Supplementary Information for:

Metalation Resistant β-Diketiminato Ligands for Thermally Robust Organoscandium Complexes

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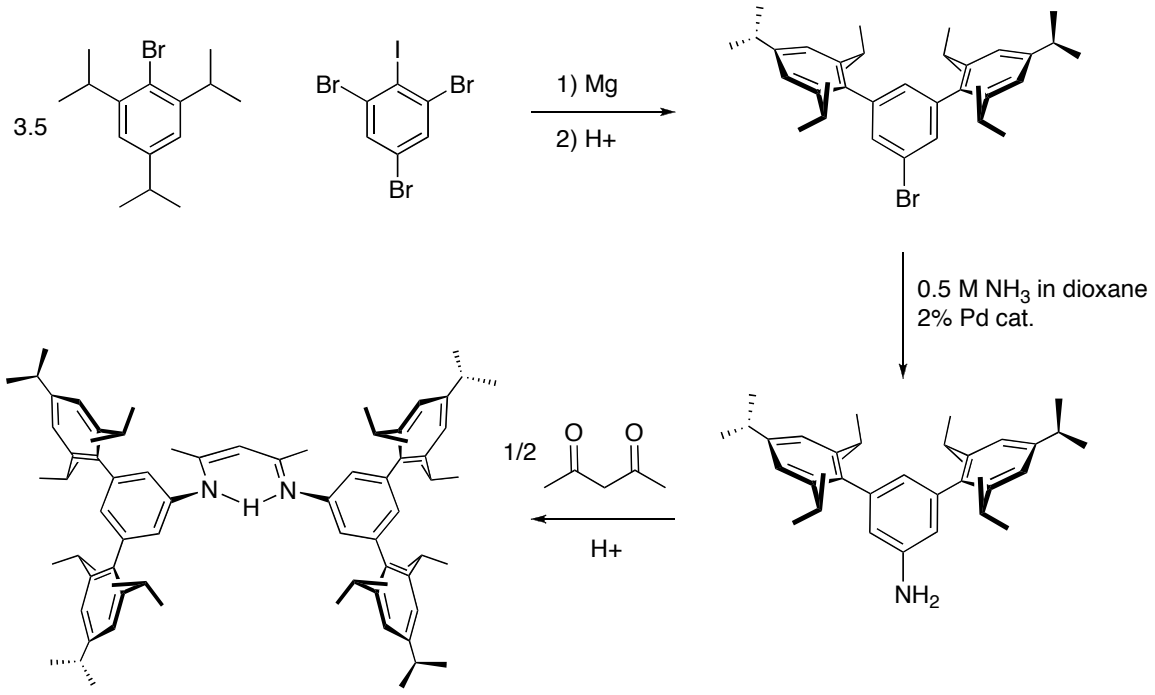
Scheme S1


3.5
Br
I
Br
Br
Br
1) Mg
2) H+
Br
0.5 M NH3 in dioxane
2% Pd cat.
NH2
1/2
O
O
H+
N
H
N

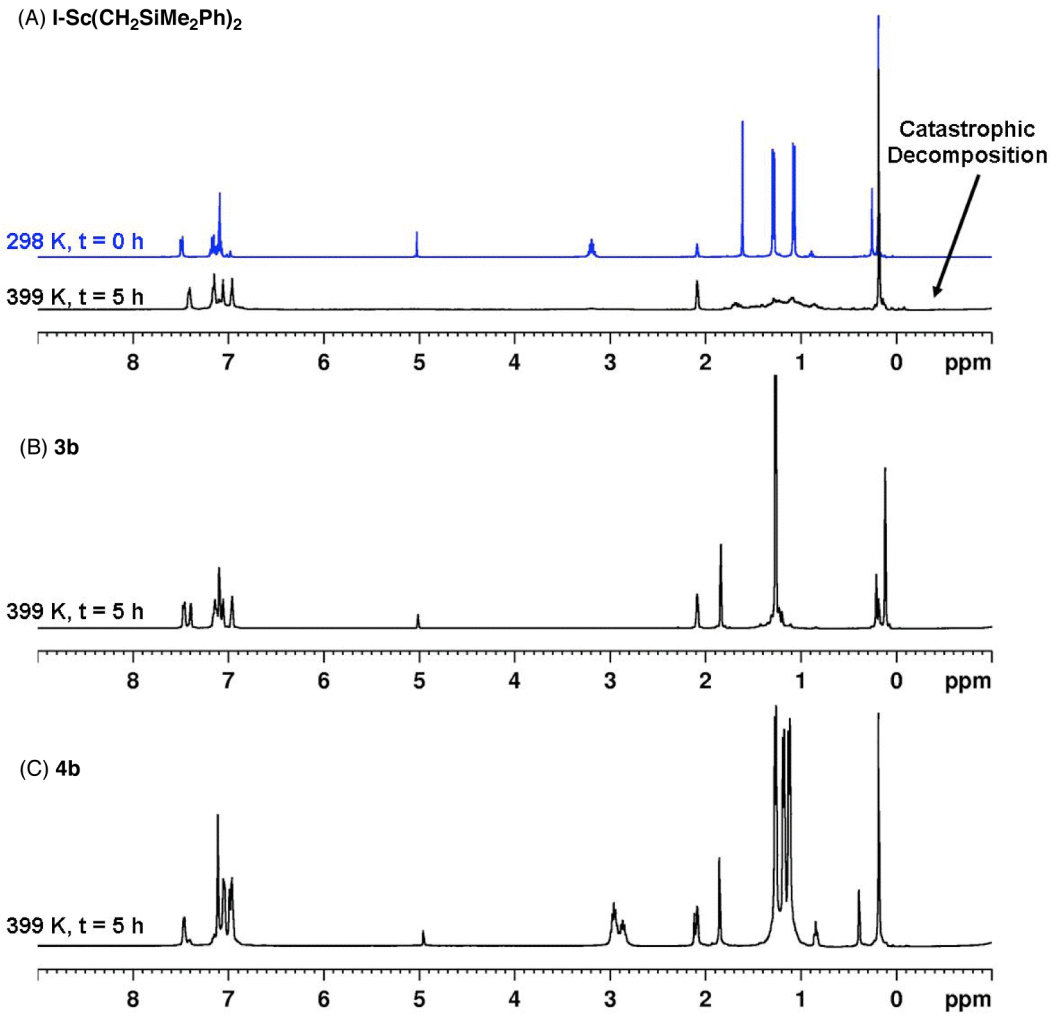


Figure S1. 400 MHz ^{1}H NMR spectroscopy depicting thermolysis of β-diketiminato scandium *bis*-alkyls (A) **I-Sc(CH$_2$SiMe$_2$Ph)$_2$**, (B) **3b** and (C) **4b**. The *bis*-alkyls supported by the previously studied 2,6-di*iso*propylphenyl ligand derivative undergo complete metalation, whereas the 3,5-substituted derivatives show no decomposition after 5 hours at 399 K.

Experimental Details

General Procedures. All operations were performed under a purified argon atmosphere using glovebox or vacuum-line techniques. Toluene, hexanes, and THF solvents were dried and purified using the Grubbs/Dow purification system[1] and were stored in evacuated 500 mL bombs over titanocene or Na/benzophenone ketal. Pentane and bromobenzene were dried over with Na, with a benzophenone indicator. Deuterated NMR solvents were dried according to their respective standard procedures. ^{1}H, $^{13}C\{^{1}H\}$, HMQC, ^{15}N, and ^{29}Si-^{1}H HMBC NMR experiments were performed on a Bruker AMX-300 and WH-400 and data are given in ppm relative to solvent signals for ^{1}H and ^{13}C signals, NH_3 for ^{15}N and $SiMe_4$ for ^{29}Si spectra. Elemental analyses were performed by Mrs. Dorothy Fox and Mr. Jianjun Li of this department.

Materials. HIPTBr (2,4,6,2”,4”,6”-hexaisopropyl-1,3’:5’,1”-terphenyl)bromide[2] bromo-2,4,6-tri*iso*propylbenzene[3] and 2,4,6-tribromo-iodobenzene[4] were prepared according to literature procedures or slight variations thereof. Pd_2dba_3 and 2-dicyclohexylphosphino-2'-(N,N-dimethylamino)biphenyl were purchased from Strem Chemicals, stored under an atmosphere of argon, and used as received. Small magnesium turnings (~1.6mm) and NaO^{t}Bu were purchased from Aldrich, stored under an atmosphere of argon, and used as received unless otherwise noted. Molecular sieves (4Å, 8-12 mesh) were purchased from EM Science and activated by drying under dynamic vacuum at 200°C for 24hours. *Para*toluenesulfonic acid monohydrate, 2,4-pentanedione, and 3,5-di*tert*butylaniline were purchased from Aldrich and used as received. $Sc(CH_2SiMe_2Ph)_3(THF)_2$[5] and $Sc(CH_2SiMe_3)_3(THF)_2$[6] were prepared as

previously described. $[HNMe_2Ph][B(C_6F_5)_4]$ and $[CPh_3][B(C_6F_5)_4]$ were generously provided by NOVA Chemicals.

Synthesis of (2,4,6,2",4",6"-hexaisopropyl-1,3':5',1"-terphenyl)aniline (HIPT-NH_2): Adapted from procedure reported by Buchwald and coworkers.[7] Pd_2dba_3 (57.0 mg, 0.0622 mmol) and 2-dicyclohexylphosphino-2'-(N,N-dimethylamino)biphenyl ligand (106 mg, 0.312 mmol) were added to a 250 mL thick-walled glass bomb. 1,4-Dioxane (30 mL) was condensed into the flask and the solution was then warmed to 50°C for 30 minutes. 3,5-Bis(2,4,6-tri*iso*propylphenyl)bromobenzene **HIPT-Br** (1.75 g, 3.12 mmol) was dissolved in dioxane (25 mL) and added *via* cannula to the premixed catalyst and ligand, followed by solid addition of NaO^tBu (420 mg, 4.36 mmol). Finally, a 0.5 M solution of ammonia in 1,4-dioxane (32 mL, 15.6 mmol) was syringed into the bomb and the flask was sealed under an atmosphere of argon. The mixture was stirred at 80°C for 4 hours, removed from heat and quenched with 100 mL of ethyl acetate. The solution was filtered over silica on a glass frit and washed with an additional 100 mL ethyl acetate. The residual solvents were removed in vacuo and the crude product was purified by flash chromatography with a gradient solvent mixture (1%-20% EtOAc/Hexanes). The purified product is isolated as a yellow powder (1.05 g, 2.11 mmol, 68 % yield). ^{1}H NMR (CD_2Cl_2): 7.03 (s, 4H, *m*-C_6H_2(trip)), 6.44 (d, $^4J_{H\text{-}H}$ = 1.3Hz, 2H, *o*-C_6H_3), 6.31 (t, $^4J_{H\text{-}H}$ = 1.3Hz, 1H, *p*-C_6H_3), 3.76 (s, 2H, NH_2), 2.91 (septet, $^3J_{H\text{-}H}$ = 6.9Hz, 2H, *p*-^{i}PrC*H*(trip)), 2.82 (septet, $^3J_{H\text{-}H}$ =6.9Hz, 4H, *o*-^{i}PrC*H*(trip)), 1.27 (d, $^3J_{H\text{-}H}$ = 6.9Hz, 12H, *p*-^{i}PrCH_3(trip)), 1.15 (d, $^3J_{H\text{-}H}$ = 6.9Hz, 12H, *o*-^{i}PrCH_3(trip)), 1.05 (d, $^3J_{H\text{-}H}$ = 6.9Hz, 12H, *o*-^{i}PrCH_3(trip)). ^{13}C{^{1}H} NMR (CD_2Cl_2): 148.43, 147.19, 146.69, 142.16, 137.99 (C_{ipso}),

122.55 (*p*-C_6H_3), 120.99 (*m*-C_6H_2(trip)), 115.10 (*o*-C_6H_3), 34.95, 30.92 (^{i}Pr*C*H(trip)), 24.93, 24.55, 24.53 (^{i}Pr*C*H_3(trip)). HRMS: Calcd. for $C_{36}H_{51}N$: 497.4021. Found: 497.3996. Anal. Calcd. for $C_{36}H_{51}N$: C, 86.86; H, 10.33; N, 2.81. Found: C, 86.70; H, 10.45; N, 2.83.

Synthesis of [H(3,5-^{t}Bu-C_6H_3)NC(Me)CHC(Me)N(3,5-^{t}Bu-C_6H_3)] (1): A Dean-Stark condenser was affixed to a 100 mL flask charged with *p*-toluenesulfonic acid monohydrate (0.92g, 4.85mmol), 2,4-pentanedione (0.50mL, 4.85mmol) and 3,5-di*tert*butylaniline (2.09g, 10.18mmol), along with toluene (60 mL). The mixture was heated at 130°C for ~48 hours and then basified with triethylamine (0.50g, 4.94mmol) to yield a yellow oil, which was crystallized in refluxing methanol to afford a pale yellow solid (1.13g, 2.37mmol, 49%). ^{1}H NMR (CD_2Cl_2): δ 12.58 (s, 1H, N··*H*··N), 7.13 (t, $^4J_{H\text{-}H}$ = 1.7Hz, 2H, *p*-C_6H_3), 6.80 (d, $^4J_{H\text{-}H}$ = 1.7Hz, 4H, *o*-C_6H_3), 4.88 (s, 1H, C*H*), 1.98 (s, 6H, CH_3), 1.31 (s, 36, C(CH_3)$_3$). ^{13}C{^{1}H} NMR (CD_2Cl_2): δ 159.94, 151.93, 145.65 (C_{ipso}), 117.90 (*p*-C_6H_3), 117.85 (*o*-C_6H_3), 97.46 (*C*H), 35.30 (C_{ipso}), 31.77 (C(*C*H_3)$_3$), 21.11 (*C*H_3). HRMS: Calcd. for $C_{33}H_{50}N_2$: 474.3974. Found: 474.3977. Anal. Calcd. for $C_{33}H_{50}N_2$: C, 83.48; H, 10.62; N, 5.90. Found: C, 83.29; H, 10.49; N, 5.88.

Synthesis of [H(3,5-trip-C_6H_3)NC(Me)CHC(Me)N(3,5-trip- C_6H_3)] (2): A 100 mL round bottom flask, fitted with a Dean-Stark condenser, was charged with 2,4-pentanedione (137 mg, 1.37 mmol), *p*-toluenesulfonic acid (260 mg, 1.37 mmol) and toluene 40 mL. This mixture was warmed to 60ºC for 30 minutes, after which time a solution of 3,5-bis(2,4,6-tri*iso*propylphenyl)aniline (1.37 g, 2.76 mmol) in toluene (25

mL) was added *via* syringe. The reaction was refluxed overnight, removing water in the Dean-Stark when necessary and the solvent volume in the reaction vessel was kept to 60-70 mL. After 24 hours, 5 Å molecular sieves were added, and the reaction was refluxed for another 48 hours. After cooling to room temperature, NEt_3 (160 mg, 1.6 mmol) was added and the solution stirred for 20 minutes. Upon removing the volatiles *in vacuo*, the yellow oily crude product was purified by column chromatography (using a basified silica column) and recrystallized in methanol to give a fine yellow powder of $^{Hipt}L_{Mw}H$ (1.05 g, 0.986 mmol, 72 % yield). ^{1}H NMR (CD_2Cl_2): 12.90 (s, 1H, N··*H*··N), 7.01 (s, 8H, *m*-C_6H_2(trip)), 6.70 (d, $^4J_{H\text{-}H}$ = 1.4Hz, 4H, *o*-C_6H_3), 6.60 (t, $^4J_{H\text{-}H}$ = 1.4Hz, 2H, *p*-C_6H_3), 4.89 (s, 1H, C*H*), 2.90 (septet, $^3J_{H\text{-}H}$ = 6.9Hz, 4H, *p*-^{i}PrC*H*(trip)), 2.77 (septet, $^3J_{H\text{-}H}$ = 6.9Hz, 8H, *o*-^{i}PrC*H*(trip)), 2.05 (s, 6H, CH_3), 1.28 (d, $^3J_{H\text{-}H}$ = 6.9Hz, 24H, *p*-^{i}PrCH_3(trip)), 1.06 (d, $^3J_{H\text{-}H}$ = 6.9Hz, 24H, *o*-^{i}PrCH_3(trip)), 1.03 (d, $^3J_{H\text{-}H}$ = 6.9Hz, 24H, *o*-^{i}PrCH_3(trip)). ^{13}C{^{1}H} NMR (CD_2Cl_2): 159.98, 148.54, 147.12, 145.93, 141.76, 137.49 (C_{ipso}), 126.83 (*p*-C_6H_3), 122.05 (*o*-C_6H_3), 120.97 (*m*-C_6H_2(trip)), 98.54 (*C*H), 34.91(*p*-^{i}Pr*C*H(trip)), 30.94 (*o*-^{i}Pr*C*H(trip)), 24.66, 24.46, 24.42 (^{i}Pr*C*H_3(trip)), 21.46 (*C*H_3). Anal. Calcd. for $C_{77}H_{106}N_2$: C, 87.27; H, 10.08; N, 2.64. Found: C, 87.12; H, 10.14; N, 2.32.

Synthesis of 3a: A cooled 50 mL round bottom flask was charged with **1** (452 mg, 1.002 mmol) and $Sc(CH_2SiMe_3)_3(THF)_2$ (477 mg, 1.002 mmol) and attached to a swivel-frit assembly. On the vacuum line, toluene (20 mL) was condensed into the flask at -78ºC. The flask was then transferred to an ice bath (0ºC) and was allowed to warm to room temperature over 3 hours. Stirring continued for one hour at room temperature. The

solvent was removed *in vacuo* and pentane (10 mL) was condensed onto the crude yellow oil. The solution was sonicated and then cooled to -78ºC to precipitate a fine yellow powder. After cold filtration, the isolated yellow powder was dried under vacuum to yield **3a** (350mg, 0.505 mmol, 51 %). ^{1}H NMR (d_8-toluene, 298K): δ 7.40 (s, 2H; *p*-C_6H_3), 7.19 (s, 4H; *o*-C_6H_3), 4.94 (s, 1H; C*H*), 1.82 (s, 6H; NCCH_3), 1.31 (s, 36H; *m*-^{t}Bu), 0.07 (s, 4H; Sc-CH_2), -0.04 (s, 18; SiMe_3). ^{13}C{^{1}H} NMR (d_8-toluene, 298K): δ 165.0 (N*C*CH_3), 153.0 (*ipso*-C_6H_3), 142.8 (*m*-C_6H_3), 120.0 (*p*-C_6H_3), 119.5 (*m*-C_6H_3), 99.8 (NC*C*H), 42.5 (Sc-*C*H_2), 34.8 (NC*C*$(CH_3)_3$), 31.1 (NCC(CH$_3$)$_3$), 22.19 (NC*C*H_3), 3.00 (SiMe_3). Anal. Calcd. For $C_{41}H_{71}N_2ScSi_2$: C, 71.04; H, 10.32; N, 4.04. Found: C, 70.45; H, 10.41; N, 4.15.

Synthesis of 3b: A 50 mL round bottom flask was charged with **1** (522 mg, 1.099 mmol) and $Sc(CH_2SiMe_2Ph)_3(THF)_2$ (700 mg, 1.099 mmol) and attached to a swivel-frit assembly. On the vacuum line, toluene (20 mL) was condensed into the flask at -78ºC. The flask was then transferred to an ice bath (0ºC) and was allowed to warm slowly to room temperature. Stirring continued for one hour at room temperature. The solvent was removed *in vacuo* and hexane (15 mL) was condensed onto the crude orange oil. The solution was sonicated and then cooled to -78ºC to precipitate the yellow product. After cold filtration, the isolated yellow powder was dried under vacuum to yield **3b** (682 mg, 0.708 mmol, 64 %). ^{1}H NMR (C_6D_6): δ 7.62-7.58 (m, 4H, *o*-C_6H_5), 7.44 (t, $^{4}J_{H\text{-}H}$ = 1.6Hz, 2H, *p*-C_6H_3), 7.26-7.17 (m, 6H, *m*/*p*-C_6H_5), 7.19 (d, $^{4}J_{H\text{-}H}$ = 1.6Hz, 4H, *o*-C_6H_3), 5.02 (s, 1H, C*H*), 1.85 (s, 6H, CH_3), 1.27 (s, 36H, C(CH_3)$_3$), 0.37 (s, 4H, Sc-CH_2), 0.25 (s, 12H, Si(CH_3)$_2$). ^{13}C{^{1}H} NMR (C_6D_6): δ 166.04, 154.05, 145.77, 143.38 (C_{ipso}), 134.18 (*o*-

C_6H_5), 128.63-128.03 (*m*/*p*-C_6H_5), 120.99 (*p*-C_6H_3), 120.28 (*o*-C_6H_3), 101.16 (*C*H), 40.49 (Sc-*C*H_2), 35.55 (C_{ipso}), 31.89 (C(*C*H_3)$_3$), 23.14 (*C*H_3), 2.45 (Si(*C*H_3)$_2$). Anal. Calcd. for $C_{51}H_{75}N_2ScSi_2$: C, 74.95; H, 9.25; N, 3.43. Found: C, 74.74; H, 8.89; N, 3.61.

Synthesis of 4a: $ScCl_3(THF)_3$ (542mg, 1.47mmol) and solid $LiCH_2SiMe_3$ (416mg, 4.423mmol) were added to a 100mL RB flask attached to a swivel-frit apparatus. Hexanes (50mL) were condensed into the flask and the mixture was stirred at 0°C for 2 hours followed by sonication and stirring at room temperature for 15min. The mixture was then cold filtered to remove LiCl and cooled to -78°C. A mixture of **2** (1.500g, 1.42mmol, dried under dynamic vacuum overnight) and hexanes (50mL) was added to the cooled flask via cannula. The resulting mixture was stirred at 0°C for 2 hours then at room temperature for a further 2 hours. Solvent evacuation and crystallization from pentane yielded **4a** as a pale yellow solid that was dried under vacuum overnight to remove residual THF (1.09g, 0.855mmol, 58%). ^{1}H NMR (C_6D_6): δ 7.20 (s, 8H, *m*-C_6H_2(trip)), 7.15 (s, 4H, *o*-C_6H_3), 7.01 (s, 2H, *p*-C_6H_3), 4.95 (s, 1H, C*H*), 3.08 (septet, $^3J_{H-H}$ = 6.8Hz, 8H, *o*-^{i}PrC*H*(trip)), 2.86 (septet, $^3J_{H-H}$ = 6.9Hz, 4H, *p*-^{i}PrC*H*(trip)), 1.90 (s, 6H, CH_3), 1.33 (d, $^3J_{H-H}$ = 6.8Hz, 24H, *o*-^{i}PrCH_3(trip)), 1.28 (d, $^3J_{H-H}$ = 6.9Hz, 24H, *p*-^{i}PrCH_3(trip)), 1.23 (d, $^3J_{H-H}$ = 6.8Hz, 24H, *o*-^{i}PrCH_3(trip)), 0.27 (s, 4H, Sc-CH_2), 0.07 (s, 18H, Si(CH_3)$_3$) . ^{13}C{^{1}H} NMR (tol-d_8): δ 166.95, 149.09, 147.13, 146.29, 143.51, 136.92 (C_{ipso}), 130.33 (*p*-C_6H_3), 125.67 (*o*-C_6H_3), 121.22 (*m*-C_6H_2(trip)), 99.54 (*C*H), 44.99 (Sc-*C*H_2), 35.18 (*o*-^{i}Pr*C*H(trip)), 31.31 (*p*-^{i}Pr*C*H(trip)), 25.13, 24.99, 24.71 (^{i}Pr*C*H_3(trip)), 23.60 (*C*H_3), 3.83 (Si(*C*H_3)$_3$). Anal. Calcd. for $C_{85}H_{127}N_2OScSi_2$: C, 79.88; H, 10.02; N, 2.19. Found: C, 79.69; H, 10.19; N, 2.12.

Synthesis of 4b: Toluene (50mL) was condensed into an evacuated 100mL RB flask attached to a swivel frit apparatus containing **2** (2.25g, 2.12mmol) and $Sc(CH_2SiMe_2Ph)_3(THF)_2$ (1.35g, 2.12mmol). The mixture was stirred at 0°C for 90min, then at room temperature for 3 hours. The solvent was removed *in vacuo* to afford a pale yellow solid (2.39g, 1.70mmol, 80%) that was further purified by recrystallization in pentane (~4mL). ^{1}H NMR (tol-d_8): δ 7.53-7.50 (m, 4H, *o*-C_6H_5), 7.14 (s, 8H, *m*-C_6H_2(trip)), 7.10-7.06 (m, 6H, *m*/*p*-C_6H_5), 6.98 (d, $^4J_{H\text{-}H}$ =1.2Hz, 4H, *o*-C_6H_3), 6.97 (t, $^4J_{H\text{-}H}$ =1.2Hz, 2H, *p*-C_6H_3), 4.92 (s, 1H, C*H*), 2.96 (septet, $^3J_{H\text{-}H}$ = 6.8Hz, 8H, *o*-^{i}PrC*H* (trip)), 2.86 (septet, $^3J_{H\text{-}H}$ = 6.9Hz, 4H, *p*-^{i}PrC*H* (trip)), 1.30 (s, 6H, CH_3), 1.29 (d, $^3J_{H\text{-}H}$ = 6.9Hz, 24H, *p*-^{i}PrC*H*$_3$(trip)), 1.22 (d, $^3J_{H\text{-}H}$ = 6.9Hz, 24H, *o*-^{i}PrC*H*$_3$(trip)), 1.15 (d, $^3J_{H\text{-}H}$ = 6.9Hz, 24H, *o*-^{i}PrC*H*$_3$(trip)), 0.44 (s, 4H, Sc-CH_2), 0.23 (s, 12H, Si(CH_3)$_2$). ^{13}C{^{1}H} NMR (tol-d_8): δ 167.78, 149.03, 147.08, 145.54, 145.34, 143.75, 136.87 (C_{ipso}), 134.00 (*o*-C_6H_5), 130.94 (*p*-C_6H_3), 129.66–127.82 (*m*/*p*-C_6H_5), 125.93 (*o*-C_6H_3), 121.20 (*m*-C_6H_2(trip)), 99.86 (*C*H), 42.86 (Sc-*C*H$_2$), 35.28 (*p*-^{i}Pr*C*H(trip)), 31.35 (*o*-^{i}Pr*C*H(trip)), 25.10, 24.90, 24.77 (^{i}Pr*C*H$_3$(trip)), 23.60 (*C*H$_3$), 2.47 (Si(*C*H$_3$)$_2$). Anal. Calcd. for $C_{95}H_{131}N_2ScSi_2$: C, 81.37; H, 9.42; N, 2.00. Found: C, 81.22; H, 9.36; N, 1.87.

Synthesis of 5b: In the glove box, a 10 mL round bottom flask charged with **4b** (25 mg, 0.019 mmol), $[HNMe_2Ph][B(C_6F_5)_4]$ (15 mg, 0.019 mmol) and bromobenzene (2 mL) and fitted to a line adapter. The flask was sonicated until all the $[HNMe_2Ph][B(C_6F_5)_4]$ had dissolved and the solvent was then removed *in vacuo* to give a yellow oil. In the glove box, pentane (2 mL) was added to the oil, and the biphasic solution was stirred for

5 minutes. The pentane layer was removed *via* syringe and then the product oil was dissolved in d_5-bromobenzene for NMR spectroscopic characterization. ^{1}H NMR (C_6D_5Br, 298 K): δ 7.48 (m, 4H; *o, m*-SiPh), 7.24 (m, 2H; *m*-$C_6H_5NMe_2$), 7.17 (s, 8H; *m*-C_6H_2), 6.89 (m, 1H; *p*-Si*Ph*), 6.67 (s, 4H, *o*-C_6H_3), 6.49 (m, 3H; *o,p*-$C_5H_5NMe_2$), 5.32 (s, 1H; NCC*H*), 2.93 (sp, 4H; *p*-^{i}PrC*H*), 2.73 (sp, 8H; *o*-^{i}PrC*H*), 2.53 (s, 6H; N*Me*$_2$), 1.93 (NCC*H*$_3$), 1.3 (d, 24H; *p*-^{i}PrC*H*$_3$), 1.20, 1.11 (d, 24H; *o*-^{i}PrC*H*), 0.34 (s, 2H; Sc-C*H*$_2$), -0.07 (s, 6H; Si*Me*$_2$). ^{13}C{^{1}H} (C_6D_5Br, 298 K): δ 168.9 (NC*C*H$_3$), 149.9 (*C*$_6$H$_5$NMe$_2$), 149.3 (*ipso*-*C*$_6$H$_3$) 146.2, 145.8, 143.7, 142.8, 140.3 (*quat*-*C*$_6$H$_2$, *C*$_6$H$_3$, Si*Ph*), 135.2, 132.9, 129.3, 129.0, 128.5, 128.1, 127.7, 125.6, 124.2 (*C*$_6$H$_3$, *C*$_6$H$_2$, Si*Ph*), 115.9 (*o*-*C*$_6$H$_5$NMe$_2$), 113.0 (*p*-*C*$_6$H$_5$NMe$_2$), 99.1 (NC*C*H), 56.1 (Sc-*C*H$_2$), 40.1(N*Me*$_2$), 34.8 (*p*-^{i}PrC*H*), 34.4 (*o*-^{i}PrC*H*$_3$) 31.9 (*o*-^{i}PrC*H*$_3$), 30.2 (*o*-^{i}PrC*H*), 25.6 (*p*-^{i}PrC*H*$_3$), 23.6 (NC*C*H$_3$), 13.6 (Si*Me*$_2$). ^{19}F NMR (C_6D_5Br); δ -131.2 (*o*-F), -161.1 (*p*-F), -164.7 (*m*-F). ^{11}B NMR (C_6D_5Br , 258 K): δ -16.9.

Synthesis of 6: An NMR tube was charged with **4b** (25 mg, 0.017 mmol) and [CPh$_3$][B(C$_6$F$_5$)$_4$] (16 mg, 0.017 mmol), along with d_5-bromobenzene (0.6 mL). The solution changed from deep orange to light yellow over ~10 seconds. ^{1}H NMR (C_6D_5Br): δ 7.4 (m, 2H; *m*-SiPh), 7.3 (b, 2H; *o*-SiPh), 7.30-7.03 (m, 11H; *p*-C_6H_3, *m*C_6H_2, *p*-SiPh), 6.73 (s, 4H; *o*-C_6H_3), 5.45 (s, 1H; NCC*H*), 2.94 (sp, 4H; *p*-^{i}PrC*H*), 2.72 (sp, 8H; *o*-^{i}PrC*H*), 2.14 (b, 2H; Ph$_3$CC*H*$_2$), 1.98 (NCC*H*$_3$), 1.32 (d, 24H; *p*-^{i}PrC*H*$_3$), 1.21, 1.12 (d, 24H; *o*-^{i}PrC*H*), 0.23 (s, 2H; Sc-C*H*$_2$), 0.20 (Ph$_3$CCH$_2$Si*Me*$_2$), -0.12 (s, 6H; Si*Me*$_2$). ^{13}C{^{1}H} (C_6D_5Br, 298 K): δ 168.9 (NC*C*H$_3$), 149.3 (*ipso*-*C*$_6$H$_3$) 146.2, 145.8, 143.7, 142.8, 140.3 (*quat*-*C*$_6$H$_2$, *C*$_6$H$_3$, Si*Ph*), 135.2, 129.3, 128.5, 128.1, 127.7, 124.2 (*C*$_6$H$_3$,

C$_6$H$_2$, Si*Ph*), 99.1 (NC*C*H), 56.1 (Sc-*C*H$_2$), 43.2 (Ph$_3$*C*CH$_2$), 35.2 (Ph$_3$C*C*H$_2$) 34.8 (*p*-^{i}PrC*H*), 34.4 (*o*-^{i}PrC*H*$_3$) 31.9 (*o*-^{i}PrC*H*$_3$), 30.2 (*o*-^{i}PrC*H*), 25.6 (*p*-^{i}PrC*H*$_3$), 23.6 (NC*C*H$_3$), 13.6 (Si*Me*$_2$) 11.2 (Ph$_3$CCH$_2$Si*Me*$_2$). ^{19}F NMR (C_6D_5Br); δ -131.1 (*o*-F), -161.0 (*p*-F), -164.9 (*m*-F). ^{11}B NMR (C_6D_5Br , 258 K): δ -16.2.

[1] Pangborn, A. B.; Giardello, M. A.; Grubbs, R. H.; Rosen, R. K.; Timmers, F. J. *Organometallics* **1996**, *15*, 1518.
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