Cover Page for Supporting Information

Manuscript Title:

Synergism between Cyclopentadienyl and Amidinate Ligands Affording the Anionic Scandium Terminal Imido Complexes

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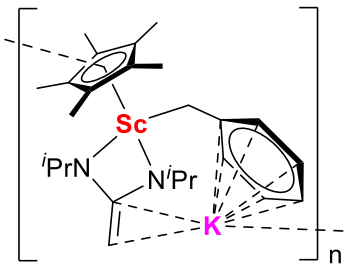
Contents:

1) Experimental Details and Characterization Data

Unless otherwise noted, all starting materials were commercially available and were used without further purification. Solvents were purified by Mbraun SPS-800 Solvent Purification System and dried over fresh Na chips and molecular sieves in a glovebox. d^8-THF was purchased from Cambridge Isotope Laboratory, degassed, and vacuum transferred to 4 Å molecular sieves. All reactions were operated under an argon atmosphere in a glovebox. The argon in the glove box was constantly circulated through a copper/molecular sieves catalyst unit. The oxygen and moisture concentrations in the glovebox atmosphere were monitored by an O_2/H_2O Combi-Analyzer to ensure that both were always below 0.1 ppm.

Organometallic samples for NMR spectroscopic measurements were prepared in a glovebox using J. Young valve NMR tubes (Wilmad 528-JY). ^{1}H and ^{13}C NMR spectra were recorded on a Bruker Avance 400 MHz, 500 MHz or 600 MHz spectrometer. ^{1}H and ^{13}C NMR spectra were reported with reference to solvent resonances of d^8-THF at 3.58 and 67.57 ppm, respectively. Elemental analyses were performed on a Vario MICRO cube elemental analyzer.

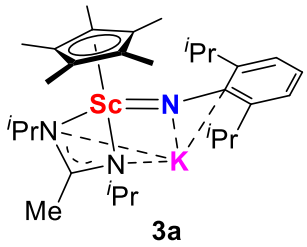
Compound **1**was prepared following the literature procedures.[1,2]



2

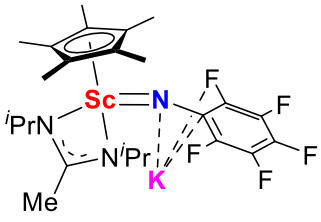
Synthesis of 2: In the glovebox, BnK (36.8 mg, 0.28 mmol) was added to an Et_2O (10 mL) solution of **1** (50.5 mg, 0.14 mmol). The solution was stirred at room temperature for 2 h upon which the color of the solution changed from red to orange-yellow, then filtered by filter funnel with fritted disc. The rest light orange powder was extracted by diethyl ether to remove KCl. After that, the volatile of filtrate was removed under reduced pressure and the residues were washed with hexane (2.5 mL × 3) thrice. The off-white solid was dried under vacuum. The single crystals of **2** suitable for X-ray analysis could be acquired by volatilization of Et_2O/hexane (1:1) at -30 °C for 2 days. Isolated Yield: 56.9 mg, 0.13 mmol, 89%. ^{1}H NMR of **2** (500 MHz, d^8-Tol) δ 0.97-0.99 (d, J = 6.30 Hz, 6H, $(CH_3)_2$CH), 1.37-1.38 (d, J = 6.05 Hz, 6H, $(CH_3)_2$CH), 1.80 (s, 2H, ScCH_2), 2.15 (s, 15H, C_5Me_5), 2.40 (s, 2H, CCH_2), 3.07-3.12 (m, 2H, $(CH_3)_2CH$), 6.07-6.10 (t, J = 7.10 Hz, 1H, Ar), 6.54-6.57 (m, 2H, Ar), 6.64-6.65 (d, J = 7.25 Hz, 2H, Ar). ^{13}C NMR of **2**

(126 MHz, d^8-Tol) δ 11.9 (CH_3 in Cp*), 25.0 ((CH_3)$_2$CH), 25.6 ((CH_3)$_2$CH), 46.7 (CCH_2), 47.4 ((CH_3)$_2$$CH$), 49.9 (Sc$CH_2$), 115.12 (Ar-$C$), 117.6 ($C_5Me_5$), 123.8 (Ar-$C$), 160.6 (Ar-$C$), 162.9 (N$C$N). Anal. Calcd for $C_{34}H_{48}KN_2OSc$ of **2**: C, 66.63; H, 8.50; N, 6.22. Found: C, 66.53; H, 8.76; N, 6.14.



3a

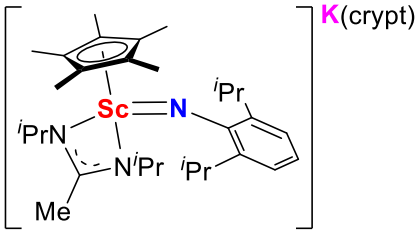
Synthesis of 3a: In the glovebox, 2,6-diisopropylaniline (132.4 μL, 0.70 mmol) was added to an Et_2O (25 mL) solution of **2** (316.1 mg, 0.70 mmol). The solution was stirred at room temperature for 30 min upon which the color of the solution changed from off-white to yellow, then the solvents were removed under reduced pressure and a pale-yellow solid was obtained. The solid was washed with hexane (5.0 mL × 3) thrice and dried under vacuum. The single crystals of **3a·Tol** suitable for X-ray analysis could be acquired by volatilization of Toluene/hexane (1:1) at -30 °C for 1 day. Isolated Yield: 307.6 mg, 0.57 mmol, 82%. ^{1}H NMR of **3a** (500 MHz, d^8-THF): δ 1.05 (d, J = 6.95 Hz, 12H, CH(CH_3)$_2$), 1.07-1.09 (d, J = 6.20 Hz, 6H, CH(CH_3)$_2$), 1.19-1.21 (d, J = 6.25 Hz, 6H, CH(CH_3)$_2$), 1.99 (s, 15H, Cp*), 2.01 (s, 3H, CH_3), 3.57-3.64 (m, 2H, CH(CH$_3$)$_2$), 3.87-3.95 (m, 2H, CH(CH$_3$)$_2$), 5.81-5.84 (t, J = 7.30 Hz, 1H, ArH), 6.52-6.54 (d, J = 7.30 Hz, 2H, ArH). ^{13}C NMR of **3a** (126 MHz, d^8-THF): δ 12.1 (CH_3 in Cp*), 12.3 (CCH_3), 25.1 ((CH_3)$_2$CH), 26.4 ((CH_3)$_2$CH), 26.6 ((CH_3)$_2$CH), 26.7 ((CH_3)$_2$$CH$), 47.6 (($CH_3$)$_2$$CH$), 107.3 (Ar-$C$), 115.2 ($C$ in Cp*), 122.1 (Ar-C), 133.6 (Ar-C), 138.3 (Ar-C), 170.1 (NCN). The single crystals of **3a·THF** suitable for elemental analysis could be acquired by volatilization of THF/hexane (1:1) at -30 °C for 1 day. Anal. Calcd. for $C_{34}H_{57}KN_3OSc$ of **3a·THF**: C, 67.18; H, 9.45; N, 6.91. Found: C, 66.56; H, 9.49; N, 6.85.



3b

Synthesis of 3b: In the glovebox, pentafluoroaniline (14.8 mg, 0.081 mmol) was added to a pre-cooled (-30 °C) Et_2O (10 mL) solution of **2** (36.4 mg, 0.081 mmol). The solution was stirred at -30 °C for 10 min upon which the color of the solution changed from off-white to yellow, then the solvents were removed under reduced pressure and a pale-yellow solid was obtained. The solid was washed with hexane (0.5 mL × 3)

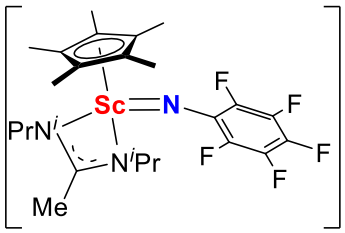
thrice and dried under vacuum. The single crystals of **3b** suitable for X-ray analysis could be acquired by volatilization of Et_2O/toluene (1:1) at -30 °C for 1 day. Isolated Yield: 35.2 mg, 0.063 mmol, 78%. ^{1}H NMR of **3b** (500 MHz, d^8-THF): δ 1.09-1.10 (d, J = 4.80 Hz, 12H, CH(CH_3)$_2$), δ 1.10-1.11 (d, J = 4.95 Hz, 12H, CH(CH_3)$_2$), 1.93 (s, 3H, CH_3), 1.98 (s, 15H, Cp*), 3.42-3.49 (m, 2H, CH(CH$_3$)$_2$). ^{13}C NMR of **3b** (126 MHz, d^8-THF): δ 11.7 (CCH$_3$), 11.8 (CH$_3$ in Cp*), 26.3 ((CH$_3$)$_2$CH), 47.9 ((CH$_3$)$_2$$C$H), 107.0 (Ar-$C$), 114.0 (Ar-$C$), 116.0 ($C$ in Cp*), 170.5 (NCN). ^{19}F NMR of **3b** (471 MHz, d^8-THF): δ -200.9 (Ar-F), δ -174.7 (Ar-F), δ -168.8 (Ar-F). **3b** was too unstable to give satisfactory elemental analysis.



4a

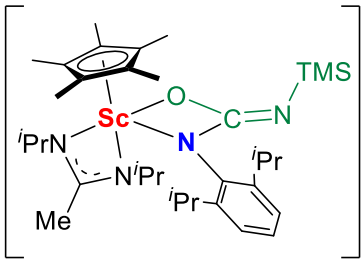
Synthesis of 4a: In the glovebox, 2,2,2-cryptand (264.2 mg, 0.70 mmol) was added to a THF (25 mL) solution of **3a** (375.6 mg, 0.70 mmol). The solution was stirred at room temperature for 30 min upon which the color of the solution changed from pale-yellow to golden yellow, then the solvents were removed under reduced pressure and a yellow solid was obtained. The solid was washed with Et_2O (3.0 mL × 3) thrice and dried under vacuum. Isolated Yield: 604.5 mg, 0.66 mmol, 95%. ^{1}H NMR of **4a** (500 MHz, d^8-THF): δ 0.99-1.00 (d, J = 6.90 Hz, 6H, CH(CH_3)$_2$), 1.05-1.06 (d, J = 6.30 Hz, 3H, CH(CH_3)$_2$), 1.09-1.10 (d, J = 6.25 Hz, 3H, CH(CH_3)$_2$), 1.11-1.12 (d, J = 6.15 Hz, 3H, CH(CH_3)$_2$), 1.12-1.13 (d, J = 6.75 Hz, 6H, CH(CH_3)$_2$), 1.16-1.17 (d, J = 6.05 Hz, 3H, CH(CH_3)$_2$), 1.86 (s, 1.5H, CH_3), 2.02 (s, 15H, Cp*), 2.09 (s, 1.5H, CH_3), 2.48-2.50 (t, J = 4.65 Hz, 12H, CH_2), 3.31-3.36 (m, 1H, CH(CH$_3$)$_2$), 3.35-3.40 (m, 1H, CH(CH$_3$)$_2$), 3.46-3.50 (m, 1H, CH(CH$_3$)$_2$), 3.47-3.48 (t, J = 4.65 Hz, 12H, CH_2), 3.52 (s, 12H, CH_2), 5.49-5.52 (t, J = 7.20 Hz, 0.5H, ArH), 6.07-6.10 (t, J = 7.40 Hz, 0.5H, ArH), 6.29-6.31 (d, J = 7.15 Hz, 1H, ArH), 6.59-6.60 (t, J = 7.45 Hz, 1H, ArH). ^{13}C NMR of **4a** (126 MHz, d^8-THF): δ 12.3 (CCH$_3$), 12.6 (CH$_3$ in Cp*), 24.7 ((CH$_3$)$_2$CH), 25.8 ((CH$_3$)$_2$CH), 26.6 ((CH$_3$)$_2$CH), 26.6 ((CH$_3$)$_2$$C$H), 26.7 (($CH_3$)$_2$CH), 26.8 (($CH_3$)$_2$CH), 28.5 ((CH$_3$)$_2$$C$H), 54.8 ($CH_2$), 68.4 ($CH_2$), 71.3 ($CH_2$), 103.3 (Ar-$C$), 112.2 (Ar-$C$), 113.4 ($C$ in Cp*), 115.3 (C in Cp*), 120.8 (Ar-C), 121.8 (Ar-C), 134.2 (Ar-C), 137.7 (Ar-C), 154.8 (Ar-C), 162.5 (Ar-C), 168.4 (NCN). The single crystals of **4a·0.25THF** suitable for X-ray analysis could be acquired by volatilization of THF/

Et_2O (1:1) under vacuum for 5 min. Anal. Calcd. for $C_{98}H_{174}K_2N_{10}O_{12.5}Sc_2$ of **4a·0.25THF**: C, 63.26; H, 9.43; N, 7.53. Found: C, 63.51; H, 9.28; N, 7.25.



4b

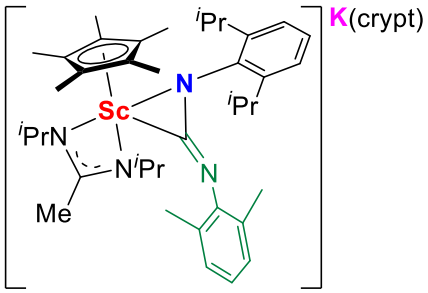
Synthesis of 4b: In the glovebox, 18-crown-6 (34.4 mg, 0.13 mmol) was added to a pre-cooled (-30 °C) Et_2O (10 mL) solution of **3b** (72.6 mg, 0.13 mmol). The solution was stirred at room temperature for 5 min upon which the color of the solution changed from pale-yellow to golden yellow, then the solvents were removed under reduced pressure and a yellow solid was obtained. The solid was washed with hexane (0.5 mL × 3) thrice and dried under vacuum. The single crystals of **4b** suitable for X-ray analysis could be acquired by volatilization of Et_2O/toluene (1:1) at -30 °C for 1 day. Isolated Yield: 69.5 mg, 0.086 mmol, 66%. ^{1}H NMR of **4b** (500 MHz, d^8-THF): δ 1.04-1.05 (d, J = 6.00 Hz, 6H, CH(CH_3)$_2$), δ 1.09-1.10 (d, J = 6.10 Hz, 6H, CH(CH_3)$_2$), 1.84 (s, 3H, CH_3), 2.00 (s, 15H, Cp*), 3.36-3.41 (m, 2H, CH(CH$_3$)$_2$), 3.57 (s, 24H, CH_2). ^{13}C NMR of **4b** (126 MHz, d^8-THF): δ 11.3 (CCH$_3$), 12.0 (CH$_3$ in Cp*), 25.9 ((CH$_3$)$_2$CH), 26.6 ((CH$_3$)$_2$CH), 48.0 ((CH$_3$)$_2$$C$H), 71.1 ($CH_2$), 106.5 (Ar-$C$), 113.7 (Ar-$C$), 115.1 ($C$ in Cp*), 128.9 (Ar-C), 169.3 (NCN). ^{19}F NMR of **4b** (471 MHz, d^8-THF): δ -205.5 (CCH$_3$), δ -176.3 (CCH$_3$), δ -169.5 (CCH$_3$). **4b** was too unstable to give satisfactory elemental analysis.



5

Synthesis of 5: In the glovebox, TMSNCO (8.9 μL, 0.065 mmol) was added to a pre-cooled (-30 °C) THF (10 mL) solution of **4a** (59.6 mg, 0.065 mmol). The solution was stirred at room temperature for 1 h upon which the color of the solution changed from golden yellow to transparence, then the solvents were removed under reduced pressure and a white solid was obtained. The solid was washed with Et_2O (0.5 mL × 3) thrice and dried under vacuum. The single crystals of **5·2THF** suitable for X-ray analysis could be acquired by volatilization of THF/ hexane (1:1) at -30 °C for 1 day. Isolated Yield: 45.6 mg, 0.044 mmol, 68%. ^{1}H NMR of **5** (500 MHz, d^8-THF): δ -0.09 (s, 9H, CH_3),

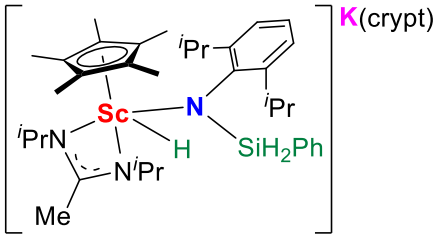
0.40-0.41 (d, J = 6.35 Hz, 3H, CH(CH_3)$_2$), 0.93-0.94 (d, J = 6.95 Hz, 3H, CH(CH_3)$_2$), 0.95-0.97 (d, J = 6.25 Hz, 3H, CH(CH_3)$_2$), 1.05-1.07 (d, J = 6.20 Hz, 3H, CH(CH_3)$_2$), 1.05-1.07 (d, J = 6.20 Hz, 3H, CH(CH_3)$_2$), 1.15-1.16 (d, J = 7.00 Hz, 3H, CH(CH_3)$_2$), 1.20-1.21 (d, J = 4.55 Hz, 3H, CH(CH_3)$_2$), 1.21-1.22 (d, J = 4.30 Hz, 3H, CH(CH_3)$_2$), 1.77 (s, 3H, CH_3), 2.03 (s, 15H, Cp*), 2.51-2.53 (t, J = 4.65 Hz, 12H, CH_2), 3.03-3.08 (m, 1H, CH(CH$_3$)$_2$), 3.16-3.21 (m, 1H, CH(CH$_3$)$_2$), 3.32-3.37 (m, 1H, CH(CH$_3$)$_2$), 3.50-3.51 (t, J = 4.65 Hz, 12H, CH_2), 3.54 (s, 12H, CH_2), 3.69-3.76 (m, 1H, CH(CH$_3$)$_2$), 6.58-6.60 (t, J = 7.50 Hz, 1H, ArH), 6.69-6.74 (m, 2H, ArH). ^{13}C NMR of **5** (126 MHz, d^8-THF): δ 3.96 (SiCH$_3$), 11.6 (CCH$_3$), 12.7 (CH$_3$ in Cp*), 23,8 ((CH$_3$)$_2$CH), 25.1 ((CH$_3$)$_2$CH), 25.8 ((CH$_3$)$_2$CH), 25.9 ((CH$_3$)$_2$CH), 26.2 ((CH$_3$)$_2$CH), 26.5 ((CH$_3$)$_2$CH), 26.6 ((CH$_3$)$_2$CH), 27.1 ((CH$_3$)$_2$CH), 27.9 ((CH_3)$_2C$H), 28.1 ((CH_3)$_2C$H), 47.8 ((CH_3)$_2C$H), 48.3 ((CH_3)$_2C$H), 54.8 (CH$_2$), 68.4 (CH$_2$), 71.3 (CH$_2$), 115.6 (C in Cp*), 120.6 (Ar-C), 121.0 (Ar-C), 121.8 (Ar-C), 144.9 (Ar-C), 145.6 (Ar-C), 151.1 (NCO), 170.4 (NCN). Anal. Calcd. for $C_{52}H_{94}KN_6O_7ScSi$ of **5**: C, 60.79; H, 9.22; N, 8.18. Found: C, 61.07; H, 9.27; N, 8.05.



6

Synthesis of 6: In the glovebox, 2,6-dimethylisonitrile (8.7 mg, 0.066 mmol) was added to a pre-cooled (-30 °C) THF (10 mL) solution of **4a** (60.5 mg, 0.066 mmol). The solution was stirred at room temperature for 1 h upon which the color of the solution changed from golden yellow to deep yellow, then the solvents were removed under reduced pressure and a yellow solid was obtained. The solid was washed with Et_2O (0.5 mL × 3) thrice and dried under vacuum. Isolated Yield: 52.6 mg, 0.050 mmol, 76%. ^{1}H NMR of **6** (500 MHz, d^8-THF): δ 0.88-0.89 (d, J = 6.40 Hz, 6H, CH(CH_3)$_2$), 1.03-1.04 (d, J = 6.85 Hz, 6H, CH(CH_3)$_2$), 1.09-1.10 (d, J = 6.35 Hz, 6H, CH(CH_3)$_2$), 1.18-1.19 (d, J = 6.80 Hz, 6H, CH(CH_3)$_2$), 1.85 (s, 3H, CH_3), 1.90 (s, 15H, Cp*), 2.20 (s, 3H, CH_3), 2.34-2.36 (t, J = 4.65 Hz, 12H, CH_2), 3.34-3.36 (t, J = 4.65 Hz, 12H, CH_2), 3.39 (s, 12H, CH_2), 3.37-3.42 (m, 2H, CH(CH$_3$)$_2$), 3.55-3.61 (m, 2H, CH(CH$_3$)$_2$), 6.16-6.19 (t, J = 7.20 Hz, 1H, ArH), 6.59-6.62 (t, J = 7.45 Hz, 1H, ArH), 6.61-6.63 (d, J = 7.20 Hz, 2H, ArH), 6.77-6.79 (d, J = 7.45 Hz, 2H, ArH). ^{13}C NMR of **6** (126

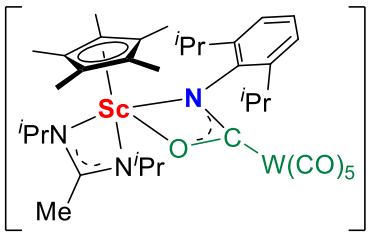
MHz, d^8-THF): δ 12.7 (CH_3 in Cp*), 13.3 (CCH_3), 22.2 (ArCH_3), 25.8 ((CH_3)$_2$CH), 26.1 ((CH_3)$_2$CH), 26.2 ((CH_3)$_2$CH), 26.4 ((CH_3)$_2$CH), 27.9 ((CH_3)$_2$CH), 48.1 ((CH_3)$_2$CH), 54.7 (CH_2), 68.3 (CH_2), 71.2 (CH_2), 115.1 (Ar-*C*), 115.6 (*C* in Cp*), 120.4 (Ar-*C*), 121.6 (Ar-*C*), 127.1 (Ar-*C*), 130.4 (Ar-*C*), 143.4 (Ar-*C*), 157.5 (Ar-*C*), 161.5(Ar-*C*), 168.9 (NCN), 218.6(*C*N). The single crystals of **6·THF** suitable for X-ray analysis could be acquired by volatilization of THF/ hexane (1:1) at -30 °C for 1 day. Anal. Calcd. for $C_{61}H_{102}KN_6O_7Sc$ of **6·THF**: C, 65.68; H, 9.22; N, 7.53. Found: C, 65.97; H, 9.43; N, 7.42.



7

Synthesis of 7: In the glovebox, phenylsilane (10.2 μL, 0.082 mmol) was added to a pre-cooled (-30 °C) THF (10 mL) solution of **4a** (75.3 mg, 0.082 mmol). The solution was stirred at room temperature for 1 h upon which the color of the solution changed from golden yellow to transparence, then the solvents were removed under reduced pressure and an off-white solid was obtained. The solid was washed with Et_2O (0.5 mL × 3) thrice and dried under vacuum. The single crystals of **7** suitable for X-ray analysis could be acquired by volatilization of THF/ hexane (1:1) at -30 °C for 1 day. Isolated Yield: 64.9 mg, 0.064 mmol, 77%. ^{1}H NMR of **7** (500 MHz, d^8-THF): δ 0.90-0.93 (m, 6H, CH(CH_3)$_2$), 1.04-1.05 (d, J = 6.25 Hz, 3H, CH(CH_3)$_2$), 1.10-1.25 (m, 15H, CH(CH_3)$_2$), 1.78 (s, 3H, CH_3), 1.97 (s, 15H, Cp*), 2.44-2.46 (t, J = 4.63 Hz, 12H, CH_2), 3.06-3.11 (m, 1H, CH(CH$_3$)$_2$), 3.43-3.45 (t, J = 4.60 Hz, 12H, CH_2), 3.48 (s, 12H, CH_2), 3.52-3.55 (m, 1H, CH(CH$_3$)$_2$), 3.61-3.68 (m, 1H, CH(CH$_3$)$_2$), 3.89-3.95 (m, 1H, CH(CH$_3$)$_2$), 5.25-5.27 (d, J = 8.45 Hz, 2H, SiH_2), 6.21 (s, 1H, ScH), 6.40-6.43 (t, J = 7.45 Hz, 1H, ArH), 6.65-6.72 (m, 2H, ArH), 6.98-7.06 (m, 3H, ArH), 7.92-7.94 (d, J = 6.85 Hz, 2H, ArH). ^{13}C NMR of **7** (126 MHz, d^8-THF): δ 12.5 (CCH_3), 13.0 (CH_3 in Cp*), 24.5 ((CH_3)$_2$CH), 24.6 ((CH_3)$_2$CH), 25.3 ((CH_3)$_2$CH), 25.8 ((CH_3)$_2$CH), 26.0 ((CH_3)$_2$CH), 26.4 ((CH_3)$_2$CH), 26.5 ((CH_3)$_2$CH), 26.7 ((CH_3)$_2$CH), 27.0 ((CH_3)$_2$CH), 27.1 ((CH_3)$_2$CH), 48.1 ((CH_3)$_2$CH), 48.3 ((CH_3)$_2$CH), 54.7 (CH_2), 68.4 (CH_2), 71.3 (CH_2), 115.8 (*C* in Cp*), 117.3 (Ar-*C*), 120.0 (Ar-*C*), 120.9 (Ar-*C*), 122.0 (Ar-*C*), 125.9 (Ar-*C*), 137.5 (Ar-*C*), 143.1 (Ar-*C*), 144.1 (Ar-*C*), 170.2 (NCN). Anal. Calcd. for $C_{54}H_{93}KN_5O_6ScSi$ of **7**: C, 63.56; H, 9.19; N, 6.86. Found: C, 63.78;

H, 9.54; N, 6.81.



8

Synthesis of 8: In the glovebox, $W(CO)_6$ (25.8 mg, 0.073 mmol) was added to a pre-cooled (-30 °C) THF (10 mL) solution of **4a** (66.9 mg, 0.073 mmol). The solution was stirred at room temperature for 1 h upon which the color of the solution changed from golden yellow to pale-yellow, then the solvents were removed under reduced pressure and an off-white solid was obtained. The solid was washed with Et_2O (0.5 mL × 3) thrice and dried under vacuum. Isolated Yield: 50.1 mg, 0.040 mmol, 54%. ^{1}H NMR of **8** (500 MHz, d^8-THF): δ 0.89-1.26 (br, 24H, CH(CH_3)$_2$), 1.77 (s, 3H, CH_3), 2.06 (s, 15H, Cp*), 2.56-2.57 (t, J = 4.65 Hz, 12H, CH_2), 3.37-3.46 (br, 2H, CH(CH$_3$)$_2$), 3.54-3.56 (br, 2H, CH(CH$_3$)$_2$), 3.54-3.56 (t, J = 4.65 Hz, 12H, CH_2), 3.60 (s, 12H, CH_2), 6.75-6.83 (m, 3H, ArH). ^{13}C NMR of **8** (126 MHz, d^8-THF): δ 12.2 (CCH$_3$), 12.8 (CH$_3$ in Cp*), 25.8 ((CH$_3$)$_2$CH), 26.1 ((CH$_3$)$_2$$C$H), 54.8 ($CH_2$), 68.5 ($CH_2$), 71.3 ($CH_2$), 117.3 ($C$ in Cp*), 123.2 (Ar-C), 150.9 (Ar-C), 172.2 (NCN), 202.8 (CO), 206.6 (CO), 235.0 (CO). The single crystals of **8·THF** suitable for X-ray analysis could be acquired by volatilization of THF/ hexane (1:1) at -30 °C for 1 day. Anal. Calcd. for $C_{58}H_{93}KN_5O_{13}ScW$ of **8·THF**: C, 52.13; H, 7.02; N, 5.24. Found: C, 51.81; H, 7.19; N, 5.28.

2) Copies of ^{1}H NMR and ^{13}C NMR Spectra

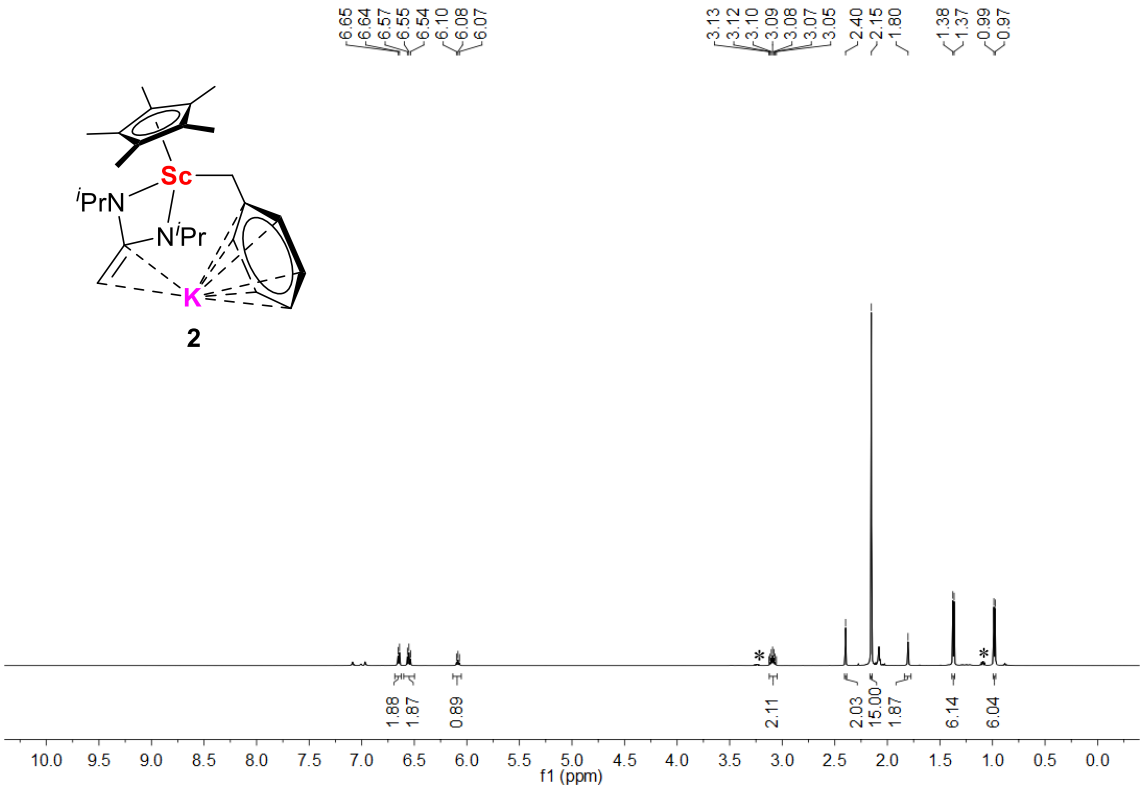


Figure S1. ^{1}H NMR spectrum of **2** (25 °C, 500 MHz, d^{8}-Tol, "*" represents the residual Et_2O).

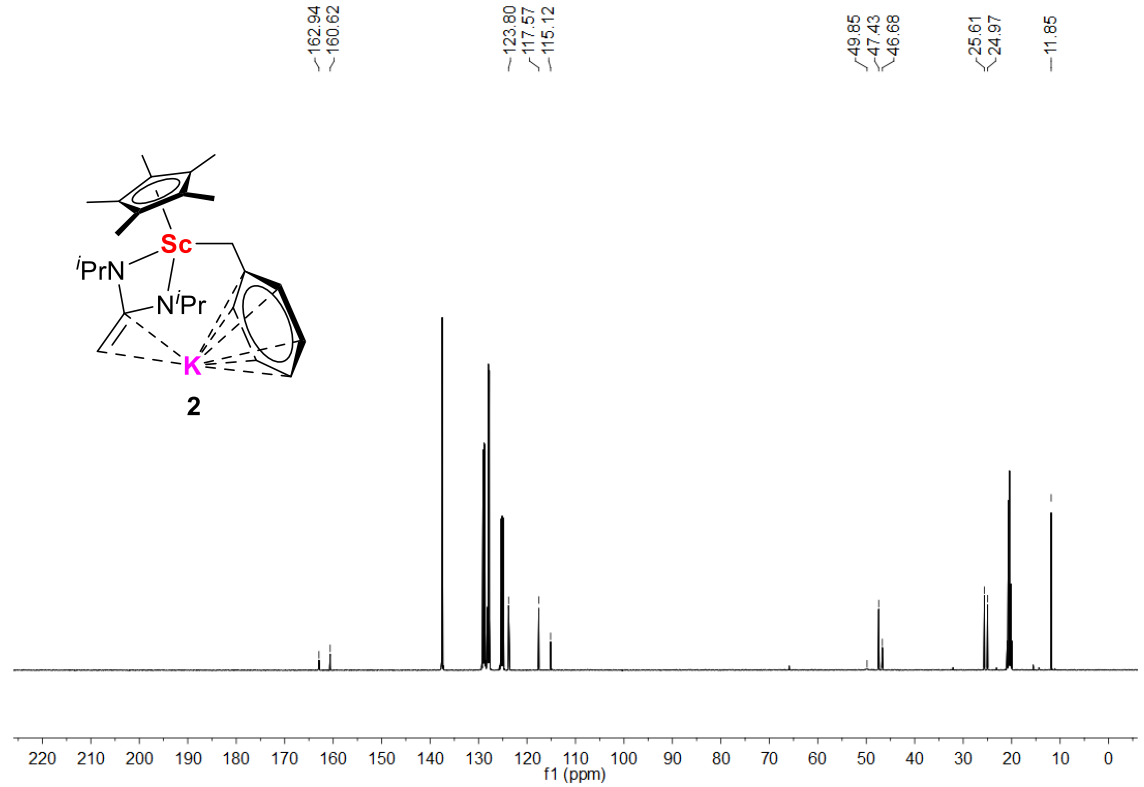


Figure S2. ^{13}C NMR spectrum of **2** (25 °C, 126 MHz, d^{8}-Tol, "*" represents the residual Et_2O).

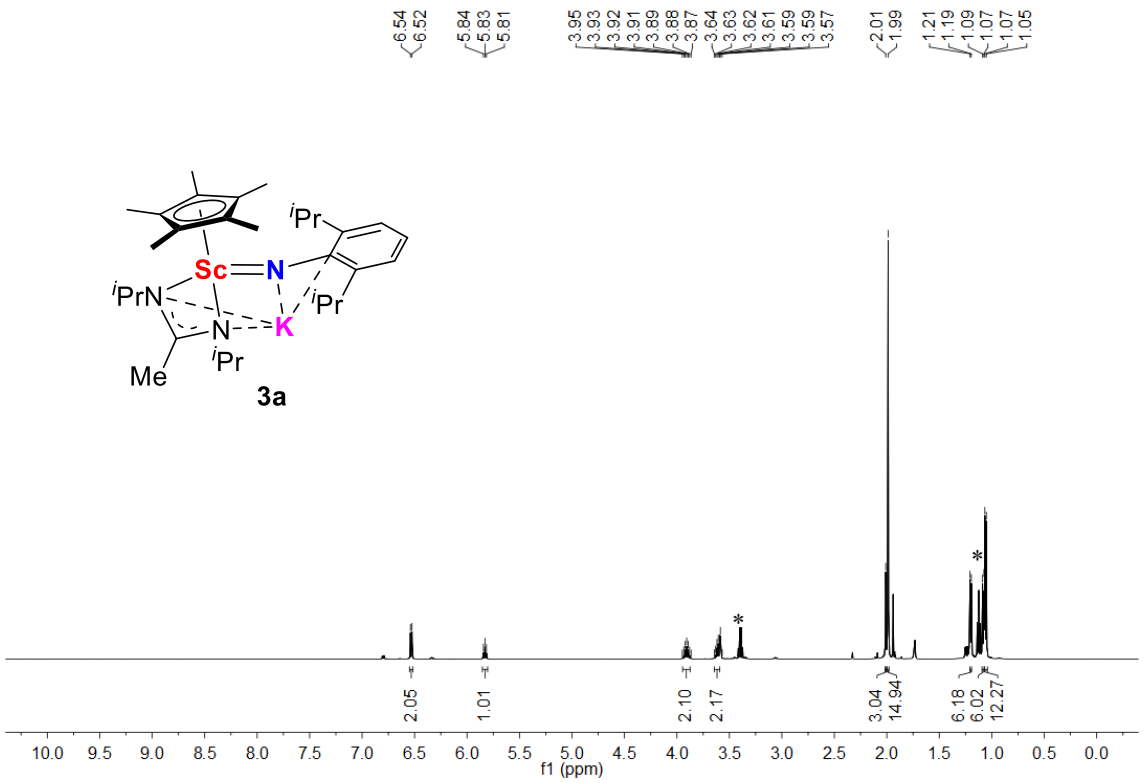


Figure S3. ^{1}H NMR spectrum of **3a** (25 °C, 500 MHz, d^{8}-THF, "*" represents the residual Et_2O).

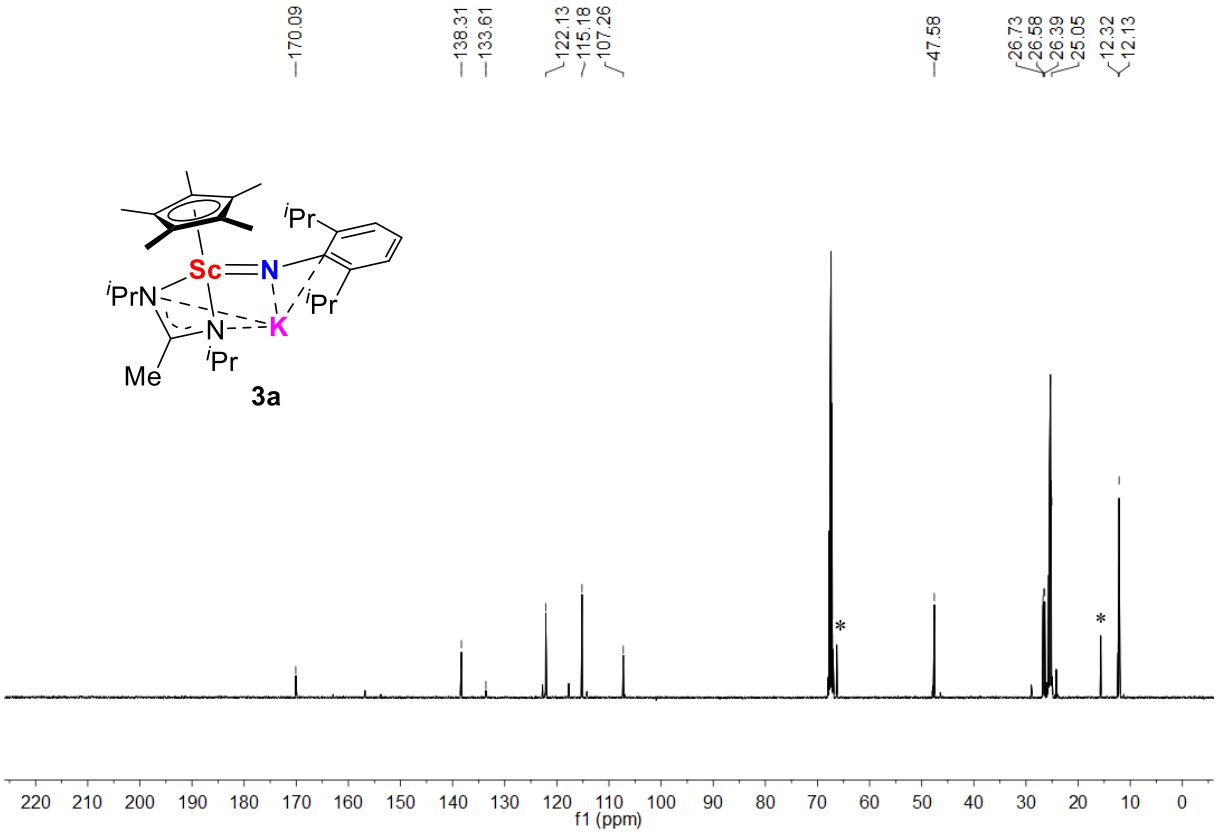


Figure S4. ^{13}C NMR spectrum of **3a** (25 °C, 126 MHz, d^{8}-THF, "*" represents the residual Et_2O).

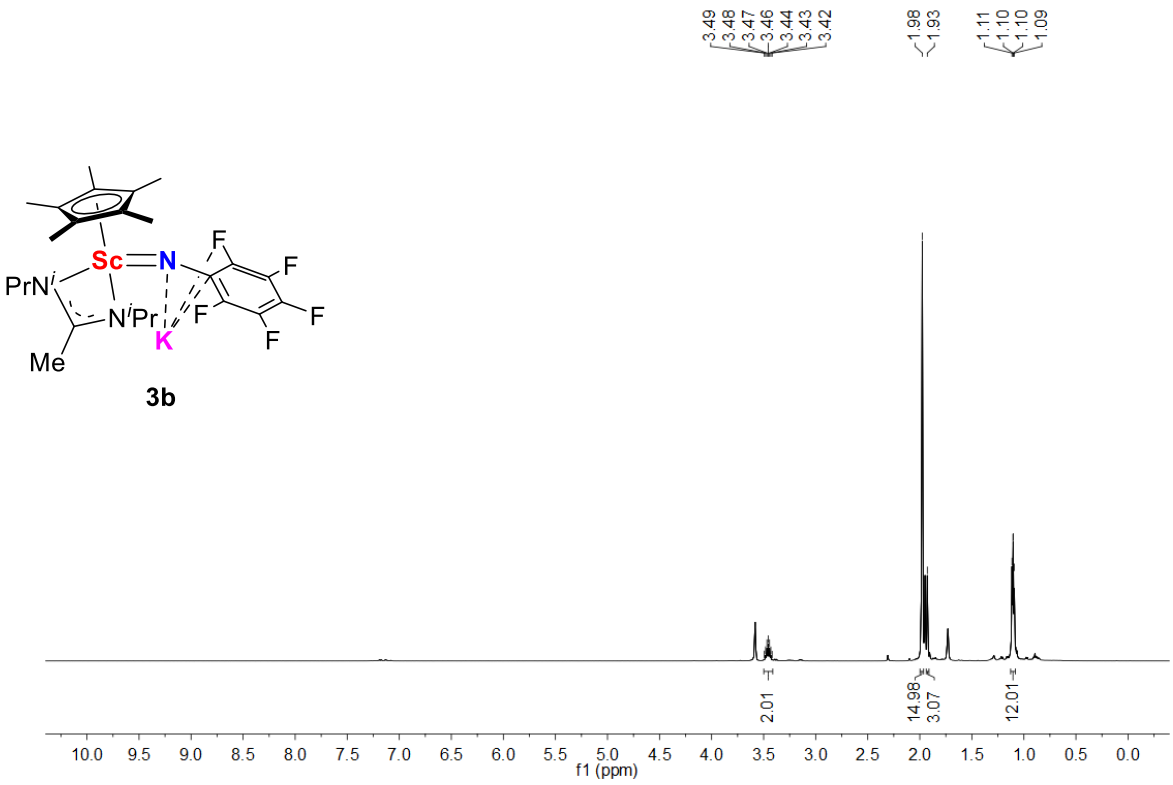


Figure S5. ^{1}H NMR spectrum of **3b** (25 °C, 500 MHz, d^{8}-THF).

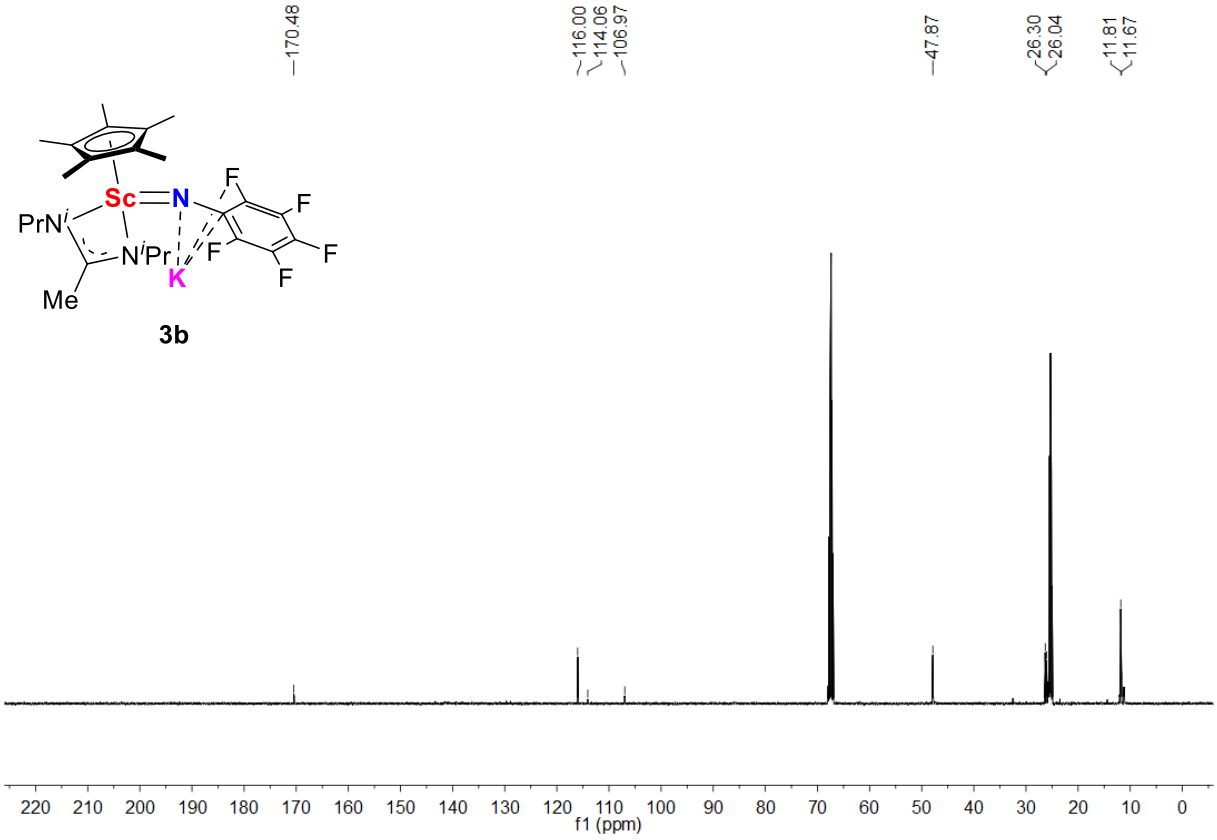


Figure S6. ^{13}C NMR spectrum of **3b** (25 °C, 126 MHz, d^{8}-THF).

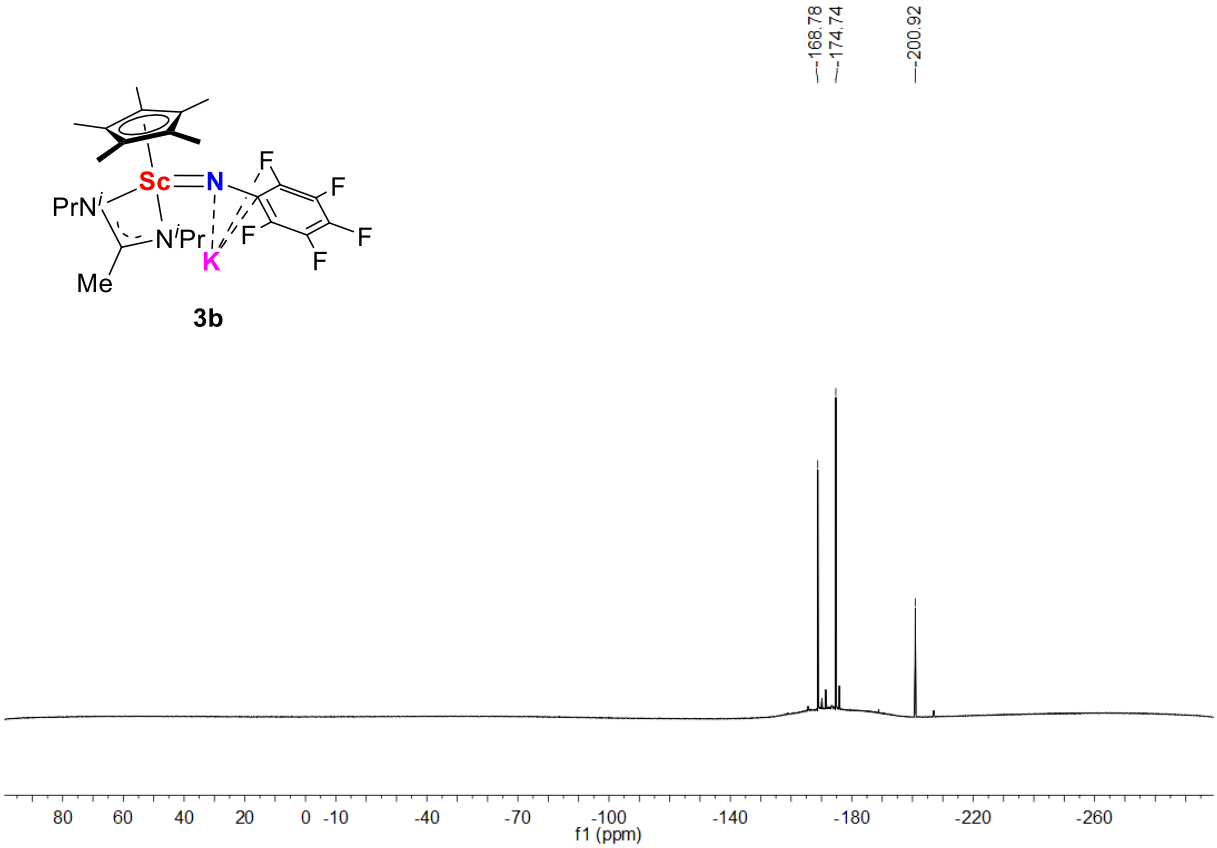


Figure S7. ^{19}F NMR spectrum of **3b** (25 °C, 471 MHz, d^8-THF).

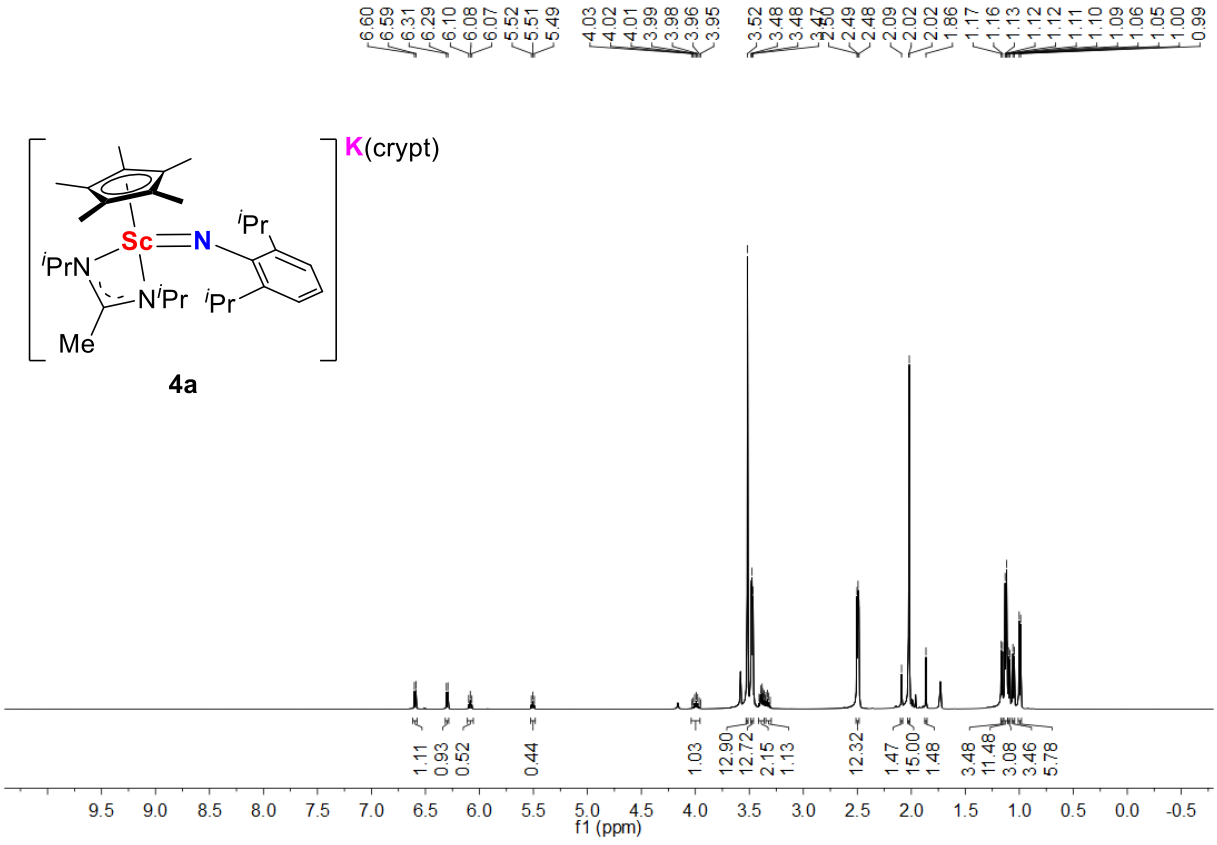


Figure S8. ^{1}H NMR spectrum of **4a** (25 °C, 500 MHz, d^8-THF).

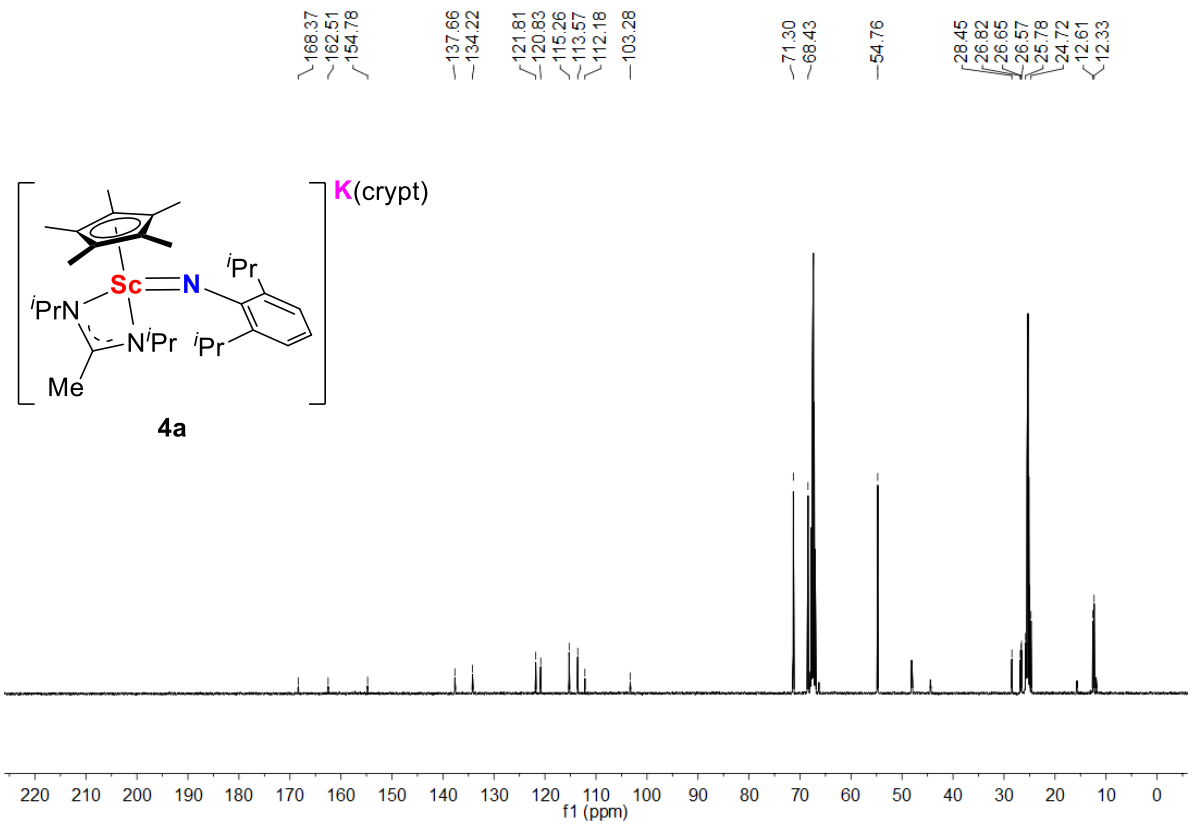


Figure S9. ^{13}C NMR spectrum of **4a** (25 °C, 126 MHz, d^8-THF).

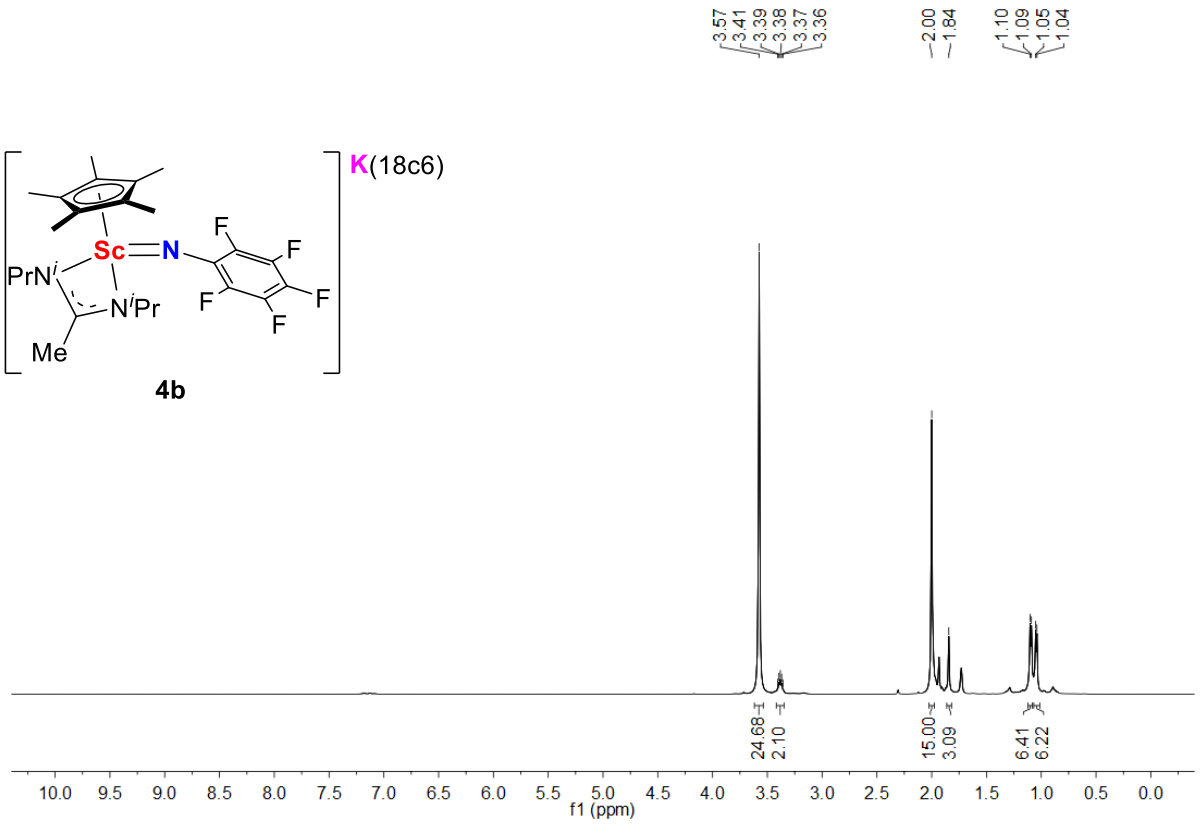


Figure S10. ^{1}H NMR spectrum of **4b** (25 °C, 500 MHz, d^8-THF).

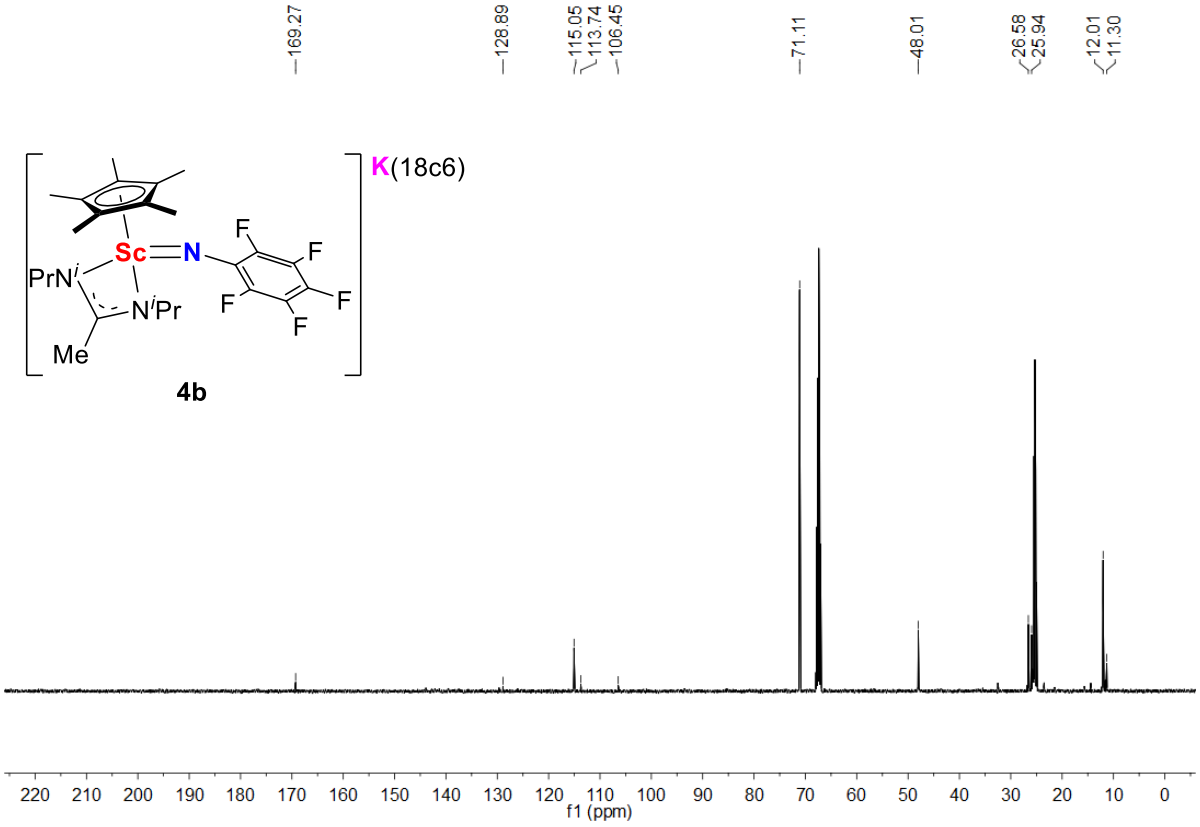


Figure S11. ^{13}C NMR spectrum of **4b** (25 °C, 126 MHz, d^8-THF).

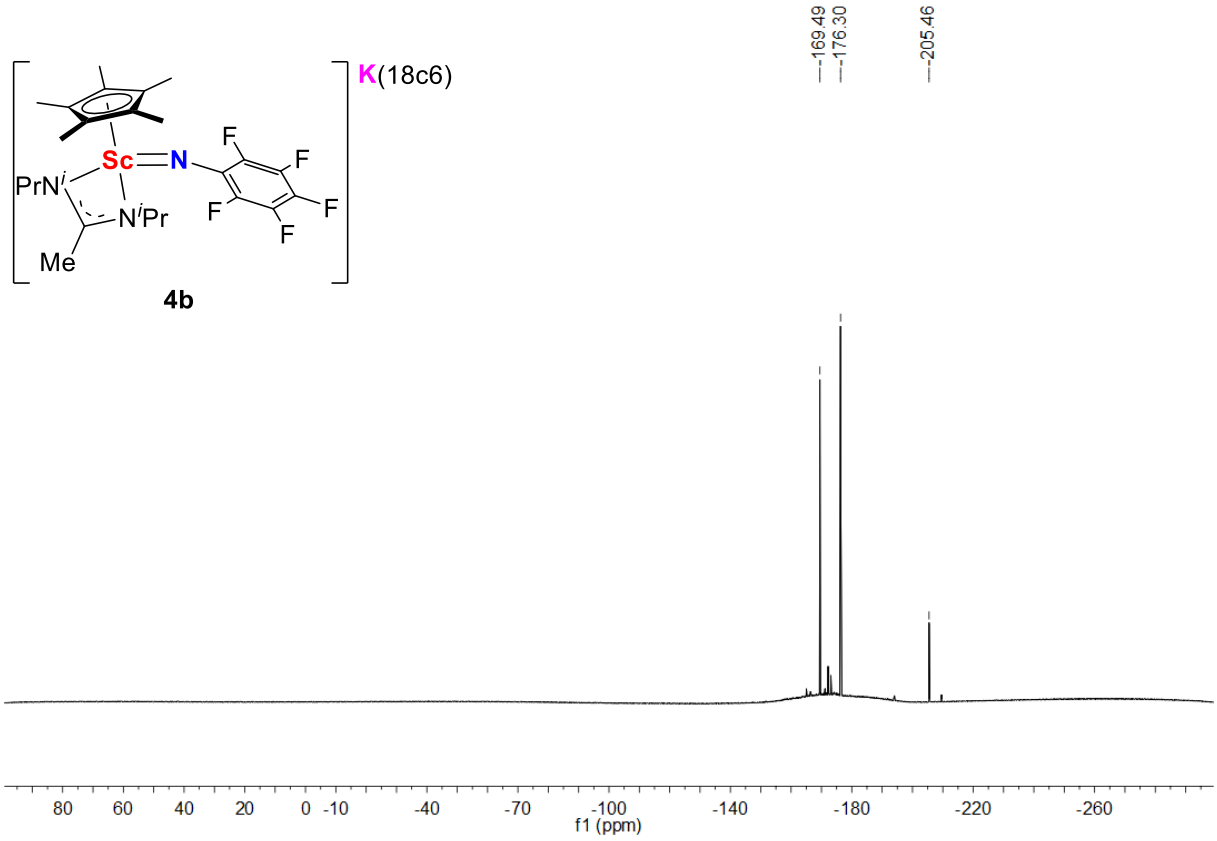


Figure S12. ^{19}F NMR spectrum of **4b** (25 °C, 471 MHz, d^8-THF).

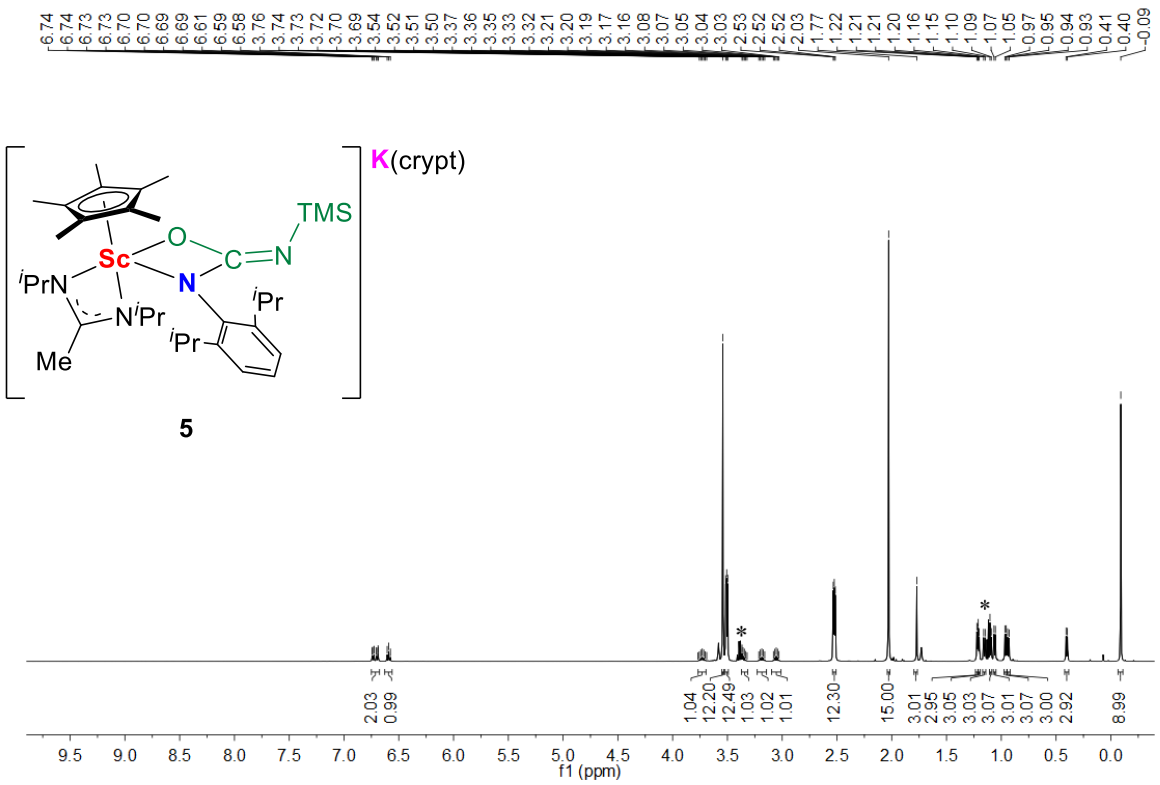


Figure S13. ^{1}H NMR spectrum of **5** (25 °C, 500 MHz, d^{8}-THF, "*" represents the residual Et_2O).

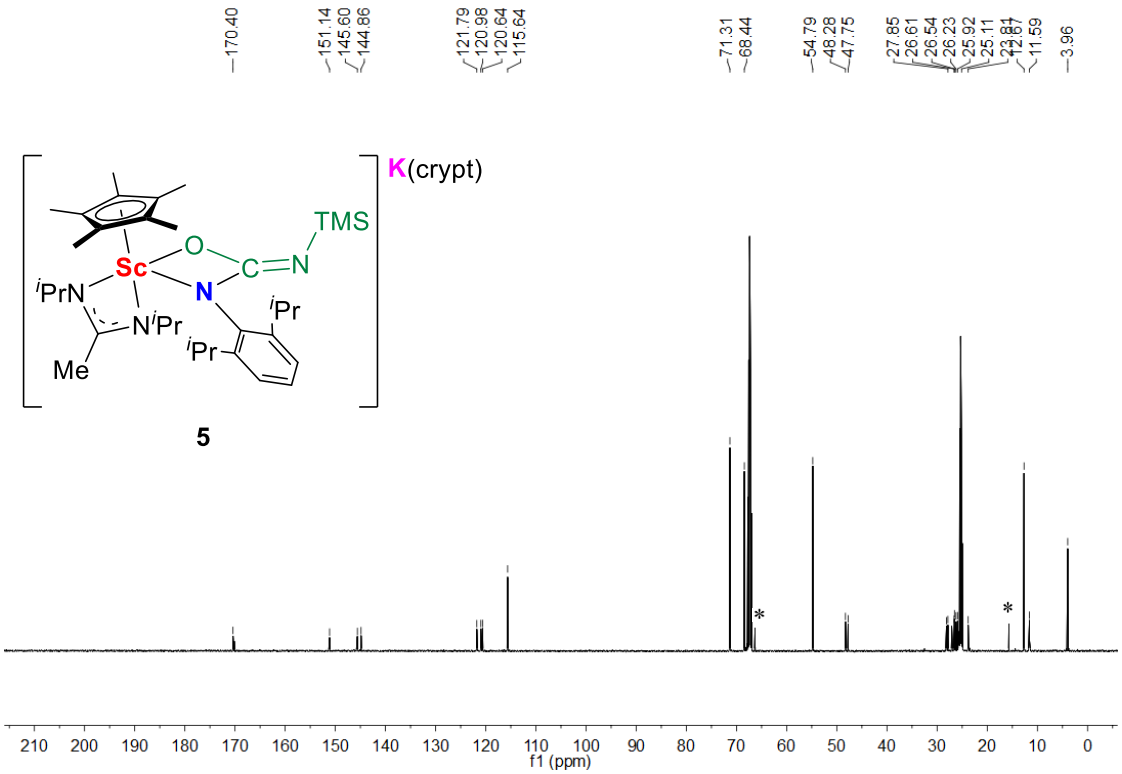


Figure S14. ^{13}C NMR spectrum of **5** (25 °C, 126 MHz, d^{8}-THF, "*" represents the residual Et_2O).

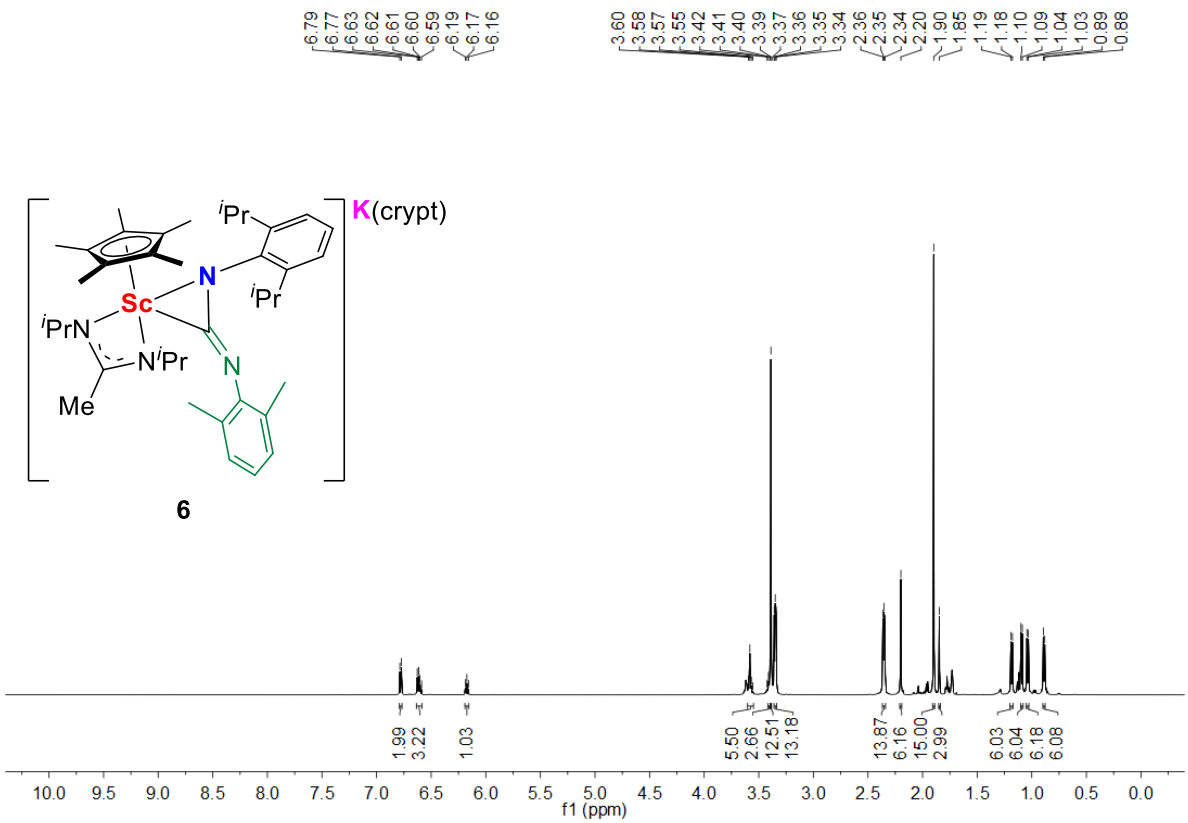


Figure S15. ^{1}H NMR spectrum of **6** (25 °C, 500 MHz, d^{8}-THF).

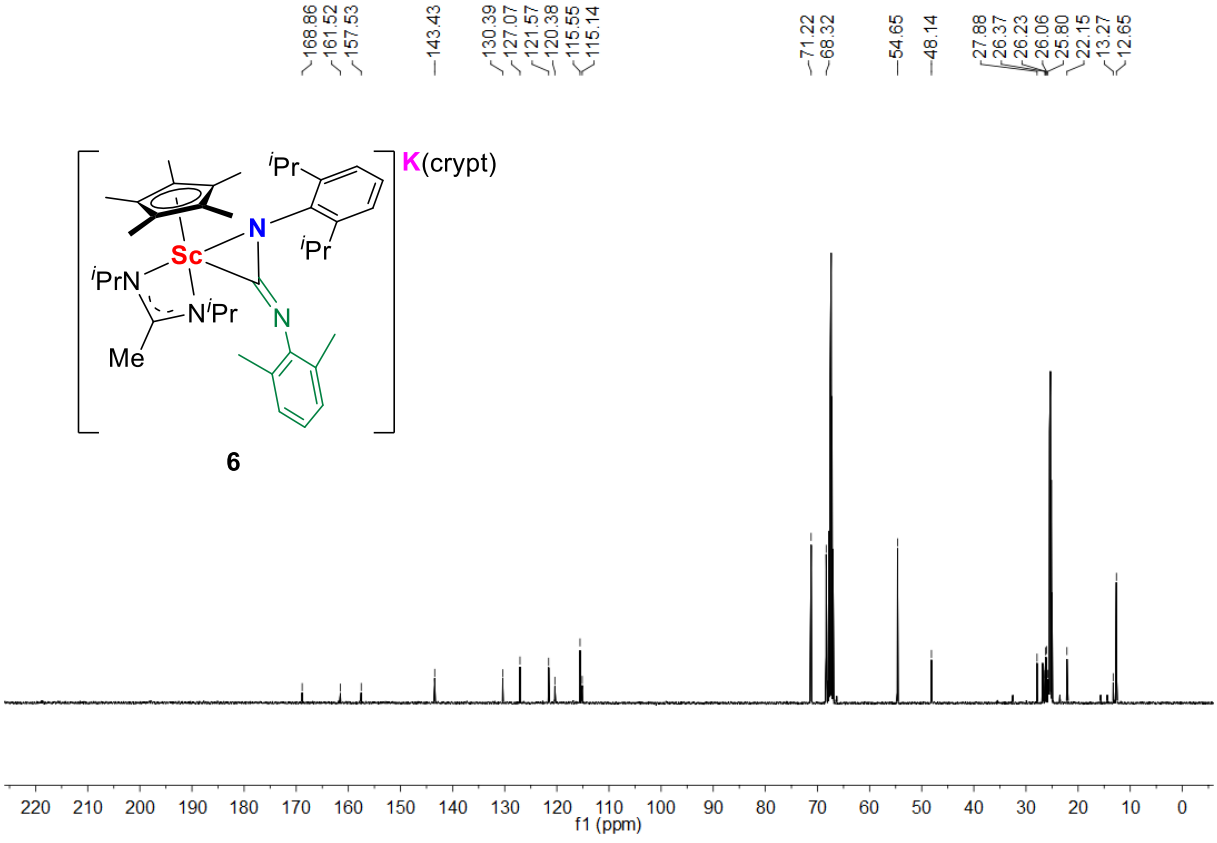


Figure S16. ^{13}C NMR spectrum of **6** (25 °C, 126 MHz, d^{8}-THF).

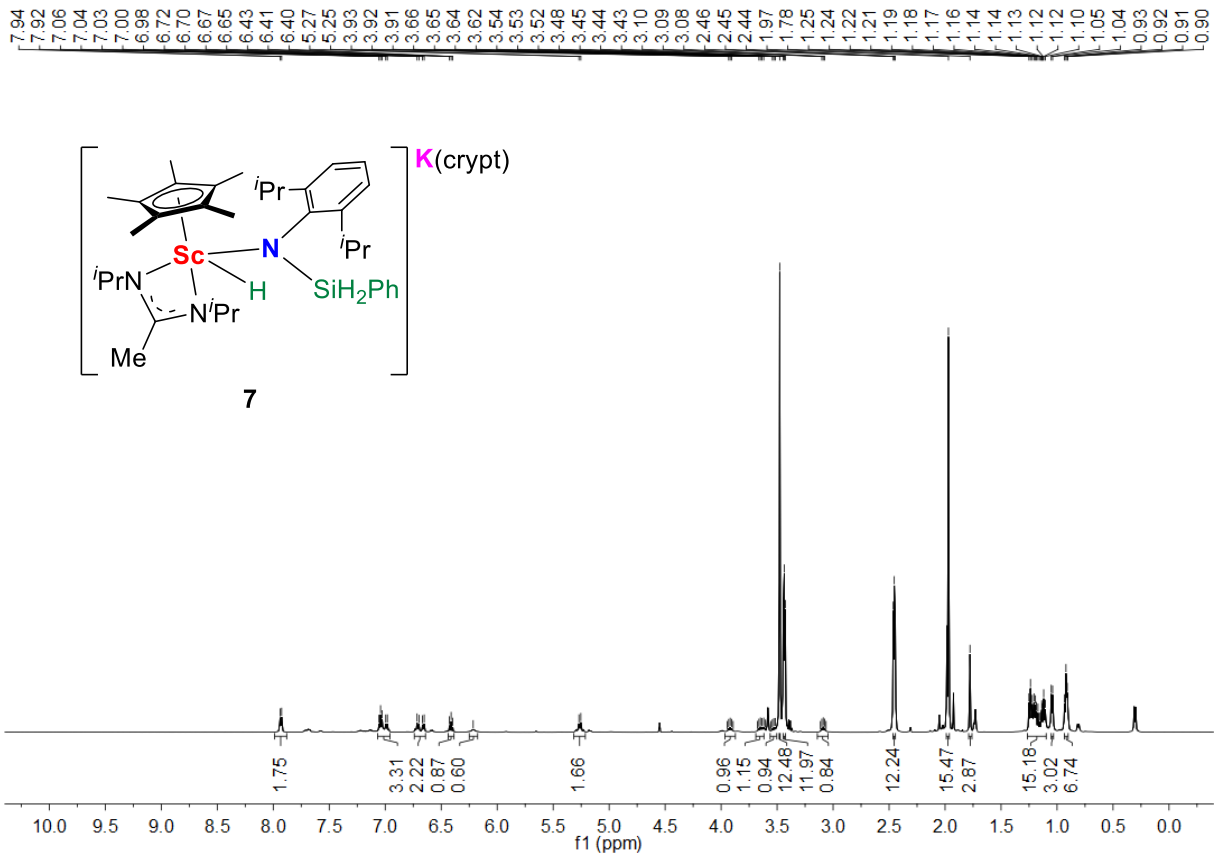


Figure S17. ^{1}H NMR spectrum of **7** (25 °C, 500 MHz, d^{8}-THF).

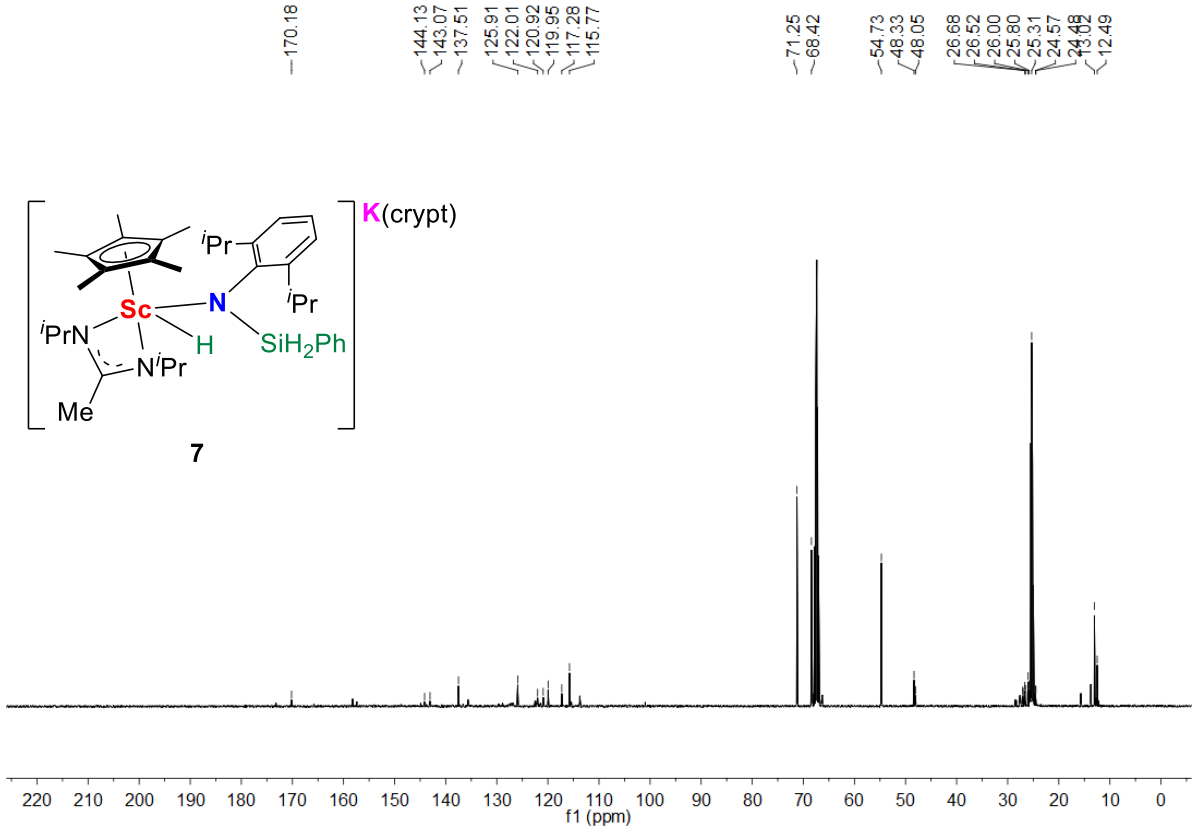


Figure S18. ^{13}C NMR spectrum of **7** (25 °C, 126 MHz, d^{8}-THF).

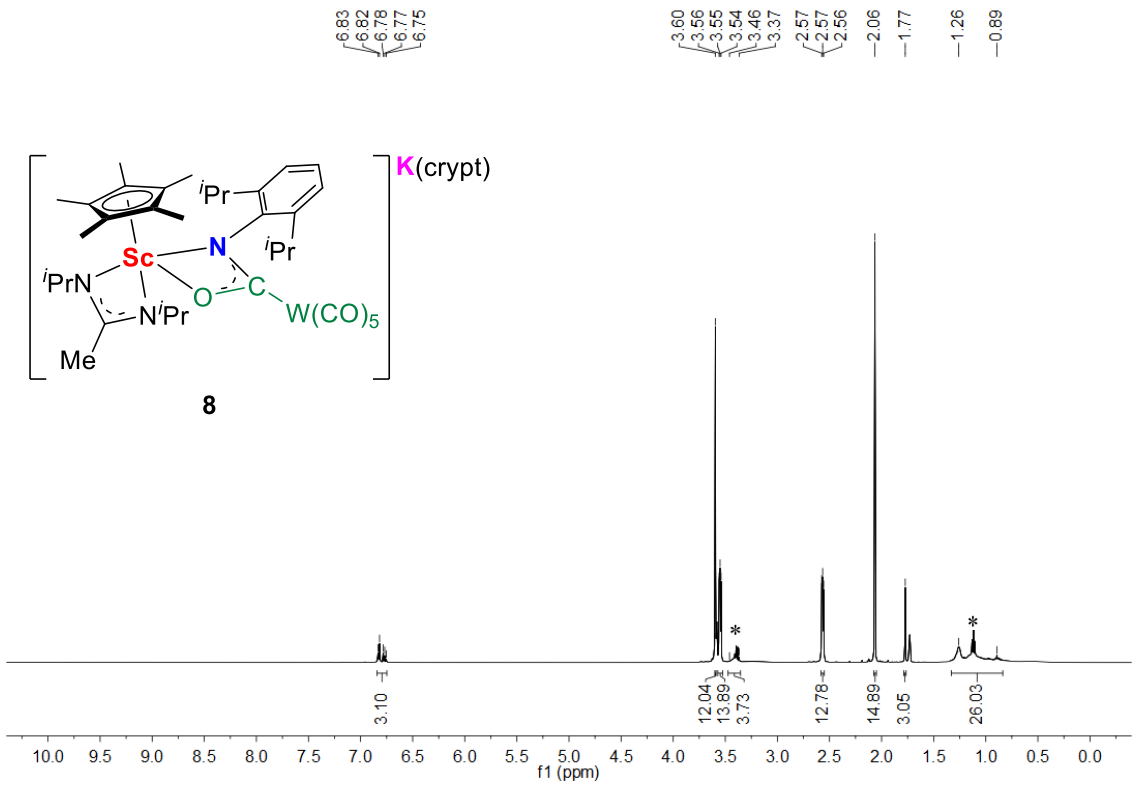


Figure S19. ^{1}H NMR spectrum of **8** (25 °C, 500 MHz, d^{8}-THF, "*" represents the residual Et_2O).

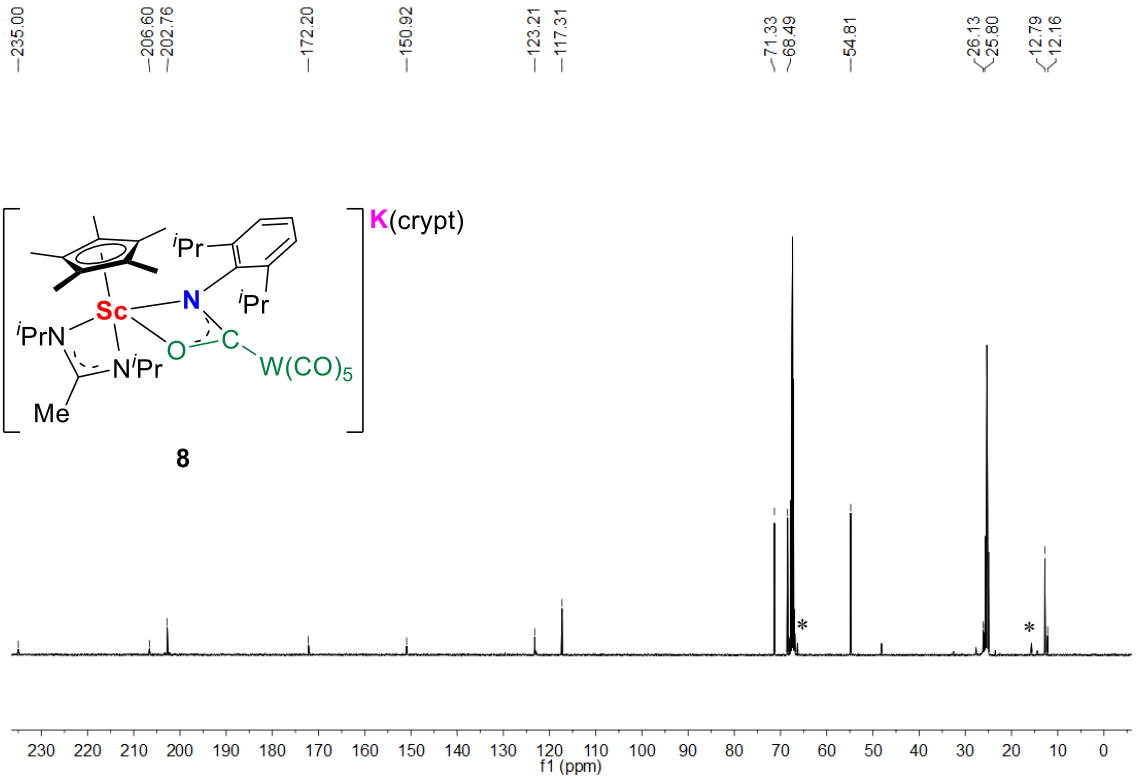


Figure S20. ^{13}C NMR spectrum of **8** (25 °C, 126 MHz, d^{8}-THF, "*" represents the residual Et_2O).

3) X-ray Crystallographic Studies

The single crystals of **2**, **3a·Tol**, **3b**, **4a·0.25THF**, **4b**, **5·2THF**, **6·THF**, **7** and **8·THF** suitable for X-ray analysis were obtained as described in the experimental details. Data collections were performed on a XtaLAB PRO 007HF(Mo): Kappa single diffractometer at 180 or 120 K. Using Olex2,[3] the structures were solved with Superflip[4] structure solution program using Charge Flipping or ShelXS-97[5] structure solution program using Direct Methods and refined with the ShelXL[6] refinement package using Least Squares minimization. Refinement was performed on F^2 anisotropically for all the non-hydrogen atoms by the full-matrix least-squares method. The hydrogen atoms were placed at the calculated positions and were included in the structure calculation without further refinement of the parameters. Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre with supplementary publication numbers: CCDC 2385556 (**2**), CCDC 2410804 (**3a·Tol**) CCDC 2385559 (**3b**), CCDC 2385558 (**4a·0.25THF**), CCDC 2385560 (**4b**), CCDC 2385563 (**5·2THF**), CCDC 2385564 (**6·THF**), CCDC 2385561 (**7**), CCDC 2385562 (**8·THF**).

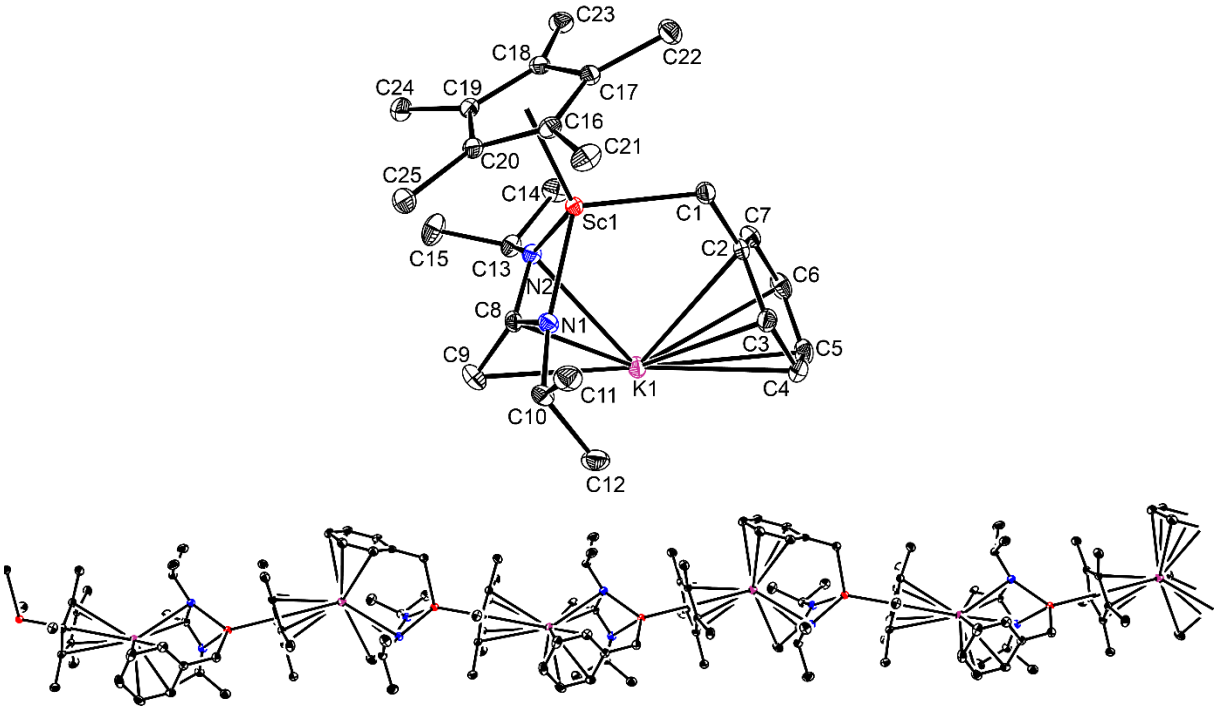
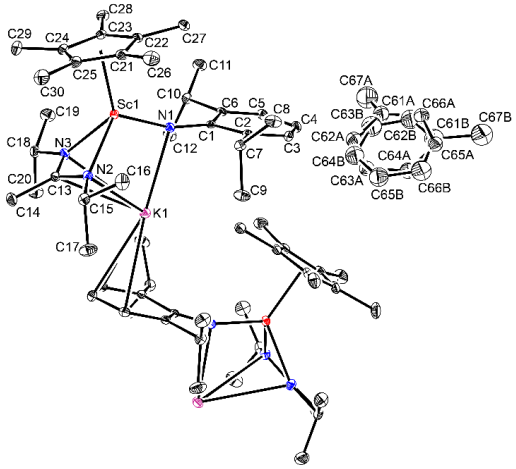


Figure S21. ORTEP drawing of repeating unit (top) and one dimensional molecular structure (bottom) of **2** with 30% thermal ellipsoids. H atoms are omitted for clarity.

Table 1 Crystal data and structure refinement for 2.

Identification code	**2**
Empirical formula	$C_{25}H_{38}KN_2Sc$
Formula weight	450.63
Temperature/K	180.00(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	9.9707(3)
b/Å	16.0110(5)
c/Å	15.9160(4)
α/°	90
β/°	93.989(2)
γ/°	90
Volume/Å^3	2534.69(13)
Z	4
ρ_{calc}g/cm^3	1.181
μ/mm^{-1}	0.467
F(000)	968.0
Crystal size/mm^3	0.2 × 0.1 × 0.1
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.678 to 54.968
Index ranges	-12 ≤ h ≤ 12, -20 ≤ k ≤ 20, -20 ≤ l ≤ 20
Reflections collected	24950
Independent reflections	5792 [R_{int} = 0.0287, R_{sigma} = 0.0266]
Data/restraints/parameters	5792/0/271
Goodness-of-fit on F^2	1.030
Final R indexes [I>=2σ (I)]	R_1 = 0.0332, wR_2 = 0.0886
Final R indexes [all data]	R_1 = 0.0401, wR_2 = 0.0919
Largest diff. peak/hole / e Å^{-3}	0.28/-0.22



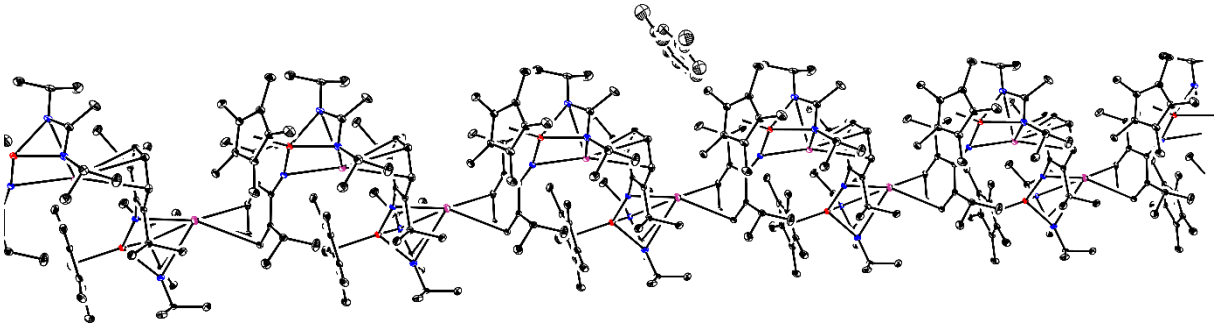


Figure S22. ORTEP drawing of repeating unit (top) and one dimensional molecular structure (bottom) of **3a·Tol** with 30% thermal ellipsoids. H atoms are omitted for clarity.

Table 2 Crystal data and structure refinement for 3a·Tol.

Identification code	**3a·Tol**
Empirical formula	$C_{67}H_{106}K_2N_6Sc_2$
Formula weight	1163.69
Temperature/K	179.99(10)
Crystal system	triclinic
Space group	P-1
a/Å	12.5098(4)
b/Å	15.3624(5)
c/Å	20.2544(7)
α/°	100.049(3)
β/°	98.550(3)
γ/°	108.603(3)
Volume/Å^3	3544.4(2)
Z	2
ρ_{calc}g/cm^3	1.090
μ/mm^{-1}	0.348
F(000)	1260.0
Crystal size/mm^3	0.1 × 0.1 × 0.1
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.186 to 50.054
Index ranges	-14 ≤ h ≤ 14, -18 ≤ k ≤ 18, -24 ≤ l ≤ 24
Reflections collected	54974
Independent reflections	12492 [R_{int} = 0.0623, R_{sigma} = 0.0507]
Data/restraints/parameters	12492/302/776
Goodness-of-fit on F^2	1.033
Final R indexes [I>=2σ (I)]	R_1 = 0.0472, wR_2 = 0.1256
Final R indexes [all data]	R_1 = 0.0615, wR_2 = 0.1329
Largest diff. peak/hole / e Å^{-3}	0.74/-0.59

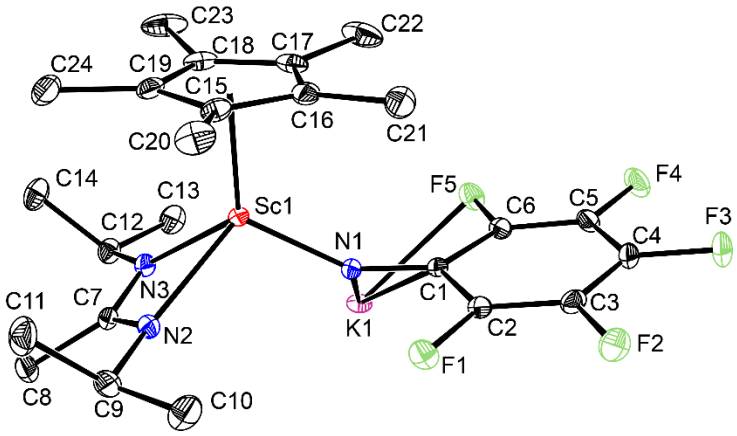


Figure S23. ORTEP drawing of **3b** with 30% thermal ellipsoids. H atoms are omitted for clarity.

Table 3 Crystal data and structure refinement for 3b.

Identification code	**3b**
Empirical formula	$C_{24}H_{32}F_5KN_3Sc$
Formula weight	541.58
Temperature/K	179.99(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	14.9082(6)
b/Å	12.6059(3)
c/Å	15.3819(6)
α/°	90
β/°	116.514(5)
γ/°	90
Volume/Å^3	2586.71(19)
Z	4
ρ_{calc}g/cm^3	1.391
μ/mm^{-1}	0.498
F(000)	1128.0
Crystal size/mm^3	0.1 × 0.1 × 0.1
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.114 to 54.968
Index ranges	$-17 \le h \le 19$, $-16 \le k \le 14$, $-19 \le l \le 19$
Reflections collected	26186
Independent reflections	5924 [R_{int} = 0.0342, R_{sigma} = 0.0305]
Data/restraints/parameters	5924/0/317
Goodness-of-fit on F^2	1.035
Final R indexes [I>=2σ (I)]	R_1 = 0.0342, wR_2 = 0.0877
Final R indexes [all data]	R_1 = 0.0445, wR_2 = 0.0919
Largest diff. peak/hole / e Å^{-3}	0.28/-0.23

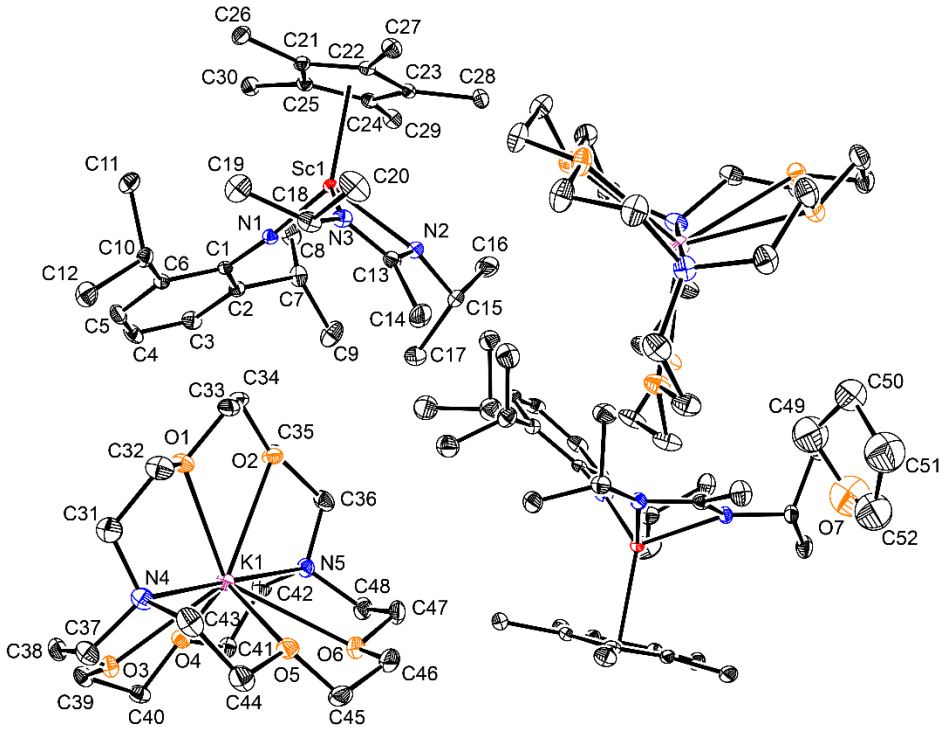


Figure S24. ORTEP drawing of **4a·0.25THF** with 30% thermal ellipsoids. H atoms are omitted for clarity.

Table 4 Crystal data and structure refinement for 4a·0.25THF.

Identification code	**4a·0.25THF**
Empirical formula	$C_{196}H_{348}K_4N_{20}O_{25}Sc_4$
Formula weight	3721.16
Temperature/K	180.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	11.8564(3)
b/Å	15.2872(4)
c/Å	31.9250(7)
α/°	95.340(2)
β/°	98.988(2)
γ/°	107.806(2)
Volume/Å^3	5380.2(2)
Z	1
ρ_{calc}g/cm^3	1.148
μ/mm^{-1}	0.262
F(000)	2024.0
Crystal size/mm^3	0.1 × 0.1 × 0.1
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.478 to 50.054
Index ranges	-13 ≤ h ≤ 14, -18 ≤ k ≤ 18, -37 ≤ l ≤ 37
Reflections collected	90386
Independent reflections	18950 [R_{int} = 0.0587, R_{sigma} = 0.0516]

Data/restraints/parameters	18950/216/1202
Goodness-of-fit on F^2	1.022
Final R indexes [I>=2σ (I)]	R_1 = 0.0449, wR_2 = 0.1005
Final R indexes [all data]	R_1 = 0.0618, wR_2 = 0.1069
Largest diff. peak/hole / e $Å^{-3}$	0.51/-0.36

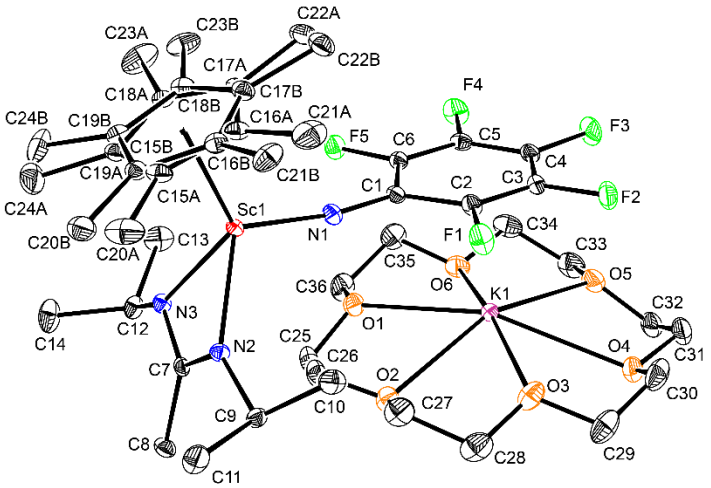


Figure S25. ORTEP drawing of **4b** with 30% thermal ellipsoids. H atoms are omitted for clarity.

Table 5 Crystal data and structure refinement for 4b.

Identification code	**4b**
Empirical formula	$C_{36}H_{56}F_5KN_3O_6Sc$
Formula weight	805.89
Temperature/K	179.99(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	9.9058(5)
b/Å	28.0102(11)
c/Å	14.9302(6)
α/°	90
β/°	96.896(4)
γ/°	90
Volume/$Å^3$	4112.6(3)
Z	4
ρ_{calc}g/cm^3	1.302
μ/mm^{-1}	0.347
F(000)	1704.0
Crystal size/mm^3	0.1 × 0.1 × 0.1
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.002 to 54.968
Index ranges	-12 ≤ h ≤ 12, -36 ≤ k ≤ 36, -19 ≤ l ≤ 19
Reflections collected	37893
Independent reflections	9391 [R_{int} = 0.0403, R_{sigma} = 0.0450]

Data/restraints/parameters	9391/289/575
Goodness-of-fit on F^2	1.034
Final R indexes [I>=2σ (I)]	R_1 = 0.0509, wR_2 = 0.1030
Final R indexes [all data]	R_1 = 0.0753, wR_2 = 0.1108
Largest diff. peak/hole / e $Å^{-3}$	0.41/-0.33

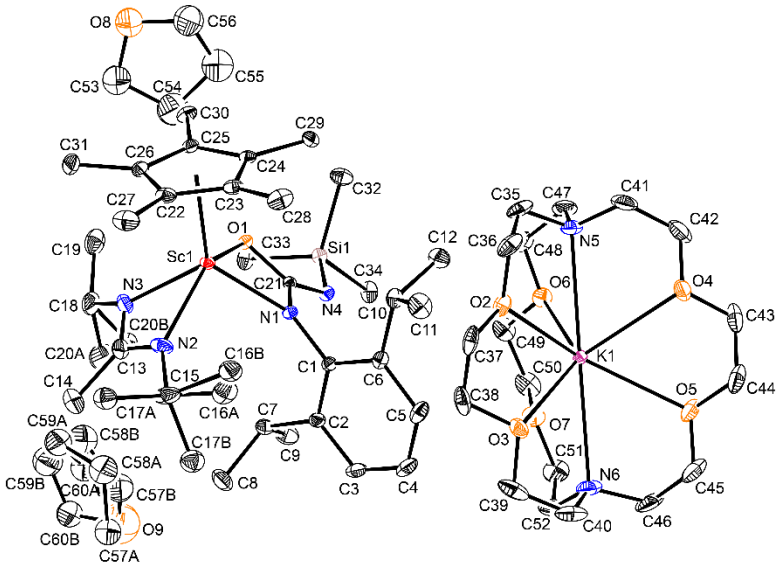


Figure S26. ORTEP drawing of **5·2THF** with 30% thermal ellipsoids. H atoms are omitted for clarity.

Table 6 Crystal data and structure refinement for 5·2THF.

Identification code	**5·2THF**
Empirical formula	$C_{60}H_{110}KN_6O_9ScSi$
Formula weight	1171.68
Temperature/K	179.99(10)
Crystal system	triclinic
Space group	P-1
a/Å	13.0622(2)
b/Å	16.5088(3)
c/Å	18.0613(3)
α/°	111.056(2)
β/°	97.391(2)
γ/°	105.329(2)
Volume/$Å^3$	3395.47(11)
Z	2
ρ_{calc}g/cm^3	1.146
μ/mm^{-1}	0.241
F(000)	1276.0
Crystal size/mm^3	0.1 × 0.1 × 0.1
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.164 to 54.968

Index ranges	$-16 \le h \le 16$, $-21 \le k \le 17$, $-22 \le l \le 23$
Reflections collected	55775
Independent reflections	15542 [R_{int} = 0.0354, R_{sigma} = 0.0350]
Data/restraints/parameters	15542/277/788
Goodness-of-fit on F^2	1.054
Final R indexes [I>=2σ (I)]	R_1 = 0.0595, wR_2 = 0.1691
Final R indexes [all data]	R_1 = 0.0727, wR_2 = 0.1779
Largest diff. peak/hole / e $Å^{-3}$	1.43/-0.80

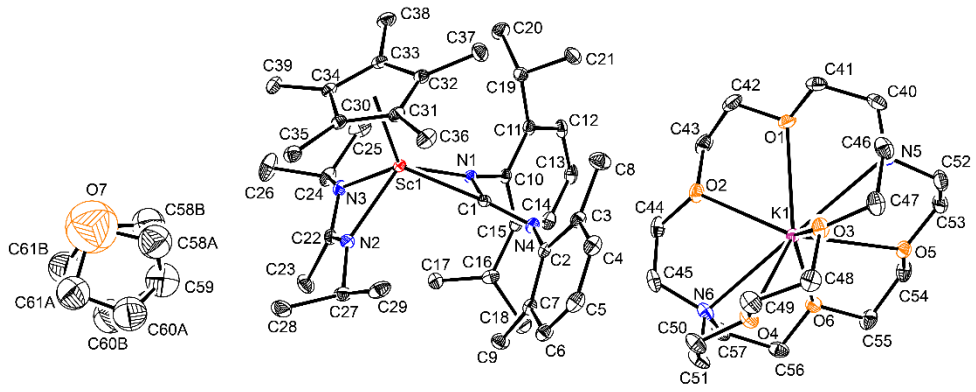


Figure S27. ORTEP drawing of **6·THF** with 30% thermal ellipsoids. H atoms are omitted for clarity.

Table 7 Crystal data and structure refinement for 6·THF.

Identification code	**6·THF**
Empirical formula	$C_{61}H_{102}KN_6O_7Sc$
Formula weight	1115.54
Temperature/K	179.99(10)
Crystal system	triclinic
Space group	P-1
a/Å	13.1083(4)
b/Å	14.0998(4)
c/Å	18.3424(5)
α/°	98.136(2)
β/°	104.412(2)
γ/°	95.120(2)
Volume/$Å^3$	3222.89(16)
Z	2
ρ_{calc}g/cm^3	1.150
μ/mm^{-1}	0.231
F(000)	1212.0
Crystal size/mm^3	0.1 × 0.1 × 0.1
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.082 to 54.97
Index ranges	$-16 \le h \le 17$, $-18 \le k \le 18$, $-23 \le l \le 23$

Reflections collected	62172
Independent reflections	14733 [R_{int} = 0.0281, R_{sigma} = 0.0258]
Data/restraints/parameters	14733/206/729
Goodness-of-fit on F^2	1.046
Final R indexes [I>=2σ (I)]	R_1 = 0.0444, wR_2 = 0.1264
Final R indexes [all data]	R_1 = 0.0525, wR_2 = 0.1314
Largest diff. peak/hole / e $Å^{-3}$	0.71/-0.58

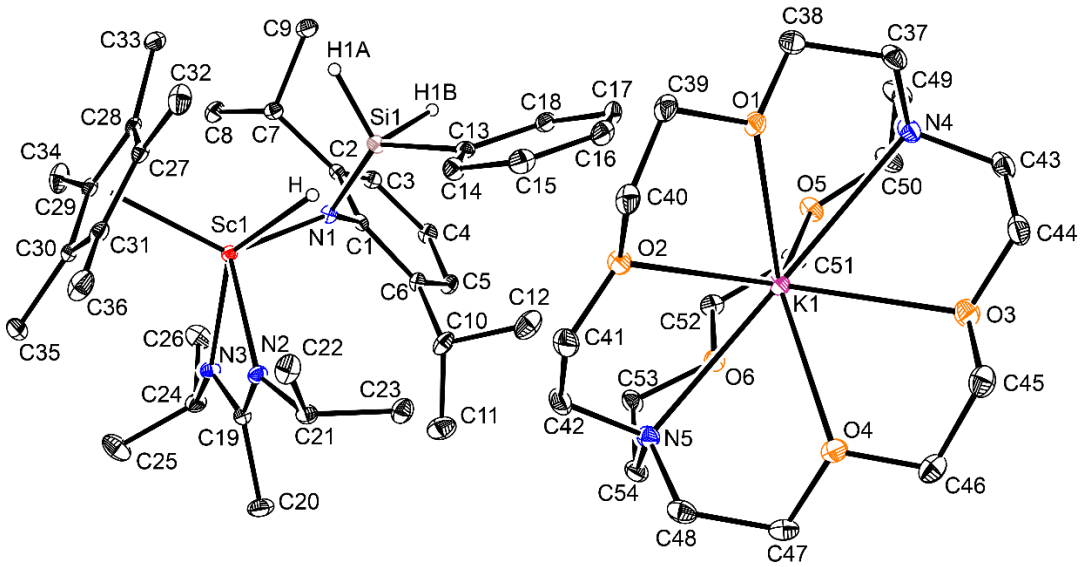


Figure S28. ORTEP drawing of **7** with 30% thermal ellipsoids. H atoms are omitted for clarity.

Table 8 Crystal data and structure refinement for 7.

Identification code	**7**
Empirical formula	$C_{54}H_{93}KN_5O_6ScSi$
Formula weight	1020.48
Temperature/K	179.99(10)
Crystal system	triclinic
Space group	P-1
a/Å	10.8384(5)
b/Å	16.2978(8)
c/Å	17.2748(7)
α/°	98.226(4)
β/°	91.222(4)
γ/°	105.732(4)
Volume/$Å^3$	2901.1(2)
Z	2
ρ_{calc}g/cm^3	1.168
μ/mm^{-1}	0.268
F(000)	1108.0
Crystal size/mm^3	0.1 × 0.1 × 0.1
Radiation	Mo Kα (λ = 0.71073)

2Θ range for data collection/°	4.064 to 50.054
Index ranges	-12 ≤ h ≤ 12, -19 ≤ k ≤ 19, -20 ≤ l ≤ 20
Reflections collected	40485
Independent reflections	10248 [R_{int} = 0.0989, R_{sigma} = 0.0916]
Data/restraints/parameters	10248/0/637
Goodness-of-fit on F^2	1.028
Final R indexes [I>=2σ (I)]	R_1 = 0.0450, wR_2 = 0.1021
Final R indexes [all data]	R_1 = 0.0663, wR_2 = 0.1095
Largest diff. peak/hole / e $Å^{-3}$	0.34/-0.29

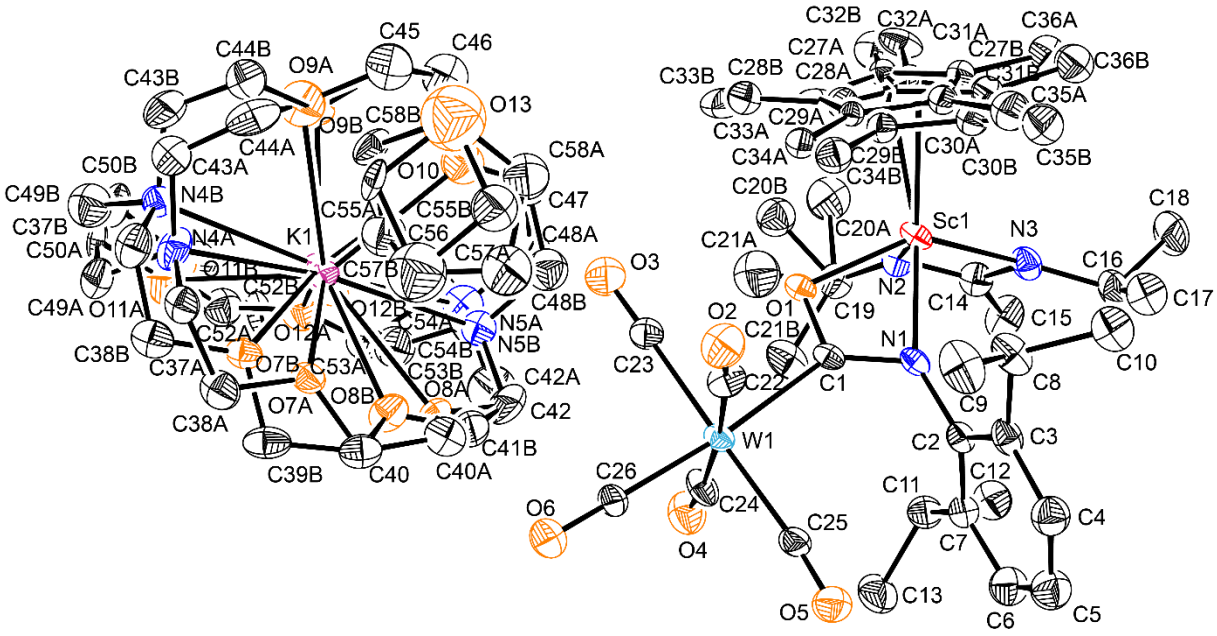


Figure S29. ORTEP drawing of **8·THF** with 30% thermal ellipsoids. H atoms are omitted for clarity.

Table 9 Crystal data and structure refinement for 8·THF.

Identification code	**8·THF**
Empirical formula	$C_{58}H_{93}KN_5O_{13}ScW$
Formula weight	1336.28
Temperature/K	180.00(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	18.5513(7)
b/Å	18.8698(6)
c/Å	20.5874(7)
α/°	90
β/°	114.089(4)
γ/°	90
Volume/$Å^3$	6579.2(4)
Z	4

ρ_{calc}g/cm^3	1.349
μ/mm^{-1}	1.973
F(000)	2776.0
Crystal size/mm^3	0.1 × 0.1 × 0.1
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.318 to 54.968
Index ranges	-24 ≤ h ≤ 19, -24 ≤ k ≤ 23, -26 ≤ l ≤ 26
Reflections collected	61204
Independent reflections	15017 [R_{int} = 0.0280, R_{sigma} = 0.0291]
Data/restraints/parameters	15017/499/1036
Goodness-of-fit on F^2	1.031
Final R indexes [I>=2σ (I)]	R_1 = 0.0547, wR_2 = 0.1362
Final R indexes [all data]	R_1 = 0.0756, wR_2 = 0.1495
Largest diff. peak/hole / e Å^{-3}	2.32/-1.71

4) Details of DFT Calculation

All calculations were carried out with GAUSSIAN 16 program package.[6] The structures of all complexes were optimized at PBE0-D3/(SDD for Sc, 6-31G* for other elements) level in gas phase. The effect of solvent was examined by performing single-point self-consistent reaction field (SCRF) calculations based on the solvation model density (SMD)[7] for gas-phase optimized structures. THF was used as solvent, and solvation free energies (ΔG_{sol}) were calculated by adding the solvation energies to the computed gas phase relative free energies (ΔG_{gas}). For all complexes, solvation free energies (ΔG_{sol}) were calculated at PBE0-D3/(SDD for Sc, def2-TZVP for other elements) level. Harmonic frequency calculations were performed at the same level for every structure to confirm it as a local minimum and to derive the thermochemical corrections for enthalpies and free energies. The intrinsic reaction coordinate (IRC) analysis was carried out throughout the pathways to confirm that all stationary points are smoothly connected to each other. All enthalpies and the Gibbs free energies in the text were given in Hartree. All distances were given in Å.

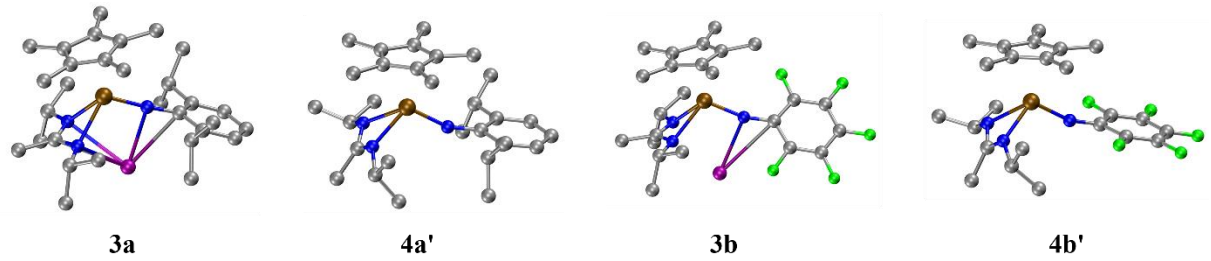


Figure S30. DFT optimized geometries of **3a**, **4a'**, **3b**, and **4b'**. Color codes for atoms: silver - C; blue - N; brown - Sc; purple - K. The H atoms are omitted for clarity.

2'
298 K, 1 atm, gas phase
Thermal correction to Enthalpy = 0.612249
Thermal correction to Gibbs Free Energy = 0.516739
Sum of electronic and thermal Enthalpies = -1130.725993
Sum of electronic and thermal Free Energies = -1130.821502
298 K, in THF
Sum of electronic and thermal Free Energies = -1131.569246

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	21	0	0.529026	-0.151452	-0.107794
2	6	0	2.796924	-0.469932	-1.208348
3	6	0	2.272183	-1.775829	-1.036033
4	6	0	3.010714	0.088018	0.078291
5	6	0	2.622997	-0.878048	1.046757
6	6	0	-2.196869	-0.680734	-1.586578
7	6	0	-0.748769	1.579992	1.212964
8	6	0	2.165981	-2.031447	0.356108
9	6	0	-3.026338	-1.810493	-1.451739
10	1	0	-2.590506	-2.797454	-1.601900
11	6	0	-1.455934	-0.335392	2.580221
12	1	0	-1.418708	0.322089	3.468057
13	6	0	3.597215	1.428583	0.415585
14	1	0	3.567103	2.111691	-0.439318
15	1	0	4.646579	1.339088	0.732605
16	1	0	3.039745	1.908737	1.226446
17	6	0	0.101280	3.142973	-0.482121
18	1	0	-0.927910	3.543703	-0.533920
19	6	0	-2.807460	0.573206	-1.380777
20	1	0	-2.189818	1.466625	-1.428294

21	6	0	2.734940	-0.672358	2.532239
22	1	0	2.063405	0.120614	2.882361
23	1	0	3.760030	-0.396497	2.814562
24	1	0	2.479517	-1.583717	3.082083
25	6	0	1.698736	-3.329276	0.954987
26	1	0	1.515289	-3.235412	2.029149
27	1	0	2.440862	-4.127090	0.811442
28	1	0	0.761907	-3.674690	0.499130
29	6	0	1.996753	-2.756611	-2.137100
30	1	0	1.205843	-3.462659	-1.860628
31	1	0	2.892847	-3.345622	-2.382606
32	1	0	1.672594	-2.250484	-3.052879
33	6	0	3.083054	0.165994	-2.540581
34	1	0	3.462304	1.186170	-2.425452
35	1	0	2.186231	0.220392	-3.171472
36	1	0	3.839039	-0.402604	-3.099117
37	6	0	-1.529227	2.499289	1.852120
38	1	0	-2.171392	2.219051	2.677817
39	1	0	-1.546859	3.538803	1.548147
40	6	0	-4.154632	0.686169	-1.068314
41	1	0	-4.577698	1.673747	-0.898437
42	6	0	-4.377135	-1.698846	-1.135935
43	1	0	-4.980949	-2.599736	-1.040485
44	6	0	-0.884948	-1.692931	2.990222
45	1	0	-0.888160	-2.374007	2.128887
46	1	0	-1.484080	-2.152232	3.786984
47	1	0	0.147103	-1.590620	3.340843
48	6	0	-4.958325	-0.447953	-0.943822
49	1	0	-6.011618	-0.357448	-0.690961
50	6	0	-2.926143	-0.493717	2.162031
51	1	0	-3.325840	0.454119	1.794803
52	1	0	-3.543527	-0.839112	3.003891
53	1	0	-3.006044	-1.218782	1.344350
54	6	0	0.626929	3.041710	-1.914781
55	1	0	1.638539	2.616877	-1.912772
56	1	0	0.671334	4.026686	-2.397269
57	1	0	-0.012923	2.385476	-2.515054
58	6	0	0.947743	4.143368	0.324487
59	1	0	0.643462	4.133160	1.374910
60	1	0	0.839096	5.165386	-0.065029
61	1	0	2.006932	3.865563	0.272206
62	7	0	-0.641772	0.218627	1.530380
63	7	0	0.075466	1.831554	0.103548
64	6	0	-0.754430	-0.808802	-1.880147

65	1	0	-0.436135	-0.061877	-2.627275
66	1	0	-0.524441	-1.800324	-2.288030

TS1

298 K, 1 atm, gas phase
Thermal correction to Enthalpy = 0.914759
Thermal correction to Gibbs Free Energy = 0.785564
Sum of electronic and thermal Enthalpies = -1653.760976
Sum of electronic and thermal Free Energies = -1653.890171
298 K, in THF
Sum of electronic and thermal Free Energies = -1654.818651

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	21	0	1.964346	-0.276870	-0.093729
2	6	0	3.982038	-0.435895	-1.612066
3	6	0	3.901982	-1.651498	-0.884152
4	6	0	4.237021	0.616399	-0.693094
5	6	0	4.310455	0.049025	0.607216
6	6	0	0.296852	1.111852	-2.068624
7	6	0	0.411453	-0.138625	1.883127
8	6	0	4.108844	-1.355237	0.487099
9	6	0	1.075256	1.980925	-2.857254
10	1	0	1.905208	1.569173	-3.426881
11	6	0	0.204450	-2.565678	1.630863
12	1	0	-0.877177	-2.395841	1.722980
13	6	0	4.452567	2.055971	-1.076353
14	1	0	4.643049	2.679078	-0.198120
15	1	0	3.586132	2.482645	-1.595776
16	1	0	5.320293	2.155878	-1.741776
17	6	0	0.840108	2.276751	1.804319
18	1	0	-0.235879	2.477353	1.673665
19	6	0	-0.783986	1.685149	-1.364612
20	1	0	-1.397173	1.036570	-0.739545
21	6	0	4.583900	0.754082	1.905639
22	1	0	4.529428	1.841065	1.793968
23	1	0	5.583338	0.508127	2.290153
24	1	0	3.850108	0.476205	2.670204
25	6	0	4.161326	-2.321003	1.635373

26	1	0	5.197440	-2.511774	1.948040
27	1	0	3.710710	-3.283873	1.374522
28	1	0	3.612201	-1.936028	2.500737
29	6	0	3.668192	-2.995940	-1.513633
30	1	0	4.469468	-3.243019	-2.223091
31	1	0	2.722158	-3.026432	-2.069540
32	1	0	3.636651	-3.793762	-0.765365
33	6	0	3.977976	-0.328154	-3.108404
34	1	0	4.895297	-0.761338	-3.532295
35	1	0	3.931339	0.716112	-3.431913
36	1	0	3.129702	-0.853337	-3.560855
37	6	0	-0.836973	-0.035118	2.600949
38	1	0	-1.039098	-0.859933	3.286164
39	1	0	-1.016586	0.925058	3.080119
40	6	0	-1.066986	3.041175	-1.456306
41	1	0	-1.911868	3.441827	-0.900721
42	6	0	0.792118	3.342734	-2.942779
43	1	0	1.415502	3.980301	-3.566674
44	6	0	0.685218	-3.222864	2.930815
45	1	0	1.747258	-3.482374	2.855351
46	1	0	0.117265	-4.137409	3.144929
47	1	0	0.563980	-2.535255	3.774362
48	6	0	-0.282097	3.886431	-2.243458
49	1	0	-0.504323	4.948261	-2.308890
50	6	0	0.419423	-3.495926	0.437250
51	1	0	0.028868	-3.042210	-0.480891
52	1	0	-0.085177	-4.457608	0.588145
53	1	0	1.490101	-3.687626	0.291991
54	6	0	1.604013	3.220196	0.877639
55	1	0	2.683282	3.091569	1.023509
56	1	0	1.352108	4.265820	1.090445
57	1	0	1.368327	3.022192	-0.171339
58	6	0	1.228731	2.563034	3.262477
59	1	0	0.731332	1.876294	3.953117
60	1	0	0.963290	3.590184	3.543607
61	1	0	2.311925	2.439616	3.383450
62	7	0	0.890229	-1.313508	1.384438
63	7	0	1.141320	0.911335	1.429082
64	6	0	0.635097	-0.320590	-1.910078
65	6	0	-5.678490	0.933188	-0.083544
66	6	0	-4.388978	0.738097	0.393955
67	6	0	-3.647540	-0.416399	-0.005340
68	6	0	-4.259384	-1.315827	-0.937804
69	6	0	-5.551979	-1.068116	-1.387891

70	6	0	-6.280272	0.041511	-0.968456
71	1	0	-6.233035	1.813902	0.234732
72	1	0	-6.010338	-1.757199	-2.093789
73	1	0	-7.288872	0.214721	-1.334119
74	6	0	-3.746047	1.706709	1.369888
75	6	0	-3.963117	1.238542	2.816993
76	6	0	-4.205360	3.159168	1.205734
77	1	0	-2.665813	1.684918	1.177929
78	1	0	-3.612563	0.210479	2.944556
79	1	0	-3.421289	1.875409	3.528869
80	1	0	-5.031715	1.271920	3.067307
81	1	0	-4.128000	3.483818	0.161983
82	1	0	-5.246265	3.299411	1.524330
83	1	0	-3.585596	3.823173	1.820985
84	6	0	-3.480307	-2.540707	-1.393099
85	6	0	-3.981717	-3.162964	-2.698945
86	6	0	-3.433835	-3.611018	-0.287844
87	1	0	-2.445801	-2.219565	-1.591344
88	1	0	-4.050580	-2.414475	-3.495498
89	1	0	-3.295103	-3.952891	-3.026721
90	1	0	-4.970838	-3.621379	-2.575384
91	1	0	-3.085955	-3.184592	0.658154
92	1	0	-4.438916	-4.018448	-0.122121
93	1	0	-2.766402	-4.438828	-0.561610
94	7	0	-2.391358	-0.600068	0.478116
95	1	0	-1.724604	-0.219807	1.573556
96	1	0	-1.922086	-1.403160	0.079295
97	1	0	-0.255638	-0.901599	-1.636754
98	1	0	1.078611	-0.747648	-2.816883

IM1

298 K, 1 atm, gas phase

Thermal correction to Enthalpy = 0.920195

Thermal correction to Gibbs Free Energy = 0.790373

Sum of electronic and thermal Enthalpies = -1653.767318

Sum of electronic and thermal Free Energies = -1653.897140

298 K, in THF

Sum of electronic and thermal Free Energies = -1654.829736

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	21	0	2.002875	0.278964	-0.021855
2	6	0	3.981659	1.194243	1.213562
3	6	0	3.833722	1.958020	0.026792
4	6	0	4.306199	-0.138927	0.846900
5	6	0	4.356658	-0.199528	-0.571309
6	6	0	0.338375	-0.136830	2.259997
7	6	0	0.539037	-0.827086	-1.752915
8	6	0	4.067093	1.099021	-1.078006
9	6	0	1.095127	-0.639371	3.337160
10	1	0	1.915735	-0.039839	3.725428
11	6	0	0.085251	1.440212	-2.553341
12	1	0	-0.975254	1.157713	-2.521781
13	6	0	4.603520	-1.245762	1.822703
14	1	0	3.751478	-1.463855	2.478114
15	1	0	5.453835	-0.979694	2.463900
16	1	0	4.862604	-2.174639	1.306915
17	6	0	1.099776	-2.949453	-0.664115
18	1	0	0.031057	-3.145970	-0.489548
19	6	0	-0.733557	-0.932241	1.799673
20	1	0	-1.344959	-0.573336	0.967426
21	6	0	4.693415	-1.386021	-1.428385
22	1	0	3.980126	-1.495486	-2.252328
23	1	0	4.664821	-2.318449	-0.856825
24	1	0	5.698298	-1.290803	-1.861872
25	6	0	4.067092	1.462762	-2.534693
26	1	0	3.553760	0.703179	-3.133107
27	1	0	5.091546	1.561874	-2.918984
28	1	0	3.551615	2.411351	-2.713778
29	6	0	3.504927	3.424263	-0.000070
30	1	0	4.285205	4.011583	0.501473
31	1	0	2.557026	3.636844	0.510427
32	1	0	3.419038	3.800720	-1.023660
33	6	0	3.974133	1.748689	2.606865
34	1	0	4.938769	2.220452	2.842453
35	1	0	3.805270	0.964357	3.350881
36	1	0	3.196359	2.507018	2.742232
37	6	0	-0.675934	-1.356115	-2.451100
38	1	0	-1.541361	-0.861334	-1.955115
39	1	0	-0.776412	-2.437413	-2.365332
40	6	0	-1.036033	-2.145798	2.405438
41	1	0	-1.881647	-2.720113	2.035808
42	6	0	0.790460	-1.858489	3.938103
43	1	0	1.391004	-2.208421	4.775163

44	6	0	0.540455	1.529215	-4.014968
45	1	0	1.575983	1.883948	-4.071642
46	1	0	-0.095815	2.223822	-4.576823
47	1	0	0.493734	0.551834	-4.506860
48	6	0	-0.279465	-2.621650	3.477909
49	1	0	-0.521852	-3.571505	3.946842
50	6	0	0.214073	2.802335	-1.873450
51	1	0	-0.153697	2.759927	-0.843560
52	1	0	-0.367968	3.562133	-2.406947
53	1	0	1.263940	3.123053	-1.852265
54	6	0	1.850500	-3.327720	0.609686
55	1	0	2.928922	-3.195578	0.462563
56	1	0	1.666027	-4.375415	0.873528
57	1	0	1.533785	-2.706196	1.451268
58	6	0	1.587511	-3.815566	-1.833380
59	1	0	1.082869	-3.556623	-2.769378
60	1	0	1.409074	-4.878766	-1.630621
61	1	0	2.663803	-3.666094	-1.979009
62	7	0	0.881468	0.470460	-1.812893
63	7	0	1.314327	-1.537595	-0.925348
64	6	0	0.699923	1.126383	1.579426
65	6	0	-6.014997	-0.554031	0.060454
66	6	0	-4.744576	-0.587127	-0.493436
67	6	0	-3.786523	0.449338	-0.196310
68	6	0	-4.226273	1.494635	0.697025
69	6	0	-5.512527	1.473954	1.222985
70	6	0	-6.424457	0.464559	0.922756
71	1	0	-6.721054	-1.346565	-0.183429
72	1	0	-5.822562	2.270943	1.897045
73	1	0	-7.424809	0.469890	1.348095
74	6	0	-4.300408	-1.709231	-1.414030
75	6	0	-5.444707	-2.458171	-2.103812
76	6	0	-3.394994	-2.705915	-0.671421
77	1	0	-3.689162	-1.242425	-2.197598
78	1	0	-6.127102	-1.765875	-2.610180
79	1	0	-5.045847	-3.157321	-2.850301
80	1	0	-6.033998	-3.048681	-1.390220
81	1	0	-2.545435	-2.177093	-0.231147
82	1	0	-3.955799	-3.201965	0.131898
83	1	0	-3.008969	-3.481644	-1.348967
84	6	0	-3.261141	2.625130	1.012287
85	6	0	-3.594166	3.422745	2.275425
86	6	0	-3.122056	3.579297	-0.188067
87	1	0	-2.273799	2.173151	1.192951

88	1	0	-3.721447	2.761416	3.139278
89	1	0	-2.786031	4.130478	2.499291
90	1	0	-4.515864	4.006281	2.155235
91	1	0	-2.898485	3.019628	-1.102051
92	1	0	-4.065046	4.117943	-0.345734
93	1	0	-2.324908	4.318750	-0.027452
94	7	0	-2.563009	0.375328	-0.755428
95	1	0	-0.672085	-1.080214	-3.509582
96	1	0	-1.997208	1.167946	-0.461553
97	1	0	-0.174158	1.572380	1.089420
98	1	0	1.144619	1.858507	2.260608

IM2

298 K, 1 atm, gas phase
Thermal correction to Enthalpy = 0.922082
Thermal correction to Gibbs Free Energy = 0.797520
Sum of electronic and thermal Enthalpies = -1653.804993
Sum of electronic and thermal Free Energies = -1653.92955
298K, in THF
Sum of electronic and thermal Free Energies = -1654.853765

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	21	0	-0.670836	-0.047571	0.236225
2	6	0	-0.977742	-0.153433	2.735381
3	6	0	-0.265212	-1.332671	2.391716
4	6	0	-2.294993	-0.266569	2.213933
5	6	0	-2.390529	-1.501904	1.529591
6	6	0	-1.673996	1.122969	-2.005708
7	6	0	-1.132452	-2.164188	1.639631
8	6	0	-2.561895	-1.217794	-2.273172
9	1	0	-3.297952	-1.033367	-1.483999
10	6	0	-3.434618	0.692297	2.413072
11	1	0	-3.137970	1.529644	3.053564
12	1	0	-4.288078	0.199382	2.899346
13	1	0	-3.789014	1.110311	1.462183
14	6	0	-1.928897	2.989373	-0.549365
15	1	0	-1.255549	3.508831	-1.255848
16	6	0	-3.672064	-2.061833	0.979394
17	1	0	-4.300311	-1.272513	0.549502

18	1	0	-4.264928	-2.548843	1.767955
19	1	0	-3.502555	-2.809766	0.197594
20	6	0	-0.813661	-3.564941	1.185287
21	1	0	-1.688955	-4.045178	0.734585
22	1	0	-0.506390	-4.190628	2.033568
23	1	0	-0.000107	-3.605418	0.450051
24	6	0	1.153295	-1.646606	2.780194
25	1	0	1.432037	-2.655294	2.456528
26	1	0	1.288372	-1.601658	3.869397
27	1	0	1.863324	-0.953323	2.314699
28	6	0	-0.451378	0.950758	3.611402
29	1	0	-0.715904	1.946874	3.240018
30	1	0	0.640568	0.910298	3.672502
31	1	0	-0.842289	0.869289	4.635991
32	6	0	-1.666072	1.786460	-3.192361
33	1	0	-1.489665	1.252312	-4.119188
34	1	0	-1.777279	2.862693	-3.250049
35	6	0	-2.056353	-2.653855	-2.168424
36	1	0	-1.335124	-2.864423	-2.968817
37	1	0	-2.882370	-3.367781	-2.260674
38	1	0	-1.551246	-2.822185	-1.214121
39	6	0	-3.232895	-0.976508	-3.626822
40	1	0	-3.591363	0.051839	-3.708317
41	1	0	-4.078524	-1.663648	-3.751102
42	1	0	-2.524849	-1.156755	-4.446535
43	6	0	-1.481315	3.375179	0.858318
44	1	0	-2.137868	2.920255	1.607389
45	1	0	-1.505945	4.463227	0.997667
46	1	0	-0.457597	3.029349	1.038811
47	6	0	-3.361765	3.471949	-0.818751
48	1	0	-3.695509	3.149415	-1.810227
49	1	0	-3.432521	4.566532	-0.765976
50	1	0	-4.043676	3.045414	-0.072749
51	7	0	-1.423727	-0.323776	-1.980924
52	7	0	-1.800049	1.560521	-0.730357
53	6	0	2.473613	0.135275	-0.303939
54	6	0	3.209425	-1.077277	-0.531838
55	6	0	4.585061	-1.041194	-0.730880
56	6	0	5.296695	0.156068	-0.710243
57	6	0	4.599422	1.341883	-0.482257
58	6	0	3.224450	1.358553	-0.280638
59	1	0	5.124349	-1.971959	-0.903033
60	1	0	6.372706	0.165950	-0.867079
61	1	0	5.151957	2.280227	-0.465652

62	7	0	1.137950	0.122300	-0.121147
63	1	0	-0.659623	-0.527278	-2.621714
64	6	0	2.429064	-2.374916	-0.573782
65	6	0	3.208903	-3.607055	-0.110898
66	6	0	1.822892	-2.604431	-1.965613
67	1	0	1.588887	-2.230723	0.113450
68	1	0	3.668559	-3.434910	0.868918
69	1	0	2.539026	-4.473405	-0.029109
70	1	0	4.006874	-3.879663	-0.814010
71	1	0	1.250471	-1.720952	-2.264483
72	1	0	2.612787	-2.770966	-2.709708
73	1	0	1.151308	-3.475299	-1.974260
74	6	0	2.472495	2.643735	0.004602
75	6	0	3.107267	3.900514	-0.596156
76	6	0	2.277266	2.811394	1.518778
77	1	0	1.476190	2.518665	-0.439292
78	1	0	3.301913	3.773273	-1.667009
79	1	0	2.437158	4.760237	-0.468576
80	1	0	4.057582	4.155274	-0.108287
81	1	0	1.764499	1.933582	1.923822
82	1	0	3.248918	2.908032	2.021224
83	1	0	1.679947	3.703293	1.754612

TS2

298 K, 1 atm, gas phase
Thermal correction to Enthalpy = 0.916218
Thermal correction to Gibbs Free Energy = 0.791506
Sum of electronic and thermal Enthalpies = -1653.773591
Sum of electronic and thermal Free Energies = -1653.898303
298 K, in THF
Sum of electronic and thermal Free Energies = -1654.822645

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	21	0	0.992079	-0.543257	-0.222964
2	6	0	2.342312	-1.807251	-1.962120
3	6	0	0.968251	-2.018698	-2.248437
4	6	0	2.642500	-2.433706	-0.730290
5	6	0	1.453072	-3.025589	-0.240509
6	6	0	-2.172129	-1.249796	2.018410

7	6	0	2.754417	1.122154	0.830282
8	6	0	0.414379	-2.776550	-1.182071
9	6	0	-2.680598	-2.558815	2.073704
10	1	0	-1.982315	-3.393478	2.051080
11	6	0	2.488568	-0.248150	2.887229
12	1	0	1.863539	-1.134560	3.052476
13	6	0	3.998197	-2.463902	-0.088993
14	1	0	4.377160	-1.450269	0.092104
15	1	0	4.730535	-2.988434	-0.718781
16	1	0	3.965366	-2.981071	0.875748
17	6	0	2.637729	2.293253	-1.297054
18	1	0	2.464536	3.201160	-0.698030
19	6	0	-3.113816	-0.202840	2.053534
20	1	0	-2.765291	0.823528	1.971132
21	6	0	1.335151	-3.843176	1.015598
22	1	0	1.786467	-3.338629	1.879738
23	1	0	1.833325	-4.817374	0.911117
24	1	0	0.286697	-4.035232	1.264931
25	6	0	-1.001148	-3.271499	-1.067294
26	1	0	-1.524993	-3.194028	-2.025443
27	1	0	-1.590261	-2.705873	-0.337485
28	1	0	-1.026924	-4.326539	-0.765591
29	6	0	0.265558	-1.532100	-3.486601
30	1	0	0.878460	-1.707035	-4.380079
31	1	0	0.036688	-0.460198	-3.441070
32	1	0	-0.686782	-2.050396	-3.635148
33	6	0	3.351540	-1.149436	-2.854453
34	1	0	4.114125	-0.632539	-2.263431
35	1	0	2.890399	-0.408610	-3.516039
36	1	0	3.861932	-1.886361	-3.492435
37	6	0	3.381316	2.326523	1.512020
38	1	0	4.005069	2.029131	2.355352
39	1	0	3.997111	2.906681	0.822918
40	6	0	-4.476869	-0.451465	2.142559
41	1	0	-5.169698	0.386401	2.147613
42	6	0	-4.047456	-2.811242	2.153869
43	1	0	-4.400671	-3.839834	2.187547
44	6	0	1.957764	0.810400	3.870402
45	1	0	2.634688	1.663411	3.984587
46	1	0	1.825528	0.361837	4.862680
47	1	0	0.988706	1.188576	3.535325
48	6	0	-4.959308	-1.759574	2.192803
49	1	0	-6.027032	-1.954384	2.249360
50	6	0	3.924023	-0.665467	3.241909

51	1	0	4.250303	-1.483961	2.594874
52	1	0	3.982288	-0.999291	4.285777
53	1	0	4.632461	0.161986	3.116936
54	6	0	1.569926	2.281664	-2.391677
55	1	0	1.691526	1.398260	-3.029583
56	1	0	1.653114	3.175618	-3.022882
57	1	0	0.568343	2.238297	-1.956569
58	6	0	4.037563	2.403475	-1.919682
59	1	0	4.821547	2.366106	-1.154638
60	1	0	4.144106	3.343084	-2.477169
61	1	0	4.208423	1.572367	-2.611094
62	7	0	2.318319	0.044701	1.477078
63	7	0	2.503697	1.102234	-0.475661
64	6	0	-0.727732	-0.962344	1.867772
65	1	0	-0.404120	-0.182787	2.564493
66	6	0	-1.650206	1.369051	-0.617529
67	6	0	-2.805159	1.016066	-1.377802
68	6	0	-3.878037	1.895499	-1.470323
69	6	0	-3.860156	3.142564	-0.851153
70	6	0	-2.721737	3.517822	-0.147315
71	6	0	-1.620536	2.671081	-0.030544
72	1	0	-4.759790	1.594778	-2.035649
73	1	0	-4.713122	3.812636	-0.926094
74	1	0	-2.690980	4.496885	0.330200
75	7	0	-0.609450	0.495550	-0.441691
76	1	0	-0.126094	-1.858626	2.054243
77	1	0	-0.767698	-0.201842	0.628078
78	6	0	-2.864319	-0.330367	-2.072625
79	6	0	-3.058409	-0.181500	-3.586745
80	6	0	-3.934214	-1.247663	-1.469896
81	1	0	-1.890558	-0.795646	-1.900966
82	1	0	-2.279642	0.455934	-4.019964
83	1	0	-3.013423	-1.160680	-4.082048
84	1	0	-4.031450	0.266841	-3.826942
85	1	0	-3.752437	-1.412349	-0.404718
86	1	0	-4.937079	-0.812965	-1.575885
87	1	0	-3.935773	-2.224547	-1.972076
88	6	0	-0.396895	3.124503	0.746754
89	6	0	-0.659860	3.129349	2.257503
90	6	0	0.123029	4.491625	0.285146
91	1	0	0.380023	2.380860	0.548207
92	1	0	-0.962117	2.134036	2.599125
93	1	0	0.238508	3.424031	2.817699
94	1	0	-1.463793	3.831569	2.515085

95	1	0	0.307247	4.494629	-0.794582
96	1	0	-0.590038	5.296365	0.506031
97	1	0	1.064645	4.739709	0.793675
98	1	0	2.587351	2.980421	1.892115

TS1'

298 K, 1 atm, gas phase

Thermal correction to Enthalpy = 0.916898

Thermal correction to Gibbs Free Energy = 0.793151

Sum of electronic and thermal Enthalpies = -1653.753156

Sum of electronic and thermal Free Energies = -1653.876903

298 K, in THF

Sum of electronic and thermal Free Energies = -1654.80486

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	21	0	-1.346893	-0.091884	-0.505887
2	6	0	-3.041669	-1.415958	-0.058754
3	6	0	-2.547662	-1.735813	-1.467877
4	6	0	-3.556711	0.028100	-0.075921
5	6	0	-3.202183	0.664931	-1.431161
6	6	0	1.766892	1.986839	-1.508144
7	6	0	-0.339556	0.922489	1.844952
8	6	0	-2.602735	-0.438388	-2.295397
9	6	0	2.933832	1.851125	-2.267803
10	1	0	3.010010	1.086316	-3.012814
11	6	0	-1.638487	2.688611	0.782192
12	1	0	-2.530999	2.291289	1.219904
13	6	0	-4.754361	0.496636	0.771241
14	1	0	-4.662290	0.109829	1.764531
15	1	0	-5.663382	0.138460	0.332886
16	1	0	-4.772210	1.565541	0.804570
17	6	0	-1.078904	-1.312574	2.325143
18	1	0	-0.560387	-1.346358	3.259773
19	6	0	1.687968	2.985195	-0.589595
20	1	0	0.793229	3.115220	-0.020430
21	6	0	-3.953034	1.890423	-1.987427
22	1	0	-4.060791	2.622769	-1.216353
23	1	0	-4.920802	1.588984	-2.332072

24	1	0	-3.398809	2.307672	-2.802341
25	6	0	-2.606353	-0.403574	-3.836412
26	1	0	-2.363298	0.582210	-4.171319
27	1	0	-3.577351	-0.674333	-4.196594
28	1	0	-1.881991	-1.097204	-4.210818
29	6	0	-2.652347	-3.124853	-2.123692
30	1	0	-2.030112	-3.156458	-2.993045
31	1	0	-3.667479	-3.311843	-2.403862
32	1	0	-2.331140	-3.871785	-1.427321
33	6	0	-3.526362	-2.480448	0.944333
34	1	0	-3.566475	-2.055073	1.923862
35	1	0	-2.846576	-3.308250	0.941782
36	1	0	-4.500693	-2.820685	0.661289
37	6	0	-0.149582	1.423913	3.089297
38	1	0	-0.198518	2.481580	3.252382
39	1	0	0.050283	0.766020	3.908127
40	6	0	2.748155	3.818623	-0.380248
41	1	0	2.678350	4.588396	0.360232
42	6	0	4.004323	2.722805	-2.042826
43	1	0	4.905810	2.628259	-2.614899
44	6	0	-1.964376	3.272330	-0.607993
45	1	0	-1.253478	4.038698	-0.380713
46	1	0	-2.743557	4.001440	-0.693066
47	1	0	-1.311656	3.107651	-1.439646
48	6	0	3.896118	3.685969	-1.096222
49	1	0	4.721296	4.343007	-0.911412
50	6	0	-1.079605	3.803992	1.684041
51	1	0	-0.855944	3.403467	2.650006
52	1	0	-1.808049	4.582441	1.779917
53	1	0	-0.187675	4.202328	1.247400
54	6	0	-1.170755	-2.730637	1.737404
55	1	0	-1.689839	-2.697023	0.802249
56	1	0	-1.700879	-3.363800	2.417296
57	1	0	-0.184948	-3.117011	1.584086
58	6	0	-2.500693	-0.755234	2.544712
59	1	0	-2.438689	0.231824	2.952996
60	1	0	-3.031433	-1.389492	3.223536
61	1	0	-3.019764	-0.721733	1.608879
62	7	0	-0.641537	1.607632	0.639308
63	7	0	-0.352108	-0.438249	1.393574
64	6	0	0.596304	0.987044	-1.714340
65	1	0	0.649835	-1.718048	-1.166085
66	1	0	-0.207723	1.623682	-1.410500
67	6	0	2.163288	-1.274197	0.238264

68	6	0	3.190110	-1.693692	-0.613890
69	6	0	4.483425	-1.856079	-0.118357
70	6	0	4.739354	-1.578529	1.228186
71	6	0	3.702405	-1.129501	2.063135
72	6	0	2.441406	-0.970634	1.576879
73	1	0	5.270482	-2.188984	-0.762555
74	1	0	5.724744	-1.707874	1.621513
75	1	0	3.905658	-0.909143	3.089551
76	7	0	0.822635	-1.181957	-0.339195
77	1	0	0.350468	1.052317	-2.751851
78	1	0	1.024921	0.011838	-1.033002
79	6	0	2.870114	-1.977409	-2.097625
80	6	0	1.399836	-2.421250	-2.226787
81	6	0	3.789348	-3.095210	-2.625863
82	1	0	3.024906	-1.088024	-2.671328
83	1	0	0.760374	-1.643978	-1.862971
84	1	0	1.174568	-2.616153	-3.254717
85	1	0	1.242975	-3.310145	-1.652709
86	1	0	4.810327	-2.788628	-2.538917
87	1	0	3.633902	-3.985684	-2.053429
88	1	0	3.561182	-3.288016	-3.653917
89	6	0	1.329749	-0.453052	2.503743
90	6	0	1.950370	0.476833	3.562601
91	6	0	0.641819	-1.641383	3.198481
92	1	0	0.607527	0.089475	1.930120
93	1	0	2.428054	1.301806	3.075659
94	1	0	1.182816	0.842015	4.211887
95	1	0	2.673185	-0.066487	4.134640
96	1	0	0.211875	-2.285495	2.460260
97	1	0	1.363164	-2.185812	3.770724
98	1	0	-0.127843	-1.278081	3.846819

IM1'

298 K, 1 atm, gas phase

Thermal correction to Enthalpy = 0.781838

Thermal correction to Gibbs Free Energy = 0.670774

Sum of electronic and thermal Enthalpies = -1382.451978

Sum of electronic and thermal Free Energies = -1382.563043

298 K, in THF

Sum of electronic and thermal Free Energies = -1383.287072

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	21	0	0.707072	-0.067805	0.149036
2	6	0	0.475297	-1.304047	1.955012
3	6	0	-0.663681	-0.272870	1.873775
4	6	0	1.806845	-0.525174	2.069018
5	6	0	1.510303	0.976301	1.899737
6	6	0	2.260874	-0.339802	-2.080510
7	6	0	-0.005926	1.151953	1.882744
8	6	0	2.749562	1.863385	-1.145104
9	1	0	3.445307	1.430113	-0.454962
10	6	0	3.036726	-1.032165	2.853365
11	1	0	3.208490	-2.062713	2.620617
12	1	0	2.856897	-0.928599	3.903029
13	1	0	3.898089	-0.457643	2.580970
14	6	0	2.023715	-2.571416	-1.070706
15	1	0	2.417198	-3.073130	-1.928659
16	6	0	2.489227	2.084057	2.307614
17	1	0	3.474266	1.824520	1.980617
18	1	0	2.482262	2.193512	3.370286
19	1	0	2.192608	3.005125	1.850694
20	6	0	-0.693842	2.396898	2.464361
21	1	0	-0.176406	3.274979	2.140969
22	1	0	-0.679307	2.346139	3.532269
23	1	0	-1.707868	2.434119	2.122490
24	6	0	-2.103984	-0.511065	2.366023
25	1	0	-2.747525	0.249214	1.973226
26	1	0	-2.125393	-0.476160	3.436127
27	1	0	-2.439062	-1.469609	2.033344
28	6	0	0.310010	-2.756214	2.450253
29	1	0	1.158775	-3.334295	2.145447
30	1	0	-0.578154	-3.179487	2.033470
31	1	0	0.241355	-2.763219	3.519232
32	6	0	3.312434	-0.509359	-2.918656
33	1	0	3.870382	0.340809	-3.253556
34	1	0	3.586960	-1.490769	-3.244329
35	6	0	2.057994	3.073508	-0.490341
36	1	0	1.370108	3.508508	-1.186049
37	1	0	2.794133	3.798296	-0.215388
38	1	0	1.527207	2.754448	0.382305
39	6	0	3.497989	2.328746	-2.408386
40	1	0	3.972304	1.489865	-2.872750
41	1	0	4.238256	3.052982	-2.138616

42	1	0	2.801741	2.768676	-3.092367
43	6	0	0.962045	-3.466324	-0.395980
44	1	0	0.562901	-2.965136	0.461652
45	1	0	1.413353	-4.387679	-0.091422
46	1	0	0.172590	-3.668096	-1.089833
47	6	0	3.159502	-2.286850	-0.076275
48	1	0	3.896800	-1.670220	-0.544030
49	1	0	3.605652	-3.210956	0.226653
50	1	0	2.764933	-1.783375	0.781874
51	7	0	1.734077	0.864074	-1.515010
52	7	0	1.398094	-1.308334	-1.483312
53	6	0	-2.023483	0.156781	-0.945317
54	6	0	-2.581375	1.370439	-0.523436
55	6	0	-3.879764	1.396035	-0.002368
56	6	0	-4.617083	0.208745	0.096665
57	6	0	-4.056905	-1.004468	-0.328302
58	6	0	-2.760041	-1.028544	-0.852933
59	1	0	-4.308619	2.321229	0.320581
60	1	0	-5.608288	0.226229	0.497950
61	1	0	-4.620397	-1.911284	-0.252409
62	7	0	-0.661482	0.117353	-1.481330
63	1	0	-0.468148	0.959785	-1.983870
64	6	0	-1.769985	2.677249	-0.623115
65	6	0	-2.193238	3.626151	0.513180
66	6	0	-2.040498	3.350416	-1.979843
67	1	0	-0.725796	2.458740	-0.535804
68	1	0	-2.004634	3.157846	1.456579
69	1	0	-1.632559	4.535290	0.448072
70	1	0	-3.236998	3.843900	0.425028
71	1	0	-1.746468	2.692091	-2.769951
72	1	0	-3.084196	3.568716	-2.066649
73	1	0	-1.479219	4.259151	-2.045089
74	6	0	-2.138321	-2.355006	-1.330425
75	6	0	-3.251910	-3.293505	-1.832334
76	6	0	-1.389141	-3.024071	-0.161564
77	1	0	-1.451697	-2.158722	-2.127675
78	1	0	-3.771234	-2.829212	-2.644832
79	1	0	-2.819061	-4.213653	-2.165293
80	1	0	-3.938812	-3.489835	-1.035953
81	1	0	-0.615034	-2.371844	0.186009
82	1	0	-2.074519	-3.220707	0.636060
83	1	0	-0.956568	-3.944385	-0.495187

TS2'
298 K, 1 atm, gas phase
Thermal correction to Enthalpy = 0.776889
Thermal correction to Gibbs Free Energy = 0.665689
Sum of electronic and thermal Enthalpies = -1382.409341
Sum of electronic and thermal Free Energies = -1382.520541
298 K, in THF
Sum of electronic and thermal Free Energies = -1383.35521

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	21	0	-0.849787	-0.120617	0.102913
2	6	0	-1.431608	1.118058	2.270029
3	6	0	-0.079733	0.703868	2.425296
4	6	0	-2.237709	-0.049020	2.194378
5	6	0	-1.390404	-1.178832	2.316882
6	6	0	-2.605008	-0.797856	-1.595985
7	6	0	-0.056558	-0.715764	2.443171
8	6	0	-1.431789	-2.955929	-1.566686
9	1	0	-2.387330	-3.507745	-1.635020
10	6	0	-3.731128	-0.132373	2.054034
11	1	0	-4.192441	0.859088	2.079878
12	1	0	-4.168056	-0.720988	2.872959
13	1	0	-4.023099	-0.604860	1.108400
14	6	0	-3.186233	1.576295	-1.652354
15	1	0	-3.369294	1.407977	-2.727875
16	6	0	-1.889999	-2.590575	2.412995
17	1	0	-2.530027	-2.847599	1.561429
18	1	0	-2.480063	-2.730731	3.330115
19	1	0	-1.064024	-3.308171	2.445741
20	6	0	1.177507	-1.542571	2.660662
21	1	0	1.093344	-2.533319	2.199093
22	1	0	1.377706	-1.695388	3.731266
23	1	0	2.055974	-1.051342	2.227972
24	6	0	1.123278	1.565848	2.696754
25	1	0	1.922849	1.418761	1.961356
26	1	0	1.542117	1.338190	3.686689
27	1	0	0.866680	2.629510	2.692047
28	6	0	-1.955200	2.526518	2.326369
29	1	0	-2.833639	2.654478	1.685181

30	1	0	-1.210554	3.260929	2.002804
31	1	0	-2.254108	2.796505	3.349252
32	6	0	-3.593695	-1.192693	-2.452129
33	1	0	-3.684435	-2.225160	-2.768177
34	1	0	-4.317472	-0.492559	-2.850786
35	6	0	-0.505821	-3.767956	-0.660532
36	1	0	0.448247	-3.242999	-0.524001
37	1	0	-0.288448	-4.748649	-1.102414
38	1	0	-0.949696	-3.922437	0.325013
39	6	0	-0.828460	-2.886743	-2.981198
40	1	0	-1.441679	-2.248107	-3.622271
41	1	0	-0.755985	-3.884766	-3.435077
42	1	0	0.180135	-2.456155	-2.934273
43	6	0	-2.423393	2.894621	-1.527522
44	1	0	-2.186652	3.100083	-0.476786
45	1	0	-3.012697	3.736741	-1.913708
46	1	0	-1.479985	2.841149	-2.081137
47	6	0	-4.556311	1.684308	-0.962377
48	1	0	-5.060798	0.713597	-0.968958
49	1	0	-5.200535	2.420254	-1.463633
50	1	0	-4.428780	1.995130	0.081428
51	7	0	-1.645117	-1.644175	-1.010494
52	7	0	-2.376738	0.503990	-1.139899
53	6	0	2.335039	0.380019	-0.576691
54	6	0	3.413647	-0.486326	-0.224468
55	6	0	4.655544	0.052633	0.098460
56	6	0	4.884059	1.425503	0.073208
57	6	0	3.857392	2.265905	-0.340198
58	6	0	2.603595	1.771108	-0.694830
59	1	0	5.466025	-0.610883	0.390573
60	1	0	5.855181	1.829054	0.347758
61	1	0	4.043368	3.336169	-0.408916
62	7	0	1.053850	-0.083686	-0.799137
63	1	0	0.042310	-1.139920	-1.302908
64	6	0	3.180360	-1.986505	-0.233448
65	6	0	4.105832	-2.783971	0.688218
66	6	0	3.255027	-2.543280	-1.665550
67	1	0	2.159024	-2.146955	0.131185
68	1	0	4.094670	-2.382848	1.707413
69	1	0	3.780510	-3.830297	0.729175
70	1	0	5.143221	-2.778791	0.330937
71	1	0	2.597438	-1.993415	-2.347300
72	1	0	4.277993	-2.453847	-2.051991
73	1	0	2.963831	-3.600795	-1.694677

74	6	0	1.540812	2.698742	-1.259973
75	6	0	2.103484	3.685259	-2.291257
76	6	0	0.786073	3.450378	-0.159800
77	1	0	0.818496	2.053637	-1.772949
78	1	0	2.686339	3.164033	-3.058211
79	1	0	1.283075	4.219991	-2.785803
80	1	0	2.752630	4.440108	-1.829164
81	1	0	0.233409	2.748258	0.470232
82	1	0	1.480431	4.004423	0.485181
83	1	0	0.064756	4.158695	-0.584245

IM2'

298 K, 1 atm, gas phase

Thermal correction to Enthalpy = 0.782799

Thermal correction to Gibbs Free Energy = 0.670976

Sum of electronic and thermal Enthalpies = -1382.425420

Sum of electronic and thermal Free Energies = -1382.537243

298 K, in THF

Sum of electronic and thermal Free Energies = -1383.369012

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	21	0	-0.741093	-0.451088	0.404358
2	6	0	-0.742000	-2.584609	1.090966
3	6	0	-0.537840	-2.499666	-0.370814
4	6	0	-2.030578	-1.928333	1.388698
5	6	0	-2.680069	-1.541028	0.120571
6	6	0	-0.469331	2.770955	0.858526
7	6	0	-1.730049	-1.863788	-0.964508
8	6	0	-2.276374	2.985646	-0.787848
9	1	0	-2.950093	2.742767	0.008433
10	6	0	-2.848804	-2.245471	2.660078
11	1	0	-2.197720	-2.260342	3.506911
12	1	0	-3.320034	-3.198845	2.551039
13	1	0	-3.598947	-1.490483	2.798944
14	6	0	0.084735	1.444077	2.946428
15	1	0	0.697770	2.296709	3.161368
16	6	0	-4.210149	-1.458490	-0.061940
17	1	0	-4.642126	-0.969258	0.787810

18	1	0	-4.613331	-2.445451	-0.148212
19	1	0	-4.439921	-0.900958	-0.944594
20	6	0	-2.196886	-2.137082	-2.406382
21	1	0	-2.897868	-1.386145	-2.704403
22	1	0	-2.662522	-3.098044	-2.446830
23	1	0	-1.356737	-2.117765	-3.067416
24	6	0	0.356826	-3.482574	-1.151745
25	1	0	0.543056	-3.091493	-2.130074
26	1	0	-0.140844	-4.425158	-1.231676
27	1	0	1.288829	-3.613540	-0.640454
28	6	0	-0.103323	-3.662717	1.980131
29	1	0	-0.178906	-3.369194	3.008959
30	1	0	0.926468	-3.776794	1.718263
31	1	0	-0.614747	-4.590377	1.838001
32	6	0	-0.221961	3.987872	1.390959
33	1	0	-0.361408	4.863686	0.798698
34	1	0	0.116507	4.066182	2.402334
35	6	0	-2.776774	2.334372	-2.091205
36	1	0	-2.105592	2.572946	-2.888541
37	1	0	-3.753639	2.706036	-2.323627
38	1	0	-2.819352	1.273469	-1.963759
39	6	0	-2.218761	4.510811	-0.969376
40	1	0	-1.870936	4.968327	-0.066236
41	1	0	-3.196692	4.879546	-1.201648
42	1	0	-1.548192	4.748050	-1.769952
43	6	0	0.887559	0.156189	3.203408
44	1	0	0.272574	-0.691940	2.986612
45	1	0	1.195700	0.124013	4.226529
46	1	0	1.751999	0.141642	2.570709
47	6	0	-1.156926	1.461418	3.851189
48	1	0	-1.717535	2.353628	3.667931
49	1	0	-0.852096	1.435906	4.877486
50	1	0	-1.760741	0.607028	3.635799
51	7	0	-0.936738	2.480093	-0.456857
52	7	0	-0.331218	1.484679	1.534622
53	6	0	1.900862	0.100640	-0.661663
54	6	0	1.555567	-0.072435	-2.008434
55	6	0	2.576184	-0.232041	-2.965622
56	6	0	3.927144	-0.201459	-2.570839
57	6	0	4.260349	-0.025210	-1.220255
58	6	0	3.237569	0.121887	-0.272287
59	1	0	2.328138	-0.371830	-4.000557
60	1	0	4.702233	-0.318199	-3.302560
61	1	0	5.287737	-0.003353	-0.918004

62	7	0	1.007813	0.250213	0.325441
63	1	0	-0.357630	2.752484	-1.231710
64	6	0	0.079263	-0.079157	-2.439885
65	6	0	-0.084744	-0.965614	-3.688915
66	6	0	-0.352330	1.362070	-2.770086
67	1	0	-0.527789	-0.461238	-1.644538
68	1	0	0.222708	-1.964224	-3.459613
69	1	0	-1.110359	-0.968245	-3.994387
70	1	0	0.522913	-0.578356	-4.481407
71	1	0	-0.231166	1.975454	-1.901900
72	1	0	0.257736	1.740950	-3.564086
73	1	0	-1.379002	1.371911	-3.074291
74	6	0	3.540885	0.290226	1.233325
75	6	0	4.910787	0.961362	1.429585
76	6	0	3.546849	-1.099309	1.905599
77	1	0	2.783107	0.898576	1.680818
78	1	0	4.907651	1.923027	0.962387
79	1	0	5.104483	1.074327	2.477438
80	1	0	5.672223	0.352384	0.990799
81	1	0	2.592042	-1.563473	1.768089
82	1	0	4.307792	-1.707169	1.462744
83	1	0	3.742118	-0.990477	2.952472

TS3'

298 K, 1 atm, gas phase

Thermal correction to Enthalpy = 0.775967

Thermal correction to Gibbs Free Energy = 0.661536

Sum of electronic and thermal Enthalpies = -1382.353927

Sum of electronic and thermal Free Energies = -1382.468359

298 K, in THF

Sum of electronic and thermal Free Energies = -1383.300771

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	21	0	-0.663744	-0.052520	0.073839
2	6	0	-1.143680	-0.380854	2.525989
3	6	0	-0.418287	-1.533878	2.125054
4	6	0	-2.422529	-0.427539	1.907746
5	6	0	-2.480101	-1.594062	1.108112
6	6	0	-1.500197	1.331042	-2.114507
7	6	0	-1.237855	-2.281264	1.242513

8	6	0	-2.303592	-1.011947	-1.662808
9	1	0	-2.361216	-0.790386	-0.592211
10	6	0	-3.565695	0.525205	2.115768
11	1	0	-3.307566	1.296582	2.849067
12	1	0	-4.454576	0.002188	2.495459
13	1	0	-3.850168	1.032901	1.185262
14	6	0	-1.840718	3.060696	-0.513971
15	1	0	-1.116066	3.632704	-1.122278
16	6	0	-3.724813	-2.083534	0.422781
17	1	0	-4.315633	-1.249623	0.025224
18	1	0	-4.374604	-2.631829	1.121092
19	1	0	-3.507441	-2.759594	-0.410910
20	6	0	-0.899312	-3.639253	0.684462
21	1	0	-1.745034	-4.064141	0.132987
22	1	0	-0.656367	-4.343747	1.490778
23	1	0	-0.037168	-3.624165	0.005816
24	6	0	0.967446	-1.901787	2.578949
25	1	0	1.260049	-2.880692	2.183934
26	1	0	1.027169	-1.957972	3.674351
27	1	0	1.713367	-1.179120	2.228490
28	6	0	-0.670612	0.631583	3.533406
29	1	0	-0.901032	1.660969	3.237740
30	1	0	0.414139	0.570356	3.664868
31	1	0	-1.132114	0.462802	4.517154
32	6	0	-1.405002	2.099507	-3.232017
33	1	0	-0.483343	2.621819	-3.462620
34	1	0	-2.248879	2.261370	-3.892049
35	6	0	-1.820497	-2.446329	-1.857701
36	1	0	-1.780906	-2.694351	-2.926371
37	1	0	-2.496744	-3.157243	-1.370057
38	1	0	-0.815918	-2.579783	-1.448831
39	6	0	-3.693850	-0.820471	-2.272193
40	1	0	-4.041260	0.206386	-2.139871
41	1	0	-4.406276	-1.505767	-1.797311
42	1	0	-3.677404	-1.038878	-3.348193
43	6	0	-1.488632	3.310561	0.950389
44	1	0	-2.198975	2.798704	1.608067
45	1	0	-1.514366	4.381670	1.186901
46	1	0	-0.482585	2.935366	1.167812
47	6	0	-3.247704	3.585904	-0.835072
48	1	0	-3.514538	3.359593	-1.872386
49	1	0	-3.313410	4.672042	-0.687114
50	1	0	-3.982909	3.102952	-0.179569
51	7	0	-1.263526	-0.115345	-2.205459

52	7	0	-1.710793	1.652548	-0.815991
53	6	0	2.511876	0.134372	-0.231568
54	6	0	3.252224	-1.062679	-0.518961
55	6	0	4.638575	-1.028029	-0.619572
56	6	0	5.356384	0.152252	-0.440767
57	6	0	4.654268	1.322129	-0.153111
58	6	0	3.268811	1.339764	-0.045059
59	1	0	5.181214	-1.946789	-0.839152
60	1	0	6.440713	0.161196	-0.522285
61	1	0	5.211625	2.247199	-0.012901
62	7	0	1.166705	0.123646	-0.142257
63	1	0	-1.179472	0.586911	-3.393517
64	6	0	2.466547	-2.340007	-0.732823
65	6	0	3.202857	-3.619994	-0.332751
66	6	0	1.956377	-2.433452	-2.177922
67	1	0	1.581975	-2.247079	-0.094173
68	1	0	3.594933	-3.544147	0.687779
69	1	0	2.522195	-4.480669	-0.376613
70	1	0	4.045424	-3.838753	-1.001829
71	1	0	1.412914	-1.518481	-2.432874
72	1	0	2.794551	-2.542748	-2.878540
73	1	0	1.280235	-3.290378	-2.312158
74	6	0	2.508958	2.604151	0.304858
75	6	0	3.193558	3.901282	-0.133448
76	6	0	2.210724	2.636167	1.811173
77	1	0	1.544816	2.534009	-0.215544
78	1	0	3.460846	3.869210	-1.195678
79	1	0	2.522947	4.755197	0.026416
80	1	0	4.109789	4.097213	0.439395
81	1	0	1.664331	1.732472	2.098112
82	1	0	3.145999	2.673020	2.385455
83	1	0	1.605485	3.511252	2.086496

4b'

298 K, 1 atm, gas phase

Thermal correction to Enthalpy = 0.782128

Thermal correction to Gibbs Free Energy = 0.669327

Sum of electronic and thermal Enthalpies = -1382.459996

Sum of electronic and thermal Free Energies = -1382.572796

298 K, in THF

Sum of electronic and thermal Free Energies = -1383.399405

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	21	0	-0.798193	-0.262584	0.146594
2	6	0	-1.819315	-0.383398	2.461089
3	6	0	-0.652257	-1.192486	2.470394
4	6	0	-2.772747	-0.998102	1.602509
5	6	0	-2.191250	-2.175945	1.076269
6	6	0	-1.892847	0.455643	-2.126992
7	6	0	-0.879704	-2.297450	1.609761
8	6	0	-0.595888	-1.403492	-3.027860
9	1	0	-1.235927	-1.532422	-3.919229
10	6	0	-4.169545	-0.542229	1.298732
11	1	0	-4.348874	0.478359	1.653403
12	1	0	-4.919601	-1.191872	1.773469
13	1	0	-4.360882	-0.545672	0.219258
14	6	0	-2.804727	2.406944	-1.006217
15	1	0	-2.445697	3.007642	-1.859441
16	6	0	-2.878637	-3.133576	0.144696
17	1	0	-3.189816	-2.640159	-0.784811
18	1	0	-3.774282	-3.572336	0.607300
19	1	0	-2.213969	-3.959765	-0.129999
20	6	0	0.066648	-3.445712	1.398071
21	1	0	0.129911	-3.749582	0.346420
22	1	0	-0.241552	-4.330613	1.973826
23	1	0	1.077398	-3.179220	1.718184
24	6	0	0.605223	-0.931199	3.252219
25	1	0	0.817263	-1.742605	3.962280
26	1	0	0.520164	-0.003683	3.828857
27	1	0	1.468889	-0.817304	2.587259
28	6	0	-2.014228	0.861200	3.286093
29	1	0	-3.000316	1.304319	3.111257
30	1	0	-1.267065	1.633970	3.067328
31	1	0	-1.946086	0.640767	4.360074
32	6	0	-2.131897	1.079136	-3.491344
33	1	0	-1.411431	1.887015	-3.661581
34	1	0	-2.020161	0.348228	-4.293927
35	6	0	-0.216277	-2.799702	-2.535429
36	1	0	0.461619	-2.714994	-1.678096
37	1	0	0.296642	-3.369611	-3.319581
38	1	0	-1.106726	-3.351522	-2.217925

39	6	0	0.666632	-0.627589	-3.430963
40	1	0	0.417924	0.323100	-3.915151
41	1	0	1.284039	-1.209548	-4.127424
42	1	0	1.246716	-0.398685	-2.529717
43	6	0	-2.394446	3.143904	0.267929
44	1	0	-2.725962	2.581079	1.147922
45	1	0	-2.838444	4.146411	0.309207
46	1	0	-1.306211	3.239404	0.319837
47	6	0	-4.336585	2.329364	-1.100590
48	1	0	-4.656152	1.762805	-1.982283
49	1	0	-4.778878	3.332550	-1.157659
50	1	0	-4.739261	1.821700	-0.218471
51	7	0	-1.323086	-0.735502	-1.964147
52	7	0	-2.193410	1.095694	-0.999171
53	6	0	2.293188	0.600022	0.045431
54	6	0	3.358931	-0.349040	-0.122638
55	6	0	4.683081	0.075386	-0.174099
56	6	0	5.036104	1.416252	-0.058778
57	6	0	4.017958	2.353019	0.122227
58	6	0	2.681472	1.981550	0.178557
59	1	0	5.469181	-0.669959	-0.305020
60	1	0	6.077312	1.726462	-0.103543
61	1	0	4.284285	3.404586	0.219910
62	7	0	0.996160	0.238851	0.068458
63	6	0	3.038066	-1.828634	-0.220253
64	6	0	3.637466	-2.619004	0.950756
65	6	0	3.475223	-2.443735	-1.555973
66	1	0	1.947269	-1.901637	-0.152753
67	1	0	3.299124	-2.210232	1.909287
68	1	0	3.346442	-3.677515	0.905370
69	1	0	4.734437	-2.572298	0.939555
70	1	0	3.037456	-1.899266	-2.398048
71	1	0	4.567214	-2.413277	-1.669022
72	1	0	3.160209	-3.494097	-1.626970
73	6	0	1.578639	2.992718	0.414127
74	6	0	1.911531	4.424133	-0.012197
75	6	0	1.137796	2.959282	1.885746
76	1	0	0.726570	2.645592	-0.185924
77	1	0	2.270627	4.458222	-1.047261
78	1	0	1.018855	5.058809	0.063621
79	1	0	2.683372	4.873639	0.626456
80	1	0	0.877782	1.934134	2.167428
81	1	0	1.954046	3.301232	2.535719
82	1	0	0.265410	3.604337	2.064173

83	1	0	-3.134119	1.510902	-3.555673

$ArNH_2$ (Ar = 2,6-$C_6H_3{}^iPr_2$)
298 K, 1 atm, gas phase
Thermal correction to Enthalpy = 0.306030
Thermal correction to Gibbs Free Energy = 0.251866
Sum of electronic and thermal Enthalpies = -523.020398
Sum of electronic and thermal Free Energies = -523.074562
298 K, in THF
Sum of electronic and thermal Free Energies = -523.2655464

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.224977	0.248575	0.094386
2	6	0	0.000002	-0.431783	0.261602
3	6	0	1.224991	0.248595	0.094434
4	6	0	1.197643	1.589227	-0.283380
5	6	0	-0.000005	2.263308	-0.481083
6	6	0	-1.197643	1.589217	-0.283408
7	1	0	2.133043	2.122824	-0.420558
8	1	0	-0.000003	3.308422	-0.774745
9	1	0	-2.133057	2.122789	-0.420584
10	7	0	-0.000036	-1.775459	0.671160
11	1	0	-0.826507	-2.295470	0.418060
12	1	0	0.826711	-2.295310	0.418636
13	6	0	2.542147	-0.488995	0.292914
14	6	0	3.704557	0.417530	0.709344
15	6	0	2.921629	-1.278483	-0.972825
16	1	0	2.402338	-1.201305	1.117513
17	1	0	3.437507	1.037419	1.570847
18	1	0	4.573706	-0.191342	0.980261
19	1	0	4.015705	1.080276	-0.105939
20	1	0	2.121502	-1.953964	-1.296655
21	1	0	3.112446	-0.586073	-1.800309
22	1	0	3.826599	-1.874879	-0.809597
23	6	0	-2.542111	-0.489054	0.292837
24	6	0	-2.921802	-1.278156	-0.973072
25	6	0	-3.704422	0.417388	0.709693
26	1	0	-2.402113	-1.201608	1.117200
27	1	0	-2.121739	-1.953534	-1.297289

28	1	0	-3.826733	-1.874615	-0.809867
29	1	0	-3.112778	-0.585495	-1.800307
30	1	0	-3.437224	1.036953	1.571385
31	1	0	-4.015637	1.080443	-0.105314
32	1	0	-4.573575	-0.191536	0.980482

Methylbenzene

298 K, 1 atm, gas phase

Thermal correction to Enthalpy = 0.136779

Thermal correction to Gibbs Free Energy = 0.099372

Sum of electronic and thermal Enthalpies = -271.334576

Sum of electronic and thermal Free Energies = -271.371983

298 K, in THF

Sum of electronic and thermal Free Energies = -271.4689561

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.910275	0.000000	-0.011502
2	6	0	0.194141	-1.199214	-0.008802
3	1	0	0.734613	-2.143044	-0.017030
4	6	0	0.194141	1.199214	-0.008802
5	1	0	0.734613	2.143044	-0.017030
6	6	0	-1.197502	1.202223	0.002062
7	1	0	-1.734969	2.146322	0.002035
8	6	0	-1.197502	-1.202223	0.002062
9	1	0	-1.734969	-2.146322	0.002035
10	6	0	-1.899078	-0.000000	0.008118
11	1	0	-2.985098	-0.000000	0.013751
12	6	0	2.418720	0.000000	0.009348
13	1	0	2.825289	0.885696	-0.488936
14	1	0	2.825289	-0.885695	-0.488938
15	1	0	2.796060	-0.000001	1.039212

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