

Supporting Information

Cationic terminal hydrido rare earth complexes bearing an amidinate ancillary Ligand

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General Methods.

All reactions were carried out under a dry and oxygen-free argon atmosphere using Schlenk techniques and an Mbraun glovebox. The argon was purified by being passed through a Dryclean column (4 Å molecular sieves, Nikka Seiko Co.) and a Gasclean GC-XR column (Nikka Seiko Co.). The nitrogen in the glovebox was constantly circulated through a copper/molecular sieves (4 Å) catalyst unit. The oxygen and moisture concentrations in the glovebox atmosphere were monitored by O₂/H₂O Combi-Analyzer (Mbraun) to ensure both were always below 0.1 ppm. THF, toluene, hexane were obtained from Kanato Kagaku Co. and purified by use of an Mbraun SPS-800 solvent purification system, and dried over fresh Na chips in the glovebox. C₆D₅Cl and N,N'-diisopropylcarbodiimide were distilled from CaH₂ under argon and dried over molecular sieves (4 Å) in the glovebox. THF-*d*₈ was distilled from Na/K alloy/benzophenone ketyl, degassed by the freeze-pump-thaw method (three times), and dried over fresh Na chips in the glovebox. LnCl₃ (Ln = Y, Lu) were purchased from Strem Chemicals Ltd. LiCH₂SiMe₃ (1.0 M in pentane) was purchased from Aldrich. The pentane solvent was removed under vacuum and the so obtained solid LiCH₂SiMe₃ was used without further purification. H₂ gas was purchased from Suzuki Shokan Co., Ltd. and used without further purification. Other commercially available reagents were purchased and used without purification. The complexes (NCN)Ln(CH₂SiMe₃)₂(THF) (**1-Ln**, Ln = Y, Lu; NCN = PhC(NC₆H₃(Pr₂-2,6)₂)^[1] and [NEt₃H][BPh₄]^[2]) were synthesized according to the published procedures. Complexes [(NCN)Ln(CH₂SiMe₃)(THF)₃][BPh₄] (Ln = Y, **2-Y**; Lu, **2-Lu**) were generated in situ from the reaction of **1-Ln** with [NEt₃H][BPh₄] in a THF solution, as monitored by ¹H NMR.^[1b]

Samples for NMR spectroscopic measurements were prepared in the glovebox by use of J. Young valve NMR tubes. (¹H, ¹¹B, ¹³C) NMR spectra were recorded on JNM-EX 300 or JNM-EX 400. ¹H and ¹³C NMR spectra of complexes were recorded using TMS as an internal standard. The chemical shifts for ¹¹B NMR spectra was recorded based on external BF₃·OEt₂ standard. The elemental analyses were performed on a MICRO CORDER JM10 apparatus.

[(NCN)YH(THF)₃][BPh₄] (3-Y): Solid [NEt₃H][BPh₄] (90 mg, 0.21 mmol) was added in several portions to a THF solution (4 mL) of (NCN)Y(CH₂SiMe₃)₂(THF) (**1-Y**) (165 mg, 0.21 mmol) at room temperature. The colorless mixture was stirred for 1h. After filtration, the mixture was charged into a glass tube in a medium-pressure autoclave with a magnetic stirring bar. The autoclave was transferred outside of the glovebox and pressurized with H₂ to 10 atm. The mixture was stirred at 0 °C for 18 h. Pressure was released and the autoclave was returned to the glovebox. After filtration, the solution was concentrated to ~2 mL, layered with hexane (4 mL), and kept at -30°C to give **3-Y** (168 mg, 0.158 mmol, 75% yield) as colorless crystalline solid. ¹H NMR (400 MHz, THF-*d*₈, 25°C): δ = 0.79 (d, *J* = 6.6 Hz, 12H, CH(CH₃)₂), 1.17 (d, *J* = 6.6 Hz, 12H, CH(CH₃)₂), 1.69 (br, THF), 3.47

(m, 4H, $\text{CH}(\text{CH}_3)_2$), 3.59 (br, THF), 6.68 (t, 7.2 Hz, 4H, p-BPh₄), 6.82 (m, 8H + 4H, m-BPh₄ + Ar-H), 7.00 (m, 5H + 2H, Ph-H + Ar-H), 7.23 (br, 8H, o-BPh₄), 7.50 (d, $J_{\text{Y-H}} = 73.4$ Hz, 1H, Y-H). ¹³C NMR (100 MHz, THF-*d*₈, 25°C): $\delta = 24.35$ (s, $\text{CH}(\text{CH}_3)_2$), 26.44 (s, $\text{CH}(\text{CH}_3)_2$), 28.91 (s, $\text{CH}(\text{CH}_3)_2$), 68.38 (s, THF), 122.06 (s, p-BPh₄), 125.10 (s, Ar), 125.51 (s, Ph), 125.90 (q, 2.8 Hz, m-BPh₄), 127.75 (s, Ph), 130.48 (s, Ar), 132.19 (s, Ph), 132.43 (s, Ar), 137.31 (s, o-BPh₄), 142.78 (s, *ispo*-Ar), 145.27 (s, *ispo*-Ph), 165.40 (q, 49.4 Hz, ipso-BPh₄), 176.66 (s, NCN). ¹¹B NMR (127 MHz, THF-*d*₈, 25°C): $\delta = -6.79$. Anal. Calcd. for (**3-Y**) C₆₇H₈₄B₁N₂O₂Y₁ (1065.13): C, 75.55; H, 7.95; N, 2.63. Found: C, 75.92; H, 8.05; N, 2.88.

[(NCN)LuH(THF)₃][BPh₄] (3-Lu): A procedure analogous to **3-Y** using [NEt₃H][BPh₄] (115 mg, 0.27 mmol) and (NCN)Lu(CH₂SiMe₃)₂(THF) (**1-Lu**) (232 mg, 0.27 mmol) gave **3-Lu** (273 mg, 0.237 mmol, 88% yield) as colorless crystalline solid. Single crystals of **3-Lu**·2THF, suitable for X-ray analysis, were grown from THF/hexane solution at -30°C. ¹H NMR (400 MHz, THF-*d*₈, 25°C): $\delta = 0.80$ (d, $J = 6.8$ Hz, 12H, $\text{CH}(\text{CH}_3)_2$), 1.16 (d, $J = 6.8$ Hz, 12H, $\text{CH}(\text{CH}_3)_2$), 1.69 (br, THF), 3.40 (m, 4H, $\text{CH}(\text{CH}_3)_2$), 3.54 (br, THF), 6.67 (t, 7.2 Hz, 4H, p-BPh₄), 6.81 (t, 7.4 Hz, 8H, m-BPh₄), 6.91 (m, 4H, Ar-H), 7.02 (m, 5H + 2H, Ph-H + Ar-H), 7.22 (br, 8H, o-BPh₄), 12.28 (s, 1H, Lu-H). ¹³C NMR (100 MHz, THF-*d*₈, 25°C): $\delta = 23.97$ (s, $\text{CH}(\text{CH}_3)_2$), 26.42 (s, $\text{CH}(\text{CH}_3)_2$), 29.15 (s, $\text{CH}(\text{CH}_3)_2$), 68.38 (s, THF), 122.11 (s, p-BPh₄), 125.05 (s, Ar), 125.35 (s, Ph), 125.90 (q, 2.8 Hz, m-BPh₄), 126.23 (s, Ar), 128.11 (s, Ph), 131.06 (s, Ar), 131.42 (s, Ph), 132.01 (s, Ar), 137.36 (s, o-BPh₄), 143.13 (s, *ispo*-Ar), 165.35 (q, 49.4 Hz, ipso-BPh₄), 177.43 (s, NCN). ¹¹B NMR (127 MHz, THF-*d*₈, 25°C): $\delta = -6.51$. Anal. Calcd. for (**3-Lu**) C₆₇H₈₄B₁N₂O₃Lu₁ (1151.19): C, 69.90; H, 7.35; N, 2.43. Found: C, 70.28; H, 7.71; N, 2.38.

[(NCN)YH(THF)₂]₂[BPh₄]₂ (4-Y): Solid of **3-Y** (50 mg, 0.047 mmol) was dissolved in C₆H₅Cl (3 mL) and was stirred at room temperature for 30 min. After removal of all the volatiles under vacuum, the residue was washed with hexane (3 x 1 mL) to give **4-Y** (44 mg, 0.022 mmol, 94% yield) as white solid. Single crystals of **4-Y**·4C₆H₅Cl suitable for X-ray analysis were grown from C₆H₅Cl at -30°C. ¹H NMR (400 MHz, C₆D₅Cl, including 25 μL THF-*d*₈, 25°C): $\delta = 0.91$ (br, 12H, $\text{CH}(\text{CH}_3)_2$), 1.11 (br, 12H, $\text{CH}(\text{CH}_3)_2$), 1.25 (br, 24H, $\text{CH}(\text{CH}_3)_2$), 1.54 (br, THF), 2.92 (br, 4H, $\text{CH}(\text{CH}_3)_2$), 3.33 (br, 4H, $\text{CH}(\text{CH}_3)_2$), 3.58 (br, THF), 6.78 (br, 8H, p-BPh₄), 7.04 (m, 16H + 8H, m-BPh₄ + Ar-H), 7.23 (m, 10H + 4H, Ph-H + Ar-H), 7.55 (t, $J_{\text{Y-H}} = 29.0$ Hz, 2H, Y-H), 7.89 (br, 16H, o-BPh₄). Due to the poor solubility in C₆D₅Cl, informative ¹³C NMR spectrum was not obtained. Anal. Calcd. for (**4-Y**) C₁₂₆H₁₅₂B₂N₄O₄Y₂ (1986.04): C, 76.20; H, 7.71; N, 2.82. Found: C, 75.97; H, 7.57; N, 3.16. The ¹H NMR of **4-Y** in THF-*d*₈ was identical with that of **3-Y**.

[(NCN)LuH(THF)₂]₂[BPh₄]₂ (4-Lu): A procedure analogous to **4-Y** using **3-Lu** (50 mg, 0.043 mmol) gave **4-Lu** (45 mg, 0.021 mmol, 96% yield). Single crystals of **4-Lu**·4C₆H₅Cl suitable for X-ray analysis were grown from C₆H₅Cl at -30°C. ¹H NMR (400 MHz, C₆D₅Cl, including 25 μL THF-*d*₈, 25°C): $\delta = 0.93$ (m, 24H, $\text{CH}(\text{CH}_3)_2$), 1.20 (br, 24H, $\text{CH}(\text{CH}_3)_2$), 1.54 (br, THF), 3.38 (m,

8H, $CH(CH_3)_2$), 3.58 (br, THF), 6.74 (br, 8H, p-BPh₄), 7.03 (m, 16H + 8H, m-BPh₄ + Ar-H), 7.19 (m, 10H + 4H, Ph-H + Ar-H), 7.84 (br, 16H, o-BPh₄), 12.52 (br, 2H, Lu-H). Due to the poor solubility in C₆D₅Cl, informative ¹³C NMR spectrum was not obtained. Anal. Calcd. for (**4-Lu**) C₁₂₆H₁₅₂B₂N₄O₄Lu₂ (2158.17): C, 70.12; H, 7.10; N, 2.60. Found: C, 70.09; H, 7.19; N, 2.66.

[(NCN)Lu{CH(NⁱPr)₂}(THF)₂][BPh₄] (5-Lu**):** The THF solution (1 mL) of N,N'-diisopropylcarbodiimide (5.5 mg, 0.043 mmol) was added dropwise to a THF solution (4 mL) of [(NCN)LuH(THF)₃][BPh₄] (**3-Lu**) (50 mg, 0.043 mmol) at room temperature. The colorless mixture was stirred for 10 min. After filtration, the solution was concentrated to ~1 mL, layered with hexane (3 mL), and kept at -30°C to give **5-Lu** (47 mg, 0.039 mmol, 90% yield) as colorless crystalline solid. Single crystals of **5-Lu**·2THF, suitable for X-ray analysis, were grown from THF/hexane solution at -30°C. ¹H NMR (400 MHz, THF-*d*₈, 25°C): δ = 0.79 (d, *J* = 6.8 Hz, 12H, CH(CH₃)₂), 0.99 (br, 12H, CH(CH₃)₂), 1.16 (d, *J* = 6.8 Hz, 12H, CH(CH₃)₂), 1.69 (br, THF), 3.16 (m, 4H, CH(CH₃)₂), 3.47 (m, 2H, CH(CH₃)₂), 3.54 (br, THF), 6.66 (t, 7.2 Hz, 4H, p-BPh₄), 6.81 (m, 8H + 4H, m-BPh₄ + Ar-H), 7.01 (m, 5H + 2H, Ph-H + Ar-H), 7.23 (br, 8H, o-BPh₄), 8.90 (s, 1H, H-NCN). ¹³C NMR (100 MHz, THF-*d*₈, 25°C): δ = 24.07 (s, CH(CH₃)₂), 25.13 (s, CH(CH₃)₂), 26.47 (s, CH(CH₃)₂), 29.19 (s, CH(CH₃)₂), 51.62 (s, CH(CH₃)₂), 68.38 (s, THF), 122.01 (s, p-BPh₄), 125.07 (s, Ar), 125.90 (m, m-BPh₄), 126.29 (s, Ph), 128.06 (s, Ph), 131.17 (s, Ar), 131.69 (s, Ph), 131.71 (s, Ar), 137.36 (s, o-BPh₄), 142.72 (s, *isop*-Ar), 143.34 (s, *isop*-Ph), 165.40 (q, 49.4 Hz, ipso-BPh₄), 170.69 (s, H-NCN), 179.21 (s, Ph-NCN). ¹¹B NMR (127 MHz, THF-*d*₈, 25°C): δ = -6.50. Anal. Calcd. for (**5-Lu**) C₇₀H₉₀B₁N₄O₂Lu₁ (1205.29): C, 69.76; H, 7.53; N, 4.65. Found: C, 69.37; H, 7.56; N, 4.49.

[(NCN)Lu(THF)₄][BPh₄]₂ (6-Lu**):** Solid [NEt₃H][BPh₄] (21 mg, 0.05 mmol) was added in one portion to a THF solution (4 mL) of [(NCN)LuH(THF)₃][BPh₄] (**3-Lu**) (57 mg, 0.05 mmol) at room temperature. The colorless mixture was stirred for 10 min. After filtration, the solution was concentrated to ~1 mL, layered with hexane (3 mL), and kept at -30°C to give **6-Lu** (71 mg, 0.046 mmol, 92% yield) as colorless crystalline solid. Single crystals of **6-Lu**·THF, suitable for X-ray analysis, were grown from THF/hexane solution at -30°C. ¹H NMR (400 MHz, THF-*d*₈, 25°C): δ = 0.74 (d, *J* = 6.8 Hz, 12H, CH(CH₃)₂), 1.16 (d, *J* = 6.8 Hz, 12H, CH(CH₃)₂), 1.69 (br, THF), 2.78 (m, 4H, CH(CH₃)₂), 3.54 (br, THF), 6.71 (t, 7.2 Hz, 8H, p-BPh₄), 6.84 (m, 16H + 4H, m-BPh₄ + Ar-H), 7.14 (m, 5H + 2H, Ph-H + Ar-H), 7.26 (br, 16H, o-BPh₄). ¹³C NMR (100 MHz, THF-*d*₈, 25°C): δ = 24.07 (s, CH(CH₃)₂), 26.54 (s, CH(CH₃)₂), 29.55 (s, CH(CH₃)₂), 68.39 (s, THF), 122.22 (s, p-BPh₄), 126.04 (m, m-BPh₄), 126.12 (s), 128.29 (s), 128.45 (s), 129.37 (s), 131.97 (s), 132.54 (s), 137.30 (s, o-BPh₄), 141.49 (s), 142.59 (s), 165.25 (q, 49.4 Hz, ipso-BPh₄), 181.52 (s, NCN). ¹¹B NMR (127 MHz, THF-*d*₈, 25°C): δ = -6.48. Anal. Calcd. for (**6-Lu**) C₉₅H₁₁₁B₂N₂O₄Lu₁ (1541.52): C, 74.02; H, 7.26; N, 1.82. Found: C, 73.58; H, 7.43; N, 1.98.

X-ray Crystallographic Studies

Single crystals suitable for X-ray analysis were obtained as described in the preparation. The crystals were manipulated in the glovebox under a microscope in the glovebox. Data collection was performed at -110°C on a Bruker SMART APEX diffractometer with a CCD area detector, using graphite monochromated Mo K α radiation ($\lambda = 0.71073 \text{ \AA}$). The determination of the crystal class and unit cell parameters was carried out by the SMART program package.^[3] The raw frame data were processed using SAINT^[4] and absorption corrections using SADABS^[5] to yield the reflection data file. The structures were solved by using SHELX-97^[6] or SUPERFLIP.^[7] Refinements were performed on F^2 anisotropically for all the non-hydrogen atoms by the full-matrix least-squares method using SHELXL-97 program.^[6] The SQUEEZE^[8] routine of the program PLATON^[9] was implemented to remove the contributions of the disordered solvents (THF in **3-Lu**, **5-Lu**, **6-Lu**; C₆H₅Cl in **4-Y** and **4-Lu**) to the observed structure factors. The hydrides in **3-Lu**, **4-Y** and **4-Lu** were located by difference Fourier syntheses. The coordinates and isotropic parameters of the hydrides in **4-Y** and **4-Lu** were refined, while the parameters of the hydride in **3-Lu** were not further refined. Other hydrogen atoms were placed at the calculated positions and were included in the structure calculation without further refinement of the parameters. The residual electron densities were of no chemical significance. Crystal data and analysis results are listed in STable 1-3.

CCDC numbers 829248 (**3-Lu**), 829249 (**5-Lu**), 829250 (**6-Lu**), 829251 (**4-Y**) and 829252 (**4-Lu**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

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Table 1. Crystal data and structure refinement for **3-Lu**

Identification code	3-Lu
Empirical formula	C ₆₇ H ₈₄ B Lu N ₂ O ₃
Formula weight	1151.14
Temperature	163(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P21/c
a	20.966(6) Å
b	11.804(3) Å
c	27.217(7) Å
α	90°
β	92.748(5)°
γ	90°
Volume	6728(3) Å ³
Z, Calculated density	4, 1.136 Mg/m ³
Absorption coefficient	1.508 mm ⁻¹
F(000)	2400
Crystal size	0.42 x 0.38 x 0.20 mm
Theta range for data collection	1.75 to 25.00°
Limiting indices	-24 ≤ h ≤ 24, -14 ≤ k ≤ 13, -32 ≤ l ≤ 21
Reflections collected / unique	35869 / 11829 [R(int) = 0.0346]
Completeness to theta	(25.00°) 100 %
Absorption correction	Empirical
Max. and min. transmission	0.7524 and 0.5700
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	11829 / 19 / 644
Goodness-of-fit on F ²	1.050
Final R indices [I > 2σ(I)]	R1 = 0.0476, wR2 = 0.1270
R indices (all data)	R1 = 0.0575, wR2 = 0.1327
Largest diff. peak and hole	2.582 and -0.875 e. Å ⁻³

Table 2. Crystal data and structure refinement for **4-Y** and **4-Lu**

Identification code	4-Y	4-Lu
Empirical formula	C126 H152 B2 N4 O4 Y2	C126 H152 B2 N4 O4 Lu2
Formula weight	1985.96	2158.08
Temperature	163(2) K	163(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system, space group	Triclinic, P-1	Triclinic, P-1
a	15.062(5) Å	15.0119(15) Å
b	16.053(5) Å	16.0338(16) Å
c	16.125(5) Å	16.0949(15) Å
α	115.236(5) $^\circ$	115.524(2) $^\circ$
β	106.900(5) $^\circ$	106.633(2) $^\circ$
γ	98.019(5) $^\circ$	98.134(2) $^\circ$
Volume	3214.3(18) Å ³	3188.7(5) Å ³
Z, Calculated density	1, 1.026 Mg/m ³	1, 1.124 Mg/m ³
Absorption coefficient	0.945 mm ⁻¹	1.586 mm ⁻¹
F(000)	1056	1120
Crystal size	0.35 x 0.32 x 0.15 mm	0.30 x 0.25 x 0.16 mm
Theta range for data collection	1.47 to 25.00 $^\circ$	1.48 to 25.00 $^\circ$
Limiting indices	-17 \leq h \leq 17, -18 \leq k \leq 18, -19 \leq l \leq 11	-17 \leq h \leq 16, -18 \leq k \leq 19, -19 \leq l \leq 18
Reflections collected / unique	16980 / 11136 [R(int) = 0.0450]	17464 / 11039 [R(int) = 0.0493]
Completeness to theta	(25.00 $^\circ$) 98.3 %	(25.00 $^\circ$) 98.4 %
Absorption correction	Empirical	Empirical
Max. and min. transmission	0.8713 and 0.7333	0.7969 and 0.6068
Refinement method	Full-matrix least-squares on F ²	Full-matrix least-squares on F ²
Data / restraints / parameters	11136 / 1 / 627	11039 / 1 / 624
Goodness-of-fit on F ²	0.875	0.945
Final R indices [I \geq 2 σ (I)]	R1 = 0.0625, wR2 = 0.1269	R1 = 0.0569, wR2 = 0.1107
R indices (all data)	R1 = 0.1090, wR2 = 0.1415	R1 = 0.0840, wR2 = 0.1192
Largest diff. peak and hole	0.381 and -0.301 e. Å ⁻³	1.368 and -0.698 e. Å ⁻³

STable 3. Crystal data and structure refinement for **5-Lu** and **6-Lu**

Identification code	5-Lu	6-Lu
Empirical formula	C70 H90 B Lu N4 O2	C95 H111 B2 Lu1 N2 O4
Formula weight	1205.24	1541.45
Temperature	163(2) K	163(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system, space group	Triclinic, P-1	Monoclinic, P21/c
a	12.306(4) Å	14.5937(15) Å
b	12.971(5) Å	40.384(4) Å
c	23.504(8) Å	28.730(3) Å
α	77.098(7)°	90°
β	86.501(6)°	91.444(2)°
γ	80.166(6)°	90°
Volume	3602(2) Å ³	16926(3) Å ³
Z, Calculated density	2, 1.110 Mg/m ³	8, 1.210 Mg/m ³
Absorption coefficient	1.411 mm ⁻¹	1.217 mm ⁻¹
F(000)	1260	6464
Crystal size	0.40 x 0.35 x 0.32 mm	0.25 x 0.20 x 0.15 mm
Theta range for data collection	1.63 to 25.00°	1.40 to 25.00°
Limiting indices	-13 ≤ h ≤ 14, -15 ≤ k ≤ 14, -26 ≤ l ≤ 27	-17 ≤ h ≤ 16, -48 ≤ k ≤ 48, -31 ≤ l ≤ 34
Reflections collected / unique	19316 / 12412 [R(int) = 0.0672]	92044 / 29679 [R(int) = 0.1086]
Completeness to theta	(25.00°) 97.7 %	(25.00°) 99.6 %
Absorption correction	Empirical	Empirical
Max. and min. transmission	0.6609 and 0.6022	0.8385 and 0.7507
Refinement method	Full-matrix least-squares on F ²	Full-matrix least-squares on F ²
Data / restraints / parameters	12412 / 6 / 696	29679 / 0 / 1875
Goodness-of-fit on F ²	0.949	0.903
Final R indices [I > 2σ(I)]	R1 = 0.0758, wR2 = 0.1548	R1 = 0.0628, wR2 = 0.1207
R indices (all data)	R1 = 0.1173, wR2 = 0.1718	R1 = 0.1137, wR2 = 0.1369
Largest diff. peak and hole	2.015 and -2.148 e. Å ⁻³	2.186 and -0.734 e. Å ⁻³

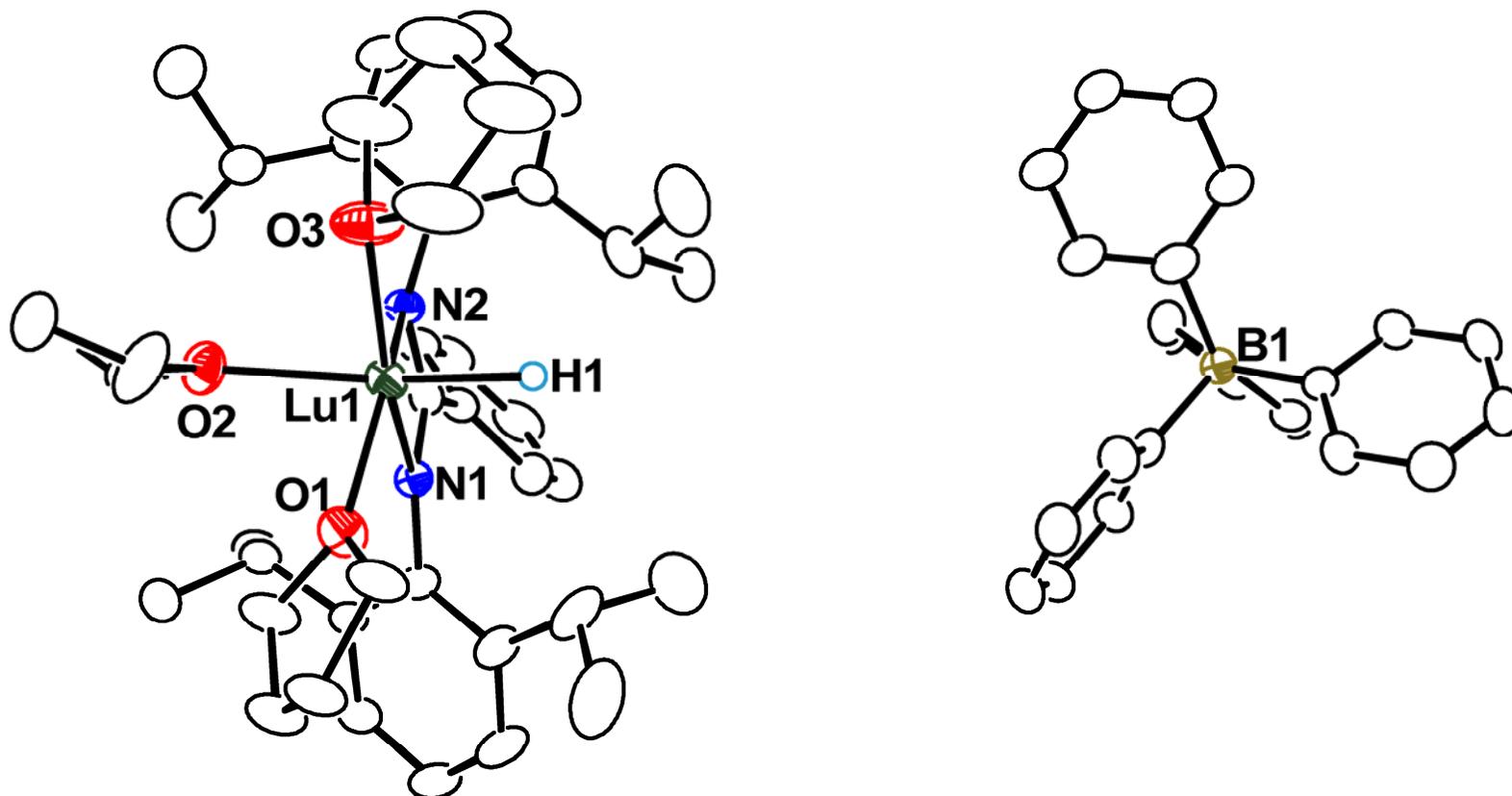


Figure 1. Ortep drawing of $[(NCN)Lu(H)(THF)_3][BPh_4]$ (**3-Lu**) with thermal ellipsoids at the 30% probability level.

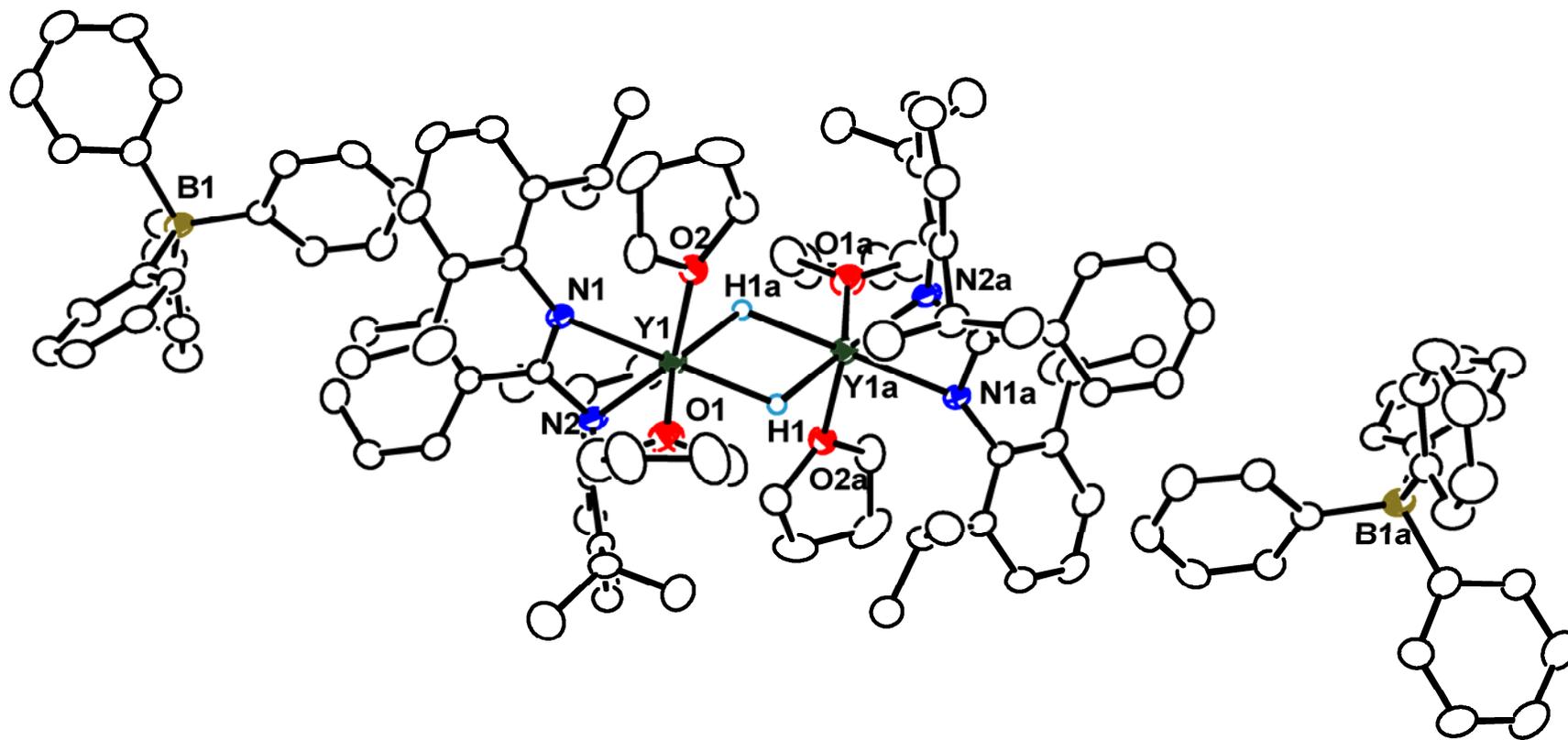


Figure 2. Ortep drawing of $[(\text{NCN})\text{Y}(\mu\text{-H})(\text{THF})_2]_2[\text{BPh}_4]_2$ (**4-Y**) with thermal ellipsoids at the 30% probability level.

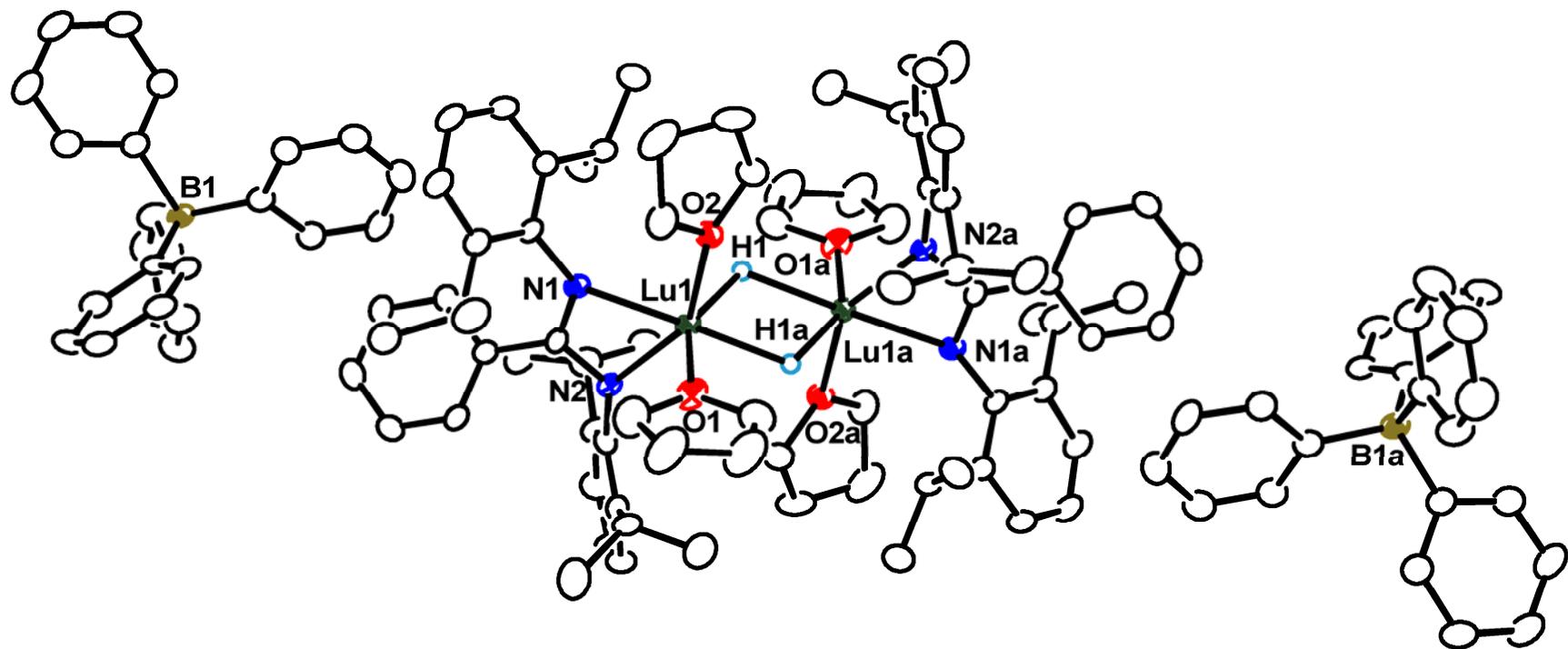


Figure 3. Ortep drawing of $[(\text{NCN})\text{Lu}(\mu\text{-H})(\text{THF})_2]_2[\text{BPh}_4]_2$ (**4-Lu**) with thermal ellipsoids at the 30% probability level.

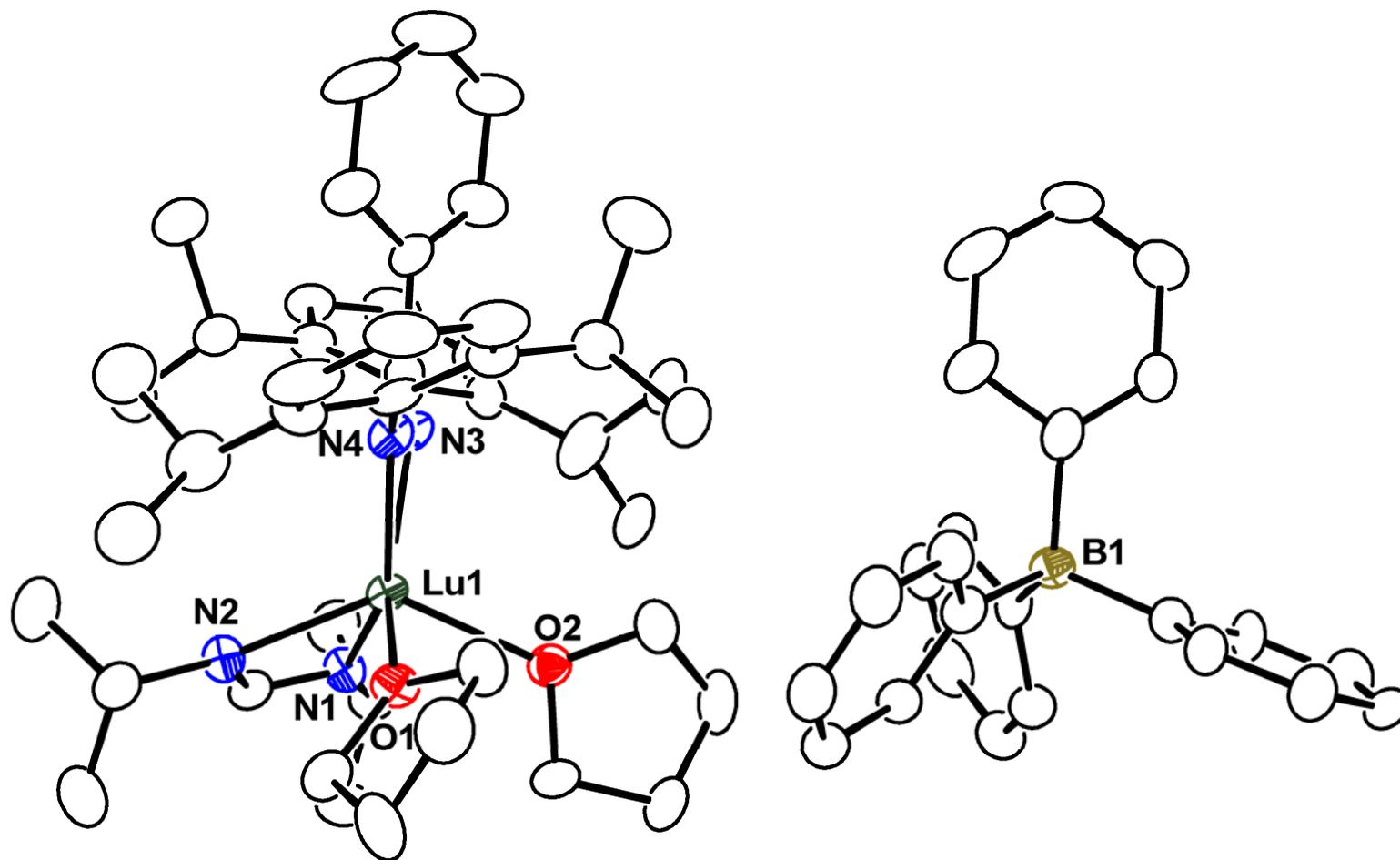


Figure 4. Ortep drawing of $[(\text{NCN})\text{Ln}\{\text{CH}(\text{N}^i\text{Pr}_2)_2\}(\text{THF})_2][\text{BPh}_4]$ (**5-Lu**) with thermal ellipsoids at the 30% probability level.

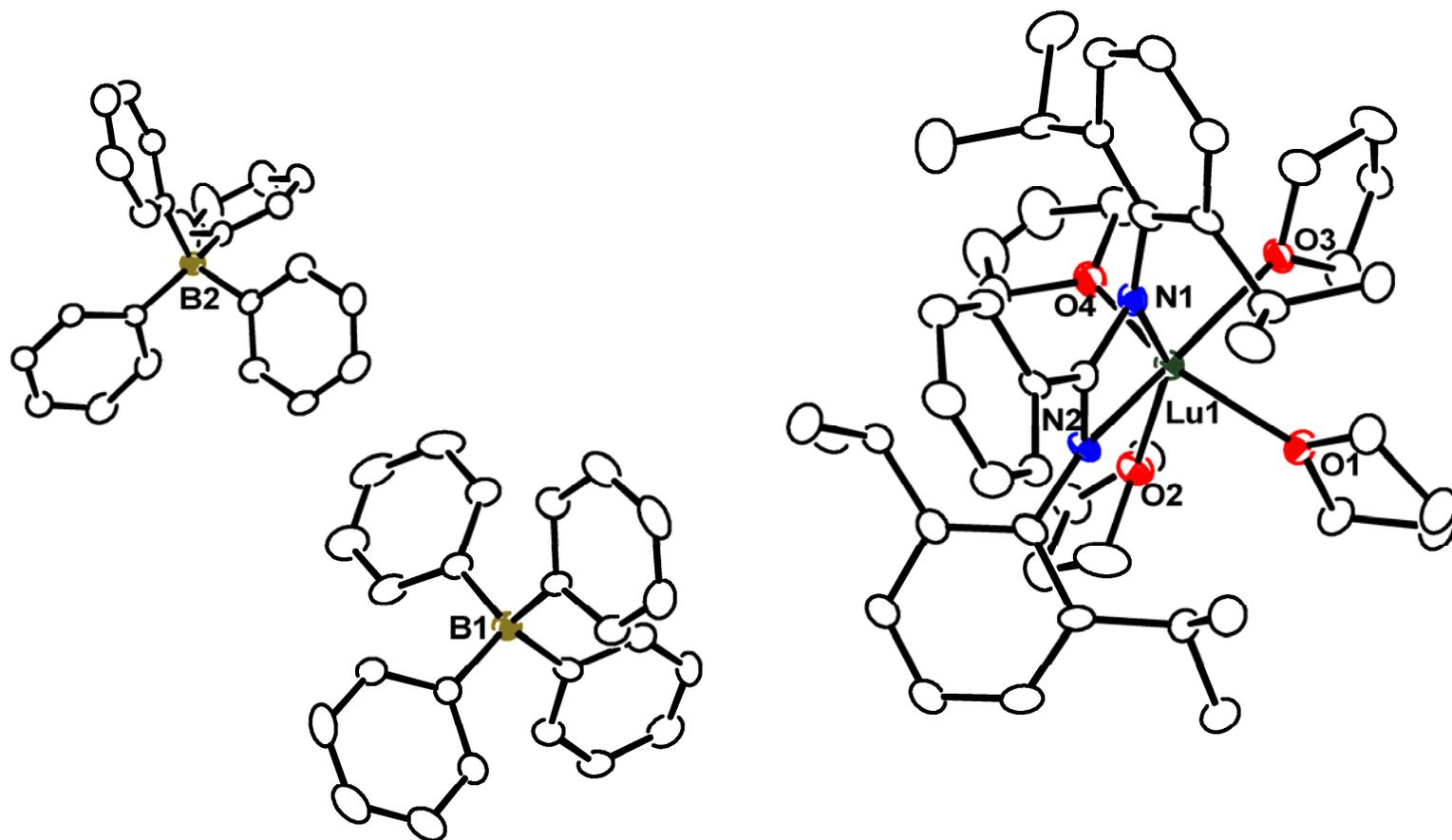


Figure 5. Ortep drawing of [(NCN)Lu(THF)₄][BPh₄]₂ (**6-Lu**) with thermal ellipsoids at the 30% probability level