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Supporting Information

A scandium terminal imido complex: synthesis, structure and DFT studies

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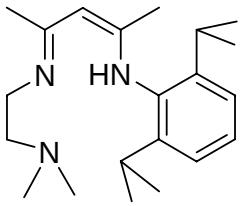
Contents

General Procedures. All operations were carried out under an atmosphere of argon using Schlenk techniques or in a nitrogen filled glovebox. THF was distilled from Na-benzophenoneketyl and degassed by freeze-thaw-vacuum prior to use. Toluene, hexane, and C_6D_6 were dried over Na/K alloy, distilled under vacuum, and stored in the glovebox. 2,6-Diisopropylaniline was purchased from Aldrich, dried over 4Å molecular sieves, distilled under vacuum and degassed by freeze-thaw-vacuum prior to use. *n*-BuLi (2.5 M solution in hexane) and MeLi (1.6 M solution in diethyl ether) were purchased from Acros and directly used. The ligand precursor, $CH_3C(2,6\text{-}(^iPr)_2C_6H_3NH)CHC(CH_3)(NCH_2CH_2NMe_2)$(**LH**), was synthesized as we previously reported.[1] ^1H and ^{13}C NMR spectra were recorded on a Varian 400 MHz spectrometer at 400 MHz and 100 MHz respectively. All chemical shifts were reported in δ units with references to the residual solvent resonance of the deuterated solvents for proton and carbon chemical shifts. Elemental analysis was performed by the Analytical Laboratory of Shanghai Institute of Organic Chemistry.



LH

Synthesis of the lithium salt of ligand. A solution of **LH** (2.00 g, 6.11 mmol) in 10 mL of THF was added by 2.5 M *n*-BuLi solution (2.70 mL, 6.75 mmol) at -78 ^oC, and then the reaction mixture was gradually warmed to room temperature. After stirring at room temperature for 4 hours, the volatiles were removed under vacuum to give a yellow solid. The solid was washed by 3 mL of cold hexane and dried under vacuum to give the lithium salt of ligand as a yellow solid (1.95 g, 5.81 mmol, 95 % yield). ^1H NMR (400 MHz, C_6D_6, 25 ^oC): δ (ppm) 7.23-7.21 (m, 2H, Ar*H*), 7.14-7.12 (m, 1H, Ar*H*), 4.94 (s, 1H, MeC(N)C*H*), 3.41 (sp, $^3J_{HH}$ = 6.8 Hz, 2H, ArC*H*Me$_2$), 3.15 (t, $^3J_{HH}$ = 6.0 Hz, 2H, NCH_2), 2.03 (t, $^3J_{HH}$ = 6.0 Hz, 2H, NCH_2), 1.94 (s, 3H, *Me*C(N)CH),

1.88 (s, 3H, *Me*C(N)CH), 1.62 (s, 6H, N*Me*$_2$), 1.29 (d, $^3J_{HH}$ = 6.8 Hz, 6H, ArCH*Me*$_2$), 1.13 (d, $^3J_{HH}$ = 6.8 Hz, 6H, ArCH*Me*$_2$) ^{13}C NMR (100 MHz, C_6D_6, 25 °C): δ (ppm) 165.1, 162.2 (imine *C*), 150.2, 141.1, 123.3, 122.9 (Ar*C*), 93.6 (MeC(N)*C*H), 62.4, 45.7 (N*C*H$_2$), 44.1 (N*Me*$_2$), 28.1, 25.3, 23.5, 22.8, 20.7 (Ar^i*Pr* and *Me*C).

Synthesis of $LScCl_2$ (1). $ScCl_3(THF)_3$ (221 mg, 0.601 mmol) and the lithium salt of ligand (201 mg, 0.599 mmol) were mixed in 5 mL of THF at room temperature. The reaction mixture was stirred for 4 hours at room temperature. The volatiles were removed under vacuum, and the residue was extracted with 5 mL of toluene. Concentration of the extract solution in vacuo to approximately 1 mL and cooling to -35 °C afforded **1** as a pale yellow crystalline solid (217 mg, 0.489 mmol, 81 % yield). **1** is soluable in toluene and benzene, and insoluable in hexane. Anal. Calcd for $C_{21}H_{34}Cl_2N_3Sc$: C, 56.76; H, 7.71; N, 9.46. Found: C, 56.10; H, 7.89; N, 9.30. ^{1}H NMR (400 MHz, C_6D_6, 25 ^{o}C): δ (ppm) 7.19-7.15 (m, 3H, Ar*H*), 5.00 (s, 1H, MeC(N)C*H*), 3.35 (sp, $^3J_{HH}$ = 7.0 Hz, 2H, ArC*H*Me$_2$), 2.83 (t, $^3J_{HH}$ = 6.2 Hz, 2H, NC*H*$_2$), 2.33 (t, $^3J_{HH}$ = 6.2 Hz, 2H, NC*H*$_2$), 2.24 (s, 6H, N*Me*$_2$), 1.61 (s, 3H, *Me*C(N)CH), 1.59 (d, $^3J_{HH}$ = 6.4 Hz, 6H, ArCH*Me*$_2$), 1.54 (s, 3H, *Me*C(N)CH), 1.16 (d, $^3J_{HH}$ = 6.8 Hz, 6H, ArCH*Me*$_2$). ^{13}C NMR (100 MHz, C_6D_6, 25 °C): δ (ppm) 167.6, 166.6 (imine *C*), 145.8, 142.5, 126.6, 124.2 (Ar*C*), 100.2 (MeC(N)*C*H), 57.5, 47.7 (N*C*H$_2$), 46.1 (N*Me*$_2$), 28.6, 25.2, 24.7, 24.3, 23.0 (Ar^i*Pr* and *Me*C).

Synthesis of LSc(Me)(NHAr) (2). A solution of **1** (148 mg, 0.333 mmol) in 5 mL of THF was added by 1.6 M MeLi solution (0.480 mL, 0.766 mmol) at -78 ^{o}C, and then the reaction mixture was gradually warmed to room temperature. After stirring at room temperature for 4 hours, the volatiles were removed under vacuum. The residue was extracted by 5 mL of toluene. The extraction was added by 2,6-diisopropylaniline (59 mg, 0.333 mmol) at room temperature. The reaction mixture was stirring at room temperature for 24 hours. The volatiles were removed under vacuum, and the residue was washed by cold hexane (0.5 mL x 4) and dried under vacuum to give **2** as a pale

yellow solid (90 mg, 47% yield). **2** is soluble in toluene and benzene, and nearly insoluble in hexane. Anal. Calcd for $C_{34}H_{55}N_4Sc$: C, 72.30; H, 9.82; N, 9.92. Found: C, 72.44; H, 10.13; N, 9.93. ^{1}H NMR (400 MHz, C_6D_6, 25 ^{o}C): δ (ppm) 7.18-7.14 (m, 5H, Ar*H*), 6.89 (t, $^3J_{HH}$ = 8.0 Hz, 1H, Ar*H*), 5.70 (s, br, 1H, ArN*H*Sc), 4.99 (s, 1H, MeC(N)C*H*), 3.65 (sp, $^3J_{HH}$ = 6.8 Hz, 1H, ArC*H*Me$_2$), 3.09 (sp, $^3J_{HH}$ = 6.8 Hz, 1H, ArC*H*Me$_2$), 2.99-2.90 (m, 3H, ArC*H*Me$_2$ and NC*H$_2$*), 2.79 (m, 1H, NC*H$_2$*), 2.31 (m, 1H, NC*H$_2$*), 2.20 (m, 1H, NC*H$_2$*), 2.12 (s, 3H, *Me*C(N)CH), 2.04 (s, 3H, *Me*C(N)CH), 1.69 (s, 3H, N*Me$_2$*), 1.68 (s, 3H, N*Me$_2$*), 1.38 (d, $^3J_{HH}$ = 7.2 Hz, 6H, ArCH*Me$_2$*), 1.37 (d, $^3J_{HH}$ = 6.8 Hz, 3H, ArCH*Me$_2$*), 1.26 (d, $^3J_{HH}$ = 6.8 Hz, 6H, ArCH*Me$_2$*), 1.24 (d, $^3J_{HH}$ = 6.8 Hz, 3H, ArCH*Me$_2$*), 1.14 (d, J_{HH} = 6.8 Hz, 3H, ArCH*Me$_2$*), 1.13 (d, J_{HH} = 6.4 Hz, 3H, ArCH*Me$_2$*), -0.50 (s, 3H, Sc*Me*). ^{13}C NMR (100 MHz, C_6D_6, 25 °C): δ (ppm) 166.7, 166.6 (imine *C*), 150.9, 146.0, 143.6, 142.3, 133.4, 125.9. 124.3, 124.0, 122.9, 116.1 (Ar*C*), 99.3 (MeC(N)*C*H), 57.3, 47.5 (N*C*H$_2$), 45.8. 45.4 (N*Me$_2$*), 29.8, 28.5, 28.1, 23.2 (Ar^i*Pr*, *Me*C and Sc*Me*).

Synthesis of LSc(NAr)(DMAP) (3). **2** (129 mg, 0.228 mmol) and 4-(dimethylamino)pyridine (DMAP) (27.8 mg, 0.228 mmol, 1 equiv.) were mixed in 5 mL of toluene. The reaction mixture was stirred for 2 days at 50 ^{o}C, and then the volatiles were removed under vacuum. The residue was washed by cold hexane (1mL x 4) and dried under vacuum to give a red solid. Recrystallization of the red solid in 1 mL of toluene at - 35 ^{o}C afforded **3** as dark red crystals (97.0 mg, 0.128 mmol, 56%). **3** was sparingly soluble in toluene and benzene, and insoluble in hexane. Anal. Calcd for $C_{40}H_{61}N_6Sc$: C, 71.61; H, 9.16; N, 12.53. Found: C, 70.89; H, 8.95; N, 12.28. ^{1}H NMR (400 MHz, C_6D_6, 25 ^{o}C): δ (ppm) 7.88 ppm (d, $^3J_{HH}$ = 8.0 Hz, 1H, ortho *H* of DMAP), 7.24 (d, $^3J_{HH}$ = 7.6 Hz, 2H, ortho *H* of DMAP and Ar*H*), 7.11 (m, 1H, Ar*H*), 7.01 (t, $^3J_{HH}$ = 7.2 Hz, 1H, Ar*H*), 6.93-6.87 (m, 3H, ArH), 5.97 (dd, $^3J_{HH}$ = 7.6 Hz, $^4J_{HH}$ = 2.8 Hz, 1H, *meta H* of DMAP), 5.47 (br, 1H, *meta H* of DMAP), 5.05 (s, 1H, MeC(N)C*H*), 3.82 (sp, $^3J_{HH}$ = 6.8 Hz, 1H, ArC*H*Me$_2$), 3.49-3.36 (m, 3H, ArC*H*Me$_2$ and NC*H$_2$*), 3.30 (sp, $^3J_{HH}$ = 6.8 Hz, 1H, ArC*H*Me$_2$), 3.20 (m, 1H, NC*H$_2$*), 3.05 (m,

1H, NC*H*$_2$), 2.34 (s, 6H, CH$_2$N*Me*$_2$ or CN*Me*$_2$), 1.91 (s, 6H, CH$_2$N*Me*$_2$ or CN*Me*$_2$), 1.82 (s, 3H, *Me*C(N)CH), 1.73 (s, 3H, *Me*C(N)CH), 1.45 (d, $^3J_{HH}$ = 6.8 Hz, 3H, ArCH*Me*$_2$), 1.41 (d, $^3J_{HH}$ = 6.8 Hz, 6H, ArCH*Me*$_2$), 1.39 (d, $^3J_{HH}$ = 6.8 Hz, 6H, ArCH*Me*$_2$), 1.21 (d, $^3J_{HH}$ = 6.8 Hz, 3H, ArCH*Me*$_2$), 1.12 (d, $^3J_{HH}$ = 6.8 Hz, 3H, ArCH*Me*$_2$), 1.01(d, $^3J_{HH}$ = 6.8 Hz, 3H, ArCH*Me*$_2$). ^{13}C NMR (100 MHz, C_6D_6, 25 °C): δ (ppm) 166.2, 165.6 (imine *C*), 152.6, 151.8, 148.2, 143.5, 142.8, 142.2, 133.6, 125.0, 123.8, 123.3, 123.0, 114.7, 109.8, 106.6 (Ar*C* and DMAP's *C*), 98.5 (MeC(N)*C*H), 58.4, 48.2, 38.5 (N*C*H$_2$, N*Me*$_2$ and CN*Me*$_2$), 28.8, 28.2, 28.0, 25.5, 25.3, 25.0, 24.9, 24.8, 24.7, 24.2, 22.9 (Ar^i*Pr* and *Me*C)

X-ray Crystallography. Suitable single crystals of **2** and **3** for X-ray diffraction were grown from the toluene solution, and sealed in thin-walled glass capillaries. Data collection was performed at 20 °C on a Bruker SMART diffractometer with graphite-monochromated Mo Kα radiation (λ = 0.71073 Å). The SMART program package was used to determine the unit-cell parameters. The absorption correction was applied using SADABS. The structures were solved by direct methods and refined on F^2 by full-matrix least squares techniques with anisotropic thermal parameters for non-hydrogen atoms. Hydrogen atoms were placed at calculated positions and were included in the structure calculation excepted for the hydrogen atom of anilide functional group in **2**, which was located in Fourier map. All calculations were carried out using the SHELXS-97 program. The software used is listed in the references.[2]

Crystal data for **2**: C41H63N4Sc, M_r = 656.91 (containing a toluene molecule), T = 293(2) K, Monoclinic, P2(1) / c, a = 16.543(3) Å, b = 15.790(3) Å, c = 15.938(3) Å, β = 100.323(3) °, V = 4095.9(11) Å^3, Z = 4, F(000) = 1432, 21031 reflections collected, 7614 unique reflections, R1 = 0.0729, wR2 = 0.1752 (I > 2σ(I)).

Table **S1** Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **2**.U (eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Sc(1)	2945(1)	8478(1)	8737(1)	43(1)
N(1)	1624(2)	8637(2)	8223(2)	43(1)
N(2)	2547(2)	8712(2)	9942(2)	61(1)
N(3)	4096(2)	8201(2)	9807(3)	62(1)
N(4)	3604(2)	9291(2)	8119(2)	52(1)
C(1)	295(3)	9370(3)	8052(3)	77(2)
C(2)	1124(2)	9129(3)	8561(3)	50(1)
C(3)	1305(3)	9461(3)	9389(3)	60(1)
C(4)	1943(3)	9224(3)	10053(3)	63(1)
C(5)	1898(3)	9573(4)	10929(3)	93(2)
C(6)	3084(3)	8374(4)	10725(3)	89(2)
C(7)	3734(3)	7797(3)	10469(3)	81(2)
C(11)	1288(2)	8179(2)	7454(3)	43(1)
C(12)	890(2)	7408(3)	7537(3)	52(1)
C(13)	578(3)	6967(3)	6800(3)	66(1)
C(14)	666(3)	7258(3)	6011(3)	75(2)
C(15)	1071(3)	8002(3)	5940(3)	65(1)
C(16)	1380(2)	8483(3)	6649(3)	52(1)
C(17)	809(3)	7038(3)	8387(3)	63(1)
C(18)	-68(3)	7074(4)	8535(4)	105(2)
C(19)	1137(4)	6132(3)	8487(4)	94(2)
C(20)	1795(3)	9315(3)	6516(3)	62(1)
C(21)	1191(3)	9952(3)	6022(4)	91(2)
C(22)	2526(3)	9197(4)	6072(3)	85(2)
C(31)	4495(3)	9026(3)	10110(3)	81(2)
C(32)	4747(3)	7661(3)	9589(4)	94(2)
C(33)	3104(3)	7230(3)	8143(3)	69(1)
C(40)	3893(2)	10087(3)	7941(3)	49(1)
C(41)	3517(2)	10813(3)	8190(3)	50(1)
C(42)	3824(3)	11596(3)	8025(3)	70(1)
C(43)	4486(3)	11693(3)	7623(3)	77(2)
C(44)	4840(3)	10984(4)	7362(3)	77(2)
C(45)	4563(3)	10177(3)	7507(3)	62(1)
C(46)	2793(3)	10763(3)	8642(3)	59(1)
C(47)	2046(3)	11243(3)	8175(4)	86(2)
C(48)	3011(3)	11080(3)	9565(3)	80(2)
C(49)	5003(3)	9431(3)	7203(4)	86(2)

C(50)	5053(4)	9460(5)	6263(5)	142(3)
C(51)	5839(4)	9308(5)	7749(5)	145(3)
C(52)	2273(10)	2000(6)	5438(9)	271(9)
C(53)	1652(6)	1883(7)	4607(8)	201(7)
C(54)	1534(11)	1454(10)	3843(11)	299(9)
C(55)	2205(11)	1036(12)	3701(11)	323(9)
C(56)	2800(7)	1141(6)	4538(9)	192(5)
C(57)	2975(8)	1524(8)	5334(9)	209(6)
C(58)	2224(11)	2543(11)	6082(10)	264(9)

Table **S2**. Bond lengths (Å) and angles (^{o}) for **2**.

Sc(1)-N(4)	2.047(3)
Sc(1)-N(2)	2.171(4)
Sc(1)-N(1)	2.206(3)
Sc(1)-C(33)	2.221(4)
Sc(1)-N(3)	2.359(4)
N(1)-C(2)	1.318(5)
N(1)-C(11)	1.446(5)
N(2)-C(4)	1.322(6)
N(2)-C(6)	1.494(6)
N(3)-C(7)	1.452(6)
N(3)-C(32)	1.463(6)
N(3)-C(31)	1.500(5)
N(4)-C(40)	1.391(5)
N(4)-H(4)	0.838(18)
C(1)-C(2)	1.511(6)
C(1)-H(1A)	0.9600
C(1)-H(1B)	0.9600
C(1)-H(1C)	0.9600
C(2)-C(3)	1.402(6)
C(3)-C(4)	1.404(6)
C(3)-H(3)	0.9300
C(4)-C(5)	1.515(6)
C(5)-H(5A)	0.9600
C(5)-H(5B)	0.9600
C(5)-H(5C)	0.9600
C(6)-C(7)	1.520(7)
C(6)-H(6A)	0.9700
C(6)-H(6B)	0.9700
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700

C(11)-C(12)	1.401(5)
C(11)-C(16)	1.403(6)
C(12)-C(13)	1.384(6)
C(12)-C(17)	1.503(6)
C(13)-C(14)	1.371(6)
C(13)-H(13)	0.9300
C(14)-C(15)	1.367(6)
C(14)-H(14)	0.9300
C(15)-C(16)	1.382(6)
C(15)-H(15)	0.9300
C(16)-C(20)	1.515(6)
C(17)-C(18)	1.512(6)
C(17)-C(19)	1.527(7)
C(17)-H(17)	0.9800
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(20)-C(22)	1.518(6)
C(20)-C(21)	1.532(6)
C(20)-H(20)	0.9800
C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600
C(22)-H(22A)	0.9600
C(22)-H(22B)	0.9600
C(22)-H(22C)	0.9600
C(31)-H(31A)	0.9600
C(31)-H(31B)	0.9600
C(31)-H(31C)	0.9600
C(32)-H(32A)	0.9600
C(32)-H(32B)	0.9600
C(32)-H(32C)	0.9600
C(33)-H(33A)	0.9600
C(33)-H(33B)	0.9600
C(33)-H(33C)	0.9600
C(40)-C(41)	1.396(5)
C(40)-C(45)	1.415(5)
C(41)-C(42)	1.380(6)
C(41)-C(46)	1.506(5)
C(42)-C(43)	1.373(6)
C(42)-H(42)	0.9300

C(43)-C(44)	1.362(7)
C(43)-H(43)	0.9300
C(44)-C(45)	1.388(6)
C(44)-H(44)	0.9300
C(45)-C(49)	1.509(6)
C(46)-C(47)	1.526(6)
C(46)-C(48)	1.534(6)
C(46)-H(46)	0.9800
C(47)-H(47A)	0.9600
C(47)-H(47B)	0.9600
C(47)-H(47C)	0.9600
C(48)-H(48A)	0.9600
C(48)-H(48B)	0.9600
C(48)-H(48C)	0.9600
C(49)-C(51)	1.509(8)
C(49)-C(50)	1.515(8)
C(49)-H(49)	0.9800
C(50)-H(50A)	0.9600
C(50)-H(50B)	0.9600
C(50)-H(50C)	0.9600
C(51)-H(51A)	0.9600
C(51)-H(51B)	0.9600
C(51)-H(51C)	0.9600
C(52)-C(58)	1.351(12)
C(52)-C(57)	1.418(12)
C(52)-C(53)	1.535(13)
C(53)-C(54)	1.376(14)
C(53)-H(53)	0.9300
C(54)-C(55)	1.346(15)
C(54)-H(54)	0.9300
C(55)-C(56)	1.518(13)
C(55)-H(55)	0.9300
C(56)-C(57)	1.388(12)
C(56)-H(56)	0.9300
C(57)-H(57)	0.9300
C(58)-H(58A)	0.9600
C(58)-H(58B)	0.9600
C(58)-H(58C)	0.9600
N(4)-Sc(1)-N(2)	126.23(15)
N(4)-Sc(1)-N(1)	109.12(13)
N(2)-Sc(1)-N(1)	82.63(13)
N(4)-Sc(1)-C(33)	103.75(17)
N(2)-Sc(1)-C(33)	127.25(17)
N(1)-Sc(1)-C(33)	97.34(14)

N(4)-Sc(1)-N(3)	91.94(14)
N(2)-Sc(1)-N(3)	74.04(14)
N(1)-Sc(1)-N(3)	155.10(13)
C(33)-Sc(1)-N(3)	90.10(15)
C(2)-N(1)-C(11)	117.8(3)
C(2)-N(1)-Sc(1)	124.6(3)
C(11)-N(1)-Sc(1)	117.6(2)
C(4)-N(2)-C(6)	117.2(4)
C(4)-N(2)-Sc(1)	125.4(3)
C(6)-N(2)-Sc(1)	116.7(3)
C(7)-N(3)-C(32)	109.4(4)
C(7)-N(3)-C(31)	111.3(4)
C(32)-N(3)-C(31)	106.4(4)
C(7)-N(3)-Sc(1)	102.8(3)
C(32)-N(3)-Sc(1)	118.0(3)
C(31)-N(3)-Sc(1)	108.8(3)
C(40)-N(4)-Sc(1)	153.7(3)
C(40)-N(4)-H(4)	109(3)
Sc(1)-N(4)-H(4)	97(3)
C(2)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
N(1)-C(2)-C(3)	124.2(4)
N(1)-C(2)-C(1)	120.3(4)
C(3)-C(2)-C(1)	115.5(4)
C(4)-C(3)-C(2)	127.9(4)
C(4)-C(3)-H(3)	116.0
C(2)-C(3)-H(3)	116.1
N(2)-C(4)-C(3)	123.1(4)
N(2)-C(4)-C(5)	120.6(5)
C(3)-C(4)-C(5)	116.3(5)
C(4)-C(5)-H(5A)	109.5
C(4)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(4)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
N(2)-C(6)-C(7)	109.5(4)
N(2)-C(6)-H(6A)	109.8
C(7)-C(6)-H(6A)	109.8
N(2)-C(6)-H(6B)	109.8

C(7)-C(6)-H(6B)	109.8
H(6A)-C(6)-H(6B)	108.2
N(3)-C(7)-C(6)	109.6(4)
N(3)-C(7)-H(7A)	109.8
C(6)-C(7)-H(7A)	109.8
N(3)-C(7)-H(7B)	109.8
C(6)-C(7)-H(7B)	109.8
H(7A)-C(7)-H(7B)	108.2
C(12)-C(11)-C(16)	120.9(4)
C(12)-C(11)-N(1)	118.1(4)
C(16)-C(11)-N(1)	121.0(4)
C(13)-C(12)-C(11)	117.8(4)
C(13)-C(12)-C(17)	119.3(4)
C(11)-C(12)-C(17)	122.9(4)
C(14)-C(13)-C(12)	121.6(5)
C(14)-C(13)-H(13)	119.2
C(12)-C(13)-H(13)	119.2
C(15)-C(14)-C(13)	119.9(5)
C(15)-C(14)-H(14)	120.0
C(13)-C(14)-H(14)	120.0
C(14)-C(15)-C(16)	121.3(5)
C(14)-C(15)-H(15)	119.4
C(16)-C(15)-H(15)	119.4
C(15)-C(16)-C(11)	118.4(4)
C(15)-C(16)-C(20)	118.2(4)
C(11)-C(16)-C(20)	123.4(4)
C(12)-C(17)-C(18)	111.6(4)
C(12)-C(17)-C(19)	111.8(4)
C(18)-C(17)-C(19)	110.6(4)
C(12)-C(17)-H(17)	107.5
C(18)-C(17)-H(17)	107.5
C(19)-C(17)-H(17)	107.5
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(17)-C(19)-H(19A)	109.5
C(17)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(17)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5

C(16)-C(20)-C(22)	112.2(4)
C(16)-C(20)-C(21)	111.8(4)
C(22)-C(20)-C(21)	110.0(4)
C(16)-C(20)-H(20)	107.5
C(22)-C(20)-H(20)	107.5
C(21)-C(20)-H(20)	107.5
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
N(3)-C(31)-H(31A)	109.5
N(3)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
N(3)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
N(3)-C(32)-H(32A)	109.5
N(3)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
N(3)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
Sc(1)-C(33)-H(33A)	109.5
Sc(1)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
Sc(1)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(41)-C(40)-N(4)	119.7(4)
C(41)-C(40)-C(45)	119.0(4)
N(4)-C(40)-C(45)	121.2(4)
C(42)-C(41)-C(40)	118.9(4)
C(42)-C(41)-C(46)	119.4(4)
C(40)-C(41)-C(46)	121.8(4)
C(43)-C(42)-C(41)	122.8(5)
C(43)-C(42)-H(42)	118.6

C(41)-C(42)-H(42)	118.6
C(44)-C(43)-C(42)	118.2(5)
C(44)-C(43)-H(43)	120.9
C(42)-C(43)-H(43)	120.9
C(43)-C(44)-C(45)	122.1(5)
C(43)-C(44)-H(44)	118.9
C(45)-C(44)-H(44)	118.9
C(44)-C(45)-C(40)	118.9(4)
C(44)-C(45)-C(49)	118.1(4)
C(40)-C(45)-C(49)	123.0(4)
C(41)-C(46)-C(47)	112.5(4)
C(41)-C(46)-C(48)	111.8(4)
C(47)-C(46)-C(48)	109.7(4)
C(41)-C(46)-H(46)	107.5
C(47)-C(46)-H(46)	107.5
C(48)-C(46)-H(46)	107.5
C(46)-C(47)-H(47A)	109.5
C(46)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
C(46)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
C(46)-C(48)-H(48A)	109.5
C(46)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(46)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
C(51)-C(49)-C(45)	111.1(5)
C(51)-C(49)-C(50)	111.5(5)
C(45)-C(49)-C(50)	114.2(5)
C(51)-C(49)-H(49)	106.5
C(45)-C(49)-H(49)	106.5
C(50)-C(49)-H(49)	106.5
C(49)-C(50)-H(50A)	109.5
C(49)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
C(49)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
C(49)-C(51)-H(51A)	109.5
C(49)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(49)-C(51)-H(51C)	109.5

H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
C(58)-C(52)-C(57)	125.9(15)
C(58)-C(52)-C(53)	127.6(14)
C(57)-C(52)-C(53)	105.7(11)
C(54)-C(53)-C(52)	142.1(15)
C(54)-C(53)-H(53)	108.9
C(52)-C(53)-H(53)	108.9
C(55)-C(54)-C(53)	113.5(18)
C(55)-C(54)-H(54)	123.2
C(53)-C(54)-H(54)	123.3
C(54)-C(55)-C(56)	102.9(15)
C(54)-C(55)-H(55)	128.5
C(56)-C(55)-H(55)	128.5
C(57)-C(56)-C(55)	147.8(13)
C(57)-C(56)-H(56)	106.1
C(55)-C(56)-H(56)	106.1
C(56)-C(57)-C(52)	107.3(12)
C(56)-C(57)-H(57)	126.4
C(52)-C(57)-H(57)	126.3
C(52)-C(58)-H(58A)	109.5
C(52)-C(58)-H(58B)	109.5
H(58A)-C(58)-H(58B)	109.5
C(52)-C(58)-H(58C)	109.4
H(58A)-C(58)-H(58C)	109.5
H(58B)-C(58)-H(58C)	109.5

Table **S3**. Anisotropic displacement parameters (A^2 x 10^3) for **2**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Sc(1)	37(1)	43(1)	50(1)	-1(1)	8(1)	-5(1)
N(1)	39(2)	43(2)	47(2)	-5(2)	10(2)	-3(2)
N(2)	57(2)	79(3)	49(2)	-9(2)	11(2)	-12(2)
N(3)	54(2)	60(2)	68(3)	8(2)	0(2)	-4(2)
N(4)	46(2)	47(2)	68(3)	3(2)	22(2)	-1(2)
C(1)	56(3)	82(4)	93(4)	-12(3)	11(3)	19(3)
C(2)	42(2)	46(3)	66(3)	-1(2)	19(2)	-3(2)
C(3)	56(3)	60(3)	71(4)	-17(3)	27(3)	-3(2)
C(4)	66(3)	72(3)	57(3)	-19(3)	23(3)	-29(3)

C(5)	96(4)	120(5)	68(4)	-40(3)	29(3)	-25(4)
C(6)	85(4)	126(5)	53(3)	6(3)	4(3)	-25(4)
C(7)	71(3)	94(4)	71(4)	19(3)	-10(3)	-2(3)
C(11)	36(2)	46(2)	46(3)	0(2)	3(2)	5(2)
C(12)	48(2)	57(3)	48(3)	-4(2)	1(2)	-4(2)
C(13)	77(3)	53(3)	61(3)	-6(3)	-6(3)	-11(2)
C(14)	86(4)	73(4)	56(3)	-15(3)	-13(3)	2(3)
C(15)	87(3)	61(3)	44(3)	0(2)	5(3)	10(3)
C(16)	53(2)	51(3)	51(3)	-1(2)	5(2)	10(2)
C(17)	65(3)	63(3)	59(3)	2(3)	5(3)	-23(2)
C(18)	85(4)	133(5)	104(5)	12(4)	40(4)	-20(4)
C(19)	113(4)	83(4)	79(4)	18(3)	4(4)	-23(3)
C(20)	80(3)	53(3)	55(3)	4(2)	13(3)	3(2)
C(21)	112(4)	64(3)	95(4)	23(3)	14(4)	13(3)
C(22)	90(4)	97(4)	73(4)	3(3)	30(3)	-2(3)
C(31)	69(3)	75(4)	91(4)	-1(3)	-11(3)	-18(3)
C(32)	64(3)	94(4)	115(5)	3(4)	-10(3)	18(3)
C(33)	63(3)	60(3)	82(4)	-12(3)	4(3)	3(2)
C(40)	48(2)	52(3)	44(3)	5(2)	2(2)	-10(2)
C(41)	48(2)	44(3)	55(3)	0(2)	4(2)	-4(2)
C(42)	73(3)	55(3)	81(4)	9(3)	6(3)	1(3)
C(43)	92(4)	57(3)	82(4)	10(3)	15(3)	-23(3)
C(44)	73(3)	85(4)	79(4)	6(3)	29(3)	-27(3)
C(45)	56(3)	66(3)	65(3)	2(3)	17(3)	-17(2)
C(46)	56(3)	44(3)	78(4)	-6(2)	10(3)	-1(2)
C(47)	56(3)	82(4)	115(5)	-7(3)	6(3)	13(3)
C(48)	77(3)	85(4)	83(4)	-13(3)	24(3)	-7(3)
C(49)	79(4)	78(4)	117(5)	-13(3)	59(4)	-21(3)
C(50)	123(6)	187(8)	120(7)	-46(6)	37(5)	11(5)
C(51)	118(6)	138(7)	169(8)	-27(5)	2(6)	50(5)
C(52)	490(20)	97(7)	316(18)	25(10)	304(18)	-82(12)
C(53)	138(7)	201(11)	240(14)	161(12)	-27(8)	-76(7)
C(56)	212(11)	136(8)	258(14)	83(9)	124(11)	-31(7)

Table **S4**. Torsion angles [deg] for **2**.

N(4)-Sc(1)-N(1)-C(2)	-95.0(3)
N(2)-Sc(1)-N(1)-C(2)	30.9(3)
C(33)-Sc(1)-N(1)-C(2)	157.6(3)
N(3)-Sc(1)-N(1)-C(2)	51.3(5)
N(4)-Sc(1)-N(1)-C(11)	84.0(3)
N(2)-Sc(1)-N(1)-C(11)	-150.2(3)

C(33)-Sc(1)-N(1)-C(11)	-23.4(3)
N(3)-Sc(1)-N(1)-C(11)	-129.8(3)
N(4)-Sc(1)-N(2)-C(4)	74.0(4)
N(1)-Sc(1)-N(2)-C(4)	-34.3(3)
C(33)-Sc(1)-N(2)-C(4)	-127.9(4)
N(3)-Sc(1)-N(2)-C(4)	154.5(4)
N(4)-Sc(1)-N(2)-C(6)	-95.8(4)
N(1)-Sc(1)-N(2)-C(6)	155.9(3)
C(33)-Sc(1)-N(2)-C(6)	62.3(4)
N(3)-Sc(1)-N(2)-C(6)	-15.3(3)
N(4)-Sc(1)-N(3)-C(7)	165.4(3)
N(2)-Sc(1)-N(3)-C(7)	38.1(3)
N(1)-Sc(1)-N(3)-C(7)	17.0(5)
C(33)-Sc(1)-N(3)-C(7)	-90.9(3)
N(4)-Sc(1)-N(3)-C(32)	-74.1(4)
N(2)-Sc(1)-N(3)-C(32)	158.6(4)
N(1)-Sc(1)-N(3)-C(32)	137.6(4)
C(33)-Sc(1)-N(3)-C(32)	29.7(4)
N(4)-Sc(1)-N(3)-C(31)	47.2(3)
N(2)-Sc(1)-N(3)-C(31)	-80.0(3)
N(1)-Sc(1)-N(3)-C(31)	-101.1(4)
C(33)-Sc(1)-N(3)-C(31)	151.0(3)
N(2)-Sc(1)-N(4)-C(40)	-21.3(7)
N(1)-Sc(1)-N(4)-C(40)	73.6(7)
C(33)-Sc(1)-N(4)-C(40)	176.6(7)
N(3)-Sc(1)-N(4)-C(40)	-92.8(7)
C(11)-N(1)-C(2)-C(3)	165.2(4)
Sc(1)-N(1)-C(2)-C(3)	-15.8(6)
C(11)-N(1)-C(2)-C(1)	-14.6(6)
Sc(1)-N(1)-C(2)-C(1)	164.4(3)
N(1)-C(2)-C(3)-C(4)	-13.0(7)
C(1)-C(2)-C(3)-C(4)	166.9(4)
C(6)-N(2)-C(4)-C(3)	-167.8(4)
Sc(1)-N(2)-C(4)-C(3)	22.4(6)
C(6)-N(2)-C(4)-C(5)	10.8(6)
Sc(1)-N(2)-C(4)-C(5)	-158.9(3)
C(2)-C(3)-C(4)-N(2)	9.7(7)
C(2)-C(3)-C(4)-C(5)	-169.0(4)
C(4)-N(2)-C(6)-C(7)	179.6(4)
Sc(1)-N(2)-C(6)-C(7)	-9.8(5)
C(32)-N(3)-C(7)-C(6)	177.5(4)
C(31)-N(3)-C(7)-C(6)	60.1(5)
Sc(1)-N(3)-C(7)-C(6)	-56.3(4)
N(2)-C(6)-C(7)-N(3)	46.2(5)

C(2)-N(1)-C(11)-C(12)	-83.7(4)
Sc(1)-N(1)-C(11)-C(12)	97.3(3)
C(2)-N(1)-C(11)-C(16)	98.4(4)
Sc(1)-N(1)-C(11)-C(16)	-80.7(4)
C(16)-C(11)-C(12)-C(13)	-1.3(6)
N(1)-C(11)-C(12)-C(13)	-179.2(4)
C(16)-C(11)-C(12)-C(17)	177.2(4)
N(1)-C(11)-C(12)-C(17)	-0.7(6)
C(11)-C(12)-C(13)-C(14)	1.3(7)
C(17)-C(12)-C(13)-C(14)	-177.2(4)
C(12)-C(13)-C(14)-C(15)	0.1(8)
C(13)-C(14)-C(15)-C(16)	-1.7(7)
C(14)-C(15)-C(16)-C(11)	1.8(7)
C(14)-C(15)-C(16)-C(20)	-177.8(4)
C(12)-C(11)-C(16)-C(15)	-0.2(6)
N(1)-C(11)-C(16)-C(15)	177.6(4)
C(12)-C(11)-C(16)-C(20)	179.3(4)
N(1)-C(11)-C(16)-C(20)	-2.9(6)
C(13)-C(12)-C(17)-C(18)	-71.9(6)
C(11)-C(12)-C(17)-C(18)	109.6(5)
C(13)-C(12)-C(17)-C(19)	52.5(6)
C(11)-C(12)-C(17)-C(19)	-125.9(4)
C(15)-C(16)-C(20)-C(22)	-59.1(5)
C(11)-C(16)-C(20)-C(22)	121.4(5)
C(15)-C(16)-C(20)-C(21)	65.0(5)
C(11)-C(16)-C(20)-C(21)	-114.5(5)
Sc(1)-N(4)-C(40)-C(41)	-16.1(9)
Sc(1)-N(4)-C(40)-C(45)	164.2(5)
N(4)-C(40)-C(41)-C(42)	178.6(4)
C(45)-C(40)-C(41)-C(42)	-1.7(6)
N(4)-C(40)-C(41)-C(46)	-0.6(6)
C(45)-C(40)-C(41)-C(46)	179.1(4)
C(40)-C(41)-C(42)-C(43)	0.2(7)
C(46)-C(41)-C(42)-C(43)	179.4(4)
C(41)-C(42)-C(43)-C(44)	1.4(8)
C(42)-C(43)-C(44)-C(45)	-1.4(8)
C(43)-C(44)-C(45)-C(40)	-0.1(8)
C(43)-C(44)-C(45)-C(49)	-179.3(5)
C(41)-C(40)-C(45)-C(44)	1.7(6)
N(4)-C(40)-C(45)-C(44)	-178.6(4)
C(41)-C(40)-C(45)-C(49)	-179.2(5)
N(4)-C(40)-C(45)-C(49)	0.5(7)
C(42)-C(41)-C(46)-C(47)	57.5(6)
C(40)-C(41)-C(46)-C(47)	-123.4(5)

C(42)-C(41)-C(46)-C(48)	-66.5(5)
C(40)-C(41)-C(46)-C(48)	112.7(5)
C(44)-C(45)-C(49)-C(51)	72.3(7)
C(40)-C(45)-C(49)-C(51)	-106.8(6)
C(44)-C(45)-C(49)-C(50)	-54.9(7)
C(40)-C(45)-C(49)-C(50)	126.0(5)
C(58)-C(52)-C(53)-C(54)	175.1(17)
C(57)-C(52)-C(53)-C(54)	4.5(18)
C(52)-C(53)-C(54)-C(55)	-8(3)
C(53)-C(54)-C(55)-C(56)	6.8(19)
C(54)-C(55)-C(56)-C(57)	-8(3)
C(55)-C(56)-C(57)-C(52)	5(2)
C(58)-C(52)-C(57)-C(56)	-172.0(12)
C(53)-C(52)-C(57)-C(56)	-1.2(11)

Crystal data for **3**: C47H69N6Sc, M_r = 763.04 (containing a toluene molecule), T = 293(2) K, Monoclinic, C2/c, a = 25.451(4) Å, b = 11.1475(16) Å, c = 34.342(5) Å, β = 105.936(3) °, V = 9369(2) Å^3, Z = 8, F(000) = 3312, 24126 refelections collected, 8790 unique refelections, R1 = 0.0759, wR2 = 0.1797 ($I > 2\sigma(I)$)

Table **S5** Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **3**. U (eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Sc(1)	4061(1)	6207(1)	5804(1)	55(1)
N(1)	3372(2)	5769(4)	6065(2)	58(1)
N(2)	3399(2)	6558(5)	5252(2)	61(2)
N(3)	4483(2)	7247(4)	5358(2)	62(1)
N(4)	4448(2)	7535(5)	6301(2)	68(2)
N(5)	5422(3)	9911(6)	7131(2)	99(2)
N(6)	4489(2)	4809(4)	5854(2)	60(1)
C(1)	2539(3)	4583(7)	6039(2)	107(3)
C(2)	2912(3)	5241(6)	5846(2)	72(2)
C(3)	2744(3)	5254(6)	5415(2)	76(2)
C(4)	2943(3)	5916(6)	5143(2)	67(2)
C(5)	2594(3)	5874(7)	4715(2)	99(3)
C(6)	3519(3)	7315(7)	4949(2)	88(2)
C(7)	4038(3)	8030(6)	5117(2)	77(2)
C(11)	3448(2)	5889(6)	6489(2)	62(2)
C(12)	3255(2)	6932(6)	6636(2)	65(2)
C(13)	3336(3)	7068(7)	7050(2)	84(2)
C(14)	3621(3)	6226(8)	7319(2)	89(2)
C(15)	3814(3)	5216(8)	7177(2)	87(2)
C(16)	3734(3)	5020(7)	6762(2)	78(2)
C(17)	3937(4)	3863(8)	6622(2)	109(3)
C(18)	3643(5)	2751(8)	6727(3)	172(5)
C(19)	4552(4)	3727(9)	6799(3)	176(5)
C(20)	2931(3)	7874(6)	6343(2)	75(2)
C(21)	3084(3)	9155(6)	6487(2)	109(3)
C(22)	2326(3)	7714(8)	6268(3)	133(4)
C(31)	4976(3)	7979(6)	5523(2)	89(2)
C(32)	4624(3)	6308(6)	5100(2)	84(2)
C(33)	4391(3)	8734(8)	6265(2)	84(2)
C(34)	4695(3)	9550(7)	6527(2)	84(2)
C(35)	5100(3)	9164(7)	6863(3)	79(2)
C(36)	5147(3)	7930(7)	6915(2)	87(2)

C(37)	4827(3)	7188(7)	6631(3)	88(2)
C(38)	5831(3)	9484(7)	7491(2)	108(3)
C(39)	5403(4)	11192(7)	7060(3)	156(4)
C(40)	4726(2)	3732(6)	5830(2)	57(2)
C(41)	4428(3)	2728(6)	5630(2)	64(2)
C(42)	4682(3)	1646(6)	5603(2)	78(2)
C(43)	5234(3)	1483(6)	5772(2)	85(2)
C(44)	5533(3)	2440(6)	5972(2)	77(2)
C(45)	5297(3)	3550(5)	6011(2)	60(2)
C(46)	5654(3)	4573(6)	6225(2)	79(2)
C(47)	5995(3)	4275(8)	6654(2)	120(3)
C(48)	6028(3)	5040(7)	5971(2)	101(3)
C(49)	3823(3)	2857(6)	5431(2)	81(2)
C(50)	3703(3)	3045(9)	4994(3)	137(4)
C(51)	3470(3)	1829(8)	5516(3)	148(4)
C(52)	2278(6)	3620(13)	7123(4)	209(6)
C(53)	2168(5)	4773(12)	7124(4)	219(6)
C(54)	1693(6)	5122(12)	6824(5)	222(6)
C(55)	1361(6)	4337(14)	6541(4)	227(6)
C(56)	1544(7)	3206(14)	6601(5)	261(8)
C(57)	2001(5)	2749(11)	6848(4)	204(5)
C(58)	2737(7)	3078(17)	7387(6)	396(13)

Table **S6**. Bond lengths (Å) and angles (^{o}) for **3**.

Sc(1)-N(6)	1.881(5)
Sc(1)-N(2)	2.198(5)
Sc(1)-N(1)	2.232(5)
Sc(1)-N(4)	2.271(5)
Sc(1)-N(3)	2.396(5)
N(1)-C(2)	1.341(8)
N(1)-C(11)	1.424(7)
N(2)-C(4)	1.327(7)
N(2)-C(6)	1.437(8)
N(3)-C(31)	1.473(7)
N(3)-C(32)	1.478(7)
N(3)-C(7)	1.488(7)
N(4)-C(37)	1.327(8)
N(4)-C(33)	1.347(8)
N(5)-C(35)	1.341(8)
N(5)-C(39)	1.448(9)
N(5)-C(38)	1.461(8)

N(6)-C(40)	1.357(7)
C(1)-C(2)	1.489(9)
C(1)-H(1A)	0.9600
C(1)-H(1B)	0.9600
C(1)-H(1C)	0.9600
C(2)-C(3)	1.427(9)
C(3)-C(4)	1.390(9)
C(3)-H(3)	0.9300
C(4)-C(5)	1.494(8)
C(5)-H(5A)	0.9600
C(5)-H(5B)	0.9600
C(5)-H(5C)	0.9600
C(6)-C(7)	1.514(8)
C(6)-H(6A)	0.9700
C(6)-H(6B)	0.9700
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(11)-C(16)	1.405(8)
C(11)-C(12)	1.408(8)
C(12)-C(13)	1.388(8)
C(12)-C(20)	1.529(8)
C(13)-C(14)	1.374(9)
C(13)-H(13)	0.9300
C(14)-C(15)	1.369(9)
C(14)-H(14)	0.9300
C(15)-C(16)	1.400(9)
C(15)-H(15)	0.9300
C(16)-C(17)	1.516(10)
C(17)-C(19)	1.524(11)
C(17)-C(18)	1.541(11)
C(17)-H(17)	0.9800
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(20)-C(22)	1.500(9)
C(20)-C(21)	1.526(9)
C(20)-H(20)	0.9800
C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600
C(22)-H(22A)	0.9600

C(22)-H(22B)	0.9600
C(22)-H(22C)	0.9600
C(31)-H(31A)	0.9600
C(31)-H(31B)	0.9600
C(31)-H(31C)	0.9600
C(32)-H(32A)	0.9600
C(32)-H(32B)	0.9600
C(32)-H(32C)	0.9600
C(33)-C(34)	1.361(9)
C(33)-H(33)	0.9300
C(34)-C(35)	1.389(9)
C(34)-H(34)	0.9300
C(35)-C(36)	1.389(9)
C(36)-C(37)	1.365(9)
C(36)-H(36)	0.9300
C(37)-H(37)	0.9300
C(38)-H(38A)	0.9600
C(38)-H(38B)	0.9600
C(38)-H(38C)	0.9600
C(39)-H(39A)	0.9600
C(39)-H(39B)	0.9600
C(39)-H(39C)	0.9600
C(40)-C(41)	1.421(8)
C(40)-C(45)	1.428(8)
C(41)-C(42)	1.383(8)
C(41)-C(49)	1.510(8)
C(42)-C(43)	1.377(8)
C(42)-H(42)	0.9300
C(43)-C(44)	1.381(8)
C(43)-H(43)	0.9300
C(44)-C(45)	1.397(8)
C(44)-H(44)	0.9300
C(45)-C(46)	1.516(8)
C(46)-C(47)	1.528(9)
C(46)-C(48)	1.548(9)
C(46)-H(46)	0.9800
C(47)-H(47A)	0.9600
C(47)-H(47B)	0.9600
C(47)-H(47C)	0.9600
C(48)-H(48A)	0.9600
C(48)-H(48B)	0.9600
C(48)-H(48C)	0.9600
C(49)-C(50)	1.461(10)
C(49)-C(51)	1.534(9)

C(49)-H(49)	0.9800
C(50)-H(50A)	0.9600
C(50)-H(50B)	0.9600
C(50)-H(50C)	0.9600
C(51)-H(51A)	0.9600
C(51)-H(51B)	0.9600
C(51)-H(51C)	0.9600
C(52)-C(53)	1.316(12)
C(52)-C(57)	1.401(12)
C(52)-C(58)	1.404(13)
C(53)-C(54)	1.409(12)
C(53)-H(53)	0.9300
C(54)-C(55)	1.406(13)
C(54)-H(54)	0.9300
C(55)-C(56)	1.341(13)
C(55)-H(55)	0.9300
C(56)-C(57)	1.337(13)
C(56)-H(56)	0.9300
C(57)-H(57)	0.9300
C(58)-H(58A)	0.9709
C(58)-H(58B)	0.9712
C(58)-H(58C)	0.9708
N(6)-Sc(1)-N(2)	120.9(2)
N(6)-Sc(1)-N(1)	106.34(19)
N(2)-Sc(1)-N(1)	83.3(2)
N(6)-Sc(1)-N(4)	110.5(2)
N(2)-Sc(1)-N(4)	127.2(2)
N(1)-Sc(1)-N(4)	93.8(2)
N(6)-Sc(1)-N(3)	96.3(2)
N(2)-Sc(1)-N(3)	74.6(2)
N(1)-Sc(1)-N(3)	154.35(18)
N(4)-Sc(1)-N(3)	89.28(19)
C(2)-N(1)-C(11)	117.8(6)
C(2)-N(1)-Sc(1)	122.2(4)
C(11)-N(1)-Sc(1)	119.4(4)
C(4)-N(2)-C(6)	117.1(6)
C(4)-N(2)-Sc(1)	123.4(4)
C(6)-N(2)-Sc(1)	117.7(4)
C(31)-N(3)-C(32)	107.5(5)
C(31)-N(3)-C(7)	109.1(5)
C(32)-N(3)-C(7)	110.7(5)
C(31)-N(3)-Sc(1)	120.4(4)
C(32)-N(3)-Sc(1)	105.4(4)
C(7)-N(3)-Sc(1)	103.5(4)

C(37)-N(4)-C(33)	113.7(6)
C(37)-N(4)-Sc(1)	121.0(5)
C(33)-N(4)-Sc(1)	124.3(5)
C(35)-N(5)-C(39)	120.7(7)
C(35)-N(5)-C(38)	122.5(7)
C(39)-N(5)-C(38)	116.6(7)
C(40)-N(6)-Sc(1)	169.6(5)
C(2)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
N(1)-C(2)-C(3)	122.9(6)
N(1)-C(2)-C(1)	122.2(7)
C(3)-C(2)-C(1)	114.8(7)
C(4)-C(3)-C(2)	130.0(7)
C(4)-C(3)-H(3)	115.0
C(2)-C(3)-H(3)	115.0
N(2)-C(4)-C(3)	123.3(6)
N(2)-C(4)-C(5)	122.2(7)
C(3)-C(4)-C(5)	114.5(7)
C(4)-C(5)-H(5A)	109.5
C(4)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(4)-C(5)-H(5C)	109.4
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
N(2)-C(6)-C(7)	111.6(6)
N(2)-C(6)-H(6A)	109.3
C(7)-C(6)-H(6A)	109.3
N(2)-C(6)-H(6B)	109.3
C(7)-C(6)-H(6B)	109.3
H(6A)-C(6)-H(6B)	107.9
N(3)-C(7)-C(6)	110.8(5)
N(3)-C(7)-H(7A)	109.4
C(6)-C(7)-H(7A)	109.5
N(3)-C(7)-H(7B)	109.5
C(6)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	108.1
C(16)-C(11)-C(12)	119.9(7)
C(16)-C(11)-N(1)	121.2(6)
C(12)-C(11)-N(1)	118.8(6)
C(13)-C(12)-C(11)	119.2(7)

C(13)-C(12)-C(20)	120.0(7)
C(11)-C(12)-C(20)	120.7(6)
C(14)-C(13)-C(12)	121.0(8)
C(14)-C(13)-H(13)	119.5
C(12)-C(13)-H(13)	119.5
C(15)-C(14)-C(13)	119.8(7)
C(15)-C(14)-H(14)	120.1
C(13)-C(14)-H(14)	120.1
C(14)-C(15)-C(16)	121.6(7)
C(14)-C(15)-H(15)	119.2
C(16)-C(15)-H(15)	119.2
C(15)-C(16)-C(11)	118.3(7)
C(15)-C(16)-C(17)	119.4(7)
C(11)-C(16)-C(17)	122.3(7)
C(16)-C(17)-C(19)	111.0(8)
C(16)-C(17)-C(18)	112.4(7)
C(19)-C(17)-C(18)	109.8(7)
C(16)-C(17)-H(17)	107.9
C(19)-C(17)-H(17)	107.8
C(18)-C(17)-H(17)	107.8
C(17)-C(18)-H(18A)	109.4
C(17)-C(18)-H(18B)	109.6
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.4
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(17)-C(19)-H(19A)	109.5
C(17)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(17)-C(19)-H(19C)	109.4
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(22)-C(20)-C(21)	109.0(6)
C(22)-C(20)-C(12)	112.0(6)
C(21)-C(20)-C(12)	112.7(6)
C(22)-C(20)-H(20)	107.6
C(21)-C(20)-H(20)	107.7
C(12)-C(20)-H(20)	107.7
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.4
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5

C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.4
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
N(3)-C(31)-H(31A)	109.5
N(3)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
N(3)-C(31)-H(31C)	109.4
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
N(3)-C(32)-H(32A)	109.5
N(3)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
N(3)-C(32)-H(32C)	109.4
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
N(4)-C(33)-C(34)	125.1(7)
N(4)-C(33)-H(33)	117.5
C(34)-C(33)-H(33)	117.4
C(33)-C(34)-C(35)	120.0(7)
C(33)-C(34)-H(34)	120.0
C(35)-C(34)-H(34)	120.0
N(5)-C(35)-C(36)	120.8(8)
N(5)-C(35)-C(34)	123.5(7)
C(36)-C(35)-C(34)	115.6(8)
C(37)-C(36)-C(35)	119.6(8)
C(37)-C(36)-H(36)	120.2
C(35)-C(36)-H(36)	120.2
N(4)-C(37)-C(36)	125.8(7)
N(4)-C(37)-H(37)	117.1
C(36)-C(37)-H(37)	117.1
N(5)-C(38)-H(38A)	109.5
N(5)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
N(5)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
N(5)-C(39)-H(39A)	109.6
N(5)-C(39)-H(39B)	109.4
H(39A)-C(39)-H(39B)	109.5
N(5)-C(39)-H(39C)	109.4
H(39A)-C(39)-H(39C)	109.5

H(39B)-C(39)-H(39C)	109.5
N(6)-C(40)-C(41)	122.6(6)
N(6)-C(40)-C(45)	121.0(6)
C(41)-C(40)-C(45)	116.3(6)
C(42)-C(41)-C(40)	121.4(6)
C(42)-C(41)-C(49)	119.4(6)
C(40)-C(41)-C(49)	119.2(6)
C(43)-C(42)-C(41)	122.0(7)
C(43)-C(42)-H(42)	119.0
C(41)-C(42)-H(42)	119.0
C(42)-C(43)-C(44)	117.8(7)
C(42)-C(43)-H(43)	121.1
C(44)-C(43)-H(43)	121.1
C(43)-C(44)-C(45)	122.6(7)
C(43)-C(44)-H(44)	118.7
C(45)-C(44)-H(44)	118.7
C(44)-C(45)-C(40)	119.8(6)
C(44)-C(45)-C(46)	119.7(6)
C(40)-C(45)-C(46)	120.4(5)
C(45)-C(46)-C(47)	114.2(6)
C(45)-C(46)-C(48)	111.1(6)
C(47)-C(46)-C(48)	110.0(6)
C(45)-C(46)-H(46)	107.1
C(47)-C(46)-H(46)	107.0
C(48)-C(46)-H(46)	107.1
C(46)-C(47)-H(47A)	109.5
C(46)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
C(46)-C(47)-H(47C)	109.4
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
C(46)-C(48)-H(48A)	109.5
C(46)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(46)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
C(50)-C(49)-C(41)	112.2(6)
C(50)-C(49)-C(51)	109.6(7)
C(41)-C(49)-C(51)	114.8(7)
C(50)-C(49)-H(49)	106.6
C(41)-C(49)-H(49)	106.6
C(51)-C(49)-H(49)	106.6
C(49)-C(50)-H(50A)	109.5

C(49)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
C(49)-C(50)-H(50C)	109.4
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
C(49)-C(51)-H(51A)	109.5
C(49)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(49)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
C(53)-C(52)-C(57)	127.6(14)
C(53)-C(52)-C(58)	124.0(14)
C(57)-C(52)-C(58)	108.2(12)
C(52)-C(53)-C(54)	114.1(13)
C(52)-C(53)-H(53)	123.0
C(54)-C(53)-H(53)	123.0
C(55)-C(54)-C(53)	124.5(13)
C(55)-C(54)-H(54)	117.8
C(53)-C(54)-H(54)	117.8
C(56)-C(55)-C(54)	111.2(13)
C(56)-C(55)-H(55)	124.5
C(54)-C(55)-H(55)	124.3
C(57)-C(56)-C(55)	131.3(15)
C(57)-C(56)-H(56)	114.3
C(55)-C(56)-H(56)	114.3
C(56)-C(57)-C(52)	110.6(12)
C(56)-C(57)-H(57)	124.7
C(52)-C(57)-H(57)	124.7
C(52)-C(58)-H(58A)	110.6
C(52)-C(58)-H(58B)	110.9
H(58A)-C(58)-H(58B)	108.3
C(52)-C(58)-H(58C)	110.5
H(58A)-C(58)-H(58C)	108.3
H(58B)-C(58)-H(58C)	108.2

Table **S7**. Anisotropic displacement parameters (A^2 x 10^3) for **3**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12

Sc(1)	58(1)	49(1)	56(1)	3(1)	15(1)	7(1)
N(1)	64(4)	62(3)	51(4)	6(3)	21(3)	9(3)
N(2)	67(4)	69(4)	48(3)	15(3)	17(3)	17(3)
N(3)	80(4)	57(3)	55(4)	-2(3)	29(3)	7(3)
N(4)	78(4)	69(4)	56(4)	-12(3)	19(3)	2(3)
N(5)	117(5)	71(5)	90(5)	-16(4)	-5(4)	2(4)
N(6)	65(3)	43(3)	74(4)	0(3)	21(3)	10(3)
C(1)	83(6)	146(8)	97(6)	10(6)	31(5)	-30(5)
C(2)	63(5)	76(5)	85(6)	-4(4)	32(5)	3(4)
C(3)	68(5)	86(5)	70(5)	-8(4)	11(4)	-8(4)
C(4)	61(5)	83(5)	52(5)	-1(4)	8(4)	10(4)
C(5)	94(6)	119(7)	71(6)	6(5)	0(5)	3(5)
C(6)	86(6)	99(6)	73(5)	14(5)	13(5)	19(5)
C(7)	111(6)	63(5)	65(5)	15(4)	38(5)	10(5)
C(11)	59(4)	68(5)	66(5)	13(4)	27(4)	7(3)
C(12)	51(4)	81(5)	61(5)	9(4)	14(4)	8(4)
C(13)	95(6)	97(6)	62(5)	3(5)	26(5)	1(5)
C(14)	99(6)	106(6)	57(5)	8(5)	14(4)	-7(5)
C(15)	89(6)	107(7)	67(6)	40(5)	26(5)	14(5)
C(16)	78(5)	91(6)	73(6)	27(5)	35(4)	17(4)
C(17)	148(8)	103(7)	92(6)	42(6)	58(6)	63(6)
C(18)	249(13)	90(7)	181(11)	22(7)	66(10)	37(8)
C(19)	160(10)	149(9)	242(13)	105(9)	94(9)	84(8)
C(20)	67(5)	85(6)	76(5)	6(4)	27(4)	21(4)
C(21)	133(7)	85(6)	111(7)	4(5)	35(6)	32(5)
C(22)	92(7)	161(9)	141(9)	50(7)	21(6)	36(6)
C(31)	86(5)	96(6)	94(6)	-22(5)	44(5)	-30(5)
C(32)	93(5)	81(5)	85(5)	-5(5)	38(4)	5(4)
C(33)	101(6)	91(6)	64(5)	1(5)	29(4)	21(5)
C(34)	110(6)	67(5)	71(6)	-14(5)	18(5)	13(5)
C(35)	97(6)	61(5)	82(6)	-8(4)	28(5)	14(4)
C(36)	90(6)	77(6)	85(6)	3(5)	11(5)	5(5)
C(37)	115(7)	70(5)	87(6)	7(5)	42(6)	11(5)
C(38)	115(7)	122(7)	71(6)	-11(5)	0(5)	8(5)
C(39)	190(10)	67(6)	161(10)	-29(6)	-35(8)	16(6)
C(40)	65(4)	49(4)	61(4)	2(4)	26(3)	2(4)
C(41)	70(5)	48(4)	75(5)	1(4)	21(4)	-2(4)
C(42)	94(6)	48(4)	95(6)	-3(4)	30(5)	-5(4)
C(43)	99(6)	55(5)	100(6)	4(4)	26(5)	16(4)
C(44)	71(5)	75(5)	80(5)	1(4)	12(4)	19(4)
C(45)	67(4)	51(4)	66(4)	-1(3)	25(4)	12(3)
C(46)	72(5)	83(5)	79(6)	-27(4)	18(4)	13(4)
C(47)	134(7)	153(8)	64(6)	-33(6)	11(5)	-26(6)
C(48)	102(6)	93(6)	107(7)	-14(5)	28(5)	-17(5)

C(49)	84(6)	68(5)	88(6)	-10(4)	19(5)	-4(4)
C(50)	93(7)	169(9)	128(9)	19(8)	-4(6)	3(6)
C(51)	95(7)	130(8)	225(12)	13(8)	57(7)	-39(6)

Table **S8**. Torsion angles [deg] for **3**.

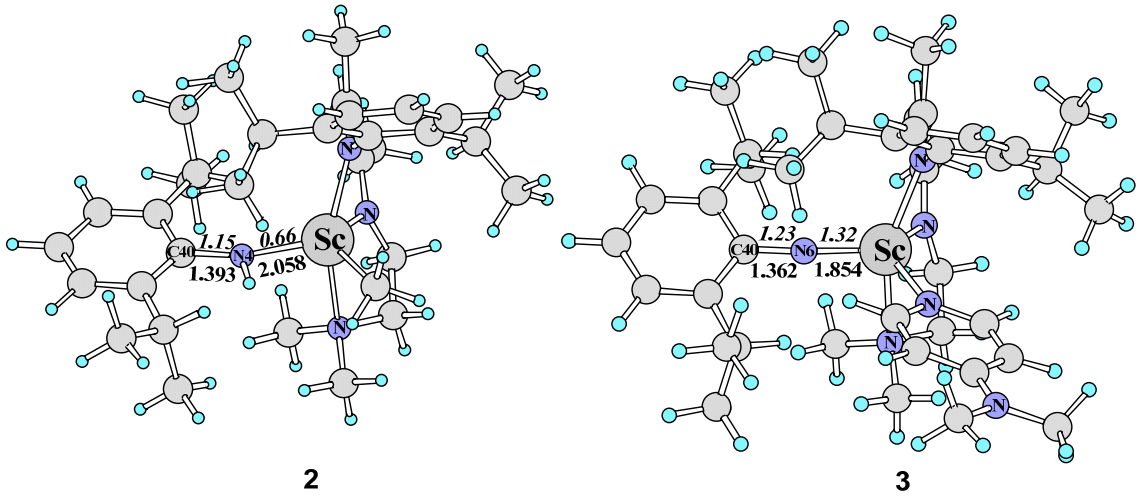
N(6)-Sc(1)-N(1)-C(2)	-85.2(5)
N(2)-Sc(1)-N(1)-C(2)	35.1(5)
N(4)-Sc(1)-N(1)-C(2)	162.1(5)
N(3)-Sc(1)-N(1)-C(2)	65.8(7)
N(6)-Sc(1)-N(1)-C(11)	85.5(5)
N(2)-Sc(1)-N(1)-C(11)	-154.2(5)
N(4)-Sc(1)-N(1)-C(11)	-27.2(5)
N(3)-Sc(1)-N(1)-C(11)	-123.5(5)
N(6)-Sc(1)-N(2)-C(4)	68.3(5)
N(1)-Sc(1)-N(2)-C(4)	-36.8(5)
N(4)-Sc(1)-N(2)-C(4)	-126.6(5)
N(3)-Sc(1)-N(2)-C(4)	156.4(5)
N(6)-Sc(1)-N(2)-C(6)	-96.1(5)
N(1)-Sc(1)-N(2)-C(6)	158.8(5)
N(4)-Sc(1)-N(2)-C(6)	69.0(5)
N(3)-Sc(1)-N(2)-C(6)	-8.0(5)
N(6)-Sc(1)-N(3)-C(31)	-87.1(5)
N(2)-Sc(1)-N(3)-C(31)	152.5(5)
N(1)-Sc(1)-N(3)-C(31)	120.8(6)
N(4)-Sc(1)-N(3)-C(31)	23.4(5)
N(6)-Sc(1)-N(3)-C(32)	34.4(4)
N(2)-Sc(1)-N(3)-C(32)	-86.0(4)
N(1)-Sc(1)-N(3)-C(32)	-117.7(5)
N(4)-Sc(1)-N(3)-C(32)	144.9(4)
N(6)-Sc(1)-N(3)-C(7)	150.8(4)
N(2)-Sc(1)-N(3)-C(7)	30.4(4)
N(1)-Sc(1)-N(3)-C(7)	-1.3(7)
N(4)-Sc(1)-N(3)-C(7)	-98.7(4)
N(6)-Sc(1)-N(4)-C(37)	-17.2(6)
N(2)-Sc(1)-N(4)-C(37)	176.4(5)
N(1)-Sc(1)-N(4)-C(37)	91.8(5)
N(3)-Sc(1)-N(4)-C(37)	-113.7(5)
N(6)-Sc(1)-N(4)-C(33)	151.3(5)
N(2)-Sc(1)-N(4)-C(33)	-15.1(6)
N(1)-Sc(1)-N(4)-C(33)	-99.7(5)
N(3)-Sc(1)-N(4)-C(33)	54.8(6)

N(2)-Sc(1)-N(6)-C(40)	-13(3)
N(1)-Sc(1)-N(6)-C(40)	79(2)
N(4)-Sc(1)-N(6)-C(40)	179(9)
N(3)-Sc(1)-N(6)-C(40)	-89(2)
C(11)-N(1)-C(2)-C(3)	168.8(6)
Sc(1)-N(1)-C(2)-C(3)	-20.4(9)
C(11)-N(1)-C(2)-C(1)	-11.9(9)
Sc(1)-N(1)-C(2)-C(1)	158.9(5)
N(1)-C(2)-C(3)-C(4)	-11.2(12)
C(1)-C(2)-C(3)-C(4)	169.4(7)
C(6)-N(2)-C(4)-C(3)	-172.4(6)
Sc(1)-N(2)-C(4)-C(3)	23.1(9)
C(6)-N(2)-C(4)-C(5)	6.0(9)
Sc(1)-N(2)-C(4)-C(5)	-158.5(5)
C(2)-C(3)-C(4)-N(2)	10.1(12)
C(2)-C(3)-C(4)-C(5)	-168.4(7)
C(4)-N(2)-C(6)-C(7)	177.9(6)
Sc(1)-N(2)-C(6)-C(7)	-16.7(7)
C(31)-N(3)-C(7)-C(6)	-178.8(5)
C(32)-N(3)-C(7)-C(6)	63.0(7)
Sc(1)-N(3)-C(7)-C(6)	-49.5(6)
N(2)-C(6)-C(7)-N(3)	46.5(8)
C(2)-N(1)-C(11)-C(16)	93.2(7)
Sc(1)-N(1)-C(11)-C(16)	-77.9(7)
C(2)-N(1)-C(11)-C(12)	-90.1(7)
Sc(1)-N(1)-C(11)-C(12)	98.8(6)
C(16)-C(11)-C(12)-C(13)	-2.0(10)
N(1)-C(11)-C(12)-C(13)	-178.7(6)
C(16)-C(11)-C(12)-C(20)	-178.6(6)
N(1)-C(11)-C(12)-C(20)	4.7(9)
C(11)-C(12)-C(13)-C(14)	2.7(11)
C(20)-C(12)-C(13)-C(14)	179.3(6)
C(12)-C(13)-C(14)-C(15)	-2.1(11)
C(13)-C(14)-C(15)-C(16)	0.8(12)
C(14)-C(15)-C(16)-C(11)	-0.2(11)
C(14)-C(15)-C(16)-C(17)	-177.6(7)
C(12)-C(11)-C(16)-C(15)	0.8(10)
N(1)-C(11)-C(16)-C(15)	177.4(6)
C(12)-C(11)-C(16)-C(17)	178.1(7)
N(1)-C(11)-C(16)-C(17)	-5.2(10)
C(15)-C(16)-C(17)-C(19)	-59.6(9)
C(11)-C(16)-C(17)-C(19)	123.1(8)
C(15)-C(16)-C(17)-C(18)	63.7(11)
C(11)-C(16)-C(17)-C(18)	-113.5(8)

C(13)-C(12)-C(20)-C(22)	-80.0(9)
C(11)-C(12)-C(20)-C(22)	96.6(8)
C(13)-C(12)-C(20)-C(21)	43.4(9)
C(11)-C(12)-C(20)-C(21)	-140.0(6)
C(37)-N(4)-C(33)-C(34)	2.2(10)
Sc(1)-N(4)-C(33)-C(34)	-167.1(5)
N(4)-C(33)-C(34)-C(35)	-0.5(12)
C(39)-N(5)-C(35)-C(36)	175.0(8)
C(38)-N(5)-C(35)-C(36)	-0.7(12)
C(39)-N(5)-C(35)-C(34)	-6.6(12)
C(38)-N(5)-C(35)-C(34)	177.7(7)
C(33)-C(34)-C(35)-N(5)	179.1(7)
C(33)-C(34)-C(35)-C(36)	-2.5(11)
N(5)-C(35)-C(36)-C(37)	-177.8(7)
C(34)-C(35)-C(36)-C(37)	3.7(11)
C(33)-N(4)-C(37)-C(36)	-0.8(11)
Sc(1)-N(4)-C(37)-C(36)	168.9(6)
C(35)-C(36)-C(37)-N(4)	-2.2(12)
Sc(1)-N(6)-C(40)-C(41)	-22(3)
Sc(1)-N(6)-C(40)-C(45)	158(2)
N(6)-C(40)-C(41)-C(42)	178.8(6)
C(45)-C(40)-C(41)-C(42)	-1.6(9)
N(6)-C(40)-C(41)-C(49)	0.6(9)
C(45)-C(40)-C(41)-C(49)	-179.9(6)
C(40)-C(41)-C(42)-C(43)	0.4(11)
C(49)-C(41)-C(42)-C(43)	178.6(7)
C(41)-C(42)-C(43)-C(44)	0.3(11)
C(42)-C(43)-C(44)-C(45)	0.2(11)
C(43)-C(44)-C(45)-C(40)	-1.5(10)
C(43)-C(44)-C(45)-C(46)	-178.2(7)
N(6)-C(40)-C(45)-C(44)	-178.3(6)
C(41)-C(40)-C(45)-C(44)	2.1(9)
N(6)-C(40)-C(45)-C(46)	-1.7(9)
C(41)-C(40)-C(45)-C(46)	178.8(6)
C(44)-C(45)-C(46)-C(47)	-55.4(9)
C(40)-C(45)-C(46)-C(47)	128.0(7)
C(44)-C(45)-C(46)-C(48)	69.7(8)
C(40)-C(45)-C(46)-C(48)	-106.9(7)
C(42)-C(41)-C(49)-C(50)	-78.7(9)
C(40)-C(41)-C(49)-C(50)	99.5(8)
C(42)-C(41)-C(49)-C(51)	47.3(10)
C(40)-C(41)-C(49)-C(51)	-134.5(7)
C(57)-C(52)-C(53)-C(54)	4(3)
C(58)-C(52)-C(53)-C(54)	178.3(17)

C(52)-C(53)-C(54)-C(55)	-1(2)
C(53)-C(54)-C(55)-C(56)	2(2)
C(54)-C(55)-C(56)-C(57)	-7(3)
C(55)-C(56)-C(57)-C(52)	10(3)
C(53)-C(52)-C(57)-C(56)	-8(3)
C(58)-C(52)-C(57)-C(56)	177.1(16)

Theoretical Calculation. Density functional theory (DFT)[3] studies have been performed with the Gaussian03 program[4] using the B3LYP[5] method. The 6-311G* basis set was used for the C, H and N, and the LanL2DZ basis set with Effective Core Potential (ECP)[6] was used for the Sc. The NBO charges and the Wiberg bond order were calculated by NBO natural bonding analysis.[7] The structure of **2** and **3** obtained by the X-ray diffraction was used as the initio structure to do the optimization. The molecule orbitals were depicted using isodensity at 0.04 au.



2 **3**

Bond angle(in degree): Sc-N4-C40 155.1 Sc-N6-C40 170.3

Fig. S1. The optimized structures of **2** and **3** with selected bond length and Wiberg bond order (in italic). Calculated at B3LYP/6-311G*/Lanl2DZ level.

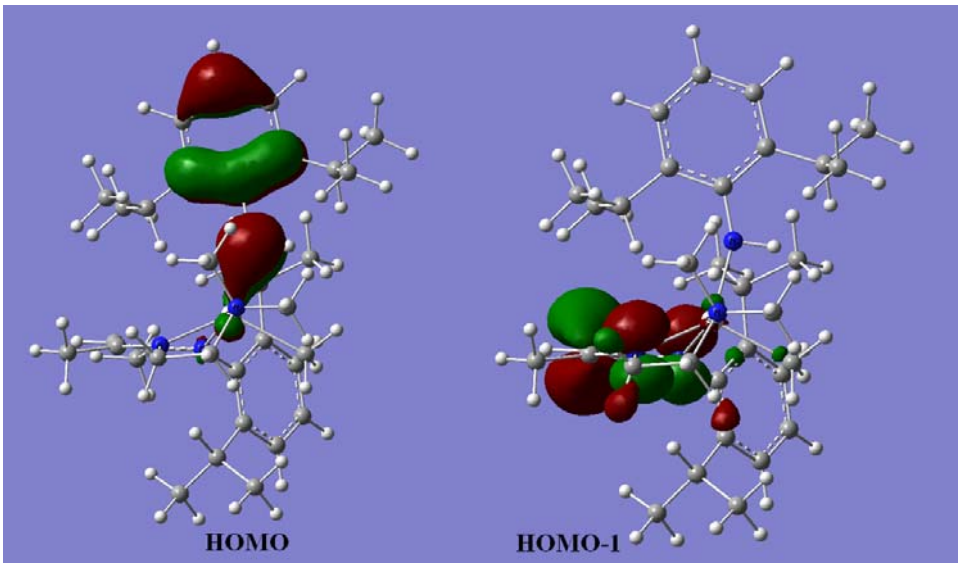


Fig. S2. HOMO and HOMO-1 of **2**. Calculated at B3LYP/6-311G*/Lanl2DZ level.

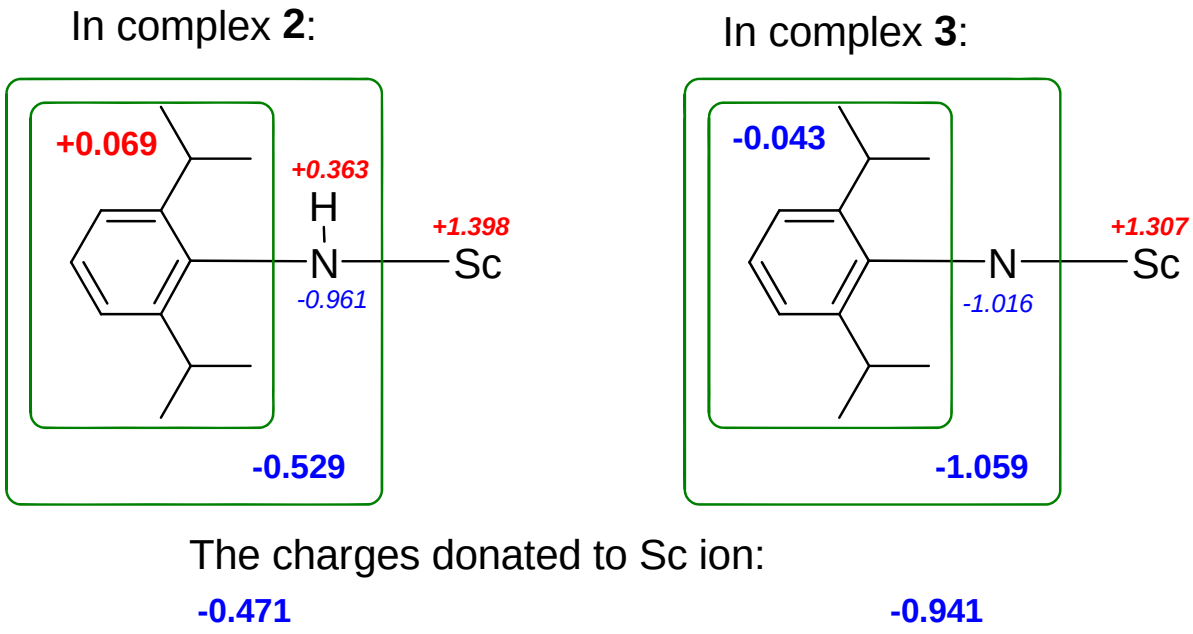


Fig. S3. The NBO charge distribution in anilido group and imido group of **2** and **3**, respectively. Calculated at B3LYP/6-311G*/Lanl2DZ level.

Calculated total energies and geometrical coordinates calculated at B3LYP/6-311G*/Lanl2DZ level:

2

E(RB+HF-LYP) =-1594.67391779 Hartree

Sc,0,0.1801800247,0.7765296504,-0.746946193
N,0,1.7065364523,-0.2238105687,0.5474413787
N,0,1.0026437415,2.6104157864,0.1934372009
N,0,-0.7417899958,2.6921365458,-1.9780423709
N,0,-1.6614165447,-0.0949599565,-0.4592647253
C,0,2.7363710505,-0.6864150498,2.7471559068
C,0,2.0131109209,0.2183533898,1.7667499467
C,0,1.7427628022,1.5252381739,2.2224095333
C,0,1.4048305266,2.6579840711,1.4656649128
C,0,1.552452824,3.9961022807,2.1657419594
C,0,0.8975038445,3.8761032074,-0.5349456158
C,0,0.4038860797,3.6250016051,-1.9540211289
C,0,2.3945341226,-1.4039366534,0.0787245649
C,0,3.6837876832,-1.2449770029,-0.4896984013
C,0,4.3650874604,-2.379638241,-0.9346342288
C,0,3.8009436404,-3.6455046299,-0.840996038
C,0,2.5284106391,-3.7852600555,-0.3073312447
C,0,1.801600839,-2.6832495574,0.1565740233
C,0,4.3498337594,0.1216929769,-0.6473501014
C,0,5.6151135525,0.2578089604,0.2203209663
C,0,4.6797272619,0.4271378739,-2.1204137871
C,0,0.3976631091,-2.9149111952,0.7067999558
C,0,0.3930085553,-3.8144199271,1.9570529575
C,0,-0.5288004431,-3.5089673824,-0.3698022967
C,0,-1.9005190849,3.2295922662,-1.2384286015
C,0,-1.1412228419,2.4368249157,-3.3728464592
C,0,0.8364522676,-0.0500082364,-2.7161600569
C,0,-2.8429059946,-0.3540168534,0.2315108025
C,0,-3.0124365098,0.103720398,1.568447596
C,0,-4.2179275659,-0.1292603569,2.2312188858
C,0,-5.2674673101,-0.8113120897,1.6318785273
C,0,-5.0974858904,-1.2869866714,0.3367755863
C,0,-3.9167799103,-1.0831684412,-0.3757880239
C,0,-1.9007451244,0.819654321,2.3233447942
C,0,-1.4019814583,-0.0120903601,3.5187002024
C,0,-2.3100558161,2.2302559766,2.7814359101

C,0,-3.8121899766,-1.6015762091,-1.8100039401
C,0,-4.587422887,-2.9032605953,-2.0689745773
C,0,-4.2398773983,-0.5203496398,-2.8218113127
H,0,-1.7016537717,-0.5708487037,-1.3615707022
H,0,2.1733751429,-1.6073639212,2.9089565446
H,0,2.8790877566,-0.1942151439,3.7083682437
H,0,3.7143543694,-0.98646881,2.3671116383
H,0,1.989868081,1.7155407732,3.2581620742
H,0,2.3204227965,4.6109834252,1.6863806813
H,0,1.8360960045,3.866349312,3.2088003832
H,0,0.6219647557,4.5709971296,2.1366151382
H,0,1.8679794797,4.3849206312,-0.6029653991
H,0,0.2235154303,4.5789847054,-0.0302192301
H,0,0.1410367753,4.5819781859,-2.4316631235
H,0,1.1996188951,3.1703112525,-2.5502694346
H,0,5.355604276,-2.2707533209,-1.3654140028
H,0,4.3473185779,-4.5163538009,-1.1899211124
H,0,2.0854698168,-4.7742178556,-0.2463926989
H,0,3.6397916432,0.8792527761,-0.3119326328
H,0,5.3999491322,0.1124194588,1.2814222422
H,0,6.0539332426,1.2541488188,0.1062126861
H,0,6.3787477527,-0.4721683673,-0.0648246303
H,0,5.0650163246,1.4471310454,-2.2208416834
H,0,3.7961434584,0.3320202719,-2.7536620542
H,0,5.4441517843,-0.2490787125,-2.5144685258
H,0,-0.0190252264,-1.9469750763,0.9895503597
H,0,0.7570152021,-4.8210603153,1.7307568841
H,0,-0.6227185146,-3.9132183288,2.3512248053
H,0,1.0215659334,-3.4132266307,2.7558005728
H,0,-0.5154087507,-2.9062862781,-1.2799107692
H,0,-1.5588160913,-3.5522268045,-0.0059101666
H,0,-0.2280445543,-4.5248981608,-0.6429563292
H,0,-2.2232026956,4.196142979,-1.6525439845
H,0,-1.6575949922,3.3621232087,-0.1855393053
H,0,-2.7237814819,2.5201150047,-1.2990668503
H,0,-1.5100888807,3.3561961756,-3.8505868458
H,0,-1.9345766238,1.6908953225,-3.3974735145
H,0,-0.2954991068,2.0563954892,-3.9409365337
H,0,1.4080907411,-0.9750373267,-2.5716387705
H,0,1.49385276,0.626422857,-3.2828577128
H,0,0.0080276871,-0.3045857524,-3.3926355491
H,0,-4.3360906224,0.2274827607,3.2506613755
H,0,-6.1969708564,-0.9804457294,2.1660292148
H,0,-5.91076604,-1.8338500013,-0.1281724433

H,0,-1.0506558401,0.9381983439,1.6478577342
H,0,-2.1960020762,-0.163260126,4.2558051423
H,0,-0.5681623321,0.4871341379,4.0204409324
H,0,-1.0613713013,-0.9990632089,3.1967126256
H,0,-2.6775639861,2.832113288,1.9460313709
H,0,-1.4606495601,2.7521478262,3.2338265186
H,0,-3.1075755194,2.1944115125,3.5290303257
H,0,-2.7638075,-1.8494859564,-2.0145218077
H,0,-4.3398434981,-3.6709483198,-1.3319973956
H,0,-4.3405551445,-3.2949904088,-3.0600927456
H,0,-5.6702348069,-2.7530841016,-2.0467819909
H,0,-5.3013784053,-0.2840344223,-2.702165582
H,0,-4.0816814034,-0.8522931572,-3.8533676298
H,0,-3.6809968467,0.4068215652,-2.6747416538

3

E(RB+HF-LYP) = -1936.50616089 Hartree

Sc,0,-0.3985818385,-0.1846977742,0.9327761189
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N,0,-1.0979618224,-1.6777147052,2.4615438641
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N,0,1.7458844164,0.7426357949,0.6278423433
N,0,5.4668295438,2.6180014505,0.0425446666
N,0,-1.5973728651,0.9367619726,0.0715199088
C,0,-0.9266878161,-4.1248006232,-1.373504147
C,0,-0.8434265214,-3.1075645019,-0.2454119317
C,0,-1.7123215832,-3.3660876854,0.8374227014
C,0,-1.7634051485,-2.7802024615,2.1123484512
C,0,-2.6250741467,-3.499717074,3.1352266191
C,0,-1.1074949506,-1.2939767569,3.8707108105
C,0,-0.2190003329,-0.0755642102,4.0961612174
C,0,0.9991803214,-2.039819472,-1.3323401164
C,0,2.278386596,-2.566478004,-1.0098949561
C,0,3.2972604132,-2.4909172575,-1.961581806
C,0,3.0829347205,-1.9078807666,-3.2052215624
C,0,1.8287879528,-1.4031638075,-3.5136264546
C,0,0.7674794322,-1.4625184576,-2.6026795527
C,0,-0.6001030484,-0.9439074188,-3.0404501881
C,0,-1.1438490635,-1.7367199562,-4.2456091735
C,0,-0.5771754301,0.5578692534,-3.3686573511
C,0,2.5446584514,-3.2417770964,0.3352569312
C,0,3.9734084667,-3.0224523749,0.8626784736

C,0,2.2546691208,-4.7554832916,0.2839928764
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C,0,-1.8697198719,1.5076386318,3.2556091348
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C,0,4.2628417205,2.0079975723,0.2296010127
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C,0,1.9195218037,1.7083439255,-0.2969549344
C,0,5.6130940276,3.6495910902,-0.9766047656
C,0,6.6231418258,2.2166739904,0.8315642559
C,0,-2.640738369,1.634758669,-0.4582177913
C,0,-3.8766173851,0.9871296371,-0.8189156178
C,0,-4.9215195085,1.7232986269,-1.370909963
C,0,-4.8239107038,3.0950433272,-1.5937519696
C,0,-3.6448419009,3.7404873928,-1.2386711829
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H,0,-1.7215271437,-3.8277892102,-2.0648282711
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H,0,-2.3549942824,-4.226936347,0.7025302723
H,0,-2.019816265,-3.8985102711,3.9557880024
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H,0,-3.362461813,-2.8262465883,3.5817413809
H,0,-0.728956215,-2.0965056083,4.5187009706
H,0,-2.1221710792,-1.0760443246,4.2286635766
H,0,-0.3458687346,0.289367443,5.1289303859
H,0,0.8316025965,-0.364455083,3.9845074158
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H,0,3.8886469417,-1.8568274856,-3.9316080573
H,0,1.6604005514,-0.9615371332,-4.4908471845
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H,0,-2.1663611486,-1.4232058712,-4.4751537391
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H,0,4.7102599266,-3.6078312503,0.3047711524
H,0,4.0425063563,-3.3442446908,1.9066689043
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H,0,2.8884436225,-5.24644312,-0.4614614859
H,0,0.2919164257,2.5911587454,4.3063737082
H,0,0.2949134989,2.8653059957,2.5487227469
H,0,1.4762921498,1.765671847,3.2710768737
H,0,-2.5905263285,0.7284926676,3.0202536412
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H,0,-2.0524145352,1.8757755881,4.2773960461
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H,0,4.888079963,0.6444682304,1.8216844342
H,0,3.1533027453,3.1081124307,-1.2989911097
H,0,1.0386291451,1.970550655,-0.867294118
H,0,5.4054925423,3.2611264355,-1.9792542476
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H,0,6.4564834828,2.3758642958,1.9022964777
H,0,7.4830885208,2.8136716979,0.5364942125
H,0,6.8758030449,1.1624092781,0.6746732872
H,0,-5.8460782621,1.2158381477,-1.6346261135
H,0,-5.6510921876,3.6471233284,-2.0297509512
H,0,-3.5629988679,4.8132360608,-1.4022677842
H,0,-0.6500900157,3.1062677322,0.179595229
H,0,-0.3548176852,3.5936466445,-2.2598418628
H,0,0.3626342509,4.8735999804,-1.2605665181
H,0,-1.1895826573,5.1284938753,-2.0636513114
H,0,-2.2273148498,5.7370618616,0.2771663033
H,0,-0.6535567584,5.4448438254,1.0179160648
H,0,-2.0893900502,4.5829904495,1.5975521891
H,0,-3.0573822494,-0.9195013507,-0.4305601103
H,0,-4.2763330522,-0.2191632975,1.6075886197
H,0,-4.8555461476,-1.7917915214,1.0333531828
H,0,-5.8146405497,-0.3279420652,0.747546375
H,0,-4.7449459849,-2.3425808049,-1.4736087447
H,0,-4.2628441003,-1.0987721081,-2.6375882662
H,0,-5.8065650221,-0.9757494184,-1.7933411691

To confirm the reliability of the method used in the calculation, the structures of **2** and **3** were fully optimized using the methods and basis sets listed in Table S9. These methods gave similar results, which are consistent well with the experimental values (bond lengths (Å) and bond angle (^{o})). Fig S3 and Fig S4 show the HOMO and HOMO-1 of **2** and **3**, respectively (calculated at BP86/6-311G**/SDD level), they are similar to those calculated at B3LYP/6-311G*/Lanl2DZ level. Therefore, the calculation results are not sensitive to the selection of basis sets (Lanl2DZ vs. SDD, 6-311G* vs. 6-311G**) and the exchange-correlation functional (B3LYP vs. BP86).[8]

Table **S9.** Selected bond lengths (Å) and bond angles (^{o}) of **2** and **3**.

Complex **2**	C40-N4	N4-Sc	C40-N4-Sc	N4-H
B3LYP/Lanl2DZ/6-311G*	1.393	2.058	155.1	1.021
B3LYP/Lanl2DZ/6-311G**	1.394	2.057	155.2	1.021
B3LYP/SDD/6-311G*	1.394	2.060	155.3	1.021
B3LYP/SDD/6-311G**	1.394	2.058	155.8	1.021
BP86/SDD/6-311G*	1.397	2.062	155.0	1.033
BP86/SDD/6-311G**	1.397	2.059	155.4	1.033
Exp.	1.391	2.047	153.7	

Complex **3**	C40-N6	N6-Sc	C40-N6-Sc
B3LYP/Lanl2DZ/6-311G*	1.362	1.854	170.3
B3LYP/Lanl2DZ/6-311G**	1.363	1.855	169.2
B3LYP/SDD/6-311G*	1.362	1.853	168.8
B3LYP/SDD/6-311G**	1.362	1.854	168.7
BP86/SDD/6-311G*	1.365	1.863	167.8
BP86/SDD/6-311G**	1.365	1.864	167.8
Exp.	1.357	1.881	169.6

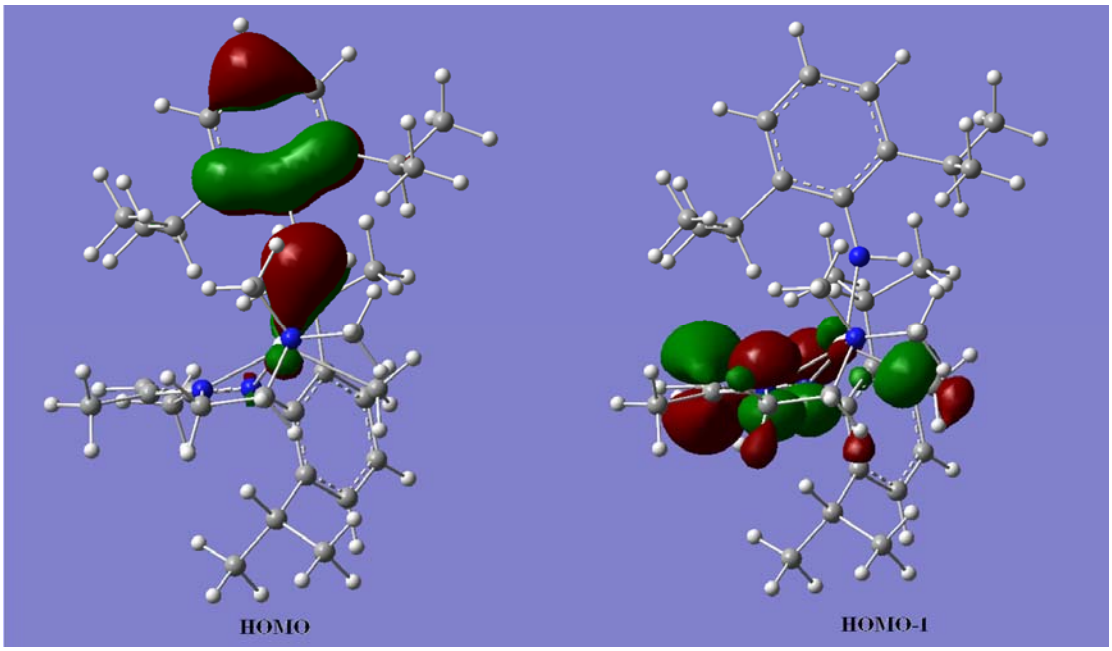

Fig. S3. HOMO and HOMO-1 of **2**. Calculated at BP86/6-311G**/SDD level.

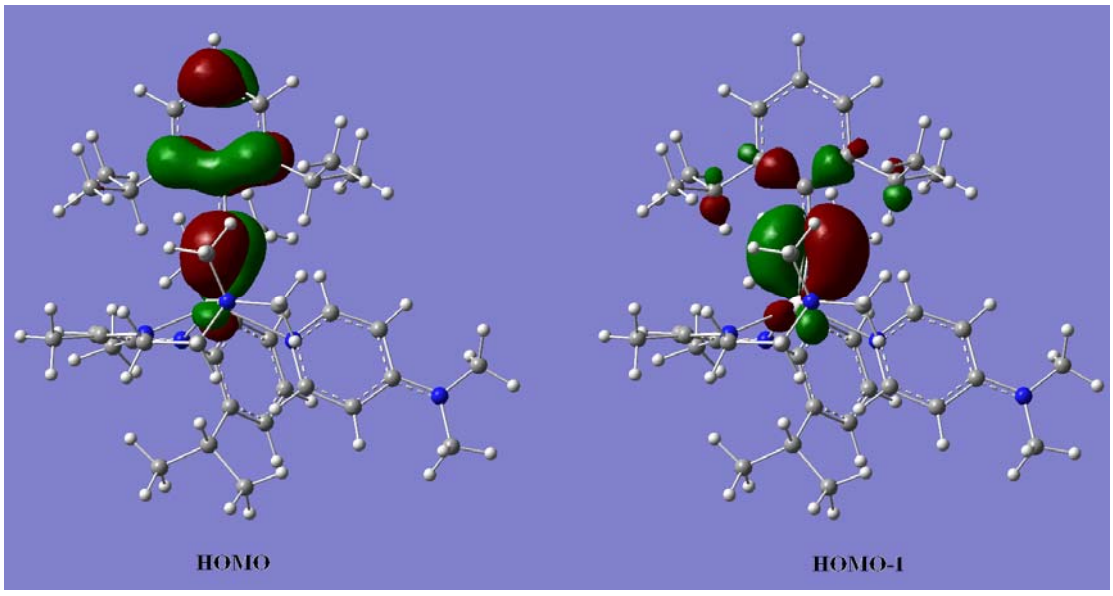

Fig. S4. HOMO and HOMO-1 of **3**. Calculated at BP86/6-311G**/SDD level.

Calculated total energies and geometrical coordinates at BP86/6-311G**/SDD level:

2

E(RB-P86) = -1595.02653535 Hartree

Sc,0.1863558784,0.770665171,-0.76087173 87
N,1.7035618807,-0.2181981237,0.5474879435
N,1.0061729666,2.60974022 95,0.1766370077
N,-0.7517464902,2.6734320003,-1.9769890701
N,-1.654325 7444,-0.1012128392,-0.4597524571
C,2.7384648992,-0.6827113612,2.756347 228
C,2.0105653866,0.2244903216,1.7791619811
C,1.7354711503,1.53793240 98,2.2305374102
C,1.4018215557,2.6729620174,1.4613034081
C,1.548723966 2,4.0205085415,2.1489015205
C,0.9021348449,3.8769643897,-0.5599904862
C,0.3962886978,3.6143534396,-1.9779105296
C,2.394230655,-1.4002738161, 0.0823263847
C,3.6973632245,-1.244207284,-0.4748223565
C,4.3788997245, -2.3860545227,-0.9257411685
C,3.8029393218,-3.6563389648,-0.846387176
C,2.5170429188,-3.7930176307,-0.3220462561
C,1.788787817,-2.6836841815 ,0.1453081972
C,4.3692530592,0.1240097334,-0.617047096
C,5.6481725438, 0.2357651771,0.2423897864
C,4.6888575023,0.4439238705,-2.0943867573
C, 0.3773491086,-2.9057909974,0.6871346945
C,0.3646701534,-3.8048882761,1 .9432813839
C,-0.5439146214,-3.5021319324,-0.3990467223
C,-1.902829419 4,3.2160774372,-1.2163576289
C,-1.1757267892,2.4162001906,-3.371018278 1
C,0.8588783033,-0.0429421984,-2.7309691749
C,-2.8387986348,-0.359995 0933,0.2334425628
C,-3.005361896,0.1012020834,1.5783978521
C,-4.215159 8314,-0.1337901481,2.2484020823
C,-5.2719156685,-0.8220438266,1.648713 401
C,-5.1049155649,-1.3003944329,0.345352186
C,-3.9201817318,-1.09284 25664,-0.3742252244
C,-1.8874514659,0.8199031512,2.3270335475
C,-1.387 0691529,-0.0109175843,3.5282959549
C,-2.2987395687,2.2356982226,2.7824 161252

C,-3.8147142705,-1.6016180132,-1.8138255105
C,-4.5886872667,-2. 9077789172,-2.079382919
C,-4.251140778,-0.5079464136,-2.8162322356
H,- 1.6984509347,-0.5918636096,-1.367702976
H,2.2177793861,-1.6474391229,2 .8546202911
H,2.8143250544,-0.2142909814,3.7466537809
H,3.7552312821,- 0.9129383857,2.4010870656
H,1.9811670372,1.7349077577,3.2747734051
H,2 .3333909707,4.6284453514,1.6668319949
H,1.8206494141,3.8952226618,3.20 47637622
H,0.6147198199,4.6055320357,2.0985205637
H,1.8813867188,4.388 3641898,-0.6364371319
H,0.2240872867,4.5891498346,-0.0511197727
H,0.12 16038147,4.5744671886,-2.4651800803
H,1.1905605522,3.145895949,-2.5833 501155
H,5.3812008085,-2.2754076342,-1.3502880775
H,4.3511647438,-4.53 41195396,-1.1991712053
H,2.0616289392,-4.7863057919,-0.2696602833
H,3. 6554869021,0.8835494577,-0.2606558194
H,5.4409677524,0.064804873,1.310 2815883
H,6.0939022383,1.2398187618,0.1429964183
H,6.4074616356,-0.499 5452031,-0.0732273514
H,5.0986425621,1.4641241193,-2.1862468064
H,3.78 74581093,0.3721176179,-2.7209992315
H,5.4394198964,-0.2527212677,-2.50 40066233
H,-0.037856465,-1.9231433163,0.9638018723
H,0.7447141667,-4.8 152242226,1.7162448139
H,-0.663112778,-3.9120159954,2.327307984
H,0.98 66318914,-3.3921207489,2.7534445243
H,-0.5217588318,-2.8916363447,-1.3 147809889
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H,-1.6343748518,3.3527560329,-0.1596887594
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H,-0.3299057846,2.0258160587,-3.9511726 924
H,1.4583158697,-0.9590940306,-2.57334952
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H,0.0302298178,-0.3212374419,-3.4115915845
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H,-1.0430906856,-1.0056374272,3.20508 50441
H,-2.6714304821,2.8381838361,1.9386474341
H,-1.4428987067,2.7616 09638,3.2384182333
H,-3.1035443949,2.1936828844,3.5351495386
H,-2.7535 128618,-1.84203729,-2.0197850384
H,-4.3228450204,-3.688279677,-1.34971 25408
H,-4.3566241425,-3.2862715875,-3.0883571459
H,-5.679592272,-2.75 58627457,-2.0331871452
H,-5.3229184953,-0.2823646055,-2.6886354162
H,- 4.0880974197,-0.8280573157,-3.8595903888
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3

E(RB-P86) = -1936.86659171 Hartree

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N,-1.1109748096,-1.6969691787, 2.4443223855
N,-0.5127559794,0.9805402166,3.0631602738
N,1.7418945687, 0.7174256364,0.6191083456
N,5.459793941,2.6311577911,-0.009715504
N,-1 .5647582691,0.933105656,0.0504644874
C,-0.9051494315,-4.1553546144,-1. 3988568505
C,-0.8490423446,-3.1495216493,-0.2574358498
C,-1.7267623411 ,-3.406904797,0.8246541359
C,-1.7822823478,-2.8114451233,2.1038592622
C,-2.6407819914,-3.5267300304,3.1359187557
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C,5.5911570449,3.6556567481,-1.0453930162
C,6.6278633 8,2.2485960657,0.7809723234
C,-2.6296572459,1.6562516737,-0.4044440219
C,-3.8965938698,1.0298411425,-0.7256464109
C,-4.9698208396,1.79797646 8,-1.192090591
C,-4.8736247544,3.1853675608,-1.3639893899
C,-3.6630425 081,3.812227317,-1.0488754565
C,-2.556222137,3.0934067298,-0.577483831 4
C,-1.2618595639,3.8355855875,-0.2596710236
C,-0.5628850519,4.3400234 841,-1.5411669514
C,-1.460518614,4.9986245684,0.7349581595
C,-4.075258 2902,-0.4697061919,-0.5195730565
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C,-4.6438776689,-1.1916552325,-1.7573305957
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H,-1.2964295437,-5.1240320227,-1.0579304585
H,0 .0797422898,-4.3068291182,-1.8625823537
H,-2.3740117272,-4.2751892237, 0.6912707323
H,-2.0244809099,-3.92582189,3.9603248108
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