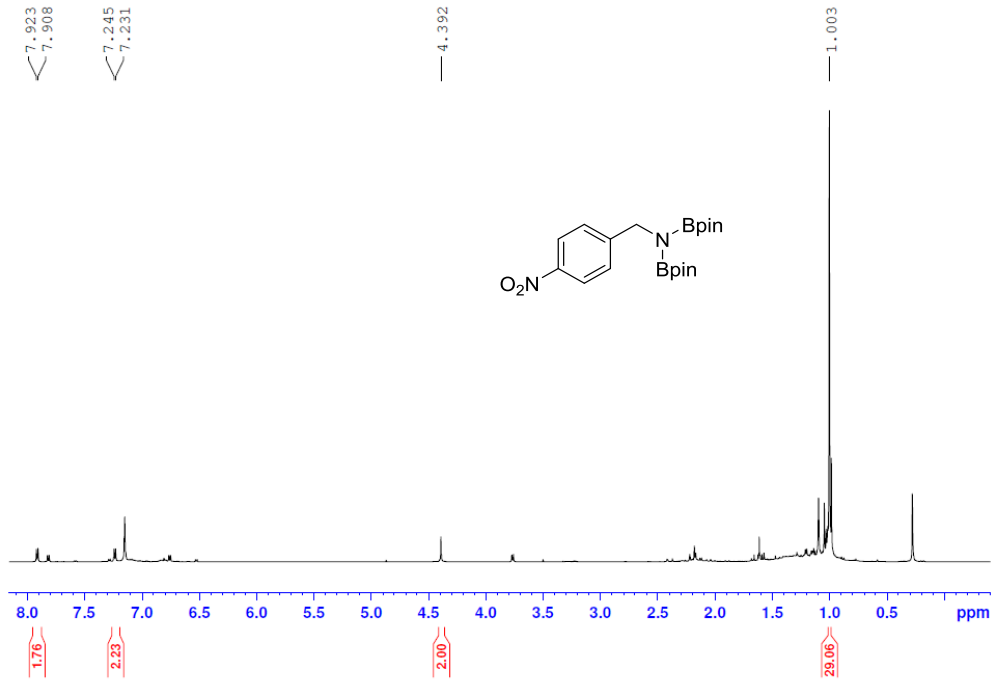
^{1}H NMR (C_6D_6, 600 MHz): δ 7.52 (d, *J* = 7.8 Hz, 2H, Ar-*H*), 7.07 (d, *J* = 7.8 Hz, 2H, Ar-*H*), 4.61 (s, 2H, Ar-CH_2), 2.15 (s, 3H, Ar-CH_3), 1.05 (s, 24H, C(CH_3)$_2$)。



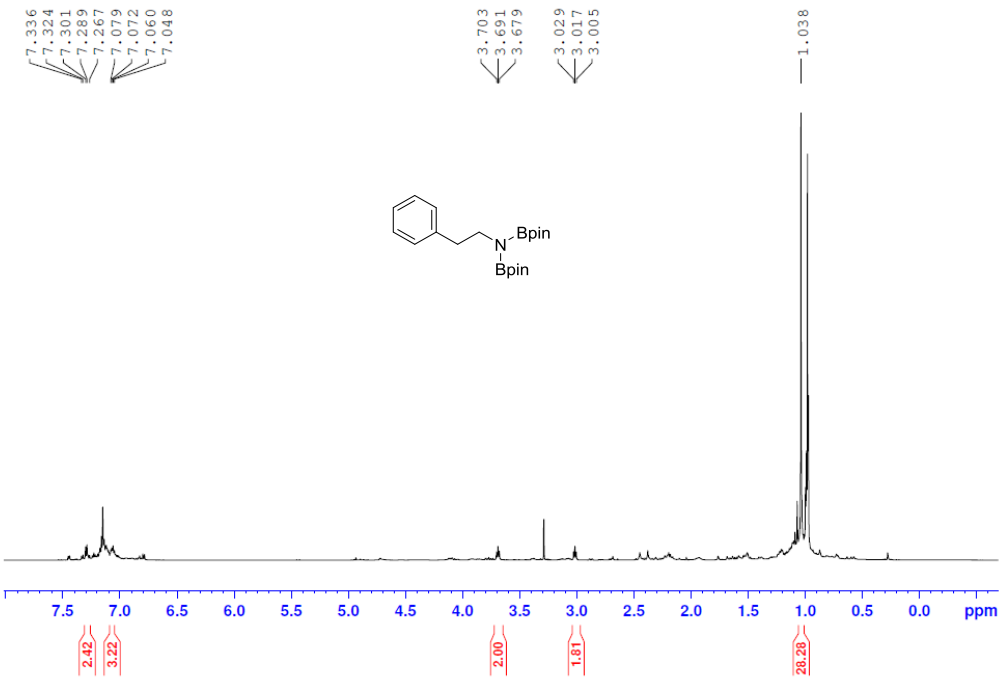
^{1}H NMR (C_6D_6, 600 MHz): δ 7.41 (m, 2H, Ar-*H*), 6.88 (m, 2H, Ar-*H*), 4.46 (s, 2H, Ar-CH_2), 1.02 (s, 24H, C(CH_3)$_2$)。



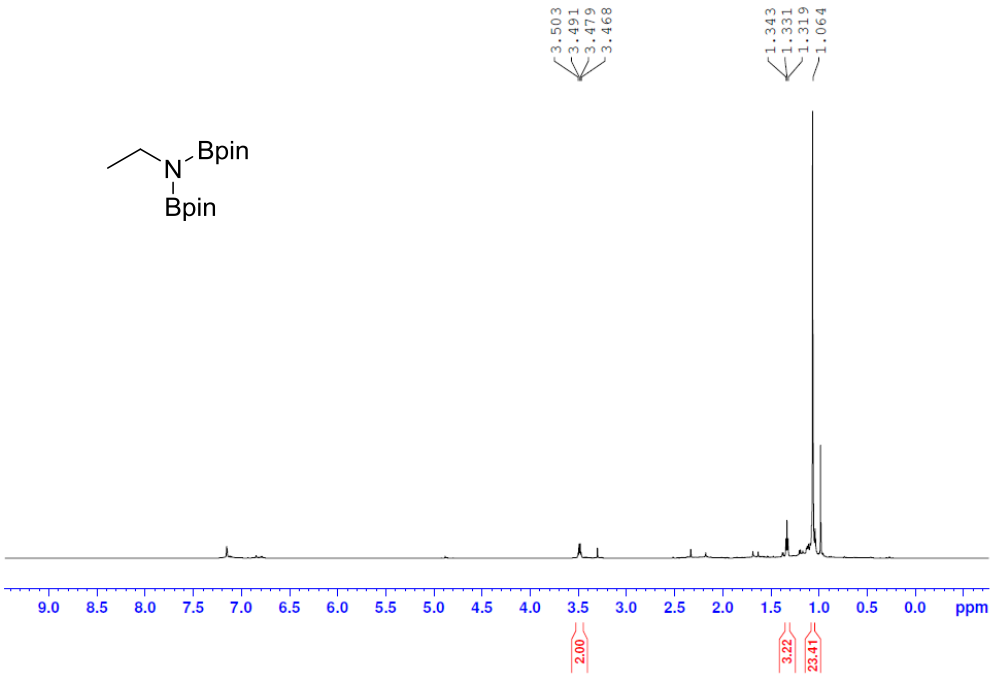
^{1}H NMR (C_6D_6, 600 MHz): δ 7.91 (d, *J*= 8.4 Hz, 2H, Ar-*H*), 7.23 (d, *J* = 8.4 Hz, 2H, Ar-*H*), 4.39 (s, 2H, Ar-CH_2), 1.03 (s, 24H, C(CH_3)$_2$)。



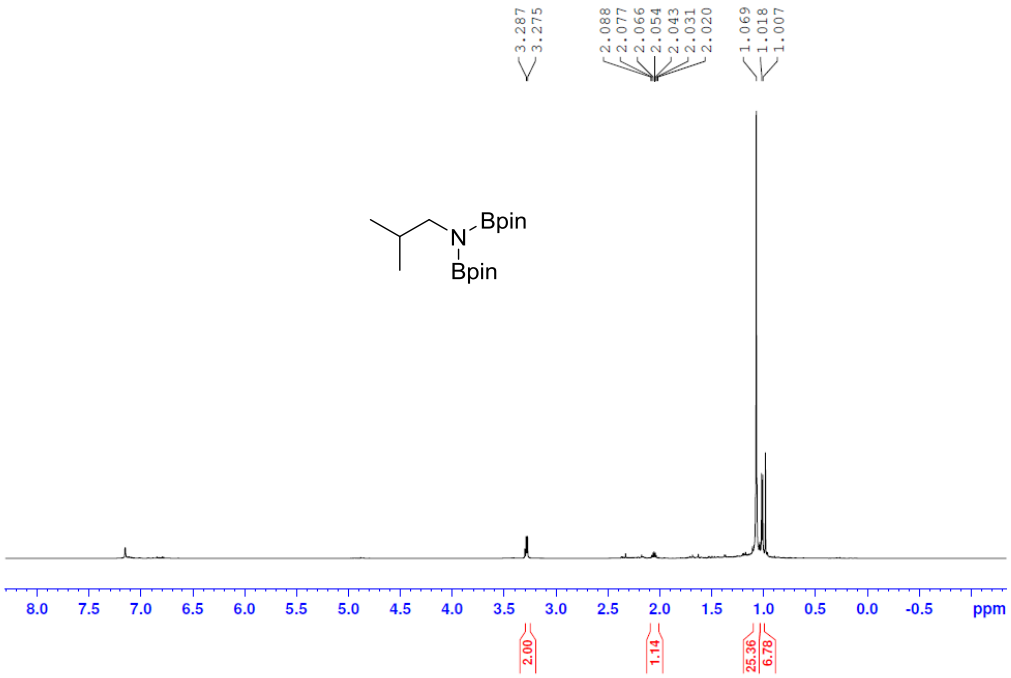
^{1}H NMR (C_6D_6, 600 MHz): δ 7.33 (m, 3H, Ar-*H*), 7.23 (m, 2H, Ar-*H*), 3.77 (t, *J*= 7.2 Hz, 2H, ArCH_2), 3.02 (t, *J*= 8.4 Hz, 3H, NCH_3), 1.04 (s, 24H, C(CH_3)$_2$)。



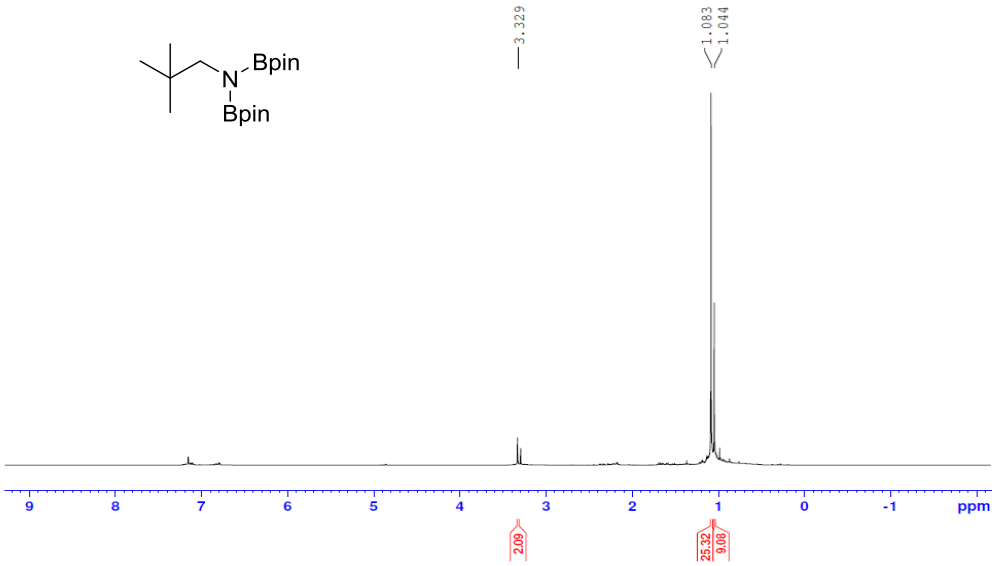
^{1}H NMR (C_6D_6, 600 MHz): δ 3.77 (q, *J*= 7.2 Hz, 2H, NCH_2), 1.33 (t, *J*= 7.2 Hz, 3H, CH_2CH_3), 1.06 (s, 24H, $C(CH_3)_2$)。



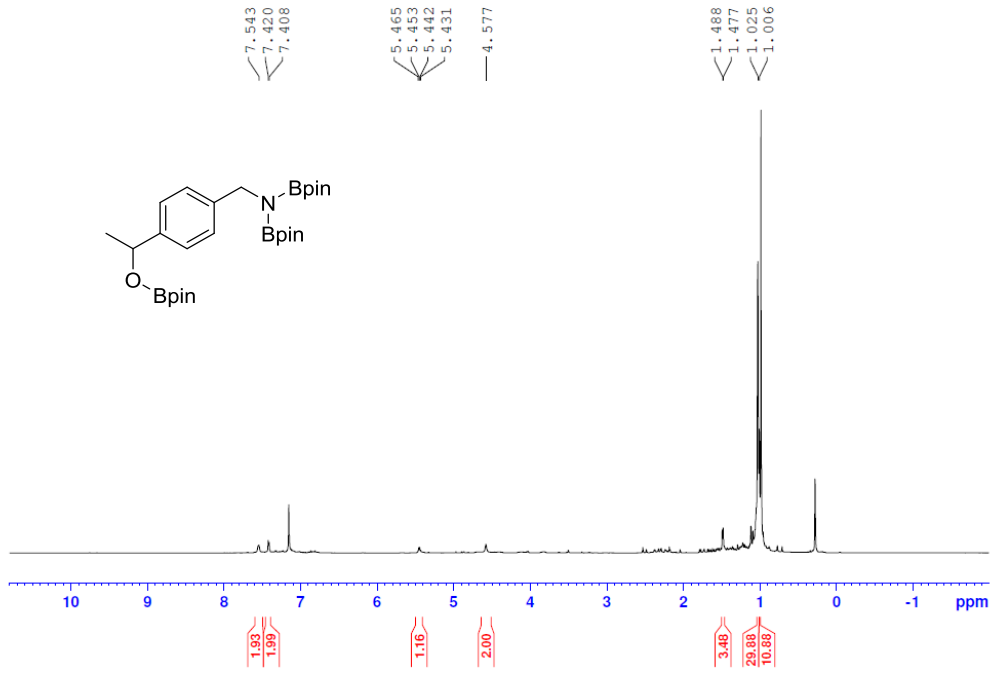
^{1}H NMR (C_6D_6, 600 MHz): δ 3.28 (d, *J*= 7.2 Hz, 2H, NCH_2), 2.05 (m, 1H, CH(CH_3)$_2$), 1.06 (s, 24H, $C(CH_3)_2$), 1.08 (d, *J* = 7.2 Hz, 6H, CH(CH_3)$_2$)。



^{1}H NMR (C_6D_6, 600 MHz): δ 3.32 (s, 2H, NCH_2), 1.08 (s, 24H, C(CH_3)$_2$), 1.04 (s, 9H, C(CH_3)$_3$)。



^{1}H NMR (C_6D_6, 600 MHz): δ 7.54 (m, 2H, Ar-*H*), 7.42 (m, 2H, Ar-*H*), 5.45 (q, *J*= 6.6 Hz, 1H, Ar-C*H*), 4.58 (s, 2H, Ar-CH_2), 1.48 (d, *J* = 6.6 Hz, 3H, OCH_3), 1.03 (s, 24H, N-Bpin-CH_3), 1.01 (s, 12H, O-Bpin-CH_3) .

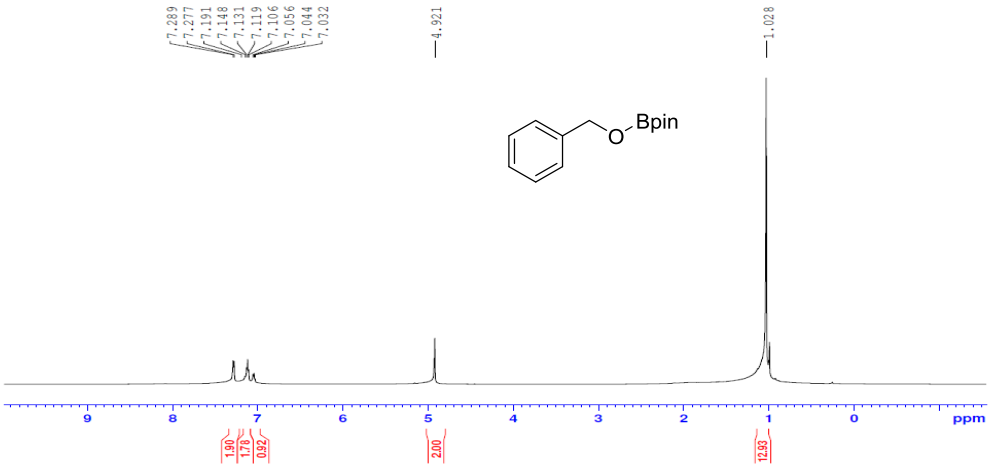


General procedure for catalytic hydroboration of ketones or aldehydes.

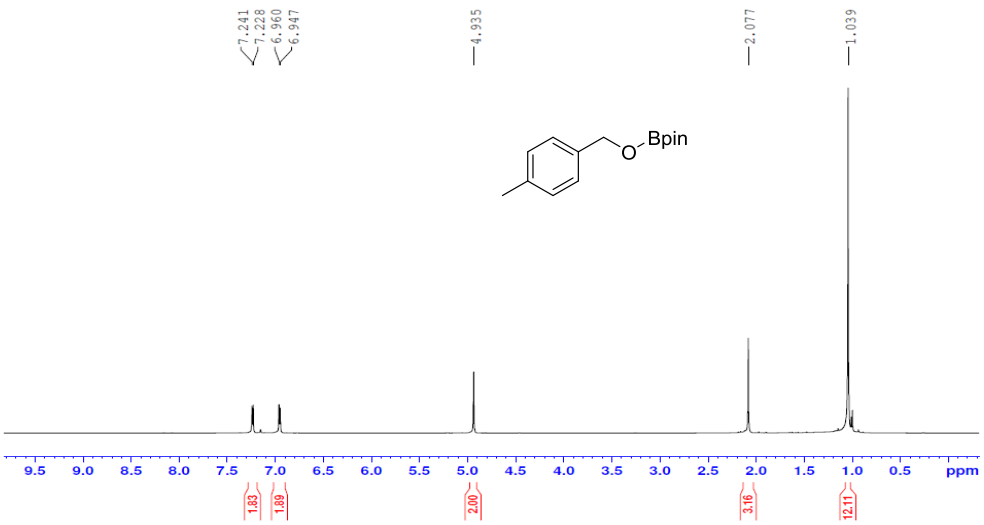
In a glovebox, ketones or aldehydes (1 mmol) was added to a solution of catalyst (0.1 or 1 mol%) and HBpin (1.1 mmol for aldehydes and 1.5 mol for ketones) in C_6D_6 (0.50 mL) at room temperature for the required time. The progress of the reaction was monitored by ^{1}H NMR.

NMR data of the crude reaction.

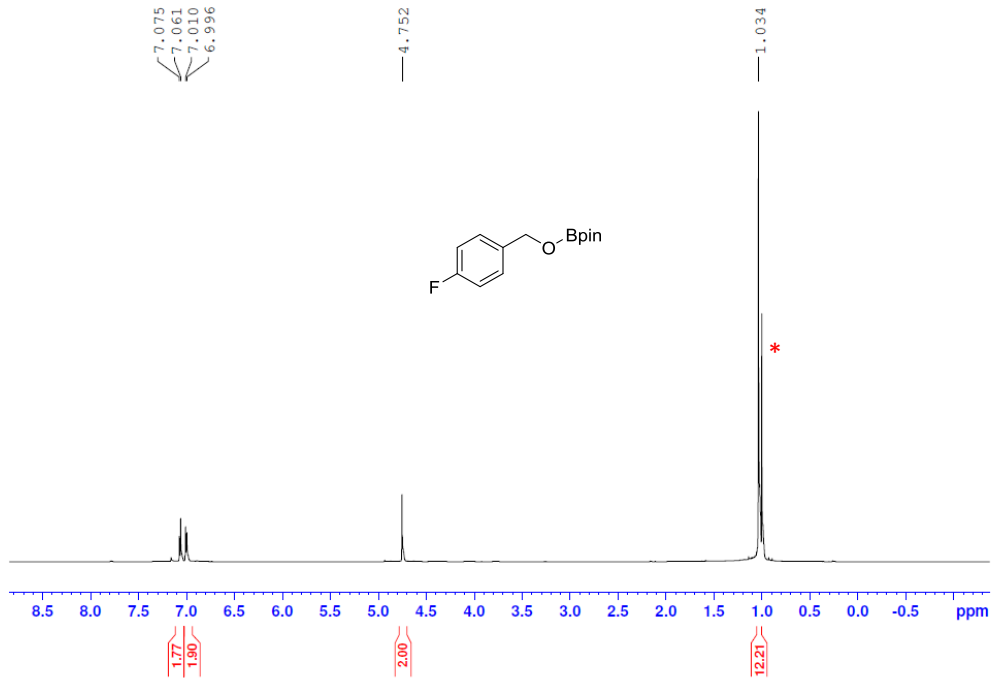
^{1}H NMR (C_6D_6, 600MHz): δ 7.27 (m, 2H, Ar-*H*) , 7.15 (m, 2H, Ar-*H*), 7.04 (m, 1H, Ar-*H*), 4.92 (s, 2H, Ar-CH_2), 1.08 (s, 12H, C(CH_3)$_2$)。



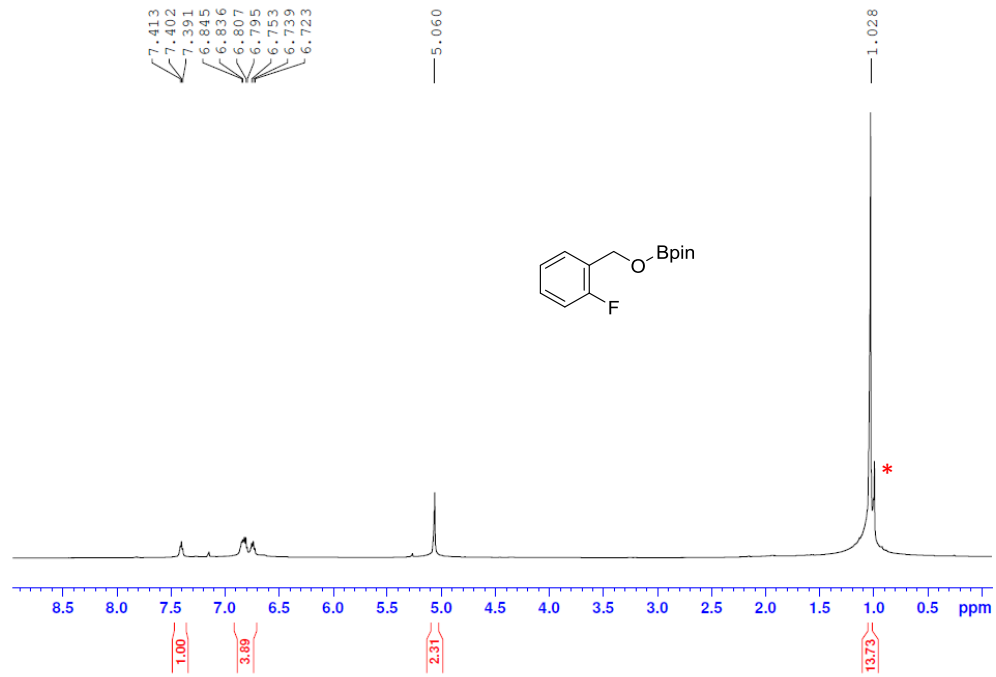
^{1}H NMR (C_6D_6, 600MHz): δ 7.23 (d, *J* = 7.8 Hz, 2H, Ar-*H*), 6.95 (d, *J* = 7.8 Hz, 2H, Ar-*H*), 4.93 (s, 2H, Ar-CH_2), 2.07 (s, 3H, Ar-CH_3), 1.03 (s, 12H, C(CH$_3$)$_2$)。



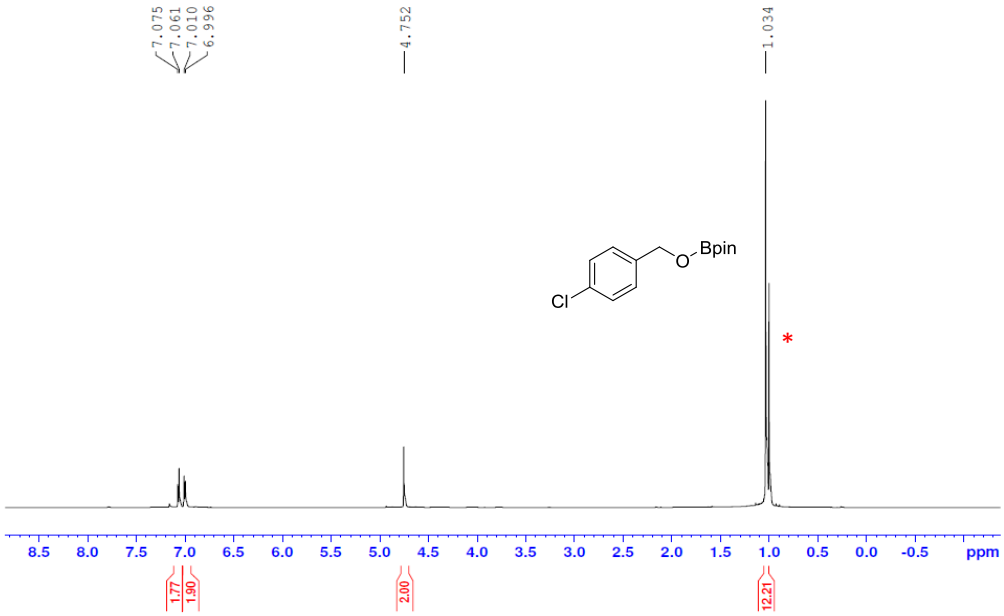
^{1}H NMR (C_6D_6, 600MHz): δ 7.07 (d, *J* = 8.4 Hz, 2H, Ar-*H*), 6.99 (d, *J*= 8.4 Hz, 2H, Ar-*H*), 4.75 (s, 2H, Ar-CH_2), 1.03 (s, 12H, C(CH_3)$_2$)。



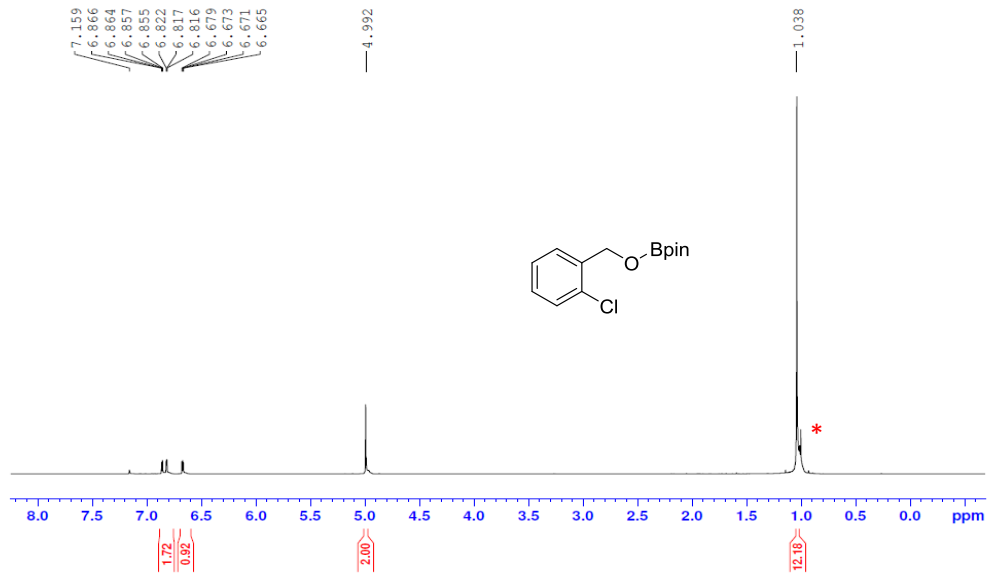
^{1}H NMR (C_6D_6, 600MHz): δ 7.40 (m, 1H, Ar-*H*), 6.80 (m, 3H, Ar-*H*), 5.06 (s, 2H, Ar-CH_2), 1.03 (s, 12H, C(CH_3)$_2$)。



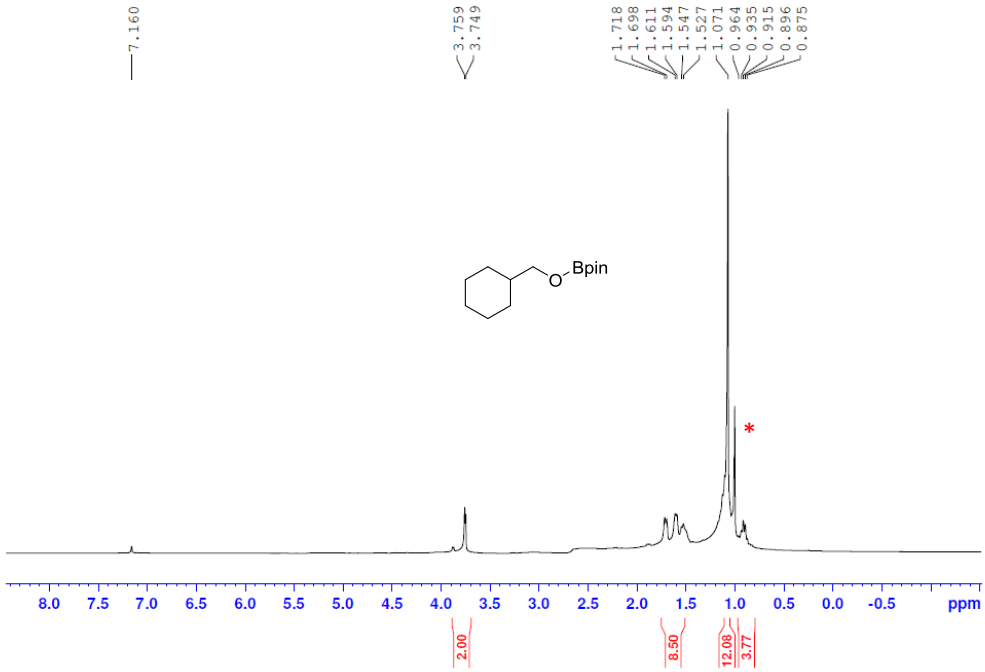
^{1}H NMR (C_6D_6, 600MHz): δ 7.53 (d, *J*= 7.2 Hz, 1H, Ar-*H*), 7.08 (d, *J* = 7.2 Hz, 1H, Ar-*H*), 6.92 (t, *J* = 7.5 Hz, 1H, Ar-*H*), 6.80 (m, 1H, Ar-*H*), 5.12 (s, 2H, Ar-CH_2), 1.04 (s, 12H, C(CH_3)$_2$)。



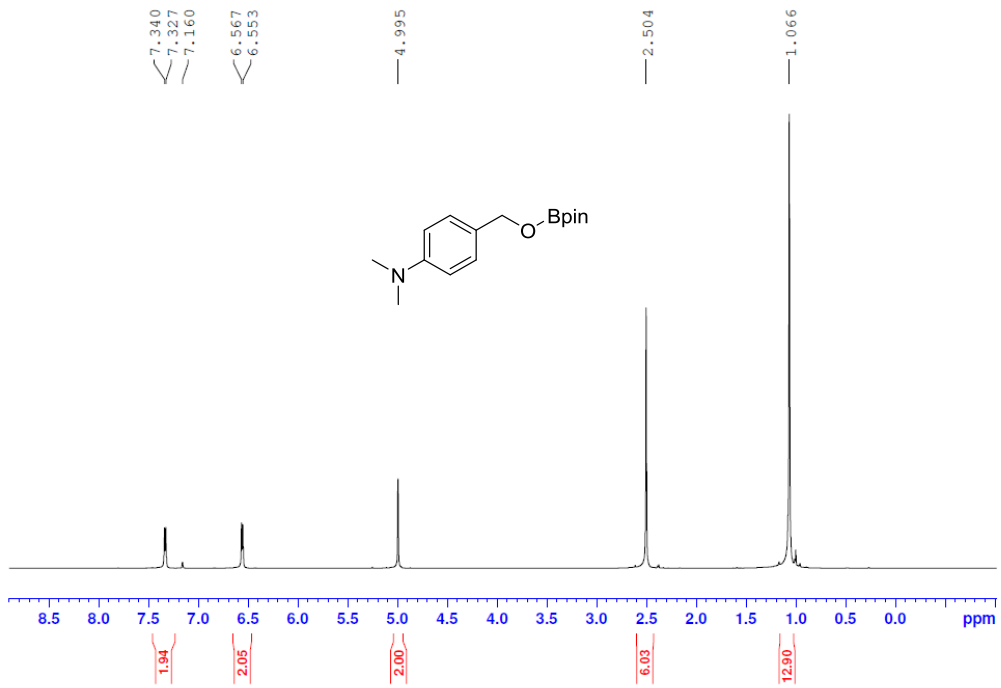
^{1}H NMR (C_6D_6, 600MHz): δ 6.85 (m, 2H, Ar-*H*), 6.67 (m, 1H, Ar-*H*), 4.99 (s, 2H, ArCH_2), 1.03 (s, 12H, C(CH_3)$_2$)。



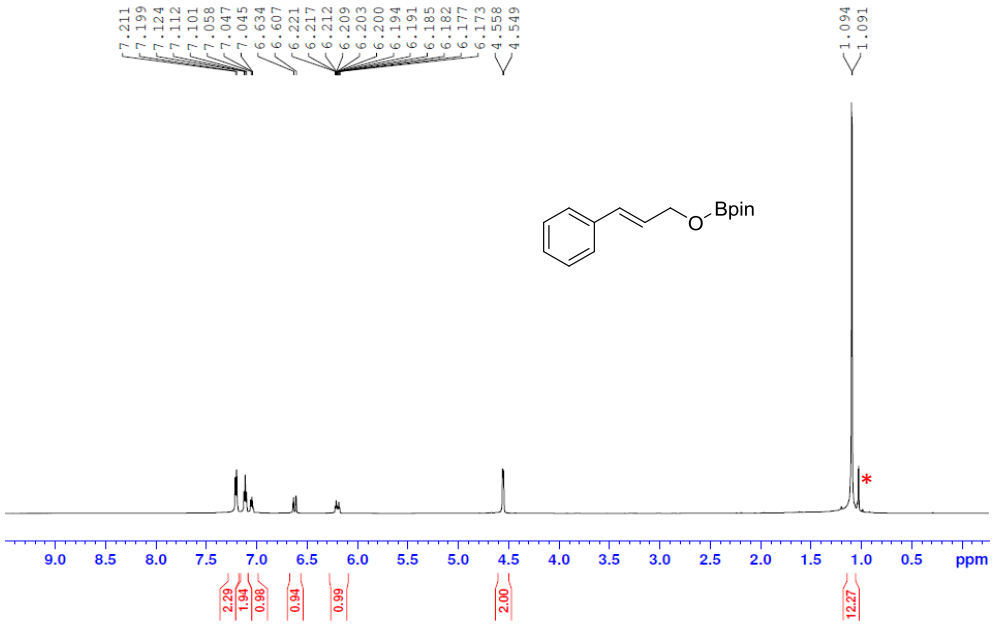
^{1}H NMR (C_6D_6, 600MHz): δ 3.75 (d, *J*= 18 Hz, 2H, OCH_2), 1.61 (m, 8H, Cy*H*) 1.03 (s, 12H, C(CH_3)$_2$), 0.91 (m, 3H, Cy*H*)。



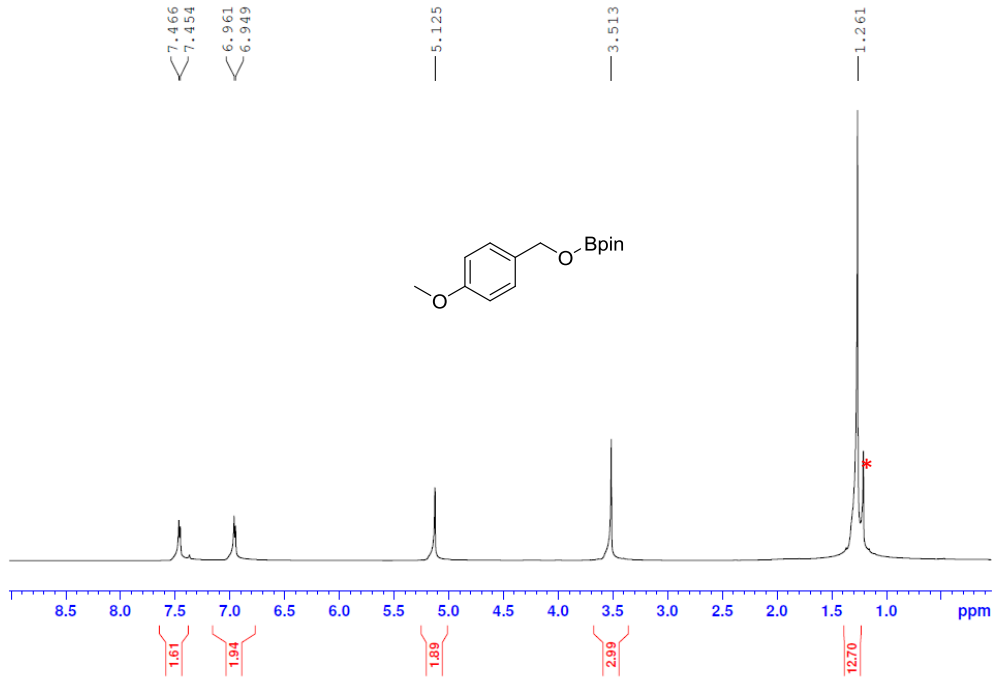
^{1}H NMR (C_6D_6, 600MHz): δ 7.33 (d, *J*= 7.8 Hz, 2H, Ar-*H*), 6.56 (d, *J*= 7.8 Hz,2H, Ar-*H*), 4.99 (s, 2H, Ar-CH_2), 2.50 (s, 6H, NCH_3), 1.07 (s, 12H, C(CH_3)$_2$).



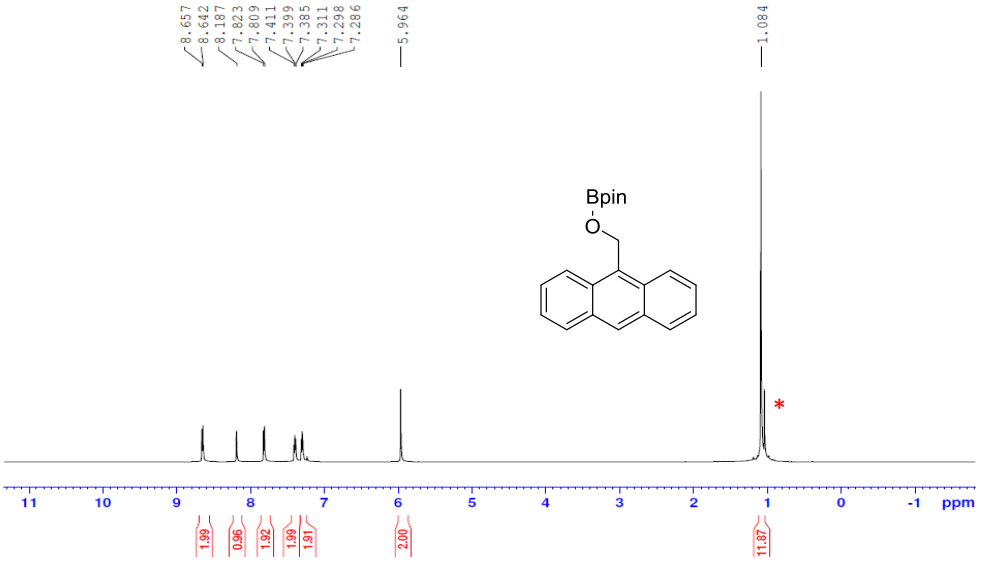
^{1}H NMR (C_6D_6, 600MHz): δ 7.20 (m, 2H, Ar-*H*), 7.11 (m, 2H, Ar-*H*), 7.04 (m, 2H, Ar-*H*), 6.62 (m, 1H, Ar-C*H*=CH), 6.20 (m, 1H, Ar-CH=C*H*), 4.54 (d, *J*= 5.4 Hz, 2H, CH=CHCH_2), 1.09 (s, 12H, C(CH_3)$_2$)。



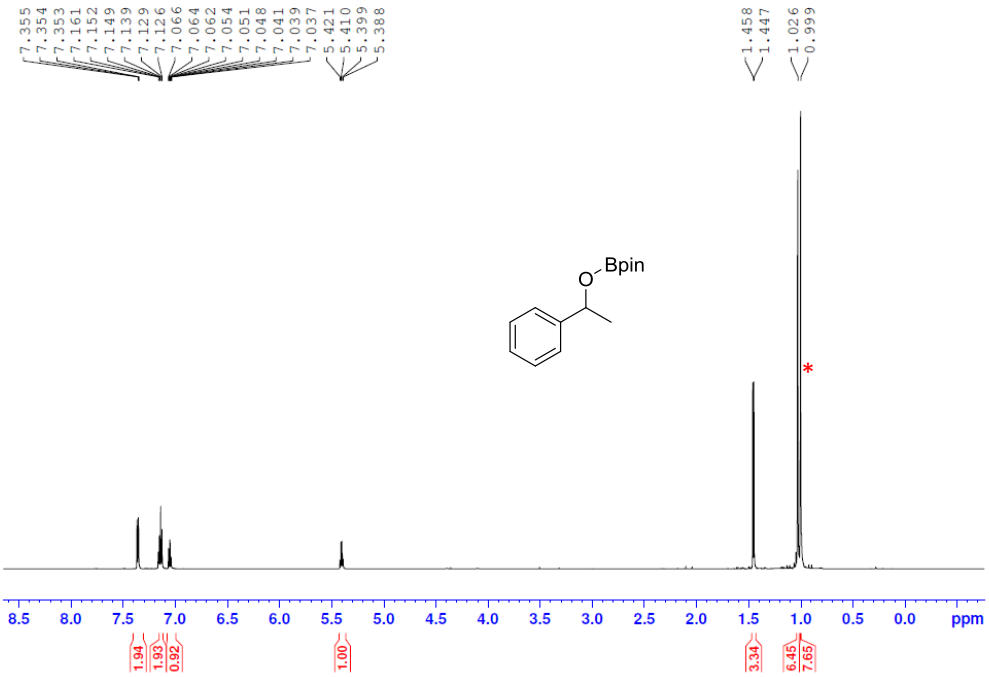
^{1}H NMR (C_6D_6, 600MHz): δ 7.46 (d, *J* = 7.2 Hz, 2H, Ar-*H*), 6.95 (d, *J* = 7.2 Hz, 2H, Ar-*H*), 5.13 (s, 2H, Ar-CH_2), 3.51 (s, 3H, OCH_3), 1.26 (s, 12H, C(CH_3)$_2$)。



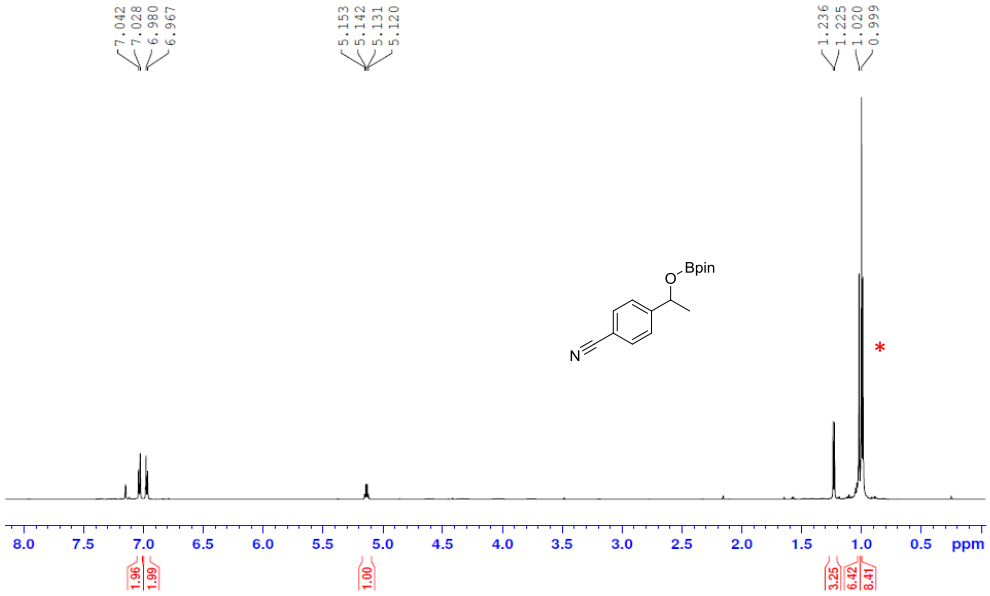
^{1}H NMR (C_6D_6, 600MHz): δ 8.65 (d, *J* = 9 Hz, 2H, Ar-*H*), 8.19 (s, 1H, Ar-*H*), 7.82 (d, *J* = 9 Hz, 2H, Ar-*H*), 7.40 (t, *J* = 7.5 Hz, 2H, Ar-*H*), 7.30 (t, *J* = 7.5 Hz, 2H, Ar-*H*), 5.96 (s, 2H, Ar-CH_2), 1.08 (s, 12H, C(CH_3)$_2$).



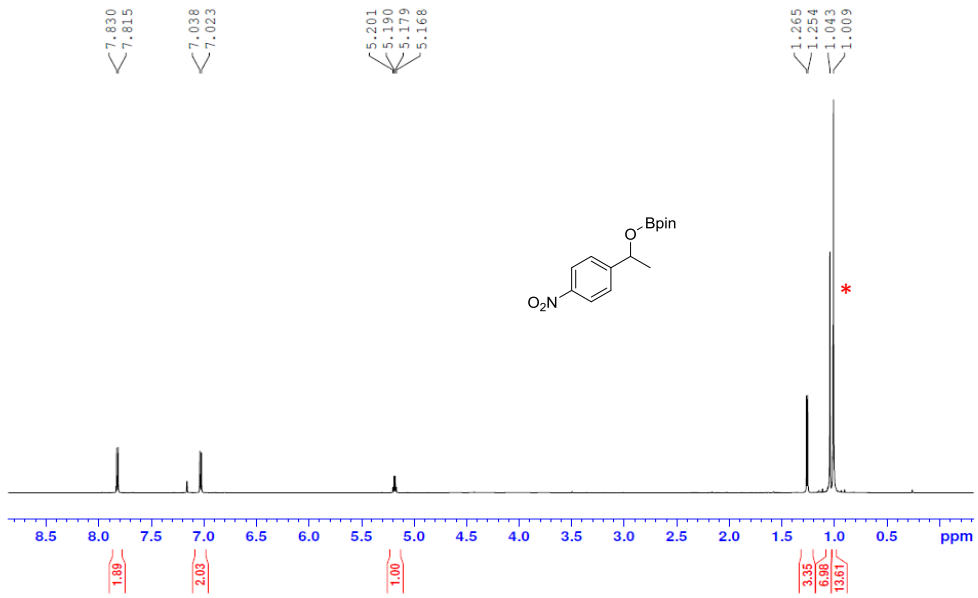
^{1}H NMR (C_6D_6, 600MHz): δ 7.35 (m, 2H, Ar-*H*) , 7.03-7.16 (m, 3H, Ar-*H*), 5.40 (q, *J* = 6.6 Hz, 1H, Ar-C*H*), 1.45 (d, *J*= 6.6 Hz, 3H, CHCH_3), 1.02 (s, 6H, C(CH_3)$_2$), 1.00 (s, 6H, C(CH_3)$_2$)。



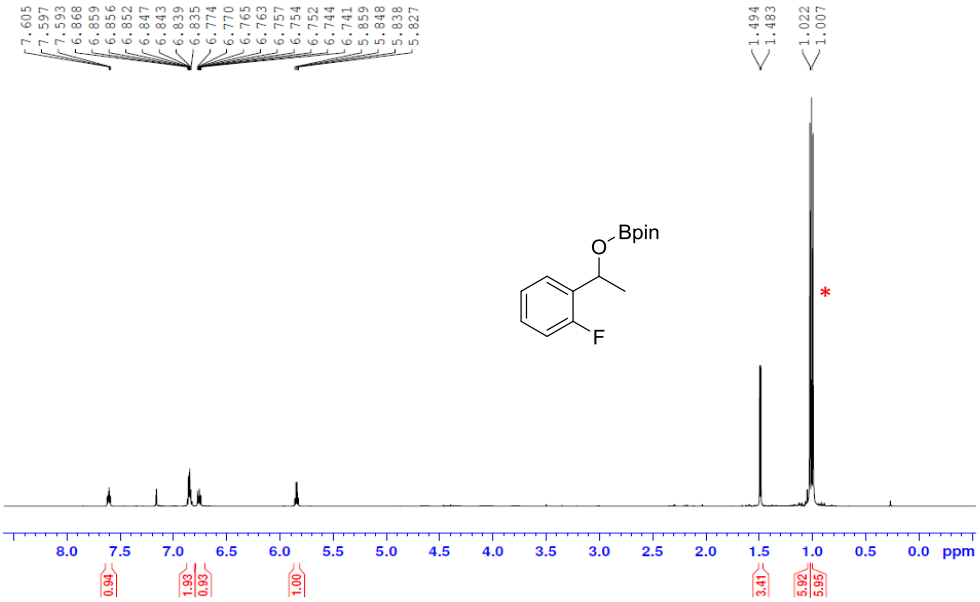
^{1}H NMR (C_6D_6, 600MHz): δ 7.03 (d, *J* = 8.4 Hz, 2H, Ar-*H*) , 6.97 (d, *J*= 8.4 Hz, 2H, Ar-*H*), 5.14 (q, *J*= 6.6 Hz, 1H, Ar-C*H*), 1.23 (d, *J* = 6.6 Hz, 3H, CHCH_3), 1.02 (s, 6H, C(CH_3)$_2$), 0.99 (s, 6H, C(CH_3)$_2$)。



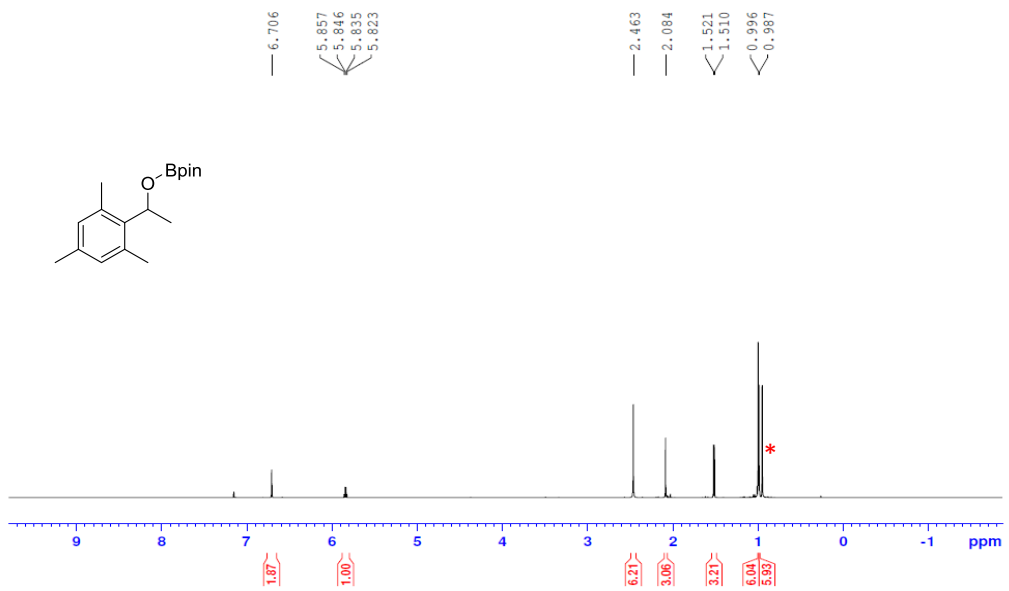
^{1}H NMR (C_6D_6, 600MHz): δ 7.83 (d, *J* = 9.0 Hz, 2H, Ar-*H*) , 7.03 (d, *J*= 9.0 Hz, 2H, Ar-*H*), 5.18 (q, *J* = 6.6 Hz, 1H, Ar-C*H*), 1.26 (d, *J* = 6.6 Hz, 3H, CHCH_3), 1.04 (s, 6H, C(CH_3)$_2$), 1.01 (s, 6H, C(CH_3)$_2$)。



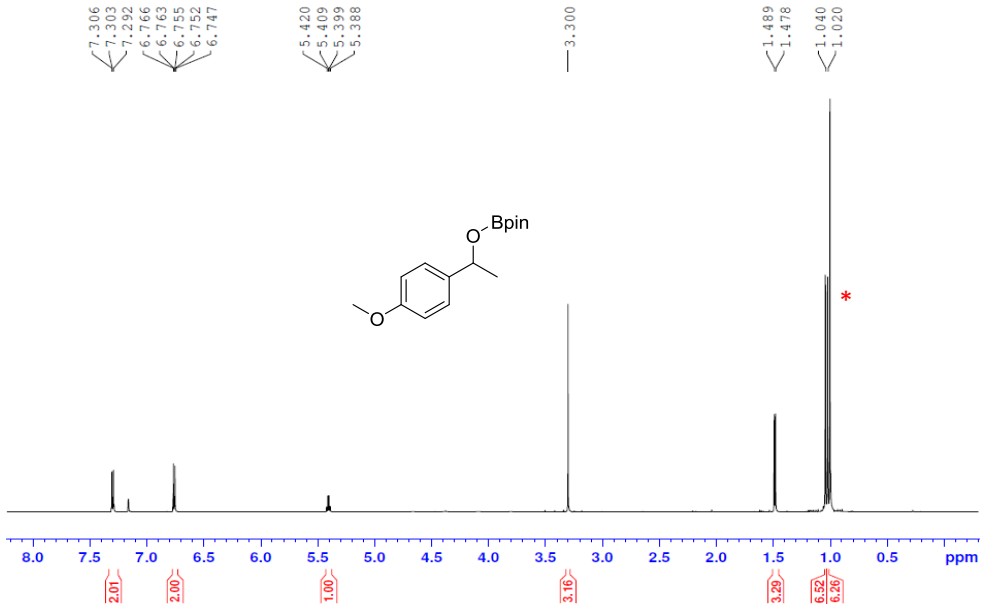
^{1}H NMR (C_6D_6, 600MHz): δ 7.60 (m, 1H, Ar-*H*) , 6.74-6.83 (m, 3H, Ar-*H*), 5.84 (q, *J* = 6.6 Hz, 1H, Ar-C*H*), 1.49 (d, *J* = 6.6 Hz, 3H, CHCH_3), 1.02 (s, 6H, C(CH_3)$_2$), 1.01 (s, 6H, C(CH_3)$_2$)。



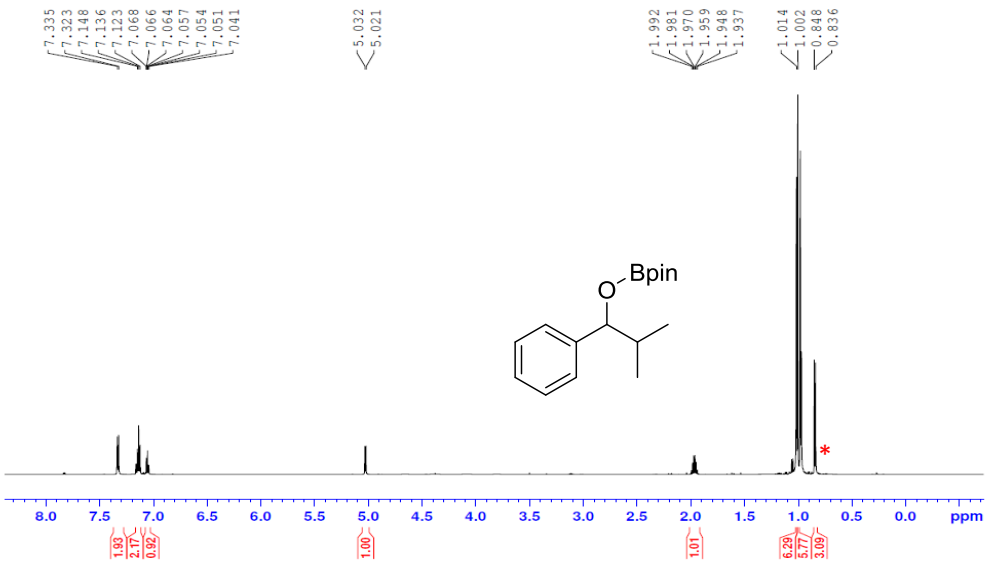
^{1}H NMR (C_6D_6, 600MHz): δ 6.71 (s, 2H, Ar-*H*), 5.84 (q, *J* = 6.6 Hz, 1H, Ar-C*H*), 2.46 (s, 6H, Ar-CH_3), 2.08 (s, 6H, Ar-CH_3), 1.51 (d, *J* = 6.6 Hz, 3H, CHCH_3), 0.99 (s, 6H, C(CH_3)$_2$), 0.98 (s, 6H, C(CH_3)$_2$)。



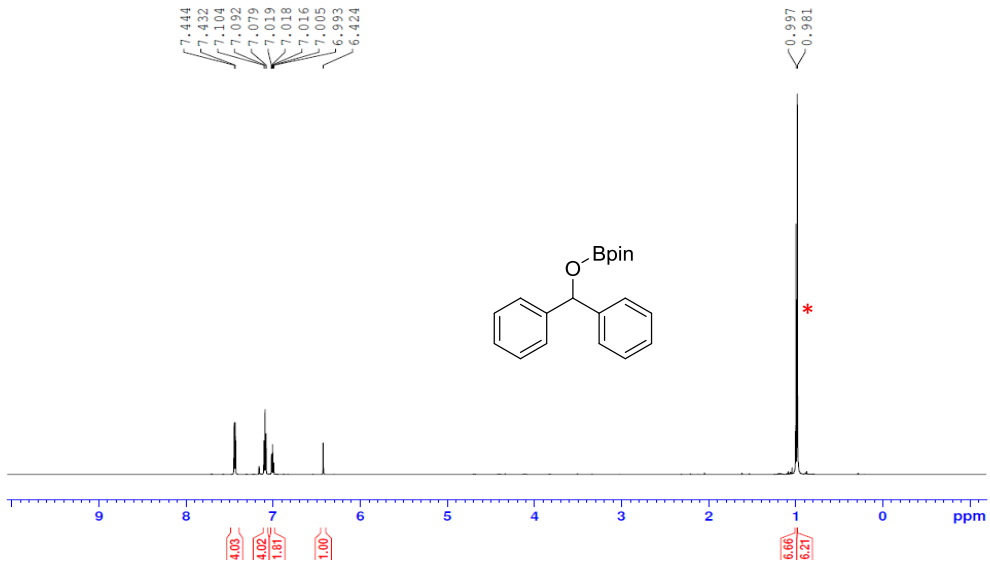
^{1}H NMR (C_6D_6, 600MHz): δ 7.03 (m, 2H, Ar-*H*) , 6.75 (m, 2H, Ar-*H*), 5.41 (q, *J* = 6.6 Hz, 1H, Ar-C*H*), 3.30 (s, 3H, OCH_3), 1.48 (d, *J*= 6.6 Hz, 3H, CHCH_3), 1.04 (s, 6H, C(CH_3)$_2$), 1.02 (s, 6H, C(CH_3)$_2$)。



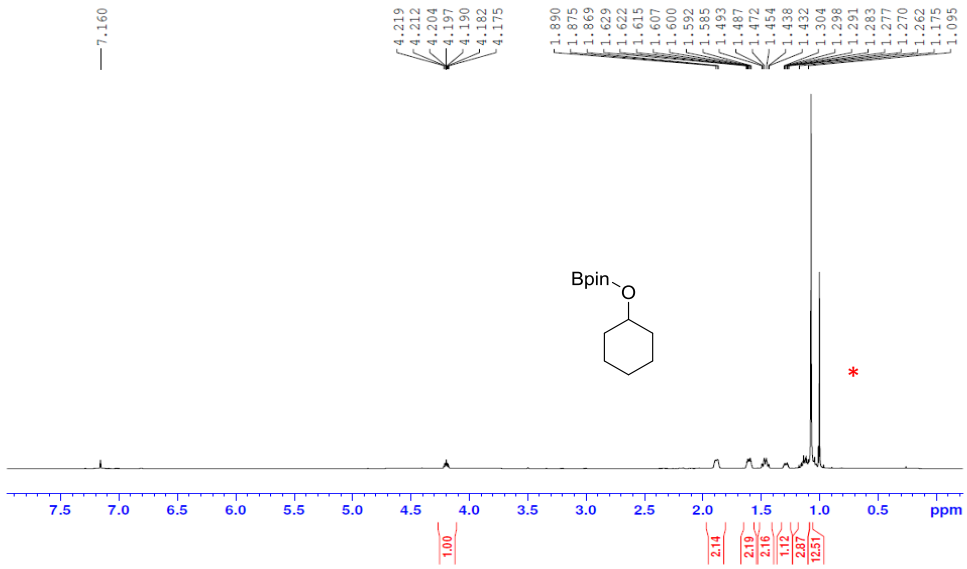
^{1}H NMR (C_6D_6, 600MHz): δ 7.33 (m, 2H, Ar-*H*), 7.04-7.14 (m, 3H, Ar-*H*), 5.03 (d, *J* = 6.6 Hz, 1H, Ar-C*H*), 1.97 (sept, *J* = 6.6 Hz, 1H, C*H*(CH$_3$)), 1.01 (s, 6 H, C(CH_3)$_2$), 0.99 (s, 6H, C(CH_3)$_2$), 0.84 (d, *J* = 6.6 Hz, 3H, CH(CH_3))。



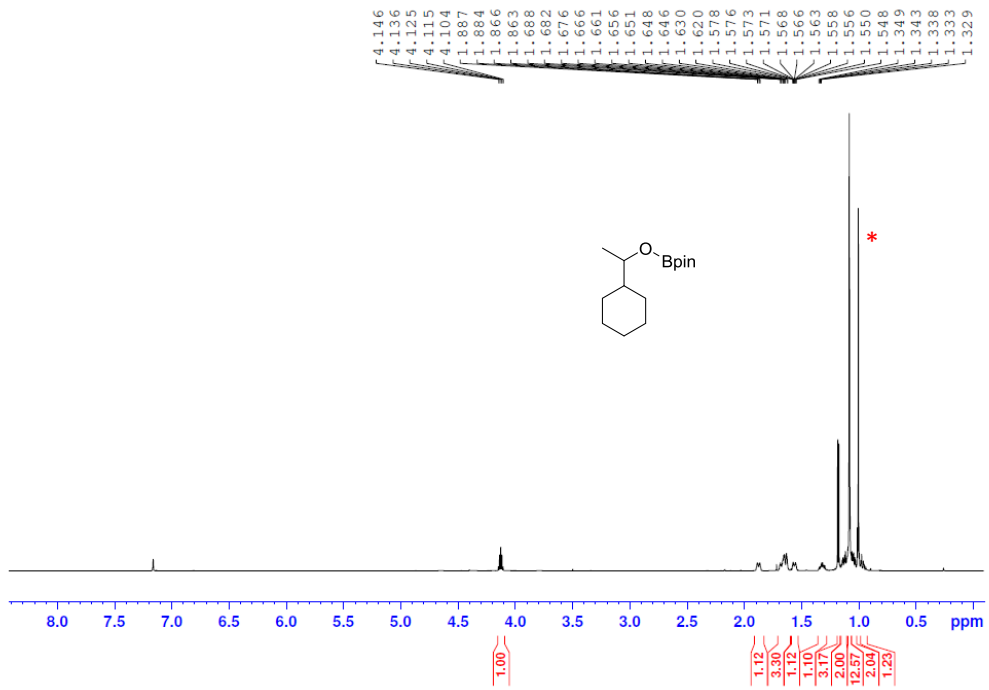
^{1}H NMR (C_6D_6, 600MHz): δ 7.69 (d, *J* = 7.2 Hz, 4H, Ar-*H*), 7.12 (t, *J*= 7.2 Hz, 4H, Ar-*H*), 6.95 (t, *J* = 7.2 Hz, 2H, Ar-*H*), 6.42 (s, 1H, Ar-C*H*), 0.99 (s, 6H, C(CH_3)$_2$), 0.98 (s, 6H, C(CH_3)$_2$)。



^{1}H NMR (C_6D_6, 600MHz): δ 4.19 (m, 1H, OC*H*), 1.86-1.89 (m, 2H, C_6H_{11}), 1.61 (m, 2H, C_6H_{11}), 1.48 (m, 2H, C_6H_{11}), 1.28 (m, 2H, C_6H_{11}), 1.16 (m, 2H, C_6H_{11}), 1.07 (s, 12H, C(CH_3)$_2$)。



^{1}H NMR (C_6D_6, 600MHz): δ 4.12 (m, 1H, OC*H*), 1.86-1.88 (m, 1H, C_6H_{11}), 1.66 (m, 3H, C_6H_{11}), 1.56 (m, 1H, C_6H_{11}), 1.31 (m, 1H, C_6H_{11}), 1.18 (d, 3H, OCHCH_3), 1.13 (m, 2H, C_6H_{11}), 1.08 (s, 12H, C(CH_3)$_2$) 1.04 (m, 2H, C_6H_{11}), 0.97 (m, 1H, C_6H_{11})。



Computational Studies

The computational studies were completed using Gaussian 09.D01[S5] program package. The geometries of Mg(I) dimer and Mg(II) dimer were optimized in gas by employing the BP86[S6] and B3LYP[S7] density functionals with 6-31G*[S8] basis set for C, H and 6-311+G*[S9] basis set for Mg, N, respectively. Single point energy for the optimized geometries in gas have further been calculated using the same methods with basis set def2-TZVP[S10]. The geometries of the stationary points in alkyne catalytic reaction were optimized in gas at the B3LYP/6-31G* level. Single point energies of the stationary points in gas have further been calculated at B3LYP/def2-TZVP level. All reactant, product and intermediate have been identified as minimum (no imaginary frequency) or transition state (only one imaginary frequency) by performing analytical vibrational frequencies. Thermal corrections to enthalpy and Gibbs free energy were calculated at 298.15K and 1atm. A continuum solvation model (SMD)[S11] and its parameterized level M05-2X[S12]/6-31G* was used to calculate solvent effect in toluene. The difference between the Gibbs free energy in toluene and the Gibbs free energy in gas is the Gibbs free energy of dissolution[S13].

Table S5 Gibbs free energy change of magnesium(I) complexes disproportionation reaction [a]

$LMg—MgL \longrightarrow LMgL + Mg(cr)$ [c] (I) (I) (II) (0)				
Compound	gas		Toluene [f]	
	BP86 [d]	B3LYP [e]	BP86 [d]	B3LYP [e]
$[(^{DippPh}Nacnac)Mg]_2$	-14.3	-16.0	-8.9	-10.7
$[(^{DippTol'}Nacnac)Mg]_2$ [b]	-5.5	-5.6	0.1	-0.2
$[(^{DippXyl}Nacnac)Mg]_2$ (**4b**)	-0.3	-1.8	5.9	4.3
$[(^{Ar}Nacnac)Mg]_2$ (**7**)	1.4	2.6	8.7	9.7

[a] unit: kcal/mol, state: 298.15K and 1atm; [b] Tol' = 2-methylphenyl; [c] the Gibbs free energy of solid magnesium was calculated by subtracting the vaporization Gibbs free

energy change of 27.0 kcal/mol[S14] from the Gibbs free energy of gaseous magnesium we calculated with DFT; [d] BP86/def2-TZVP//BP86/6-31G* (C, H); 6-311+G* (N, Mg) level; [e] B3LYP/def2-TZVP//B3LYP/6-31G* (C, H); 6-311+G* (N, Mg) level; [f] SMD model at M05-2X/6-31G* level.

Table S6: E_{el} represents the single point energies at def2-TZVP. Thermal corrections to enthalpy (H_{corr}) and Gibbs free energy (G_{corr}) were calculated at 298.15K and 1atm. ΔG_{sol} are calculated by employing the SMD model at M05-2X/6-31G* level. The optimized Cartesian coordinates are also given.

phenylacetylene (B3LYP)
E_{el} = -308.5119961
H_{corr}= 0.116932
G_{corr}= 0.079071
ΔG_{sol}= -0.009568338

C	-1.51256100	-1.20856800	-0.00001300
C	-0.11995200	-1.21309500	0.00001000
C	0.59423700	-0.00002200	0.00003000
C	-0.11993100	1.21308400	0.00001200
C	-1.51252500	1.20859100	-0.00001400
C	-2.21301500	0.00001300	-0.00002300
H	-2.05302000	-2.15127700	-0.00002100
H	0.42854300	-2.14997900	0.00002100
H	0.42860800	2.14994200	0.00002300
H	-2.05298200	2.15130200	-0.00002400
H	-3.29961200	0.00003700	-0.00004200
C	2.02418600	-0.00001500	0.00006800
C	3.23423200	0.00000100	0.00001300
H	4.30044400	0.00003800	-0.00045900

HBpin (B3LYP)
E_{el} = -412.0320046
H_{corr}= 0.201984
G_{corr}= 0.158359
ΔGsol= -0.00655846

B	-0.00007100	1.94494200	-0.00035500
H	-0.00025300	3.13486700	-0.00032600
O	-1.08610200	1.20090400	-0.36752200
O	1.08622900	1.20116200	0.36656500
C	-0.78923700	-0.19149000	-0.04498300

C	0.78924100	-0.19149200	0.04502600
C	-1.37972600	-1.07413000	-1.14309000
H	-1.14054600	-2.12925900	-0.96739700
H	-2.46942100	-0.97057500	-1.14828500
H	-1.01063100	-0.79279000	-2.13191900
C	-1.48003700	-0.48320900	1.29355200
H	-2.54921100	-0.27221500	1.19415500
H	-1.36098600	-1.53070600	1.58961600
H	-1.08481000	0.15102900	2.09318000
C	1.48004300	-0.48415600	-1.29329100
H	2.54929600	-0.27361400	-1.19385600
H	1.36053400	-1.53174500	-1.58884600
H	1.08522900	0.14988100	-2.09328300
C	1.37967700	-1.07329600	1.14380000
H	1.14084900	-2.12860900	0.96870900
H	2.46934500	-0.96942400	1.14926300
H	1.01017500	-0.79143500	2.13233400

LMgH (B3LYP)

E_{el} = -1283.2051030

H_{corr}= 0.562568

G_{corr}= 0.46717

ΔGsol= -0.02909754

N	1.97440700	0.00028500	0.34936600
N	-1.03145100	0.00020100	0.39241400
C	2.96604400	0.00021200	2.60738700
C	1.76934200	0.00022500	1.67124600
C	0.49788000	0.00022600	2.28162400
C	-0.79085500	0.00013400	1.70818200
C	-1.95946700	-0.00014600	2.67761000
C	3.31374000	0.00013000	-0.16481000
C	3.94792600	-1.22605000	-0.45734700
C	5.23212800	-1.20400300	-1.01280100
C	5.87689700	-0.00015500	-1.28668700
C	5.23236300	1.20383700	-1.01288100
C	3.94816500	1.22617100	-0.45742300
C	3.25515900	2.54331900	-0.19505500
C	3.25465300	-2.54304600	-0.19491400
C	-2.38511000	-0.00007500	-0.09582200
C	-3.02590700	-1.23022200	-0.38253200
C	-4.30821100	-1.20254200	-0.94355600
C	-4.95146500	-0.00058800	-1.22133700
C	-4.30866700	1.20162400	-0.94359700

C	-3.02638100	1.22982100	-0.38256900
C	-2.34577600	2.57476600	-0.13476800
C	-3.20696500	3.52841800	0.71490400
C	-1.94553400	3.24316300	-1.46618600
C	-2.34477900	-2.57490300	-0.13470200
C	-1.94416500	-3.24311700	-1.46609600
C	-3.20566100	-3.52892400	0.71487200
H	2.65182700	-0.00013800	3.65292400
H	3.59810500	0.87793300	2.43403300
H	3.59855400	-0.87707700	2.43354900
H	0.51344300	0.00017900	3.36460100
H	-2.59643500	0.87696900	2.52060500
H	-1.61600400	0.00016700	3.71393500
H	-2.59570200	-0.87785400	2.52091000
H	5.72596100	-2.14676600	-1.23627500
H	6.87375900	-0.00027200	-1.71906100
H	5.72636800	2.14649000	-1.23643300
H	2.35370900	2.65498000	-0.81247200
H	3.91790700	3.38212500	-0.42893700
H	2.93533600	2.64704900	0.84819200
H	2.93462700	-2.64659300	0.84828600
H	3.91728600	-3.38200200	-0.42858700
H	2.35327800	-2.65463600	-0.81246400
H	-4.80887700	-2.13958600	-1.17294400
H	-5.94653100	-0.00078500	-1.65833100
H	-4.80970000	2.13846700	-1.17301000
H	-1.42561500	2.38614900	0.42696600
H	-4.12510000	3.82310500	0.19360600
H	-2.64910900	4.44533800	0.93924400
H	-3.49832500	3.06877300	1.66621200
H	-1.29570100	2.59340400	-2.06433700
H	-1.41412300	4.18509400	-1.28276600
H	-2.82931100	3.46878900	-2.07460000
H	-1.42474200	-2.38594000	0.42711800
H	-1.41239700	-4.18484300	-1.28265500
H	-1.29455000	-2.59310600	-2.06422000
H	-2.82779300	-3.46906500	-2.07460200
H	-4.12363400	-3.82396800	0.19349700
H	-3.49728200	-3.06939900	1.66615800
H	-2.64745700	-4.44562300	0.93924900
Mg	0.45215700	0.00067300	-1.02132700
H	0.43952700	0.00150000	-2.74036100

int1a (B3LYP)

E_{el} = -1591.714579
H_{corr}= 0.681893
G_{corr} = 0.568517
ΔGsol= -0.03336604

N	0.37818000	-1.36180700	0.49987600
N	-2.49676700	-0.45983800	0.56092500
C	-2.65784200	-1.75206600	0.86495200
C	-1.59928000	-2.66042000	1.06551900
C	-0.21715600	-2.51737700	0.80174500
H	-1.90404700	-3.65859600	1.35671300
C	-0.89224600	1.97936300	-1.29585100
C	0.22010000	2.40182900	-1.04572900
H	-0.24360500	1.59338100	2.09065700
H	-1.89706300	1.73534800	-1.57116600
Mg	-0.63463600	0.42614400	0.86481000
C	1.51798200	2.91669600	-0.73690100
C	2.63086100	2.56574200	-1.52329400
C	1.68057800	3.79705200	0.35011000
C	3.88338500	3.09726900	-1.22962700
H	2.50584700	1.87444000	-2.35004400
C	2.93841600	4.32250700	0.63274700
H	0.82248100	4.04269400	0.96585300
C	4.03888300	3.97730500	-0.15604400
H	4.74008200	2.82043900	-1.83717000
H	3.06057400	4.99983500	1.47308000
H	5.01859600	4.38960100	0.06971900
C	1.75026000	-1.34273600	0.07631800
C	2.77017700	-0.99825900	1.00030200
C	2.07085200	-1.58478600	-1.28538900
C	4.08884600	-0.90139200	0.53850900
C	3.40519800	-1.46780600	-1.69329200
C	4.41223000	-1.12828400	-0.79493600
H	4.87710700	-0.64588600	1.24173100
H	3.65955400	-1.65232500	-2.73426800
H	5.44294500	-1.04789200	-1.13096800
C	-3.62450800	0.33128100	0.18192500
C	-4.07751900	0.30383100	-1.15863000
C	-4.21730000	1.20680700	1.11947400
C	-5.11726300	1.16197500	-1.53972000
C	-5.25748600	2.04236600	0.69608700
C	-5.70710300	2.02835600	-0.62252800
H	-5.46419600	1.14461300	-2.57056500
H	-5.71765300	2.71371900	1.41737800

H	-6.51177900	2.68918700	-0.93339900
C	-4.06275800	-2.31711300	1.00366600
H	-4.67429800	-1.69178800	1.66240300
H	-4.57397400	-2.34640300	0.03483700
H	-4.04070500	-3.33263900	1.40495500
C	0.58922400	-3.80535200	0.83918000
H	1.59541300	-3.64385600	1.23262700
H	0.08509200	-4.55941500	1.44859300
H	0.70095300	-4.21677800	-0.17095200
C	2.48964200	-0.76623200	2.48474200
H	1.40666000	-0.80620600	2.63390700
C	1.01528800	-1.96683400	-2.32381600
H	0.05748600	-2.07499200	-1.80729600
C	-3.46179700	-0.63354500	-2.17418500
H	-2.36699800	-0.58973700	-2.16333400
H	-3.72593500	-1.68111800	-1.98154600
H	-3.80726000	-0.39070100	-3.18413100
C	-3.75332400	1.23618600	2.55732900
H	-3.84242800	0.25175600	3.03317100
H	-2.70016000	1.53113000	2.64236200
H	-4.35062500	1.94498100	3.13963000
C	2.96112700	0.62084900	2.95902200
H	2.70113500	0.76447900	4.01445800
H	4.04833600	0.73338300	2.86609100
H	2.48051200	1.41850200	2.38590500
C	3.11643200	-1.87484200	3.35555100
H	4.20986000	-1.87880800	3.26974300
H	2.86524400	-1.71765300	4.41135800
H	2.75787100	-2.86979700	3.06943700
C	0.83837600	-0.86733700	-3.39003200
H	1.76501500	-0.70915100	-3.95542900
H	0.05795400	-1.14958700	-4.10772900
H	0.55162600	0.08655800	-2.93613600
C	1.33180800	-3.31418200	-3.00398700
H	0.51495500	-3.60333700	-3.67612600
H	2.24734600	-3.25685500	-3.60438800
H	1.46933200	-4.11785400	-2.27258500

ts2a (B3LYP)

E_{el} = -1591.694591

H_{corr}= 0.680279

G_{corr}= 0.567034

ΔG_{sol}= -0.0319865

N	1.43125800	-1.14446800	0.09956500
N	-1.54416200	-1.79244400	0.12457500
C	-1.03573400	-3.01449800	0.29832900
C	0.34286500	-3.30973500	0.35962500
C	1.47384700	-2.46898500	0.27720400
H	0.57195300	-4.35772800	0.50845100
C	-0.83480900	1.22972200	-1.76946600
C	-0.98602600	2.10027400	-0.88559300
H	-0.68747000	1.35599800	0.95837800
H	-0.89744600	1.00533400	-2.81876700
Mg	-0.35633000	-0.11545000	0.01317200
C	-1.23882100	3.44065200	-0.39049500
C	-1.17764400	4.46653700	-1.35635000
C	-1.57728700	3.76709500	0.92859800
C	-1.45620000	5.78347100	-1.00239200
H	-0.91069400	4.21766400	-2.37893900
C	-1.85838800	5.08719100	1.27410900
H	-1.60067300	2.97307400	1.66657700
C	-1.79908000	6.09929900	0.31433400
H	-1.40054700	6.56419800	-1.75617700
H	-2.12120800	5.32587200	2.30107300
H	-2.01311000	7.12823400	0.59059200
C	2.65242000	-0.38608200	0.05583200
C	3.19354500	0.15055800	1.25167100
C	3.26752500	-0.11243600	-1.19235800
C	4.35099900	0.93453200	1.17280000
C	4.42795900	0.67087900	-1.21303500
C	4.97306000	1.19192600	-0.04425100
H	4.77168800	1.35051500	2.08475400
H	4.91096600	0.87902900	-2.16449700
H	5.87358500	1.79935600	-0.08246300
C	-2.96318100	-1.60957000	0.06134700
C	-3.62780300	-1.70615200	-1.18058500
C	-3.67114400	-1.25080700	1.22870300
C	-5.00488000	-1.46198600	-1.22916200
C	-5.04769900	-1.01567000	1.13629300
C	-5.71638800	-1.12123700	-0.08104100
H	-5.52019500	-1.53746000	-2.18407200
H	-5.59660500	-0.74307700	2.03480000
H	-6.78530000	-0.93301400	-0.13593400
C	-1.97963700	-4.19546100	0.46000500
H	-2.63940900	-4.04925800	1.32252200
H	-2.63017100	-4.30589000	-0.41396100
H	-1.42802800	-5.12717600	0.60054700

C	2.81823600	-3.16005800	0.43636300
H	3.28118300	-2.88102500	1.38958800
H	2.70862000	-4.24622800	0.41627300
H	3.51858100	-2.86209600	-0.34855000
C	2.55366600	-0.08345400	2.61955200
H	1.70467200	-0.76007700	2.48241000
C	2.70674200	-0.63709500	-2.51301100
H	1.77719700	-1.17032200	-2.29159200
C	-2.87236600	-2.06074200	-2.44014900
H	-2.03913900	-1.37024500	-2.61402400
H	-2.43647700	-3.06642600	-2.39537600
H	-3.53379500	-2.02390700	-3.31150100
C	-2.96048500	-1.11411400	2.55512900
H	-2.43803300	-2.03459700	2.84170200
H	-2.20519200	-0.31830700	2.52303500
H	-3.67131600	-0.86987200	3.35096600
C	2.00472200	1.22853900	3.21540900
H	1.52862200	1.03728500	4.18523400
H	2.80739700	1.95849300	3.37610400
H	1.25888500	1.68066500	2.55385300
C	3.52511800	-0.75723100	3.60947600
H	4.37731200	-0.10806100	3.84276000
H	3.01261600	-0.98001500	4.55294800
H	3.92616500	-1.69688600	3.21320300
C	2.36298200	0.51356500	-3.47956700
H	3.26143900	1.05751400	-3.79434200
H	1.88154800	0.12231600	-4.38467400
H	1.68477100	1.23463900	-3.01206100
C	3.66192500	-1.63684000	-3.19532600
H	3.21606700	-2.02271800	-4.12022600
H	4.61469200	-1.16208300	-3.45863200
H	3.88491000	-2.49246300	-2.54900700

int3a (B3LYP)

E_{el} = -1591.779118

H_{corr}= 0.687788

G_{corr}= 0.572147

ΔG_{sol}= -0.03450702

N	2.08103200	-0.52269500	0.03815600
N	-0.41530200	-2.20255300	0.04181300
C	0.50596200	-3.17058800	0.08454100
C	1.89851500	-2.94591100	0.10777900
C	2.63152400	-1.74091200	0.08399200

H	2.50289300	-3.84392300	0.14511100
C	-1.16661400	1.47789900	-0.03202100
C	-2.51842400	1.40024600	-0.02343600
H	-2.99493900	0.41539000	-0.00089800
H	-0.76433600	2.49886900	-0.05670400
Mg	0.06016300	-0.21141300	0.00433500
C	-3.51060800	2.49733800	-0.04150300
C	-3.15942500	3.85988300	-0.05790500
C	-4.88012400	2.17655500	-0.04168200
C	-4.13461400	4.85288200	-0.07440200
H	-2.10991900	4.14077900	-0.05703600
C	-5.85974200	3.16852800	-0.05840000
H	-5.17298200	1.12848200	-0.02887300
C	-5.49158600	4.51439700	-0.07488000
H	-3.83657100	5.89867000	-0.08664100
H	-6.91092900	2.89017100	-0.05839800
H	-6.25083200	5.29208700	-0.08760100
C	2.91196100	0.65071100	0.00266400
C	3.24330500	1.31087600	1.21101500
C	3.30248300	1.19414300	-1.24597400
C	3.97365700	2.50362700	1.14399300
C	4.03115300	2.38941600	-1.25713400
C	4.36974600	3.04256400	-0.07594600
H	4.23302400	3.02075200	2.06415300
H	4.33439700	2.81904200	-2.20823500
H	4.93554100	3.96995500	-0.10663600
C	-1.80961000	-2.53676100	0.02167500
C	-2.47581200	-2.66938600	-1.21527600
C	-2.52118000	-2.63076000	1.23694200
C	-3.85219500	-2.92281600	-1.21453300
C	-3.89673400	-2.88502900	1.19329000
C	-4.56276900	-3.03345500	-0.02135100
H	-4.36915800	-3.02834000	-2.16540400
H	-4.44849100	-2.96107500	2.12727300
H	-5.63137700	-3.22966400	-0.03804100
C	0.05691100	-4.62156500	0.10813000
H	-0.58930600	-4.81833900	0.97047900
H	-0.53252600	-4.86258400	-0.78348000
H	0.91092200	-5.30026300	0.15237900
C	4.14376700	-1.87201700	0.10959800
H	4.56898000	-1.32797900	0.95975400
H	4.45097800	-2.91756700	0.17596200
H	4.58791500	-1.43629700	-0.79215100
C	2.80146100	0.77727700	2.57228500

H	2.35135900	-0.20780900	2.41459500
C	2.91429400	0.53725400	-2.56929200
H	2.49089900	-0.44622000	-2.34300500
C	-1.72842300	-2.52263500	-2.52042600
H	-1.32815300	-1.50746700	-2.64403900
H	-0.87507400	-3.20677900	-2.59201100
H	-2.39033200	-2.71936700	-3.36926500
C	-1.82216900	-2.44269100	2.56348300
H	-0.97377800	-3.12534800	2.68851000
H	-1.42396500	-1.42473500	2.66846400
H	-2.51543700	-2.61112300	3.39312600
C	1.72144400	1.68193500	3.20043300
H	1.37914000	1.26785100	4.15670600
H	2.11057900	2.68905600	3.39190100
H	0.85007100	1.78608800	2.54306100
C	3.98272800	0.58655000	3.54284900
H	4.45884600	1.54081600	3.79618600
H	3.63604700	0.13348300	4.47920500
H	4.75339800	-0.06590200	3.11668900
C	1.82206000	1.35350800	-3.29116500
H	2.18706800	2.35247800	-3.55781500
H	1.51116600	0.85161800	-4.21556500
H	0.93442100	1.48766300	-2.66124900
C	4.12237900	0.30771300	-3.49714900
H	3.81044900	-0.23262100	-4.39873100
H	4.57411800	1.25230600	-3.82130500
H	4.90389100	-0.28109300	-3.00343000

int4a (B3LYP)
E_{el} = -2003.808567
H_{corr}= 0.891941
G_{corr}= 0.751083
ΔG_{sol}= -0.03792876

N	2.76216200	0.09602500	-0.32906800
N	0.88789200	2.44030200	-0.78376800
C	2.01047100	2.93065900	-1.32146000
C	3.22827000	2.22540700	-1.41462300
C	3.59723300	0.95349300	-0.92658000
H	4.03177600	2.77518100	-1.88936900
C	-1.63377500	0.29730500	1.92275100
H	-1.74027200	1.38020700	1.80519100
Mg	0.79249800	0.56178700	0.02922800
C	-2.66514700	-0.27244900	2.81945100

C	-2.70541500	-1.63166900	3.18587400
C	-3.66411700	0.57144000	3.33837300
C	-3.70242400	-2.12088800	4.02588600
H	-1.94044800	-2.30685100	2.81288400
C	-4.66357400	0.08461800	4.18013500
H	-3.65142300	1.62590000	3.06971500
C	-4.68904600	-1.26648900	4.52833300
H	-3.70826800	-3.17437000	4.29570600
H	-5.42275900	0.76144700	4.56487000
H	-5.46481300	-1.65052900	5.18564900
C	3.27270200	-1.13092300	0.22679800
C	3.23081000	-2.32729600	-0.53229000
C	3.74271600	-1.14633600	1.56481900
C	3.69471100	-3.51048200	0.05674000
C	4.18264300	-2.35916400	2.10777500
C	4.16973300	-3.53422200	1.36345200
H	3.67920900	-4.43127300	-0.52039600
H	4.54069400	-2.38241700	3.13375900
H	4.52176800	-4.46442200	1.80175000
C	-0.27542200	3.27696700	-0.68280200
C	-0.51073900	3.97001300	0.52676300
C	-1.20476800	3.34787900	-1.74201100
C	-1.67565700	4.73376000	0.65445700
C	-2.35601400	4.12863300	-1.57271900
C	-2.59736100	4.81641900	-0.38734300
H	-1.85555600	5.27055100	1.58306600
H	-3.07057300	4.19121800	-2.39049200
H	-3.49642500	5.41666600	-0.27580900
C	2.01748900	4.35176400	-1.85951200
H	1.28141400	4.47561800	-2.66094000
H	1.74503400	5.06488200	-1.07337400
H	3.00118000	4.62331300	-2.24763400
C	5.06819200	0.59977000	-1.06600700
H	5.56442500	1.25952900	-1.78101900
H	5.57656100	0.70605700	-0.09994400
H	5.20894300	-0.43660800	-1.38122200
C	2.70445900	-2.37381600	-1.96618100
H	2.29546100	-1.38640400	-2.20380800
C	3.75998000	0.10566400	2.44081000
H	3.49127300	0.96058500	1.81297100
C	0.47014100	3.88802600	1.67436800
H	0.50534000	2.87877800	2.10622800
H	1.49169400	4.13725000	1.36604400
H	0.18234900	4.57437300	2.47684900

C	-1.01104700	2.58714000	-3.03477700
H	-1.46394200	1.58974800	-2.97378300
H	-1.49968200	3.11089200	-3.86371000
H	0.04303500	2.45489500	-3.29146000
C	1.56735200	-3.40189900	-2.12820200
H	1.15776700	-3.35461500	-3.14454800
H	1.92623300	-4.42560900	-1.96812500
H	0.74702800	-3.22199400	-1.42731100
C	3.82651000	-2.66318700	-2.98415600
H	4.28210600	-3.64418100	-2.80371100
H	3.42557500	-2.66457200	-4.00494700
H	4.62326500	-1.91342600	-2.93859400
C	2.71065300	0.01172000	3.56797000
H	2.92653800	-0.82901500	4.23807300
H	2.71094800	0.92813000	4.17119700
H	1.70026100	-0.13241200	3.16867600
C	5.15626100	0.39506700	3.02595100
H	5.14885400	1.34445000	3.57441500
H	5.47249900	-0.38613900	3.72694300
H	5.91835400	0.46319600	2.24139300
C	-0.64422200	-0.34625300	1.25959800
H	-0.62201300	-1.43237600	1.41902600
B	-1.52211000	-1.26901600	-1.98438200
O	-1.86382800	-2.44734600	-1.39402300
O	-2.56561800	-0.58016900	-2.52828200
H	-0.39629000	-0.88138600	-2.06344900
C	-3.27637500	-2.68794100	-1.69063700
C	-3.79647500	-1.24846900	-2.09731100
C	-3.93113400	-3.28450500	-0.44688900
C	-3.30386900	-3.70203300	-2.84142100
C	-4.34455300	-0.43277600	-0.92135200
C	-4.78182600	-1.22048500	-3.26399400
H	-5.00358400	-3.44141500	-0.61039000
H	-3.47761300	-4.25677700	-0.22852600
H	-3.80019600	-2.64625700	0.42917600
H	-2.76689800	-4.60394600	-2.53187400
H	-4.32829900	-3.98490600	-3.10514800
H	-2.81128700	-3.30774100	-3.73589900
H	-4.50306100	0.59885000	-1.25125800
H	-5.30165400	-0.83160400	-0.56912100
H	-3.64406100	-0.41198600	-0.08239400
H	-5.70308400	-1.75546700	-3.00703100
H	-5.04667900	-0.18320100	-3.49226600
H	-4.35914900	-1.66712800	-4.16678900

ts5a (B3LYP)
E_{el} = -2003.796477
H_{corr}= 0.890699
G_{corr}= 0.755279
∆Gsol= -0.03614431

N	2.53212200	0.67586500	-0.13621900
N	0.19333300	2.43145500	-0.98107600
C	1.21848100	3.23415200	-1.28971500
C	2.57893100	2.90207000	-1.12204900
C	3.18885500	1.76468300	-0.54989000
H	3.27197000	3.67484000	-1.43125800
C	-1.97999300	-0.11434800	1.31485800
H	-2.41871900	0.73168600	0.77763200
Mg	0.49253600	0.53123000	-0.28325100
C	-2.75321000	-0.47849600	2.51950800
C	-2.42472200	-1.57034300	3.34515800
C	-3.87472500	0.29630100	2.86806600
C	-3.18716200	-1.87101800	4.47009500
H	-1.56433000	-2.18613500	3.09930500
C	-4.63797900	-0.00140000	3.99580600
H	-4.14357600	1.14295400	2.23976600
C	-4.29724200	-1.08803100	4.80281000
H	-2.91572600	-2.71992500	5.09275200
H	-5.49966100	0.61335900	4.24367900
H	-4.88975500	-1.32478100	5.68262500
C	3.24549600	-0.40278100	0.49734700
C	3.68911400	-1.50626200	-0.27458400
C	3.42510900	-0.39102200	1.90365800
C	4.31869900	-2.57125400	0.38187200
C	4.05213900	-1.48653300	2.50906000
C	4.50135800	-2.56962200	1.76060400
H	4.66900300	-3.41923400	-0.20068200
H	4.19050200	-1.48986500	3.58718000
H	4.98889000	-3.40897600	2.24957500
C	-1.14976100	2.92598800	-1.09911400
C	-1.74599000	3.56125200	0.01354100
C	-1.88326700	2.71597600	-2.28596500
C	-3.07368100	3.99204200	-0.08611700
C	-3.20786700	3.16734300	-2.34381000
C	-3.80472500	3.79998300	-1.25685200
H	-3.53338400	4.48615300	0.76684700
H	-3.77467100	3.01342800	-3.25912700

H	-4.83394600	4.14298200	-1.32119900
C	0.93350700	4.61800000	-1.84949800
H	0.31956800	4.55638400	-2.75435200
H	0.36849200	5.22197100	-1.13081100
H	1.85847000	5.14521300	-2.09115800
C	4.69523200	1.84723100	-0.37172600
H	5.11770800	2.65841900	-0.96851800
H	4.94117500	2.03878200	0.67980200
H	5.18859900	0.91141300	-0.64389200
C	3.51999500	-1.56944300	-1.79234100
H	2.93461100	-0.69701100	-2.09977000
C	2.94486300	0.76528800	2.77999500
H	2.58097200	1.55898800	2.12035100
C	-0.97661100	3.76423000	1.29862600
H	-0.71306100	2.80599500	1.76443900
H	-0.03743800	4.30679900	1.14115300
H	-1.57417000	4.32891400	2.02104200
C	-1.28121700	1.99927800	-3.47273500
H	-1.29919200	0.91300000	-3.32032400
H	-1.85719600	2.20995700	-4.37988100
H	-0.24237200	2.29147600	-3.65458600
C	2.74911800	-2.82763400	-2.23844800
H	2.58349900	-2.80109200	-3.32264600
H	3.31352700	-3.74165800	-2.01735300
H	1.77497700	-2.90718800	-1.74724600
C	4.87682100	-1.49413700	-2.52271500
H	5.51407400	-2.34817900	-2.26371700
H	4.72668800	-1.50793900	-3.60898800
H	5.42765500	-0.58121900	-2.27241800
C	1.76774600	0.33850300	3.68027000
H	2.06587700	-0.46097800	4.36906300
H	1.41762500	1.18532500	4.28317300
H	0.92128500	-0.02873100	3.09000500
C	4.08183400	1.36549900	3.63042500
H	3.72246300	2.24355300	4.18010000
H	4.45847000	0.64752000	4.36820300
H	4.93018700	1.67739700	3.01087200
C	-0.86362100	-0.69681600	0.80968500
H	-0.48448100	-1.56041600	1.36913800
B	-0.83068800	-1.42336900	-1.36627400
O	-0.69591500	-2.77518500	-1.07876800
O	-2.02457000	-1.12544900	-2.00684800
H	0.14244600	-0.79419000	-1.75628200
C	-1.80975900	-3.47009300	-1.70038900

C	-2.86326000	-2.31218400	-1.96370700
C	-2.28228200	-4.56745300	-0.74650200
C	-1.26373300	-4.10298300	-2.98917700
C	-3.89087200	-2.14085000	-0.83825100
C	-3.59515600	-2.40325000	-3.30477200
H	-3.14445100	-5.10362500	-1.15986500
H	-1.47436900	-5.29085700	-0.59544300
H	-2.55839100	-4.16190700	0.22912300
H	-0.43132300	-4.76574900	-2.73286400
H	-2.02657300	-4.69360100	-3.50797300
H	-0.88620200	-3.34060200	-3.67752800
H	-4.44915300	-1.21476700	-1.00903900
H	-4.60411600	-2.97240800	-0.82346300
H	-3.41729800	-2.06873800	0.14161600
H	-4.20008000	-3.31561800	-3.36146500
H	-4.26786700	-1.54574200	-3.40903000
H	-2.90130700	-2.39065600	-4.14832700

int6 (B3LYP)

E_{el} = -2003.813605

H_{corr}= 0.891567

G_{corr}= 0.759396

ΔGsol= -0.0361288

N	2.15459700	0.11984300	-1.04947600
N	-0.50546600	1.21128000	-2.06639100
C	0.29649200	1.53551100	-3.08962000
C	1.66379100	1.20271200	-3.17628000
C	2.53745100	0.62912300	-2.22537600
H	2.14628300	1.51781000	-4.09351800
C	-1.49429500	0.49679000	1.61704400
H	-2.36601700	0.58908300	0.96528700
Mg	0.15792800	-0.09728900	-0.65315300
C	-1.37579100	1.56572100	2.62459800
C	-0.53723600	1.46119500	3.74982900
C	-2.16375600	2.72242700	2.48552700
C	-0.47703000	2.48600200	4.69018000
H	0.05449700	0.56238300	3.89687400
C	-2.09949300	3.75091600	3.42431400
H	-2.82583000	2.80989900	1.62733900
C	-1.25467500	3.63687700	4.52949700
H	0.17153000	2.38435000	5.55622900
H	-2.71400300	4.63818900	3.29676000
H	-1.20816500	4.43384800	5.26678500

C	3.13846700	-0.32253900	-0.09437100
C	3.46463500	-1.69977400	-0.00272300
C	3.71697500	0.61527800	0.79872000
C	4.36135500	-2.10784200	0.99307900
C	4.60201800	0.14977000	1.77845300
C	4.92520200	-1.19918500	1.88201500
H	4.62289100	-3.15955600	1.06980800
H	5.04643300	0.85921000	2.47188200
H	5.61538900	-1.53999500	2.64931500
C	-1.83883500	1.74263500	-2.02259000
C	-2.05112800	3.01700100	-1.45044600
C	-2.92348800	0.97018800	-2.48853900
C	-3.35947800	3.50643000	-1.36278200
C	-4.21605000	1.49969600	-2.38151700
C	-4.43957700	2.75540100	-1.82397300
H	-3.52678400	4.49077400	-0.93105100
H	-5.05526500	0.91017800	-2.74279000
H	-5.44987100	3.14904400	-1.75070700
C	-0.27357400	2.32757200	-4.25415500
H	-1.15978900	1.83386000	-4.66659500
H	-0.59375700	3.32445800	-3.93175200
H	0.46441100	2.44530400	-5.05008800
C	4.00995100	0.65524400	-2.59698900
H	4.13464000	0.73268900	-3.67958000
H	4.50085000	1.52445300	-2.14346400
H	4.53650400	-0.23184900	-2.23971800
C	2.91562200	-2.74487600	-0.97384700
H	2.15733800	-2.26018100	-1.59712700
C	3.40837600	2.11097500	0.73551800
H	2.76291700	2.28757500	-0.12976700
C	-0.89606900	3.84228100	-0.93115400
H	-0.37520200	3.33813500	-0.10793400
H	-0.14326800	4.03924000	-1.70326200
H	-1.25042100	4.80744500	-0.55620700
C	-2.71774300	-0.40802100	-3.07253800
H	-2.55648300	-1.14447300	-2.27453100
H	-3.60429100	-0.72176500	-3.63337500
H	-1.85742800	-0.44877200	-3.74865300
C	2.23730600	-3.92584100	-0.25322900
H	1.83392300	-4.62789500	-0.99302100
H	2.95144600	-4.48159200	0.36647700
H	1.40857800	-3.60348900	0.38396000
C	4.02154400	-3.26426500	-1.91734700
H	4.81141300	-3.77645500	-1.35494700

H	3.60461400	-3.98078100	-2.63513400
H	4.49086100	-2.45423500	-2.48599400
C	2.64080700	2.58515400	1.98420300
H	3.23687100	2.44537900	2.89405000
H	2.39758500	3.65174000	1.90616400
H	1.70304400	2.03685600	2.11742600
C	4.68186300	2.95877900	0.54232700
H	4.41933400	4.01581200	0.41526900
H	5.34935300	2.88750900	1.40913500
H	5.25278300	2.64311800	-0.33773000
C	-0.71693100	-0.60321100	1.45033200
H	0.14946200	-0.72931500	2.10945500
B	-1.15533600	-1.87299700	0.49071900
O	-0.93390400	-3.11916600	1.17620800
O	-2.53424200	-1.83670700	0.03492300
H	-0.42102800	-1.85208600	-0.62470100
C	-2.03185200	-3.98613100	0.84966800
C	-3.21155400	-2.96461500	0.61655900
C	-2.23694900	-4.95455100	2.01655300
C	-1.67960000	-4.77848300	-0.42156700
C	-3.86933800	-2.51271300	1.93277300
C	-4.29345500	-3.43784100	-0.35719100
H	-3.11698600	-5.58915500	1.85631600
H	-1.36216000	-5.60715400	2.11059000
H	-2.35784300	-4.41955900	2.96149600
H	-0.74319500	-5.32041800	-0.25471700
H	-2.45628300	-5.50864300	-0.67580400
H	-1.53816600	-4.11232600	-1.27823700
H	-4.51290700	-1.65067200	1.72766400
H	-4.48678900	-3.30276600	2.37583500
H	-3.11729700	-2.20779400	2.66616900
H	-4.78929700	-4.34372300	0.01211900
H	-5.05576900	-2.65870700	-0.46855600
H	-3.87960500	-3.64614800	-1.34690300

product (B3LYP)

E_{el} = -720.6157158

H_{corr}= 0.324704

G_{corr}= 0.262255

ΔGsol= -0.01520395

C	1.53820400	0.26847900	-0.01563900
H	1.19852200	1.29807900	-0.13562000
C	2.99860000	0.10968500	-0.00815100

C	3.63724300	-1.13299000	0.16556900
C	3.80616500	1.24793700	-0.18247100
C	5.02504600	-1.22871100	0.16246600
H	3.04110000	-2.02981800	0.30573300
C	5.19680600	1.15399200	-0.18688000
H	3.32961600	2.21630600	-0.31748700
C	5.81238900	-0.08622500	-0.01436000
H	5.49775000	-2.19793000	0.29892600
H	5.79882200	2.04829700	-0.32466700
H	6.89624200	-0.16484100	-0.01657100
C	0.59434600	-0.68875900	0.10033800
H	0.89647800	-1.72980000	0.21762000
B	-0.91658400	-0.36639100	0.05696000
O	-1.89646400	-1.32356600	0.19041100
O	-1.42774800	0.90105900	-0.12381700
C	-3.16973300	-0.69643400	-0.12634700
C	-2.86063400	0.83394000	0.11381900
C	-4.24258600	-1.29516200	0.78167200
C	-3.47267400	-1.03392700	-1.59268700
C	-3.09091900	1.27985900	1.56444100
C	-3.55467700	1.79757100	-0.84740200
H	-5.21187800	-0.81164000	0.61384800
H	-4.35436100	-2.36196900	0.56252700
H	-3.98045500	-1.19456200	1.83728800
H	-3.47179100	-2.12167200	-1.71321700
H	-4.45165800	-0.65310800	-1.90234100
H	-2.71105300	-0.61974800	-2.26082400
H	-2.66981500	2.28099800	1.69957200
H	-4.15714400	1.31764200	1.81186300
H	-2.59426800	0.60721100	2.27084800
H	-4.64407800	1.74178800	-0.73965700
H	-3.24532600	2.82373400	-0.62400700
H	-3.29554500	1.58750500	-1.88759500

int1b (B3LYP)

E_{el} = -1591.719374

H_{corr}= 0.681798

G_{corr}= 0.561559

ΔGsol= -0.03658928

N	-0.62873800	-2.21362200	0.52786600
N	-2.14702000	0.39133400	0.45088600
C	-1.05752800	-3.50492600	2.58531500
C	-1.27888000	-2.29447200	1.69430700

C	-2.17762200	-1.32021300	2.17762600
C	-2.58529700	-0.09071300	1.61975400
C	-3.58542600	0.71502500	2.42924100
C	0.25160500	-3.27450800	0.12769200
C	-0.25421900	-4.33867300	-0.64937300
C	0.62641800	-5.33797000	-1.07770000
C	1.98092600	-5.28779700	-0.75657700
C	2.47110700	-4.22284700	-0.00500400
C	1.62532400	-3.20048900	0.44115800
C	2.19084000	-2.03447300	1.21911700
C	-1.71547800	-4.39850600	-1.03048300
C	-2.60500400	1.66916800	-0.02706300
C	-3.70246000	1.72812500	-0.92063300
C	-4.07056200	2.97126800	-1.44899200
C	-3.38150700	4.13274000	-1.11486600
C	-2.30262800	4.06212700	-0.23930200
C	-1.89312000	2.84459600	0.31738400
C	-0.68319000	2.81842600	1.24962900
C	-0.83894200	3.78296600	2.44152100
C	0.62150800	3.11553100	0.48279000
C	-4.47305500	0.47824900	-1.34130200
C	-4.21324300	0.13574800	-2.82262000
C	-5.98447600	0.59869600	-1.06731000
H	-1.65139700	-3.43810600	3.49901300
H	-0.00164200	-3.59640100	2.86289900
H	-1.32318800	-4.43114900	2.06428700
H	-2.62531200	-1.55312200	3.13591400
H	-4.46836800	0.95876800	1.82926800
H	-3.15164500	1.66952400	2.74665200
H	-3.90677100	0.16963300	3.31877800
H	0.24000700	-6.16148900	-1.67365000
H	2.65233800	-6.07189100	-1.09594400
H	3.52957200	-4.17381000	0.23958800
H	2.21554200	-1.11945200	0.61139200
H	3.22074300	-2.24020000	1.52688000
H	1.60766500	-1.80800100	2.11804900
H	-2.37705300	-4.37319000	-0.15688400
H	-1.93184500	-5.31395400	-1.58961200
H	-2.00237600	-3.54983500	-1.66590700
H	-4.90915900	3.02881900	-2.13806000
H	-3.68142100	5.08787100	-1.53782400
H	-1.76199900	4.97045200	0.01383800
H	-0.59804800	1.80775900	1.66050700
H	-0.86782400	4.82939800	2.11613400

H	0.00754500	3.67638700	3.13028800
H	-1.75883600	3.58656300	3.00395600
H	0.78559700	2.40620100	-0.33593100
H	1.48526700	3.05613800	1.15622700
H	0.60322800	4.12154400	0.04679200
H	-4.10416000	-0.35870100	-0.73988400
H	-4.72791400	-0.79225000	-3.10068100
H	-3.14339700	0.00847300	-3.02550800
H	-4.57882700	0.93160700	-3.48235200
H	-6.44470200	1.39106100	-1.66880400
H	-6.18583200	0.82284200	-0.01359900
H	-6.49235200	-0.34055700	-1.31649100
C	3.95722300	1.02202200	-1.41128200
C	5.19282200	1.46264700	-0.84231900
C	5.28159300	2.71608100	-0.20705200
C	6.34140700	0.65108200	-0.91039900
C	6.48760200	3.14230600	0.34384800
H	4.39835800	3.34536100	-0.15464700
C	7.54366300	1.08482200	-0.35720200
H	6.27695400	-0.31516500	-1.40120000
C	7.62171000	2.32993100	0.27136500
H	6.54295200	4.11240900	0.83056800
H	8.42312800	0.44926800	-0.41763700
H	8.56140800	2.66570900	0.70147900
H	-0.17268900	-0.31087900	-2.30228900
C	2.91366600	0.64884400	-1.90134200
H	1.98281600	0.32358700	-2.32134100
Mg	-0.83872600	-0.62867300	-0.74542400

ts2b (B3LYP)
E_{el} =-1591.690133
H_{corr}= 0.677893
G_{corr}= 0.562395
ΔGsol= -0.03324515

N	0.35006200	-2.22067800	0.41823700
N	-2.00542700	-0.29452200	0.36218200
C	-0.00291700	-4.09516900	1.97781300
C	-0.45954000	-2.81443700	1.29955500
C	-1.73922400	-2.33960900	1.66029600
C	-2.44910800	-1.19016400	1.25179800
C	-3.80995200	-0.98702300	1.89482000
C	1.64610100	-2.77042700	0.14656700
C	1.81328300	-3.65210600	-0.94217900

C	3.09681800	-4.13257900	-1.22678500
C	4.19526700	-3.74745600	-0.46188600
C	4.01913600	-2.86251600	0.59990200
C	2.75357900	-2.35635800	0.91743000
C	2.58746700	-1.36883400	2.04901100
C	0.63660500	-4.06199300	-1.79722800
C	-2.80386100	0.85472200	0.02389700
C	-3.66585300	0.80353900	-1.10073200
C	-4.36343500	1.96233900	-1.46331300
C	-4.22448500	3.14729300	-0.74849200
C	-3.37554900	3.18612100	0.35274100
C	-2.65470400	2.05703500	0.76020200
C	-1.73155600	2.16743700	1.97334400
C	-2.49080400	2.60076600	3.24332900
C	-0.55351400	3.12437200	1.70204000
C	-3.86270800	-0.46601900	-1.92846800
C	-3.36662500	-0.28538400	-3.37687900
C	-5.33025100	-0.93952100	-1.91654300
H	-0.77166900	-4.48479600	2.64794600
H	0.91089800	-3.92755300	2.55831600
H	0.23656400	-4.86512000	1.23622400
H	-2.25907500	-2.95526000	2.38379300
H	-4.59091900	-0.87537600	1.13622700
H	-3.82476400	-0.07063800	2.49441600
H	-4.07039200	-1.82591600	2.54304600
H	3.23000500	-4.81539500	-2.06267200
H	5.18498600	-4.13078700	-0.69546500
H	4.87481200	-2.55328500	1.19606600
H	2.24328000	-0.39593200	1.67663300
H	3.53882000	-1.21162600	2.56706200
H	1.85257700	-1.70259500	2.79056800
H	-0.16798200	-4.51487400	-1.20596100
H	0.94488400	-4.78701400	-2.55684900
H	0.20071200	-3.19887600	-2.31701300
H	-5.02649300	1.93390700	-2.32421900
H	-4.77385800	4.03584000	-1.04851800
H	-3.26638700	4.11369700	0.90893000
H	-1.30999400	1.17629800	2.16648000
H	-2.89678200	3.61424400	3.14401800
H	-1.81712400	2.59861600	4.10847200
H	-3.32867500	1.93074300	3.46618400
H	0.03779900	2.79693700	0.84112100
H	0.11126800	3.16878000	2.57357900
H	-0.90863500	4.14254400	1.50179300

H	-3.26269100	-1.26015900	-1.47356300
H	-3.49489500	-1.21705700	-3.94152700
H	-2.30541400	-0.01765200	-3.40253400
H	-3.92968600	0.49878200	-3.89700500
H	-5.99300300	-0.20795800	-2.39352700
H	-5.69722200	-1.10234000	-0.89691400
H	-5.42958900	-1.88341600	-2.46566100
C	2.37829100	1.71943200	-0.88134500
C	3.53024400	2.54229700	-0.72510300
C	3.41953600	3.94721200	-0.76075200
C	4.80009400	1.95932300	-0.53567200
C	4.55104600	4.74376300	-0.61115400
H	2.44217600	4.39621400	-0.90737400
C	5.92553900	2.76428100	-0.38563800
H	4.88423300	0.87720500	-0.50999200
C	5.80494300	4.15613400	-0.42303000
H	4.45588500	5.82571800	-0.64088000
H	6.90003900	2.30613400	-0.24047200
H	6.68601800	4.78132900	-0.30634900
H	-0.00799900	-0.38718300	-2.46198400
C	1.38105200	1.00539700	-0.99470200
H	0.72908100	0.37593600	-1.92432000
Mg	-0.22272500	-0.55057600	-0.59733900

int3b (B3LYP)
E_{el} = -1590.558119
H_{corr}= 0.664810
G_{corr}= 0.548248
ΔGsol= -0.03715445

N	0.43603400	2.47378800	-0.00137700
N	-1.91331100	0.57788500	-0.01623900
C	-0.25353800	4.84126300	-0.01502500
C	-0.57056900	3.35563900	-0.01465900
C	-1.93767700	3.00928500	-0.02807700
C	-2.56548200	1.74544600	-0.02855300
C	-4.08352400	1.74931400	-0.04349000
C	1.79369000	2.93805700	0.01041800
C	2.45520900	3.12267500	1.24252300
C	3.79604400	3.52274700	1.23212000
C	4.47638600	3.72626300	0.03377700
C	3.81769300	3.52036700	-1.17621900
C	2.47732600	3.12003500	-1.21001900
C	1.78715300	2.87389700	-2.53169300

C	1.74122800	2.87977500	2.55208700
C	-2.64344300	-0.66283200	-0.01405000
C	-2.97241200	-1.27848000	1.21796000
C	-3.61443700	-2.52226500	1.19339500
C	-3.92176400	-3.15477300	-0.00720900
C	-3.57768200	-2.54775100	-1.21084100
C	-2.93495400	-1.30439200	-1.24211900
C	-2.53283300	-0.70116600	-2.58627800
C	-3.72322400	-0.56341800	-3.55435000
C	-1.39257300	-1.51231700	-3.23631000
C	-2.60673900	-0.64821100	2.56029900
C	-1.46766800	-1.43301600	3.24400700
C	-3.81677300	-0.51290400	3.50377500
H	-1.16572100	5.44082100	-0.03068300
H	0.35605900	5.11184600	-0.88403600
H	0.32907300	5.11735300	0.87072900
H	-2.61777300	3.85198300	-0.03869400
H	-4.46650800	1.21229100	-0.91787600
H	-4.47724100	2.76734100	-0.05997900
H	-4.48365300	1.23462800	0.83670800
H	4.30960800	3.66995500	2.17929200
H	5.51791500	4.03581700	0.04282200
H	4.34823700	3.66585000	-2.11427500
H	1.48090000	1.82461100	-2.63759700
H	2.45580100	3.10570000	-3.36625000
H	0.88033400	3.47879000	-2.64848000
H	0.83129200	3.48333000	2.64993100
H	2.39393500	3.11567100	3.39803200
H	1.43529500	1.83019000	2.65618200
H	-3.87229600	-3.00678000	2.13153300
H	-4.42002200	-4.12064600	-0.00458100
H	-3.80672500	-3.05184700	-2.14618000
H	-2.15227800	0.30792100	-2.39904200
H	-4.13441500	-1.54013700	-3.83432000
H	-3.40640900	-0.06377900	-4.47754300
H	-4.53623700	0.02489900	-3.11359300
H	-0.52303800	-1.59215100	-2.57343200
H	-1.06968100	-1.04110500	-4.17277500
H	-1.71866000	-2.53265500	-3.47059600
H	-2.23663800	0.36312300	2.36503700
H	-1.16672500	-0.94210400	4.17766200
H	-0.58577400	-1.51314100	2.59755700
H	-1.78488600	-2.45352300	3.48951200
H	-4.21738500	-1.49078400	3.79466200

H	-4.63095900	0.05390700	3.03773100
H	-3.52500600	0.00842100	4.42318800
Mg	0.11658600	0.46536100	0.00224600
C	1.39317600	-1.12704900	0.01215600
C	2.15372400	-2.09339600	0.01517500
C	3.03770500	-3.21585700	0.01797300
C	2.53721700	-4.52706500	0.15114400
C	4.42996400	-3.03744600	-0.11304600
C	3.40161200	-5.61889100	0.15291200
H	1.46588600	-4.67234800	0.25204200
C	5.28822200	-4.13414800	-0.11093700
H	4.82277700	-2.03039200	-0.21559200
C	4.77948700	-5.42856000	0.02188200
H	2.99855000	-6.62317100	0.25665600
H	6.35925000	-3.97839700	-0.21310000
H	5.45177300	-6.28249800	0.02335400

H_2 (B3LYP)
E_{el} = -1.179648115
H_{corr}= 0.01345
G_{corr}= -0.001342
ΔG_{sol}= 0.000548692

H	0.00000000	0.00000000	0.37139400
H	0.00000000	0.00000000	-0.37139400

ts4b (B3LYP)
E_{el} = -2002.52347
H_{corr}= 0.866134
G_{corr}= 0.733366
ΔGsol= -0.03852667

N	0.84928000	2.52556600	-0.45814700
N	2.25755700	-0.15196900	-0.74300300
C	2.04664400	4.34181200	-1.62375300
C	1.87142700	2.88028400	-1.24850100
C	2.84313600	1.98850700	-1.74874500
C	3.09796800	0.63755900	-1.42421400
C	4.44972200	0.09791300	-1.85480900
C	0.08022500	3.54909600	0.19767900
C	-1.16140800	3.95277000	-0.33203900
C	-1.90162600	4.92275700	0.35548200
C	-1.43657200	5.47745100	1.54408600
C	-0.21418300	5.05957100	2.06589300
C	0.55752900	4.09426800	1.41095000

C	1.86745400	3.63938600	2.01188600
C	-1.71068500	3.34037900	-1.59705800
C	2.70843700	-1.44025000	-0.27164100
C	2.51723300	-2.60951400	-1.04758600
C	2.91930700	-3.83972400	-0.51049500
C	3.48991700	-3.93411700	0.75335100
C	3.66696200	-2.78043500	1.50932900
C	3.28628400	-1.52537200	1.02145900
C	3.49147200	-0.29913500	1.91003100
C	4.96377400	-0.11489400	2.32618100
C	2.58038500	-0.35344900	3.15342100
C	1.89965700	-2.59440300	-2.44504800
C	0.59246000	-3.41058500	-2.49503900
C	2.88370400	-3.11441800	-3.51428500
H	2.82826900	4.46379800	-2.37632200
H	2.31731600	4.94226300	-0.74808500
H	1.11294100	4.76064400	-2.01280300
H	3.58900400	2.44690700	-2.38635800
H	5.07232100	-0.11241700	-0.97761200
H	4.97853800	0.81652000	-2.48392600
H	4.35132300	-0.84356200	-2.40078300
H	-2.85799100	5.23896000	-0.05397500
H	-2.02495900	6.22846500	2.06430300
H	0.15084100	5.48302900	2.99870000
H	1.85166800	2.56806100	2.24818100
H	2.07465500	4.18095200	2.94009000
H	2.71759700	3.79534300	1.33740600
H	-2.52760000	3.95057100	-1.99562000
H	-2.12235700	2.34128000	-1.39982500
H	-0.94835100	3.24433400	-2.37786200
H	2.77915200	-4.74230900	-1.09898400
H	3.79179000	-4.90059600	1.14810200
H	4.10760300	-2.85430000	2.50020900
H	3.21007500	0.58783300	1.33481900
H	5.31796500	-0.94634000	2.94635800
H	5.08274600	0.80619200	2.90923900
H	5.62232600	-0.04872900	1.45287100
H	1.52463500	-0.45378100	2.87386700
H	2.69145300	0.55670400	3.75543600
H	2.82945700	-1.20911300	3.79165300
H	1.65641500	-1.55633800	-2.69651600
H	0.18877500	-3.40909600	-3.51552900
H	-0.17606800	-3.00225200	-1.83260000
H	0.76957900	-4.45641500	-2.21695100

H	3.12108000	-4.17287900	-3.35518300
H	3.82989400	-2.56228600	-3.51374500
H	2.44102600	-3.02202500	-4.51305400
Mg	0.42515800	0.55869500	-0.18472900
C	-2.41892700	-1.57627600	2.71509900
C	-3.46027600	-2.50846200	2.81595900
C	-1.72337300	-1.19604600	3.87846000
C	-3.79723900	-3.05323700	4.05332100
H	-3.99974300	-2.79938200	1.91994000
C	-2.06530400	-1.74497300	5.11083300
H	-0.92295000	-0.46635800	3.80400400
C	-3.10316700	-2.67569200	5.20413000
H	-4.60634200	-3.77564100	4.11699100
H	-1.52310900	-1.44057300	6.00202900
H	-3.37077200	-3.10040500	6.16774900
C	-1.23063100	-0.33189100	0.68442600
C	-1.98331200	-0.98185500	1.46400100
H	-3.32576100	-1.47534100	0.53275000
B	-2.57505800	-0.83190600	-0.26522600
O	-3.31570500	0.28654600	-0.82334200
O	-2.19922100	-1.71053400	-1.36645800
C	-3.96095400	-0.25361600	-1.98731800
C	-2.85756200	-1.23531600	-2.55161000
C	-4.34402800	0.89663400	-2.92152500
C	-5.24741700	-0.98710500	-1.55928900
C	-1.81441200	-0.50167100	-3.41505600
C	-3.40528100	-2.43590400	-3.32984600
H	-4.80096800	0.51741300	-3.84349700
H	-5.07519300	1.54290900	-2.42397000
H	-3.48293400	1.51132400	-3.19169200
H	-5.87535600	-0.29142500	-0.99287000
H	-5.81914100	-1.34299000	-2.42347700
H	-5.03276200	-1.84595900	-0.91677500
H	-0.96682700	-1.16998000	-3.59475200
H	-2.21714300	-0.19614200	-4.38780900
H	-1.44719600	0.39615600	-2.90527200
H	-3.98381200	-2.11305300	-4.20420900
H	-2.57689300	-3.05878400	-3.68469200
H	-4.04332100	-3.05955600	-2.69933400

int5b (B3LYP)

E_{el} = -2002.619496

H_{corr}= 0.871103

G_{corr}= 0.737906

ΔGsol= -0.03686529

N	0.57927900	1.85211500	-1.55275100
N	1.42887300	-1.02651500	-1.26379400
C	1.18114200	2.80074900	-3.75175700
C	1.06735600	1.63909400	-2.77855900
C	1.52290800	0.38871700	-3.24528400
C	1.77567200	-0.80631800	-2.53827800
C	2.53689700	-1.87302200	-3.30795300
C	0.28598800	3.18912700	-1.12776500
C	-1.02644600	3.69255200	-1.24839600
C	-1.30344400	4.97482300	-0.76040900
C	-0.31129900	5.74780700	-0.16212500
C	0.98058400	5.23986200	-0.04673400
C	1.30019900	3.96229400	-0.52084200
C	2.70679900	3.42786200	-0.37588900
C	-2.11237600	2.87153800	-1.90107500
C	1.95410200	-2.18469700	-0.58632800
C	1.16777900	-3.35512800	-0.45567700
C	1.69516700	-4.44436200	0.24982900
C	2.96010400	-4.39418900	0.82439900
C	3.72061800	-3.23617900	0.69985800
C	3.24412700	-2.12048800	0.00194200
C	4.12365600	-0.87325800	-0.07881300
C	5.49812300	-1.16209200	-0.71441800
C	4.30457100	-0.22995700	1.31018400
C	-0.22842600	-3.47730000	-1.06050000
C	-1.28730000	-3.77050000	0.01832500
C	-0.28574600	-4.54633900	-2.17071400
H	1.47429400	2.45492700	-4.74520000
H	1.93040700	3.52305900	-3.40722500
H	0.23584600	3.34657800	-3.83388500
H	1.83608900	0.37713300	-4.28217700
H	3.57964100	-1.92154300	-2.97526400
H	2.53544300	-1.65663500	-4.37851900
H	2.10973200	-2.86605900	-3.14615600
H	-2.31371900	5.36644200	-0.85329800
H	-0.54390800	6.74025300	0.21428500
H	1.75884800	5.83880300	0.42063400
H	2.73758200	2.52179800	0.24178800
H	3.35601100	4.17405200	0.09310800
H	3.15108700	3.15831600	-1.34122000
H	-3.06193200	3.41587800	-1.89765400
H	-2.27249900	1.91714600	-1.38710600

H	-1.87125200	2.62764100	-2.94337100
H	1.10116200	-5.34918000	0.34894900
H	3.34982000	-5.25053000	1.36853000
H	4.70613700	-3.19509100	1.15650900
H	3.61653200	-0.14209100	-0.71469000
H	6.09401800	-1.84330700	-0.09584200
H	6.06942000	-0.23232900	-0.82313600
H	5.40270500	-1.61640000	-1.70678600
H	3.34333400	0.02239700	1.76867900
H	4.89659900	0.69060800	1.23352600
H	4.82900500	-0.90619500	1.99585000
H	-0.48420800	-2.51697600	-1.51934100
H	-2.28530400	-3.79859300	-0.43331900
H	-1.28396800	-3.00083700	0.79661600
H	-1.11339400	-4.73979300	0.50030400
H	-0.06034200	-5.54413800	-1.77561900
H	0.42968900	-4.33905300	-2.97398400
H	-1.28782500	-4.58239600	-2.61486500
Mg	0.15426800	0.28068400	-0.28939600
C	0.10070700	0.63161500	3.28107000
C	0.43178900	0.07821400	4.53131600
C	0.93264400	1.64382200	2.76875900
C	1.57251800	0.48391100	5.22091100
H	-0.21300000	-0.68904100	4.95412600
C	2.06654600	2.06395000	3.46553000
H	0.64528100	2.15234300	1.85101900
C	2.39749400	1.47877600	4.68971600
H	1.81542700	0.02973400	6.17836800
H	2.68130700	2.86414100	3.06088200
H	3.27948100	1.80719200	5.23321700
C	-1.30535700	0.08495900	1.23433600
C	-1.11811900	0.18293300	2.57469700
H	-1.92651300	-0.09109200	3.26535800
B	-2.73742700	-0.31328300	0.79926100
O	-3.83926100	-0.42308100	1.62851200
O	-3.07389100	-0.58123500	-0.52460100
C	-4.93655100	-0.99846400	0.88085000
C	-4.51873400	-0.71257000	-0.61915900
C	-6.23232300	-0.32260000	1.33325100
C	-4.98658100	-2.49162700	1.23516000
C	-5.05857600	0.62025700	-1.15500500
C	-4.84237200	-1.83175800	-1.60858600
H	-7.09135100	-0.69076000	0.76025300
H	-6.40922200	-0.54826000	2.38983900

H	-6.18069500	0.76333500	1.22772100
H	-5.10154800	-2.59173800	2.31905300
H	-5.82988900	-2.99706500	0.75197500
H	-4.06311500	-3.00208200	0.94834200
H	-4.59840500	0.82797000	-2.12610800
H	-6.14492300	0.59010400	-1.29085100
H	-4.81551500	1.44751900	-0.48150700
H	-5.92482900	-1.98800500	-1.68297000
H	-4.47144100	-1.56077400	-2.60263200
H	-4.37505700	-2.77595300	-1.32042100

int1c (B3LYP)
E_{el} = -720.5442766
H_{corr}= 0.321021
G_{corr}= 0.253282
ΔGsol= -0.014455583

C	1.71752700	-1.69011500	-0.06834700
C	2.74761200	-0.69768900	-0.04441600
C	4.04916000	-1.03010000	0.37571200
C	2.47047700	0.62423600	-0.44386400
C	5.04904800	-0.06090900	0.39607100
H	4.26286400	-2.04943100	0.68244100
C	3.47804200	1.58584500	-0.41912900
H	1.46635500	0.88320600	-0.76571900
C	4.76744200	1.24856900	-0.00050600
H	6.05060400	-0.32834200	0.72202000
H	3.25532600	2.60315600	-0.72961200
H	5.54978500	2.00259200	0.01627300
C	0.84474100	-2.52926900	-0.08979200
H	0.05931500	-3.24922700	-0.13500000
O	-2.34524700	-1.15979400	-0.89729900
O	-1.27798000	0.86963600	-0.96206700
H	-0.82728000	-0.71143800	-2.49457300
C	-3.04058200	-0.33371700	0.08401100
C	-2.05101500	0.88766400	0.27817200
C	-3.28202700	-1.17883800	1.33382200
C	-4.38132200	0.05445300	-0.55388500
C	-1.05315500	0.69581500	1.42633100
C	-2.72363000	2.25502400	0.39469500
H	-3.76863700	-0.58783700	2.11812400
H	-3.94012800	-2.01770800	1.08525200
H	-2.35056000	-1.58675200	1.73261000
H	-4.92436700	-0.85750600	-0.82044200

H	-5.00305900	0.63800500	0.13330200
H	-4.23417600	0.63668200	-1.46890100
H	-0.30902300	1.49746200	1.38900300
H	-1.55178700	0.73839200	2.40048800
H	-0.52265100	-0.25667400	1.34274500
H	-3.34910100	2.30762300	1.29316900
H	-1.95665900	3.03226800	0.47152200
H	-3.34391000	2.47988200	-0.47577900
B	-1.42620000	-0.36777900	-1.52704800

ts2c (B3LYP)
E_{el} = -720.4746746
H_{corr}= 0.318108
G_{corr}= 0.255335
ΔGsol= -0.016142256

C	1.26956900	-0.82965300	-0.16606800
C	2.59919400	-0.26868300	-0.04389000
C	3.66882900	-1.15281300	-0.28453700
C	2.86652300	1.06423900	0.29182600
C	4.98084000	-0.69986800	-0.18772200
H	3.46078900	-2.18599000	-0.54555500
C	4.18387700	1.50786600	0.38586600
H	2.04061100	1.74374100	0.47687700
C	5.24323800	0.63097300	0.14746500
H	5.79994900	-1.38831400	-0.37523000
H	4.38130200	2.54358900	0.64674000
H	6.26867600	0.98172600	0.22185800
C	0.36404600	-1.66639000	-0.35976800
H	-0.02520600	-2.63674100	-0.59336400
O	-1.31004200	0.14595900	-1.16650600
O	-1.33385900	-0.29382100	1.15149100
H	0.41696700	0.64492400	0.20040000
C	-2.58915100	0.55727800	-0.65104400
C	-2.69717500	-0.26537900	0.69153200
C	-3.65394400	0.23193800	-1.69963900
C	-2.54300300	2.07600300	-0.40859800
C	-3.16905800	-1.71199600	0.45950800
C	-3.55114300	0.38350400	1.78248700
H	-4.66026600	0.45409500	-1.32491100
H	-3.48534100	0.83834300	-2.59607900
H	-3.61497200	-0.81927200	-1.99551000
H	-2.24372600	2.57087200	-1.33829600
H	-3.51658400	2.47632700	-0.10385700

H	-1.80945500	2.32992600	0.36347500
H	-2.99653600	-2.29047300	1.37308200
H	-4.23674600	-1.76104800	0.21744300
H	-2.61520800	-2.18575800	-0.35724100
H	-4.58978500	0.50729100	1.45281800
H	-3.55314400	-0.25110800	2.67541300
H	-3.15508800	1.36074100	2.06834700
B	-0.51017300	-0.17841800	-0.01816000

Mg(g) (B3LYP)
E_{el} = -200.091537792
H_{corr}= 0.002360
G_{corr}=-0.014489

[(^{DippPh}Nacnac)Mg]$_2$（B3LYP）
E_{el} = -2407.907354
H_{corr}= 0.996599
G_{corr}=0.842414
ΔGsol= -0.04491142

Mg	-1.21986500	0.77628000	0.33475200
C	-3.37901900	4.03716500	2.49556000
N	-1.81534800	2.36962100	1.55425100
Mg	1.42249600	0.22296100	-0.58009100
C	-3.07899600	2.76792100	1.71218900
N	-3.20428400	0.15171100	0.09630100
N	2.94949600	-1.17818700	-0.29705000
C	-4.19493200	2.08534000	1.18643600
N	2.64032100	1.37086600	-1.84156100
C	-4.26441800	0.85815900	0.49402400
C	0.11533400	3.88410400	1.50428700
C	-0.76535400	3.06208600	2.22554300
C	-5.66447000	0.33241200	0.21825700
C	1.39962200	4.32175500	3.51498200
C	1.18566000	4.51017500	2.14783900
C	0.53542300	3.49344200	4.23587400
C	-0.53395400	2.86455500	3.59719200
C	-3.40113500	-1.12446200	-0.53321100
C	-3.45707800	-2.29560900	0.26483300
C	-3.57624100	-3.53737600	-0.37105500
C	-3.64108300	-3.63906400	-1.75797600
C	-3.45435300	-1.21803400	-1.94689500
C	-3.57845200	-2.48445800	-2.53236200
C	-3.37565200	0.01188100	-2.84972800

C	-4.64311800	0.18711800	-3.71042200
C	-2.12192000	-0.02658700	-3.74618600
C	-3.37390600	-2.24249000	1.78982700
C	-4.56326800	-2.94971000	2.46880800
C	-2.03809600	-2.82310700	2.29613700
C	5.17402800	-2.20761900	-0.58330000
C	4.14967500	-1.12245000	-0.87448200
C	4.56241100	-0.10695900	-1.76378300
C	3.88281300	1.04443000	-2.20732200
C	4.64266700	1.93707900	-3.17724200
C	2.07026500	2.59934000	-2.28503400
C	1.05122000	2.59495200	-3.25102600
C	0.43179700	3.78617800	-3.63696300
C	0.81479200	5.00014600	-3.06240300
C	1.82214300	5.01226700	-2.09347500
C	2.44058300	3.82370000	-1.70316200
C	2.62926400	-2.26947700	0.58108500
C	2.02839100	-3.44120300	0.05479800
C	1.63959500	-4.45279600	0.94157600
C	1.83166200	-4.32745200	2.31472000
C	2.42129400	-3.17262800	2.82085800
C	2.82742900	-2.13042400	1.97791400
C	3.46172800	-0.88249200	2.58931300
C	4.73839800	-1.21018400	3.38924200
C	2.45752500	-0.11048800	3.46796500
C	1.78090900	-3.62698300	-1.44146400
C	0.27414000	-3.62650000	-1.76730800
C	2.45011700	-4.90217400	-1.99194700
H	-3.17039600	3.90427900	3.56272600
H	-4.42699600	4.32556400	2.38673200
H	-2.74825300	4.86389300	2.15140400
H	-5.15224700	2.54922500	1.39164700
H	-0.04439100	4.02958500	0.43967700
H	-5.83971900	-0.60249800	0.76228300
H	-5.80202500	0.10547700	-0.84324800
H	-6.42506800	1.05440500	0.52363400
H	1.85292600	5.14783100	1.57356600
H	0.69639100	3.33084100	5.29868100
H	-3.61749800	-4.44128900	0.23130300
H	-3.73728500	-4.61231900	-2.23232400
H	-3.62472000	-2.56701600	-3.61544600
H	-3.29183600	0.89346100	-2.20612300
H	-5.54618200	0.25227500	-3.09365100
H	-4.77628000	-0.65090100	-4.40496400

H	-4.57574200	1.10527900	-4.30668700
H	-1.21137400	-0.11514400	-3.14300600
H	-2.04940400	0.89054200	-4.34410000
H	-2.15059900	-0.87636700	-4.43897700
H	-3.40631300	-1.19103200	2.09045200
H	-4.51083300	-2.82090100	3.55667600
H	-4.56611100	-4.02706800	2.26510800
H	-5.52278600	-2.54528900	2.12656000
H	-1.97215300	-2.74395800	3.38862400
H	-1.18007800	-2.29487300	1.86528700
H	-1.93797200	-3.88171500	2.02855700
H	5.40279600	-2.24780600	0.48701800
H	6.10324900	-2.03264200	-1.12997900
H	4.78922700	-3.19532200	-0.85699900
H	5.56349900	-0.22671400	-2.16024300
H	4.89492800	2.89967300	-2.71921200
H	4.03200200	2.15856900	-4.05933600
H	5.57008500	1.46095700	-3.50331800
H	0.75331300	1.64975200	-3.69640600
H	-0.35183200	3.76298800	-4.39008800
H	2.12562500	5.95097000	-1.63630600
H	1.17550100	-5.35380900	0.54847300
H	1.52320700	-5.12457800	2.98626700
H	2.56813400	-3.07574200	3.89365700
H	3.75336100	-0.22014100	1.76812900
H	5.20362100	-0.28798100	3.75805200
H	5.47638900	-1.73815800	2.77468800
H	4.52007900	-1.84136600	4.25903600
H	2.13170100	-0.71384700	4.32440100
H	1.56484400	0.17076300	2.89824100
H	2.91006800	0.80970800	3.85690900
H	2.22783800	-2.77459600	-1.96216700
H	-0.23938000	-4.46747500	-1.28682400
H	0.11442200	-3.71116600	-2.84945400
H	-0.21297200	-2.70758000	-1.42290500
H	3.52657100	-4.91690700	-1.78671700
H	2.31229300	-4.96446000	-3.07825800
H	2.01685900	-5.80828800	-1.55229600
H	2.23219100	4.81121800	4.01290800
H	0.33275100	5.92596600	-3.36382500
H	-1.19716400	2.20656000	4.15320000
H	3.21023800	3.82932600	-0.93562200

[(^{DippPh}Nacnac)$_2$Mg] (B3LYP)

E_{el} = -2207.796495
H_{corr}= 0.995392
G_{corr}= 0.855118
ΔGsol= -0.03638193

N	1.26083100	0.27188000	1.40984900
N	-0.88671100	-1.93349900	1.44229300
C	1.61596100	-0.42915500	2.49322800
C	1.00497700	-1.62469400	2.93263900
C	-0.17295900	-2.27805500	2.51828400
Mg	-0.00010300	-0.66620600	-0.00002500
N	0.88613500	-1.93388600	-1.44223600
N	-1.26081100	0.27205800	-1.40998800
C	-1.61624900	-0.42907200	-2.49320400
C	-1.00561500	-1.62485000	-2.93245700
C	0.17221400	-2.27841800	-2.51812900
H	1.48562700	-2.07894500	3.79104200
H	-1.48649400	-2.07916000	-3.79070200
C	-1.83841000	1.58851000	-1.26578400
C	-1.17453500	2.68998300	-1.87225400
C	-3.04789100	1.79146400	-0.55606000
C	-1.76398800	3.95780300	-1.79418100
C	-3.58904700	3.08396700	-0.50389500
C	-2.96757700	4.16044700	-1.12485400
H	-1.27289900	4.80201800	-2.26899000
H	-4.52130500	3.24442300	0.03113200
H	-3.41104500	5.15189800	-1.08086100
C	2.14348100	-2.55871300	-1.21189000
C	3.19136600	-2.48691600	-2.14752800
C	2.38153100	-3.22364400	0.00233800
C	4.42659100	-3.07924600	-1.88465200
C	3.62067500	-3.81042300	0.26440700
C	4.64968700	-3.74583300	-0.67707000
H	5.22008700	-3.01257100	-2.62502600
H	3.77754900	-4.32378400	1.20979100
H	5.61280000	-4.20519200	-0.47263600
C	1.83877900	1.58815800	1.26549500
C	3.04839200	1.79071100	0.55588400
C	1.17518900	2.68983900	1.87187300
C	3.58991800	3.08305800	0.50368500
C	1.76500900	3.95748700	1.79378600
C	2.96869300	4.15975500	1.12451600
H	4.52229200	3.24321000	-0.03123100
H	1.27416300	4.80185300	2.26857800

H	3.41246000	5.15107300	1.08052400
C	-2.14417400	-2.55808900	1.21194900
C	-2.38233500	-3.22301000	-0.00226300
C	-3.19204200	-2.48608400	2.14758800
C	-3.62158600	-3.80956700	-0.26432200
C	-4.42737100	-3.07820000	1.88472500
C	-4.65058700	-3.74476900	0.67715400
H	-3.77855200	-4.32292100	-1.20969400
H	-5.22085400	-3.01137300	2.62509900
H	-5.61378200	-4.20395800	0.47272700
C	-2.79197200	0.02823600	-3.34842700
H	-3.73276800	-0.16632200	-2.82120300
H	-2.76107500	1.09942800	-3.55594500
H	-2.81894700	-0.51144300	-4.29759100
C	0.57020400	-3.47659900	-3.37453900
H	1.28712600	-3.19929100	-4.15496700
H	1.03332300	-4.26429900	-2.77417600
H	-0.31228700	-3.88574600	-3.87343800
C	2.79158100	0.02811000	3.34861400
H	3.73245000	-0.16663400	2.82158700
H	2.76076900	1.09933200	3.55599800
H	2.81830700	-0.51145400	4.29784900
C	-0.57138100	-3.47596800	3.37486500
H	-1.28835400	-3.19832500	4.15512800
H	-1.03461400	-4.26366200	2.77458000
H	0.31092800	-3.88524900	3.87397600
C	3.80049700	0.66742400	-0.15414800
H	3.27507700	-0.27234300	0.03628400
C	-0.14004600	2.52876100	2.63476900
H	-0.59067100	1.58519600	2.31048500
C	-3.80015300	0.66848400	0.15428600
H	-3.27505000	-0.27146200	-0.03613600
C	0.14074500	2.52859400	-2.63501600
H	0.59110200	1.58490200	-2.31073500
H	1.58624400	-3.28005100	0.73739400
H	-1.58705300	-3.27957500	-0.73731700
H	3.03440500	-1.94720500	-3.07652200
H	-3.03497200	-1.94639500	3.07657700
C	3.81891400	0.89446100	-1.67920200
H	4.29512300	1.84933800	-1.93191800
H	4.37869800	0.09583900	-2.17645900
H	2.80530700	0.90622000	-2.09296300
C	5.24498100	0.50197400	0.36236500
H	5.70656800	-0.38064700	-0.09510400

H	5.86473300	1.37139700	0.11193500
H	5.28026400	0.37590200	1.44955500
C	-1.14239900	3.65682000	2.32873500
H	-2.11689000	3.41877100	2.76993300
H	-0.82106300	4.61417900	2.75675200
H	-1.28263800	3.79453700	1.25311200
C	0.08024900	2.42965000	4.15955500
H	0.58731800	3.32568700	4.53898200
H	-0.88346100	2.34478100	4.67696100
H	0.68262000	1.55886900	4.43361800
C	-0.07934100	2.42966500	-4.15984600
H	-0.58628800	3.32578400	-4.53924500
H	0.88444300	2.34479600	-4.67711400
H	-0.68171600	1.55895800	-4.43411400
C	1.14333400	3.65639100	-2.32879300
H	2.11780400	3.41816300	-2.76993700
H	0.82224800	4.61386300	-2.75674700
H	1.28351800	3.79397700	-1.25314600
C	-5.24480900	0.50338800	-0.36185100
H	-5.70653600	-0.37904600	0.09583800
H	-5.86425500	1.37301800	-0.11138000
H	-5.28039100	0.37718900	-1.44901600
C	-3.81813600	0.89576000	1.67931100
H	-4.29394800	1.85084500	1.93199100
H	-4.37808300	0.09741200	2.17682300
H	-2.80442700	0.90722900	2.09283200

$[(^{DippTol'}Nacnac)Mg]_2$ (B3LYP)
E_{el} = -2486.566907
H_{corr}= 1.055463
G_{corr}= 0.893877
ΔGsol= -0.04514449

Mg	-1.21695000	0.75993700	0.21891700
C	-3.16723200	4.31619500	2.06042000
N	-1.73838500	2.42679100	1.36812300
Mg	1.39483400	-0.03267200	-0.62392600
C	-2.95325400	2.97722300	1.37190800
N	-3.23460200	0.29975400	-0.11398500
N	2.82397400	-1.52706200	-0.31006700
C	-4.08992300	2.39393100	0.77489000
N	2.64740400	0.93976800	-1.99083100
C	-4.23952100	1.13745400	0.15130000
C	0.18363400	3.94514400	1.44040400

C	-0.68145900	3.05600000	2.09471900
C	-5.66351000	0.74276100	-0.20844900
C	1.47222000	4.22996900	3.46234000
C	1.25044200	4.53643200	2.11960800
C	0.62552900	3.32886300	4.11031100
C	-0.45336200	2.72708700	3.45061400
C	-1.34770900	1.74849500	4.17508300
C	-3.52499100	-0.99882300	-0.65531700
C	-3.73222000	-2.08864400	0.22883600
C	-3.95776400	-3.36066500	-0.31120800
C	-3.97647500	-3.57138900	-1.68707400
C	-3.52859200	-1.20562900	-2.05786600
C	-3.75879100	-2.49820000	-2.54599900
C	-3.28230900	-0.07218300	-3.05211800
C	-4.46657200	0.12949200	-4.01910400
C	-1.97951000	-0.29694900	-3.84595100
C	-3.70319300	-1.91829100	1.74736000
C	-5.01368100	-2.37996700	2.41493200
C	-2.49434100	-2.64619700	2.36992500
C	4.90631400	-2.79652000	-0.68928000
C	3.96210400	-1.64490500	-0.99491600
C	4.37725400	-0.76020900	-2.01315300
C	3.78380000	0.43236700	-2.47306300
C	4.50967500	1.15505500	-3.59735400
C	2.17879300	2.20091800	-2.46991100
C	1.20192300	2.24192300	-3.47530700
C	0.67067400	3.45598300	-3.91424500
C	1.10904400	4.64921000	-3.33987700
C	2.07344400	4.61223700	-2.33053700
C	2.61989900	3.40561600	-1.87528300
C	3.64313200	3.39577400	-0.76423800
C	2.50438500	-2.48085300	0.71581900
C	1.76373800	-3.64582300	0.39153100
C	1.37961100	-4.50665100	1.42725000
C	1.71041700	-4.24100700	2.75318500
C	2.44018700	-3.09626700	3.06029100
C	2.84776900	-2.20149200	2.06285000
C	3.64422700	-0.95927400	2.45943900
C	4.97121900	-1.32012900	3.15716400
C	2.81211500	-0.00915900	3.34324200
C	1.36320500	-3.98503000	-1.04374300
C	-0.16393600	-3.90838500	-1.23657400
C	1.88918200	-5.36566800	-1.48593400
H	-2.91187200	4.25723700	3.12427500

H	-4.20453900	4.64633800	1.97140700
H	-2.51696400	5.08292500	1.62480500
H	-5.00167100	2.97185500	0.86573100
H	0.00969200	4.16683400	0.39071700
H	-5.97361300	-0.14349200	0.35612600
H	-5.74771600	0.48219600	-1.26783300
H	-6.36441500	1.55162300	0.00942700
H	1.90342600	5.23116500	1.59813500
H	0.80262900	3.08291400	5.15519300
H	-0.99322300	1.58165900	5.19732000
H	-1.37834100	0.77805900	3.66431300
H	-2.38510800	2.10139400	4.23263400
H	-4.11947000	-4.20124500	0.35899300
H	-4.15546100	-4.56602000	-2.08722900
H	-3.76661300	-2.66612000	-3.62008900
H	-3.16289200	0.85398700	-2.48106400
H	-5.40337300	0.31439500	-3.48197300
H	-4.61900700	-0.74882400	-4.65750400
H	-4.27972000	0.98797200	-4.67560600
H	-1.12102500	-0.39406900	-3.17184600
H	-1.79061400	0.54667800	-4.52152900
H	-2.03510300	-1.20816100	-4.45391700
H	-3.58797200	-0.85146800	1.96100000
H	-4.98164700	-2.18207200	3.49322200
H	-5.17934700	-3.45557700	2.28150600
H	-5.88373800	-1.85683900	2.00213400
H	-2.45841000	-2.47615200	3.45342800
H	-1.54825000	-2.29885800	1.93928400
H	-2.55243400	-3.72853500	2.20306400
H	5.22363800	-2.76987900	0.35860100
H	5.79606000	-2.75815400	-1.32163500
H	4.41229000	-3.76153100	-0.84121000
H	5.30712300	-1.02718000	-2.50077000
H	4.79511100	2.17014200	-3.30067100
H	3.85734400	1.25690600	-4.47204200
H	5.41125800	0.61618900	-3.89697300
H	0.86482800	1.30425000	-3.90874800
H	-0.08093500	3.46577200	-4.69938400
H	2.41446000	5.54277200	-1.88128000
H	3.27540500	2.84713400	0.11155200
H	3.88009000	4.41616200	-0.44588200
H	4.57968000	2.91243900	-1.06665200
H	0.80771800	-5.40021100	1.19016200
H	1.40203400	-4.92251000	3.54187600

H	2.69850600	-2.89086700	4.09619200
H	3.89501800	-0.41742400	1.54226500
H	5.54895900	-0.41243000	3.37006700
H	5.59023600	-1.97617200	2.53479500
H	4.79867000	-1.83423800	4.11012200
H	2.52903200	-0.48964100	4.28785400
H	1.89059700	0.30259900	2.83930100
H	3.38458700	0.89461400	3.58511800
H	1.81504600	-3.23715000	-1.70294300
H	-0.68217700	-4.64243900	-0.60845400
H	-0.43279900	-4.11306800	-2.28002700
H	-0.55550400	-2.91911500	-0.97583200
H	2.97607700	-5.44407900	-1.37007800
H	1.64823300	-5.54345400	-2.54098500
H	1.43544400	-6.17584700	-0.90290000
H	2.29890400	4.68398700	4.00220700
H	0.70495100	5.60176100	-3.67185100

[($^{DippTol'}$Nacnac)$_2$Mg] (B3LYP)
E_{el} = -2286.442095
H_{corr}= 1.05426
G_{corr}= 0.9092
ΔGsol= -0.03649411

N	1.01458800	0.51857400	1.65238500
N	-1.21791000	-1.64737700	1.61842200
C	1.10567200	0.00407000	2.88764800
C	0.33428600	-1.06112300	3.39870000
C	-0.78970400	-1.73945100	2.87646200
Mg	-0.05939200	-0.58724800	0.18905200
N	0.89438800	-1.98292400	-1.09693900
N	-1.19588000	0.26629800	-1.40269200
C	-1.66347300	-0.64403200	-2.25460600
C	-1.21488600	-1.98832000	-2.32216700
C	0.01612600	-2.54884000	-1.94318200
H	0.57971900	-1.33359300	4.41778600
H	-1.82098000	-2.62502200	-2.95806500
C	-1.51394500	1.65671500	-1.62440900
C	-0.55128300	2.46056200	-2.29419600
C	-2.74262000	2.22582200	-1.20254900
C	-0.84180000	3.80988600	-2.52675400
C	-2.98088500	3.58263000	-1.46448600
C	-2.04725000	4.37475100	-2.12034600
H	-0.11535000	4.42932000	-3.04251100

H	-3.92351900	4.02245900	-1.14963100
H	-2.25545700	5.42359900	-2.31546000
C	2.25024500	-2.41544600	-1.20793600
C	2.91057800	-2.24529600	-2.43916300
C	2.95681600	-2.99991100	-0.13100200
C	4.22401600	-2.66545700	-2.63207800
C	4.28538000	-3.39771100	-0.34141100
C	4.92195600	-3.24743700	-1.57348000
H	4.70115200	-2.52563500	-3.59876900
H	4.82385300	-3.85581300	0.48559000
H	5.94914300	-3.57804500	-1.70139000
C	1.69840100	1.77345400	1.41928200
C	3.03881900	1.81319800	0.96083000
C	1.00362800	2.98774200	1.68549600
C	3.66025900	3.05960800	0.79355200
C	1.67674800	4.20216800	1.50609400
C	2.99696600	4.24756400	1.06800500
H	4.69025700	3.09273500	0.44912700
H	1.16001500	5.13310700	1.71360800
H	3.50039700	5.20249800	0.94033900
C	-2.47466600	-2.26470000	1.29725200
C	-2.56266000	-3.58302300	0.79702800
C	-3.64938300	-1.52210300	1.47882800
C	-3.82759800	-4.08666500	0.46370400
C	-4.90035400	-2.04515000	1.15078000
C	-4.99076600	-3.33456700	0.62805000
H	-3.89612200	-5.10059700	0.07512400
H	-5.79488100	-1.44665800	1.30397500
H	-5.95555400	-3.75650100	0.35968600
C	-2.75162000	-0.31172800	-3.26810400
H	-3.72802500	-0.60596800	-2.86427300
H	-2.79397900	0.75194900	-3.50353400
H	-2.59785800	-0.87249800	-4.19371000
C	0.32128400	-3.90414700	-2.57824200
H	0.85263700	-3.79619900	-3.52962900
H	0.94476100	-4.52282700	-1.92711600
H	-0.61360200	-4.43438700	-2.78130200
C	2.12695500	0.55707800	3.87661000
H	3.11968900	0.15741600	3.64132900
H	2.20213700	1.64464200	3.83665100
H	1.88147500	0.26027800	4.89864700
C	-1.55071700	-2.59822700	3.87784100
H	-0.98948500	-2.70415700	4.80863800
H	-2.51924100	-2.14272400	4.11443200

H	-1.76195000	-3.59498200	3.47973400
C	-1.34627200	-4.46553800	0.67040100
H	-0.51511100	-3.93624000	0.20264500
H	-0.99349900	-4.80641600	1.65371800
H	-1.57155000	-5.35755400	0.07689700
C	3.86135800	0.56670900	0.64647200
H	3.23645200	-0.31133500	0.83035000
C	-0.44000900	3.00721300	2.19266700
H	-0.93485100	2.11599200	1.79016600
C	2.31340600	-3.25210800	1.21007500
H	1.49450400	-3.97599200	1.13606100
H	3.04735500	-3.65326900	1.91712500
H	1.88959200	-2.34770900	1.65728300
C	-3.84491000	1.43009400	-0.50563700
H	-3.52425500	0.38732400	-0.44016000
C	0.75189500	1.86915300	-2.83088000
H	1.01297400	1.01519700	-2.19637800
C	-1.22768400	4.23940300	1.71229600
H	-2.28849500	4.11820900	1.95537800
H	-0.89063000	5.15572800	2.21199100
H	-1.14276800	4.38392500	0.63198900
C	-0.52934600	2.92577300	3.73275200
H	0.02971800	3.74812500	4.19674400
H	-1.57557200	3.00969800	4.05271700
H	-0.14044100	1.98325100	4.12451300
C	5.11644500	0.44537800	1.53680100
H	5.62441600	-0.50624500	1.33997500
H	5.83050400	1.25129900	1.32888400
H	4.87671700	0.48823400	2.60371600
C	4.28837300	0.53837000	-0.83321800
H	4.92387200	1.39867200	-1.07637300
H	4.85422600	-0.37228800	-1.05002600
H	3.42236800	0.56210100	-1.50011700
C	1.93330300	2.85427100	-2.79820600
H	2.85789400	2.33308100	-3.06996100
H	1.80478800	3.67161100	-3.51815100
H	2.07175400	3.29075200	-1.80414000
C	0.56182500	1.32461700	-4.26350800
H	0.27045600	2.13034400	-4.94896200
H	1.49788900	0.88816400	-4.63424800
H	-0.20991500	0.55020000	-4.30583400
C	-4.09035900	1.93280100	0.93090100
H	-4.38471200	2.98867200	0.93655000
H	-4.89988000	1.36396600	1.40445100

H	-3.19452300	1.83309100	1.55174700
C	-5.17482800	1.46646800	-1.28939800
H	-5.90137600	0.78483300	-0.83075900
H	-5.61583300	2.47032100	-1.28353000
H	-5.04550800	1.17034100	-2.33441900
H	-3.56319200	-0.52335000	1.89315500
H	2.36746100	-1.76726200	-3.25052000

[(^{DippXyl}Nacnac)Mg]$_2$ (B3LYP)

E_{el} = -2565.224412

H_{corr}= 1.114513

G_{corr}= 0.949871

∆Gsol= -0.04463199

Mg	1.38918400	-0.35461300	-0.45062100
C	4.26512300	-2.61826700	-3.03613300
N	3.17816200	0.68333800	-0.07372000
Mg	-1.38927000	-0.35427800	0.45074900
C	3.67557300	-1.61200200	-2.05835800
N	2.36175000	-1.60961700	-1.82669100
N	-2.36206400	-1.60897700	1.82703100
C	4.59319000	-0.72608500	-1.45866300
N	-3.17812600	0.68377000	0.07372500
C	4.37073600	0.34382400	-0.56840600
C	1.23074600	-3.78782800	-1.98271900
C	1.53366500	-2.52918600	-2.54629200
C	5.60483500	1.13879400	-0.17092900
C	0.38446400	-4.65483900	-2.68489400
C	-0.15992400	-4.29024700	-3.91539200
C	0.14058400	-3.04207900	-4.45840800
C	0.98266200	-2.14621900	-3.78887300
C	1.29789400	-0.79715200	-4.39297900
C	1.81317200	-4.19763500	-0.65033100
C	3.21536700	1.67729200	2.18911200
C	3.07811600	1.83016400	0.78639700
C	2.59078200	4.18466500	1.09316400
C	2.70730200	4.04218000	2.47291700
C	3.01843200	2.79547700	3.00898200
C	2.76884200	3.09668200	0.22924900
C	2.63836800	3.31301500	-1.27831800
C	3.66924600	4.33143500	-1.80633600
C	1.21211500	3.74088800	-1.67434900
C	3.57039800	0.33472700	2.82640100
C	2.37370200	-0.25983800	3.59230800

C	4.80444200	0.42712100	3.74559800
C	-4.26554700	-2.61714400	3.03667400
C	-3.67587200	-1.61109700	2.05874500
C	-4.59337200	-0.72512800	1.45893900
C	-4.37077200	0.34453000	0.56842200
C	-5.60476400	1.13951900	0.17067100
C	-1.53410800	-2.52865800	2.54662400
C	-1.23148600	-3.78740100	1.98310700
C	-0.38518400	-4.65446700	2.68518200
C	0.15947400	-4.28985700	3.91555900
C	-0.14079200	-3.04162100	4.45854900
C	-0.98286300	-2.14569100	3.78909200
C	-1.29780500	-0.79653300	4.39315300
C	-1.81428900	-4.19724600	0.65090000
C	-3.07782200	1.83042200	-0.78660100
C	-3.21498900	1.67733400	-2.18929800
C	-3.01782500	2.79535300	-3.00934300
C	-2.70654600	4.04209900	-2.47346900
C	-2.59006800	4.18479200	-1.09373300
C	-2.76833700	3.09698100	-0.22964900
C	-2.63791600	3.31354600	1.27789000
C	-3.66887100	4.33199500	1.80570800
C	-1.21170900	3.74155900	1.67392900
C	-3.57019600	0.33472500	-2.82640200
C	-2.37357400	-0.26014200	-3.59219000
C	-4.80419200	0.42718900	-3.74565700
H	3.85519600	-2.47532200	-4.04214200
H	4.01942500	-3.64433700	-2.74195300
H	5.35188600	-2.52420500	-3.09127500
H	5.62624600	-0.87098600	-1.75055400
H	6.49335200	0.77483500	-0.69145300
H	5.78365000	1.06904300	0.90745500
H	5.47886900	2.20198800	-0.39807600
H	0.15570100	-5.62890200	-2.25831400
H	-0.81321300	-4.97573700	-4.44874000
H	-0.28119100	-2.75247600	-5.41815600
H	2.37329700	-0.65925200	-4.55800400
H	0.97572000	0.02321800	-3.73927200
H	0.79152600	-0.67586400	-5.35583000
H	2.90820600	-4.14326800	-0.64434200
H	1.52551200	-5.22376900	-0.40025300
H	1.46218600	-3.54751200	0.16149200
H	2.35581100	5.16057800	0.67586000
H	2.56188000	4.89845000	3.12647700

H	3.11586600	2.68906600	4.08643200
H	2.84263600	2.35716600	-1.77035900
H	3.59253200	4.42053900	-2.89684400
H	4.69544200	4.03321500	-1.56419300
H	3.50442800	5.32817300	-1.37989100
H	1.13024100	3.84402400	-2.76353100
H	0.94631800	4.70637200	-1.22785200
H	0.46430500	3.01113700	-1.34682500
H	3.81612200	-0.36248700	2.01932300
H	1.51002700	-0.40058500	2.93305400
H	2.06401500	0.39708500	4.41471800
H	2.63134300	-1.23716700	4.01784500
H	5.67064900	0.84728100	3.22202100
H	5.08003700	-0.56970900	4.11032500
H	4.61169600	1.05596700	4.62268900
H	-5.35225000	-2.52261400	3.09218200
H	-3.85520500	-2.47446300	4.04254600
H	-4.02041400	-3.64330800	2.74232900
H	-5.62643900	-0.86980200	1.75090100
H	-5.47845500	2.20287800	0.39682600
H	-6.49322200	0.77623800	0.69177100
H	-5.78392900	1.06883600	-0.90759900
H	-0.15661600	-5.62858900	2.25863100
H	0.81277600	-4.97539300	4.44883300
H	0.28116600	-2.75201300	5.41821500
H	-0.97511400	0.02373600	3.73956800
H	-0.79167000	-0.67545800	5.35615400
H	-2.37320400	-0.65825200	4.55785400
H	-2.90937100	-4.14364500	0.64549300
H	-1.52606300	-5.22311400	0.40039400
H	-1.46420000	-3.54663700	-0.16090900
H	-3.11520000	2.68877300	-4.08678300
H	-2.56095900	4.89823800	-3.12716300
H	-2.35497100	5.16074000	-0.67658000
H	-2.84215400	2.35776000	1.77006600
H	-3.50415700	5.32864000	1.37900800
H	-3.59212100	4.42136600	2.89619300
H	-4.69504800	4.03361900	1.56368200
H	-0.46383500	3.01183500	1.34649700
H	-1.12989000	3.84479300	2.76310600
H	-0.94596000	4.70702900	1.22737100
H	-3.81604700	-0.36233200	-2.01922600
H	-2.63136200	-1.23748700	-4.01759900
H	-1.50993400	-0.40093500	-2.93289900

H	-2.06375000	0.39660800	-4.41468800
H	-4.61129700	1.05588200	-4.62282400
H	-5.67035100	0.84757400	-3.22218200
H	-5.07994200	-0.56964500	-4.11025400

[(^{DippXyl}Nacnac)$_2$Mg] (B3LYP)

E_{el} = -2365.090528

H_{corr}= 1.113672

G_{corr}= 0.962265

∆Gsol= -0.03501177

C	1.16154000	-3.51726000	3.01677800
N	-0.89427700	0.38790600	1.65864900
Mg	-0.01194200	-0.61856000	-0.02927500
C	0.64310900	-2.26362600	2.31927200
N	1.24886800	-1.82266800	1.20622900
N	-1.34730100	-1.76650200	-1.26039500
C	-0.46127500	-1.65138300	2.93534700
N	0.89346800	0.34729400	-1.71009100
C	-1.00821900	-0.35217400	2.76119100
C	2.92139900	-3.23125200	0.01865400
C	2.59831000	-2.27411500	1.00797100
C	-1.70862500	0.16271700	4.01693700
C	4.25742000	-3.61972900	-0.14584000
C	5.26942500	-3.09978900	0.65652800
C	4.94245800	-2.17980000	1.64918100
C	3.62203500	-1.75500400	1.83979700
C	3.32045700	-0.76554300	2.94216500
C	1.85880600	-3.88587200	-0.82704700
C	-2.75200700	2.03024900	1.44445100
C	-1.39049400	1.74603100	1.73862800
C	-1.05438000	4.06644600	2.36889300
C	-2.39770200	4.34016600	2.14519900
C	-3.22702500	3.32877600	1.67186300
C	-0.52451900	2.78416700	2.16810300
C	0.96064600	2.56539100	2.45108900
C	1.26599900	2.55916300	3.96341200
C	1.84123500	3.61502600	1.74567400
C	-3.72241300	0.97502500	0.90929300
C	-4.73357900	1.56168800	-0.09500900
C	-4.50765800	0.24110300	2.01870500
C	-1.47853100	-3.32844100	-3.18216900
C	-0.83451500	-2.16940300	-2.42880400
C	0.27490500	-1.58808400	-3.07416700

C	0.94495500	-0.36239700	-2.84246800
C	1.73741000	0.14688700	-4.04109100
C	-2.69549200	-2.19367800	-0.99255300
C	-2.97787300	-3.25398500	-0.10323800
C	-4.31303900	-3.61315300	0.12643200
C	-5.36108100	-2.96508300	-0.52060000
C	-5.07448100	-1.94258500	-1.42240700
C	-3.75594800	-1.54288100	-1.66980600
C	-3.48598800	-0.43938000	-2.66577300
C	-1.87804600	-4.04715400	0.55574600
C	1.48522600	1.66783800	-1.77155500
C	2.87455700	1.86580500	-1.55576700
C	3.41074600	3.14451800	-1.76559800
C	2.61716500	4.21784800	-2.14874800
C	1.24711800	4.02879400	-2.29726100
C	0.65654000	2.77263400	-2.10891800
C	-0.85341300	2.63394400	-2.30804000
C	-1.22768300	2.43874800	-3.79278400
C	-1.63859800	3.82494000	-1.72833400
C	3.82946500	0.77145200	-1.07424700
C	4.48208900	1.18333500	0.26123500
C	4.94783400	0.43334900	-2.08347600
H	2.06188100	-3.31129400	3.60514800
H	1.42717800	-4.29005500	2.28900100
H	0.40486300	-3.91814300	3.69582400
H	-0.81947000	-2.16399000	3.82150600
H	-2.29822400	-0.64154600	4.46774600
H	-2.35601100	1.01965900	3.84121900
H	-0.95567700	0.45599500	4.75735800
H	4.49596900	-4.36039700	-0.90585600
H	6.29942200	-3.41772600	0.51806400
H	5.72170100	-1.77524200	2.29163500
H	2.90038000	-1.25314300	3.83171500
H	2.58943200	-0.01869900	2.62423400
H	4.23251900	-0.24865700	3.25696500
H	1.01836700	-4.23258600	-0.21789700
H	2.27249000	-4.74903200	-1.35968400
H	1.44973800	-3.20038600	-1.57695800
H	-0.40103200	4.86025100	2.71916400
H	-2.79356400	5.33687600	2.32225800
H	-4.26977000	3.55350800	1.47375600
H	1.23062500	1.58199200	2.05385400
H	2.33685700	2.39820300	4.13745500
H	0.71853100	1.77103300	4.48850000

H	0.99238100	3.51780500	4.42093900
H	2.90086400	3.37898300	1.89282300
H	1.67602600	4.61984800	2.15202500
H	1.64803900	3.64888200	0.66999700
H	-3.13218100	0.21795400	0.38321900
H	-4.24444400	2.15477200	-0.87411400
H	-5.47397600	2.20144400	0.39926100
H	-5.28366400	0.74788700	-0.57587600
H	-3.85693900	-0.34559000	2.66961700
H	-5.22789000	-0.44975600	1.56638300
H	-5.06210200	0.95470200	2.64164500
H	-0.80564700	-3.70545000	-3.95594300
H	-2.41069400	-3.02193900	-3.66912100
H	-1.73046600	-4.14991700	-2.50505800
H	0.55478900	-2.07733800	-3.99908700
H	1.32231200	1.09140100	-4.40632200
H	1.70943800	-0.57581700	-4.85896000
H	2.77888400	0.34781600	-3.78811000
H	-4.52323600	-4.43163300	0.81107300
H	-6.38964500	-3.26350000	-0.33602500
H	-5.88327000	-1.44314800	-1.95121400
H	-2.87713100	0.35704300	-2.22787300
H	-4.42379600	0.00067800	-3.01838500
H	-2.93640500	-0.79730200	-3.54436000
H	-1.17746400	-4.45159600	-0.18316300
H	-2.29564200	-4.88850200	1.11887600
H	-1.29843800	-3.43335300	1.25011400
H	4.47683600	3.29807000	-1.62309800
H	3.05801600	5.19756200	-2.31405200
H	0.62365200	4.87362700	-2.57268300
H	-1.17270500	1.73611300	-1.76801600
H	-0.84980900	3.27060700	-4.40022700
H	-2.31760700	2.40547300	-3.91103400
H	-0.82259800	1.50803100	-4.19962100
H	-1.36246600	4.02676100	-0.68965900
H	-2.71270800	3.61143000	-1.75614800
H	-1.48121000	4.74071800	-2.31051600
H	3.25164100	-0.14090800	-0.89910100
H	5.12581400	0.38027900	0.63136500
H	3.72949700	1.39745300	1.02426000
H	5.09832000	2.08210500	0.14100000
H	5.57783500	1.30747500	-2.28826800
H	4.55990500	0.07263100	-3.04036700
H	5.59009800	-0.35353600	-1.67170700

[(^{Ar}Nacnac)Mg]$_2$ (B3LYP)
E_{el} = -4256.940678
H_{corr}= 1.681254
G_{corr}= 1.441377
∆Gsol= -0.08320979

Mg	4.49564300	10.30167200	10.74987600
C	0.70063700	12.34068800	11.84385700
H	0.30159500	13.24538000	11.37954700
H	0.66799400	12.47158000	12.93028000
H	0.03725900	11.50398000	11.60477000
N	2.74834400	10.94839400	11.73735300
N	4.97820500	12.29709000	10.23724700
C	2.12254600	12.07293500	11.37186400
C	4.03497500	13.23937400	10.13847100
C	2.70469400	13.08713400	10.58544200
H	2.05533800	13.92774200	10.37403400
C	2.08743300	10.10209500	12.68907100
C	4.36852600	14.59772200	9.54004600
H	4.85059100	14.50655300	8.56265500
H	5.06589400	15.13651000	10.19013000
H	3.46779800	15.20558700	9.42899600
C	1.21448300	9.08859700	12.22617800
C	0.54713200	8.29031300	13.15575200
H	-0.13369000	7.52494100	12.79028000
C	0.73499500	8.43971300	14.53453000
C	1.63738500	9.41042700	14.96587200
H	1.82221400	9.51295200	16.03131800
C	2.31686300	10.25378500	14.07532800
C	0.99723400	8.86409400	10.74779700
H	0.56231300	9.73979100	10.24992700
H	0.33152400	8.01317800	10.57720300
H	1.94267400	8.64684200	10.23485400
C	-0.02669800	7.58639500	15.52295400
H	-0.13975300	6.55701900	15.16419600
H	-1.03805000	7.97940200	15.69432600
H	0.47745400	7.55247100	16.49474500
C	3.27814900	11.32191600	14.61780000
H	3.73566800	11.78392600	13.73568200
C	2.53109500	12.45140300	15.33997100
C	2.01079500	12.29973400	16.63521500
H	2.16678900	11.37018700	17.17413200
C	1.13675600	14.55857300	16.60448000

H	0.59912300	15.36733800	17.09225600
C	1.31941700	13.33776600	17.25918600
H	0.92752200	13.19400400	18.26295700
C	1.66075600	14.73070300	15.32373300
H	1.53721700	15.67748000	14.80384200
C	2.35285700	13.68708800	14.70155900
H	2.76215200	13.83812800	13.70560900
C	4.44235300	10.74309000	15.44297700
C	5.16735400	11.55851000	16.32703400
H	4.85481100	12.58548200	16.48896000
C	6.27972600	11.06947100	17.01335900
H	6.81992700	11.72407500	17.69239100
C	6.69628800	9.74980200	16.83212500
H	7.55943800	9.36732300	17.37028100
C	5.99013600	8.92897800	15.95267000
H	6.29970500	7.89794000	15.79871000
C	4.87767000	9.42159000	15.26573500
H	4.33736800	8.76691000	14.59126900
C	6.29685900	12.61187300	9.76652700
C	7.31268900	13.04363900	10.65171600
C	8.57839300	13.34401900	10.13281300
H	9.36132500	13.65918300	10.81795100
C	8.86886900	13.25025000	8.76989800
C	7.86038500	12.79030000	7.91971800
H	8.06623200	12.68224200	6.85688800
C	6.59028700	12.44974800	8.39348300
C	5.54746600	11.92362600	7.43520100
H	4.68376700	12.59362900	7.34223700
H	5.15635300	10.95428100	7.76992700
H	5.97574800	11.78812500	6.43722200
C	10.24092200	13.60739600	8.24438000
H	10.98165800	12.83361500	8.48697100
H	10.60649200	14.54471900	8.67993900
H	10.23335300	13.72499800	7.15554000
C	7.04201700	13.21105900	12.15129600
H	6.17653300	12.57949800	12.37777700
C	6.63663600	14.63422800	12.55596900
C	7.08172500	15.78106900	11.88458500
H	7.71646700	15.67912400	11.00965100
C	6.70836100	17.05690700	12.31921500
H	7.06664200	17.93176300	11.78229900
C	5.87821300	17.20897500	13.42990900
H	5.58473600	18.20067300	13.76397300
C	5.42634700	16.07357200	14.10744400

H	4.77297100	16.17218400	14.97043400
C	5.80618400	14.80354000	13.67444700
H	5.45910000	13.92708000	14.21588400
C	8.19989100	12.67513500	13.00465500
C	9.20103000	13.50259000	13.53001200
H	9.14989400	14.57584400	13.37126600
C	10.25714600	12.96613600	14.27143200
H	11.02338100	13.62719400	14.66888800
C	9.32458700	10.75963300	14.00420200
H	9.35290700	9.69053900	14.19798000
C	8.27596700	11.29792700	13.25894800
H	7.50129800	10.63922200	12.87197100
Mg	5.65645100	7.65210100	10.11824800
C	9.45137500	5.61310900	9.02397000
H	9.85059500	4.70867800	9.48863600
H	9.48376300	5.48166200	7.93760000
H	10.11474400	6.44998700	9.26245600
N	7.40371400	7.00547400	9.13065100
N	5.17388100	5.65667800	10.63092200
C	8.02953800	5.88094900	9.49613900
C	6.11722500	4.71450500	10.72975700
C	7.44747100	4.86680200	10.28269000
H	8.09688700	4.02625100	10.49414100
C	8.06448600	7.85165300	8.17872300
C	5.78386400	3.35620500	11.32840400
H	5.30194300	3.44746900	12.30585800
H	5.08644400	2.81727200	10.67850100
H	6.68465600	2.74842600	11.43940400
C	8.93759700	8.86515000	8.64133200
C	9.60475900	9.66332700	7.71152600
H	10.28566900	10.42874500	8.07674200
C	9.41659000	9.51379600	6.33280300
C	8.51409800	8.54305300	5.90175100
H	8.32908600	8.44038300	4.83635200
C	7.83478100	7.69981300	6.79252800
C	9.15528900	9.08972600	10.11964200
H	9.58964700	8.21377500	10.61754400
H	9.82170000	9.94015000	10.28995200
H	8.21013700	9.30779600	10.63276400
C	10.17810800	10.36698000	5.34412900
H	10.29133700	11.39637400	5.70278300
H	11.18938500	9.97387900	5.17253600
H	9.67372100	10.40087700	4.37245900
C	6.87336500	6.63165500	6.25033700

H	6.41617800	6.16955600	7.13257700
C	7.62024600	5.50227200	5.52782900
C	8.13987600	5.65396800	4.23232000
H	7.98341100	6.58344700	3.69342000
C	9.01438100	3.39530300	4.26275100
H	9.55193500	2.58661900	3.77475600
C	8.83115700	4.61603800	3.60807000
H	9.22252800	4.75982100	2.60409700
C	8.49103000	3.22313600	5.54375800
H	8.61499800	2.27640800	6.06363700
C	7.79902700	4.26665000	6.16621400
H	7.39021600	4.11556700	7.16235600
C	5.70884000	7.21046700	5.42560400
C	4.98345800	6.39499000	4.54190500
H	5.29590700	5.36799500	4.37993900
C	3.45437600	8.20370200	4.03728000
H	2.59101900	8.58615600	3.49943900
C	4.16091000	9.02458300	4.91637100
H	3.85144000	10.05564500	5.07036300
C	5.27364300	8.53199400	5.60290000
H	5.81424600	9.18672200	6.27707800
C	3.85530200	5.34176500	11.10178600
C	2.83945700	4.90971400	10.21675700
C	1.57388700	4.60906200	10.73584600
H	0.79095700	4.29363300	10.05082600
C	1.28356400	4.70282600	12.09879000
C	2.29203300	5.16312900	12.94880400
H	2.08629900	5.27120200	14.01165500
C	3.56198500	5.50395600	12.47485100
C	4.60479600	6.03038300	13.43297600
H	5.46864100	5.36056500	13.52592000
H	4.99567400	6.99977600	13.09811900
H	4.17658600	6.16589000	14.43098500
C	-0.08830900	4.34532400	12.62453300
H	-0.82905900	5.11945900	12.38310600
H	-0.45419500	3.40852000	12.18813300
H	-0.08027900	4.22655900	13.71324600
C	3.10996500	4.74215700	8.71716100
H	3.97514400	5.37404500	8.49041700
C	3.51586400	3.31907100	8.31272200
C	3.07103400	2.17219100	8.98421600
H	2.43617500	2.27407800	9.85907100
C	3.44479500	0.89640200	8.54979300
H	3.08671000	0.02151600	9.08679100

C	4.27508900	0.74442000	7.43919400
H	4.56887400	-0.24724000	7.10528700
C	4.72670000	1.87985900	6.76155200
H	5.38017800	1.78132000	5.89863200
C	4.34646800	3.14984400	7.19434800
H	4.69336000	4.02632900	6.65283100
C	1.95172000	5.27740700	7.86386300
C	0.95112800	4.44935100	7.33840900
H	1.00294600	3.37612200	7.49707800
C	-0.10531000	4.98517900	6.59699100
H	-0.87110200	4.32365300	6.19946300
C	0.82580000	7.19226200	6.86444600
H	0.79677500	8.26135800	6.67078400
C	1.87474200	6.65459000	7.60969500
H	2.64891200	7.31379200	7.99681300
C	10.32481200	11.59331100	14.51019200
H	11.14261000	11.17745400	15.09296900
C	-0.17385600	6.35797500	6.35833300
H	-0.99190100	6.77335000	5.77555800
C	3.87082900	6.88400300	3.85598600
H	3.33032800	6.22935900	3.17723200

[(^{Ar}Nacnac)$_2$Mg] (B3LYP)
E_{el} = -4056.796902
H_{corr}= 1.679655
G_{corr}= 1.450905
ΔGsol= -0.07200093

C	3.81280100	11.59614500	8.42092700
H	4.49850600	12.44626000	8.41850800
H	2.81452900	11.97035000	8.66828500
H	3.76009000	11.18279300	7.40952800
N	3.73580600	9.31567200	9.41035200
N	5.44631600	9.21519400	11.98581000
C	4.26050800	10.55051100	9.43269000
C	5.69209800	10.46541600	11.57205900
C	5.23928500	11.00412500	10.34914200
H	5.61216800	11.99840000	10.13747600
C	2.65419300	9.09805500	8.47829400
C	6.54403000	11.39345300	12.42604900
H	7.45726800	10.88431100	12.75104400
H	6.01589900	11.71376100	13.32550100
H	6.82234800	12.29004400	11.86757000
C	2.97432200	8.61474500	7.18613300

C	1.98493700	8.50289900	6.21076500
H	2.26646500	8.14590300	5.22199400
C	0.65114300	8.83129700	6.47026700
C	0.33504400	9.22462200	7.76710500
H	-0.70344100	9.42770900	8.01558600
C	1.30029500	9.37004000	8.78015800
C	4.38828200	8.25295700	6.83146100
H	5.06661000	9.11322000	6.87589500
H	4.42895100	7.84142300	5.82257700
H	4.80473000	7.49793300	7.50764200
C	-0.39766900	8.74339900	5.38648600
H	-0.39853800	7.75459900	4.91280000
H	-0.21513200	9.48093000	4.59393700
H	-1.40080600	8.92838700	5.78488100
C	0.80943400	9.80495800	10.16453700
H	1.62612400	9.60365000	10.86816200
C	0.47812000	11.29955000	10.29228800
C	0.33417800	11.84301900	11.57987900
H	0.47851300	11.20272100	12.44644000
C	-0.21694600	14.01395600	10.66181500
H	-0.48387900	15.05796000	10.80340400
C	-0.00892000	13.18225100	11.76527300
H	-0.10895100	13.57475400	12.77374300
C	-0.08246200	13.48802400	9.37776500
H	-0.24488400	14.12081800	8.50876400
C	0.25822400	12.14336400	9.19548200
H	0.35095600	11.75138600	8.18812600
C	-0.37949400	8.92005600	10.59013100
C	-1.68910300	9.40540400	10.69488100
H	-1.89108400	10.45542200	10.51192900
C	-2.74569800	8.55603300	11.03734500
H	-3.75291700	8.95854500	11.11154300
C	-2.51165300	7.20379200	11.28047900
H	-3.33258500	6.54196900	11.54423600
C	-1.20907000	6.70679300	11.17887000
H	-1.00643400	5.65565800	11.35718000
C	-0.15728100	7.55666800	10.83848500
H	0.84786700	7.15070300	10.75337400
C	5.60637000	8.93365200	13.39256500
C	4.60799700	9.31388100	14.33283900
C	4.70748900	8.86363500	15.65630600
H	3.90805800	9.11185600	16.34918600
C	5.78096400	8.10106400	16.11542800
C	6.79427800	7.81203500	15.20149700

H	7.66891400	7.25564100	15.53408800
C	6.72904100	8.20903500	13.86215100
C	7.89170400	7.87220400	12.96392800
H	8.33475500	8.76913200	12.51895800
H	7.60212300	7.20890200	12.14433200
H	8.67705200	7.36359900	13.53319000
C	5.83955000	7.60100400	17.54006000
H	5.43085200	6.58476600	17.62434600
H	5.25896300	8.23994000	18.21413400
H	6.87020000	7.56558800	17.91097800
C	3.43943400	10.24336600	13.96720000
H	3.31027500	10.17642600	12.88239000
C	3.73783000	11.71981700	14.27931600
C	3.29168600	12.70887500	13.39117000
H	2.77419800	12.41647000	12.48332700
C	3.50807900	14.06326000	13.64860200
H	3.15226800	14.80595100	12.93897000
C	4.17995400	14.46006400	14.80635000
H	4.35247400	15.51390300	15.00868600
C	4.63502200	13.48729100	15.69754900
H	5.16685100	13.77983600	16.59952000
C	4.41852300	12.13187200	15.43525300
H	4.80155700	11.38943500	16.12796800
C	2.10666700	9.79505400	14.59209300
C	1.58344700	10.36068100	15.76366500
H	2.11182300	11.17241600	16.25332300
C	0.37784900	9.90631900	16.30499900
H	-0.00466100	10.36168000	17.21522100
C	0.16145300	8.32506400	14.50092400
H	-0.39512700	7.55160400	13.97973100
C	1.37144200	8.77405600	13.97086300
H	1.74663900	8.32721700	13.05486900
Mg	5.15792800	7.93214400	10.21233600
C	9.26803800	6.57789100	9.60346100
H	9.68405000	5.60118200	9.85576100
H	9.65263100	6.87115800	8.62719900
H	9.63950300	7.30735900	10.33560900
N	7.03763600	7.54174000	9.07872000
N	4.76812600	5.83434900	10.45594300
C	7.74530800	6.56682200	9.66233500
C	5.87057600	5.10828100	10.69802900
C	7.19819400	5.51015400	10.42372100
H	7.94552100	4.82912300	10.81082200
C	7.72560900	8.34384900	8.08733000

C	5.75802700	3.72651000	11.32989300
H	5.17269300	3.74528900	12.25349400
H	5.25688900	3.03297000	10.64867200
H	6.74717600	3.32263000	11.55428500
C	8.30746900	9.58375500	8.44098400
C	8.88861300	10.39651000	7.46082800
H	9.31382700	11.35133600	7.76724900
C	8.97894500	10.00299100	6.12890500
C	8.48974800	8.73600800	5.80685900
H	8.59616300	8.38925600	4.78350500
C	7.86534400	7.89508800	6.73867400
C	8.45937800	10.02459500	9.87479000
H	9.49166100	9.84815100	10.20972600
H	8.26187500	11.09453100	9.98713700
H	7.80033100	9.48042000	10.54472500
C	9.58749800	10.90026000	5.07664400
H	10.37717000	11.53299900	5.49681100
H	10.02041900	10.31879200	4.25524400
H	8.83533100	11.57015300	4.63793300
C	7.49073200	6.46999900	6.30274000
H	6.71983900	6.11932700	6.99877000
C	8.68804500	5.51390900	6.47319600
C	9.92026300	5.75849800	5.84786100
H	10.05593800	6.65875700	5.25728400
C	10.83415600	3.69654100	6.73228100
H	11.66165900	2.99898800	6.83172100
C	10.98219100	4.86352800	5.97786900
H	11.92752500	5.07766300	5.48557900
C	9.61360700	3.43825900	7.35528000
H	9.47884600	2.53490100	7.94499500
C	8.55328000	4.34063400	7.22648200
H	7.61337100	4.13066900	7.72687200
C	6.89398400	6.32108400	4.88022100
C	6.88516200	5.05498900	4.26920900
H	7.36209900	4.21796000	4.76815900
C	5.68923000	5.90650600	2.34414400
H	5.22958500	5.74920900	1.37211800
C	5.69404200	7.17193600	2.92910000
H	5.23759400	8.01374800	2.41418100
C	6.28607800	7.37419300	4.17874200
H	6.27578600	8.36979700	4.60480600
C	3.51226400	5.19910200	10.79337600
C	2.76002300	4.44543200	9.86108600
C	1.60356800	3.78029400	10.30261900

H	1.03035700	3.21003900	9.57736000
C	1.16017300	3.82649000	11.62267700
C	1.88677800	4.61821500	12.51561800
H	1.55672800	4.70259500	13.54935900
C	3.04160700	5.30036800	12.12761800
C	3.79154000	6.10561600	13.15469700
H	4.80427000	5.72479300	13.33015300
H	3.90712300	7.14588500	12.84565700
H	3.26326100	6.10794700	14.11203300
C	-0.04431400	3.03350000	12.07678200
H	-0.63035800	3.58101300	12.82398700
H	-0.70496200	2.79068200	11.23772000
H	0.25685300	2.08407100	12.54003200
C	3.16569200	4.28051900	8.38977300
H	3.77010700	5.15686700	8.12514600
C	4.04779200	3.05106600	8.13968200
C	3.86617500	1.84018200	8.82421400
H	3.11895200	1.77458300	9.60873900
C	4.63573900	0.71599700	8.51521100
H	4.47658200	-0.20971200	9.06259500
C	5.60078800	0.77770300	7.50877600
H	6.19852400	-0.09689400	7.26609200
C	5.78730300	1.97426900	6.81436100
H	6.53362200	2.03745400	6.02722300
C	5.01889200	3.09708100	7.12948400
H	5.15978400	4.01659200	6.56621500
C	1.92798800	4.28205200	7.46535200
C	1.67095800	3.26332300	6.53852400
H	2.36506400	2.43705900	6.43382800
C	0.52112600	3.28547400	5.74252600
H	0.34726300	2.47954200	5.03379700
C	-0.15297100	5.34868600	6.78157200
H	-0.85995700	6.16475300	6.89673600
C	1.00019700	5.33150500	7.56373400
H	1.16832500	6.13516100	8.27411200
C	-0.33830300	8.88720400	15.67744700
H	-1.28203400	8.54301800	16.09233400
C	-0.40032000	4.32334400	5.86480200
H	-1.30163600	4.33453700	5.25717800
C	6.28948200	4.84691600	3.02458300
H	6.30168900	3.85236100	2.58597400

Mg(g) (BP86)

E_{el} = -200.082482378

H_{corr}= 0.002360
G_{corr}= -0.014489

[(^{DippPh}Nacnac)Mg]$_2$ (BP86)
E_{el} = -2407.822491
H_{corr}= 0.970088
G_{corr}= 0.813779
ΔGsol= -0.0450758

Mg	-1.22806300	0.77716200	0.26220700
C	-3.28039200	4.26203400	2.21344300
N	-1.77277100	2.45419200	1.40812600
Mg	1.42784200	0.15405200	-0.58973100
C	-3.02749000	2.92644700	1.52158700
N	-3.23862200	0.21842400	0.04294500
N	2.94375600	-1.26103300	-0.28724400
C	-4.16829300	2.26032200	1.00899300
N	2.67702000	1.29102300	-1.85697600
C	-4.28494900	0.99281300	0.38593300
C	0.34822000	3.69395100	1.33753600
C	-0.69896100	3.10581900	2.08394200
C	-5.69957000	0.50265900	0.10689500
C	1.53195100	4.26434300	3.39321000
C	1.44895400	4.27213200	1.99104700
C	0.50306400	3.66605800	4.14111800
C	-0.59919000	3.08683000	3.49479500
C	-3.47666400	-1.08609000	-0.51589000
C	-3.57183100	-2.21443800	0.35184900
C	-3.71879900	-3.49376500	-0.21794500
C	-3.77310300	-3.67325700	-1.60588000
C	-3.52271400	-1.25828700	-1.93049500
C	-3.67328100	-2.55951400	-2.44839500
C	-3.39918200	-0.07740500	-2.89638800
C	-4.62740300	0.04975100	-3.82687800
C	-2.09932400	-0.17341300	-3.72834100
C	-3.49597900	-2.07077900	1.87394100
C	-4.70637400	-2.71389800	2.58780500
C	-2.17052700	-2.65146800	2.41954100
C	5.14958500	-2.34951100	-0.57802800
C	4.14625300	-1.24636300	-0.88731200
C	4.55888600	-0.25890300	-1.81784100
C	3.90697800	0.91623500	-2.26136300
C	4.66925800	1.75833500	-3.28072700
C	2.15604000	2.56348300	-2.22723700

C	0.94663700	2.63894100	-2.95767500
C	0.36635600	3.88300200	-3.25616100
C	0.97497200	5.07402800	-2.82692900
C	2.17168800	5.00936200	-2.09169400
C	2.75355700	3.76939600	-1.78786500
C	2.61446100	-2.32547500	0.62341200
C	2.04593000	-3.53387500	0.12207300
C	1.63568200	-4.51719700	1.04232000
C	1.78044500	-4.33065000	2.42325900
C	2.34141800	-3.14122400	2.90326700
C	2.76403400	-2.12280500	2.02639800
C	3.36825200	-0.83877500	2.59904600
C	4.65259100	-1.11834100	3.41301800
C	2.34088500	-0.05875100	3.45054000
C	1.84138700	-3.76625100	-1.37737300
C	0.35103500	-3.61308300	-1.76020500
C	2.38640700	-5.13289100	-1.84896400
H	-3.20909700	4.17462900	3.31225000
H	-4.28541000	4.64233600	1.96963800
H	-2.53057200	5.01136000	1.90476800
H	-5.11505300	2.78500800	1.16496900
H	0.28427400	3.70914200	0.24358800
H	-5.91049600	-0.42499100	0.66916300
H	-5.83182600	0.25480500	-0.96110200
H	-6.44902700	1.25856200	0.38971900
H	2.24314900	4.73231100	1.39235200
H	0.56121300	3.64267100	5.23568300
H	-3.79048800	-4.36719700	0.44124600
H	-3.89094400	-4.67742100	-2.02913300
H	-3.71067900	-2.70116800	-3.53544500
H	-3.34156800	0.84529700	-2.29034700
H	-5.56676000	0.13914100	-3.25252100
H	-4.72532400	-0.82862900	-4.49103400
H	-4.53449800	0.94493600	-4.46911500
H	-1.21141500	-0.21543900	-3.06983600
H	-1.99680800	0.70235100	-4.39631300
H	-2.09381900	-1.08201800	-4.35840800
H	-3.50610500	-0.99146100	2.10970600
H	-4.65659200	-2.52268700	3.67552500
H	-4.72996500	-3.81001800	2.44526900
H	-5.66336500	-2.30819900	2.21325400
H	-2.10268300	-2.50900000	3.51427400
H	-1.29288300	-2.16558800	1.95569100
H	-2.09403200	-3.73452800	2.21144600

H	5.34149300	-2.41004900	0.50808800
H	6.10645100	-2.17883000	-1.09608200
H	4.75887000	-3.33777800	-0.88037900
H	5.54974900	-0.42386000	-2.25038600
H	5.14242900	2.64182800	-2.81599100
H	3.99219900	2.13518300	-4.06680900
H	5.46642700	1.16254700	-3.75399400
H	0.47705600	1.71032300	-3.30064600
H	-0.56581000	3.91870800	-3.83187400
H	2.65238400	5.93149000	-1.74435500
H	1.19077800	-5.44671000	0.66773600
H	1.45634200	-5.11001500	3.12250700
H	2.45330500	-2.99563300	3.98456500
H	3.65127900	-0.19530200	1.74593100
H	5.09949800	-0.17071400	3.76599000
H	5.41010700	-1.64802200	2.80779000
H	4.44157300	-1.74057600	4.30236300
H	2.01619900	-0.64856700	4.32807800
H	1.43990600	0.19163500	2.86084600
H	2.77530200	0.88839400	3.81901600
H	2.40186300	-2.98250800	-1.91807600
H	-0.27344400	-4.36384400	-1.24259600
H	0.21098800	-3.74363200	-2.84947000
H	-0.03812100	-2.61609600	-1.48147900
H	3.45049400	-5.26365900	-1.58112500
H	2.29656000	-5.22091700	-2.94721800
H	1.82486100	-5.97516500	-1.40485000
H	2.39182600	4.71698300	3.89945000
H	0.52081200	6.04311700	-3.06049600
H	-1.38886100	2.59735100	4.07674700
H	3.66982200	3.72010400	-1.18853100

[(^{DippPh}Nacnac)$_2$Mg] (BP86)

E_{el} = -2207.716904

H_{corr}= 0.968510

G_{corr}= 0.825527

ΔGsol= -0.03648791

N	0.90495000	-1.95159400	-1.44630100
C	-1.60782100	-0.44583500	-2.51855500
N	1.25153000	0.25912400	1.42464200
C	0.18752300	-2.30961000	-2.53063200
N	-0.90477200	-1.95166200	1.44627500
C	-0.99582400	-1.65301000	-2.94775400

C	2.47897800	-3.10663500	0.03875800
C	2.17984200	-2.54313700	-1.22357300
C	0.57960100	-3.52261600	-3.37511700
C	4.73804700	-3.66247300	-0.69429900
C	3.74199500	-3.66090400	0.29636800
C	-3.82045400	0.64932200	0.10173500
C	3.19789100	-2.53186400	-2.20843100
C	4.45720900	-3.09148900	-1.94732300
C	-1.83063600	1.57806200	-1.28554700
C	-1.73870200	3.96232100	-1.80249700
C	-2.95963700	4.16632300	-1.14766700
N	-1.25153600	0.25894300	-1.42464100
Mg	0.00008000	-0.68452300	0.00001300
C	-2.77472800	0.02711000	-3.38085600
C	-3.59838700	3.08196200	-0.53844300
C	-3.05820000	1.78067200	-0.59039000
C	-3.83415700	0.85344000	1.63416100
C	-5.27065400	0.50520100	-0.41708600
C	0.18097800	2.51649900	-2.62001000
C	-0.01781000	2.41034000	-4.15167400
C	1.18338600	3.64556700	-2.30001300
C	-0.57932600	-3.52251600	3.37524800
C	-0.18735300	-2.30953800	2.53066100
C	0.99593800	-1.65283000	2.94777300
C	1.60783400	-0.44559600	2.51858400
C	2.77467200	0.02743400	3.38093100
C	1.83052600	1.57828900	1.28551000
C	1.14829200	2.68588100	1.87856200
C	1.73837100	3.96257400	1.80229700
C	2.95932300	4.16663000	1.14752600
C	3.59820000	3.08227500	0.53841000
C	3.05811800	1.78095000	0.59041400
C	3.82052800	0.64960800	-0.10155200
C	5.27068000	0.50566300	0.41743200
C	3.83435700	0.85360000	-1.63399700
C	-0.18123100	2.51663000	2.61979800
C	-1.18371900	3.64559500	2.29966000
C	0.01750300	2.41056800	4.15147000
C	-2.17966100	-2.54321700	1.22359200
C	-3.19767800	-2.53198700	2.20848400
C	-4.45700100	-3.09161400	1.94739800
C	-4.73787600	-3.66255500	0.69436400
C	-3.74185600	-3.66094400	-0.29633700
C	-2.47883800	-3.10667000	-0.03875200

C	-1.14852500	2.68568200	-1.87871900
H	-1.48262100	-2.11759100	-3.81027800
H	1.70891100	-3.11238700	0.81729300
H	1.11185700	-4.27994200	-2.77690000
H	1.23728500	-3.24832500	-4.21920300
H	-0.32618800	-3.98120800	-3.80598200
H	5.72240500	-4.09853700	-0.49182100
H	3.94447400	-4.09852300	1.28090200
H	-3.29570800	-0.29956300	-0.10779900
H	2.99805200	-2.05929900	-3.17588600
H	5.22721800	-3.07235300	-2.72768900
H	-1.23049900	4.81395300	-2.26829300
H	-3.40411000	5.16734700	-1.10476900
H	-3.72853300	-0.12452000	-2.84347600
H	-2.82219000	-0.53376600	-4.32753800
H	-2.71072600	1.10316900	-3.60858300
H	-4.54699300	3.24190600	-0.01222200
H	-4.31357500	1.81314100	1.90273700
H	-2.81076600	0.85966700	2.04811000
H	-4.39538600	0.03941700	2.12484500
H	-5.74342000	-0.38767000	0.02984700
H	-5.30913300	0.39739900	-1.51545700
H	-5.88698800	1.38343100	-0.14925300
H	0.62327500	1.56138100	-2.28057300
H	-0.61975000	1.52989900	-4.43230900
H	0.96104500	2.32450000	-4.65923700
H	-0.52529700	3.31164000	-4.54382600
H	0.86608500	4.61127500	-2.73619700
H	2.17127500	3.40480000	-2.73193100
H	1.31057100	3.78404200	-1.21343700
H	-1.23668800	-3.24812800	4.21955700
H	0.32655700	-3.98119800	3.80582800
H	-1.11184500	-4.27979500	2.77722000
H	1.48274700	-2.11734100	3.81033100
H	2.71092600	1.10360700	3.60817300
H	3.72855700	-0.12471000	2.84382500
H	2.82178900	-0.53304300	4.32786600
H	1.23006700	4.81419000	2.26801400
H	3.40372200	5.16768400	1.10457400
H	4.54683200	3.24226000	0.01224800
H	3.29583100	-0.29930100	0.10799700
H	5.30906000	0.39805600	1.51582600
H	5.88698200	1.38389100	0.14950900
H	5.74355600	-0.38724900	-0.02930200

H	4.39574000	0.03960200	-2.12455100
H	4.31367200	1.81333700	-1.90261700
H	2.81100400	0.85964700	-2.04804000
H	-0.62343400	1.56145600	2.28040600
H	-2.17161800	3.40479400	2.73152900
H	-1.31084000	3.78396200	1.21306300
H	-0.86650200	4.61135900	2.73578900
H	-0.96134500	2.32434700	4.65897600
H	0.52461500	3.31206500	4.54365500
H	0.61978600	1.53036800	4.43212900
H	-2.99781400	-2.05945500	3.17595000
H	-5.22698500	-3.07251400	2.72778900
H	-5.72224000	-4.09861200	0.49190100
H	-3.94436600	-4.09852900	-1.28087900
H	-1.70880000	-3.11238100	-0.81731400

[($^{DippTol'}$Nacnac)Mg]$_2$ (BP86)
E_{el} = -2486.476854
H_{corr}= 1.027631
G_{corr}= 0.865413
ΔGsol= -0.04564127

Mg	-1.23724700	0.75497100	0.20096300
C	-3.34855200	4.41441600	1.69113100
N	-1.84263400	2.51326300	1.17888000
Mg	1.43530300	-0.03379600	-0.50310600
C	-3.08605200	3.02380000	1.12636500
N	-3.23665500	0.22754700	-0.17729000
N	2.85549700	-1.53615000	-0.13256800
C	-4.19743500	2.34699800	0.56594800
N	2.76538300	0.95777000	-1.79894500
C	-4.28902300	1.04546500	0.01388600
C	0.04063200	4.09594300	1.11499500
C	-0.81630500	3.25142100	1.85195900
C	-5.68484800	0.57090100	-0.36928000
C	1.28281000	4.64144000	3.13005100
C	1.07969200	4.79450200	1.75003400
C	0.44629600	3.78274400	3.86091600
C	-0.60590600	3.07497300	3.24792500
C	-1.48425400	2.14126100	4.05222400
C	-3.46481400	-1.09969700	-0.68509600
C	-3.63990200	-2.17762000	0.23226700
C	-3.79649100	-3.48076200	-0.27789700
C	-3.77732300	-3.73231800	-1.65544500

C	-3.43473900	-1.34548300	-2.08965600
C	-3.59273800	-2.66826300	-2.54699100
C	-3.22245000	-0.22112700	-3.10618300
C	-4.36647300	-0.13933500	-4.14302000
C	-1.85939700	-0.36812800	-3.82143800
C	-3.64938400	-1.95611600	1.74697300
C	-4.96531900	-2.43726400	2.39990400
C	-2.43101700	-2.63037600	2.41968100
C	4.99463600	-2.76837700	-0.35078400
C	4.05984000	-1.62572500	-0.72552300
C	4.53449600	-0.71830600	-1.70566500
C	3.94543800	0.46295700	-2.21782700
C	4.70805600	1.18023900	-3.32520600
C	2.31354700	2.21480400	-2.31249200
C	1.32825400	2.24140000	-3.32263100
C	0.81554400	3.45755200	-3.80152000
C	1.28256700	4.66735500	-3.26585200
C	2.25180500	4.64463900	-2.24947100
C	2.77643200	3.43712000	-1.74832700
C	3.77934900	3.44182000	-0.61505800
C	2.45530800	-2.54565900	0.81209400
C	1.84322800	-3.74785900	0.34635000
C	1.36825800	-4.67274000	1.29544800
C	1.49046400	-4.43606500	2.67112800
C	2.09558800	-3.25502800	3.11620900
C	2.58412100	-2.29418000	2.20887900
C	3.23826800	-1.01899400	2.74457200
C	4.49521400	-1.32627400	3.59053100
C	2.23394400	-0.16330600	3.54994600
C	1.65956000	-4.02801400	-1.14761100
C	0.20074000	-3.75464900	-1.58079100
C	2.08686200	-5.45676600	-1.54940400
H	-3.09933300	4.46546300	2.76638700
H	-4.40312000	4.70533700	1.56354100
H	-2.71176800	5.16455200	1.18841400
H	-5.14050300	2.89877000	0.60451200
H	-0.11848500	4.19851100	0.03527100
H	-5.96161700	-0.33505800	0.19943200
H	-5.73174400	0.29248500	-1.43688000
H	-6.43949000	1.34925700	-0.17537800
H	1.72732100	5.45423700	1.16197300
H	0.60920300	3.65359900	4.93845500
H	-1.16688100	2.11449100	5.10884600
H	-1.44229700	1.10874300	3.65658700

H	-2.54895000	2.43935000	4.02376500
H	-3.93559600	-4.31462500	0.42085800
H	-3.90316100	-4.75366100	-2.03279900
H	-3.57100700	-2.86664800	-3.62547800
H	-3.20385100	0.73401600	-2.55050400
H	-5.35221400	-0.02352300	-3.65802800
H	-4.40996900	-1.04741300	-4.77208400
H	-4.21460400	0.72452700	-4.81599100
H	-1.02858500	-0.36113300	-3.09171400
H	-1.70104600	0.46330700	-4.53349100
H	-1.80489700	-1.31655500	-4.38736500
H	-3.56867400	-0.86834500	1.92387900
H	-4.96332500	-2.21091500	3.48207600
H	-5.09851800	-3.52913800	2.28803600
H	-5.84714700	-1.94570400	1.95124000
H	-2.42835400	-2.43178000	3.50783500
H	-1.47782500	-2.26101600	2.00006900
H	-2.44984700	-3.72653500	2.27700900
H	5.17326300	-2.78472400	0.73930700
H	5.96425700	-2.67819500	-0.86538100
H	4.55188000	-3.74735700	-0.60813700
H	5.51061900	-0.96830200	-2.13020500
H	4.95078600	2.22139700	-3.04860500
H	4.08996800	1.23733700	-4.23986800
H	5.64566500	0.65633100	-3.56906100
H	0.97390300	1.28800600	-3.73111100
H	0.05689200	3.45608000	-4.59251300
H	2.61494500	5.59028400	-1.82685200
H	3.34922400	2.98477400	0.29612100
H	4.08233900	4.47290900	-0.36357600
H	4.69215500	2.86691400	-0.85364500
H	0.89017500	-5.59661700	0.94924800
H	1.11552200	-5.17077600	3.39294900
H	2.19266700	-3.07108700	4.19316500
H	3.56441900	-0.42188000	1.87332900
H	4.97854800	-0.38783800	3.91939100
H	5.23773900	-1.90930000	3.01671700
H	4.24147100	-1.90790500	4.49606200
H	1.87553500	-0.70367500	4.44588600
H	1.35097100	0.09710900	2.93725100
H	2.70357000	0.77906900	3.88688300
H	2.30283900	-3.32264800	-1.70350600
H	-0.50525200	-4.41916300	-1.05057100
H	0.07651700	-3.91960900	-2.66722600

H	-0.10061500	-2.71446500	-1.35620700
H	3.12186200	-5.67897700	-1.23233700
H	2.03168800	-5.57524300	-2.64699100
H	1.42835000	-6.22475800	-1.10406100
H	2.09007900	5.18255400	3.63640900
H	0.89532700	5.62412600	-3.63364700

[($^{DippTol'}$Nacnac)$_2$Mg] (BP86)

E_{el} = -2286.358457

H_{corr}= 1.025777

G_{corr}=0.878301

∆Gsol= -0.0367035

N	1.02389400	0.53433800	1.64650200
N	-1.17570100	-1.67367200	1.62434000
C	1.13136700	0.02562400	2.89499600
C	0.37529200	-1.05671300	3.41259200
C	-0.74225400	-1.76083200	2.89313400
Mg	-0.04483100	-0.58817700	0.18463800
N	0.92658600	-1.97142100	-1.11492400
N	-1.22078900	0.25167300	-1.39053000
C	-1.68414300	-0.66846200	-2.25401100
C	-1.19978100	-2.00507000	-2.33930100
C	0.05090700	-2.55030800	-1.97229300
H	0.63249900	-1.32609100	4.44035300
H	-1.80235600	-2.65643600	-2.98046400
C	-1.57016900	1.63789400	-1.60400700
C	-0.61646600	2.46914100	-2.27048500
C	-2.81844600	2.18242800	-1.17889400
C	-0.93720400	3.82001900	-2.50262000
C	-3.08710500	3.54169300	-1.44112900
C	-2.16412900	4.36016700	-2.09816700
H	-0.21383500	4.46025400	-3.01806900
H	-4.04872800	3.96261300	-1.12409900
H	-2.39726900	5.41304700	-2.29426400
C	2.29043700	-2.38381000	-1.22476800
C	2.95074200	-2.22981500	-2.46808900
C	3.01105900	-2.93308900	-0.12667100
C	4.27905300	-2.63313300	-2.65149100
C	4.35389100	-3.31427900	-0.32991000
C	4.99109000	-3.18130000	-1.57303700
H	4.75862100	-2.50558800	-3.62890100
H	4.90331200	-3.74816300	0.51523100
H	6.03255900	-3.49922900	-1.69470900

C	1.69063600	1.79952200	1.40631900
C	3.03886800	1.85567200	0.94726300
C	0.97036300	3.01063300	1.66009700
C	3.64409500	3.11719700	0.76907700
C	1.62845300	4.24120800	1.47092200
C	2.95721300	4.30411300	1.03433700
H	4.68306000	3.16219900	0.42183200
H	1.08844900	5.17251900	1.66897400
H	3.44980300	5.27388200	0.89854200
C	-2.42501300	-2.31338500	1.30694800
C	-2.48554400	-3.63639800	0.79035000
C	-3.62181500	-1.59432800	1.50542500
C	-3.74829300	-4.16871900	0.45946800
C	-4.86934600	-2.14737400	1.17939600
C	-4.93386800	-3.44110500	0.64125200
H	-3.79526100	-5.18916600	0.05835800
H	-5.78417400	-1.56707200	1.34682100
H	-5.89867200	-3.88622100	0.37352300
C	-2.79328100	-0.33980500	-3.24936600
H	-3.77603100	-0.59378000	-2.81047200
H	-2.81231500	0.72894300	-3.51150300
H	-2.67967700	-0.93236400	-4.17151500
C	0.38129200	-3.89746900	-2.61991600
H	0.89716200	-3.77625600	-3.58859100
H	1.03773000	-4.50631900	-1.97628000
H	-0.55129700	-4.45504100	-2.81015600
C	2.14817300	0.61187900	3.87259500
H	3.16353900	0.25969900	3.61419700
H	2.17489400	1.71201000	3.83746000
H	1.93331800	0.29459900	4.90523200
C	-1.49191600	-2.63767600	3.89129500
H	-0.92654600	-2.74048800	4.83078000
H	-2.47767100	-2.19870000	4.13046000
H	-1.68882600	-3.64379000	3.48273100
C	-1.24288200	-4.48334200	0.64620700
H	-0.43487800	-3.92700500	0.14505300
H	-0.84898300	-4.79705900	1.63311900
H	-1.45369100	-5.39939600	0.06796500
C	3.87456100	0.61322700	0.63866500
H	3.25734700	-0.27786600	0.84926200
C	-0.47927800	3.00387900	2.15751100
H	-0.95740500	2.09475700	1.74404500
C	2.36505900	-3.16627700	1.21936500
H	1.54324800	-3.90173400	1.15649100

H	3.10478900	-3.55102800	1.94307300
H	1.92665700	-2.25006000	1.65436400
C	-3.89918100	1.35930000	-0.47372000
H	-3.55228800	0.31241900	-0.41832500
C	0.70099000	1.89984200	-2.80329000
H	0.97600300	1.04364700	-2.15792900
C	-1.28393600	4.22717500	1.67197200
H	-2.35372800	4.08822000	1.90655000
H	-0.96311500	5.15500200	2.18167500
H	-1.19045400	4.37565500	0.58347000
C	-0.57707200	2.91218200	3.70075600
H	-0.02867700	3.74744800	4.17533200
H	-1.63491500	2.97894200	4.01721300
H	-0.17235200	1.96492600	4.09153800
C	5.15025400	0.52443500	1.50972000
H	5.67702500	-0.42697400	1.31257100
H	5.85041800	1.34834000	1.27841300
H	4.92657800	0.57576900	2.58936800
C	4.27281400	0.57053500	-0.85291400
H	4.89790500	1.44301500	-1.12045700
H	4.84829300	-0.34468100	-1.07304400
H	3.38496700	0.57704500	-1.50682000
C	1.86550900	2.91003600	-2.77226100
H	2.80749300	2.40403200	-3.04898500
H	1.71799200	3.73201400	-3.49764100
H	1.99832100	3.35153100	-1.76964800
C	0.51703000	1.34224100	-4.23641200
H	0.20137300	2.14477200	-4.92914400
H	1.46855500	0.92186000	-4.61234600
H	-0.24398000	0.54407400	-4.26956200
C	-4.13272500	1.85327400	0.97235000
H	-4.45230000	2.91152400	0.98376300
H	-4.92907900	1.26235600	1.46207200
H	-3.21641400	1.77205300	1.58234300
C	-5.24380000	1.38032400	-1.24067500
H	-5.95899600	0.67723400	-0.77566900
H	-5.70420200	2.38530300	-1.21761200
H	-5.12366100	1.09646100	-2.29972000
H	-3.55281600	-0.58915300	1.93322100
H	2.39373000	-1.77250500	-3.29436000

$[(^{DippXyl}Nacnac)Mg]_2$ (BP86)

E_{el} = -2565.129816

H_{corr}= 1.084875

G_{corr}= 0.91698
∆Gsol= -0.04521207

Mg	1.39846600	-0.31620900	-0.47173600
C	4.32266300	-2.51945900	-3.09274800
N	3.17675500	0.75072300	-0.09289900
Mg	-1.38693600	-0.37577000	0.43714100
C	3.72485200	-1.52237500	-2.10647100
N	2.40230700	-1.54761700	-1.86002800
N	-2.33327800	-1.65242900	1.82425700
C	4.62893600	-0.61389100	-1.50474300
N	-3.21177100	0.61132100	0.05830600
C	4.38778000	0.44375500	-0.59501500
C	1.32325500	-3.76229900	-1.99053800
C	1.59243800	-2.49390400	-2.57126300
C	5.60268100	1.26207900	-0.17693800
C	0.49510100	-4.66314800	-2.68784400
C	-0.06457700	-4.32176200	-3.92748800
C	0.19924500	-3.06202600	-4.48413000
C	1.02288300	-2.13179200	-3.82131100
C	1.29934400	-0.77305700	-4.42918400
C	1.91814000	-4.13346300	-0.64958400
C	3.20366100	1.69848600	2.19823500
C	3.05544000	1.87982600	0.79168400
C	2.51134700	4.22781200	1.15036600
C	2.63983800	4.05833800	2.53451600
C	2.98392400	2.80072600	3.04679900
C	2.71131100	3.15646800	0.25787000
C	2.57175700	3.39405400	-1.24854100
C	3.58790700	4.44074600	-1.76235100
C	1.13354900	3.80779700	-1.63253400
C	3.58509400	0.34252900	2.79747700
C	2.38050200	-0.31329200	3.50816800
C	4.79386100	0.43731000	3.75559400
C	-4.21385000	-2.73154900	3.02944700
C	-3.65932900	-1.70564000	2.04741200
C	-4.60533400	-0.85088200	1.43126100
C	-4.40993100	0.23503400	0.54404900
C	-5.65804600	1.00856100	0.13953100
C	-1.47965800	-2.52341300	2.57941500
C	-1.10141600	-3.78192000	2.04051700
C	-0.23473900	-4.60405100	2.78698600
C	0.25472500	-4.19614100	4.03611800
C	-0.11781200	-2.94671500	4.55214800

C	-0.97940100	-2.09244700	3.83796500
C	-1.36477000	-0.73951200	4.39718800
C	-1.62754300	-4.23163900	0.69467300
C	-3.13997100	1.76430100	-0.80050200
C	-3.27346600	1.60718700	-2.21143900
C	-3.09851200	2.73612300	-3.03487000
C	-2.81314300	3.99638500	-2.49378700
C	-2.70139400	4.14175300	-1.10550300
C	-2.85954400	3.04359800	-0.23743300
C	-2.73909600	3.25402600	1.27441400
C	-3.76822200	4.28231400	1.79846600
C	-1.30672700	3.66966200	1.67830900
C	-3.59251900	0.24868000	-2.84056700
C	-2.35345600	-0.34426900	-3.54679600
C	-4.79276700	0.31271100	-3.81163200
H	3.88533800	-2.39451300	-4.09979200
H	4.10638500	-3.55903100	-2.78723900
H	5.41458900	-2.39780100	-3.17060900
H	5.67276400	-0.73380200	-1.80687900
H	6.50599500	0.94196600	-0.71971600
H	5.79301100	1.15840900	0.90682600
H	5.44156700	2.33832600	-0.36234600
H	0.29290600	-5.64772700	-2.24817300
H	-0.70452400	-5.03569500	-4.45827200
H	-0.23689000	-2.78830500	-5.45282100
H	2.37903200	-0.60216200	-4.59704000
H	0.95539400	0.04438300	-3.76678700
H	0.78265000	-0.66379700	-5.39800800
H	3.01769700	-4.02135400	-0.63515600
H	1.67681900	-5.17772800	-0.38696200
H	1.52699800	-3.48613700	0.16003800
H	2.25039900	5.21489800	0.74972100
H	2.47766700	4.90457400	3.21198800
H	3.09055500	2.67201500	4.13070100
H	2.79206700	2.43802500	-1.75707500
H	3.50322800	4.55391500	-2.85891700
H	4.62824100	4.15093600	-1.53006400
H	3.40887800	5.43312200	-1.30882200
H	1.04546200	3.93618100	-2.72732700
H	0.85220300	4.76607000	-1.15857000
H	0.39180700	3.05280600	-1.31727200
H	3.87420100	-0.32105700	1.96246700
H	1.53273500	-0.45892900	2.81289900
H	2.02445600	0.31600700	4.34508700

H	2.65372800	-1.30383400	3.91535400
H	5.66567500	0.91084500	3.26928400
H	5.09525400	-0.57180200	4.09138800
H	4.55559700	1.02781700	4.65921800
H	-5.31419700	-2.69645100	3.06356700
H	-3.82881600	-2.55363000	4.05000300
H	-3.90241100	-3.75504700	2.75441400
H	-5.64541800	-1.03346800	1.71440200
H	-5.56438800	2.07625800	0.40627000
H	-6.55685300	0.60221000	0.62950100
H	-5.80931200	0.97383900	-0.95434300
H	0.05128200	-5.58138800	2.37861700
H	0.92387400	-4.85064900	4.60605100
H	0.26359600	-2.62115900	5.52774600
H	-1.02091600	0.08171700	3.73919900
H	-0.91643300	-0.58311600	5.39340700
H	-2.45993800	-0.62181300	4.49272700
H	-2.73216700	-4.21472800	0.65190000
H	-1.29262500	-5.25765800	0.46525500
H	-1.27268100	-3.57291900	-0.12217500
H	-3.19419200	2.62652700	-4.12185400
H	-2.68425800	4.86324400	-3.15204000
H	-2.48720700	5.13043900	-0.68187500
H	-2.95654300	2.28714800	1.76302500
H	-3.58590700	5.28853200	1.37796300
H	-3.70387000	4.36440700	2.89915500
H	-4.80266500	3.99472700	1.53824200
H	-0.55909100	2.92070900	1.36107000
H	-1.22915800	3.78625200	2.77525400
H	-1.02445800	4.63331600	1.21613600
H	-3.86394700	-0.44198300	-2.02163000
H	-2.58040700	-1.33820800	-3.97389800
H	-1.50985600	-0.46656100	-2.84196900
H	-2.01268600	0.31350800	-4.36810400
H	-4.57020900	0.93295200	-4.69918900
H	-5.68988600	0.73709700	-3.32589800
H	-5.04664400	-0.70066500	-4.17276600

[(^{DippXyl}Nacnac)$_2$Mg] (BP86)

E_{el} = -2365.003372

H_{corr}= 1.083366

G_{corr}= 0.930108

ΔGsol= -0.03529797

C	1.16568700	-3.57032000	2.98555300
N	-0.86365800	0.38213700	1.67664000
Mg	-0.01807100	-0.61737300	-0.03213600
C	0.65168300	-2.29805800	2.31230000
N	1.25301600	-1.84648400	1.18791100
N	-1.39136000	-1.74592200	-1.25376200
C	-0.44513700	-1.67450600	2.94940800
N	0.86429800	0.35899200	-1.72613000
C	-0.98225900	-0.36393100	2.78925500
C	2.91329700	-3.22967300	-0.05786300
C	2.60000800	-2.30558000	0.97807000
C	-1.66824300	0.17002000	4.04727000
C	4.25153100	-3.63245700	-0.23632900
C	5.27453100	-3.15777100	0.59426600
C	4.95702200	-2.26806500	1.62831300
C	3.63486000	-1.82986100	1.83697400
C	3.34433900	-0.87003900	2.97196600
C	1.83651500	-3.82795700	-0.93040500
C	-2.69996000	2.05446300	1.45210600
C	-1.33892700	1.74821100	1.76526800
C	-0.96659800	4.07537600	2.39781200
C	-2.31013700	4.37348100	2.15418500
C	-3.15735900	3.36936500	1.67037600
C	-0.45451600	2.77590700	2.20731900
C	1.02599500	2.52538100	2.50267800
C	1.32806100	2.55480500	4.01964100
C	1.93454600	3.53592300	1.76824200
C	-3.67021000	1.00276100	0.90244100
C	-4.72315400	1.60673300	-0.05161000
C	-4.41167000	0.20427100	2.00362100
C	-1.57246500	-3.30382200	-3.18701700
C	-0.90001000	-2.15157200	-2.44319100
C	0.21335400	-1.57398400	-3.10105700
C	0.91097800	-0.35680400	-2.86823600
C	1.75466100	0.12211800	-4.04658500
C	-2.74136300	-2.16467600	-0.96905500
C	-3.01891000	-3.22532400	-0.06526200
C	-4.36085400	-3.58060800	0.18004100
C	-5.41921100	-2.92790000	-0.46342300
C	-5.13689100	-1.90357300	-1.37755800
C	-3.81191400	-1.50784800	-1.64328300
C	-3.54096400	-0.40697000	-2.64548200
C	-1.90821000	-4.01035000	0.59038500
C	1.46079500	1.68059000	-1.77473400

C	2.86135400	1.87990400	-1.58747300
C	3.38478800	3.18175500	-1.73136700
C	2.56990400	4.27422600	-2.03655100
C	1.19211700	4.07650300	-2.18304900
C	0.61381200	2.79850600	-2.05607700
C	-0.89102100	2.63521000	-2.28560900
C	-1.20576400	2.36907200	-3.77807100
C	-1.71408200	3.83950000	-1.78420800
C	3.83889000	0.76345300	-1.20997700
C	4.43419400	1.03269500	0.19083200
C	4.99962100	0.60100900	-2.22067300
H	2.06102600	-3.37869600	3.60344700
H	1.45241700	-4.32675500	2.23498800
H	0.39157500	-3.99665600	3.64432000
H	-0.80423200	-2.19792700	3.84120600
H	-2.22847300	-0.64005300	4.54479300
H	-2.34838000	1.01062700	3.85244100
H	-0.90399000	0.51764600	4.76633300
H	4.48198100	-4.35177500	-1.03215400
H	6.30883200	-3.48719100	0.44369600
H	5.74723500	-1.89460800	2.29195700
H	2.96080400	-1.38878200	3.87201500
H	2.57670700	-0.13013500	2.69133700
H	4.26032900	-0.33287200	3.27279500
H	0.96878000	-4.15775800	-0.33297900
H	2.22604400	-4.69918800	-1.48593900
H	1.45201000	-3.10474400	-1.67444900
H	-0.29512000	4.86466000	2.75495700
H	-2.69357600	5.38627500	2.32346200
H	-4.20192000	3.61315100	1.45240200
H	1.27035200	1.51411700	2.12853100
H	2.40229900	2.36906300	4.20356600
H	0.75285600	1.79200800	4.57101000
H	1.07718300	3.54179600	4.45072200
H	2.99692400	3.27263200	1.91797000
H	1.79432000	4.56222300	2.15550600
H	1.73527000	3.55119800	0.68419200
H	-3.07158500	0.27025800	0.32789800
H	-4.26601800	2.24575300	-0.82679900
H	-5.46873400	2.21471800	0.49341300
H	-5.27404300	0.79207000	-0.55128200
H	-3.72597300	-0.40266400	2.61409900
H	-5.13586100	-0.48630000	1.53581500
H	-4.96643700	0.88568200	2.67624400

H	-0.92490600	-3.67615700	-3.99679100
H	-2.53260900	-2.99410400	-3.63715200
H	-1.80072000	-4.13847700	-2.50190900
H	0.48396900	-2.06882800	-4.03802900
H	1.60872500	1.19699300	-4.24156900
H	1.50780200	-0.43934400	-4.96111000
H	2.82907000	-0.01885400	-3.83738300
H	-4.56750300	-4.40260800	0.87653500
H	-6.45540900	-3.22494200	-0.26622000
H	-5.95540300	-1.39889200	-1.90604200
H	-2.93881900	0.40454800	-2.20051600
H	-4.48554300	0.02612900	-3.01618100
H	-2.96853000	-0.76578900	-3.52057900
H	-1.18609100	-4.38982000	-0.15492200
H	-2.31516700	-4.87530100	1.14274700
H	-1.33966600	-3.38881800	1.30482600
H	4.46196900	3.33612500	-1.59878000
H	3.00129400	5.27548900	-2.14915500
H	0.54935200	4.93391900	-2.40772700
H	-1.21511800	1.74459700	-1.71348100
H	-0.82588000	3.19636600	-4.40642900
H	-2.29768200	2.29624200	-3.93602000
H	-0.75096000	1.42966900	-4.13382400
H	-1.47381900	4.09480400	-0.73853900
H	-2.79199800	3.60408800	-1.83835900
H	-1.55315400	4.73771500	-2.40910800
H	3.28210100	-0.19039000	-1.16777600
H	5.12260000	0.22053400	0.47987700
H	3.64358600	1.10081200	0.95588600
H	4.99740300	1.98434700	0.20241700
H	5.65796100	1.48940600	-2.22157700
H	4.64730600	0.45474000	-3.25615600
H	5.61773800	-0.27208100	-1.94449900

$[(^{Ar}Nacnac)Mg]_2$ (BP86)
E_{el} = -4256.803835
H_{corr}= 1.635554
G_{corr}= 1.390319
ΔGsol= -0.08400169

Mg	4.50657700	10.30888100	10.76383500
C	0.69808300	12.34622600	11.88641400
H	0.27700900	13.24821500	11.41460700
H	0.67756500	12.48926700	12.98168700

H	0.03765900	11.48972100	11.66589200
N	2.75901100	10.95991100	11.76109100
N	4.98455400	12.31275800	10.25928500
C	2.11962100	12.09172500	11.40017100
C	4.03753400	13.26771600	10.15999200
C	2.70244900	13.11326400	10.61161300
H	2.04567900	13.96132000	10.40067900
C	2.10370000	10.10773100	12.71466400
C	4.38474200	14.62510400	9.56234300
H	4.87256600	14.52847800	8.57737400
H	5.09544300	15.16056000	10.21759000
H	3.48372000	15.24882700	9.45064700
C	1.23804700	9.07833600	12.24872600
C	0.57786600	8.26798700	13.18600500
H	-0.09765400	7.48549000	12.81833700
C	0.76451900	8.42293000	14.57285600
C	1.66365800	9.40900300	15.00594200
H	1.85288600	9.51495100	16.08041000
C	2.33577600	10.26306100	14.10880000
C	1.02702100	8.85768600	10.76645500
H	0.56952100	9.73419200	10.26950800
H	0.37928600	7.98411900	10.58499600
H	1.98801800	8.66878000	10.24830900
C	0.00746000	7.56446300	15.56552800
H	-0.12894700	6.53387900	15.19170900
H	-1.00327400	7.97192100	15.76243300
H	0.53096300	7.50934600	16.53615300
C	3.29395000	11.34131200	14.64350300
H	3.75973700	11.79532900	13.74639600
C	2.53714500	12.47908600	15.34801100
C	2.00538000	12.33497100	16.64823500
H	2.16671300	11.40283300	17.20046600
C	1.11046700	14.59976200	16.58706500
H	0.55859800	15.41628500	17.06633600
C	1.29801400	13.38035400	17.25993000
H	0.89616000	13.24297000	18.27057200
C	1.64591600	14.76406500	15.30084000
H	1.51787600	15.71246800	14.76616400
C	2.35432800	13.71373200	14.69085000
H	2.77350800	13.85551500	13.68677500
C	4.45056400	10.76828600	15.48733000
C	5.15224100	11.58572900	16.40000400
H	4.82066800	12.61629200	16.56625900
C	6.26072400	11.09590700	17.10810600

H	6.78506800	11.75288400	17.81150800
C	6.69496800	9.77442100	16.91988000
H	7.55679600	9.39010000	17.47692100
C	6.01204400	8.95240800	16.01030400
H	6.33778500	7.91772000	15.85004600
C	4.90381300	9.44514900	15.30163600
H	4.37586800	8.79010000	14.60146200
C	6.30573400	12.62797300	9.78961900
C	7.32478000	13.06300300	10.68258400
C	8.60002100	13.36265500	10.16631300
H	9.38674100	13.67711000	10.86336100
C	8.89635400	13.26600100	8.79561000
C	7.88437900	12.80053200	7.93824900
H	8.09596900	12.68764400	6.86722400
C	6.60456100	12.45928900	8.40990700
C	5.55868400	11.92577100	7.45523500
H	4.68373700	12.59664800	7.36379100
H	5.16679000	10.94867100	7.80116200
H	5.98592500	11.78426000	6.44799100
C	10.27202600	13.62598500	8.27148400
H	11.03173100	12.87642800	8.56607900
H	10.61612700	14.59904400	8.66729500
H	10.27932700	13.68983800	7.16939600
C	7.04355400	13.23457900	12.18191400
H	6.16645700	12.59785300	12.40672000
C	6.64149300	14.66414200	12.57848300
C	7.09281700	15.80841300	11.88956400
H	7.72696900	15.68910200	11.00405600
C	6.72863800	17.09762700	12.31769800
H	7.09215900	17.97288000	11.76654000
C	5.90132600	17.26502800	13.43869400
H	5.61377500	18.26974100	13.76882000
C	5.44314000	16.13204800	14.13264200
H	4.79009800	16.24349200	15.00572600
C	5.81371000	14.84823500	13.70657700
H	5.46181600	13.97029100	14.26181500
C	8.20335200	12.70134500	13.03937500
C	9.20102300	13.54151800	13.57301600
H	9.13333600	14.62455200	13.42014900
C	10.26883400	13.00762600	14.31439800
H	11.03461400	13.67903800	14.72040300
C	9.35351500	10.77993900	14.02945800
H	9.39402700	9.70102700	14.21725100
C	8.29307100	11.31507400	13.28405700

H	7.51733100	10.64720100	12.88717300
Mg	5.64478600	7.64488000	10.10443800
C	9.45357900	5.60751600	8.98269100
H	9.87476600	4.70582600	9.45496600
H	9.47403900	5.46387900	7.88749300
H	10.11390500	6.46421800	9.20271800
N	7.39263600	6.99383100	9.10771800
N	5.16683700	5.64096900	10.60903300
C	8.03201300	5.86208100	9.46882300
C	6.11392900	4.68612900	10.70876600
C	7.44910200	4.84061600	10.25742500
H	8.10589200	3.99263800	10.46861000
C	8.04791100	7.84599000	8.15411600
C	5.76669700	3.32884600	11.30663000
H	5.27858400	3.42566800	12.29143600
H	5.05624500	2.79314800	10.65131000
H	6.66775600	2.70525300	11.41874500
C	8.91349400	8.87547500	8.61997300
C	9.57351300	9.68589100	7.68263700
H	10.24904000	10.46839700	8.05027100
C	9.38666000	9.53101800	6.29581100
C	8.48752200	8.54491000	5.86280600
H	8.29800700	8.43911300	4.78837300
C	7.81569800	7.69068600	6.76000400
C	9.12449700	9.09621200	10.10222900
H	9.58179600	8.21968300	10.59930600
H	9.77234400	9.96970100	10.28365600
H	8.16346800	9.28532700	10.62024700
C	10.14348800	10.38958100	5.30304900
H	10.28048500	11.41996900	5.67717300
H	11.15395900	9.98180800	5.10543000
H	9.61948600	10.44524300	4.33272000
C	6.85764400	6.61229300	6.22539100
H	6.39176900	6.15842800	7.12253600
C	7.61460000	5.47440800	5.52122400
C	8.14705300	5.61847100	4.22127400
H	7.98625600	6.55068400	3.66902200
C	9.04148700	3.35350400	4.28279500
H	9.59343600	2.53689000	3.80376700
C	8.85449700	4.57296600	3.60987600
H	9.25687700	4.71032000	2.59944000
C	8.50541000	3.18927300	5.56876800
H	8.63304400	2.24084500	6.10349400
C	7.79688900	4.23971800	6.17844200

H	7.37724100	4.09800600	7.18233000
C	5.70113500	7.18526200	5.38141800
C	5.00051300	6.36841000	4.46742600
H	5.33280500	5.33823300	4.30024400
C	3.45692400	8.17931300	3.94866600
H	2.59518300	8.56372300	3.39155300
C	4.13877000	9.00072200	4.85961400
H	3.81224000	10.03500300	5.02088700
C	5.24689100	8.50790000	5.56837200
H	5.77385200	9.16254600	6.26968900
C	3.84555900	5.32575200	11.07840800
C	2.82677300	4.89044300	10.18527300
C	1.55140400	4.59084400	10.70125800
H	0.76491800	4.27616100	10.00405000
C	1.25466000	4.68787600	12.07184700
C	2.26637600	5.15360100	12.92936200
H	2.05445600	5.26681400	14.00028900
C	3.54632900	5.49475400	12.45799400
C	4.59184400	6.02859600	13.41286800
H	5.46618100	5.35712900	13.50596200
H	4.98487800	7.00491900	13.06607800
H	4.16384100	6.17170500	14.41956300
C	-0.12115600	4.32805300	12.59569600
H	-0.88101300	5.07684600	12.29958200
H	-0.46463300	3.35429400	12.20108200
H	-0.12904700	4.26577100	13.69786000
C	3.10835300	4.71854400	8.68604800
H	3.98552800	5.35519700	8.46131400
C	3.51043900	3.28889200	8.28983300
C	3.05931300	2.14478900	8.97916000
H	2.42525800	2.26432500	9.86470800
C	3.42352600	0.85548000	8.55134700
H	3.06016000	-0.01964100	9.10282000
C	4.25066200	0.68780800	7.43026100
H	4.53822700	-0.31698400	7.10039200
C	4.70862600	1.82062100	6.73589500
H	5.36151200	1.70897900	5.86271800
C	4.33803300	3.10453200	7.16164100
H	4.68975600	3.98233200	6.60606300
C	1.94873900	5.25162900	7.82824800
C	0.95128100	4.41131900	7.29442000
H	1.01904900	3.32830100	7.44736600
C	-0.11641900	4.94504900	6.55276800
H	-0.88203700	4.27353500	6.14662300

C	0.79858400	7.17285100	6.83780700
H	0.75800000	8.25174800	6.64994700
C	1.85892000	6.63787700	7.58347500
H	2.63449600	7.30585500	7.98049700
C	10.35078700	11.62567000	14.54399700
H	11.17978100	11.21051800	15.12854900
C	-0.19847900	6.32698600	6.32308600
H	-1.02738700	6.74202000	5.73833200
C	3.89212600	6.85833000	3.75921900
H	3.36862700	6.20180100	3.05476700

[(^{Ar}Nacnac)$_2$Mg] (BP86)

E_{el} = -4056.671128

H_{corr}= 1.633744

G_{corr}= 1.399914

ΔGsol= -0.07245593

C	3.78943300	11.60465900	8.42759000
H	4.46751800	12.47257400	8.42332400
H	2.77512600	11.96793200	8.67050200
H	3.74337800	11.18109400	7.40934500
N	3.72339500	9.31898700	9.42734500
N	5.45046800	9.20886000	11.99444500
C	4.24900800	10.56622200	9.44409300
C	5.69537100	10.47452700	11.58857900
C	5.23447200	11.01951700	10.36364700
H	5.61013200	12.02364500	10.15113700
C	2.64082300	9.09861200	8.49619100
C	6.54892800	11.39300900	12.45425300
H	7.46523800	10.87197500	12.78429800
H	6.01281200	11.71067100	13.36271000
H	6.83534300	12.30183800	11.90150400
C	2.95940600	8.58889700	7.20533100
C	1.96124100	8.47094600	6.22666400
H	2.24184900	8.09308300	5.23507000
C	0.62232400	8.81655100	6.48391000
C	0.30691400	9.22831400	7.78570800
H	-0.73975800	9.43673300	8.03994600
C	1.28086200	9.38337500	8.79862000
C	4.37451100	8.20478500	6.86684400
H	5.07048800	9.06334600	6.90724800
H	4.42438100	7.77132100	5.85669000
H	4.78043300	7.44940600	7.56652900
C	-0.42929900	8.73736400	5.39707800

H	-0.35874000	7.78814000	4.83599000
H	-0.31108900	9.55708600	4.66220100
H	-1.44864000	8.81416700	5.81409900
C	0.80348800	9.83649900	10.18367900
H	1.63477300	9.63581300	10.88795800
C	0.48107000	11.33644400	10.29702700
C	0.35847800	11.90235400	11.58592500
H	0.51387200	11.26688500	12.46642900
C	-0.20381500	14.07227800	10.63530100
H	-0.46768900	15.12803500	10.76538200
C	0.01982900	13.25346000	11.75544700
H	-0.06550500	13.66575900	12.76720100
C	-0.09042200	13.52286500	9.34984500
H	-0.26604000	14.14789200	8.46642200
C	0.24515200	12.16690700	9.18300700
H	0.32175600	11.74939500	8.17351600
C	-0.38968300	8.96018900	10.62575200
C	-1.69598100	9.46747400	10.76957900
H	-1.88356900	10.53337700	10.60634100
C	-2.76246800	8.62367400	11.12680500
H	-3.77017400	9.04265700	11.23153700
C	-2.54094100	7.25662900	11.34661200
H	-3.37212300	6.59752000	11.62260700
C	-1.24114900	6.73892200	11.20585800
H	-1.04677300	5.67350500	11.36561500
C	-0.17922100	7.58221900	10.84888700
H	0.82598900	7.15957500	10.72854800
C	5.60833600	8.91793200	13.39995600
C	4.60655600	9.30255700	14.34797400
C	4.69957500	8.83599200	15.67435800
H	3.89050000	9.08457600	16.37202500
C	5.77246000	8.05402100	16.13041800
C	6.79081900	7.76268600	15.20934400
H	7.66885300	7.19185500	15.54041400
C	6.73030200	8.17354500	13.86535200
C	7.88693900	7.83669000	12.95545200
H	8.31514200	8.73954300	12.48520500
H	7.59145600	7.15358300	12.13843700
H	8.69282000	7.34003300	13.52389900
C	5.82398300	7.53843100	17.55348300
H	5.40223000	6.51718600	17.62858600
H	5.24336500	8.18044300	18.23886800
H	6.86161500	7.48801400	17.92937800
C	3.44967000	10.25024300	13.98160600

H	3.32159000	10.18777900	12.88475500
C	3.76797900	11.72330800	14.30512800
C	3.32277700	12.73405300	13.42793300
H	2.79080900	12.45560900	12.51177800
C	3.55751900	14.08958300	13.70523500
H	3.20417600	14.85281900	13.00219800
C	4.24386800	14.46491000	14.87175300
H	4.43037400	15.52280200	15.08918300
C	4.69687500	13.46977700	15.75200200
H	5.24198100	13.74659200	16.66204700
C	4.46427300	12.11282000	15.46964900
H	4.84970800	11.34575800	16.14995300
C	2.10789200	9.82395500	14.60953100
C	1.62425200	10.36694800	15.81842300
H	2.19725500	11.14948700	16.32738300
C	0.40523100	9.93472300	16.36738500
H	0.05239300	10.37227100	17.30878600
C	0.09514600	8.42602400	14.49620100
H	-0.50399800	7.68961900	13.94970400
C	1.32011000	8.85063000	13.95917200
H	1.66646500	8.42137500	13.01224200
Mg	5.16381400	7.93926100	10.20951600
C	9.28042600	6.59067400	9.57415200
H	9.70995400	5.60950000	9.82687100
H	9.65261300	6.88499700	8.58208600
H	9.66141100	7.33323500	10.30228700
N	7.03560200	7.55489500	9.06919600
N	4.76618700	5.83597100	10.42644100
C	7.75684200	6.57121900	9.64846200
C	5.87427200	5.10697100	10.69416500
C	7.20819500	5.51238600	10.41865000
H	7.96341300	4.82929100	10.81564200
C	7.71537900	8.36261200	8.07559500
C	5.74849400	3.73829300	11.35463000
H	5.12332500	3.77911000	12.26303400
H	5.26843100	3.01800100	10.66929200
H	6.73940400	3.34183200	11.62520700
C	8.29642300	9.61276500	8.42930500
C	8.86971000	10.43226200	7.43882200
H	9.29733400	11.39702000	7.74485200
C	8.95112000	10.03773700	6.09686200
C	8.46056300	8.76153300	5.77503200
H	8.55561200	8.41164700	4.74060700
C	7.84443000	7.91360500	6.71804800

C	8.44765200	10.04729500	9.86817700
H	9.49062600	9.87996700	10.20408500
H	8.23470200	11.12232600	9.99239500
H	7.78880500	9.48318400	10.54047500
C	9.54726700	10.94142200	5.03804600
H	10.35328300	11.57357500	5.45118700
H	9.96587600	10.35973700	4.19785200
H	8.78528300	11.62375200	4.61335200
C	7.46589200	6.48527600	6.29220400
H	6.68690600	6.13849600	6.99962000
C	8.66449900	5.52792900	6.47020000
C	9.90682300	5.78123300	5.85064000
H	10.04275900	6.69570600	5.26384300
C	10.82334400	3.70413600	6.73479000
H	11.65854400	3.00187600	6.83692500
C	10.97565300	4.88234500	5.98355600
H	11.93216800	5.10286800	5.49542500
C	9.59226500	3.43830300	7.35290400
H	9.45469700	2.52425400	7.94225200
C	8.52479700	4.34415400	7.22170900
H	7.57261500	4.13096300	7.71944400
C	6.87256800	6.33147900	4.86699100
C	6.88840000	5.06255000	4.24454000
H	7.38735700	4.22614400	4.74481900
C	5.66995300	5.91216500	2.31518900
H	5.20973600	5.75246000	1.33364300
C	5.65127300	7.18113600	2.91226800
H	5.17616400	8.02507500	2.39837700
C	6.24247300	7.38629500	4.17058000
H	6.21949700	8.38700700	4.61042100
C	3.50614500	5.20080600	10.75225200
C	2.77579900	4.41516500	9.81655900
C	1.60473400	3.75351500	10.24789700
H	1.04596000	3.16152400	9.51359100
C	1.12791400	3.83076200	11.56485600
C	1.83218200	4.65664900	12.45844300
H	1.47325900	4.76962200	13.48989500
C	2.99889300	5.34061300	12.07792600
C	3.72112400	6.19314800	13.08986300
H	4.75165600	5.84320600	13.28501800
H	3.81660900	7.23646700	12.74528600
H	3.18153900	6.21591100	14.05074400
C	-0.08183900	3.03530800	12.01236800
H	-0.66351400	3.57437800	12.78162900

H	-0.75542200	2.80968300	11.16712300
H	0.21811100	2.06664800	12.45771900
C	3.22161300	4.21945000	8.35877300
H	3.84118300	5.09814500	8.09106200
C	4.10560800	2.97917300	8.15540400
C	3.91523000	1.78802200	8.88711900
H	3.15591100	1.75801000	9.67610500
C	4.68747500	0.64466500	8.62148100
H	4.52177600	-0.26786300	9.20602800
C	5.66398200	0.66815600	7.61313800
H	6.26599400	-0.22343900	7.40419300
C	5.85922400	1.84510700	6.87231400
H	6.61777200	1.87873400	6.08221400
C	5.08743300	2.98702300	7.14288100
H	5.23280000	3.89306400	6.54140600
C	2.00292100	4.20308800	7.40555300
C	1.75437600	3.15078100	6.50210400
H	2.45149800	2.30977600	6.44015500
C	0.61410300	3.15819100	5.67886000
H	0.44444200	2.32504700	4.98669100
C	-0.06472000	5.27206600	6.64511100
H	-0.77225900	6.10431800	6.72142700
C	1.07842900	5.26938200	7.45588300
H	1.24346600	6.09867900	8.15252400
C	-0.36490400	8.96355000	15.70939800
H	-1.32282600	8.63786900	16.13064700
C	-0.30469200	4.21434500	5.75115900
H	-1.20106500	4.21459100	5.12018800
C	6.29284100	4.85207600	2.99123900
H	6.32343500	3.85320900	2.54078900

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