Supplementary Information for:

**Metalation Resistant β -Diketiminato Ligands for Thermally Robust
Organoscandium Complexes**

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Scheme S1

S2

Figure S1

S3

Experimental Details

S4-S12

Scheme S1

Figure S1. 400 MHz ^1H NMR spectroscopy depicting thermolysis of β -diketiminato scandium *bis*-alkyls (A) $\text{I-Sc}(\text{CH}_2\text{SiMe}_2\text{Ph})_2$, (B) **3b** and (C) **4b**. The *bis*-alkyls supported by the previously studied 2,6-diisopropylphenyl 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 system¹ 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. ¹H, ¹³C{¹H}, HMQC, ¹⁵N, and ²⁹Si-¹H HMBC NMR experiments were performed on a Bruker AMX-300 and WH-400 and data are given in ppm relative to solvent signals for ¹H and ¹³C signals, NH₃ for ¹⁵N and SiMe₄ for ²⁹Si 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)bromide² bromo-2,4,6-triisopropylbenzene³ and 2,4,6-tribromo-iodobenzene⁴ were prepared according to literature procedures or slight variations thereof. Pd₂dba₃ and 2-di(tert-butyl)phosphino-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'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. Paratoluenesulfonic acid monohydrate, 2,4-pentanedione, and 3,5-ditertbutylaniline were purchased from Aldrich and used as received. Sc(CH₂SiMe₂Ph)₃(THF)₂⁵ and Sc(CH₂SiMe₃)₃(THF)₂⁶ were prepared as

previously described. $[\text{HNMe}_2\text{Ph}][\text{B}(\text{C}_6\text{F}_5)_4]$ and $[\text{CPh}_3][\text{B}(\text{C}_6\text{F}_5)_4]$ were generously provided by NOVA Chemicals.

Synthesis of (2,4,6,2'',4'',6''-hexaisopropyl-1,3':5',1''-terphenyl)aniline (HIPT-NH₂): Adapted from procedure reported by Buchwald and coworkers.⁷ Pd_2dba_3 (57.0 mg, 0.0622 mmol) and 2-di(tert-butyl)phosphino-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-triisopropylphenyl)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*t*Bu (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). ¹H NMR (CD_2Cl_2): 7.03 (s, 4H, *m*-C₆H₂(trip)), 6.44 (d, ⁴*J*_{H-H} = 1.3Hz, 2H, *o*-C₆H₃), 6.31 (t, ⁴*J*_{H-H} = 1.3Hz, 1H, *p*-C₆H₃), 3.76 (s, 2H, NH₂), 2.91 (septet, ³*J*_{H-H} = 6.9Hz, 2H, *p*-ⁱPrCH(trip)), 2.82 (septet, ³*J*_{H-H} = 6.9Hz, 4H, *o*-ⁱPrCH(trip)), 1.27 (d, ³*J*_{H-H} = 6.9Hz, 12H, *p*-ⁱPrCH₃(trip)), 1.15 (d, ³*J*_{H-H} = 6.9Hz, 12H, *o*-ⁱPrCH₃(trip)), 1.05 (d, ³*J*_{H-H} = 6.9Hz, 12H, *o*-ⁱPrCH₃(trip)). ¹³C{¹H} NMR (CD_2Cl_2): 148.43, 147.19, 146.69, 142.16, 137.99 (C_{ipso}),

122.55 (*p*-C₆H₃), 120.99 (*m*-C₆H₂(trip)), 115.10 (*o*-C₆H₃), 34.95, 30.92 (ⁱPrCH(trip)), 24.93, 24.55, 24.53 (ⁱPrCH₃(trip)). HRMS: Calcd. for C₃₆H₅₁N: 497.4021. Found: 497.3996. Anal. Calcd. for C₃₆H₅₁N: C, 86.86; H, 10.33; N, 2.81. Found: C, 86.70; H, 10.45; N, 2.83.

Synthesis of [H(3,5-^tBu-C₆H₃)NC(Me)CHC(Me)N(3,5-^tBu-C₆H₃)] (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-ditertbutylaniline (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%). ¹H NMR (CD₂Cl₂): δ 12.58 (s, 1H, N··H··N), 7.13 (t, ⁴J_{H-H} = 1.7Hz, 2H, *p*-C₆H₃), 6.80 (d, ⁴J_{H-H} = 1.7Hz, 4H, *o*-C₆H₃), 4.88 (s, 1H, CH), 1.98 (s, 6H, CH₃), 1.31 (s, 36, C(CH₃)₃). ¹³C{¹H} NMR (CD₂Cl₂): δ 159.94, 151.93, 145.65 (C_{ipso}), 117.90 (*p*-C₆H₃), 117.85 (*o*-C₆H₃), 97.46 (CH), 35.30 (C_{ipso}), 31.77 (C(CH₃)₃), 21.11 (CH₃). HRMS: Calcd. for C₃₃H₅₀N₂: 474.3974. Found: 474.3977. Anal. Calcd. for C₃₃H₅₀N₂: 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-C₆H₃)NC(Me)CHC(Me)N(3,5-trip-C₆H₃)] (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 60°C for 30 minutes, after which time a solution of 3,5-bis(2,4,6-triisopropylphenyl)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 $^{\text{Hipt}}\text{L}_{\text{Mw}}\text{H}$ (1.05 g, 0.986 mmol, 72 % yield). ^1H NMR (CD_2Cl_2): 12.90 (s, 1H, $\text{N}\cdots\text{H}\cdots\text{N}$), 7.01 (s, 8H, *m*- $\text{C}_6\text{H}_2(\text{trip})$), 6.70 (d, $^4J_{\text{H-H}} = 1.4\text{Hz}$, 4H, *o*- C_6H_3), 6.60 (t, $^4J_{\text{H-H}} = 1.4\text{Hz}$, 2H, *p*- C_6H_3), 4.89 (s, 1H, CH), 2.90 (septet, $^3J_{\text{H-H}} = 6.9\text{Hz}$, 4H, *p*- $^i\text{PrCH}(\text{trip})$), 2.77 (septet, $^3J_{\text{H-H}} = 6.9\text{Hz}$, 8H, *o*- $^i\text{PrCH}(\text{trip})$), 2.05 (s, 6H, CH_3), 1.28 (d, $^3J_{\text{H-H}} = 6.9\text{Hz}$, 24H, *p*- $^i\text{PrCH}_3(\text{trip})$), 1.06 (d, $^3J_{\text{H-H}} = 6.9\text{Hz}$, 24H, *o*- $^i\text{PrCH}_3(\text{trip})$), 1.03 (d, $^3J_{\text{H-H}} = 6.9\text{Hz}$, 24H, *o*- $^i\text{PrCH}_3(\text{trip})$). $^{13}\text{C}\{^1\text{H}\}$ 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*- $\text{C}_6\text{H}_2(\text{trip})$), 98.54 (CH), 34.91(*p*- $^i\text{PrCH}(\text{trip})$), 30.94 (*o*- $^i\text{PrCH}(\text{trip})$), 24.66, 24.46, 24.42 ($^i\text{PrCH}_3(\text{trip})$), 21.46 (CH_3). Anal. Calcd. for $\text{C}_{77}\text{H}_{106}\text{N}_2$: 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 $\text{Sc}(\text{CH}_2\text{SiMe}_3)_3(\text{THF})_2$ (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 -78°C . The flask was then transferred to an ice bath (0°C) 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 -78°C 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 %). ^1H NMR (d_8 -toluene, 298K): δ 7.40 (s, 2H; $p\text{-C}_6\text{H}_3$), 7.19 (s, 4H; $o\text{-C}_6\text{H}_3$), 4.94 (s, 1H; CH), 1.82 (s, 6H; NCCCH_3), 1.31 (s, 36H; $m\text{-}^t\text{Bu}$), 0.07 (s, 4H; Sc-CH_2), -0.04 (s, 18; SiMe_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (d_8 -toluene, 298K): δ 165.0 (NCCCH_3), 153.0 ($ipso\text{-C}_6\text{H}_3$), 142.8 ($m\text{-C}_6\text{H}_3$), 120.0 ($p\text{-C}_6\text{H}_3$), 119.5 ($m\text{-C}_6\text{H}_3$), 99.8 (NCCCH), 42.5 (Sc-CH_2), 34.8 ($\text{NCC}(\text{CH}_3)_3$), 31.1 ($\text{NCC}(\text{CH}_3)_3$), 22.19 (NCCCH_3), 3.00 (SiMe_3). Anal. Calcd. For $\text{C}_{41}\text{H}_{71}\text{N}_2\text{ScSi}_2$: 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 $\text{Sc}(\text{CH}_2\text{SiMe}_2\text{Ph})_3(\text{THF})_2$ (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 -78°C . The flask was then transferred to an ice bath (0°C) 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 -78°C 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 %). ^1H NMR (C_6D_6): δ 7.62-7.58 (m, 4H, $o\text{-C}_6\text{H}_5$), 7.44 (t, $^4J_{\text{H-H}} = 1.6\text{Hz}$, 2H, $p\text{-C}_6\text{H}_3$), 7.26-7.17 (m, 6H, $m/p\text{-C}_6\text{H}_5$), 7.19 (d, $^4J_{\text{H-H}} = 1.6\text{Hz}$, 4H, $o\text{-C}_6\text{H}_3$), 5.02 (s, 1H, CH), 1.85 (s, 6H, CH_3), 1.27 (s, 36H, $\text{C}(\text{CH}_3)_3$), 0.37 (s, 4H, Sc-CH_2), 0.25 (s, 12H, $\text{Si}(\text{CH}_3)_2$). $^{13}\text{C}\{^1\text{H}\}$ NMR (C_6D_6): δ 166.04, 154.05, 145.77, 143.38 (C_{ipso}), 134.18 ($o\text{-}$

C_6H_5), 128.63-128.03 (*m/p*- C_6H_5), 120.99 (*p*- C_6H_5), 120.28 (*o*- C_6H_5), 101.16 (CH), 40.49 (Sc-CH₂), 35.55 (C_{ipso}), 31.89 (C(CH₃)₃), 23.14 (CH₃), 2.45 (Si(CH₃)₂). Anal. Calcd. for C₅₁H₇₅N₂ScSi₂: C, 74.95; H, 9.25; N, 3.43. Found: C, 74.74; H, 8.89; N, 3.61.

Synthesis of 4a: ScCl₃(THF)₃ (542mg, 1.47mmol) and solid LiCH₂SiMe₃ (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%). ¹H NMR (C₆D₆): δ 7.20 (s, 8H, *m*-C₆H₂(trip)), 7.15 (s, 4H, *o*-C₆H₃), 7.01 (s, 2H, *p*-C₆H₃), 4.95 (s, 1H, CH), 3.08 (septet, ³J_{H-H} = 6.8Hz, 8H, *o*-ⁱPrCH(trip)), 2.86 (septet, ³J_{H-H} = 6.9Hz, 4H, *p*-ⁱPrCH(trip)), 1.90 (s, 6H, CH₃), 1.33 (d, ³J_{H-H} = 6.8Hz, 24H, *o*-ⁱPrCH₃(trip)), 1.28 (d, ³J_{H-H} = 6.9Hz, 24H, *p*-ⁱPrCH₃(trip)), 1.23 (d, ³J_{H-H} = 6.8Hz, 24H, *o*-ⁱPrCH₃(trip)), 0.27 (s, 4H, Sc-CH₂), 0.07 (s, 18H, Si(CH₃)₃). ¹³C{¹H} NMR (tol-d₈): δ 166.95, 149.09, 147.13, 146.29, 143.51, 136.92 (C_{ipso}), 130.33 (*p*-C₆H₃), 125.67 (*o*-C₆H₃), 121.22 (*m*-C₆H₂(trip)), 99.54 (CH), 44.99 (Sc-CH₂), 35.18 (*o*-ⁱPrCH(trip)), 31.31 (*p*-ⁱPrCH(trip)), 25.13, 24.99, 24.71 (ⁱPrCH₃(trip)), 23.60 (CH₃), 3.83 (Si(CH₃)₃). Anal. Calcd. for C₈₅H₁₂₇N₂OScSi₂: 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 $\text{Sc}(\text{CH}_2\text{SiMe}_2\text{Ph})_3(\text{THF})_2$ (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). ^1H NMR (tol- d_8): δ 7.53-7.50 (m, 4H, *o*- C_6H_5), 7.14 (s, 8H, *m*- $\text{C}_6\text{H}_2(\text{trip})$), 7.10-7.06 (m, 6H, *m/p*- C_6H_5), 6.98 (d, $^4J_{\text{H-H}} = 1.2\text{Hz}$, 4H, *o*- C_6H_3), 6.97 (t, $^4J_{\text{H-H}} = 1.2\text{Hz}$, 2H, *p*- C_6H_3), 4.92 (s, 1H, CH), 2.96 (septet, $^3J_{\text{H-H}} = 6.8\text{Hz}$, 8H, *o*- $^i\text{PrCH}(\text{trip})$), 2.86 (septet, $^3J_{\text{H-H}} = 6.9\text{Hz}$, 4H, *p*- $^i\text{PrCH}(\text{trip})$), 1.30 (s, 6H, CH_3), 1.29 (d, $^3J_{\text{H-H}} = 6.9\text{Hz}$, 24H, *p*- $^i\text{PrCH}_3(\text{trip})$), 1.22 (d, $^3J_{\text{H-H}} = 6.9\text{Hz}$, 24H, *o*- $^i\text{PrCH}_3(\text{trip})$), 1.15 (d, $^3J_{\text{H-H}} = 6.9\text{Hz}$, 24H, *o*- $^i\text{PrCH}_3(\text{trip})$), 0.44 (s, 4H, Sc- CH_2), 0.23 (s, 12H, $\text{Si}(\text{CH}_3)_2$). $^{13}\text{C}\{^1\text{H}\}$ 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*- $\text{C}_6\text{H}_2(\text{trip})$), 99.86 (CH), 42.86 (Sc- CH_2), 35.28 (*p*- $^i\text{PrCH}(\text{trip})$), 31.35 (*o*- $^i\text{PrCH}(\text{trip})$), 25.10, 24.90, 24.77 ($^i\text{PrCH}_3(\text{trip})$), 23.60 (CH_3), 2.47 ($\text{Si}(\text{CH}_3)_2$). Anal. Calcd. for $\text{C}_{95}\text{H}_{131}\text{N}_2\text{ScSi}_2$: 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), $[\text{HNMe}_2\text{Ph}][\text{B}(\text{C}_6\text{F}_5)_4]$ (15 mg, 0.019 mmol) and bromobenzene (2 mL) and fitted to a line adapter. The flask was sonicated until all the $[\text{HNMe}_2\text{Ph}][\text{B}(\text{C}_6\text{F}_5)_4]$ 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. ¹H NMR (C₆D₅Br, 298 K): δ 7.48 (m, 4H; *o*, *m*-SiPh), 7.24 (m, 2H; *m*-C₆H₅NMe₂), 7.17 (s, 8H; *m*-C₆H₂), 6.89 (m, 1H; *p*-SiPh), 6.67 (s, 4H, *o*-C₆H₃), 6.49 (m, 3H; *o,p*-C₅H₅NMe₂), 5.32 (s, 1H; NCCH), 2.93 (sp, 4H; *p*-^{*i*}PrCH), 2.73 (sp, 8H; *o*-^{*i*}PrCH), 2.53 (s, 6H; NMe₂), 1.93 (NCCH₃), 1.3 (d, 24H; *p*-^{*i*}PrCH₃), 1.20, 1.11 (d, 24H; *o*-^{*i*}PrCH), 0.34 (s, 2H; Sc-CH₂), -0.07 (s, 6H; SiMe₂). ¹³C{¹H} (C₆D₅Br, 298 K): δ 168.9 (NCCH₃), 149.9 (C₆H₅NMe₂), 149.3 (*ipso*-C₆H₃) 146.2, 145.8, 143.7, 142.8, 140.3 (*quat*-C₆H₂, C₆H₃, SiPh), 135.2, 132.9, 129.3, 129.0, 128.5, 128.1, 127.7, 125.6, 124.2 (C₆H₃, C₆H₂, SiPh), 115.9 (*o*-C₆H₅NMe₂), 113.0 (*p*-C₆H₅NMe₂), 99.1 (NCCH), 56.1 (Sc-CH₂), 40.1(NMe₂), 34.8 (*p*-^{*i*}PrCH), 34.4 (*o*-^{*i*}PrCH₃) 31.9 (*o*-^{*i*}PrCH₃), 30.2 (*o*-^{*i*}PrCH), 25.6 (*p*-^{*i*}PrCH₃), 23.6 (NCCH₃), 13.6 (SiMe₂). ¹⁹F NMR (C₆D₅Br); δ -131.2 (*o*-F), -161.1 (*p*-F), -164.7 (*m*-F). ¹¹B NMR (C₆D₅Br, 258 K): δ -16.9.

Synthesis of 6: An NMR tube was charged with **4b** (25 mg, 0.017 mmol) and [CPh₃][B(C₆F₅)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. ¹H NMR (C₆D₅Br): δ 7.4 (m, 2H; *m*-SiPh), 7.3 (b, 2H; *o*-SiPh), 7.30-7.03 (m, 11H; *p*-C₆H₃, *m*C₆H₂, *p*-SiPh), 6.73 (s, 4H; *o*-C₆H₃), 5.45 (s, 1H; NCCH), 2.94 (sp, 4H; *p*-^{*i*}PrCH), 2.72 (sp, 8H; *o*-^{*i*}PrCH), 2.14 (b, 2H; Ph₃CCH₂), 1.98 (NCCH₃), 1.32 (d, 24H; *p*-^{*i*}PrCH₃), 1.21, 1.12 (d, 24H; *o*-^{*i*}PrCH), 0.23 (s, 2H; Sc-CH₂), 0.20 (Ph₃CCH₂SiMe₂), -0.12 (s, 6H; SiMe₂). ¹³C{¹H} (C₆D₅Br, 298 K): δ 168.9 (NCCH₃), 149.3 (*ipso*-C₆H₃) 146.2, 145.8, 143.7, 142.8, 140.3 (*quat*-C₆H₂, C₆H₃, SiPh), 135.2, 129.3, 128.5, 128.1, 127.7, 124.2 (C₆H₃,

C_6H_2 , $SiPh$), 99.1 (NCCH), 56.1 (Sc-CH₂), 43.2 (Ph₃CCH₂), 35.2 (Ph₃CCH₂) 34.8 (*p*-^{*i*}PrCH), 34.4 (*o*-^{*i*}PrCH₃) 31.9 (*o*-^{*i*}PrCH₃), 30.2 (*o*-^{*i*}PrCH), 25.6 (*p*-^{*i*}PrCH₃), 23.6 (NCCH₃), 13.6 (SiMe₂) 11.2 (Ph₃CCH₂SiMe₂). ¹⁹F NMR (C₆D₅Br); δ -131.1 (*o*-F), -161.0 (*p*-F), -164.9 (*m*-F). ¹¹B NMR (C₆D₅Br, 258 K): δ -16.2.

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