*Supporting Information*

# Reduction of *tert*-butylphosphaalkyne and trimethylsilylnitrile with magnesium(I) dimers

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## Contents

## 1. Experimental

### 1.1. General considerations

All manipulations were carried out using standard Schlenk and glove box techniques under an atmosphere of high purity dinitrogen. Hexane and toluene were distilled over molten potassium. NMR spectra were acquired on a Bruker AVIII 500 MHz NMR spectrometer ($^{1}$H 500 MHz, $^{13}$C 126 MHz), Bruker AVIII 400 MHz NMR spectrometer ($^{1}$H 400 MHz, $^{31}$P 162 MHz), Bruker DPX300, or Bruker AvanceIII 400 spectrometers ($^{1}$H, $^{13}$C{$^{1}$H}, and $^{29}$Si{$^{1}$H}). NMR spectra were referenced to the resonances of the solvent used, or to external 85% $H_3PO_4$ ($^{31}$P) or trimethylsilane ($^{29}$Si). Mass spectra were recorded on an Agilent Technologies 5975D inert MSD with a solid state probe. IR spectra were recorded as Nujol mulls, using an Agilent Cary 630 spectrometer operating in attenuated total reflectance (ATR) or transmission modes. Melting points were determined in sealed glass capillaries under dinitrogen and are uncorrected.

Hexane (hex; Sigma Aldrich, HPLC grade), toluene (Sigma Aldrich, HPLC grade), benzene (Sigma aldrich, HPLC grade) were purified using an MBraun SPS-800 solvent system. THF and $Et_2O$ (Sigma Aldrich) were distilled over Na/benzophenone. $C_6D_6$ (Aldrich, 99.5%) was dried over a sodium mirror and degassed before use. All solvents were stored over 3 Å molecular sieves, under an $N_2$ atmosphere, in gas-tight ampoules.

The compounds [{($^{Ar}$L)Mg–}$_2$] (Ar = Xyl, Mes, or Dipp) and $^{t}$BuCP were prepared by literature procedures.[1-4] $Me_3SiCN$ was stored in a J. Young ampuole under nitrogen, its purity confirmed by NMR spectroscopy. Benzaldehyde and acetophenone (Sigma Aldrich) were dried using 3 Å mol sieves. All other reagents were used as received.

## 1.2. Compound synthesis

### 1.2.1. Synthesis of [{$^{Mes}$LMg}$_2${PC($^t$Bu)}], 1

A solution of $^t$BuCP (15 mg, 0.15 mmol) in toluene (1 mL) was added to a suspension of [$^{Mes}$LMg]$_2$ (132 mg, 0.15 mmol) in toluene (1 mL) at room temperature. The reaction mixture was stirred for 1 hour. The volatiles were removed under reduced pressure, and the resulting orange oil taken up into hexane (*ca.* 2 mL). The solution was filtered, and the hexane concentrated to 0.5 mL. Cooling the solution to –35 °C overnight yielded light pink crystals of **1** (110 mg, 75%).

**Elemental analysis** calcd. for $C_{63}H_{91}Mg_2N_4P$: C, 76.90; H, 9.32; N, 5.69; Found: C, 75.90; H, 9.91; N, 5.37.

**$^1$H NMR** (500 MHz, $C_6D_6$) δ = 7.09–7.04 (m, 12H, Ar*H*), 4.89 (s, 1H, NCC*H*), 4.84 (s, 1H, NCC*H*), 3.31 (sept, $^3J_{H–H}$ = 6.8 Hz, 4H, methine C*H*), 3.09 (p, $^3J_{H–H}$ = 6.8 Hz, 4H, methine C*H*), 1.69 (s, 6H, C$H_3$), 1.61 (s, 6H, C$H_3$), 1.1–1.25 (m, 48H, *iso*propyl C$H_3$), 0.65 (s, 9H, *tert*butyl $CH_3$).

**$^{13}$C NMR** (126 MHz, $C_6D_6$) δ = 169.50 (NC$CH_3$), 168.80 (NC$CH_3$), 145.15 (Ar*C*), 143.70 (Ar*C*), 142.02 (Ar*C*), 141.85 (Ar*C*), 125.63 (Ar*C*), 124.79 (Ar*C*), 123.86 (Ar*C*), 123.66 (br, possibly *C*=P) 123.35 (Ar*C*), 95.53 (nacnac α-*C*), 94.59 (nacnac α-*C*), 44.87 (d, $^2J_{C–P}$ = 20 Hz; *t*Bu*C*$CH_3$), 29.87 (Dipp *C*$(CH_3)_2$), 29.78 (Dipp *C*$(CH_3)_2$), 28.38 (NC*C*$H_3$), 28.29 (NC*C*$H_3$), 24.66 (Dipp C(*C*$H_3)_2$), 24.44 (Dipp C(*C*$H_3)_2$), 24.01 (*t*BuC(*C*$H_3)_3$), 23.81 (Dipp C(*C*$H_3)_2$), 23.65 (Dipp C(*C*$H_3)_2$).

**$^{31}$P{$^1$H} NMR** (162 MHz, $C_6D_6$) δ = 341.5 ppm.

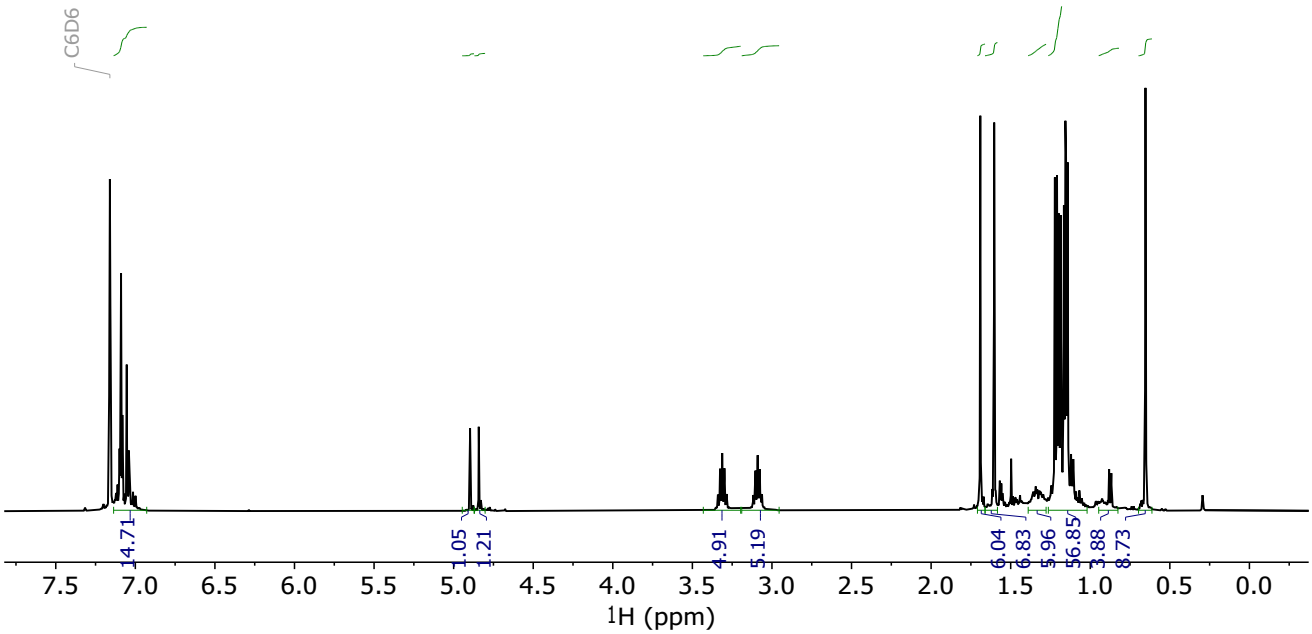



*Figure S 1. $^{1}H$ NMR (500 MHz) spectrum of **1** in $C_6D_6$.*

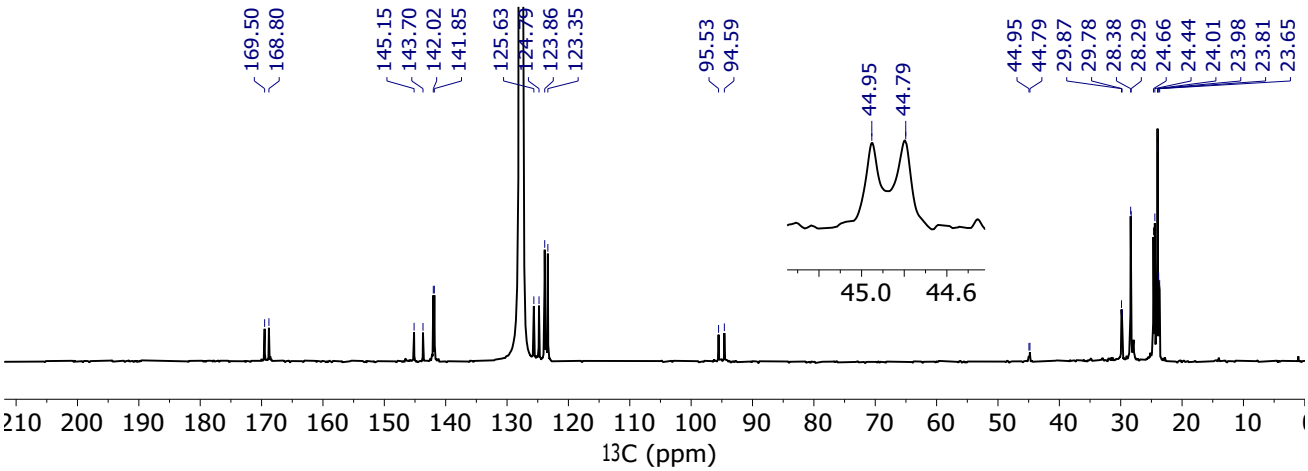



*Figure S 2. $^{13}C\{^{1}H\}$ NMR (126 MHz) spectrum of **1** in $C_6D_6$.*

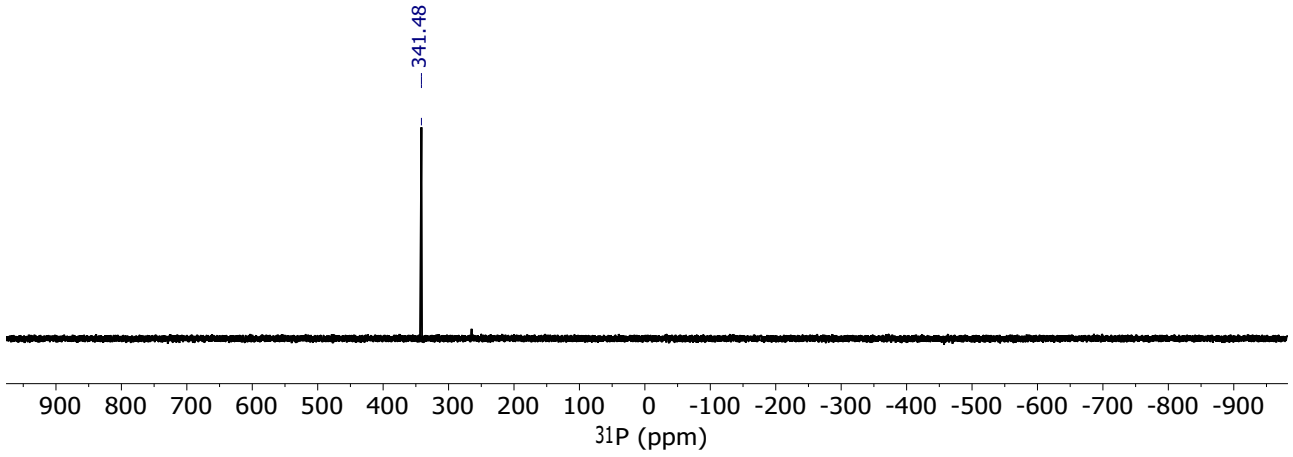



*Figure S 3. $^{31}P\{^{1}H\}$ NMR (162 MHz) spectrum of **1** in $C_6D_6$.*

### 1.2.2. Synthesis of [{$^{Mes}$LMg}$_2${cyclo-$P_2C_2(^tBu)_2$}], 2

A solution of *t*BuCP (21 mg, 0.21 mmol) in toluene (1 mL) was added to a suspension of [$^{Mes}$LMg]$_2$ (70 mg, 0.102 mmol) in toluene (1 mL) at room temperature. The solution immediately darkened from yellow to deep red. The reaction mixture was stirred overnight, filtered and concentrated to 0.5 mL. Cooling the solution to – 35 °C overnight yielded light orange crystals of **2** (48 mg, 53%). The compound was stable in the solid state over a period of weeks, however in solutions of toluene decomposes over days.

**Elemental analysis** calcd. for $C_{56}H_{76}Mg_2N_4P_2$: C, 73.44; H, 8.37; N, 6.12. Found: C, 72.91; H, 8.21; N, 6.02.

**$^1$H NMR** (500 MHz, $C_6D_6$) δ = 6.85 (s, 8H, Ar*H*), 4.82 (s, 2H, NCC*H*), 2.26 (s, 12H, Mes *para*-C$H_3$), 2.25 (s, 24H, Mes *ortho*-C$H_3$), 1.57 (s, 12H, NCC$H_3$), 1.22 (s, 18H, *t*Bu-C$H_3$).

**$^{13}$C NMR** (126 MHz, $C_6D_6$) δ = 168.75 (N*C*CH$_3$), 145.37 (Ar*C*), 138.14 (t, $^1J_{C\text{-}P}$ = 54.8 Hz, {*C*$_2$P$_2$}), 132.75 (Ar*C*), 131.96 (Ar*C*), 128.85 (Ar*C*), 94.57 (nacnac α-*C*), 36.34 (*t*Bu*C*(CH$_3$)$_3$), 32.03 (*t*BuC(*C*H$_3$)$_3$), 23.77 (NC*C*H$_3$), 20.67 (Ar*C*H$_3$), 19.90 (Ar*C*H$_3$).

**$^{31}$P{$^1$H} NMR** (162 MHz, $C_6D_6$) δ = 202.3 (s).

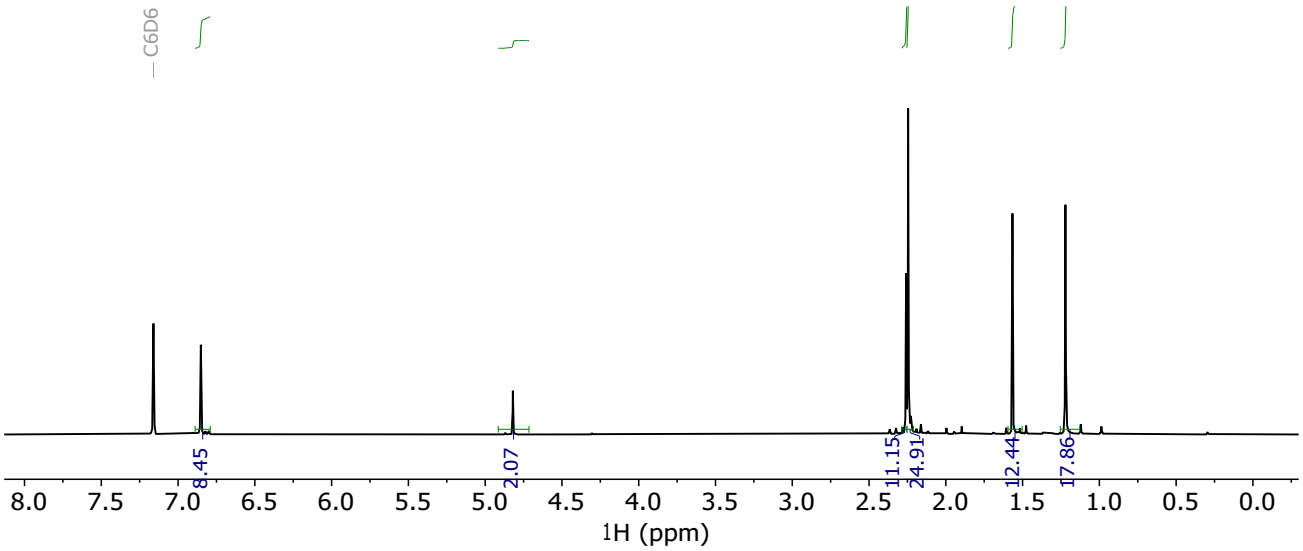



*Figure S 4. $^{1}H$ NMR (500 MHz) spectrum of **2** in $C_6D_6$.*

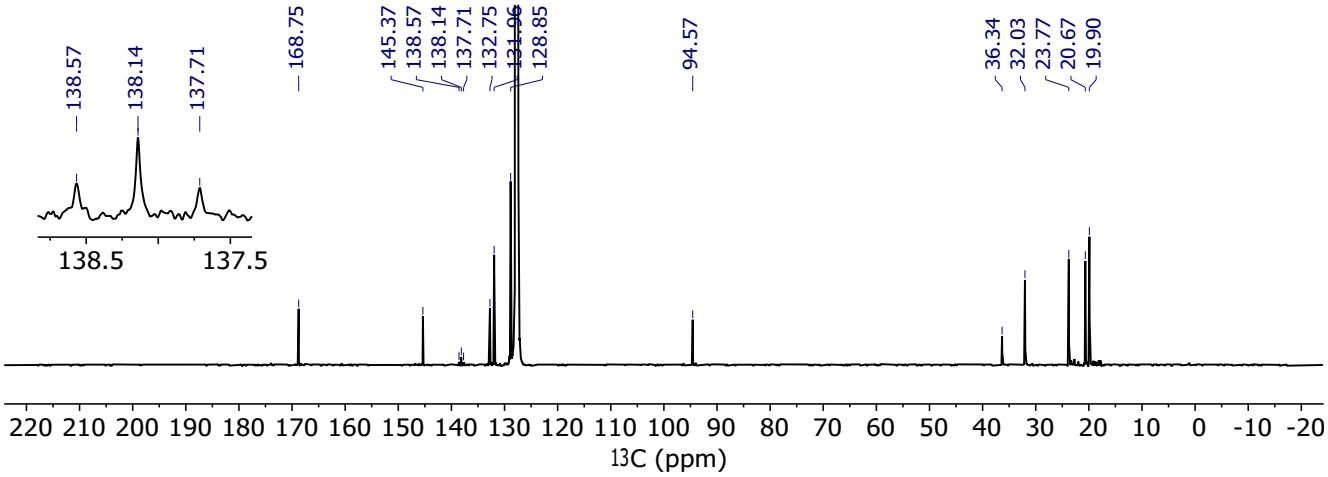



*Figure S 5. $^{13}C\{^{1}H\}$ NMR (126 MHz) spectrum of **2** in $C_6D_6$.*

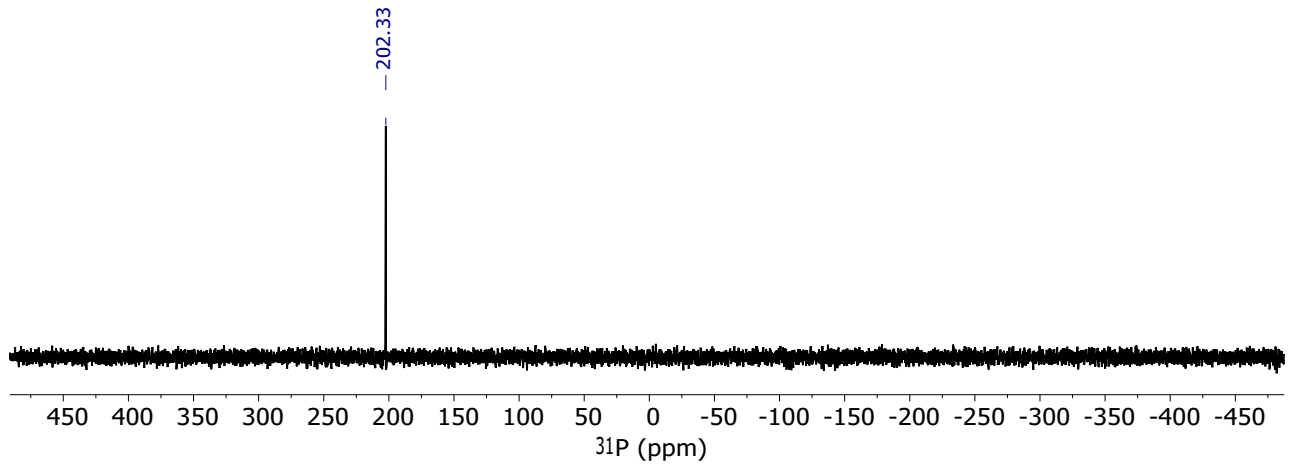



*Figure S 6. $^{31}P\{^{1}H\}$ NMR (162 MHz) spectrum of **2** in $C_6D_6$.*

### 1.2.3. Reaction monitoring during the generation of 2

The procedure outlined in section 1.2.2. was monitored by $^{31}P\{^{1}H\}$ NMR spectroscopy. Two intermediates could be observed during the generation of **2**. A singlet resonance at + 345.9 ppm and an AX spin system with doublets at 382.4 and 287.1 ppm ($J_{P\text{-}P}$ = 304 Hz). When the reaction is conducted at high concentrations colourless crystals form on the walls of the NMR tube. The crystal structure revealed one of the intermediates to be the 8-membered heterocycle **3**. Monitoring the reaction to completions shows complete consumption of the intermediates to leave **2** as the only product in both the $^{31}P$ and $^{1}H$ NMR spectra. Computations allow for the tentative assignment of the observed AX spin system as **A**, in which the steric requirement of the Mes groups prevents equivalence between the two phosphorus sites (See section 3).

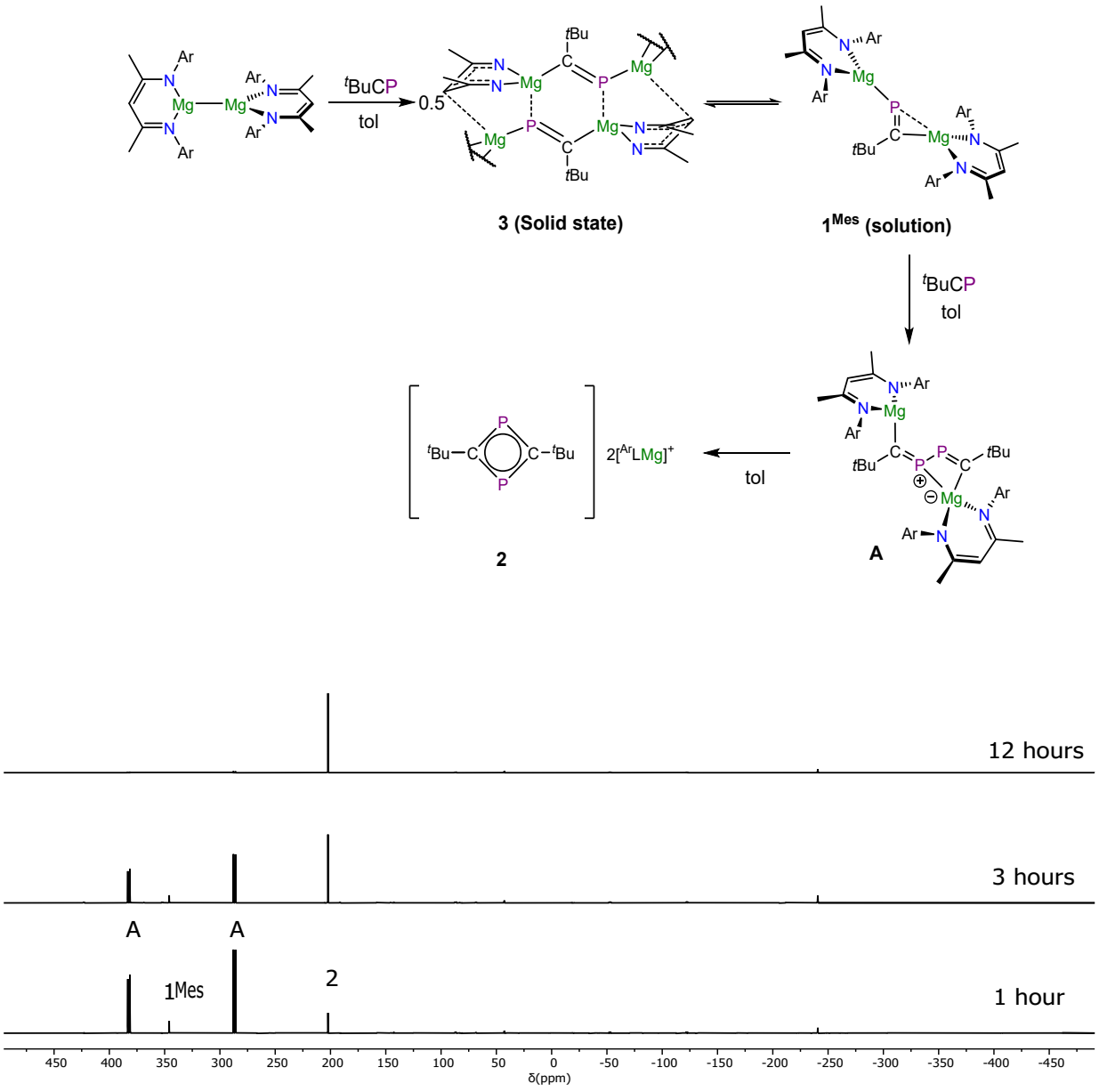



*Figure S 7. Proposed intermediates during conversion of $^{t}$BuCP to **2**. **3** is likely monomeric in solution and assignment of A is based on **6** (see computational section). Some of the ligands are truncated for clarity. Ar = Mes.*

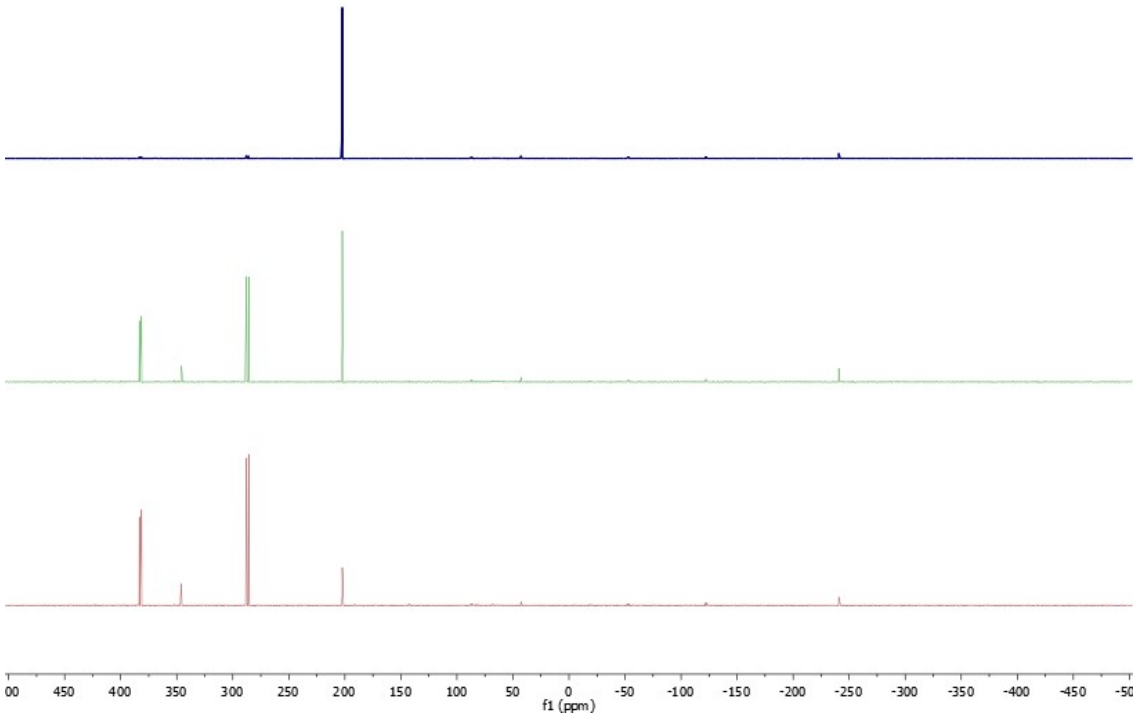



*Figure S 8. Monitoring reaction progress upon addition of $[^{Mes}Mg]_2$ to $^{t}$BuCP. Bottom: 1 hour. Middle: 3 hours. Top: 12 hours.*

### 1.2.4. Detection of proposed species 4, 5, and 6

If instead of toluene, THF is used as the solvent for the procedure outlined in 1.2.2, three new species can be observed in the $^{31}P\{^{1}H\}$ NMR spectrum.

These species are stable in THF over several days, however once the solvent is removed under reduced pressure and replaced with hexane, toluene, or benzene partial conversion to **2** can be observed. Dissolution in $Et_2O$ resulted in more complex mixtures of products. The instability of these species in all but THF made separation and characterisation unfeasible. However, if the solvent was removed immediately and replaced with hexane, followed by cooling to –35°C, red crystals formed. Refinement of the X-ray data indicated positional disorder between proposed products **5** and **6.** NMR spectroscopy performed on the crystals revealed a mixture of products, with the major product displaying the AX spin system.

**$^{31}P\{^{1}H\}$ NMR** (162 MHz, $C_6D_6$:THF) δ = 445.9, 385.8 (d, $J_{P–P}$ = 304), 351.3, 280.2 (d, $J_{P–P}$ = 296 Hz).

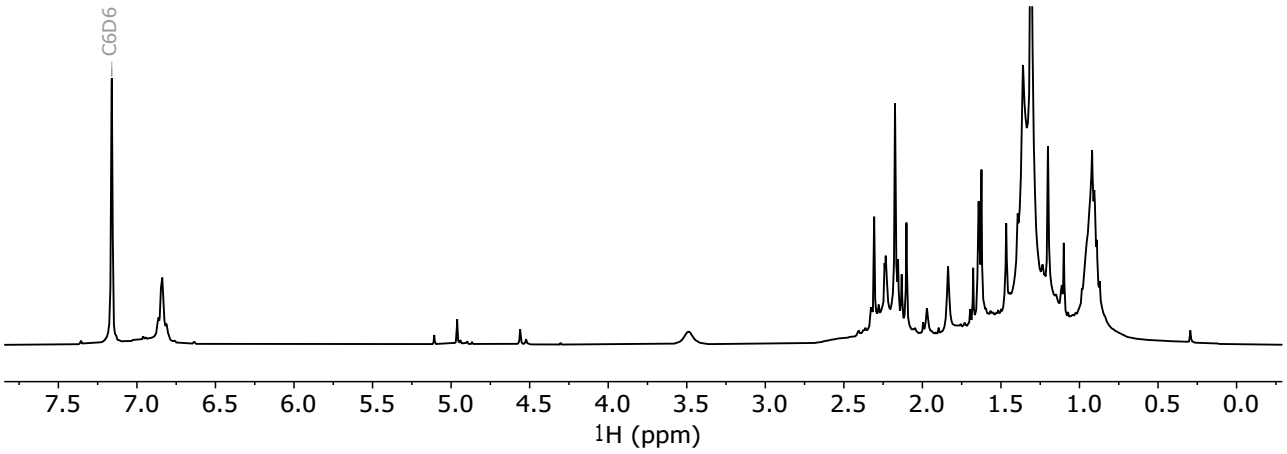



*Figure S 9. $^{1}H$ NMR spectrum (400 MHz) of reaction mixture generated from procedure 1.2.4.*

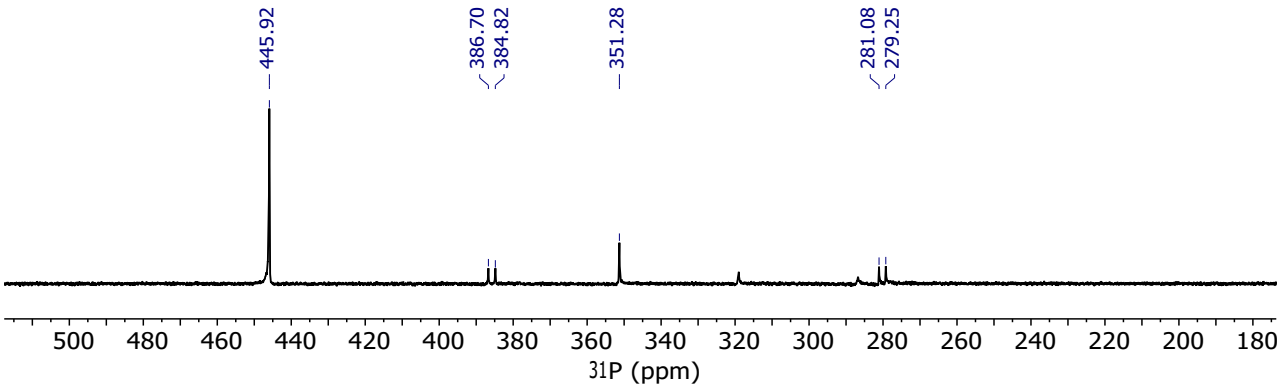



*Figure S 10. $^{31}P\{^{1}H\}$ NMR spectrum (162 MHz) of reaction mixture generated from procedure 1.2.4.*

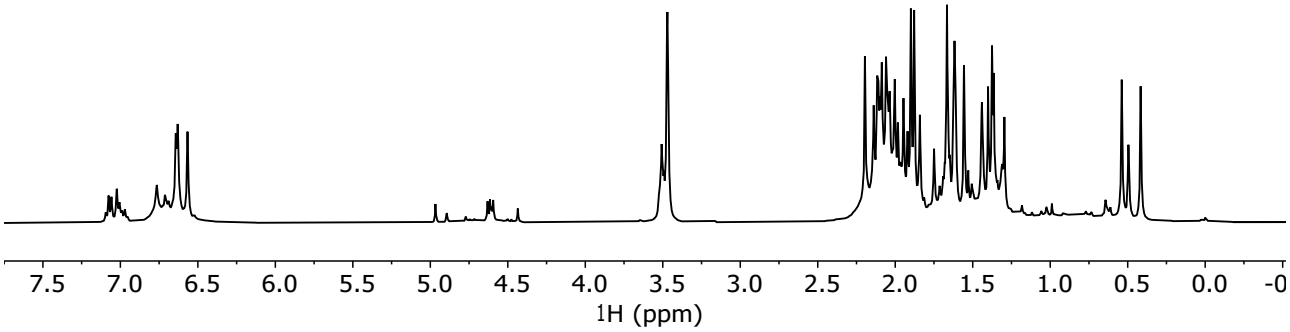



*Figure S 12. $^{1}H$ NMR spectrum (400 MHz) of the crystals containing **5** and **6**.*

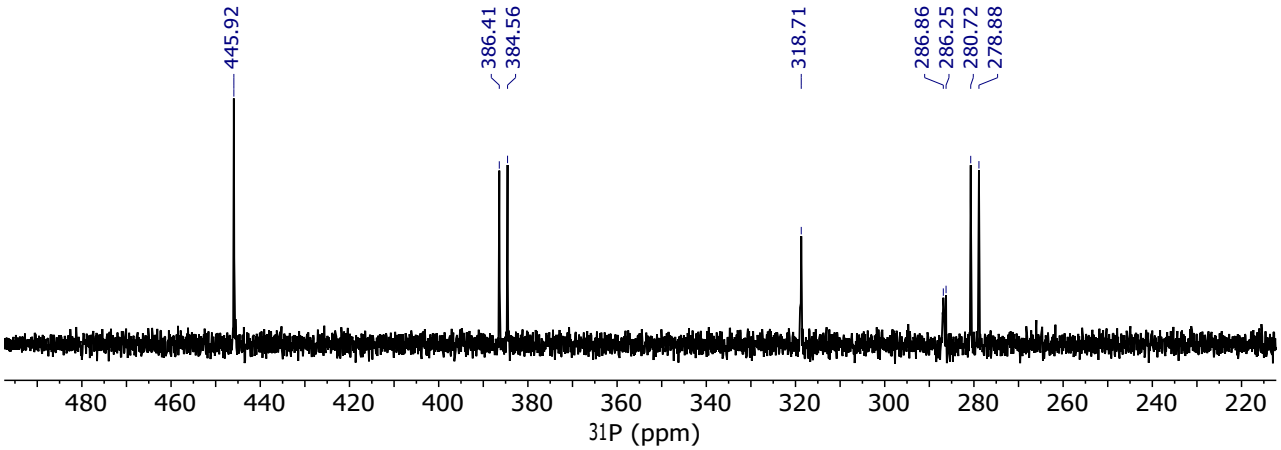



*Figure S 13 . $^{31}P\{^{1}H\}$ NMR spectrum (162 MHz) of crystals containing **5** and **6**.*

1.2.5. Synthesis of [{$^{Mes}$LMg}$_2${μ-(Me$_3$SiN=C-N=CSiMe$_3$)}], 8.

Trimethylsilyl cyanide (19 μl, 0.14 mmol) was added via micro syringe to a solution of [$^{Mes}$LMg]$_2$ (50 mg, 0.06 mmol) disolved in toluene (10 ml) at –78 °C. The resultant solution was allowed to warm to room temperature and stirred overnight. The solution was filtered, concentrated to ca 5 mL and stored at –30 °C, yielding red crystals of **8** (42mg, 65%). **M.p.** 170-173 °C (decomp).

**Elemental analysis** calc'd for $C_{54}H_{76}Mg_2N_6Si_2$: C 70.96 %, H 8.38 %, N 9.19 %. Found: C 70.91 %, H 8.46 %, N 9.12 %.

**$^1$H NMR** (400 MHz, 298 K, $C_6D_6$) δ = 6.96 (s, 4H, Ar*H*), 6.88 (s, 2H, Ar*H*), 6.83 (s, 2H, Ar*H*), 4.88 (s, 1H, NCC*H*), 4.83 (s, 1H, NCC*H*), 2.32 (s, 6H, ArC$H_3$), 2.30 (s, 6H, ArC$H_3$), 2.26 (s, 6H, ArC$H_3$), 2.19 (s, 6H, ArC$H_3$), 2.06 (s, 6H, ArC$H_3$), 1.79 (s, 6H, ArC$H_3$), 1.65 (s, 6H, NCC$H_3$), 1.61 (s, 6H, NCC$H_3$), 0.05 (s, 9H, NSi(C$H_3$)$_3$), –0.08 (s, 9H, CSi(C$H_3$)$_3$.

**$^{13}$C NMR** (75 MHz, 298 K, $C_6D_6$) δ =168.5 (N*C*CH$_3$), 167.1 (N*C*CH$_3$), 145.6 (Ar*C*), 144.9 (Ar*C*), 133.1 (Ar*C*), 132.4 (Ar*C*), 131.9 (Ar*C*), 131.5 (2 x Ar*C*), 131.4 (*C*NSi(CH$_3$)$_3$), 131.3 (Ar*C*), 129.3 ( 2x overlapping signals, Ar*C*), 129.2 (overlapping signals, Ar*C* & N*C*Si(CH$_3$)$_3$), 129.1 (Ar*C*), 95.4 (NC*C*H), 94.3 (NC*C*H), 23.0 (NC*C*H$_3$), 22.9 (NC*C*H$_3$), 21.1 (Ar*C*H$_3$), 21.0 (Ar*C*H$_3$), 19.5 (Ar*C*H$_3$), 19.4 (2 x overlapping Ar*C*H$_3$), 18.9 (Ar*C*H$_3$), –0.7 (NSi(*C*H$_3$)$_3$), –3.5 (CSi(*C*H$_3$)$_3$).

**$^{29}$Si NMR** (80MHz, 298K, $C_6D_6$) δ = 5.34 (NC*Si*(CH$_3$)$_3$), –13.73 (CN*Si*(CH$_3$)$_3$).

**IR** ν/cm$^{-1}$ (ATR): 1655 (w), 1623 (w), 1517 (m), 1550 (m), 1475 (m), 1448 (m), 1396 (s), 1246 (m), 1195 (m), 1146 (m), 1008 (m), 957 (w), 923 (w), 852 (s), 833 (s), 742 (w), 690 (w)

**EI/MS** (70eV) m/z (%): 73.0 (SiMe$_3$+, 47), 160.1 (MeCNMes$^+$, 28), 357.3 ($^{Mes}$LMg$^+$, 100), 429.3 ($^{Mes}$LMgSiMe$_2$CH$_2$+, 38).

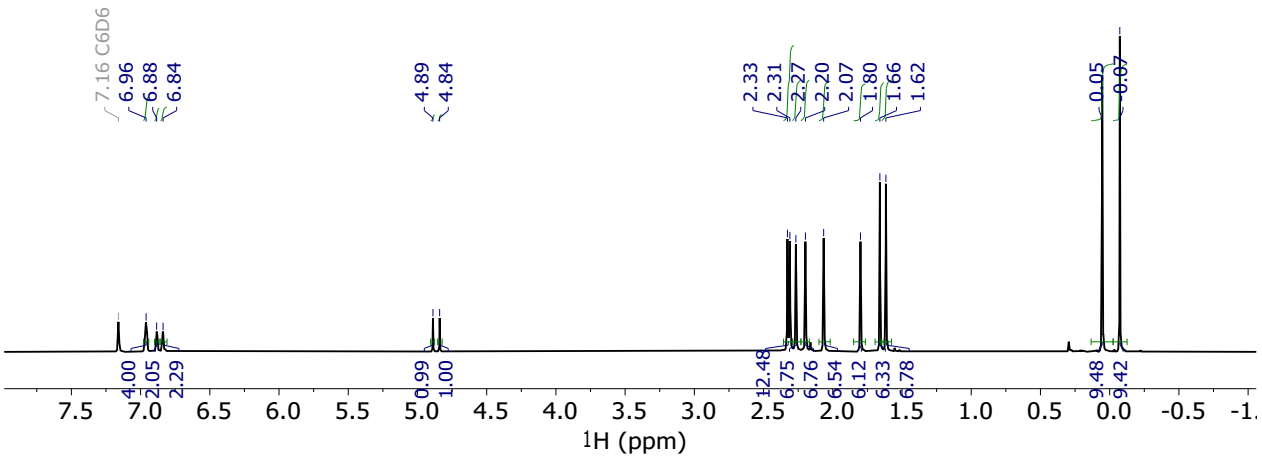



*Figure S 13: $^1$H NMR (400 MHz) spectrum of **8** in $C_6D_6$.*

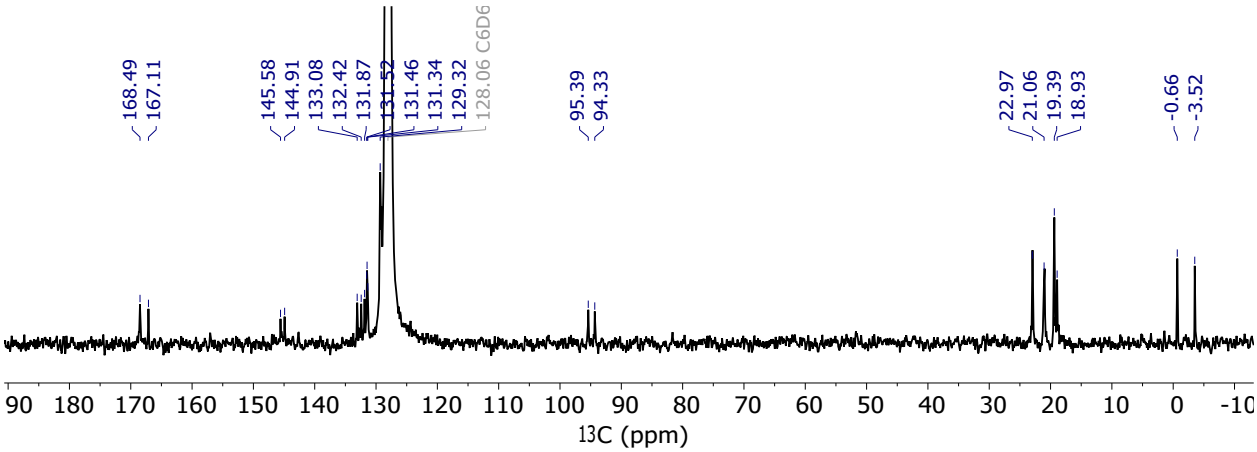



*Figure S 14: $^{13}C\{^{1}H\}$ NMR (100 MHz) spectrum of **8** in $C_6D_6$.*

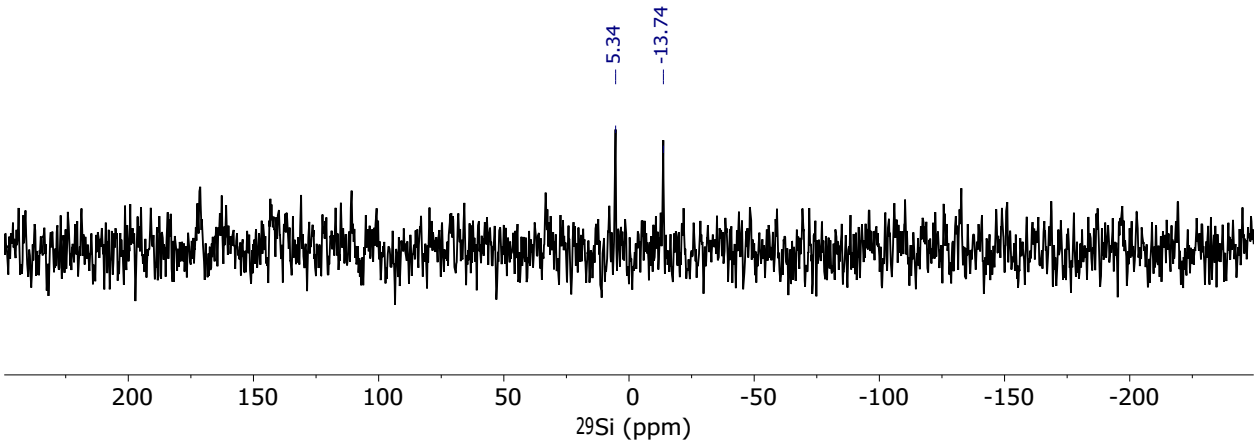



*Figure S 15: $^{29}Si\{^{1}H\}$ NMR (80 MHz) spectrum of **8** in $C_6D_6$.*

### 1.2.6. Synthesis of [{$^{Xyl}$LMg}$_2${μ-(Me$_3$SiN=C–N=CSiMe$_3$)}], 9

Trimethylsilyl cyanide (84 μL, 0.67 mmol) was added via micro syringe to a solution of [$^{Xyl}$LMg]$_2$ (200 mg, 0.30 mmol) disolved in toluene (20 ml) at –78 °C. The resultant solution was allowed to warm to room temperature and stirred overnight. The solution was filtered, concentrated to ca. 5 ml and stored at –30 °C, yielding red crystals of **8** (96 mg, 36%). M.p. 166-170 °C (decomp).

**Elemental analysis** calc'd for $C_{50}H_{68}Mg_2N_6Si_2$: C 70.00 %, H 7.99 %, N 9.80 %, found: C 69.79 %, H 8.16 %, N 9.60 %.

**$^1$H NMR** (400 MHz, 298 K, $C_6D_6$); δ =6.96-7.15 (m, 12H, Ar*H*, 4.85 (s, 1H, NCC*H*), 4.80 (s, 1H, NCC*H*), 2.32 (s, 6H, ArC$H_3$), 2.18 (s, 6H, ArC$H_3$), 2.05 (s, 6H, ArC$H_3$), 1.79 (s, 6H, ArC$H_3$), 1.61 (s, 6H, NCC$H_3$), 1.55 (s, 6H, NCC$H_3$), 0.01 (s, 9H, NSi(C$H_3$)$_3$), –0.10 (s, 9H, CSi(C$H_3$)$_3$.

**$^{13}$C NMR** (75 MHz, 298 K, $C_6D_6$); δ = 168.4 (N*C*CH$_3$), 167.0 (N*C*CH$_3$), 148.2 (Ar*C*), 147.5 (Ar*C*), 132.2 (Ar*C*), 131.9 (2 x Ar*C*), 131.7 (Ar*C*), 128.7 (Ar*C*), 128.6 (2 x Ar*C*), 124.3 (Ar*C*), 123.9 (Ar*C*), 95.3 (NC*C*H), 94.3 (NC*C*H), 23.0 (NC*C*H$_3$), 22.9 (NC*C*H$_3$), 19.6 (Ar*C*H$_3$), 19.5 (Ar*C*H$_3$), 19.3 (Ar*C*H$_3$), 18.9 (Ar*C*H$_3$), –0.7 (NSi(*C*H$_3$)$_3$), –3.7 (CSi(*C*H$_3$)$_3$) – overlapping signals led to less than expected number of resonances being assignable, C=N resonance also not observed.

**$^{29}$Si{$^1$H} NMR** (80 MHz, 298 K, $C_6D_6$); δ = 5.52 (NC*Si*(CH$_3$)$_3$), –13.72 (CN*Si*(CH$_3$)$_3$).

**IR** ν/cm$^{-1}$ (ATR): 1540 (w), 1516 (m), 1449 (m), 1388 (s), 1265 (w), 1182 (m), 1094 (w), 1012 (m), 917 (w), 831 (s), 761 (s), 746 (s), 698 (m).

**EI/MS** (70eV) m/z (%): 73.0 (SiMe$_3$+, 100), 146.1 (MeCNXyl+, 27), 329.2 ($^{Xyl}$LMg+, 69), 401.3 ($^{Xyl}$LMgSiMe$_2$CH$_2$+, 21).

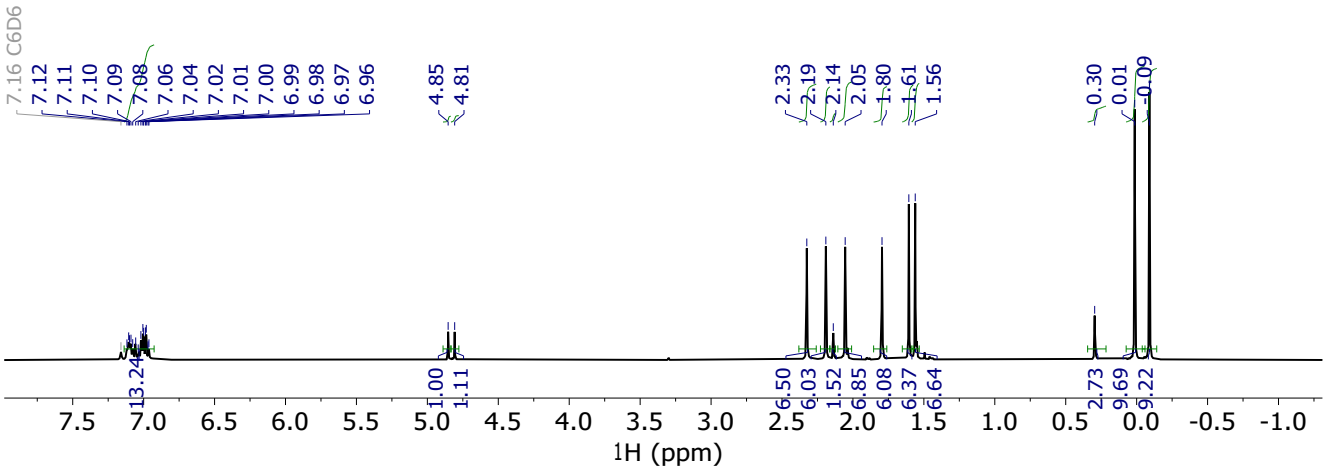



*Figure S 16: $^{1}H$ NMR spectrum (400 MHz) of **9** in $C_6D_6$.*

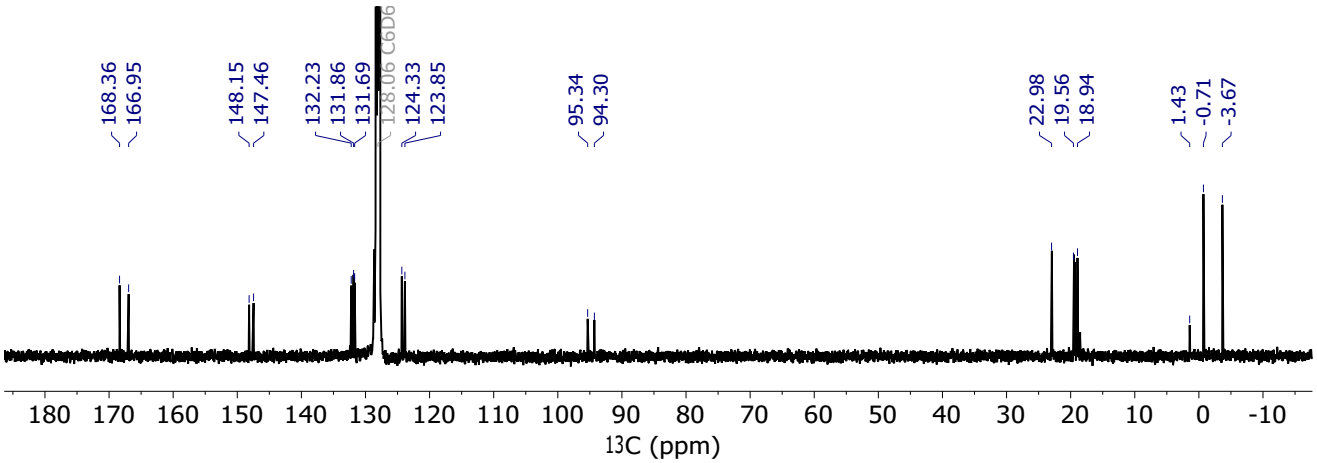



*Figure S 17: $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz) of **9** in $C_6D_6$.*

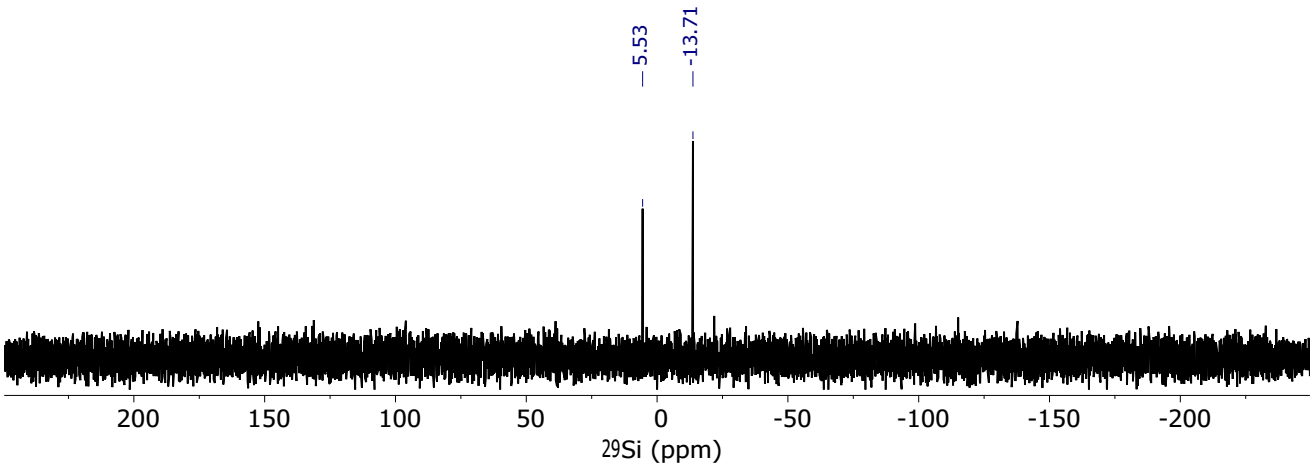



*Figure S 18: $^{29}Si\{^{1}H\}$ NMR spectrum (80 MHz) of **9** in $C_6D_6$.*

### 1.3. Catalytic Experiments

Catalytic studies were performed using the same methodology previously reported by Ma *et al*.[5]
In a glove box, a single crystal of the catalyst (weighing roughly 1 mg) was added to a solution of benzaldehyde (1 mmol) or acetophenone (1 mmol) and $Me_3SiCN$ (1.5 mmol) dissolved in $C_6D_6$ (0.5 mL) at room temperature in a J. Young NMR tube equipped with a Teflon screw cap. The progress of the reaction was monitored by $^1H$ NMR.

Blank reactions in the absence of catalyst gave no reaction for acetophenone but considerable conversion of benzaldehyde.[7] Full conversion in the absence of catalyst was shown within 2 hours. Catalytic runs using benzaldehyde as a substrate gave full conversion within the same timeframe and so the effect of the catalyst on the reaction is hard to determine.

Acetophenone showed little conversion without the catalyst (ca. 1%) even with heating for 24 h. Catalytic experiments showed complete conversion within 1.5 hours.

Catalytic run times were consistent between $[\{^{Ar}LMg\}_2]$ and $[\{^{Ar}LMg\}_2\{\mu\text{–}(Me_3SiN{=}C\text{–}N{=}CSiMe_3)\}]$.

Catalytic experiments were also conducted using the previously reported complex, $[\{^{Dipp}LMg(\mu\text{–}CN)\}_3]$,[6] as this is a by–product of the reaction of $[\{^{Dipp}LMg\}_2]$ and $Me_3SiCN$. Reaction times for this were slower (ca 6 h) but catalysis with acetophenone still proceeded.

### 1.3.1. Reactions of benzaldehyde with [{$^{Xyl}$LMg}$_2$] and [{$^{Xyl}$LMg}$_2${μ–(Me$_3$SiN=C–N=SiMe$_3$)}]

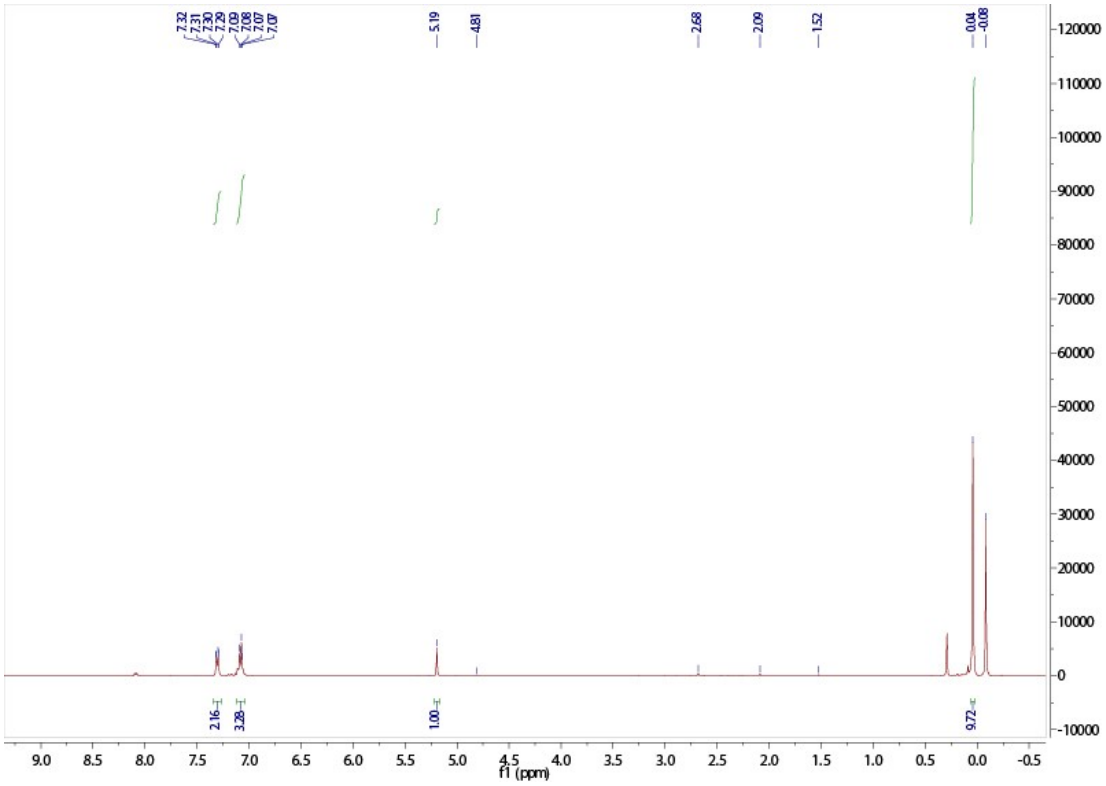



*Figure S 19. Full $^1$H NMR spectrum of the catalytic run involving benzaldehyde and Me$_3$SiCN using [{$^{Xyl}$LMg}$_2$] as the pre-catalyst.*

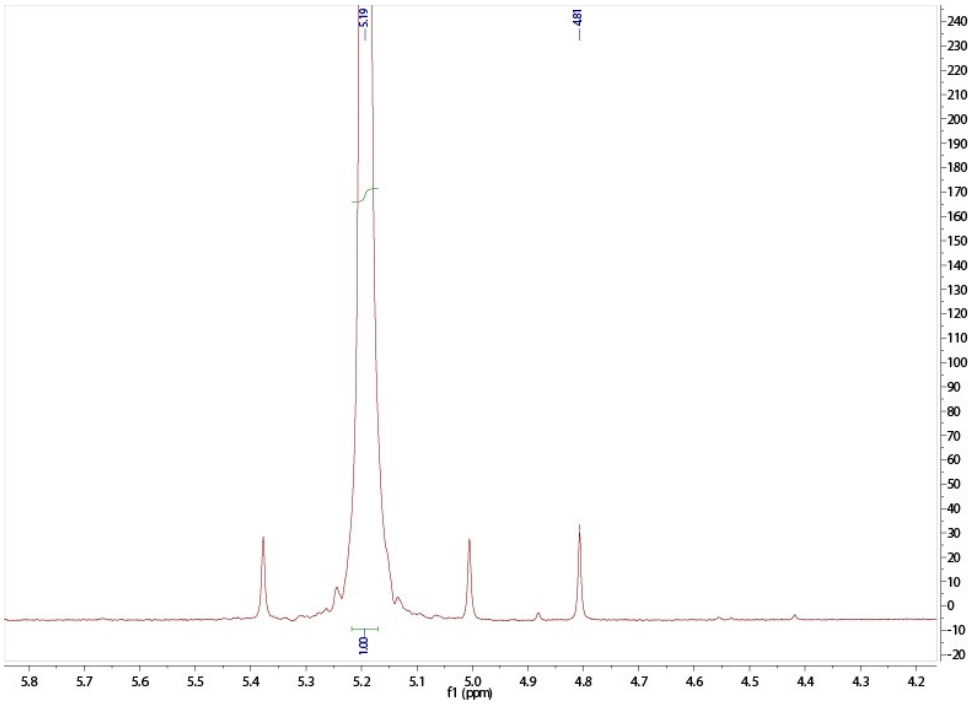



*Figure S 20. $^1$H NMR spectrum of the catalytic run involving benzaldehyde and Me$_3$SiCN using [{$^{Xyl}$LMg}$_2$] as the pre-catalyst. Zoomed in on Nacnac methine region showing no [{$^{Xyl}$LMg}$_2$] present.*

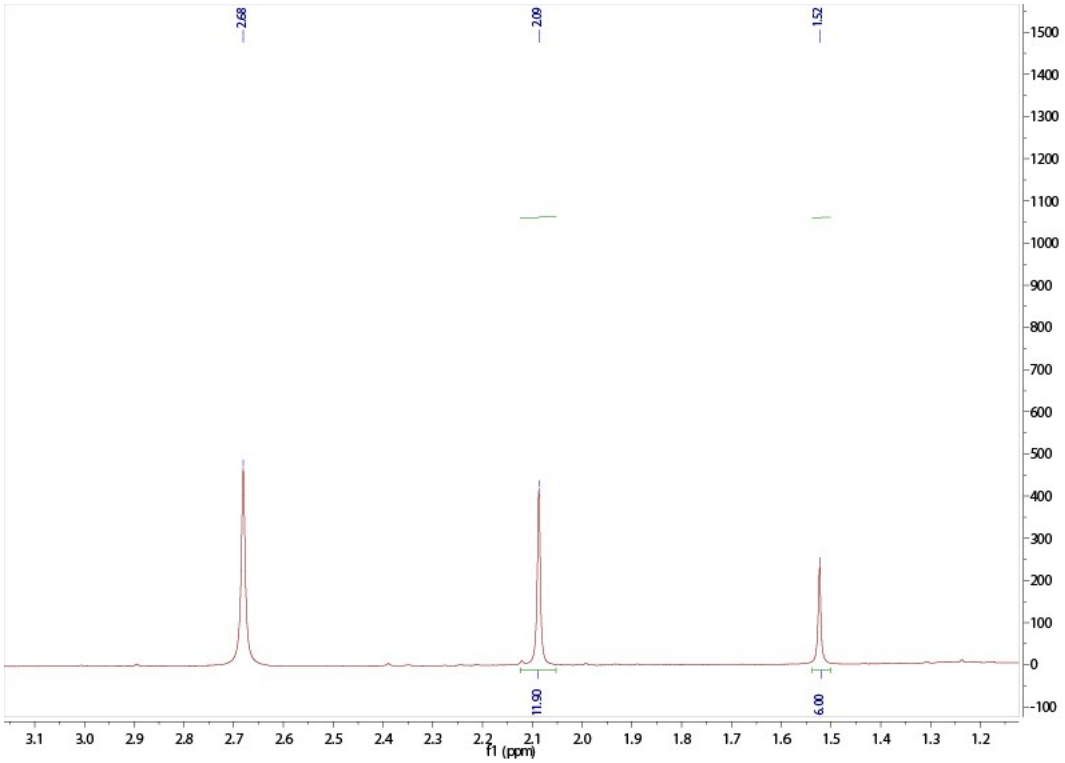



*Figure S 21. [1]H NMR spectrum of the catalytic run involving benzaldehyde and $Me_3SiCN$ using [{$^{Xyl}$LMg}$_2$] as the pre-catalyst. Zoomed in on $ArCH_3$ region showing no [{$^{Xyl}$LMg}$_2$] present.*

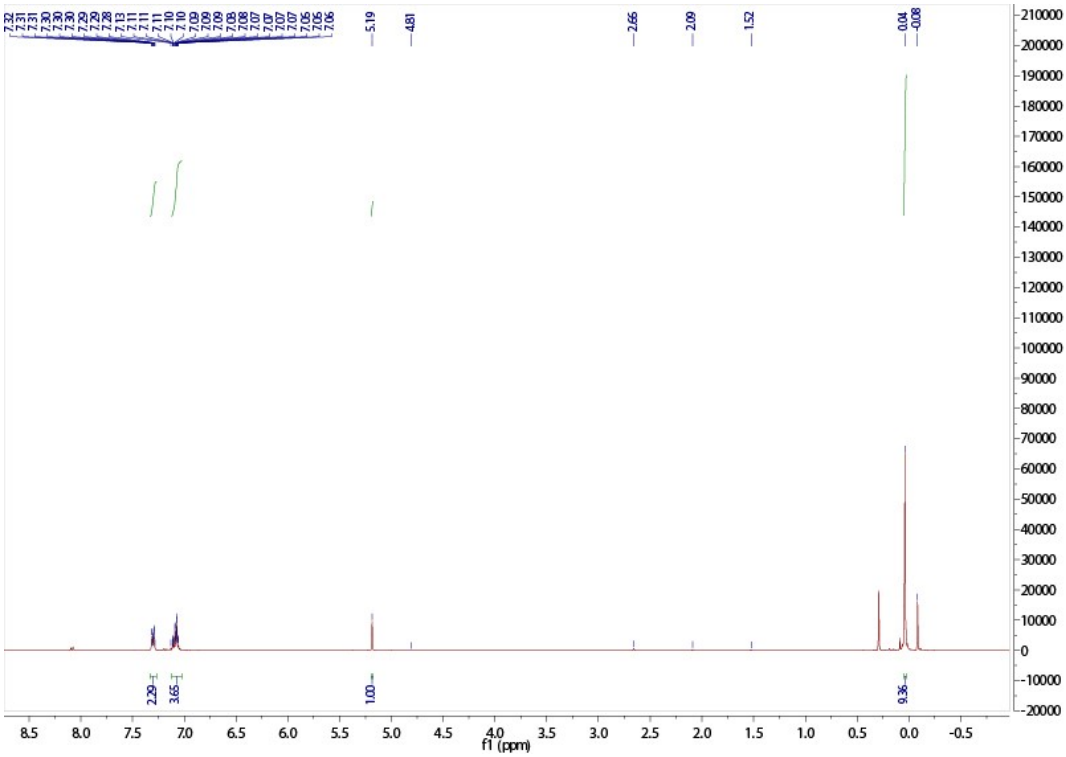



*Figure S 22. Full [1]H NMR spectrum of the catalytic run involving benzaldehyde and $Me_3SiCN$ using [{$^{Xyl}$LMg}$_2${μ–($Me_3SiN$=C–N=$SiMe_3$)}] as the pre-catalyst.*

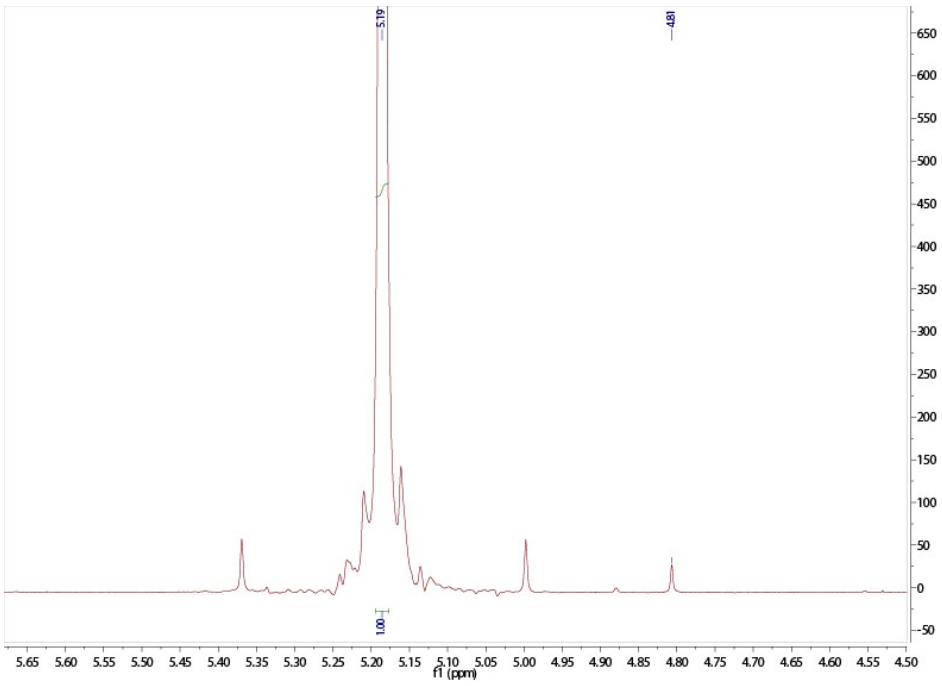



*Figure S 23. $^{1}H$ NMR spectrum of the catalytic run involving benzaldehyde and $Me_3SiCN$ using [{$^{Xyl}$LMg}$_2${μ–($Me_3SiN$=C−N=$SiMe_3$)}] as the pre-catalyst. Zoomed in on the Nacnac methine region showing no [{$^{Xyl}$LMg}$_2$] or [{$^{Xyl}$LMg}$_2${μ–($Me_3SiN$=C−N=$SiMe_3$)}] present, Same peaks shown in both runs.*

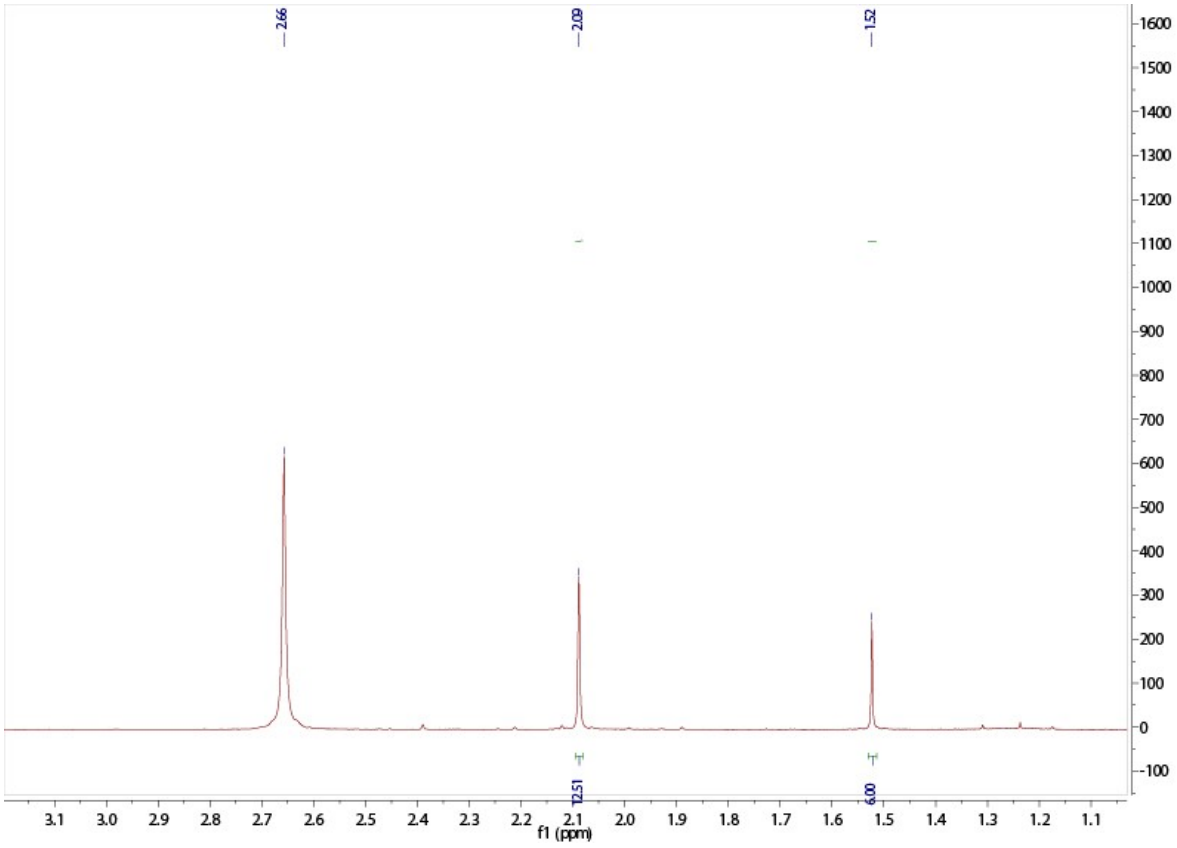



*Figure S 24. $^{1}H$ NMR spectrum of the catalytic run involving benzaldehyde and $Me_3SiCN$ using [{$^{Xyl}$LMg}$_2${μ–($Me_3SiN$=C−N=$SiMe_3$)}] as the pre-catalyst. Zoomed in on the $ArCH_3$ region showing no [{$^{Xyl}$LMg}$_2$] or [{$^{Xyl}$LMg}$_2${μ–($Me_3SiN$=C−N=$SiMe_3$)}] present. Same peaks shown in both runs.*

### 1.3.2. Reactions of acetophenone with [{$^{Xyl}$LMg}$_2$] and [{$^{Xyl}$LMg}$_2${μ–(Me$_3$SiN=C–N=CSiMe$_3$)}]

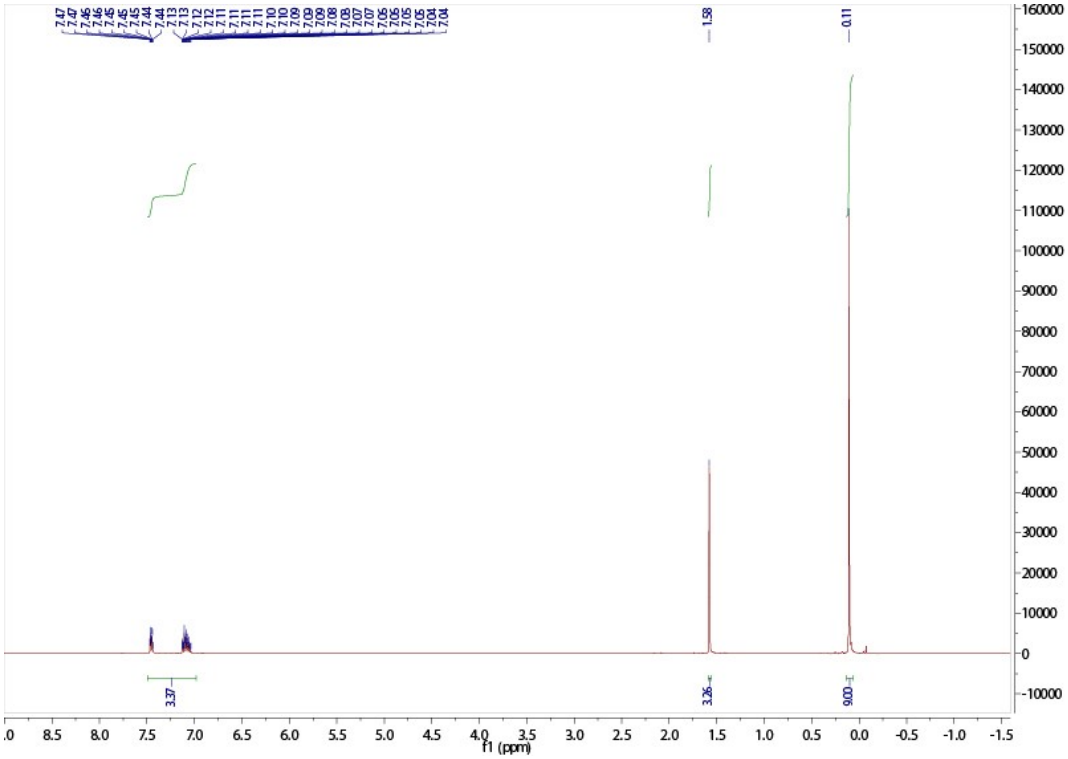



*Figure S 25. Full $^1$H NMR spectrum of the catalytic run involving acetophenone and Me$_3$SiCN using [{($^{Xyl}$L)Mg}$_2$] as the pre-catalyst.*

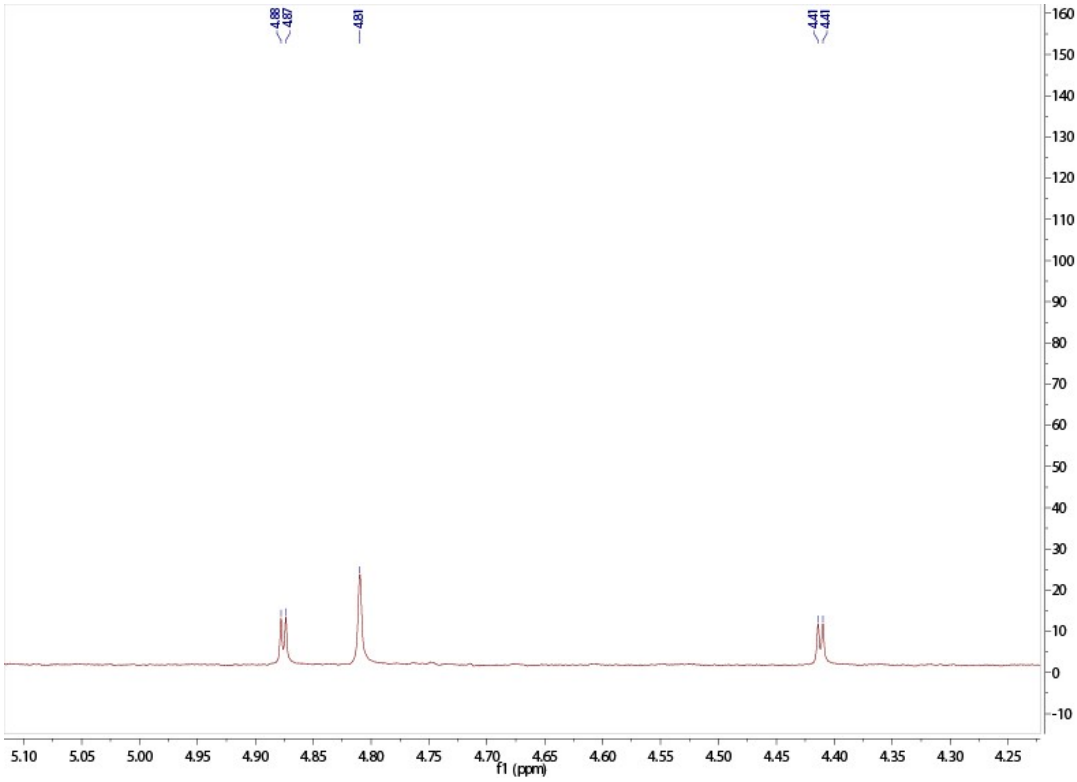



*Figure S 26. $^1$H NMR spectrum of the catalytic run involving acetophenone and Me$_3$SiCN using [{$^{Xyl}$LMg}$_2$] as the pre-catalyst. Zoomed in on Nacnac methine region showing no [{$^{Xyl}$LMg}$_2$] present.*

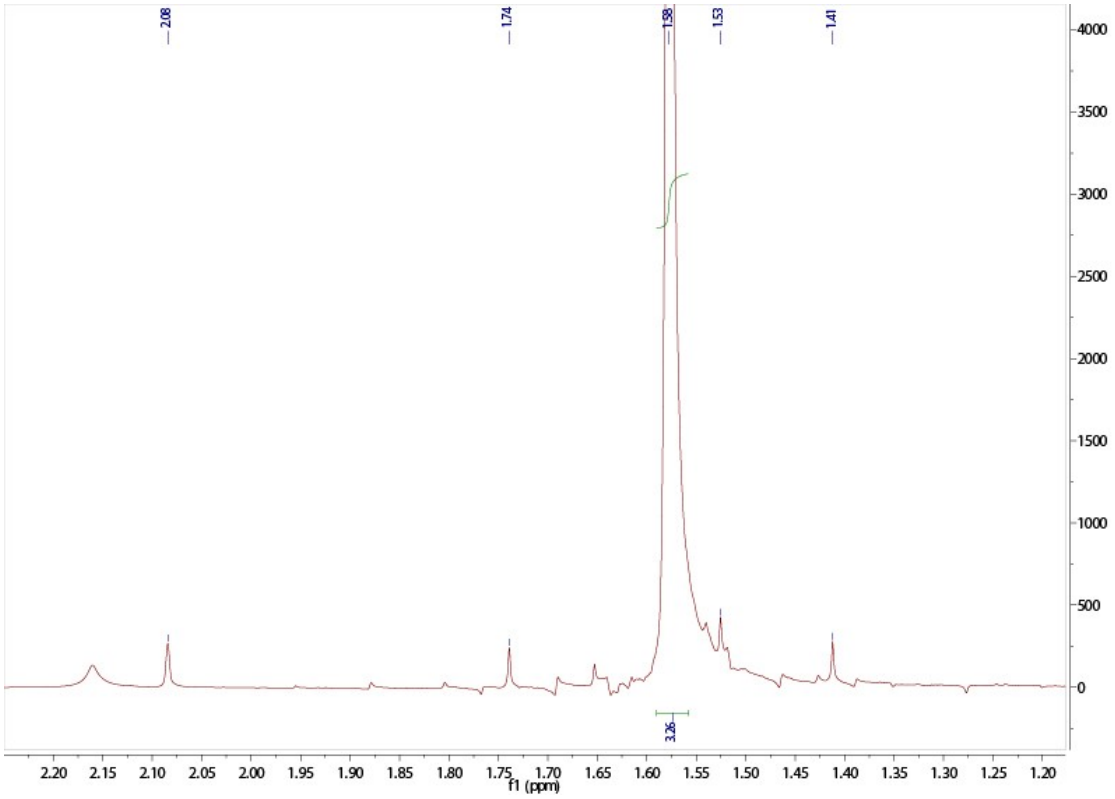



*Figure S 27. [1]H NMR spectrum of the catalytic run involving benzaldehyde and $Me_3SiCN$ using [{($^{Xyl}$L)Mg}$_2$] as the pre-catalyst. Zoomed in on $ArCH_3$ region showing no [{($^{Xyl}$L)Mg}$_2$] present.*

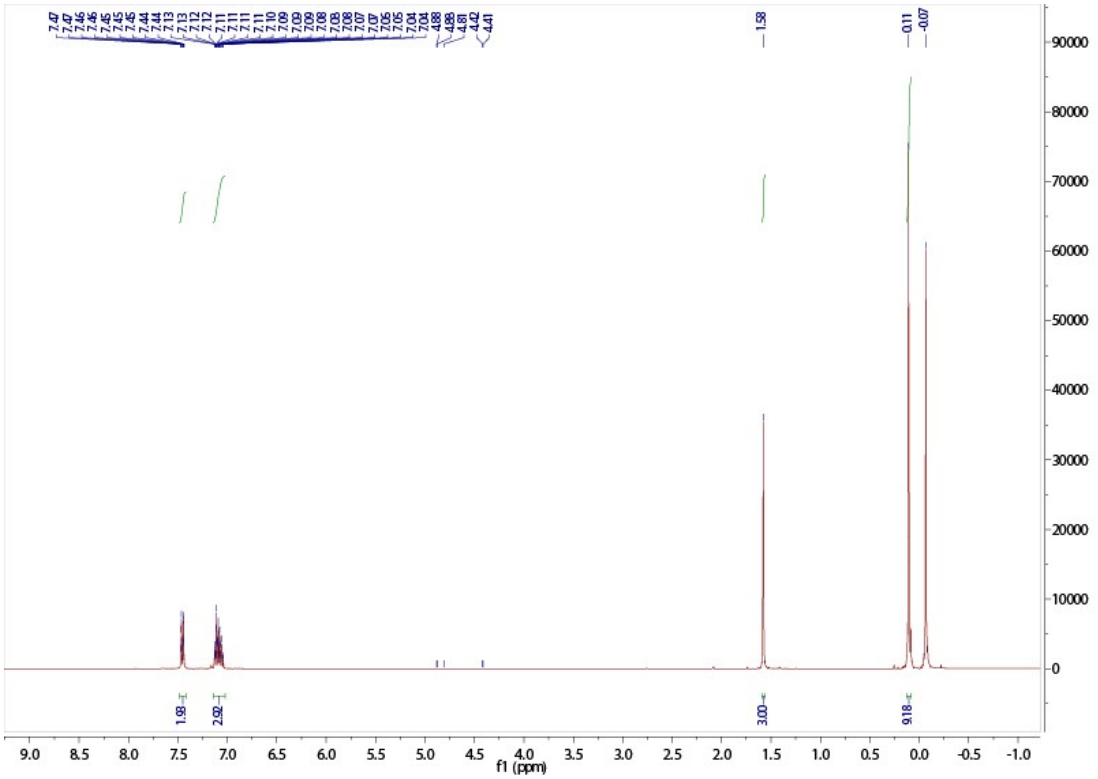



*Figure S 28. Full [1]H NMR spectrum of the catalytic run involving acetophenone and $Me_3SiCN$ using [{($^{Xyl}$L)Mg}$_2${μ–($Me_3SiN$=C–N=$SiMe_3$)}] as the pre-catalyst.*

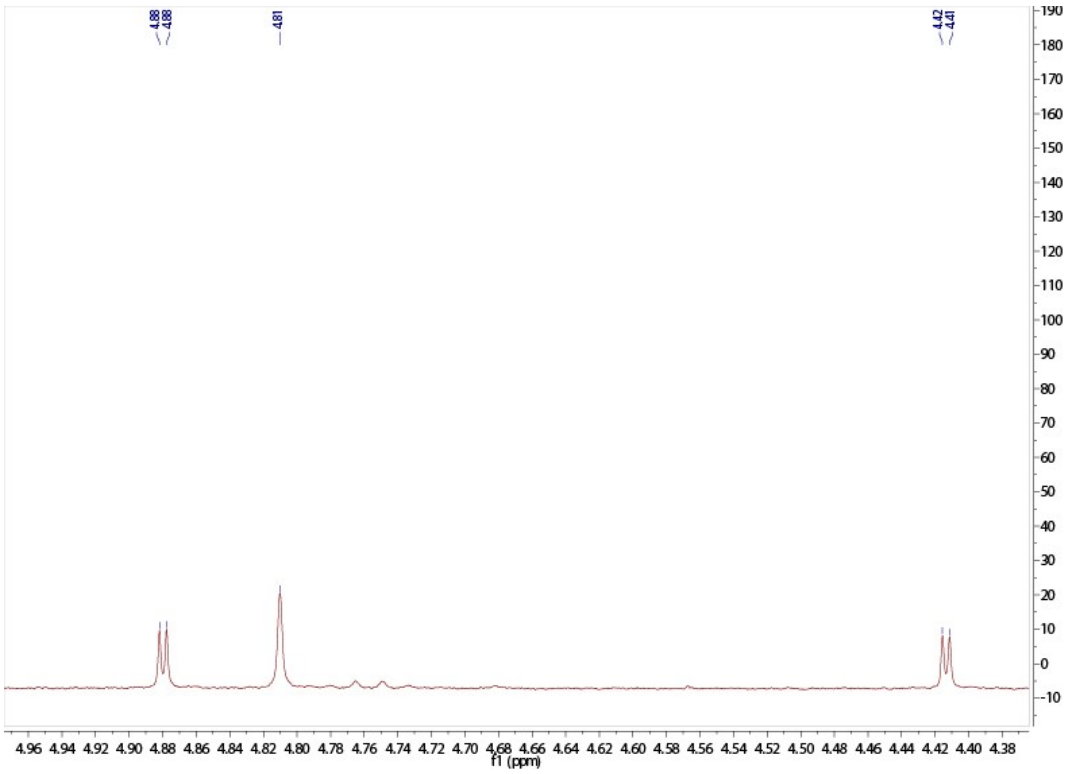



*Figure S 29. $^1$H NMR spectrum of the catalytic run involving acetophenone and $Me_3SiCN$ using [{($^{Xyl}$L)Mg}$_2${μ–($Me_3SiN$=C–N=$SiMe_3$)}] as the pre-catalyst. Zoomed in on the Nacnac methine region showing no [{($^{Xyl}$L)Mg}$_2$] or [{($^{Xyl}$L)Mg}$_2${μ–($Me_3SiN$=C–N=$SiMe_3$)}] present, Same peaks shown in both runs.*

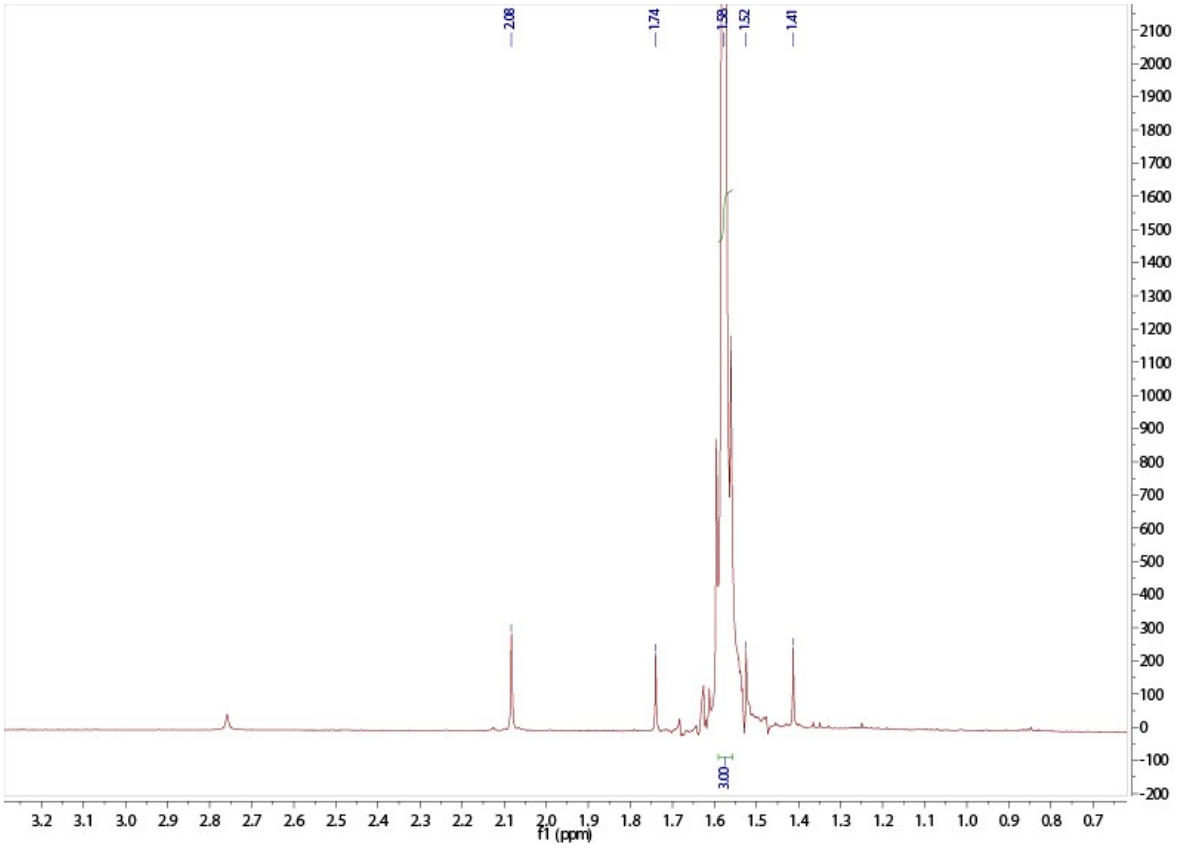



*Figure S 30. $^1$H NMR spectrum of the catalytic run involving acetophenone and $Me_3SiCN$ using [{($^{Xyl}$L)Mg}$_2${μ–($Me_3SiN$=C–N=$SiMe_3$)}] as the pre-catalyst. Zoomed in on the $ArCH_3$ region showing no [{($^{Xyl}$L)Mg}$_2$] or [{($^{Xyl}$L)Mg}$_2${μ–($Me_3SiN$=C–N=$SiMe_3$)}] present. Same peaks shown in both runs.*

### 1.3.3 Blank reaction of $Me_3SiCN$ and acetophenone

A solution of acetophenone (1 mmol) and $Me_3SiCN$ (1.5 mmol) dissolved in $C_6D_6$ (0.5 mL) at room temperature in a J. Young NMR tube equipped with a Teflon screw cap. The progress of the reaction was monitored by $^1H$ NMR.

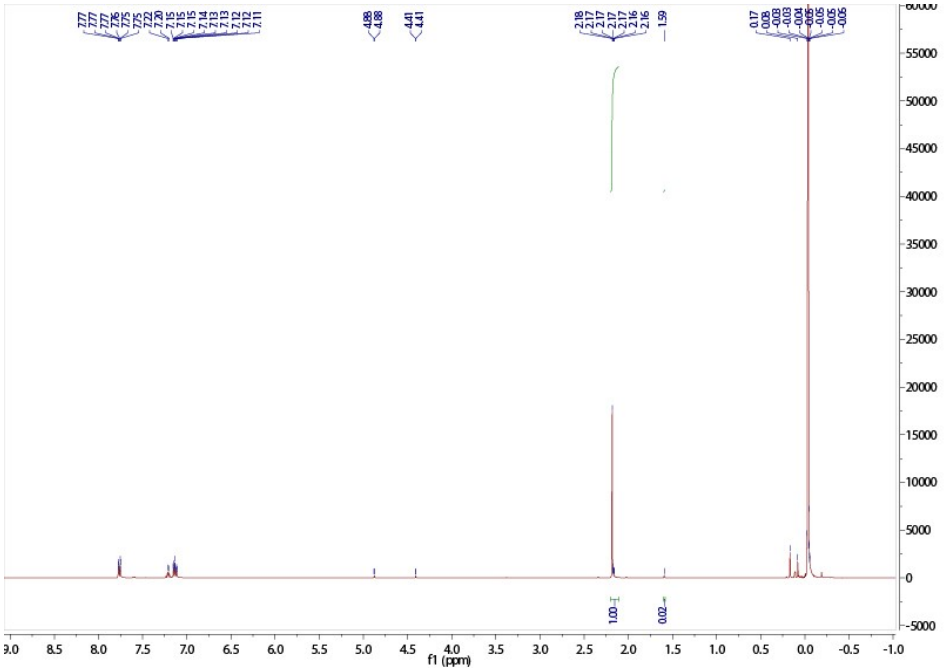



*Figure S 31. Full $^1H$ NMR spectrum of the reaction of acetophenone and $Me_3SiCN$ using no catalyst. Minimal conversion observed even after heating at 60 °C for 24h.*

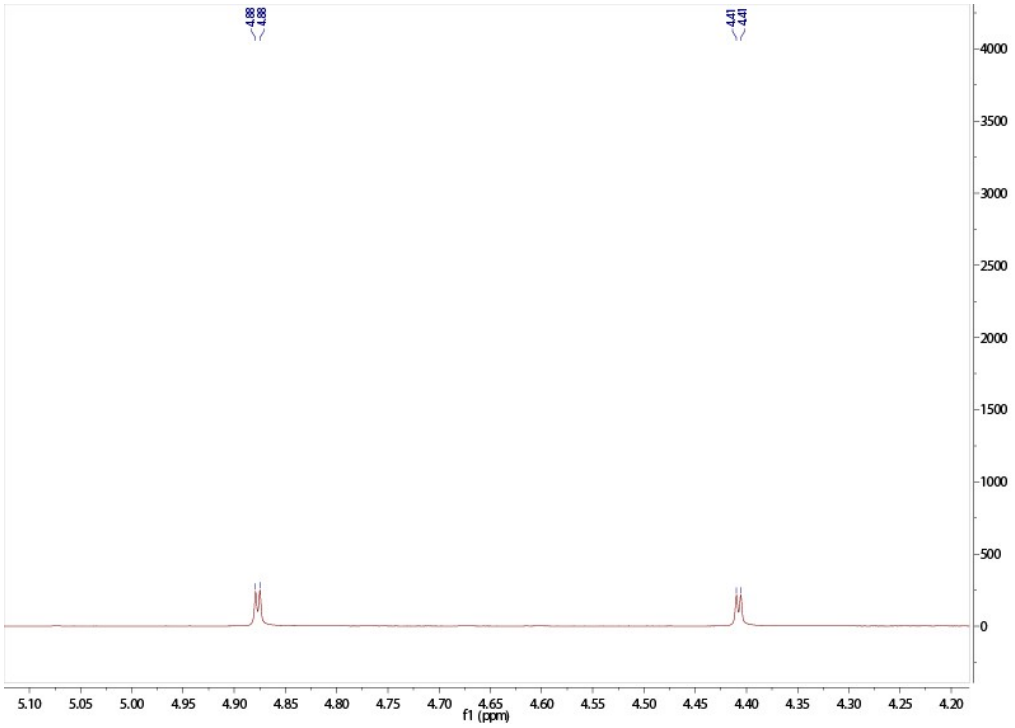



*Figure S 32. $^1H$ NMR spectrum of the reaction of acetophenone and $Me_3SiCN$ using no catalyst. Zoomed in at Nacnac methine region. Minimal conversion observed even after heating at 60 °C for 24 h.*

### 1.3.4. Reaction of acetophenone using catalytic [{($^{Dipp}$L)Mg(μ–CN)}$_3$]

In a glove box, a single crystal of the [{$^{Dipp}$LMg(μ–CN)}$_3$] (weighing roughly 1 mg) was added to a solution of benzaldehyde (1 mmol) or acetophenone (1 mmol) and TMSCN (1.5 mmol) dissolved in $C_6D_6$ (0.5 mL) at room temperature in a J. Young NMR tube equipped with a Teflon screw cap. The progress of the reaction was monitored by $^1$H NMR spectroscopy.

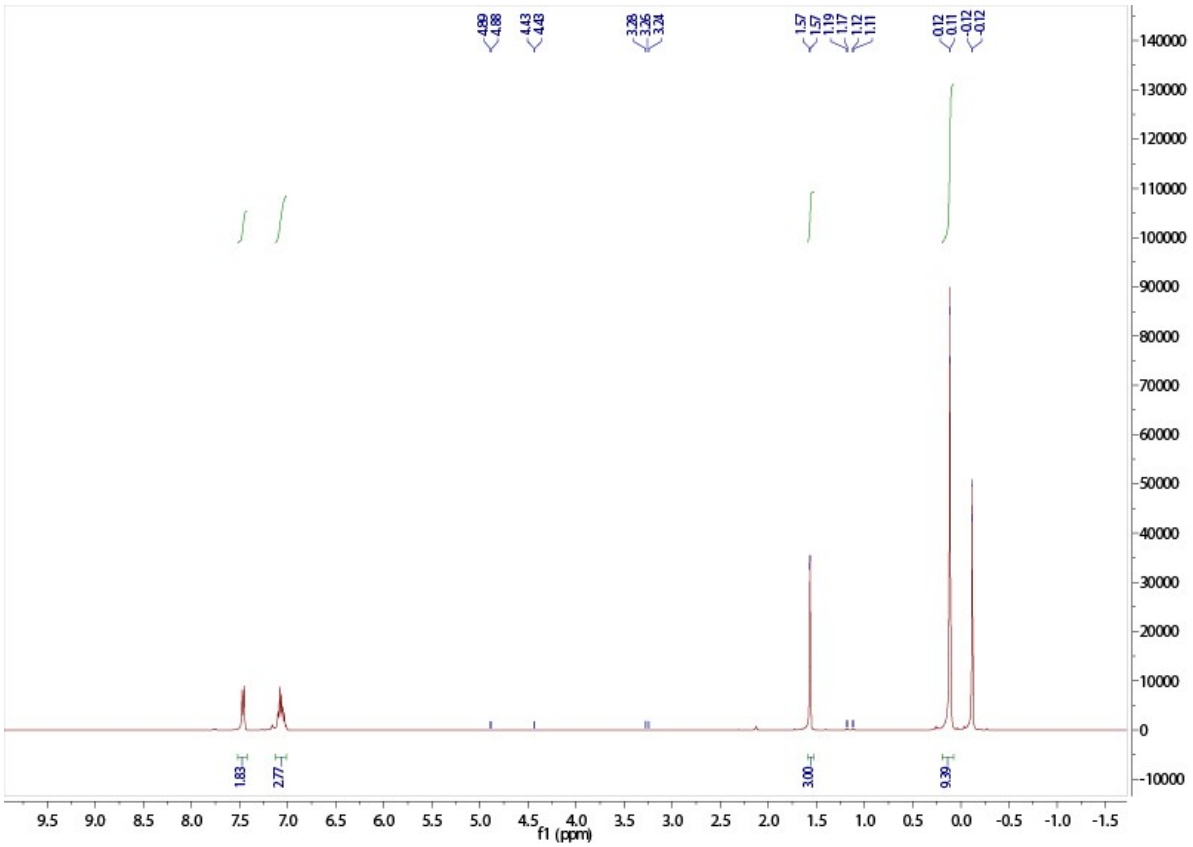



*Figure S 33. Full $^1$H NMR spectrum of the catalytic run involving acetophenone and $Me_3SiCN$ using [{($^{Dipp}$L)Mg(μ–CN)}$_3$] as the pre-catalyst.*

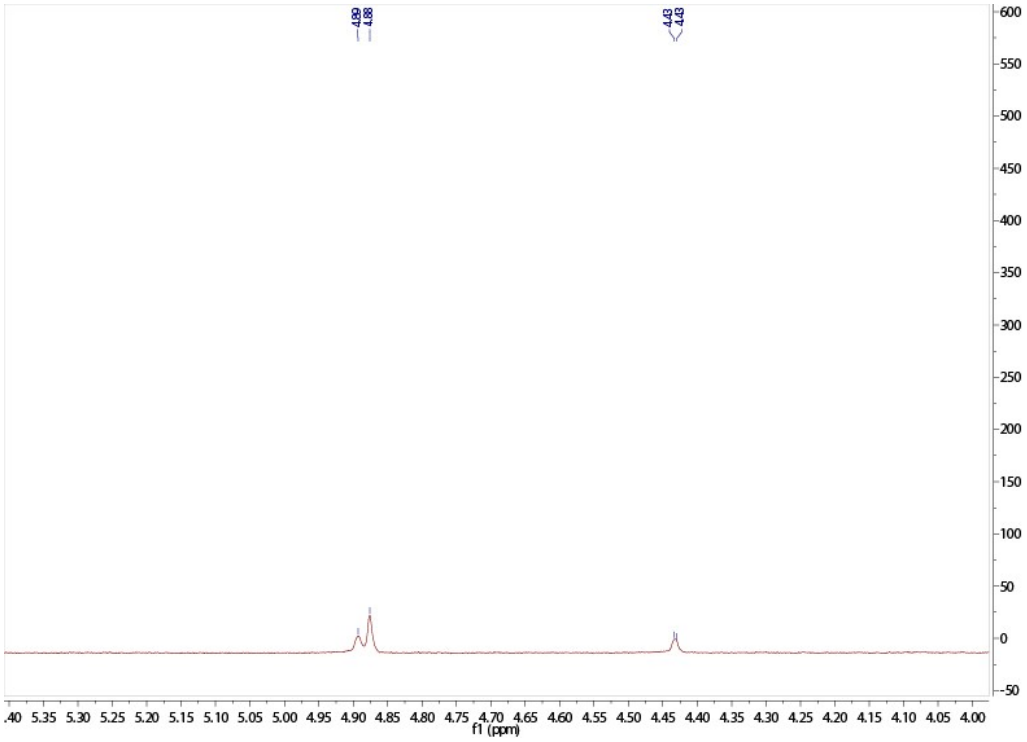



*Figure S 34. $^1$H NMR spectrum of the catalytic run involving acetophenone and $Me_3SiCN$ using [{($^{Dipp}$L)Mg(μ–CN)}$_3$] as the pre-catalyst. Zoomed in on the Nacnac methine region showing no [{($^{Dipp}$L)Mg(μ–CN)}$_3$] or [{($^{Dipp}$L)Mg}$_2$] present.*

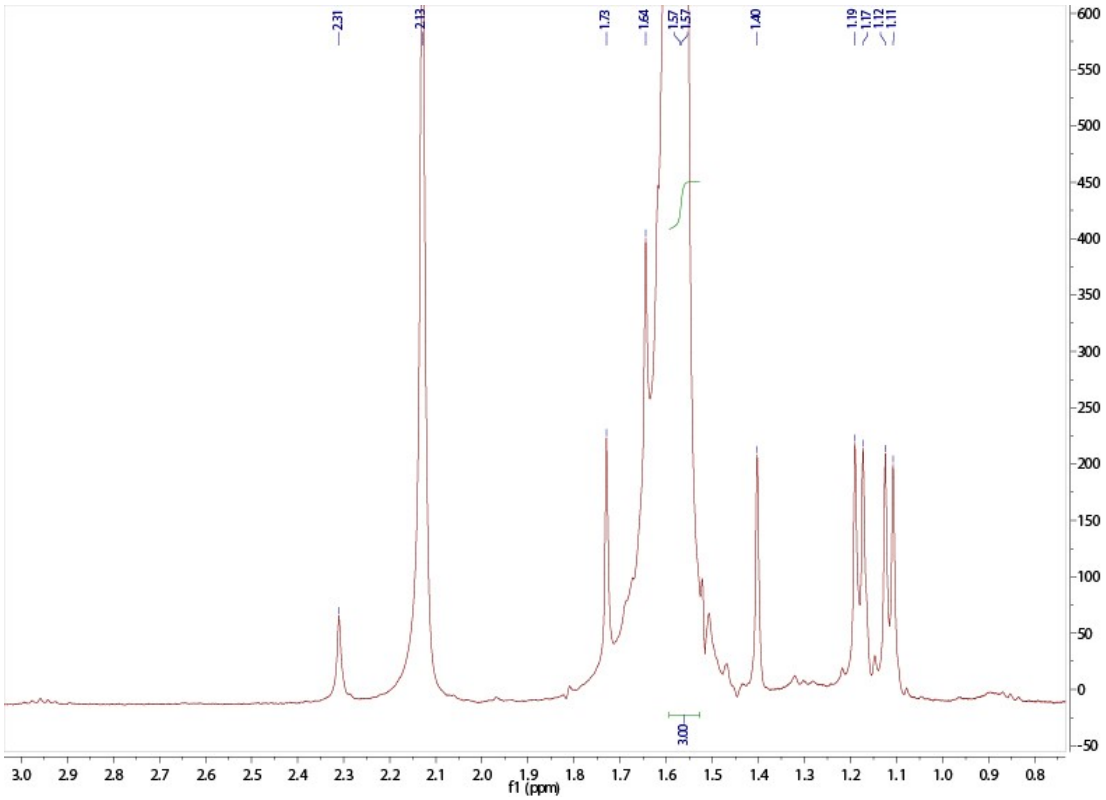



*Figure S 35. $^1$H NMR spectrum of the catalytic run involving acetophenone and $Me_3SiCN$ using [{($^{Dipp}$L)Mg(μ–CN)}$_3$] as the pre-catalyst. Zoomed in on the ArCH$Me_2$ region, showing no [{($^{Dipp}$L)Mg(μ–CN)}$_3$] or [{($^{Dipp}$L)Mg}$_2$] present.*

## 2. X-Ray Crystallography

Single-crystal X-ray diffraction data were collected using either an Oxford Diffraction Supernova dual-source diffractometer equipped with a 135 mm Atlas CCD area detector (**1**, **2**, **3**, **5/6**) or an Oxford Gemini Ultra diffractometer (**8**, **9**). Crystals were selected under Paratone-N oil, mounted on micromount loops and quench-cooled using an open flow $N_2$ cooling device. Data were collected at 150 K, unless otherwise stated, using mirror monochromated Cu Kα (λ = 1.54184 Å) or Mo Kα (λ = 0.71073 Å) radiation and processed using the CrysAlisPro package, including unit cell parameter refinement and inter-frame scaling (which was carried out using SCALE3 ABSPACK within CrysAlisPro).[8] Equivalent reflections were merged and diffraction patterns processed with the CrysAlisPro suite. Hydrogen atoms are typically included in calculated positions (riding model). Crystal data, details of data collections and refinements for all structures can be found in their CIF files and are summarized in Table S1.

**Table S1.** Selected X-ray data collection and refinement parameters for **1**, **2** and **3**.

| | **1·hexane** | **2** | **3·hexane** |
|---|---|---|---|
| Formula | $C_{69}H_{105}Mg_2N_4P$ | $C_{56}H_{76}Mg_2N_4P_2$ | $C_{108}H_{148}Mg_4N_8P_2$ |
| CCDC | 2123990 | 2123991 | 2123992 |
| Fw [g mol$^{-1}$] | 1070.15 | 915.76 | 1717.52 |
| Crystal system | monoclinic | monoclinic | Monoclinic |
| Space group | *C*2/*c* | $P2_1/n$ | $P2_1/n$ |
| *a* (Å) | 21.8841(4) | 14.9573(2) | 13.5990(1) |
| *b* (Å) | 11.3716(2) | 18.0124(2) | 22.4045(1) |
| *c* (Å) | 29.3532(5) | 19.9090(2) | 16.8412(1) |
| α (°) | 90 | 90 | 90 |
| β (°) | 111.490(2) | 92.617(1) | 94.715(1) |
| γ (°) | 90 | 90 | 90 |
| *V* (Å$^3$) | 6796.9(2) | 5358.23(11) | 5113.79(5) |
| *Z* | 4 | 4 | 2 |
| Radiation, λ (Å) | Cu Kα, 1.54184 | Cu Kα, 1.54184 | Cu Kα, 1.54184 |
| Temp (K) | 150(2) | 150(2) | 150(2) |
| $\rho_{calc}$ (g cm$^{-3}$) | 1.046 | 1.135 | 1.115 |
| μ (mm$^{-1}$) | 0.828 | 1.251 | 0.993 |
| Reflections collected | 7167 | 11189 | 10643 |
| Independent reflections | 5921 | 9244 | 9627 |
| Parameters | 376 | 597 | 569 |
| R(int) | 0.0418 | 0.0377 | 0.0375 |
| R1/wR2,[a] I ≥ 2σI (%) | 0.1115 | 0.0975 | 0.1017 |
| R1/wR2,[a] all data (%) | 0.1200 | 0.1056 | 0.1061 |
| GOF | 1.027 | 1.028 | 1.041 |

$R1 = [\Sigma||F_o| - |F_c||]/\Sigma|F_o|$; $wR2 = \{[\Sigma w[(F_o)^2 - (F_c)^2]^2]/[\Sigma w(F_o^2)^2\}^{1/2}$; $w = [\sigma^2(F_o)^2 + (AP)^2 + BP]^{-1}$, where $P = [(F_o)^2 + 2(F_c)^2]/3$ and the A and B values are 0.0593 and 4.4468 for **1·hexane**, 0.0563 and 0.8294 for **2**, and 0.0587 and 1.4411 for **3·hexane.**

**Table S2.** Selected X-ray data collection and refinement parameters for **5/6**, **8**, and **9**.

| | **5/6** | **8** | **9** |
|---|---|---|---|
| Formula | $C_{60}H_{84}Mg_2N_4OP_2$ | $C_{54}H_{76}Mg_2N_6Si_2$ | $C_{50}H_{68}Mg_2N_6Si_2$ |
| CCDC | 2123993 | 2123994 | 2123995 |
| Fw [g mol$^{-1}$] | 987.87 | 914.00 | 857.90 |
| Crystal system | triclinic | monoclinic | triclinic |
| Space group | *P*–1 | $P2_1/c$ | *P*–1 |
| *a* (Å) | 11.6939(7) | 12.195(2) | 10.7347(11) |
| *b* (Å) | 14.1088(6) | 22.685(5) | 11.2562(10) |
| *c* (Å) | 19.7110(8) | 20.460(4) | 12.2531(12) |
| α (°) | 72.352(4) | 90 | 73.388(9) |
| β (°) | 76.371(4) | 102.65(3) | 81.480(9) |
| γ (°) | 73.373(5) | 90 | 64.513(10) |
| *V* (Å$^3$) | 2929.7(3) | 5523(2) | 1280.2(2) |
| *Z* | 2 | 4 | 1 |
| Radiation, λ (Å) | Cu Kα, 1.54184 | Mo Kα, 0.71073 | Mo Kα, 0.71073 |
| Temp (K) | 150(2) | 123(2) | 123(2) |
| $\rho_{calc}$ (g cm$^{-3}$) | 1.120 | 1.099 | 1.113 |
| μ (mm$^{-1}$) | 1.190 | 0.126 | 0.132 |
| Reflections collected | 10271 | 84107 | 15265 |
| Independent reflections | 7541 | 11987 | 5030 |
| Parameters | 705 | 599 | 281 |
| R(int) | 0.0650 | 0.0418 | 0.0372 |
| R1/wR2,[a] $I \geq 2\sigma I$ (%) | 0.1663 | 0.0393 | 0.0446 |
| R1/wR2,[a] all data (%) | 0.1820 | 0.1042 | 0.1102 |
| GOF | 1.062 | 1.038 | 1.040 |

$R1 = [\Sigma||F_o| - |F_c||]/\Sigma|F_o|$; $wR2 = \{[\Sigma w[(F_o)^2 - (F_c)^2]^2]/[\Sigma w(F_o^2)^2\}^{1/2}$; $w = [\sigma^2(F_o)^2 + (AP)^2 + BP]^{-1}$, where $P = [(F_o)^2 + 2(F_c)^2]/3$ and the A and B values are 0.0940 and 0.7043 for **5/6**, 0.0493 and 3.0684 for **8**, and 0.0411 and 0.5436 for **9**.

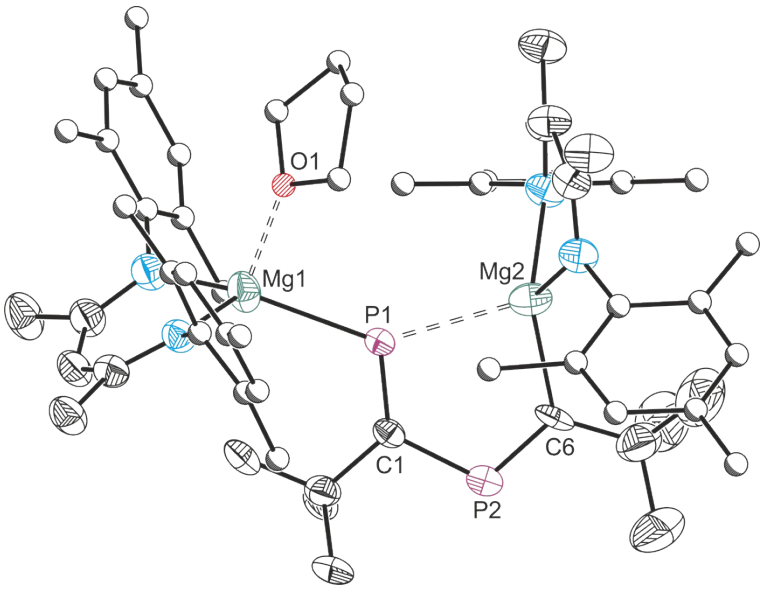



*Figure S 36. ORTEP diagram of* ***5*** *(50% thermal ellipsoids; hydrogen atoms omitted).*

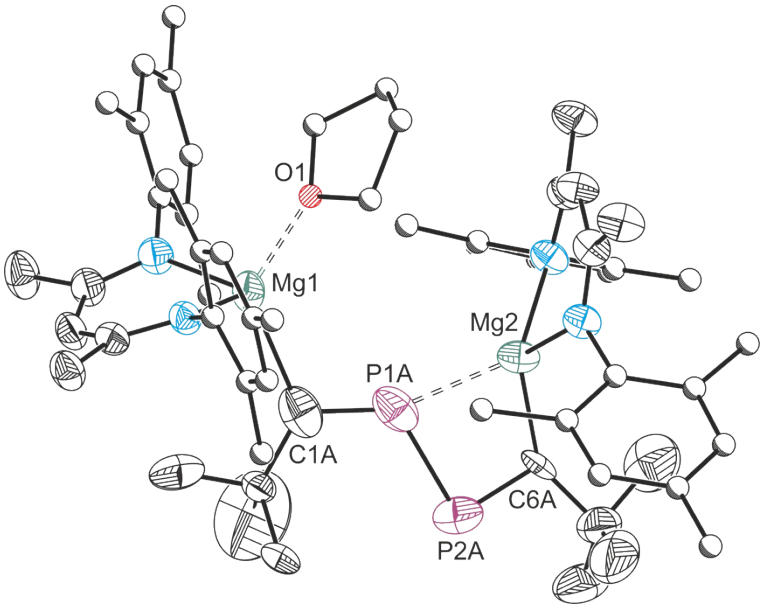



*Figure S 37. ORTEP diagram of* ***6*** *(50% thermal ellipsoids; hydrogen atoms omitted).*

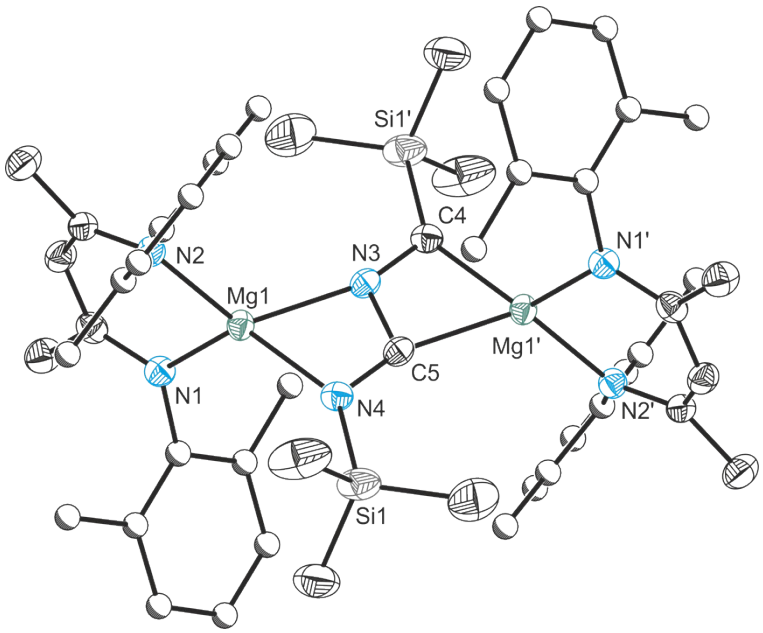



*Figure S 38. ORTEP diagram of* ***9****. (25% thermal ellipsoids; hydrogen atoms omitted). Selected bond lengths (Å) and angles (º): Mg(1)-N(1) 2.0173(15), Mg(1)-N(2) 2.0203(15), Mg(1)-C(5) 2.5708(16), Mg(1)-C(4) 2.1237(17), Mg(1)-C(5)' 2.1212(16), C(4)-Si(1) 1.8081(17), C(4)-C(5 1.312(2). C(5)-C(5)' 1.480(3), C(4)-Mg(1)-C(5)' 65.75(6), C(4)-C(5)-C(5)' 111.09(17).*

## 3. Computational Studies

Geometry optimizations were performed using Becke's 3-parameter hybrid functional,[9] combined with the nonlocal correlation functional provided by Perdew–Wang.[10] The 6-31+G(d) all-electron basis set was used for all atoms.[1`] Dispersion effects were also considered using the third generation of Grimme's dispersion corrections with the Becke-Johnson damping model.[12] Natural bond order analysis (NBO) was performed using Weinhold's methodology.[13] All calculations were performed with the Gaussian16 suite of programs.[14] Images were created using VMD.[15] Calculated $^{31}$P NMR shifts were referenced to phosphoric acid (calculated: 370.1 ppm; given a refence value of 0.0 ppm).

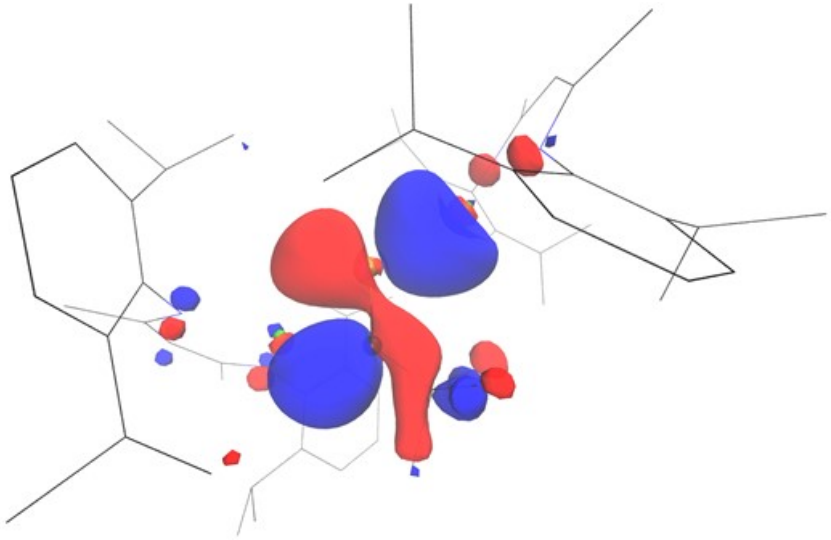
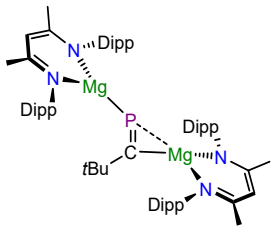


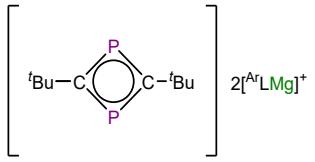
*Figure S 39. HOMO of **1**.*

*Table S 3. Calculated $^{31}P$ NMR chemical shifts of isolated and proposed species in this study, referenced to phosphoric acid (calculated at 370.1 ppm and set a reference value of 0.0 ppm). Where phosphorus environments are chemically equivalent, an average of calculated values is given. Formal charges in the structures omitted for clarity. Ar = Mes. THF = tetrahydrofuran. *proposed species*

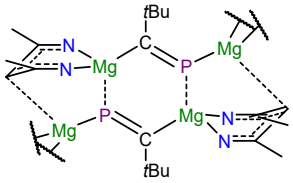
| Compound | Theoretical NMR Shift (ppm) | Observed NMR shift (ppm) |
|---|---|---|
| **1** | 361.0 | 361.0 |
| **2** | 205.9 | 202.3 |
| **3 (metallocycle)** | 388.5 | |
| **4(THF)** | 424.7 | |
| **4(THF)$_2$*** | 431.0 | 445.9 |
| **5(THF)** | 251.7, 331.5 | 251.7, 331.5 |
| **5(THF)$_2$*** | 239.7, 523.7 | |
| **6(THF)** | 283.7, 376.9 | |
| **6(THF)$_2$*** | 336.0 | 351.3 |
| **A*** | 297.7, 375.8 | 287.1, 382.4 |



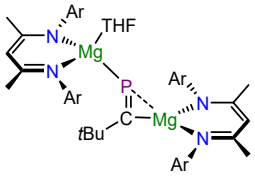

**1**



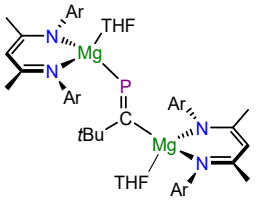

**2**



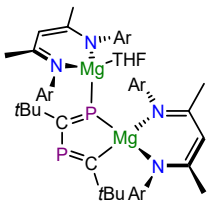

**3**



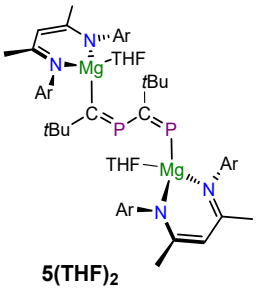

**4(THF)**



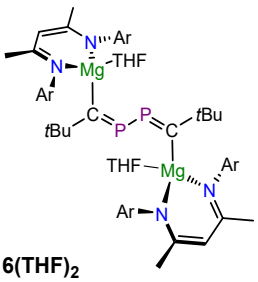

**4(THF)$_2$**



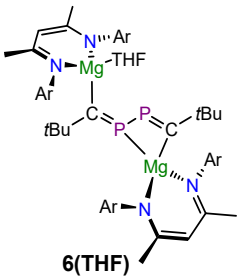

**5(THF)**



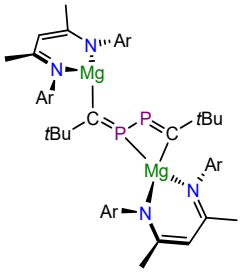

**5(THF)$_2$**




**6(THF)$_2$**




**6(THF)**




**A**

1

E(RB3PW91) = -3415.59680464 au

| | | | |
|---|---|---|---|
| Mg | 2.446643 | -0.199125 | 0.226257 |
| N | 3.671891 | -1.793683 | -0.075793 |
| N | 3.869514 | 0.871295 | 1.203208 |
| P | -0.012646 | -0.080216 | 0.234476 |
| C | 4.818027 | -1.965103 | 0.579736 |
| C | 5.390864 | -0.999559 | 1.430767 |
| H | 6.317337 | -1.299085 | 1.908154 |
| C | 5.000714 | 0.332504 | 1.662417 |
| C | 5.602356 | -3.240484 | 0.382114 |
| H | 4.940457 | -4.104309 | 0.276046 |
| H | 6.287710 | -3.408390 | 1.216652 |
| H | 6.198549 | -3.182805 | -0.536171 |
| C | 5.943408 | 1.183414 | 2.480001 |
| H | 6.111183 | 2.153509 | 2.001623 |
| H | 6.904201 | 0.683814 | 2.621078 |
| H | 5.515438 | 1.392770 | 3.466624 |
| C | 3.281425 | -2.733910 | -1.071741 |
| C | 3.914797 | -2.707926 | -2.332781 |
| C | 3.479544 | -3.599899 | -3.314944 |
| H | 3.950997 | -3.590813 | -4.294283 |
| C | 2.436357 | -4.486740 | -3.067407 |
| H | 2.109795 | -5.174583 | -3.843408 |
| C | 1.791438 | -4.468201 | -1.835431 |
| H | 0.951666 | -5.134556 | -1.662730 |
| C | 2.186865 | -3.588066 | -0.824607 |
| C | 4.962720 | -1.659847 | -2.663521 |
| H | 5.352877 | -1.252243 | -1.725956 |
| C | 6.149346 | -2.215131 | -3.454750 |
| H | 5.858127 | -2.524589 | -4.465169 |
| H | 6.593238 | -3.084030 | -2.955914 |
| H | 6.925340 | -1.448055 | -3.560366 |
| C | 4.300664 | -0.498580 | -3.416149 |
| H | 3.878807 | -0.841381 | -4.368197 |
| H | 5.025412 | 0.296928 | -3.626080 |
| H | 3.478808 | -0.066634 | -2.836049 |
| C | 1.441205 | -3.544005 | 0.495095 |
| H | 1.532625 | -2.521787 | 0.888293 |
| C | 2.078624 | -4.473262 | 1.533871 |
| H | 2.061887 | -5.512529 | 1.183060 |
| H | 1.526508 | -4.423702 | 2.480070 |
| H | 3.119269 | -4.197525 | 1.733617 |
| C | -0.052791 | -3.821442 | 0.344656 |
| H | -0.492325 | -3.205511 | -0.445104 |
| H | -0.576304 | -3.586242 | 1.274486 |
| H | -0.256903 | -4.874374 | 0.118562 |
| C | 3.627794 | 2.261707 | 1.400228 |
| C | 3.824742 | 3.133341 | 0.307836 |
| C | 3.615536 | 4.500977 | 0.499909 |
| H | 3.771077 | 5.189342 | -0.325651 |
| C | 3.195787 | 4.995326 | 1.731125 |
| H | 3.038653 | 6.062691 | 1.864496 |
| C | 2.936410 | 4.115919 | 2.776889 |
| H | 2.560337 | 4.504440 | 3.719742 |
| C | 3.131798 | 2.739861 | 2.629156 |
| C | 4.263787 | 2.586827 | -1.038540 |
| H | 3.833748 | 1.579228 | -1.135884 |
| C | 5.785223 | 2.411485 | -1.108841 |
| H | 6.083312 | 2.032561 | -2.093554 |
| H | 6.141712 | 1.703423 | -0.355517 |
| H | 6.288803 | 3.371981 | -0.945475 |
| C | 3.753224 | 3.406975 | -2.222649 |
| H | 4.267205 | 4.372423 | -2.300701 |
| H | 2.677784 | 3.596036 | -2.145250 |
| H | 3.936200 | 2.864370 | -3.156537 |
| C | 2.726607 | 1.784178 | 3.734603 |
| H | 3.195036 | 0.815260 | 3.531332 |
| C | 3.176442 | 2.238574 | 5.125586 |
| H | 4.250571 | 2.454515 | 5.153975 |
| H | 2.964929 | 1.457321 | 5.864744 |
| H | 2.647083 | 3.142660 | 5.448200 |
| C | 1.206505 | 1.573548 | 3.696470 |
| H | 0.680831 | 2.517483 | 3.885558 |
| H | 0.895967 | 0.851483 | 4.460189 |
| H | 0.871991 | 1.200341 | 2.722200 |
| C | -0.831833 | 0.000812 | -1.259593 |
| Mg | -2.506901 | 0.120507 | 0.002350 |
| N | -3.642409 | 1.826860 | 0.021557 |
| N | -3.838090 | -0.892302 | 1.183929 |
| C | -4.710573 | 2.021335 | 0.782689 |
| C | -5.267322 | 1.025008 | 1.610147 |
| H | -6.145866 | 1.330505 | 2.168815 |
| C | -4.916052 | -0.331267 | 1.737011 |
| C | -5.435871 | 3.348247 | 0.750915 |
| H | -4.775495 | 4.161238 | 0.440640 |
| H | -5.855707 | 3.577838 | 1.734653 |
| H | -6.268366 | 3.314895 | 0.037441 |
| C | -5.856700 | -1.195872 | 2.543237 |
| H | -6.162315 | -2.072025 | 1.960578 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -6.748222 | -0.639508 | 2.840184 | C | -3.456782 | -2.799990 | -2.097892 |
| H | -5.369376 | -1.578571 | 3.445003 | H | -3.156119 | -3.843864 | -2.249086 |
| C | -3.267040 | 2.765418 | -0.975053 | H | -2.554112 | -2.223197 | -1.863156 |
| C | -4.015287 | 2.843745 | -2.170370 | H | -3.862379 | -2.421255 | -3.043560 |
| C | -3.557510 | 3.685441 | -3.187071 | C | -2.572401 | -1.805730 | 3.674414 |
| H | -4.114932 | 3.755957 | -4.117170 | H | -2.973803 | -0.813056 | 3.445664 |
| C | -2.385847 | 4.421977 | -3.037271 | C | -3.079179 | -2.216187 | 5.061423 |
| H | -2.040825 | 5.066056 | -3.842515 | H | -4.165128 | -2.361162 | 5.075987 |
| C | -1.652053 | 4.323852 | -1.858784 | H | -2.829292 | -1.444206 | 5.798790 |
| H | -0.734024 | 4.894802 | -1.752933 | H | -2.617222 | -3.151868 | 5.398088 |
| C | -2.072379 | 3.498706 | -0.812066 | C | -1.042580 | -1.690905 | 3.676491 |
| C | -5.236465 | 1.964482 | -2.382683 | H | -0.579963 | -2.665025 | 3.879903 |
| H | -5.648474 | 1.707298 | -1.403342 | H | -0.711514 | -0.990186 | 4.452225 |
| C | -6.349818 | 2.650642 | -3.176190 | H | -0.678441 | -1.330006 | 2.709457 |
| H | -6.066467 | 2.817004 | -4.222105 | C | -0.221726 | 0.082942 | -2.646703 |
| H | -6.611395 | 3.621794 | -2.740569 | C | -1.322096 | 0.362071 | -3.676883 |
| H | -7.248954 | 2.023397 | -3.181074 | H | -2.055912 | -0.450369 | -3.679586 |
| C | -4.829461 | 0.641661 | -3.041021 | H | -1.846028 | 1.292498 | -3.434383 |
| H | -4.426703 | 0.811566 | -4.046173 | H | -0.905677 | 0.451809 | -4.689874 |
| H | -5.689579 | -0.034519 | -3.120230 | C | 0.457447 | -1.253983 | -2.975293 |
| H | -4.049730 | 0.137413 | -2.461333 | H | 0.860874 | -1.246443 | -3.995722 |
| C | -1.289295 | 3.413441 | 0.483732 | H | 1.282253 | -1.460957 | -2.286540 |
| H | -1.407719 | 2.394066 | 0.871959 | H | -0.249475 | -2.086353 | -2.892039 |
| C | -1.865427 | 4.363126 | 1.541100 | C | 0.809221 | 1.214876 | -2.730544 |
| H | -1.822722 | 5.402896 | 1.193362 | H | 0.329710 | 2.184798 | -2.562407 |
| H | -1.288791 | 4.290554 | 2.471445 | H | 1.590637 | 1.095866 | -1.966402 |
| H | -2.907484 | 4.122503 | 1.771458 | H | 1.300517 | 1.231661 | -3.711304 |
| C | 0.207924 | 3.649007 | 0.309849 | | | | |
| H | 0.621616 | 3.011567 | -0.475540 | 2 | | | |
| H | 0.735869 | 3.414569 | 1.238139 | E(RB3PW91) = -3481.21299097 au | | | |
| H | 0.439134 | 4.692689 | 0.067060 | P | -0.001562 | 1.537282 | 0.000027 |
| C | -3.607403 | -2.285314 | 1.382139 | C | -0.404661 | 0.157801 | -1.109622 |
| C | -3.915035 | -3.180592 | 0.336427 | P | 0.001342 | -1.243923 | 0.000524 |
| C | -3.660344 | -4.542923 | 0.516374 | C | 0.404541 | 0.159025 | 1.110087 |
| H | -3.893105 | -5.239813 | -0.285514 | C | 0.453980 | 0.184850 | 2.624840 |
| C | -3.120668 | -5.021306 | 1.704710 | C | -0.969504 | 0.075082 | 3.199712 |
| H | -2.934312 | -6.084725 | 1.833294 | H | -1.589721 | 0.916207 | 2.864853 |
| C | -2.799345 | -4.126489 | 2.720424 | H | -0.968675 | 0.092790 | 4.297592 |
| H | -2.350569 | -4.500635 | 3.637577 | H | -1.447146 | -0.858916 | 2.886160 |
| C | -3.020418 | -2.754262 | 2.577873 | C | 1.078652 | 1.502752 | 3.096399 |
| C | -4.494903 | -2.686017 | -0.975247 | H | 2.094513 | 1.617843 | 2.708846 |
| H | -4.739151 | -1.625547 | -0.846981 | H | 1.119224 | 1.545780 | 4.192216 |
| C | -5.795378 | -3.403881 | -1.347266 | H | 0.504031 | 2.367028 | 2.746775 |
| H | -6.226477 | -2.962759 | -2.253895 | C | 1.302276 | -0.985036 | 3.133815 |
| H | -6.535303 | -3.325296 | -0.542877 | H | 0.954954 | -1.942845 | 2.733081 |
| H | -5.627876 | -4.469170 | -1.545580 | H | 1.280418 | -1.043932 | 4.229559 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 2.344410 | -0.864972 | 2.821268 | C | -4.053727 | 2.881972 | -1.216806 |
| C | -0.454222 | 0.182896 | -2.624400 | C | -4.787232 | 1.766369 | -1.906813 |
| C | 0.969471 | 0.075976 | -3.199339 | H | -4.117126 | 0.926038 | -2.125363 |
| H | 1.587875 | 0.918556 | -2.864824 | H | -5.211843 | 2.105802 | -2.856653 |
| H | 0.968490 | 0.093296 | -4.297226 | H | -5.597478 | 1.359983 | -1.291302 |
| H | 1.449269 | -0.856851 | -2.885562 | C | -3.864988 | 4.108900 | -1.854107 |
| C | -1.081662 | 1.499309 | -3.096480 | H | -4.262177 | 4.245840 | -2.859110 |
| H | -2.097924 | 1.612252 | -2.709346 | C | -3.178272 | 5.158371 | -1.239384 |
| H | -1.121952 | 1.541971 | -4.192323 | C | -2.940634 | 6.457132 | -1.962292 |
| H | -0.509065 | 2.364938 | -2.746866 | H | -2.025290 | 6.409316 | -2.567238 |
| C | -1.300140 | -0.988922 | -3.132852 | H | -2.825557 | 7.290548 | -1.260909 |
| H | -0.950936 | -1.945899 | -2.731761 | H | -3.767067 | 6.696408 | -2.640649 |
| H | -1.278233 | -1.048214 | -4.228573 | C | -2.699759 | 4.956923 | 0.055497 |
| H | -2.342492 | -0.870838 | -2.820285 | H | -2.174047 | 5.765787 | 0.561155 |
| Mg | -2.161724 | 0.046940 | 0.343365 | C | -2.865611 | 3.743674 | 0.728205 |
| N | -3.422170 | -1.542581 | 0.739528 | C | -2.312158 | 3.567914 | 2.111386 |
| C | -3.087249 | -2.803272 | 0.161056 | H | -2.984101 | 2.996863 | 2.759769 |
| C | -3.537880 | -3.079803 | -1.145021 | H | -2.114449 | 4.536381 | 2.581734 |
| C | -4.528629 | -2.169408 | -1.813760 | H | -1.364988 | 3.019108 | 2.065892 |
| H | -5.544567 | -2.338095 | -1.431679 | C | -5.727243 | 2.228185 | 1.692386 |
| H | -4.549626 | -2.331620 | -2.895813 | H | -6.190302 | 2.595863 | 0.768905 |
| H | -4.305026 | -1.117551 | -1.618665 | H | -5.224558 | 3.087454 | 2.148188 |
| C | -3.072044 | -4.220272 | -1.799490 | H | -6.518824 | 1.882054 | 2.360730 |
| H | -3.405471 | -4.413716 | -2.818434 | Mg | 2.161617 | 0.051147 | -0.343233 |
| C | -2.190473 | -5.112787 | -1.184265 | N | 3.648856 | 1.414529 | -0.679812 |
| C | -1.815994 | -4.853955 | 0.132821 | C | 3.530432 | 2.702654 | -0.078414 |
| H | -1.151544 | -5.547064 | 0.645444 | C | 2.857642 | 3.749437 | -0.728361 |
| C | -2.245643 | -3.714869 | 0.818034 | C | 2.304244 | 3.572321 | -2.111386 |
| C | -1.770774 | -3.486232 | 2.222635 | H | 2.978247 | 3.004554 | -2.760532 |
| H | -0.783677 | -3.010377 | 2.214694 | H | 2.102183 | 4.540262 | -2.580952 |
| H | -1.673002 | -4.436042 | 2.759698 | H | 1.359458 | 3.019440 | -2.065755 |
| H | -2.444981 | -2.837316 | 2.787215 | C | 2.689459 | 4.962259 | -0.055647 |
| C | -1.646369 | -6.303023 | -1.927286 | H | 2.161989 | 5.770075 | -0.561160 |
| H | -2.401426 | -6.749731 | -2.583993 | C | 3.167874 | 5.164628 | 1.239226 |
| H | -1.296168 | -7.078776 | -1.237908 | C | 3.856906 | 4.116640 | 1.853685 |
| H | -0.795293 | -6.016228 | -2.559529 | H | 4.254083 | 4.254386 | 2.858572 |
| C | -4.550153 | -1.412538 | 1.430628 | C | 4.048091 | 2.890056 | 1.216262 |
| C | -5.337769 | -2.651043 | 1.788009 | C | 4.784067 | 1.776014 | 1.906187 |
| H | -5.713384 | -3.138509 | 0.880891 | H | 4.115186 | 0.935322 | 2.127222 |
| H | -6.189164 | -2.410616 | 2.428808 | H | 5.210183 | 2.117053 | 2.854781 |
| H | -4.705504 | -3.387028 | 2.295848 | H | 5.593474 | 1.369636 | 1.289607 |
| C | -5.093756 | -0.172187 | 1.823366 | C | 2.927271 | 6.462917 | 1.962000 |
| H | -5.991307 | -0.230266 | 2.429056 | H | 2.827616 | 7.298945 | 1.261302 |
| C | -4.748231 | 1.119721 | 1.382695 | H | 3.744907 | 6.695332 | 2.653206 |
| N | -3.652011 | 1.407149 | 0.679325 | H | 2.002624 | 6.419063 | 2.552951 |
| C | -3.536008 | 2.695576 | 0.078094 | C | 4.745597 | 1.129352 | -1.383296 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 5.722328 | 2.239808 | -1.693068 | N | -2.394449 | 1.885843 | -2.045072 |
| H | 5.217787 | 3.098379 | -2.148121 | N | -5.883161 | 0.908602 | 1.542224 |
| H | 6.514146 | 1.895472 | -2.362060 | N | -5.190947 | -1.953743 | 1.308673 |
| H | 6.185289 | 2.607862 | -0.769682 | C | 3.821909 | -0.952895 | 2.341890 |
| C | 5.093865 | -0.161866 | -1.823829 | C | -3.900467 | -0.708756 | -2.311666 |
| H | 5.991557 | -0.218105 | -2.429482 | C | 3.855676 | 1.547825 | 1.967353 |
| C | 4.553055 | -1.403318 | -1.430707 | C | -3.703115 | 1.778470 | -1.888269 |
| N | 3.425290 | -1.535650 | -0.739702 | C | 5.876313 | -3.811423 | 0.274953 |
| C | 3.093018 | -2.796916 | -0.160964 | C | -2.246534 | -2.089062 | -3.340710 |
| C | 3.543909 | -3.072257 | 1.145200 | C | 6.515211 | 0.293643 | -2.632977 |
| C | 3.080487 | -4.213790 | 1.799645 | C | 2.086995 | 3.075928 | 2.456551 |
| H | 3.414096 | -4.406401 | 2.818683 | C | 6.211867 | 2.083264 | -1.084132 |
| C | 2.201160 | -5.108339 | 1.184289 | C | 5.871533 | -2.153436 | -2.434470 |
| C | 1.659295 | -6.299641 | 1.927229 | C | 6.421738 | -1.033799 | -3.086594 |
| H | 2.412572 | -6.739654 | 2.590426 | H | 6.933145 | -1.243727 | -4.018568 |
| H | 1.318458 | -7.079647 | 1.237934 | C | 2.048884 | -2.180251 | 3.357494 |
| H | 0.802156 | -6.016120 | 2.552744 | C | 4.884296 | -3.305241 | -0.589014 |
| C | 1.826377 | -4.850466 | -0.132970 | C | -6.521159 | 0.446816 | 2.634392 |
| H | 1.163660 | -5.545146 | -0.645717 | C | 0.939883 | 0.150456 | -2.215935 |
| C | 2.253552 | -3.710464 | -0.818095 | C | -4.944867 | -3.165745 | 0.581916 |
| C | 1.778157 | -3.482412 | -2.222588 | C | -4.371113 | 0.513127 | -1.725287 |
| H | 0.792675 | -3.003258 | -2.214314 | H | -5.456961 | 0.600032 | -1.713806 |
| H | 1.676669 | -4.432664 | -2.758118 | C | -1.815600 | 3.142626 | -2.415926 |
| H | 2.453781 | -2.836404 | -2.788875 | C | -6.234085 | 2.204915 | 1.047628 |
| C | 4.532448 | -2.159617 | 1.814158 | C | -2.555891 | -2.157912 | -4.713414 |
| H | 5.549036 | -2.326893 | 1.433173 | C | 1.765835 | 4.012898 | 1.458198 |
| H | 4.552731 | -2.320950 | 2.896357 | C | 7.310752 | 2.249794 | -0.219244 |
| H | 4.307208 | -1.108305 | 1.618037 | C | 3.644196 | -3.964910 | -0.713309 |
| C | 5.343629 | -2.640134 | -1.787409 | C | 1.538651 | 0.144994 | -3.619005 |
| H | 6.194788 | -2.397949 | -2.427853 | C | 4.408842 | 0.230695 | 1.779588 |
| H | 4.713310 | -3.377706 | -2.295371 | H | 5.497473 | 0.216675 | 1.795840 |
| H | 5.719880 | -3.126515 | -0.879977 | C | 5.437017 | 3.191956 | -1.477681 |
| | | | | C | -1.533196 | 0.303017 | 3.625360 |
| 3 | | | | C | -5.920487 | -2.008413 | 2.433571 |
| E(RB3PW91) = -5886.91045687 au | | | | C | -1.464240 | -3.100050 | -2.743573 |
| P | 1.888319 | 0.069915 | -0.760501 | C | -3.719366 | -3.849411 | 0.722773 |
| P | -1.872745 | 0.085581 | 0.777823 | C | -6.442851 | -0.878802 | 3.093656 |
| Mg | 1.138047 | 0.263264 | 1.678345 | H | -6.953526 | -1.079921 | 4.028037 |
| Mg | -1.115061 | 0.261888 | -1.657926 | C | 2.305545 | -2.249152 | 4.740345 |
| Mg | 4.366259 | -0.289595 | -0.640510 | C | -0.925578 | 0.230859 | 2.227673 |
| Mg | -4.362914 | -0.161151 | 0.667647 | C | -5.454253 | 3.327261 | 1.386759 |
| N | 2.558022 | 1.770072 | 2.098616 | C | -5.927608 | -3.644978 | -0.307524 |
| N | 2.520183 | -1.085439 | 2.564822 | C | 5.585447 | -4.931972 | 1.063341 |
| N | -2.616141 | -0.960056 | -2.543609 | H | 6.342721 | -5.303294 | 1.750703 |
| N | 5.146167 | -2.091124 | -1.305939 | C | 1.904949 | 3.384362 | 3.818414 |
| N | 5.877381 | 0.770624 | -1.548441 | C | 4.292130 | 3.007455 | -2.431514 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 4.628961 | 2.614190 | -3.397846 | H | 1.739095 | -4.148485 | -1.691011 |
| H | 3.770449 | 3.951663 | -2.610054 | H | 3.034018 | -3.555624 | -2.743616 |
| H | 3.563940 | 2.286977 | -2.042015 | C | -6.253053 | -3.359981 | 3.027571 |
| C | 3.390259 | -5.074461 | 0.101345 | H | -6.998418 | -3.881872 | 2.416319 |
| H | 2.424498 | -5.568530 | 0.023759 | H | -6.656373 | -3.251727 | 4.036636 |
| C | 4.828205 | 2.693129 | 2.095975 | H | -5.369318 | -4.004121 | 3.064095 |
| H | 4.702591 | 3.415841 | 1.284064 | C | -7.408255 | 1.392613 | 3.414527 |
| H | 5.859553 | 2.346121 | 2.077438 | H | -6.875589 | 2.316801 | 3.662094 |
| H | 4.649275 | 3.233264 | 3.032323 | H | -7.757233 | 0.926543 | 4.338064 |
| C | 1.232492 | -3.150344 | 2.740670 | H | -8.284197 | 1.685814 | 2.823940 |
| C | -4.573642 | 3.005162 | -1.985282 | C | 7.417946 | 1.222574 | -3.415692 |
| H | -4.149127 | 3.844764 | -1.431060 | H | 6.894492 | 2.145168 | -3.687240 |
| H | -5.577012 | 2.811295 | -1.609975 | H | 7.778857 | 0.739694 | -4.325803 |
| H | -4.652104 | 3.318512 | -3.034382 | H | 8.285783 | 1.521614 | -2.816168 |
| C | -4.963895 | -1.700382 | -2.710713 | C | 7.220324 | -3.138490 | 0.364421 |
| H | -5.255604 | -1.545817 | -3.755633 | H | 7.866007 | -3.402741 | -0.483572 |
| H | -5.856505 | -1.564460 | -2.099107 | H | 7.743913 | -3.428430 | 1.280810 |
| H | -4.615162 | -2.728588 | -2.604460 | H | 7.118566 | -2.048525 | 0.339106 |
| C | 4.335503 | -5.559378 | 1.013832 | C | -7.678320 | 3.610668 | -0.292235 |
| C | -7.351537 | 2.340019 | 0.200010 | H | -8.540888 | 3.716136 | -0.946818 |
| C | -2.121901 | -3.271009 | -5.449823 | C | -7.273741 | -2.975822 | -0.392848 |
| H | -2.356124 | -3.316631 | -6.511688 | H | -7.961319 | -3.356016 | 0.374903 |
| C | -5.630438 | -4.747210 | -1.119693 | H | -7.741285 | -3.153723 | -1.366628 |
| H | -6.377475 | -5.093101 | -1.831238 | H | -7.190758 | -1.897869 | -0.225789 |
| C | 1.375181 | 4.632937 | 4.164236 | C | -1.335591 | 4.020027 | -1.427175 |
| H | 1.223284 | 4.866265 | 5.215982 | C | 0.978726 | -4.303982 | 4.880413 |
| C | 7.617986 | 3.534446 | 0.246766 | C | 1.252310 | 5.256226 | 1.847068 |
| H | 8.465920 | 3.663321 | 0.916223 | H | 1.016997 | 5.987650 | 1.076959 |
| C | -2.720632 | -3.432599 | 1.764782 | C | -1.062594 | -4.196583 | -3.508097 |
| H | -2.360590 | -2.410306 | 1.604706 | H | -0.471725 | -4.977503 | -3.033637 |
| H | -1.854283 | -4.097562 | 1.758366 | C | -4.389579 | -5.390777 | -1.059122 |
| H | -3.156688 | -3.453131 | 2.770726 | C | 0.723867 | -4.201893 | 3.505359 |
| C | 4.778976 | -2.044934 | 2.745166 | H | 0.107840 | -4.954865 | 3.018342 |
| H | 5.009740 | -1.972059 | 3.813982 | C | -3.463486 | -4.946404 | -0.107462 |
| H | 5.717034 | -1.953859 | 2.198139 | H | -2.509206 | -5.459658 | -0.014975 |
| H | 4.356142 | -3.034175 | 2.560761 | C | -6.916269 | 4.741829 | 0.027190 |
| C | 6.157215 | -3.508102 | -3.046297 | C | 1.380272 | 1.585111 | -4.161787 |
| H | 6.847868 | -4.085242 | -2.421076 | H | 0.336613 | 1.901855 | -4.117624 |
| H | 6.601853 | -3.400819 | -4.037793 | H | 1.720899 | 1.635396 | -5.205235 |
| H | 5.240956 | -4.100988 | -3.130364 | H | 1.961097 | 2.293645 | -3.566321 |
| C | -1.388662 | -4.307138 | -4.867360 | C | -4.277813 | 3.169994 | 2.306146 |
| C | -5.808602 | 4.578582 | 0.869362 | H | -4.581556 | 2.803485 | 3.293805 |
| H | -5.204211 | 5.444615 | 1.130991 | H | -3.750822 | 4.118538 | 2.441782 |
| C | -1.683813 | 3.454785 | -3.782651 | H | -3.562662 | 2.437222 | 1.914398 |
| C | 2.628679 | -3.514931 | -1.725397 | C | 5.768103 | 4.458326 | -0.980246 |
| H | 2.310971 | -2.479890 | -1.559171 | H | 5.165165 | 5.312997 | -1.279542 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 8.127136 | 1.057696 | 0.201750 | H | -3.341743 | -0.037015 | 4.788922 |
| H | 7.494895 | 0.292838 | 0.667741 | H | -3.178892 | -1.112979 | 3.388268 |
| H | 8.904041 | 1.347567 | 0.915503 | C | -1.360291 | 1.767336 | 4.094325 |
| H | 8.612071 | 0.568987 | -0.651805 | H | -0.313757 | 2.073921 | 4.033526 |
| C | -3.279556 | -1.049164 | -5.433115 | H | -1.700190 | 1.875050 | 5.133688 |
| H | -3.431671 | -0.180903 | -4.790245 | H | -1.937109 | 2.447435 | 3.462235 |
| H | -4.260794 | -1.379481 | -5.798504 | C | 0.408020 | -5.443191 | 5.685780 |
| H | -2.703248 | -0.723303 | -6.307265 | H | -0.687023 | -5.465886 | 5.622527 |
| C | 1.762975 | -3.313563 | 5.476136 | H | 0.680500 | -5.357115 | 6.742451 |
| H | 1.953088 | -3.357703 | 6.546810 | H | 0.774618 | -6.411852 | 5.322903 |
| C | 6.853251 | 4.650486 | -0.114311 | C | 7.164447 | 6.017593 | 0.438753 |
| C | 1.036135 | 5.581716 | 3.191394 | H | 6.505213 | 6.260593 | 1.282785 |
| C | -1.027332 | -2.965397 | -1.319583 | H | 7.024469 | 6.796658 | -0.318789 |
| H | -0.184766 | -2.264506 | -1.235394 | H | 8.196816 | 6.075915 | 0.798601 |
| H | -0.693030 | -3.926585 | -0.925205 | C | 0.691606 | -0.798389 | -4.497917 |
| H | -1.826287 | -2.590756 | -0.678892 | H | 0.722028 | -1.826425 | -4.121823 |
| C | -8.164341 | 1.130951 | -0.177046 | H | 1.059848 | -0.794374 | -5.532611 |
| H | -7.533613 | 0.364318 | -0.642287 | H | -0.355218 | -0.480184 | -4.503361 |
| H | -8.959364 | 1.397907 | -0.879594 | C | -4.036822 | -6.501171 | -2.014057 |
| H | -8.625096 | 0.654581 | 0.696603 | H | -4.933047 | -6.957779 | -2.446777 |
| C | 3.011432 | -0.274557 | -3.728805 | H | -3.458515 | -7.289043 | -1.517991 |
| H | 3.666980 | 0.402384 | -3.175260 | H | -3.424768 | -6.114327 | -2.839821 |
| H | 3.336407 | -0.261707 | -4.776880 | C | -7.253076 | 6.092964 | -0.549627 |
| H | 3.165784 | -1.283833 | -3.338371 | H | -7.102024 | 6.890608 | 0.186151 |
| C | 2.281737 | 2.381931 | 4.873766 | H | -8.294267 | 6.134292 | -0.885610 |
| H | 1.816969 | 1.411168 | 4.676703 | H | -6.616604 | 6.322005 | -1.414824 |
| H | 1.969041 | 2.720290 | 5.865956 | C | 3.095211 | -1.190382 | 5.465711 |
| H | 3.365555 | 2.208838 | 4.898596 | H | 4.027114 | -1.598196 | 5.878967 |
| C | 1.994285 | 3.685982 | 0.012598 | H | 2.516700 | -0.790992 | 6.307305 |
| H | 3.034232 | 3.399537 | -0.162782 | H | 3.350853 | -0.356442 | 4.810480 |
| H | 1.759308 | 4.537590 | -0.629711 | C | -0.947175 | -5.503994 | -5.670091 |
| H | 1.385412 | 2.837353 | -0.316917 | H | -1.175375 | -5.374768 | -6.732848 |
| C | -1.516797 | 3.692496 | 0.025665 | H | -1.448899 | -6.419378 | -5.330049 |
| H | -2.573084 | 3.533128 | 0.261694 | H | 0.132592 | -5.671168 | -5.575423 |
| H | -1.134546 | 4.490822 | 0.665521 | C | 3.994407 | -6.699167 | 1.938526 |
| H | -1.005900 | 2.764360 | 0.302938 | H | 4.894942 | -7.140865 | 2.377405 |
| C | 0.891010 | -3.021624 | 1.290124 | H | 3.448038 | -7.491767 | 1.414313 |
| H | 0.101939 | -2.272231 | 1.140611 | H | 3.356723 | -6.350531 | 2.761757 |
| H | 0.525099 | -3.970101 | 0.892011 | C | -1.046040 | 4.646759 | -4.144497 |
| H | 1.750380 | -2.707508 | 0.697004 | H | -0.930437 | 4.881532 | -5.200601 |
| C | -2.210204 | 2.508331 | -4.826621 | C | -0.550707 | 5.536235 | -3.182323 |
| H | -1.833410 | 1.493925 | -4.661060 | C | -0.718117 | 5.210028 | -1.831395 |
| H | -1.913564 | 2.827928 | -5.829972 | H | -0.360825 | 5.897391 | -1.068103 |
| H | -3.305514 | 2.441783 | -4.801623 | C | 0.166793 | 6.797579 | -3.591479 |
| C | -3.012424 | -0.091967 | 3.743511 | H | 1.224288 | 6.598003 | -3.811580 |
| H | -3.655934 | 0.575108 | 3.163717 | H | 0.132689 | 7.549887 | -2.796190 |

| | | | |
|---|---|---|---|
| H | -0.276309 | 7.236511 | -4.492304 |
| C | -0.708118 | -0.609732 | 4.554861 |
| H | -0.763801 | -1.655283 | 4.234180 |
| H | -1.073355 | -0.540490 | 5.588341 |
| H | 0.345842 | -0.317253 | 4.540845 |
| C | 0.431990 | 6.907291 | 3.579586 |
| H | -0.659268 | 6.830909 | 3.678922 |
| H | 0.639966 | 7.675115 | 2.826618 |
| H | 0.823350 | 7.259481 | 4.540265 |

4(THF)

E(RB3PW91) = -3408.78200840 au

| | | | |
|---|---|---|---|
| Mg | 2.584913 | 0.242142 | 0.285369 |
| N | 4.153691 | 0.177142 | -1.061885 |
| N | 3.300287 | 2.020144 | 1.070566 |
| P | 0.193928 | -0.391849 | 0.442287 |
| C | 5.343021 | 0.679291 | -0.733928 |
| C | 5.555746 | 1.564296 | 0.343616 |
| H | 6.591321 | 1.834467 | 0.525603 |
| C | 4.598174 | 2.292784 | 1.084743 |
| C | 6.565521 | 0.295527 | -1.538155 |
| H | 6.462177 | -0.710296 | -1.955983 |
| H | 7.461617 | 0.336788 | -0.911799 |
| H | 6.722184 | 0.982541 | -2.376943 |
| C | 5.104365 | 3.453377 | 1.908281 |
| H | 4.924801 | 4.399851 | 1.385041 |
| H | 6.179441 | 3.369485 | 2.088007 |
| H | 4.579248 | 3.514026 | 2.867242 |
| C | 3.949680 | -0.399520 | -2.339731 |
| C | 3.980628 | 0.406243 | -3.496530 |
| C | 3.684376 | -0.172203 | -4.733529 |
| H | 3.696996 | 0.460370 | -5.620411 |
| C | 3.345641 | -1.518700 | -4.862451 |
| C | 3.283229 | -2.287704 | -3.698083 |
| H | 2.993529 | -3.335660 | -3.766069 |
| C | 3.565442 | -1.752197 | -2.441739 |
| C | 4.252891 | 1.883303 | -3.415388 |
| H | 5.318996 | 2.118942 | -3.529748 |
| C | 3.411613 | -2.604215 | -1.213699 |
| H | 2.461460 | -2.382348 | -0.706182 |
| C | 2.354011 | 2.924381 | 1.616250 |
| C | 1.989365 | 4.091330 | 0.917834 |
| C | 0.947838 | 4.880928 | 1.415337 |
| H | 0.654358 | 5.767846 | 0.854817 |
| C | 0.268419 | 4.560641 | 2.589309 |
| C | 0.668906 | 3.414840 | 3.280691 |
| H | 0.169877 | 3.151914 | 4.212530 |
| C | 1.683141 | 2.584003 | 2.808306 |
| C | 2.678493 | 4.501095 | -0.355323 |
| H | 3.262335 | 3.682117 | -0.779859 |
| C | 2.037368 | 1.329888 | 3.554622 |
| H | 1.611328 | 0.451958 | 3.052623 |
| C | -0.835394 | 0.468615 | -0.613343 |
| Mg | -2.475592 | -0.492907 | 0.277382 |
| N | -4.434491 | -0.351711 | -0.446517 |
| N | -2.782368 | -2.515144 | 0.701229 |
| C | -5.407676 | -1.191257 | -0.107953 |
| C | -5.200298 | -2.394682 | 0.592714 |
| H | -6.097335 | -2.959735 | 0.822596 |
| C | -3.981690 | -3.064403 | 0.846172 |
| C | -6.829282 | -0.880045 | -0.522426 |
| H | -7.083430 | 0.162260 | -0.300713 |
| H | -7.541244 | -1.538043 | -0.017706 |
| H | -6.955064 | -1.005900 | -1.604213 |
| C | -4.089258 | -4.519731 | 1.246674 |
| H | -3.646846 | -5.153351 | 0.468414 |
| H | -5.131307 | -4.817404 | 1.384964 |
| H | -3.533756 | -4.730173 | 2.166329 |
| C | -4.702608 | 0.646316 | -1.418608 |
| C | -4.677596 | 0.292679 | -2.781669 |
| C | -4.880218 | 1.282896 | -3.743178 |
| H | -4.851580 | 1.005038 | -4.796196 |
| C | -5.088300 | 2.619624 | -3.393774 |
| C | -5.096981 | 2.946899 | -2.037576 |
| H | -5.251909 | 3.983407 | -1.740134 |
| C | -4.904040 | 1.983751 | -1.043762 |
| C | -4.372308 | -1.122692 | -3.183059 |
| H | -3.391022 | -1.423543 | -2.798419 |
| C | -4.900202 | 2.370001 | 0.407026 |
| H | -3.930468 | 2.147872 | 0.864314 |
| C | -1.634171 | -3.338410 | 0.851972 |
| C | -1.017672 | -3.867990 | -0.294663 |
| C | 0.119831 | -4.663002 | -0.146486 |
| H | 0.594590 | -5.070725 | -1.038313 |
| C | 0.662105 | -4.947496 | 1.109148 |
| C | 0.051209 | -4.379519 | 2.229117 |
| H | 0.470918 | -4.563783 | 3.217978 |
| C | -1.072168 | -3.557504 | 2.119478 |
| C | -1.551217 | -3.522921 | -1.654422 |
| H | -2.627479 | -3.710290 | -1.734048 |
| C | -1.625398 | -2.843273 | 3.317441 |
| H | -2.697954 | -3.020706 | 3.455977 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -0.468064 | 1.472745 | -1.681018 | H | 1.878607 | -6.648610 | 0.554724 |
| C | -1.081361 | 1.001200 | -3.008146 | C | 3.056385 | -2.126675 | -6.208559 |
| H | -0.651822 | 0.037892 | -3.309368 | H | 3.935283 | -2.653592 | -6.603633 |
| H | -2.163301 | 0.882518 | -2.906303 | H | 2.239047 | -2.854438 | -6.151978 |
| H | -0.887816 | 1.728351 | -3.809516 | H | 2.776598 | -1.361207 | -6.940114 |
| C | 1.029477 | 1.691412 | -1.879722 | C | -0.887268 | 5.392973 | 3.076023 |
| H | 1.226875 | 2.424661 | -2.671494 | H | -0.803613 | 6.432567 | 2.741817 |
| H | 1.488321 | 2.081065 | -0.962843 | H | -1.841206 | 5.004772 | 2.693258 |
| H | 1.527791 | 0.757651 | -2.166749 | H | -0.949355 | 5.393479 | 4.170173 |
| C | -1.118013 | 2.806937 | -1.273301 | H | 3.361674 | 5.343643 | -0.182947 |
| H | -2.201381 | 2.686709 | -1.168807 | H | 1.947627 | 4.822655 | -1.104919 |
| H | -0.708369 | 3.156158 | -0.317911 | H | 1.639428 | 1.357193 | 4.574494 |
| H | -0.929517 | 3.579453 | -2.032792 | H | 3.119605 | 1.175061 | 3.603548 |
| O | -2.794758 | 0.374604 | 2.150625 | H | 3.718587 | 2.414218 | -4.209783 |
| C | -1.924929 | 1.368036 | 2.741696 | H | 3.931170 | 2.289579 | -2.453199 |
| C | -3.934325 | 0.121249 | 2.988624 | H | 3.391932 | -3.667212 | -1.474550 |
| C | -2.543501 | 1.684881 | 4.098919 | H | 4.217823 | -2.433976 | -0.494073 |
| H | -0.919518 | 0.946271 | 2.783466 | H | -1.037589 | -4.090438 | -2.437146 |
| H | -1.897800 | 2.232623 | 2.070507 | H | -1.394588 | -2.453734 | -1.853481 |
| C | -4.021884 | 1.340138 | 3.892225 | H | -1.106567 | -3.145376 | 4.233433 |
| H | -4.794461 | -0.034921 | 2.334768 | H | -1.493169 | -1.761944 | 3.178053 |
| H | -3.753991 | -0.798879 | 3.557818 | H | -5.102374 | 3.438915 | 0.529663 |
| H | -2.382813 | 2.726978 | 4.388486 | H | -5.652729 | 1.810437 | 0.975973 |
| H | -2.109588 | 1.045040 | 4.876829 | H | -4.361673 | -1.226377 | -4.272573 |
| H | -4.538629 | 2.158092 | 3.377528 | H | -5.094765 | -1.840267 | -2.776982 |
| H | -4.552182 | 1.131256 | 4.826413 | | | | |
| O | 3.316631 | -1.105674 | 1.729897 | 5 | | | |
| C | 4.681304 | -1.261418 | 2.162744 | E(RB3PW91) = -3713.60836304 au | | | |
| C | 2.486416 | -2.169738 | 2.258917 | Mg | 2.228968 | -0.865873 | 0.415191 |
| C | 4.762011 | -2.680253 | 2.704767 | Mg | -2.143782 | 0.863834 | 0.035652 |
| H | 5.329341 | -1.061266 | 1.307475 | N | 2.926368 | -2.784097 | 0.659019 |
| H | 4.885236 | -0.509920 | 2.935849 | N | 4.069296 | -0.040471 | 0.818009 |
| C | 3.358759 | -2.879553 | 3.281058 | N | -3.168622 | -0.369920 | -1.314898 |
| H | 1.575705 | -1.726064 | 2.665284 | N | -1.600449 | 2.090679 | -1.586504 |
| H | 2.195690 | -2.820207 | 1.430938 | P | 0.005198 | -0.010976 | 1.110800 |
| H | 5.559409 | -2.799572 | 3.444442 | P | -2.023596 | 0.762162 | 3.371974 |
| H | 4.941564 | -3.389919 | 1.888235 | C | -0.398228 | 0.074545 | 2.761256 |
| H | 3.275897 | -2.396431 | 4.262135 | C | 0.491324 | -0.388831 | 3.925112 |
| H | 3.081703 | -3.931020 | 3.392161 | C | -2.954692 | 1.155132 | 2.020987 |
| C | -5.252830 | 3.678218 | -4.451387 | C | -4.365399 | 1.675708 | 2.291231 |
| H | -4.278587 | 3.997436 | -4.845062 | C | 4.004319 | -3.055914 | 1.384005 |
| H | -5.841513 | 3.310578 | -5.299567 | C | 4.873559 | -2.067447 | 1.891621 |
| H | -5.752978 | 4.567508 | -4.052880 | H | 5.663746 | -2.434914 | 2.537102 |
| C | 1.900748 | -5.793803 | 1.240270 | C | 4.967783 | -0.703337 | 1.548302 |
| H | 2.806979 | -5.217914 | 1.004158 | C | 4.349465 | -4.497561 | 1.669917 |
| H | 2.013870 | -6.183516 | 2.257903 | H | 3.464790 | -5.050434 | 2.003527 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 5.128979 | -4.576844 | 2.431219 | C | -2.903679 | -0.446911 | -2.616347 |
| H | 4.708486 | -4.995637 | 0.761796 | C | -2.099504 | 0.473663 | -3.312490 |
| C | 6.196884 | 0.032998 | 2.027421 | H | -1.963579 | 0.272778 | -4.369978 |
| H | 6.849559 | 0.284912 | 1.183706 | C | -1.579291 | 1.701728 | -2.853866 |
| H | 6.770072 | -0.570433 | 2.734653 | C | -3.494229 | -1.579112 | -3.427610 |
| H | 5.924881 | 0.980214 | 2.505109 | H | -3.403716 | -2.528068 | -2.888006 |
| C | 2.252033 | -3.800190 | -0.068878 | H | -2.996130 | -1.667283 | -4.396993 |
| C | 1.018984 | -4.302962 | 0.389548 | H | -4.561978 | -1.423163 | -3.613016 |
| C | 0.287001 | -5.157626 | -0.437422 | C | -0.971015 | 2.613748 | -3.895720 |
| H | -0.671190 | -5.532981 | -0.081675 | H | -1.508358 | 3.567931 | -3.930075 |
| C | 0.738530 | -5.529289 | -1.706174 | H | -1.004990 | 2.161043 | -4.889626 |
| C | 1.972815 | -5.034140 | -2.130174 | H | 0.068972 | 2.856987 | -3.650295 |
| H | 2.347888 | -5.310209 | -3.115195 | C | -4.244242 | -1.141078 | -0.800406 |
| C | 2.740680 | -4.180754 | -1.333725 | C | -5.573141 | -0.767949 | -1.079116 |
| C | 0.481762 | -3.902952 | 1.732070 | C | -6.615709 | -1.497297 | -0.499525 |
| H | -0.376077 | -4.521947 | 2.010539 | H | -7.641863 | -1.195766 | -0.706834 |
| H | 0.150376 | -2.857047 | 1.728297 | C | -6.381086 | -2.575966 | 0.351681 |
| H | 1.240693 | -3.994951 | 2.516051 | C | -5.053199 | -2.921287 | 0.618336 |
| C | -0.071121 | -6.454809 | -2.574036 | H | -4.843155 | -3.754157 | 1.288343 |
| H | -1.144400 | -6.257901 | -2.476057 | C | -3.982550 | -2.219797 | 0.065805 |
| H | 0.093981 | -7.503953 | -2.295621 | C | -5.891843 | 0.407280 | -1.964007 |
| H | 0.197916 | -6.350144 | -3.630486 | H | -6.100868 | 0.095244 | -2.996441 |
| C | 4.059612 | -3.661371 | -1.830725 | H | -5.061219 | 1.116382 | -2.006308 |
| H | 4.109553 | -3.689353 | -2.924166 | H | -6.780608 | 0.933834 | -1.600801 |
| H | 4.899407 | -4.258153 | -1.451006 | C | -7.516748 | -3.315945 | 1.005754 |
| H | 4.229249 | -2.636913 | -1.490328 | H | -7.322334 | -4.393801 | 1.047935 |
| C | 4.382163 | 1.263921 | 0.336780 | H | -8.457590 | -3.162487 | 0.466679 |
| C | 3.914599 | 2.407666 | 1.013270 | H | -7.667554 | -2.971686 | 2.037416 |
| C | 4.164808 | 3.666290 | 0.467015 | C | -2.570361 | -2.594832 | 0.405166 |
| H | 3.809719 | 4.545045 | 1.003143 | H | -2.105655 | -1.838004 | 1.050525 |
| C | 4.832236 | 3.830655 | -0.749081 | H | -1.939932 | -2.680471 | -0.486262 |
| C | 5.293718 | 2.685096 | -1.397194 | H | -2.539024 | -3.547332 | 0.942499 |
| H | 5.832771 | 2.784864 | -2.338685 | C | -1.093580 | 3.379131 | -1.257797 |
| C | 5.096723 | 1.405527 | -0.867373 | C | -1.974176 | 4.476144 | -1.195888 |
| C | 3.134854 | 2.286400 | 2.289064 | C | -1.485522 | 5.711380 | -0.766944 |
| H | 2.153509 | 1.827601 | 2.111502 | H | -2.172068 | 6.555447 | -0.710572 |
| H | 2.961092 | 3.270429 | 2.734521 | C | -0.143951 | 5.895613 | -0.421644 |
| H | 3.647714 | 1.660538 | 3.027171 | C | 0.717551 | 4.805104 | -0.539333 |
| C | 5.013299 | 5.198876 | -1.348706 | H | 1.773907 | 4.926413 | -0.307303 |
| H | 5.808227 | 5.205501 | -2.101704 | C | 0.267765 | 3.547907 | -0.950314 |
| H | 5.265319 | 5.941241 | -0.583080 | C | -3.399729 | 4.336396 | -1.653899 |
| H | 4.091064 | 5.538225 | -1.838898 | H | -4.040522 | 5.096578 | -1.196192 |
| C | 5.682787 | 0.207202 | -1.561080 | H | -3.804907 | 3.350194 | -1.419089 |
| H | 5.746076 | 0.364732 | -2.642975 | H | -3.472683 | 4.456953 | -2.743809 |
| H | 5.096252 | -0.692855 | -1.365489 | C | 0.352432 | 7.226298 | 0.077562 |
| H | 6.700563 | 0.001937 | -1.202896 | H | 0.174306 | 7.334801 | 1.155687 |

| | | | |
|---|---|---|---|
| H | -0.156498 | 8.058842 | -0.421098 |
| H | 1.429288 | 7.338865 | -0.089431 |
| C | 1.242744 | 2.413345 | -1.078326 |
| H | 1.469276 | 1.985896 | -0.095739 |
| H | 2.192009 | 2.752358 | -1.505949 |
| H | 0.836506 | 1.603901 | -1.686385 |
| O | 1.771233 | -0.929120 | -1.596507 |
| C | 0.513525 | -1.545235 | -2.002932 |
| H | -0.297547 | -0.862018 | -1.737418 |
| H | 0.409350 | -2.482740 | -1.454561 |
| C | 0.637072 | -1.717314 | -3.503055 |
| H | -0.344049 | -1.726336 | -3.983144 |
| H | 1.160221 | -2.651183 | -3.737324 |
| C | 1.479120 | -0.501187 | -3.889982 |
| H | 1.966188 | -0.597749 | -4.865049 |
| H | 0.852447 | 0.396652 | -3.898936 |
| C | 2.485506 | -0.439276 | -2.753131 |
| H | 3.337227 | -1.102659 | -2.933153 |
| H | 2.851726 | 0.563688 | -2.522374 |
| C | -0.250276 | -1.502567 | 4.693600 |
| H | -1.196527 | -1.142794 | 5.108792 |
| H | -0.469361 | -2.349417 | 4.034312 |
| H | 0.375182 | -1.862106 | 5.520846 |
| C | 1.847350 | -0.945066 | 3.492236 |
| H | 2.445303 | -0.199336 | 2.962922 |
| H | 2.422964 | -1.250888 | 4.373946 |
| H | 1.744322 | -1.826236 | 2.854819 |
| C | 0.747081 | 0.796458 | 4.878196 |
| H | 1.244059 | 1.618383 | 4.352415 |
| H | -0.185323 | 1.181198 | 5.301384 |
| H | 1.393884 | 0.474176 | 5.704289 |
| C | -5.291957 | 0.452056 | 2.423868 |
| H | -5.037288 | -0.122498 | 3.320956 |
| H | -6.339964 | 0.774888 | 2.495814 |
| H | -5.198129 | -0.211261 | 1.560929 |
| C | -4.821089 | 2.510959 | 1.088874 |
| H | -4.159022 | 3.372611 | 0.947040 |
| H | -4.804207 | 1.906043 | 0.174289 |
| H | -5.845513 | 2.885361 | 1.221851 |
| C | -4.500269 | 2.539685 | 3.556477 |
| H | -5.529781 | 2.908129 | 3.661178 |
| H | -4.250707 | 1.971466 | 4.458905 |
| H | -3.827980 | 3.404654 | 3.509723 |

5$(THF)_2$

| | | | |
|---|---|---|---|
| Mg | -3.66736600 | 0.43488500 | -0.22249000 |
| Mg | 4.03630300 | -0.51007800 | -0.27540300 |
| N | -5.16120700 | -0.81584800 | -0.91139600 |
| N | -4.67025200 | 2.12563500 | -0.85213800 |
| N | 5.87159100 | -0.18593200 | 0.67937700 |
| N | 3.69131900 | -2.17915600 | 0.95032300 |
| P | -1.16917200 | 0.16796800 | -0.11897900 |
| P | 1.43662500 | -0.33518900 | -1.42811800 |
| C | -0.39707700 | 0.06704200 | -1.63609900 |
| C | -0.94801300 | 0.00045600 | -3.07691800 |
| C | 2.48527600 | 0.85597900 | -0.88500700 |
| C | 2.34336200 | 2.33896300 | -0.56147200 |
| C | -5.96111500 | -0.43443800 | -1.91329000 |
| C | -6.05401000 | 0.88301400 | -2.40681700 |
| H | -6.71004100 | 1.01167000 | -3.25883400 |
| C | -5.56025200 | 2.08099100 | -1.84060400 |
| C | -6.87182900 | -1.46777700 | -2.55312100 |
| H | -6.31107600 | -2.37153400 | -2.81054300 |
| H | -7.34953600 | -1.07767300 | -3.45317500 |
| H | -7.65607200 | -1.77566600 | -1.85350400 |
| C | -6.12725200 | 3.38158500 | -2.37936500 |
| H | -6.73985900 | 3.87102500 | -1.61460700 |
| H | -6.74649300 | 3.21593900 | -3.26221700 |
| H | -5.32681800 | 4.08296200 | -2.63241800 |
| C | -5.38263200 | -2.08031900 | -0.28403100 |
| C | -4.56198100 | -3.18754100 | -0.57466200 |
| C | -4.77451000 | -4.38709600 | 0.11384100 |
| H | -4.13965700 | -5.23956000 | -0.11708300 |
| C | -5.75927900 | -4.51692000 | 1.09599300 |
| C | -6.54689400 | -3.39817000 | 1.38338000 |
| H | -7.31123500 | -3.46877100 | 2.15460800 |
| C | -6.37641100 | -2.18314800 | 0.71320900 |
| C | -3.45211600 | -3.07464700 | -1.58865400 |
| H | -2.94919100 | -4.03462600 | -1.73293700 |
| H | -2.69848000 | -2.34696300 | -1.26464200 |
| H | -3.82277500 | -2.73234900 | -2.56008100 |
| C | -5.97542600 | -5.83012100 | 1.80981900 |
| H | -5.03333800 | -6.37088000 | 1.94497800 |
| H | -6.64765400 | -6.48589300 | 1.24228100 |
| H | -6.42393900 | -5.68109500 | 2.79678000 |
| C | -7.19961600 | -0.97569100 | 1.09010100 |
| H | -7.93066500 | -1.22339500 | 1.86432900 |
| H | -7.73683700 | -0.55325100 | 0.23505300 |
| H | -6.55178100 | -0.17786600 | 1.46729000 |
| C | -4.39027500 | 3.35690900 | -0.18205100 |
| C | -3.26901500 | 4.12966900 | -0.54470900 |
| C | -2.95942700 | 5.26528100 | 0.21024300 |
| H | -2.09146100 | 5.85737200 | -0.07154900 |

| | | | |
|---|---|---|---|
| C | -3.72748100 | 5.65702200 | 1.31057200 |
| C | -4.83958000 | 4.87892400 | 1.64462300 |
| H | -5.45470200 | 5.16584700 | 2.49516400 |
| C | -5.18255100 | 3.73237700 | 0.92162000 |
| C | -2.41410600 | 3.72854600 | -1.71878800 |
| H | -1.97332600 | 2.74122800 | -1.55348500 |
| H | -1.59817100 | 4.43740100 | -1.87733700 |
| H | -2.99827500 | 3.66268300 | -2.64320100 |
| C | -3.34429100 | 6.86564200 | 2.13158400 |
| H | -4.20704300 | 7.28286200 | 2.65970800 |
| H | -2.91630700 | 7.65532000 | 1.50600100 |
| H | -2.59089500 | 6.60904900 | 2.88705400 |
| C | -6.35119600 | 2.87530100 | 1.34094200 |
| H | -6.89109300 | 3.32549700 | 2.17841700 |
| H | -6.00184500 | 1.88357000 | 1.64577200 |
| H | -7.06086700 | 2.71319100 | 0.52330300 |
| C | 6.55077200 | -1.15332200 | 1.29533300 |
| C | 6.02220300 | -2.42457800 | 1.59575000 |
| H | 6.70995700 | -3.11135600 | 2.07358400 |
| C | 4.67188800 | -2.84217900 | 1.56452900 |
| C | 7.97075500 | -0.87862300 | 1.76250600 |
| H | 8.56549800 | -0.41749200 | 0.96875700 |
| H | 8.46636900 | -1.79356700 | 2.09170900 |
| H | 7.96724100 | -0.17181700 | 2.59885100 |
| C | 4.34851900 | -4.11038100 | 2.33839100 |
| H | 3.73291400 | -3.86736400 | 3.21114200 |
| H | 5.25589800 | -4.60753600 | 2.68518100 |
| H | 3.76469600 | -4.81160500 | 1.73608400 |
| C | 6.39592100 | 1.14193900 | 0.68197700 |
| C | 6.12108600 | 1.98507800 | 1.77853300 |
| C | 6.52879300 | 3.32048100 | 1.72280800 |
| H | 6.30375100 | 3.97343600 | 2.56358300 |
| C | 7.20239100 | 3.84171000 | 0.61458700 |
| C | 7.48038700 | 2.98080000 | -0.45066400 |
| H | 8.00900600 | 3.36484200 | -1.32063700 |
| C | 7.08591500 | 1.64018700 | -0.43915300 |
| C | 5.39164900 | 1.44708000 | 2.98490700 |
| H | 6.03379400 | 0.79219300 | 3.58682200 |
| H | 4.53211700 | 0.84019600 | 2.68911100 |
| H | 5.04330100 | 2.25745100 | 3.63056500 |
| C | 7.58043200 | 5.30252500 | 0.55161100 |
| H | 8.46532300 | 5.46212500 | -0.07244400 |
| H | 7.79054500 | 5.70669800 | 1.54686700 |
| H | 6.76701900 | 5.90101900 | 0.12242800 |
| C | 7.38026300 | 0.73616100 | -1.61016700 |
| H | 6.45734900 | 0.31416900 | -2.01594500 |
| H | 8.00358100 | -0.11571100 | -1.31386400 |
| H | 7.89966400 | 1.27621600 | -2.40619100 |
| C | 2.34661700 | -2.62543800 | 1.17090800 |
| C | 1.60390100 | -2.07997200 | 2.23102300 |
| C | 0.30060800 | -2.53773900 | 2.44840700 |
| H | -0.26550500 | -2.12389700 | 3.28020300 |
| C | -0.29005800 | -3.50128600 | 1.63027100 |
| C | 0.45248500 | -3.99035800 | 0.55042100 |
| H | 0.00183500 | -4.72182800 | -0.11762400 |
| C | 1.75817800 | -3.56440200 | 0.30286200 |
| C | 2.19326500 | -0.98996100 | 3.08942700 |
| H | 1.53816900 | -0.75184200 | 3.93219600 |
| H | 2.31916200 | -0.07683800 | 2.49624600 |
| H | 3.18013800 | -1.25639300 | 3.48121000 |
| C | -1.69814700 | -3.98494400 | 1.87549600 |
| H | -2.39641200 | -3.58665900 | 1.13302100 |
| H | -2.06299700 | -3.68503600 | 2.86310500 |
| H | -1.76545800 | -5.07713200 | 1.81575800 |
| C | 2.53077000 | -4.06675100 | -0.88809600 |
| H | 2.80603300 | -3.21828300 | -1.52129000 |
| H | 1.93518800 | -4.76421000 | -1.48357800 |
| H | 3.45915700 | -4.57156500 | -0.59668500 |
| O | -3.88837800 | 0.42411500 | 1.87105700 |
| C | -3.61269500 | -0.86725300 | 2.50723100 |
| H | -2.92054900 | -1.41765200 | 1.86256400 |
| H | -4.55487100 | -1.41248300 | 2.57304800 |
| C | -2.96765000 | -0.52474100 | 3.84559300 |
| H | -2.31613700 | -1.32801500 | 4.19793100 |
| H | -3.73335400 | -0.34369800 | 4.60819200 |
| C | -2.21089600 | 0.77029900 | 3.51430900 |
| H | -1.95666700 | 1.36290100 | 4.39680200 |
| H | -1.29520200 | 0.54389200 | 2.95863700 |
| C | -3.19893700 | 1.49067900 | 2.60415600 |
| H | -3.95710600 | 2.05269100 | 3.15843000 |
| H | -2.73029900 | 2.15629100 | 1.87578200 |
| C | -0.60897800 | -1.38879900 | -3.67833700 |
| H | 0.47131300 | -1.55106500 | -3.72744800 |
| H | -1.03930500 | -2.19104300 | -3.07163200 |
| H | -1.01306800 | -1.46780900 | -4.69475400 |
| C | -2.46878000 | 0.20218100 | -3.18483400 |
| H | -2.78443500 | 1.16758300 | -2.78478300 |
| H | -2.77412500 | 0.17050100 | -4.23708000 |
| H | -3.02323000 | -0.58107300 | -2.66641100 |
| C | -0.26461200 | 1.09102100 | -3.93596900 |
| H | -0.52937100 | 2.08979900 | -3.57859100 |
| H | 0.82537000 | 1.00204800 | -3.90287300 |

| | | | |
|---|---|---|---|
| H | -0.58399500 | 1.00568800 | -4.98151800 |
| C | 3.65876500 | 3.05605500 | -0.93664700 |
| H | 3.85173500 | 2.96826200 | -2.01187500 |
| H | 3.60849800 | 4.12395800 | -0.68801500 |
| H | 4.51055800 | 2.62826700 | -0.40587300 |
| C | 2.12080700 | 2.46381000 | 0.96414800 |
| H | 1.20262200 | 1.94659300 | 1.25878600 |
| H | 2.95998700 | 2.02778800 | 1.51544800 |
| H | 2.04371700 | 3.51875300 | 1.25782600 |
| C | 1.19045500 | 3.05299000 | -1.29158400 |
| H | 1.17318500 | 4.11949300 | -1.03232100 |
| H | 1.31265400 | 2.97335500 | -2.37594100 |
| H | 0.22697100 | 2.62127600 | -1.02696500 |
| O | 4.78794200 | -1.37869200 | -2.03142300 |
| C | 5.60867200 | -2.57007900 | -2.05255000 |
| C | 4.43236500 | -1.07291700 | -3.39836000 |
| C | 5.13351600 | -3.38038100 | -3.28018200 |
| H | 6.65737400 | -2.26370200 | -2.14160400 |
| H | 5.46690600 | -3.06805700 | -1.09362600 |
| C | 4.13053300 | -2.44146400 | -3.99976500 |
| H | 3.58584000 | -0.38856900 | -3.35332000 |
| H | 5.28881800 | -0.58571900 | -3.88540000 |
| H | 4.65615500 | -4.31580900 | -2.98037600 |
| H | 5.98077000 | -3.63036400 | -3.92465700 |
| H | 3.10034800 | -2.71755200 | -3.75927500 |
| H | 4.24450400 | -2.45203300 | -5.08673300 |

6(THF)

E(RB3PW91) = -3713.58574133 au

| | | | |
|---|---|---|---|
| Mg | -2.400656 | 0.308813 | -0.204253 |
| N | -2.579671 | -1.545769 | 0.704773 |
| C | 1.468931 | 0.535455 | -1.422159 |
| Mg | 2.558692 | 0.069612 | 0.380277 |
| N | -3.243885 | 1.226150 | 1.444055 |
| C | 3.498542 | -0.391259 | -2.528474 |
| H | 4.143357 | 0.120912 | -1.808982 |
| H | 4.068758 | -0.506212 | -3.459502 |
| H | 3.273308 | -1.392807 | -2.146812 |
| C | 2.516822 | 1.774171 | -3.324048 |
| H | 3.099358 | 2.362822 | -2.609493 |
| H | 1.594646 | 2.319802 | -3.550474 |
| H | 3.100759 | 1.681583 | -4.249783 |
| N | 4.363226 | 1.070270 | 0.676520 |
| C | 1.374665 | -0.418612 | -3.780824 |
| H | 1.959725 | -0.553391 | -4.700280 |
| H | 0.442524 | 0.086455 | -4.048986 |
| H | 1.125529 | -1.410929 | -3.389989 |
| N | 3.374362 | -1.702152 | 1.115241 |
| C | -4.019678 | 2.399959 | 1.231245 |
| C | -3.399888 | 3.640411 | 1.012801 |
| C | -1.907004 | 3.772778 | 1.098517 |
| H | -1.592485 | 4.801350 | 0.897039 |
| H | -1.401405 | 3.120692 | 0.375994 |
| H | -1.540089 | 3.494797 | 2.094303 |
| C | -4.196068 | 4.752476 | 0.727818 |
| C | -5.586656 | 4.666698 | 0.650009 |
| C | -6.421423 | 5.869146 | 0.299495 |
| H | -6.621783 | 5.907729 | -0.779428 |
| H | -5.915067 | 6.801335 | 0.571823 |
| H | -7.390369 | 5.847602 | 0.810437 |
| C | -6.178694 | 3.420360 | 0.866902 |
| H | -7.261283 | 3.324351 | 0.795055 |
| C | -5.420570 | 2.282371 | 1.144937 |
| C | -6.082841 | 0.939015 | 1.274563 |
| H | -7.169793 | 1.031420 | 1.189101 |
| H | -5.857028 | 0.440740 | 2.223965 |
| H | -5.738562 | 0.263327 | 0.482399 |
| C | -3.659117 | 1.524080 | 3.843688 |
| H | -3.299702 | 2.555796 | 3.767973 |
| H | -3.316241 | 1.088331 | 4.785676 |
| H | -4.753496 | 1.578195 | 3.875772 |
| C | -3.196121 | 0.699511 | 2.664599 |
| C | -2.758822 | -0.611800 | 2.934206 |
| H | -2.694333 | -0.878387 | 3.984282 |
| C | -2.604659 | -1.683246 | 2.028862 |
| C | -2.500948 | -3.059283 | 2.644880 |
| H | -3.490274 | -3.521584 | 2.733301 |
| H | -2.076688 | -2.995400 | 3.650540 |
| H | -1.885140 | -3.720556 | 2.030707 |
| C | -2.753370 | -2.703466 | -0.106306 |
| C | -1.707421 | -3.125259 | -0.952608 |
| C | -0.430896 | -2.349574 | -1.042401 |
| H | 0.399063 | -2.973470 | -1.385310 |
| H | -0.146420 | -1.907737 | -0.086174 |
| H | -0.541522 | -1.523241 | -1.752907 |
| C | -1.896468 | -4.243865 | -1.761650 |
| H | -1.075386 | -4.565169 | -2.400890 |
| C | -3.103167 | -4.948879 | -1.782684 |
| C | -3.270630 | -6.162113 | -2.657555 |
| H | -2.647604 | -6.995114 | -2.306542 |
| H | -2.974962 | -5.952202 | -3.692370 |
| H | -4.309850 | -6.506645 | -2.667841 |
| C | -4.139005 | -4.485103 | -0.974372 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -5.102058 | -4.994217 | -0.997586 | C | 5.105324 | 4.342927 | -1.922128 |
| C | -3.992205 | -3.371280 | -0.140479 | C | 5.308029 | 5.477338 | -2.889551 |
| C | -5.178306 | -2.901905 | 0.659531 | H | 4.541961 | 5.464433 | -3.675742 |
| H | -6.072725 | -2.862855 | 0.027467 | H | 6.285277 | 5.415317 | -3.379482 |
| H | -5.017660 | -1.908520 | 1.082895 | H | 5.241797 | 6.449494 | -2.387557 |
| H | -5.403584 | -3.584852 | 1.489514 | C | 4.088048 | 4.390567 | -0.964665 |
| C | 2.771376 | -2.944119 | 0.761606 | H | 3.453667 | 5.273878 | -0.904806 |
| C | 1.611028 | -3.383199 | 1.429889 | C | 3.847155 | 3.333806 | -0.089185 |
| C | 1.044011 | -2.610678 | 2.586923 | C | 2.719989 | 3.426450 | 0.899079 |
| H | 0.380667 | -1.806623 | 2.247525 | H | 2.358414 | 4.456478 | 0.978867 |
| H | 1.831658 | -2.146252 | 3.185154 | H | 3.025233 | 3.087533 | 1.893501 |
| H | 0.454514 | -3.265062 | 3.235192 | H | 1.870215 | 2.808219 | 0.581849 |
| C | 0.980214 | -4.550635 | 1.003328 | C | 2.195838 | 0.381981 | -2.757227 |
| H | 0.080214 | -4.880665 | 1.519193 | P | -0.063902 | 1.165594 | -1.192923 |
| C | 1.452218 | -5.293495 | -0.080868 | P | -1.336816 | 1.562781 | -2.993744 |
| C | 0.729774 | -6.534428 | -0.530663 | C | -2.706499 | 0.906998 | -2.238620 |
| H | 0.903890 | -7.368884 | 0.161242 | C | -4.031274 | 0.743808 | -2.965734 |
| H | 1.064203 | -6.853147 | -1.523467 | C | -4.642766 | -0.602862 | -2.545337 |
| H | -0.351545 | -6.363581 | -0.575052 | H | -4.800512 | -0.639484 | -1.459416 |
| C | 2.616001 | -4.854725 | -0.711163 | H | -5.615006 | -0.763877 | -3.030451 |
| H | 3.016621 | -5.426116 | -1.547853 | H | -3.983690 | -1.437849 | -2.808699 |
| C | 3.299619 | -3.705955 | -0.296776 | C | -3.933152 | 0.790547 | -4.496320 |
| C | 4.609203 | -3.344702 | -0.944908 | H | -3.520920 | 1.747455 | -4.837115 |
| H | 4.586516 | -3.537946 | -2.022523 | H | -3.277589 | -0.005506 | -4.868666 |
| H | 5.424985 | -3.949907 | -0.525988 | H | -4.922549 | 0.664833 | -4.955793 |
| H | 4.866357 | -2.295807 | -0.785681 | C | -4.946643 | 1.884582 | -2.484897 |
| C | 4.802998 | -2.996659 | 2.627804 | H | -5.026644 | 1.901159 | -1.393964 |
| H | 3.933863 | -3.488846 | 3.077263 | H | -4.549504 | 2.855785 | -2.799528 |
| H | 5.556789 | -2.825957 | 3.399828 | H | -5.955872 | 1.766625 | -2.902829 |
| H | 5.215768 | -3.700624 | 1.896273 | H | -3.711069 | 5.712972 | 0.559572 |
| C | 4.409103 | -1.704042 | 1.950418 | O | 1.573395 | 0.602175 | 2.141515 |
| C | 5.198230 | -0.571925 | 2.245650 | C | 0.186074 | 0.978729 | 2.316767 |
| H | 5.959088 | -0.723612 | 3.004215 | C | 2.300002 | 0.779532 | 3.377724 |
| C | 5.247956 | 0.674099 | 1.589300 | C | 0.017272 | 1.217301 | 3.806713 |
| C | 6.388670 | 1.588099 | 1.976992 | H | 0.005841 | 1.874663 | 1.720927 |
| H | 7.251889 | 1.442631 | 1.318275 | H | -0.439267 | 0.169463 | 1.936155 |
| H | 6.716862 | 1.376980 | 2.998760 | C | 1.414188 | 1.674147 | 4.225635 |
| H | 6.095894 | 2.639525 | 1.900396 | H | 2.450148 | -0.204990 | 3.834067 |
| C | 4.662699 | 2.183521 | -0.152079 | H | 3.275622 | 1.198483 | 3.132538 |
| C | 5.695368 | 2.113700 | -1.108581 | H | -0.255582 | 0.283358 | 4.309755 |
| C | 6.580329 | 0.903563 | -1.257283 | H | -0.763027 | 1.953068 | 4.014873 |
| H | 6.667584 | 0.621147 | -2.312172 | H | 1.608548 | 1.554121 | 5.295535 |
| H | 6.198757 | 0.040683 | -0.706778 | H | 1.570418 | 2.726888 | 3.962044 |
| H | 7.596553 | 1.107154 | -0.894668 | $6(THF)_2$ | | | |
| C | 5.893770 | 3.196213 | -1.972131 | Mg | 4.07491300 | 0.38109200 | -0.73550500 |
| H | 6.685447 | 3.127171 | -2.717441 | N | 6.08549800 | -0.16678000 | -0.57339400 |

| | | | |
|---|---|---|---|
| C | -2.21087800 | 0.17101300 | -0.70213700 |
| Mg | -4.04545100 | -0.85523600 | -0.21141200 |
| N | 4.44100800 | 2.06019900 | 0.44458900 |
| C | -3.49077400 | 2.24054500 | -0.08210000 |
| H | -4.14803200 | 2.11205300 | -0.94878400 |
| H | -3.44292900 | 3.31113400 | 0.15213300 |
| H | -3.95143600 | 1.74145500 | 0.77641800 |
| C | -1.45353800 | 2.47449200 | -1.50506600 |
| H | -2.03826700 | 2.36629900 | -2.42506900 |
| H | -0.42998600 | 2.15212200 | -1.70922800 |
| H | -1.42682700 | 3.54037200 | -1.24323700 |
| N | -6.02669400 | -0.41664700 | -0.66980700 |
| C | -1.24297700 | 1.81212800 | 0.92681900 |
| H | -1.24975100 | 2.85592400 | 1.25922000 |
| H | -0.20434700 | 1.51995300 | 0.76046600 |
| H | -1.64596700 | 1.19746300 | 1.73503200 |
| N | -4.55733500 | -1.03151400 | 1.81013000 |
| C | 3.39060600 | 2.58647800 | 1.26011300 |
| C | 2.39665500 | 3.40478100 | 0.69251300 |
| C | 2.44673400 | 3.75757100 | -0.77242800 |
| H | 1.58947800 | 4.37255800 | -1.05787700 |
| H | 2.42698900 | 2.85197600 | -1.38792300 |
| H | 3.36133500 | 4.30618000 | -1.02665600 |
| C | 1.36170000 | 3.87379900 | 1.50536000 |
| C | 1.26724400 | 3.53163900 | 2.85652700 |
| C | 0.09227900 | 3.97961100 | 3.69177700 |
| H | -0.71751100 | 3.24102700 | 3.64545300 |
| H | -0.31327000 | 4.93203700 | 3.33633000 |
| H | 0.36779000 | 4.09851700 | 4.74442300 |
| C | 2.26399400 | 2.71268200 | 3.39483500 |
| H | 2.21961400 | 2.44301500 | 4.44767900 |
| C | 3.32232300 | 2.22751000 | 2.62068300 |
| C | 4.35706100 | 1.30955400 | 3.22407100 |
| H | 4.20308900 | 1.19694300 | 4.30051200 |
| H | 5.37917700 | 1.66505700 | 3.05949400 |
| H | 4.29811100 | 0.31452800 | 2.77061300 |
| C | 5.77922800 | 4.00921700 | 1.13868900 |
| H | 4.98475400 | 4.69763000 | 0.83529900 |
| H | 6.74842900 | 4.46173600 | 0.92214700 |
| H | 5.69048800 | 3.89296800 | 2.22385400 |
| C | 5.62842500 | 2.66409600 | 0.45001000 |
| C | 6.78743500 | 2.11925300 | -0.14901100 |
| H | 7.64914600 | 2.77489200 | -0.18339000 |
| C | 7.02479400 | 0.78311700 | -0.53248400 |
| C | 8.45594300 | 0.42669100 | -0.90247200 |
| H | 8.92931300 | -0.18262900 | -0.12720100 |
| H | 9.06217500 | 1.32307400 | -1.04593400 |
| H | 8.47385600 | -0.16776500 | -1.82116800 |
| C | 6.48623500 | -1.53464000 | -0.60273100 |
| C | 6.26717300 | -2.31395700 | -1.75448100 |
| C | 5.65550500 | -1.69943600 | -2.98898100 |
| H | 5.82760100 | -2.32401000 | -3.86997600 |
| H | 6.04863200 | -0.69763600 | -3.18033300 |
| H | 4.56941900 | -1.59377400 | -2.86947400 |
| C | 6.58453400 | -3.67571400 | -1.72758900 |
| H | 6.41600800 | -4.27023100 | -2.62322600 |
| C | 7.10182800 | -4.29169900 | -0.58611500 |
| C | 7.46408900 | -5.75791600 | -0.58485700 |
| H | 8.52551400 | -5.90643500 | -0.82118000 |
| H | 6.88450000 | -6.31497600 | -1.32729600 |
| H | 7.28454700 | -6.21335000 | 0.39430000 |
| C | 7.28871500 | -3.50393500 | 0.55393600 |
| H | 7.66429700 | -3.96839800 | 1.46352600 |
| C | 6.98863300 | -2.14010300 | 0.57122500 |
| C | 7.15212500 | -1.34118900 | 1.84191000 |
| H | 7.27137800 | -2.00140500 | 2.70500000 |
| H | 6.28640500 | -0.69617800 | 2.01175300 |
| H | 8.02587600 | -0.67950100 | 1.80974600 |
| C | -3.61552400 | -0.60418100 | 2.79426800 |
| C | -2.44091900 | -1.36417900 | 3.00144300 |
| C | -2.24572000 | -2.68151800 | 2.29396000 |
| H | -2.20758700 | -2.55143200 | 1.20744400 |
| H | -3.06508400 | -3.37518700 | 2.51275600 |
| H | -1.30736500 | -3.15234400 | 2.59696500 |
| C | -1.46870800 | -0.88762500 | 3.87850400 |
| H | -0.56822800 | -1.47580400 | 4.03177400 |
| C | -1.60929600 | 0.33108400 | 4.55245600 |
| C | -0.50508300 | 0.83306700 | 5.45031500 |
| H | -0.22755100 | 0.08373300 | 6.20032200 |
| H | -0.79530800 | 1.74693200 | 5.97610100 |
| H | 0.39378200 | 1.05553100 | 4.86496800 |
| C | -2.77751300 | 1.06043700 | 4.34118900 |
| H | -2.91026900 | 2.01251900 | 4.85147800 |
| C | -3.78858100 | 0.61725900 | 3.47657100 |
| C | -5.02283600 | 1.47169200 | 3.30013100 |
| H | -4.75115600 | 2.52741600 | 3.20179400 |
| H | -5.68812700 | 1.39119800 | 4.16928600 |
| H | -5.59776600 | 1.18464700 | 2.41915300 |
| C | -6.02786400 | -1.81978900 | 3.62791700 |
| H | -5.14625100 | -2.26479300 | 4.09717300 |
| H | -6.87090000 | -2.50863700 | 3.71628500 |
| H | -6.27523000 | -0.91798900 | 4.19757000 |

| | | | |
|---|---|---|---|
| C | -5.76016100 | -1.47242100 | 2.17448900 |
| C | -6.83651200 | -1.63291100 | 1.27175100 |
| H | -7.71234000 | -2.13034800 | 1.67129000 |
| C | -6.99726800 | -1.04933600 | -0.00381900 |
| C | -8.38146100 | -1.14322900 | -0.62524200 |
| H | -8.87990600 | -0.16921900 | -0.63103800 |
| H | -9.01449100 | -1.84624300 | -0.08084100 |
| H | -8.30891900 | -1.46157100 | -1.66987800 |
| C | -6.37055000 | 0.42130700 | -1.77245500 |
| C | -6.92973600 | 1.69719900 | -1.53527900 |
| C | -7.18313500 | 2.17750500 | -0.12663800 |
| H | -7.58019600 | 3.19599500 | -0.12685500 |
| H | -6.25492700 | 2.17168000 | 0.45134700 |
| H | -7.88999700 | 1.54159200 | 0.41633700 |
| C | -7.20781500 | 2.52642600 | -2.62439100 |
| H | -7.63898600 | 3.50790300 | -2.43779000 |
| C | -6.93955500 | 2.13908600 | -3.94118900 |
| C | -7.21856000 | 3.07175800 | -5.09603500 |
| H | -6.38561400 | 3.76863400 | -5.25327900 |
| H | -8.11465800 | 3.67474900 | -4.91726700 |
| H | -7.36286000 | 2.52123300 | -6.03072300 |
| C | -6.37205600 | 0.88075600 | -4.14912500 |
| H | -6.15093100 | 0.55739200 | -5.16427200 |
| C | -6.07534200 | 0.01846400 | -3.08858800 |
| C | -5.42111600 | -1.31532300 | -3.35044700 |
| H | -5.52638700 | -1.61041700 | -4.39809300 |
| H | -5.83624800 | -2.10300500 | -2.71620200 |
| H | -4.34666000 | -1.26620700 | -3.13183200 |
| C | -2.08698300 | 1.65979700 | -0.35674200 |
| P | -1.01987300 | -0.93735000 | -1.14764600 |
| P | 1.07766800 | -0.01811200 | -1.40172400 |
| C | 2.26572300 | -0.76359000 | -0.46087300 |
| C | 2.13971400 | -1.83913800 | 0.62524400 |
| C | 3.54460700 | -2.27849700 | 1.08738300 |
| H | 4.12190300 | -1.42759500 | 1.46464800 |
| H | 3.48870400 | -3.02028300 | 1.89333400 |
| H | 4.11163200 | -2.71896900 | 0.26224000 |
| C | 1.40160100 | -3.10316300 | 0.13270000 |
| H | 0.36832400 | -2.88362600 | -0.14407500 |
| H | 1.90590100 | -3.52778600 | -0.74201900 |
| H | 1.38940200 | -3.86753000 | 0.92063400 |
| C | 1.38692600 | -1.23299800 | 1.83196700 |
| H | 1.87360400 | -0.31614400 | 2.18159100 |
| H | 0.35682800 | -0.98007200 | 1.57112600 |
| H | 1.36727400 | -1.94857200 | 2.66444100 |
| H | 0.59618600 | 4.50601100 | 1.06251700 |
| O | -4.02563900 | -2.89202000 | -0.78453700 |
| C | -3.28347300 | -3.53677800 | -1.84853800 |
| C | -4.62503700 | -3.96055200 | -0.01100800 |
| C | -2.58800300 | -4.69312100 | -1.14020300 |
| H | -3.99471400 | -3.87771400 | -2.61305900 |
| H | -2.59859500 | -2.79531100 | -2.25993600 |
| C | -3.61769700 | -5.12900600 | -0.06625700 |
| H | -4.81015800 | -3.56531700 | 0.98407600 |
| H | -5.58532400 | -4.22033200 | -0.47159400 |
| H | -1.67310600 | -4.31884600 | -0.67295600 |
| H | -2.31928800 | -5.49954300 | -1.82711400 |
| H | -3.13648000 | -5.28593400 | 0.90177100 |
| H | -4.12342700 | -6.05871200 | -0.34109200 |
| O | 4.16602600 | 1.20355100 | -2.67722400 |
| C | 4.86071900 | 2.42805500 | -3.01587600 |
| C | 3.45453400 | 0.80052900 | -3.87117100 |
| C | 3.94627600 | 3.15725100 | -4.02403600 |
| H | 5.03383700 | 2.96321300 | -2.08569900 |
| H | 5.83017300 | 2.16272900 | -3.45450500 |
| C | 2.86151400 | 2.10829600 | -4.38175200 |
| H | 4.17399000 | 0.36142700 | -4.57570600 |
| H | 2.71359000 | 0.06125300 | -3.56833900 |
| H | 4.51628300 | 3.46821600 | -4.90384000 |
| H | 3.50127600 | 4.05164500 | -3.58237900 |
| H | 2.63648100 | 2.07421600 | -5.45068600 |
| H | 1.93414600 | 2.30638100 | -3.83763200 |
| | | | |
| A | | | |
| Mg | -2.19419600 | -0.68195400 | 0.05971800 |
| N | -3.07827000 | 1.17959700 | -0.20190500 |
| C | 1.64134600 | 0.28642500 | 1.65596200 |
| Mg | 2.71693100 | 0.81732300 | -0.08233700 |
| N | -2.49301300 | -1.16106500 | -1.92509600 |
| C | 3.47526500 | 1.43416600 | 2.91984200 |
| H | 4.25301200 | 0.98794800 | 2.29123500 |
| H | 3.92898400 | 1.63948300 | 3.89627800 |
| H | 3.17326600 | 2.39563400 | 2.48467600 |
| C | 2.76179100 | -0.86292600 | 3.61701000 |
| H | 3.47901500 | -1.33510600 | 2.93928000 |
| H | 1.93083800 | -1.55477300 | 3.77551400 |
| H | 3.25889100 | -0.70103000 | 4.58136500 |
| N | 4.43117200 | -0.11854700 | -0.67970900 |
| C | 1.24013400 | 1.12843200 | 4.00331600 |
| H | 1.70930200 | 1.33962200 | 4.97171700 |
| H | 0.38499900 | 0.47151800 | 4.17794400 |
| H | 0.86256300 | 2.07093600 | 3.59249600 |

| | | | |
|---|---|---|---|
| N | 2.71161600 | 2.10756800 | -1.64837700 |
| C | -2.38243200 | -2.54763600 | -2.26012400 |
| C | -1.12058400 | -3.12800300 | -2.48614900 |
| C | 0.12015100 | -2.27129900 | -2.49676100 |
| H | 1.01911600 | -2.87908000 | -2.62623500 |
| H | 0.22033800 | -1.71097600 | -1.56088100 |
| H | 0.09153900 | -1.53168500 | -3.30450400 |
| C | -1.04131000 | -4.50551200 | -2.71501200 |
| C | -2.17578800 | -5.32061200 | -2.72488500 |
| C | -2.06202400 | -6.81266400 | -2.92985100 |
| H | -1.99708600 | -7.33963100 | -1.96967000 |
| H | -1.16765000 | -7.07184200 | -3.50464200 |
| H | -2.93241200 | -7.21226500 | -3.45989700 |
| C | -3.41885000 | -4.71934100 | -2.50503800 |
| H | -4.31557700 | -5.33530300 | -2.50631700 |
| C | -3.54393800 | -3.34789000 | -2.26867100 |
| C | -4.89487500 | -2.72860900 | -2.00595800 |
| H | -5.67930500 | -3.48911700 | -1.98130400 |
| H | -5.16355400 | -1.98711900 | -2.76638900 |
| H | -4.90371100 | -2.19937800 | -1.04756200 |
| C | -2.87729700 | -0.74022800 | -4.31750900 |
| H | -1.92047200 | -1.19058600 | -4.60013900 |
| H | -3.08964400 | 0.08859700 | -4.99462100 |
| H | -3.63870300 | -1.51196500 | -4.46526400 |
| C | -2.83872100 | -0.28176900 | -2.87012500 |
| C | -3.17869000 | 1.06161700 | -2.62148600 |
| H | -3.41350900 | 1.65087800 | -3.49946900 |
| C | -3.36295400 | 1.71879600 | -1.38503300 |
| C | -3.95070500 | 3.11733100 | -1.43430700 |
| H | -4.95199200 | 3.12922200 | -0.99398200 |
| H | -4.02329400 | 3.48592700 | -2.45895700 |
| H | -3.33964900 | 3.81170300 | -0.85207000 |
| C | -3.50721800 | 1.83662000 | 0.99817400 |
| C | -2.59516400 | 2.61157100 | 1.74463400 |
| C | -1.21867500 | 2.90660200 | 1.20630200 |
| H | -0.68379700 | 3.60270800 | 1.85842800 |
| H | -1.25800300 | 3.34248800 | 0.20496100 |
| H | -0.61475600 | 1.99987900 | 1.12275200 |
| C | -3.00242500 | 3.12602400 | 2.97794400 |
| H | -2.29582700 | 3.71959100 | 3.55431300 |
| C | -4.28332300 | 2.89955200 | 3.49181300 |
| C | -4.67383500 | 3.41844900 | 4.85521400 |
| H | -4.20719000 | 4.38641500 | 5.06494400 |
| H | -4.35537100 | 2.72784700 | 5.64608400 |
| H | -5.75781800 | 3.53889500 | 4.94451000 |
| C | -5.17918200 | 2.16255500 | 2.71552200 |
| H | -6.18880700 | 1.99141300 | 3.08370500 |
| C | -4.81927600 | 1.63259700 | 1.47132100 |
| C | -5.84825800 | 0.89935900 | 0.64283100 |
| H | -6.56735200 | 0.37601500 | 1.27856600 |
| H | -5.38572400 | 0.17341900 | -0.02782100 |
| H | -6.41593400 | 1.59754000 | 0.01404200 |
| C | 1.66233600 | 3.08172900 | -1.70124000 |
| C | 0.46732600 | 2.77410900 | -2.37473700 |
| C | 0.28752600 | 1.42125200 | -3.01536500 |
| H | 0.23369300 | 0.63994400 | -2.24829200 |
| H | 1.12050800 | 1.15833800 | -3.67468100 |
| H | -0.64234800 | 1.37557000 | -3.58238400 |
| C | -0.54875300 | 3.73417600 | -2.41421900 |
| H | -1.46893000 | 3.49486100 | -2.93912000 |
| C | -0.41647600 | 4.97209600 | -1.77845100 |
| C | -1.53854200 | 5.98286200 | -1.79262000 |
| H | -2.26969200 | 5.76032000 | -2.57453800 |
| H | -1.16202600 | 6.99768800 | -1.95801300 |
| H | -2.07396300 | 5.99003900 | -0.83495500 |
| C | 0.76934600 | 5.23656100 | -1.08403900 |
| H | 0.88458900 | 6.18933800 | -0.57167600 |
| C | 1.81391100 | 4.31036900 | -1.03143700 |
| C | 3.09123400 | 4.60996000 | -0.28563100 |
| H | 3.04936400 | 5.59052200 | 0.19501400 |
| H | 3.96197600 | 4.59057100 | -0.95055300 |
| H | 3.28346400 | 3.86109100 | 0.49276800 |
| C | 3.48177400 | 3.06608700 | -3.77919600 |
| H | 2.51786700 | 2.97931200 | -4.28977400 |
| H | 4.27883000 | 2.93959200 | -4.51269700 |
| H | 3.52933300 | 4.08454200 | -3.38083300 |
| C | 3.59466000 | 2.05241800 | -2.65517400 |
| C | 4.63475900 | 1.10873900 | -2.75828100 |
| H | 5.23113500 | 1.17749300 | -3.65918300 |
| C | 5.02604500 | 0.10003900 | -1.85438700 |
| C | 6.18598400 | -0.78572200 | -2.26773700 |
| H | 7.02223100 | -0.69488600 | -1.56912700 |
| H | 6.54124500 | -0.54014800 | -3.26934000 |
| H | 5.87953300 | -1.83676200 | -2.24952500 |
| C | 4.96425500 | -1.08870600 | 0.22817800 |
| C | 6.01016700 | -0.73213700 | 1.10305100 |
| C | 6.67270800 | 0.62235700 | 1.01099100 |
| H | 7.21912900 | 0.85424500 | 1.92886600 |
| H | 5.94317200 | 1.41743000 | 0.83187600 |
| H | 7.38871500 | 0.66833900 | 0.18140900 |
| C | 6.43069600 | -1.66074100 | 2.06066600 |
| H | 7.23019900 | -1.38258700 | 2.74394700 |

| | | | |
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| C | 5.84895200 | -2.92625500 | 2.17072700 |
| C | 6.28225000 | -3.89090400 | 3.24862700 |
| H | 5.66593600 | -3.77389100 | 4.14859200 |
| H | 7.32334500 | -3.72540100 | 3.54189200 |
| H | 6.18297200 | -4.93021500 | 2.92063500 |
| C | 4.82342300 | -3.25899300 | 1.28047600 |
| H | 4.35794900 | -4.23967600 | 1.34750000 |
| C | 4.36458300 | -2.36077600 | 0.31368100 |
| C | 3.23242300 | -2.73037100 | -0.61100400 |
| H | 2.98791000 | -3.79281400 | -0.53313900 |
| H | 3.46789300 | -2.50369200 | -1.65577200 |
| H | 2.32498100 | -2.16925700 | -0.35809200 |
| C | 2.26509500 | 0.48324700 | 3.04246000 |
| P | 0.26394200 | -0.58383300 | 1.25520600 |
| P | -0.85667800 | -1.68712500 | 2.84724900 |
| C | -2.24515400 | -1.88229700 | 1.87384800 |
| C | -3.41229300 | -2.74354800 | 2.35492900 |
| C | -4.72470800 | -1.96774500 | 2.12530700 |
| H | -4.84783200 | -1.72143500 | 1.06684300 |
| H | -5.59193400 | -2.56538700 | 2.43163300 |
| H | -4.73271600 | -1.02947200 | 2.68830800 |
| C | -3.35576400 | -3.18208200 | 3.83301100 |
| H | -2.44920100 | -3.75804200 | 4.04475500 |
| H | -3.36639300 | -2.31509500 | 4.50174000 |
| H | -4.21843000 | -3.81219100 | 4.08068000 |
| C | -3.41652500 | -4.00827700 | 1.46071600 |
| H | -3.43979200 | -3.74817000 | 0.39910800 |
| H | -2.51788200 | -4.60777100 | 1.63590500 |
| H | -4.29394800 | -4.62812800 | 1.68403900 |
| H | -0.06430400 | -4.95127600 | -2.88943700 |

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