Electronic Supplementary Information (ESI) for: C-H Bond activation of ethylene by a zirconacycle

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Experimental.

General. All manipulations were performed under a dry argon atmosphere using standard Schlenk techniques or under a nitrogen atmosphere in a glovebox unless otherwise indicated. Water and oxygen were removed from benzene, toluene, pentane, diethyl ether, and tetrahydrofuran solvents using an IT PureSolv system. Benzene-d_6 and tetrahydrofuran-d_8 were heated to reflux over Na/K alloy and vacuum-transferred. The compounds Cp_2ZrHCl,[1] $Cp_2ZrMeCl$,[2] (*E*)-$Cp_2Zr(CH{=}CH_2SiMe_3)Cl$,[3] $LiN(SiMe_3)_2$,[4] $LiN(SiHMe_2)_2$,[5] $LiN(SiEtMe_2)_2$,[6] $B(C_6F_5)_3$,[7] $Cp_2Zr\{N(SiHMe_2)_2\}H$,[8] $Cp_2Zr(CH{=}CH_2)Cl$,[9] and $Cp_2ZrEtCl$[10] were prepared following literature procedures.

^1H, $^{13}C\{^1H\}$, ^{11}B and $^{29}Si\{^1H\}$ NMR spectra were collected on an Agilent MR400 spectrometer or a Bruker Avance III 600 spectrometer. ^{11}B NMR spectra were referenced to an external sample of $BF_3{\cdot}Et_2O$. ^{15}N chemical shifts were determined either by ^1H-^{15}N HMBC experiments on a Bruker Avance II 700 spectrometer with a Bruker Z-gradient inverse TXI $^1H/^{13}C/^{15}N$ 5mm cryoprobe or by ^1H-^{15}N CIGARAD experiments on an Agilent MR400 spectrometer; ^{15}N chemical shifts were originally referenced to liquid NH_3 and recalculated to the CH_3NO_2 chemical shift scale by adding -381.9 ppm. Assignments of resonances are supported by ^1H-^1H and heteronuclear correlation NMR experiments. Infrared spectra were measured on a Bruker IFS66v FTIR. Elemental analyses were performed using a Perkin-Elmer 2400 Series II CHN/S. X-ray diffraction data was collected on a Bruker APEX II diffractometer.

$Cp_2Zr\{N(SiHMe_2)_2\}H$ (1). The synthesis of $Cp_2Zr\{N(SiHMe_2)_2\}H$ was previously reported in reference 8; here we give the low temperature ^1H, ^{13}C and ^{29}Si NMR spectra that provide support for a β-agostic interaction. The synthetic procedure and room temperature spectroscopic data is repeated here for the reader's convenience. A suspension of $[Cp_2ZrHCl]_n$ (0.909 g, 3.53 mmol) and $LiN(SiHMe_2)_2$ (0.491 g, 3.53 mmol) was stirred for 30 min in benzene (15 mL) at

room temperature. The volatile materials were removed under reduced pressure to leave an off-white crystalline solid, which was extracted with pentane (15 mL). The pentane extract was concentrated and cooled to -30 °C, yielding crystalline $Cp_2Zr\{N(SiHMe_2)_2\}H$ (0.931 g, 2.62 mmol, 74.4%). ^{1}H NMR (benzene-d_6, 400 MHz, 25 °C): δ□5.78 (s, 10 H, C_5H_5), 5.60 (s, 1 H, ZrH), 3.78 (m, $^1J_{SiH}$ = 161.0 Hz, 2 H, SiH), 0.18 (d, $^3J_{HH}$ = 3.2 Hz, 12 H, SiH*Me*$_2$). ^{13}C{^{1}H} NMR (benzene-d_6, 125 MHz, 25 °C): δ 107.58 (C_5H_5), 1.76 (SiMe). ^{15}N{^{1}H} NMR (benzene-d_6, 61 MHz, 25 °C): δ -292.4. ^{29}Si{^{1}H} NMR (benzene-d_6, 119.3 MHz, 25 °C): δ -40.7. ^{1}H NMR (toluene-d_8, 600 MHz, -82 °C): δ□5.67 (s, 10 H, C_5H_5), 5.48 (s, 1 H, ZrH), 4.99 (s br, $^1J_{SiH}$ = 179.6 Hz, 1 H, SiH^{anagostic}), 2.13 (s br, $^1J_{SiH}$ = 129.7 Hz, 1 H, SiH^{agostic}), 0.49 (s br, 6 H, SiMe), 0.06 (s br, 6 H, SiMe). ^{13}C{^{1}H} NMR (toluene-d_8, 125 MHz, -82 °C): δ 106.58 (C_5H_5), 2.96 (SiH^{anagostic}Me$_2$), -1.13 (SiH^{agostic}Me$_2$). ^{29}Si{^{1}H} NMR (toluene-d_8, 119.3 MHz, -82 °C): δ -23.1 (SiH^{anagostic}Me$_2$), -62.9 (SiH^{agostic}Me$_2$). IR (KBr, cm^{-1}): 3099 w br, 2955 m, 2895 w, 2047 s br ($\nu_{SiH\text{-}anagostic}$), 1907 m br ($\nu_{SiH\text{-}agostic}$), 1559 m br ($\nu_{ZrH}$), 1441 w, 1246 s, 1014 s, 890 s, 798 s br, 765 s br, 650 s br. Anal. Calcd for $C_{14}H_{25}NSi_2Zr$: C, 47.40; H, 7.10; N, 3.95. Found: C, 47.02; H, 6.96; N, 3.92. mp 104-106 °C.

$Cp_2Zr\{N(SiHMe_2)_2\}Me$ (2). $Cp_2ZrMeCl$ (0.716 g, 2.63 mmol) and $LiN(SiHMe_2)_2$ (0.367 g, 0.264 mmol) were suspended in benzene (15 mL). This mixture was stirred at room temperature for 13 h. Evaporation of the volatile materials provided an off-white solid. Extraction with pentane (15 mL), concentration, and cooling of the saturated solution to -30 °C yielded crystals of $Cp_2Zr\{N(SiHMe_2)_2\}Me$. The mother liquor was further concentrated and cooled to provide a second crop of crystals in good overall yield (0.823 g, 2.23 mmol, 84.8%). ^{1}H NMR (benzene-d_6, 400 MHz, 25 °C): δ□5.82 (s, 10 H, C_5H_5), 4.44 (m, $^1J_{SiH}$ = 180.8 Hz, 2 H, SiH), 0.47 (s, 3 H, ZrMe), 0.22 (d, $^3J_{HH}$ = 3.2 Hz, 12 H, SiMe). ^{13}C{^{1}H} NMR (benzene-d_6, 125 MHz, 25 °C): δ□112.41 (C_5H_5), 34.46 (ZrMe), 1.96 (SiMe). ^{15}N{^{1}H} NMR (benzene-d_6, 61 MHz, 25 °C): δ -277.4. ^{29}Si{^{1}H} NMR (benzene-d_6, 119.3 MHz, 25 °C): δ -27.6 (SiMe). IR (KBr, cm^{-1}): 3104 m br, 2954 s br, 2074 s br (SiH), 1815 w br, 1718 w br, 1616 w br, 1247 s, 1015 s, 901 s br, 800 s br, 763 s br. Anal. Calcd for $C_{15}H_{27}Si_2NZr$: C, 48.85; H, 7.38; N, 3.80. Found: C, 49.15; H, 7.20; N, 3.79. mp 185-191 °C.

$Cp_2Zr\{\kappa^2$-N(SiHMe$_2$)SiHMeCH$_2$$\}$ (3). A benzene solution of **2** (0.332 g, 0.90 mmol) was heated at 135 °C for 3 h in a sealed reaction vessel. The color quickly turned from pale yellow to green. After 6 h, the reaction mixture was evaporated to provide **3** as an analytically pure, yellow-green oil in excellent yield (0.310 g, 0.879 mmol, 97.6%). ^{1}H NMR (benzene-d_6, 400 MHz, 25 °C): δ 5.84 (s, 5 H, C_5H_5), 5.81 (s, 5 H, C_5H_5), 4.84 (m, $^1J_{SiH}$ = 193.4 Hz, 1 H, NSi*H*Me$_2$), 4.37 (m, $^1J_{SiH}$ = 204.0 Hz, 1 H, ZrCH$_2$Si*H*Me), 1.97 (dd, $^2J_{HH}$ = 12.4 Hz, $^3J_{HH}$ = 4.4 Hz, 1 H, CH$_2$), 1.61 (dd, $^2J_{HH}$ = 12.4 Hz, $^3J_{HH}$ = 2.4 Hz, 1 H, CH$_2$), 0.28 (d, $^3J_{HH}$ = 2.4 Hz, 3 H, SiMe), 0.22 (d, $^3J_{HH}$ = 3.2 Hz, 3 H, SiMe$_2$), 0.20 (d, $^3J_{HH}$ = 3.2 Hz, 3 H, SiMe$_2$). ^{13}C{^{1}H} NMR (benzene-d_6, 125 MHz, 25 °C): δ 112.24 (C_5H_5), 112.20 (C_5H_5), 36.44 (ZrCH$_2$), 2.54 (SiMe$_2$), 2.09 (SiMe$_2$), 1.58 (CH$_2$SiH*Me*). ^{15}N{^{1}H} NMR (benzene-d_6, 61 MHz, 25 °C): δ -250.8. ^{29}Si{^{1}H} NMR (benzene-d_6, 119.3 MHz, 25 °C): δ -19.9 (NSiHMe$_2$), -68.3 (CH$_2$SiHMe). IR (KBr, cm^{-1}): 3097 w br, 2950 m br, 2895 m, 2074 s br (SiH), 1598 w br, 1441 m, 1247 s, 1168 w, 1015 s, 910 s br, 795 s br, 715 m, 678 m. Anal. Calcd for $C_{14}H_{23}Si_2NZr$: C, 47.67; H, 6.57; N, 3.97. Found: C, 47.31; H, 6.80; N, 4.00.

$Cp_2Zr\{\kappa^2$-N(SiHMe$_2$)SiMe$_2$CH$_2$CH$_2$$\}$ (4). Compound **1** (0.129 g, 0.364 mmol) was dissolved in benzene (10 mL) in a 100 mL reaction flask equipped with a Teflon valve. The solution was degassed with three freeze-pump-thaw cycles. The flask was then charged with 1 atm of ethylene, sealed, and heated at 150 °C overnight. The volatiles were removed under reduced pressure to provide analytically pure **4** as light brown oily residue (0.127 g, 0.335 mmol, 92.0%). ^{1}H NMR (benzene-d_6, 400 MHz, 25 °C): δ 5.85 (s, 10 H, C_5H_5), 3.94 (m, $^1J_{SiH}$ = 174.8 Hz, 1 H, NSi*H*Me$_2$), 1.50 (m, 2 H, CH$_2$), 1.34 (m, 2 H, CH$_2$), 0.13 (overlapping s and d, 12 H, SiMe$_2$ and SiH*Me*$_2$). ^{13}C{^{1}H} NMR (benzene-d_6, 125 MHz, 25 °C): δ 112.12 (C_5H_5), 37.86 (ZrCH$_2$), 18.70 (*C*H$_2$SiMe$_2$), 3.55 (SiMe$_2$), 1.87 (CH$_2$Si*Me*$_2$). ^{15}N{^{1}H} NMR (benzene-d_6, 61 MHz, 25 °C): δ -255.9. ^{29}Si{^{1}H} NMR (benzene-d_6, 119.3 MHz, 25 °C): δ -33.3 (*Si*Me). IR (KBr, cm^{-1}): 2951 s, 2900 s br, 2062 s br (SiH), 1800 w, 1704 w, 1602 w, 1441 s, 1406 s, 1366 m, 1247 s, 1166 s, 1015 s, 917 s br, 795 s br. Anal. Calcd for $C_{16}H_{27}Si_2NZr$: C, 50.47; H, 7.15; N, 3.68. Found: C, 50.79; H, 6.89; N, 3.63.

$Cp_2Zr\{N(SiEtMe_2)_2\}H$ (5). This compound was prepared and characterized in situ; all attempts to isolate **5** afforded mixtures of **5** and the cyclometalated $Cp_2Zr\{\kappa^2$-N(SiEtMe$_2$)SiMeEtCH$_2$$\}$

(**6**). A solution of $LiN(SiEtMe_2)_2$ (0.028 g, 0.102 mmol) in benzene-d_6 (0.5 mL) was added to Cp_2ZrHCl (0.020 g, 0.102 mmol) in an NMR tube. Cyclooctane (10 μL) was added to the NMR tube as an internal standard, and the reaction mixture was agitated on a vortex stirrer. After 75 min., $Cp_2Zr\{N(SiEtMe_2)_2\}H$ was detected. The yield was estimated by ^1H NMR spectroscopy as 52.3% based on integration relative to the internal standard. At room temperature, hindered rotation renders the $SiMe_2Et$ groups inequivalent. ^1H NMR (benzene-d_6, 400 MHz, 25 °C): δ 5.88 (s, 10 H, C_5H_5), 5.64 (s, 1 H, Zr*H*), 1.04 (t, $^3J_{HH}$ = 7.8 Hz, 3 H, $SiCH_2CH_3$), 0.98 (t, $^3J_{HH}$ = 5.2 Hz, 3 H, $SiCH_2CH_3$), 0.77 (q, $^3J_{HH}$ = 7.8 Hz, 2 H, $SiCH_2CH_3$), 0.56 (q, $^3J_{HH}$ = 5.2 Hz, 2 H, $SiCH_2CH_3$), 0.24 (s, 6 H, $SiEtMe_2$), 0.06 (s, 6 H, $SiEtMe_2$). $^{13}C\{^1H\}$ NMR (benzene-d_6, 150 MHz, 25 °C): δ 109.54 (C_5H_5), 15.25 ($SiCH_2CH_3$), 13.94 ($SiCH_2CH_3$), 9.07 ($SiCH_2CH_3$), 8.66 ($SiCH_2CH_3$), 4.58 (SiMe), 4.00 (SiMe). $^{15}N\{^1H\}$ NMR (benzene-d_6, 61 MHz, 25 °C): δ -256.7. $^{29}Si\{^1H\}$ NMR (benzene-d_6, 119.3 MHz, 25 °C): δ -6.8, -13.3.

$Cp_2Zr\{\kappa^2$-$N(SiEtMe_2)SiMeEtCH_2\}$ (6). A suspension of $[Cp_2ZrHCl]_n$ (0.087 g, 0.338 mmol) and $LiN(SiEtMe_2)_2$ (0.066 g, 0.338 mmol) was stirred for 24 h in benzene (2 mL) at room temperature. The volatile materials were removed under reduced pressure leaving an off-white solid residue, which was extracted with pentane (2 × 2 mL). The pentane extract was evaporated to dryness to yield **6** as a yellow oil (0.081 g, 0.199 mmol, 58.8%). ^1H NMR (benzene-d_6, 600 MHz, 25 °C): δ 5.84 (s, 5 H, C_5H_5), 5.83 (s, 5 H, C_5H_5), 1.86 (d, $^2J_{HH}$ = 12.1, 1 H, CH_2), 1.72 (d, $^2J_{HH}$ = 12.1 Hz, 1 H, CH_2), 1.13 (t, $^3J_{HH}$ = 7.9 Hz, 3 H, $CH_2SiMeCH_2CH_3$), 1.02 (t, $^3J_{HH}$ = 7.9 Hz, 3 H, $SiMe_2CH_2CH_3$), 0.73 (m, 1 H, $CH_2SiMeCH_2CH_3$), 0.51 (q, $^3J_{HH}$ = 8.4 Hz, 2 H, $SiMe_2CH_2CH_3$), 0.42 (m, 1 H, $CH_2SiMeCH_2CH_3$), 0.18 (s, 3 H, SiMe), 0.06 (s, 3 H, $SiMe_2$), 0.06 (s, 3 H, $SiMe_2$). $^{13}C\{^1H\}$ NMR (benzene-d_6, 150 MHz): δ 112.04 (C_5H_5), 111.97 (C_5H_5), 40.29 ($ZrCH_2$), 13.11 ($SiMe_2CH_2CH_3$), 12.07 ($CH_2SiMeCH_2CH_3$), 9.23 ($CH_2SiMeCH_2CH_3$), 8.76 ($SiMe_2CH_2CH_3$), 2.34 ($SiMe_2$), 2.33 ($SiMe_2$), 1.58 (CH_2SiMe). $^{15}N\{^1H\}$ NMR (benzene-d_6, 61 MHz, 25 °C): δ -239.1. $^{29}Si\{^1H\}$ NMR (benzene-d_6, 119.3 MHz, 25 °C): δ -4.2 ($SiMe_2Et$), -52.5 ($CH_2SiMeEt$). IR (KBr, cm^{-1}): 2951 s, 2872 s, 1459 m, 1249 s, 1180 w, 1014 s, 985 s, 794 s br. Anal. Calcd for $C_{18}H_{31}Si_2NZr$: C, 52.88; H, 7.64; N, 3.43. Found: C, 52.20; H, 7.02; N, 3.80.

$Cp_2Zr\{N(SiHMe_2)_2\}C{\equiv}CSiMe_3$ (7). $Cp_2Zr\{\kappa^2\text{-}N(SiHMe_2)SiHMeCH_2\}$ (**3**) (0.082 g, 0.231 mmol) was dissolved in benzene (5 mL), and $SiMe_3C{\equiv}CH$ (0.33 mL, 2.34 mmol) was added with a syringe. The reaction mixture was heated at 150 °C for 17 h. The volatiles were evaporated under reduced pressure to provide analytically pure **7** as a light brown microcrystalline solid (0.104 g, 0.231 mmol, 99.8%). ^{1}H NMR (benzene-d_6, 600 MHz, 25 °C): δ 6.01 (s, 10 H, C_5H_5), 4.47 (m, $^1J_{SiH}$ = 172.2 Hz, 2 H, Si*H*Me_2), 0.38 (d, $^3J_{HH}$ = 3.2 Hz, 12 H, SiH*Me*$_2$), 0.31 (s, 9 H, $SiMe_3$). $^{13}C\{^1H\}$ NMR (benzene-d_6, 150 MHz, 25 °C): δ 161.48 (Zr*C*≡CSiMe$_3$), 131.39 (ZrC≡*C*SiMe$_3$), 113.03 (C_5H_5), 1.71 ($SiHMe_2$), 0.94 ($SiMe_3$). $^{15}N\{^1H\}$ NMR (benzene-d_6, 61 MHz, 25 °C): δ -267.3. $^{29}Si\{^1H\}$ NMR (benzene-d_6, 119.3 MHz, 25 °C): δ -24.3 ($SiMe_3$), -28.3 ($SiHMe_2$). IR (KBr, cm^{-1}): 2956 m, 2897 w, 2076 m br (SiH), 2031 w (C≡C), 1442 w, 1245 s, 1018 s, 905 s br, 842 s br, 798 s br, 744 s br, 681 s br. Anal. Calcd for $C_{19}H_{33}Si_3NZr$: C, 50.61; H, 7.38; N, 3.11. Found: C, 50.24; H, 7.01; N, 2.74. mp 87-93 °C.

$Cp_2Zr\{N(SiHMe_2)_2\}CH{=}CH_2$ (8). The procedure described above for **2** was used, starting from $Cp_2Zr(CH{=}CH_2)Cl$ (0.037g, 0.130 mmol) and $LiN(SiHMe_2)_2$ (0.018 g, 0.130 mmol) to afford **8** (0.044 g, 0.114 mmol, 87.9%) as light brown gummy solid. ^{1}H NMR (benzene-d_6, 600 MHz, 25 °C): δ 7.68 (dd, $^3J_{HH}$ = 19.2 Hz, $^3J_{HH}$ = 14.4 Hz, 1 H, ZrCH), 6.39 (dd, $^3J_{HH}$ = 14.4 Hz, $^2J_{HH}$ = 3.6 Hz, 1 H, *cis*-ZrCH=CH), 5.89 (s, 10 H, C_5H_5), 5.63 ($^3J_{HH}$ = 19.2 Hz, $^2J_{HH}$ = 3.6 Hz, 1 H, *trans*-ZrCH=CH), 4.48 (m, $^1J_{SiH}$ = 186.5 Hz, 2 H, SiH), 0.24 (d, $^3J_{HH}$ = 3.0 Hz, 12 H, SiMe). $^{13}C\{^1H\}$ NMR (benzene-d_6, 150 MHz, 25 °C): δ 187.22 (ZrCH), 128.82 (ZrCH=*C*H_2), 112.78 (C_5H_5), 1.93 (SiMe). $^{15}N\{^1H\}$ NMR (benzene-d_6, 61 MHz, 25 °C): δ -274.5. $^{29}Si\{^1H\}$ NMR (benzene-d_6, 119.3 MHz, 25 °C): δ -27.3. IR (KBr, cm^{-1}): Anal. Calcd for $C_{19}H_{35}Si_3NZr$: C, 50.47; H, 7.15; N, 3.68. Found: C, 50.83; H, 7.64; N, 3.71.

$Cp_2Zr\{N(SiHMe_2)_2\}Et$ (9). The procedure described above for **2** was used, starting from $Cp_2ZrEtCl$ (0.426 g, 1.490 mmol) and $LiN(SiHMe_2)_2$ (0.208 g, 1.490 mmol) to afford **9** (0.478 g, 1.248 mmol, 83.7%) as light brown solid. ^{1}H NMR (benzene-d_6, 600 MHz, 25 °C): δ 5.84 (s, 10 H, C_5H_5), 4.46 (m, $^1J_{SiH}$ = 183.2 Hz, 2 H, SiH), 1.41 (t, $^3J_{HH}$ = 7.4 Hz, 3 H, $ZrCH_2CH_3$), 1.10 (q, $^3J_{HH}$ = 7.4 Hz, 2 H, $ZrCH_2CH_3$), 0.22 (d, $^3J_{HH}$ = 3.1 Hz, 12 H, SiMe). $^{13}C\{^1H\}$ NMR (benzene-d_6, 150 MHz, 25 °C): δ 112.38 (C_5H_5), 47.66 ($ZrCH_2$), 18.44 (CH_3), 2.28 (SiMe).

$^{15}N\{^{1}H\}$ NMR (benzene-d_6, 61 MHz, 25 °C): δ -277.4. $^{29}Si\{^{1}H\}$ NMR (benzene-d_6, 119.3 MHz, 25 °C): δ -25.8. IR (KBr, cm^{-1}): 3092 w, 2951 m, 2896 m, 2854 m, 2090 m (ν_{SiH}), 2055 m (νSiH), 1443 w, 1370 w, 1246 s, 1172 w, 1139 w, 1016 s, 901 s, 844 m, 800 s, 762 s, 699 s, 679 s, 633 m, 598 m. Anal. Calcd for $C_{16}H_{29}Si_2NZr$: C, 50.20; H, 7.64; N, 3.66. Found: C, 49.05; H, 7.00; N, 3.66. mp 79-83 °C.

$Cp_2Zr[\eta^2$-N(SiHMe$_2$)SiMe$_2$] (10). Compound **9** (0.034 g, 0.088 mmol) was dissolved in benzene-d_6 (0.6 mL) and added to a NMR tube equipped with a J. Young valve. Cyclooctane (0.5 μL) was added to the mixture as an internal standard. The reaction mixture was heated to 65 °C for 2 h to give a brown colored solution that contained a mixture of products. The NMR yield was calculated by comparison to the integration of the internal standard (37.2%). ^{1}H NMR (benzene-d_6, 600 MHz, 25 °C): δ 5.31 (s, 10 H, C_5H_5), 0.55 (s, 6 H, $SiMe_2$), -0.04 (d, $^{3}J_{HH}$ = 5.5 Hz, 6 H, SiH*Me*), -2.23 (m, $^{1}J_{SiH}$ = 89.1 Hz, 1 H, SiH). $^{13}C\{^{1}H\}$ NMR (benzene-d_6, 150 MHz, 25 °C): δ 101.14 (C_5H_5), 3.71 ($SiMe_2$), -0.16 ($SiHMe_2$). $^{15}N\{^{1}H\}$ NMR (benzene-d_6, 61 MHz, 25 °C): δ -355.6. $^{29}Si\{^{1}H\}$ NMR (benzene-d_6, 119.3 MHz, 25 °C): δ -8.7 ($SiMe_2$), -61.5 ($SiHMe_2$).

$Cp_2Zr\{\eta^2$-N(SiHMe$_2$)SiMe$_2$}PMe$_3$ (10·PMe$_3$). Compound **9** (0.022 g, 0.057 mmol) and PMe_3 (6.4 μl, 0.063 mmol) were dissolved in benzene-d_6 (0.6 mL) and added to a NMR tube equipped with a J. Young valve. Cyclooctane (0.5 μL) was added to the mixture as an internal standard. The reaction mixture was heated to 65 °C for 2.5 h to give a deep red solution, and the NMR yield was calculated by comparison to the integration of the internal standard (74.3%). ^{1}H NMR (benzene-d_6, 600 MHz, 25 °C): δ 5.40 (s, 10 H, C_5H_5), 5.18 (br, 1 H, SiH), 0.93 (d, $^{2}J_{PH}$ = 9 Hz, 9 H, PMe), 0.42 (d, $^{3}J_{HH}$ = 4.8 Hz, 6 H, SiH*Me*$_2$), 0.40 (s, 6 H, $SiMe_2$). $^{13}C\{^{1}H\}$ NMR (benzene-d_6, 150 MHz, 25 °C): δ 104.72 (C_5H_5), 20.98 (d, $^{1}J_{PC}$ = 21.8 Hz, PMe), 3.62 ($SiMe_2$ and SiHMe overlapped). $^{15}N\{^{1}H\}$ NMR (benzene-d_6, 61 MHz, 25 °C): δ -331.1. ^{31}P NMR (benzene-d_6, 243 MHz, 25 °C): δ 18.67. $^{29}Si\{^{1}H\}$ NMR (benzene-d_6, 119.3 MHz, 25 °C): δ -12.9 ($^{1}J_{SiH}$ = 177.0 Hz, $SiHMe_2$), -26.9 ($^{2}J_{PSi}$ = 74.0 Hz, $SiMe_2$).

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