Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information for:

Synthesis of Homoleptic, Divalent Lanthanide (Sm, Eu) Complexes via Oxidative Transmetallation

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General Considerations

Unless otherwise noted, all reagents were obtained from commercial suppliers. The syntheses and manipulations were conducted under argon with exclusion of oxygen and water using Schlenk techniques or in an inert atmosphere box (Vigor) under a dinitrogen (<0.1 ppm O_2/H_2O) atmosphere. The glovebox is equipped with two -35 ˚C freezers. All glassware and cannulae were stored in an oven over-night (>8 h) at a temperature of ca. 160˚C. Celite and molecular sieves were dried under vacuum at a temperature >250˚C for a minimum of 24 h. C_6D_6 was stored over 3 Å molecular sieves and then vacuum-transferred from purple sodium/benzophenone prior to use. Pyridine-d_5 was degassed by three freeze-pump-thaw cycles stored over 3 Å molecular sieves for at least 24 h prior to use. Hexanes, diethyl ether and tetrahydrofuran were purged with UHP-grade argon (Airgas) and passed through columns containing Q-5 and molecular sieves in a solvent purification system (JC Meyer Solvent Systems). All solvents in the glovebox were stored in bottles over 3 Å molecular sieves. NMR spectra were obtained on a Bruker Advance III 400 MHz spectrometer at 298 K, unless otherwise noted. ^{1}H NMR chemical shifts are reported in δ, parts per million. ^{1}H NMR are references to the residual ^{1}H resonances of the deuterated solvent. Peak position is listed, followed by peak multiplicity, integration value, and proton assignment, where applicable. Multiplicity and shape are indicated by one or more of the following abbreviations: s (singlet); d (doublet); t (triplet); q (quartet); dd (doublet of doublets); td (triplet of doublets); m (multiplet); br (broad). Infrared (IR) samples were taken on a Bruker ALPHA FTIR spectrometer from 400 to 4000 cm^{-1}. IR samples were prepared as Nujol mulls sandwiched between two KBr plates. The peaks are listed in wavenumber [cm^{-1}] and intensity by using the following abbreviations: vw (very weak); w (weak); m (medium); s (strong); vs (very strong); br (broad). UV/vis/NIR spectroscopy was performed in Teflon-valve sealed quartz cuvettes with a 1 cm path length on a Hitachi UH4150 UV–vis–NIR scanning spectrophotometer between 2500 and 240 nm. Elemental analyses were determined at Robertson Microlit Laboratories (Ledgewood, NJ).

Magnetic measurements were performed on a Quantum Design MPMS-5S magnetometer. Inside of a glovebox, a measured amount of quartz wool (10–20 mg) was loaded and packed tightly into a quartz tube. Powdered samples were loaded inside of the tube and onto the glass wool plug by tapping the compound through a glass pipet. Another pre-massed amount of quartz wool (10–20 mg) was loaded on top of the sample, and the contents were packed tightly again. The top of the tube was affixed to an Ultra Torr Swagelok adaptor while the bottom was plugged with a piece of snug tubing tightly closed with a stopper and copper wire. This was transported from the glovebox to a Schlenk line where it was sealed above and below the sample using a O_2/H_2 torch while the sample was under vacuum. The vacuum sealed tubing was taped to a straw, and the straw was loaded into the instrument. Diamagnetic corrections for the quartz wool and the complex were performed using Pascal's constants.[1]

Crystals suitable for X-ray diffraction were covered in paratone oil in a glove box and transferred to the diffractometer in a 20 mL capped vial. Crystals were mounted on a loop

with paratone oil on a Bruker D8 VENTURE diffractometer. The crystals were cooled and kept at T = 100(2) K during data collections. The structures were solved with the ShelXT structure solution program using the Intrinsic Phasing solution method and by using Olex2 as the graphical interface.[2-3] The model was refined with version 2014/7 of XL using Least Squares minimization.[4] Structures are visualized in Ortep3 and graphics are generated with POV-ray.[5]

Synthetic Procedures

Synthesis of (^{t}BuO)$_3$SiCl. This procedure was adapted from a literature procedure.[6] $SiCl_4$ (23 mL, 34 g, 200 mmol, 1.0 equiv.) was added to 300 mL of hexanes in a 3-neck, 1L round-bottom flask via syringe. The solution was stirred vigorously and cooled to 0 °C with an ice-water bath. Solid potassium *tert*-butoxide (72.1 g, 640 mmol, 3.2 equiv.) was added in small portions to the solution over 1h. Once the addition is complete, the reaction mixture was allowed to warm to room temperature and is stirred for an additional 2 h and then refluxed overnight. The reaction mixture was filtered through Celite on a glass frit and the volatiles are removed *in vacuo*. The yellowish oil was distilled (3 torr, 55°C) yielding a clear, colorless liquid (49.65 g, 176 mmol, 88%). ^{1}H NMR (400 MHz, C_6D_6): δ 1.37 (s, 27 H, *tert*-butyl -CH_3). ^{13}C NMR (400 MHz, C_6D_6): δ 74.76 (s), 30.93 (s). IR (cm^{-1}): *v* 2980 (s), 2936 (m), 2917 (m), 2876 (w), 1472 (m), 1392 (m), 1368 (s), 1244 (s), 1186 (s), 1080 (s), 1031 (m), 915 (vw), 832 (m), 806 (m), 697 (m), 637 (m). Elem anal. Found (calculated) for $C_{12}H_{27}O_3SiCl$: C, 51.20 (50.95); H, 9.70 (9.62); N, <0.10 (0.00).

Synthesis of (^{t}BuO)$_3$SiNH$_2$. In a 2-neck 5L round-bottom flask, (^{t}BuO)$_3$SiCl (29g, 102 mmol, 1.0 equiv.) was added to 500 mL of diethyl ether. The solution was stirred vigorously as anhydrous ammonia is bubbled through the solution for 20 minutes. A white precipitate was observed at this time. The flask is sealed under a slight positive pressure of ammonia and stirred overnight. The reaction mixture was subjected to these same conditions (20 minutes of bubbling anhydrous ammonia and overnight stirring) two more times in order to achieve a stoichiometric amount of ammonia. The mixture was filtered through Celite and the volatiles are removed *in vacuo*. The yellowish oil was purified via distillation (3 torr, 69°C) yielding a colorless liquid (25.8g, 97.9 mmol, 96%). ^{1}H NMR (400 MHz, C_6D_6): δ 1.39 (s, 27 H, *tert*-butyl -CH_3), 0.52 (s, 2 H, -NH_2). ^{13}C NMR (400 MHz, C_6D_6): δ 71.80 (s), 31.34 (s). IR (cm^{-1}): *v* 3497 (w), 3420 (w), 2975 (s), 2934 (m), 2874 (m), 1549 (m), 1473 (m), 1389 (m), 1365 (m), 1244 (m), 1193 (m), 1065 (s), 1027 (m), 871 (m), 830 (m), 804 (w), 794 (w), 696 (m), 640 (s). Elem anal. Found (calculated) for $C_{12}H_{28}O_3SiNLi$: C, 52.50 (54.71); H, 10.77 (11.10); N, 5.06 (5.32).

Synthesis of (^{t}BuO)$_3$SiNHLi. In a 1 L round-bottom Schlenk flask, (^{t}BuO)$_3$SiNH$_2$ (25.794g, 97.9 mmol, 1.0 equiv.) was dissolved to 200 mL of hexanes. The solution was cooled to 0°C using an ice-water bath. The solution is stirred vigorously and nBuLi (42.8 mL, 2.40 M, 103 mmol, 1.05 equiv.) was added dropwise via addition funnel over 25 minutes. After the addition was complete, the solution was allowed to warm to room temperature. The mixture was stirred for 16 h. All volatiles were removed *in vacuo* and the solid is redissolved in approximately 120 mL of n-pentane, and the solution is filtered through Celite. The solution was concentrated *in vacuo* and chilled to -80°C yielding the title compound as a white crystalline solid (23.253 g, 86.24 mmol, 88%) after decantation. ^{1}H NMR (400 MHz, C_6D_6): δ 1.56 (s, 27 H, *tert*-butyl -CH_3), -1.29 (s, 1 H, -NH). ^{13}C NMR (400 MHz, C_6D_6): δ 71.81 (s), 31.99 (s). IR (cm^{-1}): *v* 1361 (s), 1241 (s), 1213 (s), 1196 (s), 1055 (s), 1038 (s), 1018 (s), 992 (s), 956 (m), 941 (m), 931 (m), 817 (m), 694 (m),

624 (w). Elem. anal. Found (calculated) for $C_{12}H_{28}O_3SiNLi$: C, 52.05 (53.50); H, 10.48 (10.48); N, 4.99 (5.20). Carbon consistently low on multiple burns.

Synthesis of $(({}^tBuO)_3Si)_2NH$, BTTSA-H. $({}^tBuO)_3SiNHLi$ (18.5629g, 68.9 mmol, 1.0 equiv.) was slurried in 300 mL of toluene in a 1 L round-bottom Schlenk flask. Separately, $({}^tBuO)_3SiCl$ was dissolved in 100 mL of toluene and the solution is added to the stirring slurry via cannula. The reaction mixture was stirred for an hour and then the reaction is brought to reflux (after all solid is dissolved) for 24h. The mixture was filtered through Celite and the solid was washed with toluene. The filtrate was concentrated *in vacuo* and crystalized at -80°C yielding the title compound as a white crystalline solid (26.78 g, 76%) after decantation. ^1H NMR (400 MHz, C_6D_6): δ 1.46 (s, 54 H, *tert*-butyl -CH_3), 0.63 (s, 1 H, -NH). ^{13}C NMR (400 MHz, C_6D_6): δ 72.03 (s), 31.49 (s). IR (cm^{-1}): *v* 3409 (m), 3246 (w), 3192 (w), 2713 (w), 2272 (w), 1874 (w), 1365 (s), 1242 (s), 1203 (s), 1062 (s), 1002 (s), 969 (s), 934 (m), 830 (s), 800 (m), 700 (s), 624 (m). Elem. anal. Found (calculated) for $C_{24}H_{55}NO_6Si_2$: C, 54.31 (56.54); H, 10.41 (10.87); N, 2.71 (2.75). Carbon consistently low on multiple burns.

Synthesis of $(({}^tBuO)_3Si)_2NK$. $(({}^tBuO)_3Si)_2NH$ (2.045g, 3.92 mmol, 1.0 equiv.) was added to a 100 mL pear Schlenk flask with 20 mL of toluene. Potassium benzyl (548 mg, 4.12 mmol, 1.05 equiv.) was added to the flask as a solid. 30 mL toluene was added to assist in the transfer. The reaction mixture was brought to reflux for 12h. After about 1h, the solution began to turn from cherry-red to light brown. After the reflux, volatiles was removed *in vacuo* and the solid was extracted with diethyl ether. The solution is filtered over celite and crystalized at -80°C yielding white crystalline material (1.82 g, 83%). ^1H NMR (400 MHz, pyridine-d_5): δ 1.61 (s, 54 H, *tert*-butyl -CH_3). ^{13}C NMR (400 MHz, pyridine-d_5): δ 70.19 (s), 32.16 (s). IR (cm^{-1}): *v* 2713 (w), 2272 (w), 1874 (w), 1365 (s), 1242 (s), 1203 (s), 1062 (s), 1002 (s), 969 (s), 934 (m), 830 (s), 800 (m), 700 (s), 624 (m). Elem. anal. Found (calculated) for $C_{24}H_{54}NO_6Si_2K$: C, 51.39 (52.61); H, 10.02 (9.93); N, 2.54 (2.56). Carbon consistently low on multiple burns.

Synthesis of $[\{(({}^tBuO)_3Si\}_2NCu]KCl$, 1. $(({}^tBuO)_3Si)_2NK$ (917 mg, 1.67 mmol, 1.0 equiv.) was dissolved in 8 mL of THF and added to a stirring slurry of CuCl (166 mg, 1.67 mmol, 1.0 equiv.) in 2 mL THF. Upon addition, the solution adopted a yellow-orange color. The reaction mixture was stirred for 16h. The mixture was filtered through Celite and washed with THF. The volatiles were removed *in vacuo*. The resultant solid was dissolved in approximately 7 mL of *n*-pentane and filtered through Celite and the filter cake was washed with n-pentane. The volatiles are removed *in vacuo* yielding title compound as a tan solid (781 mg, 77%). XRD quality crystals were obtained by the slow evaporation of a hexanes solution at -35 °C. ^1H NMR (400 MHz, C_6D_6): δ 1.64 (s, 108 H, *tert*-butyl -CH_3). ^{13}C NMR (400 MHz, C_6D_6): δ 72.03 (s), 32.39 (s). IR (cm^{-1}): *v* 2720 (m), 2272 (w), 1364 (s), 1304 (m), 1241 (s), 1192 (s), 1065 (s), 990 (s), 909 (m), 826 (s), 813 (s), 755 (m), 684 (m), 608 (w). Elem anal. Found (calculated) for $C_{48}H_{108}N_2ClCu_2O_{12}Si_4K$: C, 46.39 (47.28); H, 8.45 (8.93); N, 2.26 (2.30). Carbon consistently low on multiple burns.

Synthesis of [{(^{t}BuO)$_3$Si}$_2$N]$_2$Sm, 2-Sm. [{(^{t}BuO)$_3$Si}$_2$NCu]KCl (200 mg, 0.164, 1.0 equiv.) was dissolved in 4 mL of THF and added to a slurry of Sm metal (24.7 mg, 0.164, 1.0 equiv.) in 1 mL of THF. The reaction mixture was stirred with a glass stir bar for 60 h. The solution changed color from yellow-tan to red to finally dark green over the reaction period. The mixture was filtered through Celite and washed with THF. The volatiles were removed *in vacuo.* The solid was extracted with 5 mL *n*-pentane and filtered through Celite. Volatiles were again removed *in vacuo* yielding the title compound as a dark green solid (131 mg, 68%). XRD quality crystals were obtained via the slow evaporation of a diethyl either solution at -35°C. No ^{1}H NMR signal observed. IR (cm^{-1}): *v* 2364 (w), 1362 (m), 1276 (m), 1261 (m), 1242 (m), 1193 (s), 1065 (s), 1058 (s), 1038 (m), 967 (m), 914 (w), 819 (w), 801 (m), 732 (w), 685 (w), 661 (w), 649 (w). Elem anal. Found (calculated) for $C_{48}H_{108}N_2O_{12}Si_4Sm$: C, 46.32 (49.36); H, 9.11 (9.32); N, 2.31 (2.40). Carbon consistently low on multiple burns.

Synthesis of [{(^{t}BuO)$_3$Si}$_2$N]$_2$Eu, 2-Eu. [{(^{t}BuO)$_3$Si}$_2$NCu]KCl (431.7 mg, 0.354, 1.0 equiv.) was dissolved in 6 mL of THF and added to a slurry of Eu metal (53.8 mg, 0.354, 1.0 equiv.) in 1 mL of THF. The reaction was stirred with a glass stir bar for 60 h. The solution color turned from yellow-tan to red to finally light green/colorless over the reaction period. The mixture was filtered through Celite and the filter was washed with THF. Volatiles were removed *in vacuo.* The product was extracted with 5 mL *n*-pentane and filtered through Celite. Volatiles were removed *in vacuo* yielding the title compound as a pale green solid (341 mg, 82%). XRD quality crystals were obtained from a concentrated diethyl either at -35°C. No ^{1}H NMR signal observed. IR (cm^{-1}): *v* 2364 (w), 1362 (m), 1276 (m), 1261 (m), 1242 (m), 1193 (s), 1065 (s), 1058 (s), 1038 (m), 967 (m), 914 (w), 819 (w), 801 (m), 732 (w), 685 (w), 661 (w), 649 (w). Elem anal. Found (calculated) for $C_{48}H_{108}N_2O_{12}Si_4Eu$: C, 48.45 (49.29); H, 9.60 (9.31); N, 2.31 (2.39). Carbon consistently low on multiple burns.

NMR Spectra

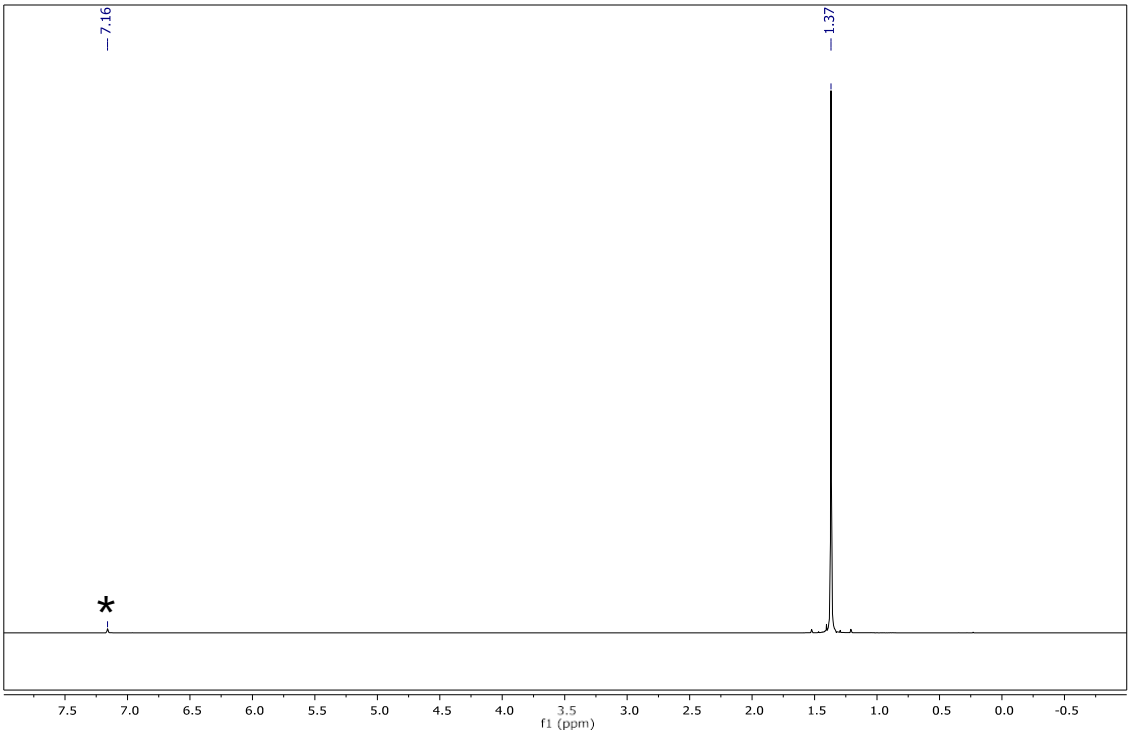

Figure S1. ^{1}H NMR for $(^{t}BuO)_3SiCl$ in C_6D_6. C_6D_5H is noted as *.

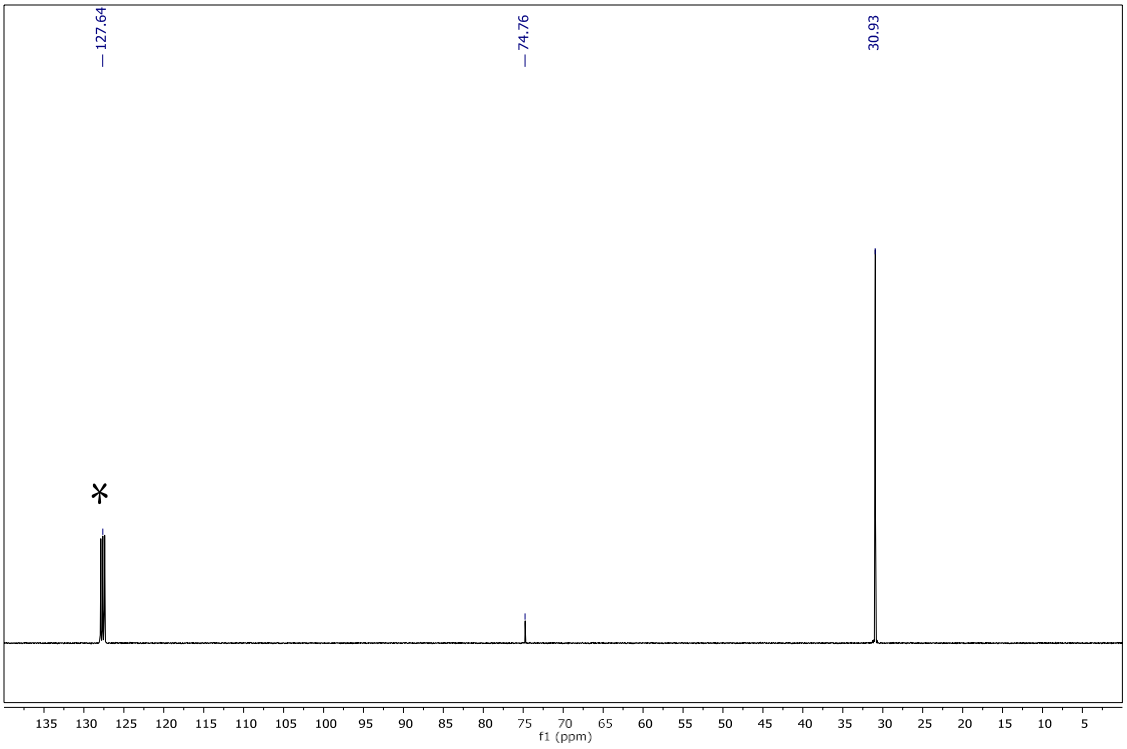

Figure S2. ^{13}C NMR for $(^{t}BuO)_3SiCl$ in C_6D_6. C_6D_5H is noted as *.

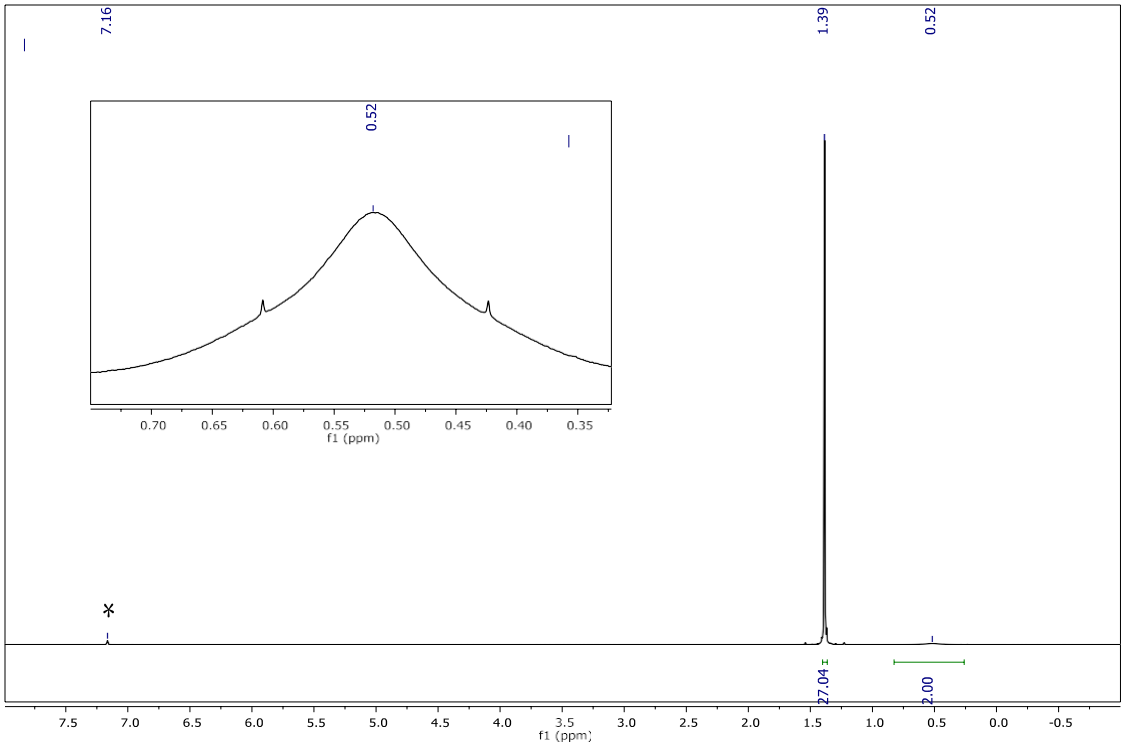

Figure S3. ^{1}H NMR for $(^{t}BuO)_3SINH_2$ in C_6D_6. Peak of C_6D_5H is noted as *.

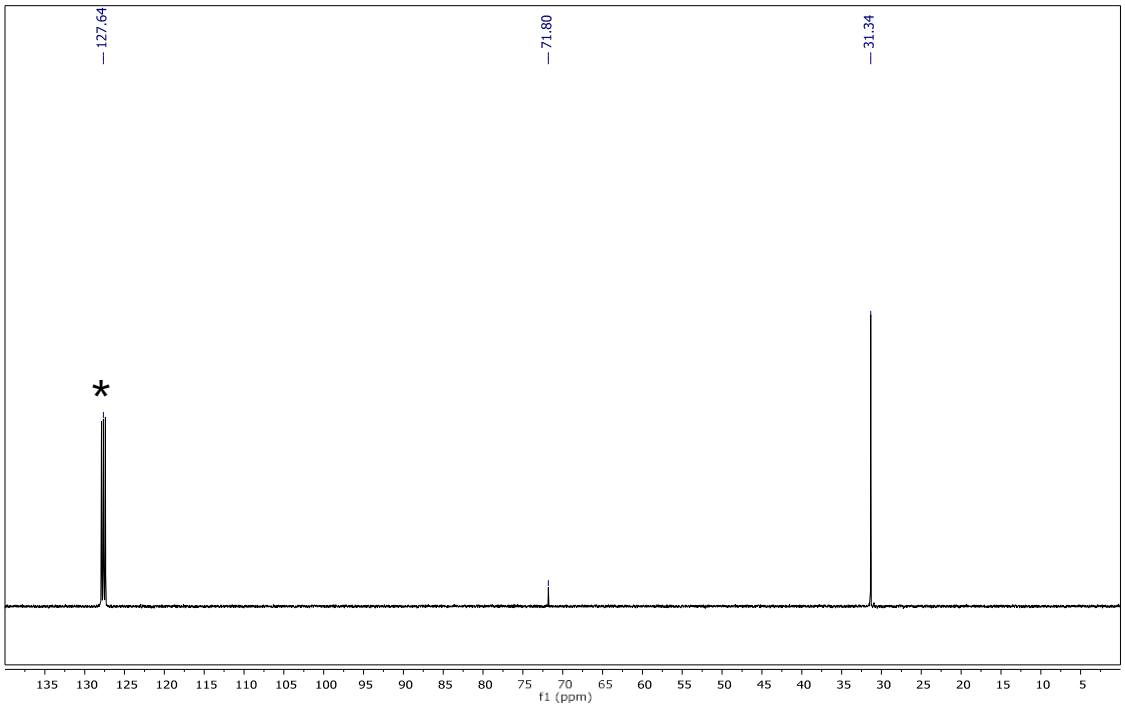

Figure S4. ^{13}C NMR for $(^{t}BuO)_3SiNH_2$ in C_6D_6. C_6D_5H is noted as *.

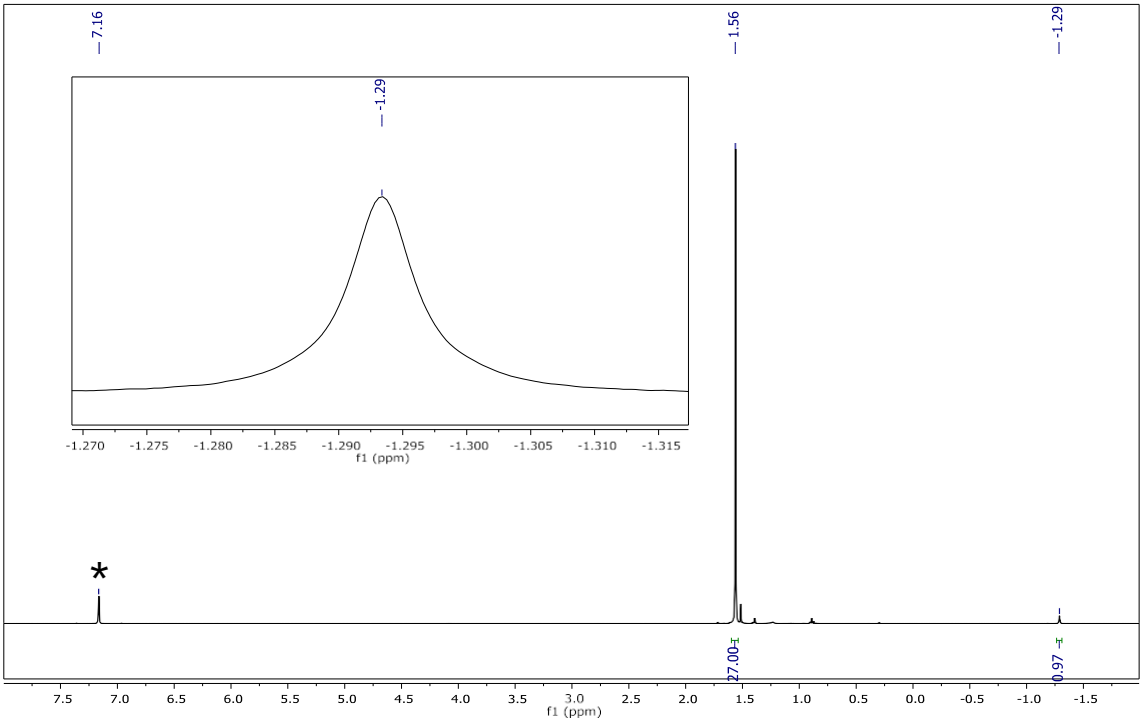

Figure S5. ^{1}H NMR for $(^{t}BuO)_3SiNHLi$ in C_6D_6. Peak of C_6D_5H is noted as *.

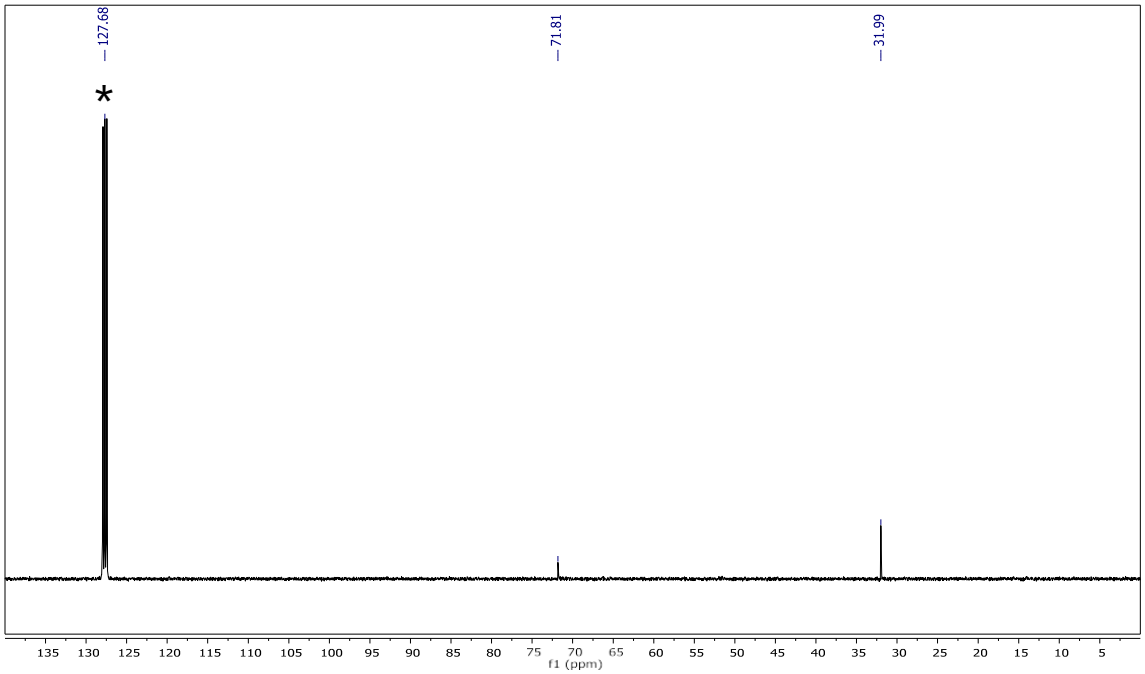

Figure S6. ^{13}C NMR for $(^{t}BuO)_3SiNHLi$ in C_6D_6. Peaks of C_6D_5H is noted as *.

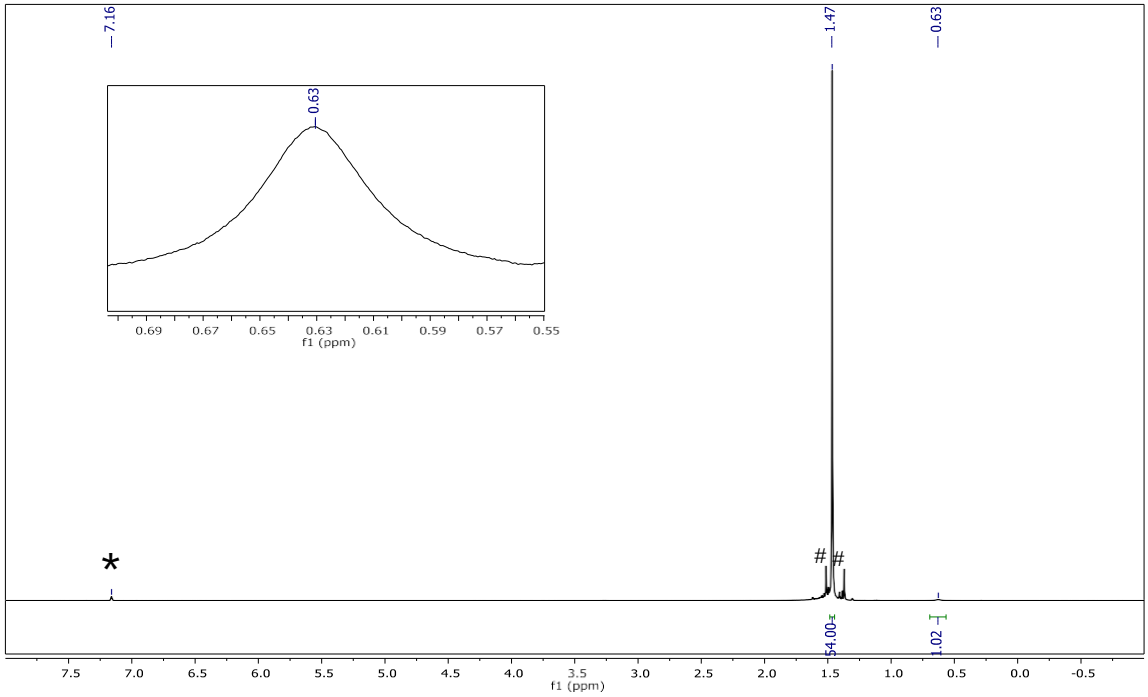

Figure S7. ^{1}H NMR for $((^{t}BuO)_3Si)_2NH$ in C_6D_6. Peak of C_6D_5H is noted as *. Unidentified impurities are marked as #.

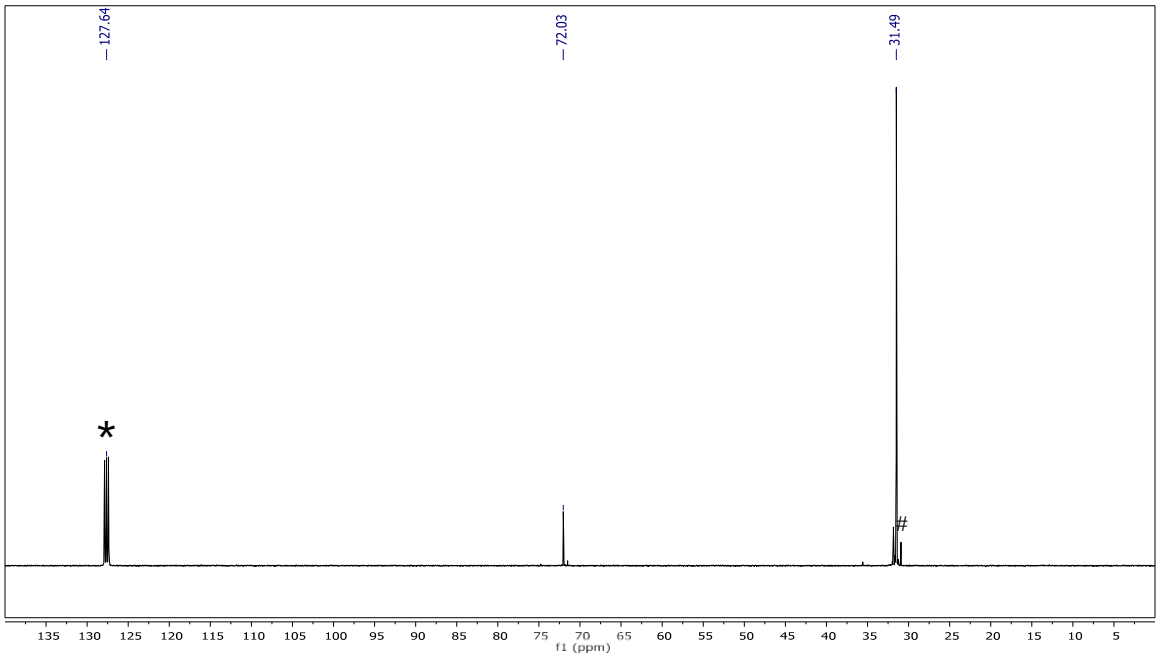

Figure S8. ^{13}C NMR for $((^{t}BuO)_3Si)_2NH$ in C_6D_6. Peak of C_6D_5H is noted as *. Unidentified impurities are marked as #.

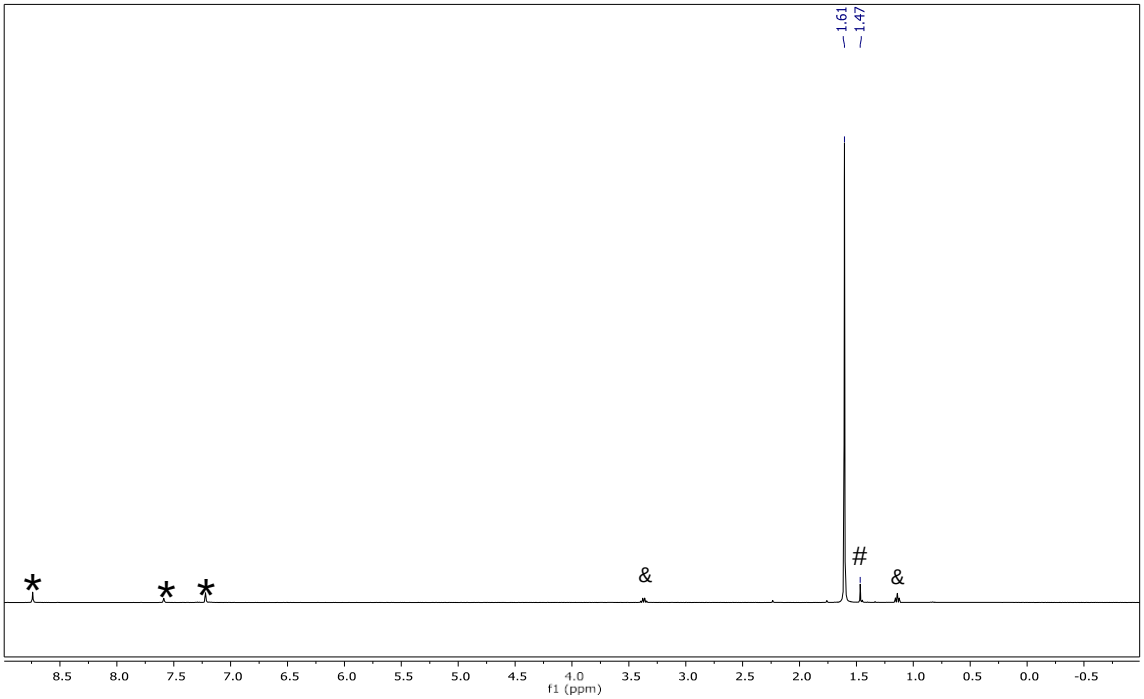

Figure S9. ^{1}H NMR for $(({}^{t}BuO)_3Si)_2NK$ in pyridine-d_5. Residual NMR solvent peaks are noted as*. **BTTSA-H** impurity is marked as #. Diethyl ether impurity is labeled with &.

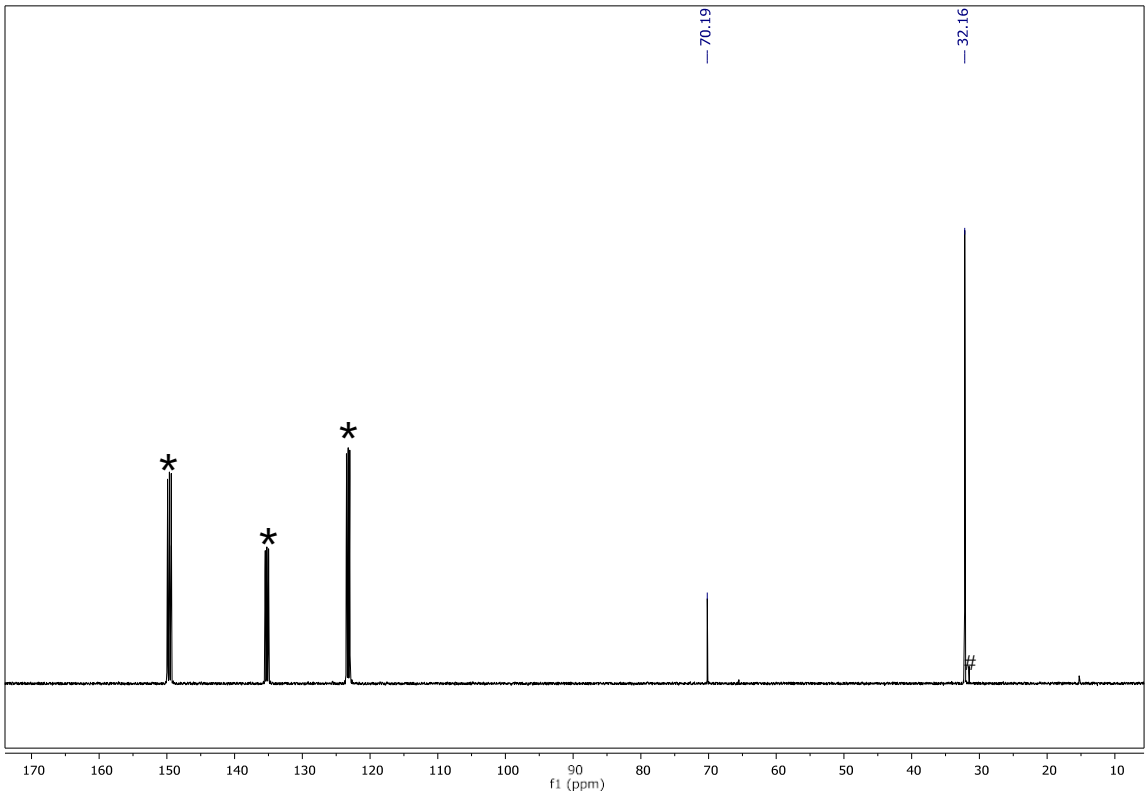

Figure S10. ^{13}C NMR for $(({}^{t}BuO)_3Si)_2NK$ in pyridine-d_5. Residual NMR solvent peaks are noted as*. **BTTSA-H** impurity are marked as #.

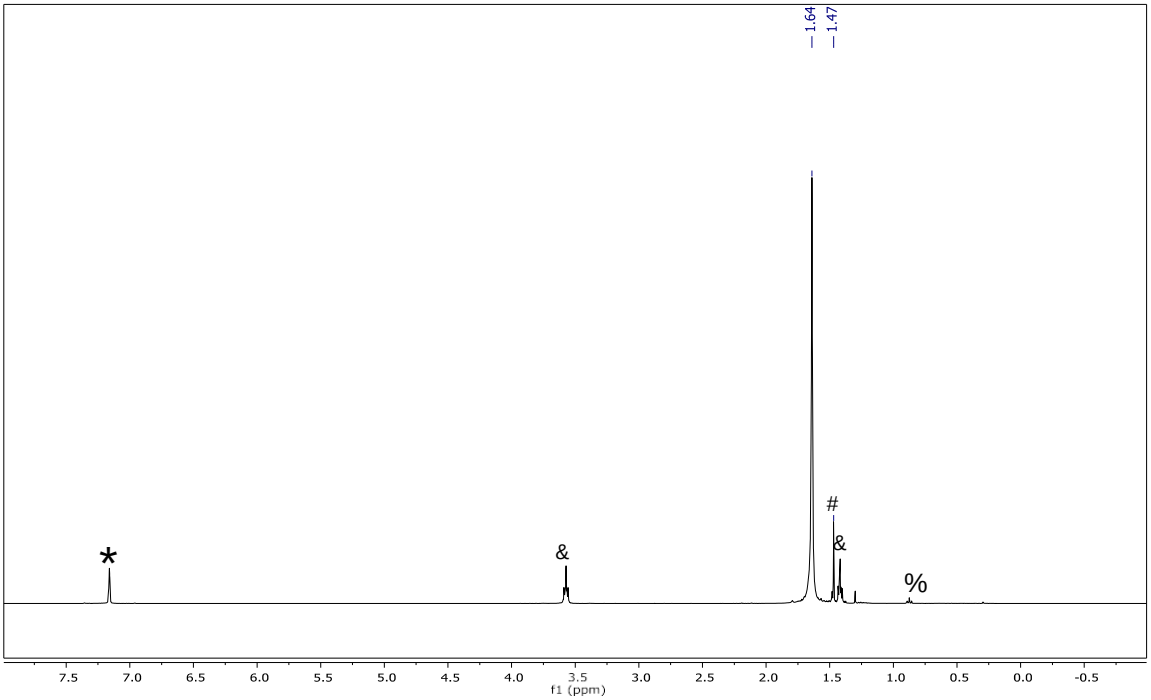

Figure S11. ^{1}H NMR for **1** in C_6D_6. Peak of C_6D_5H is noted as *. **BTTSA-H** impurity is marked as #. THF impurity is labeled with &. Pentane impurity is marked with %.

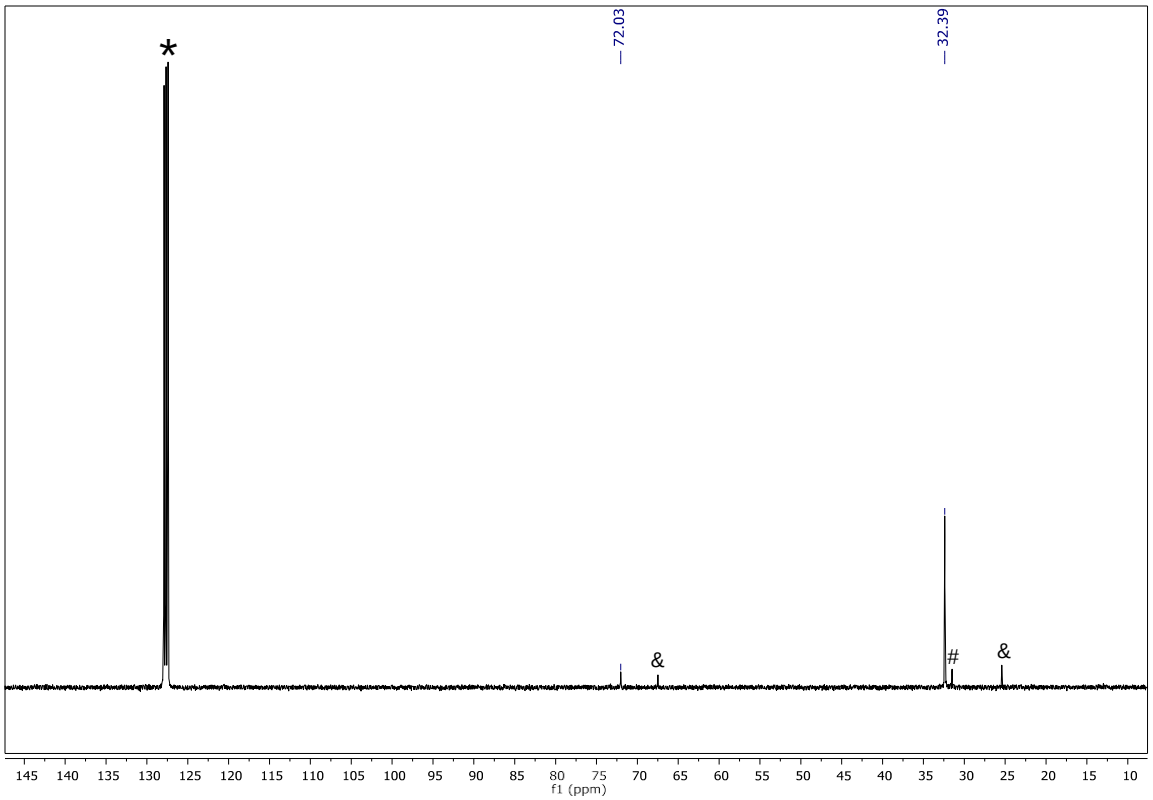

Figure S12. ^{13}C NMR for **1** in C_6D_6. Peak of C_6D_5H is noted as *. **BTTSA-H** impurity is marked as #. THF impurity is labeled with &.

Crystallographic Data

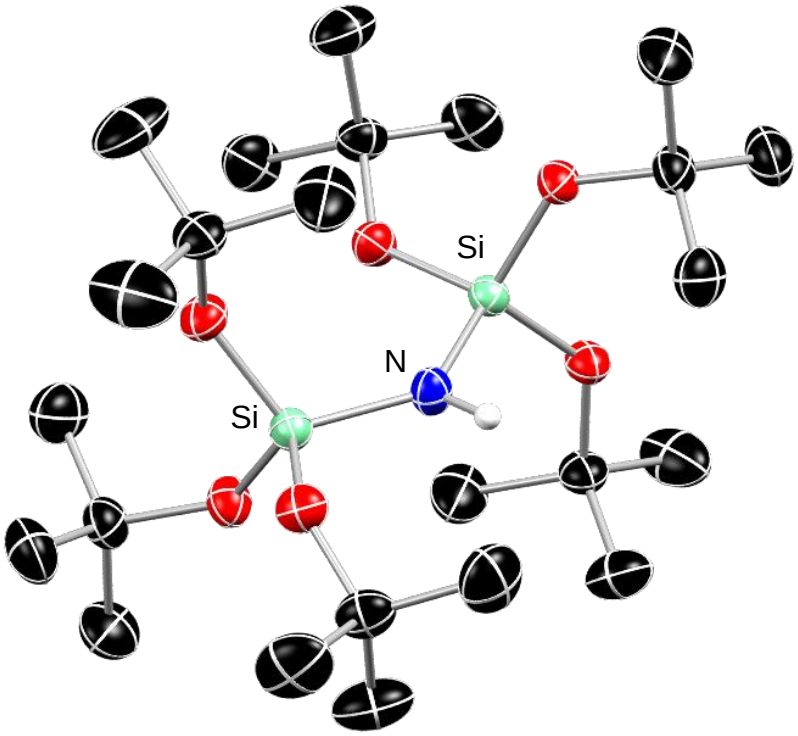

Figure S13. Molecular structure of **BTTSA-H**. Thermal ellipsoids are shown at 50% probability and H atoms (except for N–H) are omitted for clarity.

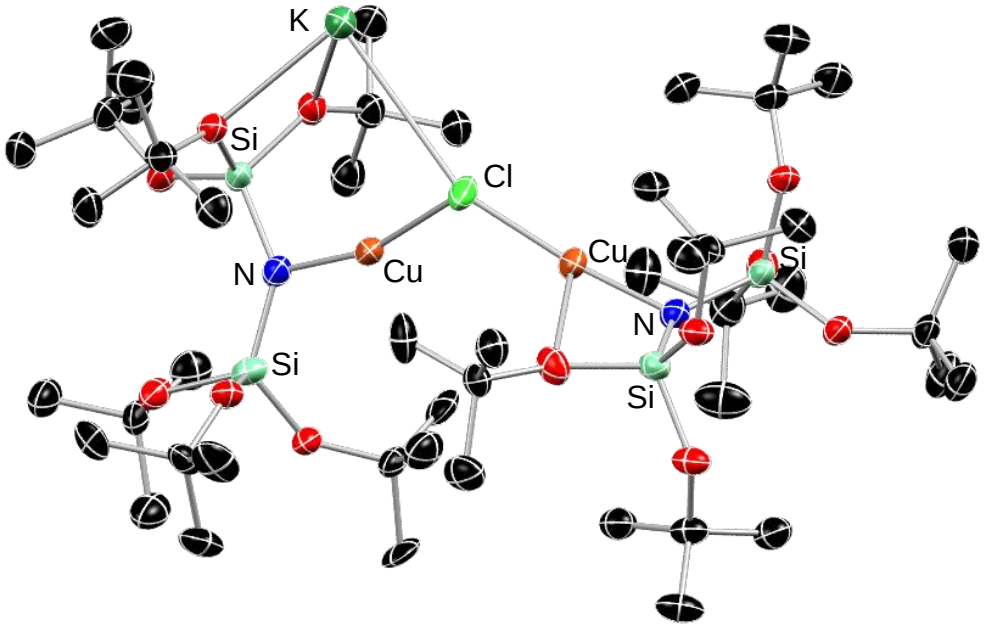

Figure S14. Molecular structure of **2**. One subunit of a polymeric chain is shown. Thermal ellipsoids are shown at 50% probability and H atoms are omitted for clarity.

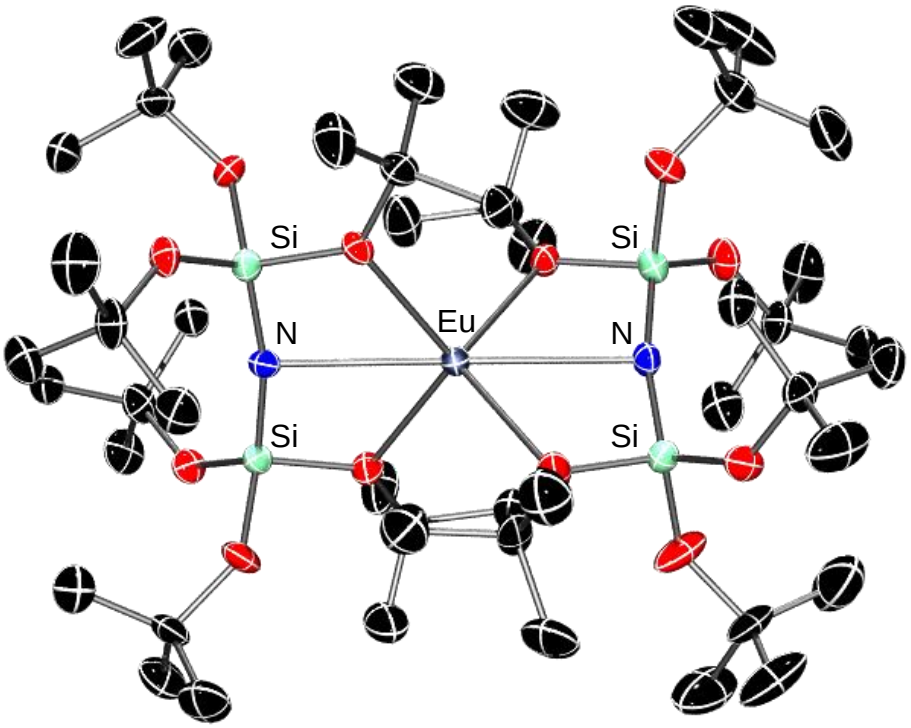

Figure S15. Molecular structure of **2-Eu.** Thermal ellipsoids are shown at 50% probability and H atoms are omitted for clarity.

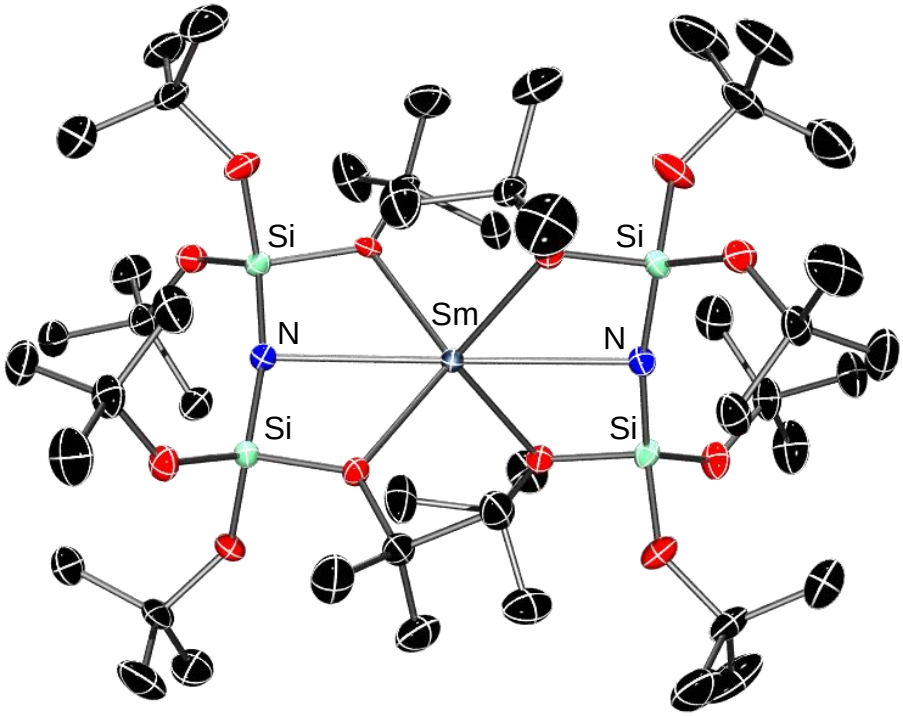

Figure S16. Molecular structure of **2-Sm**. Thermal ellipsoids are shown at 50% probability and H atoms are omitted for clarity.

Table S1. Crystal data and structure refinement for BTTSA-H.

Identification code	BTTSA-H
Empirical formula	$C_{24}H_{55}NO_6Si_2$
Formula weight	509.87
Temperature/K	185(2)
Crystal system	triclinic
Space group	P-1
a/Å	9.2019(9)
b/Å	9.4820(10)
c/Å	20.813(2)
α/°	79.543(4)
β/°	79.198(4)
γ/°	64.407(3)
Volume/Å^3	1598.4(3)
Z	2
ρ_{calc}g/cm^3	1.059
μ/mm^{-1}	0.143
F(000)	564.0
Crystal size/mm^3	0.333 × 0.258 × 0.14
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.794 to 61.016
Index ranges	-13 ≤ h ≤ 13, -13 ≤ k ≤ 13, -29 ≤ l ≤ 29
Reflections collected	41132
Independent reflections	9720 [R_{int} = 0.0413, R_{sigma} = 0.0391]
Data/restraints/parameters	9720/1/319
Goodness-of-fit on F^2	1.031
Final R indexes [I>=2σ (I)]	R_1 = 0.0438, wR_2 = 0.1021
Final R indexes [all data]	R_1 = 0.0660, wR_2 = 0.1171
Largest diff. peak/hole / e Å^{-3}	0.41/-0.29

Table S2. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for BTTSA-H. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Si2	7221.8(4)	7588.3(4)	3266.4(2)	22.18(8)
Si1	8757.5(4)	7591.3(4)	1781.8(2)	23.81(9)
O4	9015.6(10)	7301.3(11)	3391.3(4)	27.60(19)
O2	9545.6(11)	8837.9(11)	1746.2(5)	30.9(2)

O1	10221.3(11)	5851.5(11)	1842.3(5)	30.1(2)
O5	5952.0(10)	9238.9(10)	3540.7(5)	26.78(19)
N1	7323.4(13)	7635.0(13)	2436.6(5)	26.7(2)
C13	9569.1(16)	7554.1(16)	3946.4(7)	30.5(3)
O3	7918.9(12)	8007.2(11)	1109.8(5)	31.0(2)
C14	11383.4(18)	6533(2)	3891.3(9)	46.5(4)
C18	3651(2)	9282(2)	4325.3(8)	45.1(4)
C21	7133.2(17)	4622.4(15)	3610.9(7)	29.8(3)
C22	8954.1(19)	3844.7(18)	3425.3(10)	50.5(4)
C8	9975(3)	11037(2)	1872.9(12)	65.3(6)
C15	8705(2)	7079(2)	4590.4(7)	43.8(4)
C12	7587(3)	5656(2)	1000.4(10)	58.2(5)
C1	11918.1(16)	5251.9(17)	1584.6(7)	33.5(3)
C19	3463.3(18)	9754(2)	3111.8(9)	42.8(4)
C17	4204.4(15)	9978.2(15)	3659.1(7)	31.0(3)
C4	12818(2)	5624(2)	2023.2(10)	51.0(4)
C16	9237(2)	9284.0(19)	3891.0(10)	47.8(4)
C7	9122(4)	10874(2)	838.4(10)	75.3(7)
C9	6990.5(19)	7425.8(18)	837.1(7)	36.6(3)
C24	6621(3)	3916(2)	4280.6(9)	54.8(5)
C20	3778.9(19)	11715.3(17)	3662.0(10)	47.3(4)
C2	12147(2)	5962(2)	876.5(8)	49.5(4)
C3	12462(2)	3482.4(18)	1619.6(9)	47.1(4)
C5	8930.5(19)	10517.9(16)	1578.4(7)	35.4(3)
C10	7233(3)	7861(3)	99.7(9)	62.2(5)
C6	7176(2)	11304.6(19)	1865.2(12)	61.2(6)
C11	5208(2)	8248(3)	1103.3(10)	58.3(5)
C23	6250(2)	4475(2)	3096.9(9)	50.4(4)
O6	6598.3(11)	6272.3(10)	3666.8(4)	26.87(19)

Table S3. Anisotropic Displacement Parameters ($Å^2×10^3$) for BTTSA-H. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Si2	20.62(15)	20.71(16)	23.87(17)	-2.93(12)	-2.21(12)	-7.33(12)
Si1	23.81(16)	22.01(16)	24.37(17)	-1.76(13)	-2.02(13)	-8.99(13)
O4	23.5(4)	31.1(5)	28.3(5)	-6.3(4)	-4.8(3)	-9.5(4)
O2	30.0(5)	24.9(4)	38.8(5)	-2.4(4)	-3.2(4)	-13.1(4)
O1	25.4(4)	25.2(4)	35.0(5)	-1.5(4)	-0.5(4)	-8.0(4)
O5	21.6(4)	23.0(4)	33.9(5)	-6.0(4)	-1.3(4)	-7.3(3)

N1	21.5(5)	32.2(6)	26.3(5)	-3.0(4)	-3.8(4)	-10.6(4)
C13	29.3(6)	30.4(7)	33.3(7)	-6.9(5)	-9.6(5)	-10.1(5)
O3	37.2(5)	30.0(5)	27.2(5)	0.6(4)	-7.1(4)	-15.3(4)
C14	30.4(7)	56.4(10)	51.7(10)	-15.6(8)	-15.3(7)	-9.1(7)
C18	40.3(8)	44.2(9)	46.1(9)	-10.1(7)	12.2(7)	-18.2(7)
C21	34.0(7)	21.6(6)	33.6(7)	-4.4(5)	-0.4(5)	-12.3(5)
C22	35.5(8)	26.3(7)	81.9(13)	-11.6(8)	-0.5(8)	-6.0(6)
C8	73.3(13)	44.9(10)	96.6(17)	-2.9(10)	-24.6(12)	-38.1(10)
C15	48.7(9)	51.8(10)	30.7(8)	-4.1(7)	-9.7(7)	-18.6(8)
C12	80.7(14)	41.3(9)	64.4(12)	-4.0(8)	-27.0(10)	-29.8(9)
C1	24.1(6)	31.7(7)	39.6(8)	-7.6(6)	0.3(5)	-7.0(5)
C19	26.0(7)	45.0(9)	54.5(10)	-8.5(7)	-8.1(6)	-9.4(6)
C17	21.6(6)	25.5(6)	40.9(8)	-6.3(5)	1.5(5)	-6.3(5)
C4	33.7(8)	52.5(10)	67.7(12)	-16.4(9)	-10.9(8)	-13.0(7)
C16	50.5(9)	36.5(8)	65.0(11)	-9.8(8)	-15.8(8)	-21.0(7)
C7	133(2)	49.5(11)	43.4(10)	7.1(9)	-1.1(12)	-46.1(13)
C9	46.1(8)	37.3(8)	31.3(7)	-1.0(6)	-12.8(6)	-19.6(6)
C24	84.7(14)	33.7(8)	42.6(9)	-0.5(7)	6.2(9)	-28.4(9)
C20	34.7(8)	25.5(7)	73.1(12)	-11.7(7)	1.4(8)	-5.2(6)
C2	43.2(9)	50.2(10)	44.5(9)	-7.5(7)	10.5(7)	-14.9(8)
C3	37.5(8)	30.9(8)	62.1(11)	-10.3(7)	-4.9(7)	-2.5(6)
C5	43.3(8)	24.8(6)	39.1(8)	-1.7(6)	-2.1(6)	-17.0(6)
C10	88.9(15)	80.8(14)	32.6(9)	1.5(9)	-18.9(9)	-47.9(12)
C6	47.1(10)	25.3(8)	101.4(16)	-10.4(9)	3.9(10)	-9.7(7)
C11	43.8(10)	75.1(13)	61.5(12)	-8.6(10)	-16.7(9)	-25.1(9)
C23	62.1(11)	48.3(10)	54.0(10)	-12.7(8)	-11.5(9)	-30.6(9)
O6	28.6(4)	20.8(4)	29.0(5)	-3.8(3)	0.6(4)	-9.4(3)

Table S4. Bond Lengths for BTTSA-H.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Si2	O4	1.6166(9)	C18	C17	1.520(2)
Si2	O5	1.6233(9)	C21	C22	1.515(2)
Si2	N1	1.7055(12)	C21	C24	1.517(2)
Si2	O6	1.6255(10)	C21	C23	1.517(2)
Si1	O2	1.6178(10)	C21	O6	1.4432(15)
Si1	O1	1.6187(10)	C8	C5	1.511(2)
Si1	N1	1.7028(11)	C12	C9	1.516(2)
Si1	O3	1.6274(10)	C1	C4	1.516(2)
O4	C13	1.4416(16)	C1	C2	1.522(2)
O2	C5	1.4398(16)	C1	C3	1.521(2)

O1	C1	1.4418(16)	C19	C17	1.521(2)
O5	C17	1.4417(15)	C17	C20	1.521(2)
C13	C14	1.520(2)	C7	C5	1.509(2)
C13	C15	1.524(2)	C9	C10	1.516(2)
C13	C16	1.520(2)	C9	C11	1.522(2)
O3	C9	1.4346(17)	C5	C6	1.510(2)

Table S5. Bond Angles for BTTSA-H.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
O4	Si2	O5	107.46(5)	O6	C21	C24	105.56(11)
O4	Si2	N1	105.32(5)	O6	C21	C23	108.31(12)
O4	Si2	O6	114.34(5)	O1	C1	C4	108.49(12)
O5	Si2	N1	113.03(5)	O1	C1	C2	110.62(12)
O5	Si2	O6	105.41(5)	O1	C1	C3	105.01(12)
O6	Si2	N1	111.40(5)	C4	C1	C2	111.25(14)
O2	Si1	O1	106.96(5)	C4	C1	C3	110.62(13)
O2	Si1	N1	115.24(6)	C3	C1	C2	110.65(13)
O2	Si1	O3	106.44(5)	O5	C17	C18	108.85(11)
O1	Si1	N1	106.96(5)	O5	C17	C19	110.43(11)
O1	Si1	O3	113.02(5)	O5	C17	C20	105.28(11)
O3	Si1	N1	108.39(5)	C18	C17	C19	111.19(13)
C13	O4	Si2	130.82(8)	C18	C17	C20	110.75(13)
C5	O2	Si1	132.45(9)	C20	C17	C19	110.17(13)
C1	O1	Si1	132.58(9)	O3	C9	C12	110.93(13)
C17	O5	Si2	132.88(8)	O3	C9	C10	105.49(13)
Si1	N1	Si2	134.90(7)	O3	C9	C11	108.99(13)
O4	C13	C14	105.57(11)	C12	C9	C11	110.67(15)
O4	C13	C15	110.65(12)	C10	C9	C12	110.54(15)
O4	C13	C16	108.51(12)	C10	C9	C11	110.09(15)
C14	C13	C15	110.92(13)	O2	C5	C8	105.60(13)
C16	C13	C14	110.73(13)	O2	C5	C7	108.77(13)
C16	C13	C15	110.34(13)	O2	C5	C6	110.69(12)
C9	O3	Si1	135.99(9)	C7	C5	C8	110.23(16)
C22	C21	C24	111.36(14)	C7	C5	C6	111.02(17)
C22	C21	C23	110.69(14)	C6	C5	C8	110.38(16)
C24	C21	C23	109.63(14)	C21	O6	Si2	132.15(8)
O6	C21	C22	111.11(11)				

Table S6. Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for BTTSA-H.

Atom	*x*	*y*	*z*	U(eq)
H14A	11573	5426	3917	70
H14B	11839	6675	4252	70
H14C	11909	6840	3469	70
H18A	3992	8151	4321	68
H18B	2465	9796	4416	68
H18C	4139	9450	4669	68
H22A	9502	3961	3760	76
H22B	9251	4346	2998	76
H22C	9287	2724	3398	76
H8A	9862	10776	2352	98
H8B	9629	12177	1766	98
H8C	11114	10495	1692	98
H15A	7538	7744	4613	66
H15B	9132	7214	4962	66
H15C	8891	5975	4611	66
H12A	8733	5148	823	87
H12B	6946	5285	805	87
H12C	7469	5392	1479	87
H19A	3895	10149	2686	64
H19B	2281	10335	3179	64
H19C	3736	8632	3117	64
H4A	12419	6768	2010	76
H4B	13983	5177	1867	76
H4C	12635	5169	2476	76
H16A	9780	9579	3471	72
H16B	9653	9465	4254	72
H16C	8065	9924	3912	72
H7A	10263	10320	663	113
H7B	8780	12010	719	113
H7C	8448	10522	653	113
H24A	6940	2790	4272	82
H24B	5440	4442	4387	82
H24C	7151	4059	4615	82
H20A	4307	11841	4002	71
H20B	2599	12286	3756	71
H20C	4156	12138	3231	71
H2A	11512	5745	609	74
H2B	13298	5496	701	74
H2C	11777	7102	863	74

H3A	12255	3054	2076	71
H3B	13625	2988	1467	71
H3C	11854	3265	1339	71
H10A	6888	9003	4	93
H10B	6584	7536	-115	93
H10C	8383	7326	-67	93
H6A	6514	10954	1671	92
H6B	6798	12449	1767	92
H6C	7077	11021	2343	92
H11A	5049	7895	1573	87
H11B	4546	7989	866	87
H11C	4880	9389	1042	87
H23A	6581	4935	2665	76
H23B	5076	5034	3213	76
H23C	6523	3361	3081	76
H1	6379(16)	7878(18)	2334(8)	32

Table S7. Crystal data and structure refinement for BTTSA-Cu.

Identification code	BTTSA-Cu
Empirical formula	$C_{48}H_{108}ClCu_2KN_2O_{12}Si_4$
Formula weight	1219.35
Temperature/K	191.07
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	20.524(8)
b/Å	19.826(9)
c/Å	19.692(8)
α/°	90
β/°	112.541(15)
γ/°	90
Volume/Å^3	7401(6)
Z	4
ρ_{calc}g/cm^3	1.094
μ/mm^{-1}	0.777
F(000)	2624.0
Crystal size/mm^3	0.549 × 0.29 × 0.258
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.638 to 60.708
Index ranges	-26 ≤ h ≤ 28, -27 ≤ k ≤ 27, -27 ≤ l ≤ 27
Reflections collected	182799
Independent reflections	21842 [R_{int} = 0.0802, R_{sigma}= 0.0519]

Data/restraints/parameters	21842/32/741
Goodness-of-fit on F^2	1.071
Final R indexes [I>=2σ (I)]	R_1 = 0.0552, wR_2 = 0.1280
Final R indexes [all data]	R_1 = 0.1125, wR_2= 0.1719
Largest diff. peak/hole / e $Å^{-3}$	0.61/-1.03

Table S8. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$×10^3) for BTTSA-Cu. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cu1	7891.8(2)	3204.4(2)	7502.0(2)	31.70(10)
Cu2	7130.4(2)	4647.1(2)	8127.5(2)	29.79(10)
K1	7614.5(4)	1014.3(4)	5070.9(4)	35.68(16)
Cl1	7583.2(5)	3644.1(5)	8337.4(5)	46.9(2)
Si1	9083.5(4)	2597.8(5)	7114.6(4)	27.70(17)
Si2	7488.3(4)	2305.3(4)	6275.5(4)	27.79(17)
Si3	6238.4(5)	5824.7(4)	7416.9(4)	30.79(18)
Si4	6970.0(4)	5557.1(5)	9137.7(4)	29.23(18)
O1	9580.0(11)	3280.6(12)	7351.4(12)	34.6(5)
O2	9431.1(11)	2091.6(12)	7830.1(11)	33.5(5)
O3	9186.0(10)	2182.9(11)	6432.8(11)	30.9(5)
O4	7475.7(11)	1460.5(11)	6347.6(11)	31.9(5)
O5	7328.6(11)	2312.7(11)	5382.3(11)	32.8(5)
O6	6837.0(11)	2660.3(12)	6441.9(13)	35.9(5)
O10	6585.0(11)	4944.2(12)	9443.6(11)	34.5(5)
O11	7800.9(10)	5321.5(11)	9646.5(11)	32.6(5)
O12	6795.9(12)	6309.9(12)	9386.5(11)	37.9(5)
N2	6798.0(13)	5529.3(13)	8236.5(13)	28.9(5)
N1	8206.6(12)	2726.3(13)	6842.8(13)	28.5(5)
C1	9534.0(17)	4001.5(18)	7177.6(19)	38.0(7)
C2	10297.7(19)	4239(2)	7369(2)	50.7(9)
C3	9225(2)	4375(2)	7663(2)	53.1(10)
C4	9097(2)	4120(2)	6371(2)	55.9(11)
C5	9805.9(17)	2190(2)	8613.0(16)	40.5(8)
C6	9792(2)	1500(2)	8960(2)	55.3(10)
C7	10569.2(18)	2404(2)	8780.3(19)	51.0(10)
C8	9430(2)	2719(2)	8898.2(19)	53.2(10)
C9	9792.1(16)	1941.6(18)	6298.0(17)	34.7(7)
C10	10338.0(19)	1605(2)	6972(2)	52.5(10)

C11	10115.0(19)	2546(2)	6044(2)	47.8(9)
C12	9491.8(17)	1420.8(19)	5681.3(18)	39.5(7)
C13	7694.6(16)	1000.1(16)	6978.2(17)	32.8(6)
C14	7765.7(18)	1368.1(18)	7687.4(17)	37.8(7)
C15	8401.6(18)	687.9(18)	7046.1(19)	40.4(8)
C16	7126.6(19)	444.0(18)	6795(2)	44.1(8)
C17	7316.3(16)	2868.2(16)	4884.0(16)	32.0(6)
C18	8030.8(17)	2871.0(18)	4802.1(17)	36.4(7)
C19	6725.4(19)	2703.1(18)	4144.9(17)	42.1(8)
C20	7178.2(17)	3551.5(17)	5175.5(17)	35.3(7)
C37	5847.5(16)	4721.2(19)	9167.9(17)	38.1(7)
C38	5754(2)	4371(3)	9815(2)	73.6(16)
C39	5717.1(18)	4217.9(18)	8535(2)	41.4(8)
C40	5340.2(17)	5323(2)	8912(2)	45.0(9)
C41	8468.8(15)	5581.5(19)	9648.5(17)	35.9(7)
C42	8782.9(17)	5053(2)	9290.6(19)	41.9(8)
C43	8955.4(17)	5663(2)	10460.7(19)	47.0(9)
C44	8383.9(18)	6257.8(19)	9240(2)	41.2(8)
C45	6854.7(19)	6628(2)	10078.3(17)	45.0(9)
C46	7480(2)	7116(3)	10320(2)	64.2(13)
C47	6944(3)	6093(2)	10675(2)	63.2(13)
C48	6166.6(19)	7021(2)	9911.2(19)	45.8(9)
C21A	6092(7)	2644(5)	6364(4)	29.7(13)
C22A	5900(20)	1906(3)	6458(7)	37.9(12)
C23A	5662(4)	2884(5)	5585(4)	45.3(13)
C24A	5967(4)	3104(4)	6920(4)	43.9(12)
O7A	6520(2)	6034(2)	6791(2)	29.4(6)
C25A	6963(3)	5733(3)	6457(3)	28.9(11)
C26A	7746(3)	5847(6)	6947(7)	40.2(16)
C27A	6795(5)	4976(3)	6353(4)	47.2(12)
C28A	6793(7)	6083(4)	5710(5)	41.8(14)
O9A	5790(2)	6574.6(19)	7470(2)	32.0(6)
C33A	5965(3)	7281(2)	7444(3)	30.2(13)
C34A	6757(3)	7388(4)	7864(4)	42.7(14)
C35A	5542(4)	7694(3)	7797(4)	45.1(12)
C36A	5744(5)	7486(4)	6633(3)	47.8(15)
O8A	5571(3)	5294(3)	7087(3)	32.3(8)
C29A	4862(4)	5281(6)	6526(6)	32.3(18)
C30A	4641(6)	4550(6)	6295(8)	55(2)
C31A	4855(6)	5700(5)	5859(4)	51.4(19)
C32A	4380(6)	5625(11)	6854(10)	42.1(18)
C21B	6070(5)	2564(4)	6150(3)	29.7(13)

C22B	5903(15)	1974(3)	6569(5)	37.9(12)
C23B	5724(3)	2439(4)	5324(3)	45.3(13)
C24B	5820(3)	3232(3)	6342(4)	43.9(12)
O7B	6483(2)	5408.0(19)	6783.9(19)	29.4(6)
C25B	6994(3)	5547(3)	6467(3)	28.9(11)
C26B	7686(3)	5804(5)	7063(6)	40.2(16)
C27B	7122(4)	4890(3)	6124(4)	47.2(12)
C28B	6687(6)	6094(4)	5876(5)	41.8(14)
O9B	6332(2)	6593.0(19)	7265(2)	32.0(6)
C33B	6232(3)	7237(2)	7561(3)	30.2(13)
C34B	6911(3)	7443(3)	8198(4)	42.7(14)
C35B	5623(3)	7167(3)	7830(4)	45.1(12)
C36B	6034(4)	7759(3)	6936(4)	47.8(15)
O8B	5463(2)	5561(3)	7265(2)	32.3(8)
C29B	4831(4)	5481(4)	6604(5)	32.3(18)
C31B	4808(5)	6011(5)	6028(4)	51.4(19)
C32B	4186(4)	5559(10)	6824(8)	42.1(18)
C30B	4849(6)	4759(5)	6320(7)	55(2)

Table S9. Anisotropic Displacement Parameters ($Å^2×10^3$) for BTTSA-Cu. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cu1	29.30(19)	43.0(2)	27.64(18)	3.53(15)	16.29(15)	6.99(16)
Cu2	30.51(19)	39.4(2)	21.55(17)	2.16(14)	12.34(14)	8.42(15)
K1	31.6(3)	47.2(4)	29.3(3)	-1.7(3)	12.8(3)	-6.0(3)
Cl1	64.0(6)	52.8(5)	39.7(4)	17.7(4)	37.5(4)	30.1(4)
Si1	19.7(3)	44.5(5)	19.7(3)	-2.1(3)	8.5(3)	0.5(3)
Si2	20.3(4)	38.0(4)	23.7(4)	4.4(3)	6.8(3)	-0.5(3)
Si3	35.8(4)	36.4(4)	19.7(4)	0.8(3)	10.2(3)	-2.2(3)
Si4	21.6(4)	45.8(5)	20.1(3)	-4.3(3)	7.7(3)	5.6(3)
O1	23.1(10)	47.3(13)	32.7(11)	-6.0(10)	9.8(9)	-1.5(9)
O2	24.0(10)	54.8(14)	19.8(9)	-0.7(9)	6.2(8)	4.0(9)
O3	23.2(10)	48.8(13)	21.7(9)	-2.5(9)	9.6(8)	1.8(9)
O4	28.4(10)	40.9(12)	24.2(10)	6.9(9)	7.7(8)	1.6(9)
O5	30.5(11)	38.8(12)	24.1(10)	7.2(9)	5.1(8)	-3.4(9)
O6	19.7(10)	43.5(13)	43.8(13)	5.2(10)	11.3(9)	0.2(9)
O10	23.5(10)	57.4(14)	23.9(10)	4.0(9)	10.6(8)	7.3(9)
O11	22.8(10)	46.8(13)	27.1(10)	-6.0(9)	8.2(8)	4.2(9)
O12	35.1(12)	54.5(14)	22.0(10)	-7.7(9)	8.8(9)	13.2(10)

N2	25.4(12)	38.3(14)	24.2(11)	-4.4(10)	10.7(9)	1.1(10)
N1	23.5(11)	39.8(14)	24.0(11)	-0.1(10)	10.9(9)	0.5(10)
C1	29.8(15)	47.4(19)	37.5(17)	-6.3(14)	13.8(13)	-7.8(14)
C2	38.9(19)	63(2)	52(2)	-16.8(19)	20.1(17)	-16.0(17)
C3	48(2)	53(2)	67(3)	-6(2)	32(2)	0.2(18)
C4	55(2)	55(2)	43(2)	5.8(17)	1.8(18)	-16.6(19)
C5	32.1(16)	68(2)	18.0(13)	-0.6(14)	5.7(12)	10.3(15)
C6	51(2)	78(3)	28.5(17)	10.8(18)	5.1(16)	13(2)
C7	32.9(18)	83(3)	29.0(17)	-9.1(18)	3.4(14)	2.8(18)
C8	51(2)	85(3)	23.1(15)	-0.8(17)	14.4(15)	23(2)
C9	23.8(14)	57(2)	27.6(14)	-5.6(14)	14.4(12)	2.6(13)
C10	35.2(18)	89(3)	34.3(18)	-1.6(18)	14.4(15)	20.2(19)
C11	38.3(18)	65(2)	52(2)	-12.3(18)	30.1(17)	-8.6(17)
C12	33.8(16)	55(2)	35.4(16)	-10.3(15)	20.0(14)	-3.4(15)
C13	29.1(15)	37.3(16)	29.3(15)	9.6(12)	8.4(12)	4.2(12)
C14	37.3(17)	46.5(19)	29.7(15)	10.1(14)	12.9(13)	6.1(14)
C15	36.7(17)	45.4(19)	36.8(17)	6.1(14)	11.5(14)	10.3(14)
C16	39.9(18)	44(2)	46(2)	11.2(16)	14.6(16)	-1.1(15)
C17	31.4(15)	38.4(16)	22.0(13)	3.5(12)	5.6(11)	-4.6(12)
C18	37.3(17)	44.3(18)	27.5(15)	0.0(13)	12.5(13)	-3.6(14)
C19	42.8(18)	44.5(19)	25.9(15)	6.2(14)	-1.4(13)	-4.9(15)
C20	33.1(16)	42.5(18)	28.2(14)	3.6(13)	9.4(12)	-0.5(13)
C37	21.3(14)	65(2)	29.4(15)	9.5(15)	11.7(12)	5.6(14)
C38	31.9(19)	145(5)	50(2)	36(3)	22.2(18)	7(2)
C39	33.9(17)	42.3(19)	50(2)	4.2(15)	18.6(15)	-2.1(14)
C40	24.7(15)	67(2)	41.6(18)	-8.0(17)	10.7(14)	7.7(15)
C41	20.5(13)	56(2)	29.9(15)	-6.2(14)	7.8(11)	2.8(13)
C42	28.4(15)	62(2)	35.6(17)	-1.4(16)	12.9(13)	10.9(15)
C43	26.3(16)	76(3)	32.7(17)	-12.2(17)	4.8(13)	-0.9(16)
C44	30.9(16)	51(2)	43.9(19)	-8.6(16)	16.6(14)	-3.5(14)
C45	42.0(18)	65(2)	25.0(15)	-13.0(15)	9.5(13)	20.5(17)
C46	41(2)	92(3)	51(2)	-42(2)	7.2(17)	6(2)
C47	80(3)	80(3)	25.1(17)	-4.4(18)	14.5(18)	35(2)
C48	40.4(18)	62(2)	32.9(17)	-8.7(16)	11.5(14)	19.1(17)
C21A	16.9(15)	40(3)	32(4)	2(3)	10(3)	1.4(18)
C22A	27.3(16)	45(2)	43(3)	0(2)	16(4)	0(3)
C23A	25(2)	69(4)	36(3)	6(2)	5.5(19)	-3(2)
C24A	28(2)	42(3)	68(3)	-11(3)	25(3)	1.8(19)
O7A	35.8(15)	33.0(14)	22.3(13)	3.4(12)	14.5(12)	7.6(13)
C25A	44.6(19)	22(3)	26.2(15)	3.1(18)	21.0(14)	9(2)
C26A	41(2)	60(3)	32(3)	1(2)	28.1(19)	-1.0(19)
C27A	65(4)	42(3)	37(3)	-4(2)	24(2)	9(3)

C28A	63(4)	51(2)	24(4)	9(2)	31(3)	7(2)
O9A	42.0(17)	30.7(15)	27.5(14)	0.3(12)	18.0(13)	3.9(13)
C33A	36(4)	27.4(18)	34(2)	1.9(16)	20(3)	10(2)
C34A	50(4)	36(2)	41(4)	-6(3)	16(3)	-4(2)
C35A	62(3)	41(2)	41(3)	3(2)	29(2)	17(2)
C36A	71(5)	38(3)	42(4)	12(2)	30(3)	15(3)
O8A	27.7(16)	46(3)	21.0(18)	1.1(15)	6.6(12)	3.9(16)
C29A	27.8(17)	32(6)	27(2)	-2(3)	-0.1(16)	9(2)
C30A	44(6)	53(6)	42(2)	-18(4)	-11(4)	4(4)
C31A	41(3)	73(6)	29(3)	14(3)	1(2)	12(4)
C32A	8(5)	65(4)	44(2)	-2(3)	-1(4)	1(5)
C21B	16.9(15)	40(3)	32(4)	2(3)	10(3)	1.4(18)
C22B	27.3(16)	45(2)	43(3)	0(2)	16(4)	0(3)
C23B	25(2)	69(4)	36(3)	6(2)	5.5(19)	-3(2)
C24B	28(2)	42(3)	68(3)	-11(3)	25(3)	1.8(19)
O7B	35.8(15)	33.0(14)	22.3(13)	3.4(12)	14.5(12)	7.6(13)
C25B	44.6(19)	22(3)	26.2(15)	3.1(18)	21.0(14)	9(2)
C26B	41(2)	60(3)	32(3)	1(2)	28.1(19)	-1.0(19)
C27B	65(4)	42(3)	37(3)	-4(2)	24(2)	9(3)
C28B	63(4)	51(2)	24(4)	9(2)	31(3)	7(2)
O9B	42.0(17)	30.7(15)	27.5(14)	0.3(12)	18.0(13)	3.9(13)
C33B	36(4)	27.4(18)	34(2)	1.9(16)	20(3)	10(2)
C34B	50(4)	36(2)	41(4)	-6(3)	16(3)	-4(2)
C35B	62(3)	41(2)	41(3)	3(2)	29(2)	17(2)
C36B	71(5)	38(3)	42(4)	12(2)	30(3)	15(3)
O8B	27.7(16)	46(3)	21.0(18)	1.1(15)	6.6(12)	3.9(16)
C29B	27.8(17)	32(6)	27(2)	-2(3)	-0.1(16)	9(2)
C31B	41(3)	73(6)	29(3)	14(3)	1(2)	12(4)
C32B	8(5)	65(4)	44(2)	-2(3)	-1(4)	1(5)
C30B	44(6)	53(6)	42(2)	-18(4)	-11(4)	4(4)

Table S10. Bond Lengths for BTTSA-Cu.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cu1	Cl1	2.1601(11)	C9	C11	1.543(5)
Cu1	Si2	2.8572(13)	C9	C12	1.532(5)
Cu1	N1	1.909(2)	C13	C14	1.532(5)
Cu2	Cl1	2.1667(13)	C13	C15	1.535(4)
Cu2	N2	1.919(3)	C13	C16	1.543(5)
K1	$Cl1^{1}$	3.4565(17)	C17	C18	1.535(5)
K1	Si2	3.5659(16)	C17	C19	1.531(4)

K1	Si4[1]	3.6012(18)	C17	C20	1.539(5)
K1	O4	2.781(2)	C37	C38	1.527(5)
K1	O5	2.761(3)	C37	C39	1.537(5)
K1	O10[1]	2.757(2)	C37	C40	1.535(5)
K1	O11[1]	2.847(3)	C41	C42	1.535(5)
Si1	O1	1.650(2)	C41	C43	1.535(4)
Si1	O2	1.652(2)	C41	C44	1.539(5)
Si1	O3	1.655(2)	C45	C46	1.531(6)
Si1	N1	1.689(3)	C45	C47	1.539(6)
Si2	O4	1.682(2)	C45	C48	1.534(5)
Si2	O5	1.661(2)	C21A	C22A	1.545(5)
Si2	O6	1.651(2)	C21A	C23A	1.524(7)
Si2	N1	1.690(3)	C21A	C24A	1.521(7)
Si3	N2	1.687(3)	O7A	C25A	1.439(5)
Si3	O7A	1.604(4)	C25A	C26A	1.542(5)
Si3	O9A	1.773(4)	C25A	C27A	1.535(7)
Si3	O8A	1.650(5)	C25A	C28A	1.540(6)
Si3	O7B	1.722(4)	O9A	C33A	1.451(5)
Si3	O9B	1.578(4)	C33A	C34A	1.530(7)
Si3	O8B	1.591(5)	C33A	C35A	1.538(7)
Si4	O10	1.682(3)	C33A	C36A	1.538(6)
Si4	O11	1.679(2)	O8A	C29A	1.450(4)
Si4	O12	1.652(2)	C29A	C30A	1.534(13)
Si4	N2	1.672(3)	C29A	C31A	1.549(16)
O1	C1	1.464(4)	C29A	C32A	1.53(2)
O2	C5	1.448(4)	C21B	C22B	1.545(5)
O3	C9	1.449(3)	C21B	C23B	1.524(7)
O4	C13	1.466(3)	C21B	C24B	1.521(7)
O5	C17	1.469(4)	O7B	C25B	1.439(5)
O6	C21A	1.477(14)	C25B	C26B	1.541(5)
O6	C21B	1.466(10)	C25B	C27B	1.535(7)
O10	C37	1.467(4)	C25B	C28B	1.539(6)
O11	C41	1.463(4)	O9B	C33B	1.451(5)
O12	C45	1.463(4)	C33B	C34B	1.531(7)
C1	C2	1.539(5)	C33B	C35B	1.538(7)
C1	C3	1.526(5)	C33B	C36B	1.538(6)
C1	C4	1.513(5)	O8B	C29B	1.450(4)
C5	C6	1.534(6)	C29B	C31B	1.534(13)
C5	C7	1.532(5)	C29B	C32B	1.550(16)
C5	C8	1.531(5)	C29B	C30B	1.542(13)
C9	C10	1.523(5)			

[1]+X,1/2-Y,-1/2+Z

Table S11. Bond Angles for BTTSA-Cu.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
Cl1	Cu1	Si2	145.18(4)	O1	C1	C4	110.9(3)
N1	Cu1	Cl1	173.10(8)	C3	C1	C2	109.1(3)
N1	Cu1	Si2	34.85(8)	C4	C1	C2	110.4(3)
N2	Cu2	Cl1	163.75(8)	C4	C1	C3	111.1(3)
Cl1[1]	K1	Cu2[1]	34.33(2)	O2	C5	C6	105.2(3)
Cl1[1]	K1	Si2	122.53(4)	O2	C5	C7	110.4(3)
Cl1[1]	K1	Si4[1]	78.55(3)	O2	C5	C8	110.3(3)
Si2	K1	Cu2[1]	149.32(3)	C7	C5	C6	110.1(3)
Si2	K1	Si4[1]	148.68(3)	C8	C5	C6	110.5(3)
Si4[1]	K1	Cu2[1]	44.311(16)	C8	C5	C7	110.4(3)
O4	K1	Cu2[1]	160.47(5)	O3	C9	C10	112.4(2)
O4	K1	Cl1[1]	149.42(6)	O3	C9	C11	107.9(3)
O4	K1	Si2	27.32(5)	O3	C9	C12	104.8(2)
O4	K1	Si4[1]	126.28(5)	C10	C9	C11	111.0(3)
O4	K1	O11[1]	129.29(7)	C10	C9	C12	109.5(3)
O5	K1	Cu2[1]	123.34(5)	C12	C9	C11	111.1(3)
O5	K1	Cl1[1]	96.40(5)	O4	C13	C14	111.5(3)
O5	K1	Si2	26.77(4)	O4	C13	C15	107.3(2)
O5	K1	Si4[1]	148.45(5)	O4	C13	C16	106.7(2)
O5	K1	O4	53.02(6)	C14	C13	C15	110.9(3)
O5	K1	O11[1]	175.23(6)	C14	C13	C16	110.7(3)
O10[1]	K1	Cu2[1]	56.72(5)	C15	C13	C16	109.6(3)
O10[1]	K1	Cl1[1]	88.38(5)	O5	C17	C18	107.5(2)
O10[1]	K1	Si2	123.65(6)	O5	C17	C19	106.2(2)
O10[1]	K1	Si4[1]	26.69(5)	O5	C17	C20	111.7(2)
O10[1]	K1	O4	107.33(7)	C18	C17	C20	110.8(3)
O10[1]	K1	O5	123.41(7)	C19	C17	C18	110.0(3)
O10[1]	K1	O11[1]	52.66(7)	C19	C17	C20	110.5(3)
O11[1]	K1	Cu2[1]	52.84(4)	O10	C37	C38	105.7(3)
O11[1]	K1	Cl1[1]	81.15(5)	O10	C37	C39	109.3(2)
O11[1]	K1	Si2	156.24(5)	O10	C37	C40	111.2(3)
O11[1]	K1	Si4[1]	27.10(5)	C38	C37	C39	110.0(4)
Cu1	Cl1	Cu2	117.04(4)	C38	C37	C40	110.0(3)
Cu1	Cl1	K1[2]	158.64(4)	C40	C37	C39	110.6(3)
Cu2	Cl1	K1[2]	81.53(3)	O11	C41	C42	108.4(3)
O1	Si1	O2	103.84(12)	O11	C41	C43	105.9(3)
O1	Si1	O3	112.35(12)	O11	C41	C44	112.8(2)

O1	Si1	N1	115.68(13)	C42	C41	C43	109.3(3)
O2	Si1	O3	104.02(12)	C42	C41	C44	109.7(3)
O2	Si1	N1	114.91(12)	C43	C41	C44	110.5(3)
O3	Si1	N1	105.62(12)	O12	C45	C46	108.8(3)
O4	Si2	N1	118.28(12)	O12	C45	C47	110.9(3)
O5	Si2	O4	95.45(11)	O12	C45	C48	106.2(3)
O5	Si2	N1	117.62(12)	C46	C45	C47	111.0(3)
O6	Si2	O4	111.59(12)	C46	C45	C48	109.8(3)
O6	Si2	O5	111.12(12)	C48	C45	C47	110.1(3)
O6	Si2	N1	103.05(13)	O6	C21A	C22A	108.1(14)
N2	Si3	O9A	114.41(16)	O6	C21A	C23A	106.0(8)
N2	Si3	O7B	104.22(16)	O6	C21A	C24A	111.5(8)
O7A	Si3	N2	120.75(18)	C23A	C21A	C22A	109.9(5)
O7A	Si3	O9A	100.2(2)	C24A	C21A	C22A	111.1(5)
O7A	Si3	O8A	110.6(2)	C24A	C21A	C23A	110.2(4)
O8A	Si3	N2	108.3(2)	C25A	O7A	Si3	136.1(4)
O8A	Si3	O9A	100.7(3)	O7A	C25A	C26A	110.0(3)
O9B	Si3	N2	115.36(18)	O7A	C25A	C27A	108.5(4)
O9B	Si3	O7B	103.63(19)	O7A	C25A	C28A	107.3(4)
O9B	Si3	O8B	117.8(2)	C27A	C25A	C26A	110.7(4)
O8B	Si3	N2	109.35(18)	C27A	C25A	C28A	110.8(4)
O8B	Si3	O7B	104.7(2)	C28A	C25A	C26A	109.4(4)
Cu2	Si4	$K1^2$	71.61(4)	C33A	O9A	Si3	131.8(4)
O10	Si4	Cu2	89.33(9)	O9A	C33A	C34A	109.9(4)
O10	Si4	$K1^2$	47.42(8)	O9A	C33A	C35A	107.9(4)
O11	Si4	Cu2	82.84(8)	O9A	C33A	C36A	108.3(4)
O11	Si4	$K1^2$	50.55(8)	C34A	C33A	C35A	110.4(4)
O11	Si4	O10	95.42(12)	C34A	C33A	C36A	110.7(5)
O12	Si4	Cu2	153.06(9)	C36A	C33A	C35A	109.6(4)
O12	Si4	$K1^2$	135.16(9)	C29A	O8A	Si3	138.6(7)
O12	Si4	O10	111.21(12)	O8A	C29A	C30A	109.8(7)
O12	Si4	O11	111.09(12)	O8A	C29A	C31A	108.4(9)
O12	Si4	N2	111.28(13)	O8A	C29A	C32A	106.9(8)
N2	Si4	Cu2	42.14(9)	C30A	C29A	C31A	110.5(7)
N2	Si4	$K1^2$	113.56(10)	C30A	C29A	C32A	112.3(10)
N2	Si4	O10	114.79(13)	C32A	C29A	C31A	108.7(11)
N2	Si4	O11	112.14(12)	O6	C21B	C22B	108.3(11)
C1	O1	Si1	139.2(2)	O6	C21B	C23B	115.6(6)
C5	O2	Si1	134.9(2)	O6	C21B	C24B	101.7(6)
C9	O3	Si1	134.23(18)	C23B	C21B	C22B	109.8(4)
Si2	O4	K1	103.31(9)	C24B	C21B	C22B	111.1(4)
C13	O4	K1	117.60(18)	C24B	C21B	C23B	110.1(4)

C13	O4	Si2	133.0(2)	C25B	O7B	Si3	133.3(3)
Si2	O5	K1	104.74(10)	O7B	C25B	C26B	110.2(3)
C17	O5	K1	120.10(17)	O7B	C25B	C27B	107.8(4)
C17	O5	Si2	131.3(2)	O7B	C25B	C28B	107.9(4)
C21A	O6	Si2	148.7(4)	C27B	C25B	C26B	110.8(4)
C21B	O6	Si2	134.1(3)	C27B	C25B	C28B	110.8(4)
Si4	O10	K1[2]	105.89(10)	C28B	C25B	C26B	109.4(4)
C37	O10	K1[2]	117.6(2)	C33B	O9B	Si3	136.6(3)
C37	O10	Si4	130.17(19)	O9B	C33B	C34B	109.8(4)
Si4	O11	K1[2]	102.35(10)	O9B	C33B	C35B	108.5(4)
C41	O11	K1[2]	123.93(18)	O9B	C33B	C36B	107.8(4)
C41	O11	Si4	129.8(2)	C34B	C33B	C35B	110.3(4)
C45	O12	Si4	135.6(2)	C34B	C33B	C36B	110.8(5)
Si3	N2	Cu2	110.51(13)	C36B	C33B	C35B	109.6(4)
Si4	N2	Cu2	102.08(13)	C29B	O8B	Si3	133.7(6)
Si4	N2	Si3	142.48(16)	O8B	C29B	C31B	110.6(7)
Si1	N1	Cu1	117.18(14)	O8B	C29B	C32B	107.7(9)
Si1	N1	Si2	133.53(16)	O8B	C29B	C30B	106.9(6)
Si2	N1	Cu1	104.94(13)	C31B	C29B	C32B	110.4(7)
O1	C1	C2	105.8(3)	C31B	C29B	C30B	111.5(9)
O1	C1	C3	109.4(3)	C30B	C29B	C32B	109.6(8)

[1]+X,1/2-Y,-1/2+Z; [2]+X,1/2-Y,1/2+Z

Table S12. Hydrogen Atom Coordinates (Å×10[4]) and Isotropic Displacement Parameters (Å[2]×10[3]) for BTTSA-Cu.

Atom	*x*	*y*	*z*	U(eq)
H2A	10581.13	4133.69	7885.03	76
H2B	10302.36	4726.73	7292.03	76
H2C	10496.18	4006.85	7052.69	76
H3A	8748.2	4207.7	7563.59	80
H3B	9205.32	4859.32	7555.4	80
H3C	9523.7	4299.2	8181.11	80
H4A	9318.55	3893.13	6072.51	84
H4B	9067.79	4605.44	6268.76	84
H4C	8621.23	3938.95	6249.67	84
H6A	9302.97	1371.52	8858.89	83
H6B	10055.59	1526.4	9493.11	83
H6C	10010.28	1162.05	8751.13	83
H7A	10816.18	2041.62	8638.41	76
H7B	10808	2494.91	9307.54	76

H7C	10571.74	2813.28	8501.82	76
H8A	9433.1	3154.12	8662.57	80
H8B	9674.62	2764.89	9432	80
H8C	8941.49	2578.12	8782.68	80
H10A	10542.78	1942.43	7359.94	79
H10B	10711.47	1407.76	6840.56	79
H10C	10110.8	1249.94	7149.08	79
H11A	9753.87	2755.13	5612.44	72
H11B	10506.8	2390.02	5916.99	72
H11C	10289.26	2878.37	6442.34	72
H12A	9289.58	1042.91	5855.55	59
H12B	9870.04	1254.67	5537.22	59
H12C	9123.69	1631.52	5256.58	59
H14A	8148.16	1699.41	7811.26	57
H14B	7872.07	1040.84	8088.49	57
H14C	7322.19	1599.46	7615.89	57
H15A	8338.93	437.58	6596.21	61
H15B	8566.82	380.2	7467.64	61
H15C	8750.2	1046.69	7117.8	61
H16A	6684.89	638.87	6786.96	66
H16B	7285.23	89.29	7169.4	66
H16C	7048.98	250.85	6311.94	66
H18A	8410.68	2925.89	5286.91	55
H18B	8044.32	3245.23	4482.72	55
H18C	8093.35	2443.54	4584.53	55
H19A	6812.51	2259.83	3976.02	63
H19B	6713.37	3046.74	3782.54	63
H19C	6272.08	2697.01	4202.89	63
H20A	6711.49	3545.43	5202.92	53
H20B	7195.82	3912.1	4842.53	53
H20C	7539.44	3631.97	5666.48	53
H38A	6095.94	4001.99	9991.67	110
H38B	5274.74	4189.12	9657.05	110
H38C	5832.35	4696.68	10213.31	110
H39A	5758.4	4451.36	8115.11	62
H39B	5242.52	4026.69	8389.66	62
H39C	6067.14	3854.93	8698.4	62
H40A	5423.47	5632.29	9324.51	67
H40B	4852.27	5159.96	8733.01	67
H40C	5421.02	5559.38	8514.18	67
H42A	8807.36	4616.34	9531.58	63
H42B	9258.23	5193.11	9344.46	63

H42C	8483.52	5013.72	8767.21	63
H43A	8750.66	5992.77	10693.44	70
H43B	9419.47	5821.86	10495.54	70
H43C	9006.67	5228.13	10711.69	70
H44A	8074.92	6195.94	8722.05	62
H44B	8847.17	6416.75	9272.24	62
H44C	8175.71	6591.43	9464.1	62
H46A	7921.35	6860.18	10472.42	96
H46B	7475.55	7388.72	10733.77	96
H46C	7443.36	7413.35	9909.2	96
H47A	6535.89	5789.55	10509.25	95
H47B	6976.82	6317.29	11130.37	95
H47C	7374.67	5833.44	10763.51	95
H48A	6121.37	7368.05	9541.68	69
H48B	6173.52	7234.92	10362.5	69
H48C	5765.23	6710.44	9722.76	69
H22A	6013.63	1616.09	6115.04	57
H22B	5393.83	1875.01	6353.74	57
H22C	6169.04	1758.13	6963.02	57
H23A	5775.41	3356.83	5533.77	68
H23B	5157.93	2843.37	5486.79	68
H23C	5775.3	2606.98	5232.85	68
H24A	6229.46	2933.01	7417.99	66
H24B	5462.01	3113.33	6825.51	66
H24C	6128.07	3560.59	6875.78	66
H26A	7827.64	6327.47	7063.92	60
H26B	8041.21	5697.08	6685.17	60
H26C	7866.34	5587.83	7402.71	60
H27A	6922.91	4760.93	6834.64	71
H27B	7065.15	4770.6	6090.47	71
H27C	6289.46	4914.09	6066.92	71
H28A	6295.67	6007.72	5396.82	63
H28B	7092.3	5895.05	5471.15	63
H28C	6881.42	6567.81	5787.49	63
H34A	6896.32	7211.62	8364.64	64
H34B	6864.66	7870.91	7884.09	64
H34C	7018.12	7149.74	7611.54	64
H35A	5037	7613.21	7528.62	68
H35B	5643.73	8174.45	7776.35	68
H35C	5677.35	7555.9	8310.92	68
H36A	5978.54	7192.22	6396.6	72
H36B	5882.28	7955.61	6605.45	72

H36C	5231.76	7442.36	6381.54	72
H30A	4937.12	4363.41	6050.92	82
H30B	4145.88	4539.63	5955.76	82
H30C	4700.07	4279.83	6731.64	82
H31A	4977.34	6169.58	6011.02	77
H31B	4383.86	5682.62	5467.78	77
H31C	5200.55	5513.75	5677.93	77
H32A	4412.63	5387.35	7302.47	63
H32B	3891.7	5612.81	6496.46	63
H32C	4527.99	6094.93	6973.55	63
H22D	6061.17	1549.15	6427.71	57
H22E	5393.77	1953.88	6446.8	57
H22F	6149.45	2043.75	7099.58	57
H23D	5791.66	2834.58	5059.63	68
H23E	5217.7	2359.72	5186.15	68
H23F	5938.37	2043.35	5195.31	68
H24D	6035.33	3302.32	6875.12	66
H24E	5304.93	3224.64	6183.32	66
H24F	5956.88	3600.28	6092.27	66
H26D	7593.62	6224.91	7272.82	60
H26E	8033.62	5887.25	6844.07	60
H26F	7868.84	5464.95	7452.41	60
H27D	7326.86	4551.85	6510.18	71
H27E	7447.25	4976.71	5877.07	71
H27F	6672.61	4722.48	5764.74	71
H28D	6239.7	5936.73	5505.22	63
H28E	7020.68	6188.28	5640.86	63
H28F	6605.68	6507.32	6105.67	63
H34D	7015.83	7115.54	8599.25	64
H34E	6850.89	7891.45	8375.27	64
H34F	7301.73	7453.31	8028.6	64
H35D	5180.25	7091.19	7407.18	68
H35E	5585.49	7580.37	8084.57	68
H35F	5715.29	6783.38	8167.9	68
H36D	6406.81	7778.23	6741.46	72
H36E	5979.99	8203.51	7126.19	72
H36F	5588.33	7627.34	6543.3	72
H31D	4814.71	6463.17	6231.91	77
H31E	4375.08	5953.33	5589.48	77
H31F	5218.7	5955.12	5895.74	77
H32D	4213.25	5223.31	7198.34	63
H32E	3751.22	5491.67	6389.54	63

H32F	4186.13	6013	7021.22	63
H30D	5268.45	4703.63	6202.87	82
H30E	4424.63	4680.95	5876.75	82
H30F	4863.38	4432.68	6699.8	82

Table S13. Atomic Occupancy for BTTSA-Cu.

Atom	***Occupancy***	**Atom**	***Occupancy***	**Atom**	***Occupancy***
C21A	0.444(5)	C22A	0.444(5)	H22A	0.444(5)
H22B	0.444(5)	H22C	0.444(5)	C23A	0.444(5)
H23A	0.444(5)	H23B	0.444(5)	H23C	0.444(5)
C24A	0.444(5)	H24A	0.444(5)	H24B	0.444(5)
H24C	0.444(5)	O7A	0.472(3)	C25A	0.472(3)
C26A	0.472(3)	H26A	0.472(3)	H26B	0.472(3)
H26C	0.472(3)	C27A	0.472(3)	H27A	0.472(3)
H27B	0.472(3)	H27C	0.472(3)	C28A	0.472(3)
H28A	0.472(3)	H28B	0.472(3)	H28C	0.472(3)
O9A	0.481(3)	C33A	0.481(3)	C34A	0.481(3)
H34A	0.481(3)	H34B	0.481(3)	H34C	0.481(3)
C35A	0.481(3)	H35A	0.481(3)	H35B	0.481(3)
H35C	0.481(3)	C36A	0.481(3)	H36A	0.481(3)
H36B	0.481(3)	H36C	0.481(3)	O8A	0.463(4)
C29A	0.463(4)	C30A	0.463(4)	H30A	0.463(4)
H30B	0.463(4)	H30C	0.463(4)	C31A	0.463(4)
H31A	0.463(4)	H31B	0.463(4)	H31C	0.463(4)
C32A	0.463(4)	H32A	0.463(4)	H32B	0.463(4)
H32C	0.463(4)	C21B	0.556(5)	C22B	0.556(5)
H22D	0.556(5)	H22E	0.556(5)	H22F	0.556(5)
C23B	0.556(5)	H23D	0.556(5)	H23E	0.556(5)
H23F	0.556(5)	C24B	0.556(5)	H24D	0.556(5)
H24E	0.556(5)	H24F	0.556(5)	O7B	0.528(3)
C25B	0.528(3)	C26B	0.528(3)	H26D	0.528(3)
H26E	0.528(3)	H26F	0.528(3)	C27B	0.528(3)
H27D	0.528(3)	H27E	0.528(3)	H27F	0.528(3)
C28B	0.528(3)	H28D	0.528(3)	H28E	0.528(3)
H28F	0.528(3)	O9B	0.519(3)	C33B	0.519(3)
C34B	0.519(3)	H34D	0.519(3)	H34E	0.519(3)
H34F	0.519(3)	C35B	0.519(3)	H35D	0.519(3)
H35E	0.519(3)	H35F	0.519(3)	C36B	0.519(3)
H36D	0.519(3)	H36E	0.519(3)	H36F	0.519(3)
O8B	0.537(4)	C29B	0.537(4)	C31B	0.537(4)

H31D	0.537(4)	H31E	0.537(4)	H31F	0.537(4)
C32B	0.537(4)	H32D	0.537(4)	H32E	0.537(4)
H32F	0.537(4)	C30B	0.537(4)	H30D	0.537(4)
H30E	0.537(4)	H30F	0.537(4)		

Table S14. Solvent masks information for BTTSA-Cu.

Number	X	Y	Z	Volume	Electron count	Content
1	0.000	0.000	0.000	619.8	97.0	?
2	0.000	0.500	0.500	619.8	97.0	?

Table S15. Crystal data and structure refinement for 2-Sm.

Identification code	2-Sm
Empirical formula	$C_{2.34}H_{5.27}N_{0.1}O_{0.59}Si_{0.2}Sm_{0.05}$
Formula weight	56.98
Temperature/K	106.92
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	21.438(5)
b/Å	15.090(3)
c/Å	21.412(4)
α/°	90
β/°	111.444(6)
γ/°	90
Volume/Å^3	6447(2)
Z	82
ρ_{calc}g/cm^3	1.203
μ/mm^{-1}	1.035
F(000)	2496.0
Crystal size/mm^3	0.158 × 0.126 × 0.109
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.694 to 56.564
Index ranges	-28 ≤ h ≤ 28, -20 ≤ k ≤ 20, -28 ≤ l ≤ 28
Reflections collected	85838
Independent reflections	15980 [R_{int} = 0.1689, R_{sigma} = 0.1267]
Data/restraints/parameters	15980/60/679
Goodness-of-fit on F^2	1.010
Final R indexes [I>=2σ (I)]	R_1 = 0.0714, wR_2 = 0.1099
Final R indexes [all data]	R_1 = 0.1395, wR_2 = 0.1360
Largest diff. peak/hole / e Å^{-3}	1.34/-1.44

Table S16. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 2-Sm. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Sm1	5021.2(2)	6202.6(2)	7472.7(2)	19.38(9)
Si1	4146.1(9)	4341.0(11)	7284.0(8)	23.1(4)
Si2	5775.5(9)	4287.4(11)	7996.4(8)	22.9(4)
Si3	4813.2(8)	7928.1(11)	6469.8(8)	20.8(4)
Si4	5367.0(8)	8241.4(11)	8087.0(8)	21.2(4)

O2	3855(2)	4029(3)	6502(2)	47.6(14)
O3	3712.3(19)	3781(3)	7631.6(19)	30.2(10)
O4	6061.1(19)	5233(3)	7776(2)	23.4(9)
O5	6163(2)	3453(3)	7812(2)	31.4(10)
O6	6071(2)	4331(3)	8820(2)	31.2(10)
O8	4010(2)	8098(3)	6082(2)	30.5(10)
O9	5170(2)	8494(3)	6040.4(19)	25.4(9)
O10	5224.7(19)	7288(3)	8433.9(18)	21.8(9)
O11	6180(2)	8386(3)	8434.7(19)	24.7(9)
O12	5057(2)	9069(3)	8370.5(19)	25.9(9)
N1	4962(2)	4424(3)	7638(2)	22.0(11)
N2	5081(2)	7972(3)	7291(2)	21.5(11)
C00K	5382(3)	7018(4)	9126(3)	30.4(15)
C00L	6640(3)	9096(4)	8763(3)	28.1(14)
C00N	6720(3)	5544(5)	7824(3)	31.8(16)
C00O	4250(3)	4062(4)	8831(3)	34.6(16)
C00P	4445(3)	9563(4)	8149(3)	31.9(15)
C00Q	3844(3)	3424(4)	8289(3)	29.7(15)
C00R	4999(3)	6161(4)	9090(3)	36.0(16)
C00S	3586(3)	8732(5)	5618(3)	33.1(15)
C00T	5537(3)	2108(4)	7416(3)	37.5(17)
C00U	5994(3)	2808(4)	7287(3)	32.2(15)
C00V	6386(4)	3740(5)	9382(3)	38.1(16)
C00W	6365(3)	8471(4)	6712(3)	33.9(16)
C00X	6644(4)	6521(5)	7677(4)	51(2)
C00Y	3450(4)	3332(5)	6094(3)	41.0(18)
C01A	5176(4)	7710(5)	9511(3)	48(2)
C01B	5909(3)	9013(5)	5526(3)	40.3(18)
C01C	6136(3)	6797(5)	9445(3)	45.7(19)
C01D	3725(4)	9664(5)	5911(4)	50(2)
C01E	4205(4)	2547(4)	8340(4)	50(2)
C01F	3691(4)	8703(5)	4944(3)	51(2)
C01G	7250(4)	5335(6)	8487(4)	57(2)
C01H	2877(3)	8452(5)	5519(4)	57(2)
C01I	5989(4)	2898(5)	9295(4)	56(2)
C01J	6374(4)	4247(6)	9989(3)	59(2)
C01K	6914(4)	5086(5)	7277(4)	52(2)
C01L	6583(4)	9326(5)	9432(3)	49(2)
C01M	4381(4)	9957(5)	8779(4)	50(2)
C01N	3156(4)	3275(6)	8331(4)	62(3)
C01O	3785(5)	2453(6)	6286(5)	85(3)
C01P	3363(5)	3591(7)	5381(4)	80(3)

C01Q	2761(4)	3298(6)	6147(4)	71(3)
C01R	7101(4)	3544(7)	9446(4)	79(3)
C010	3847(3)	8958(5)	7786(4)	40.4(18)
C011	5648(4)	3234(5)	6600(3)	44.7(19)
C012	5796(3)	8957(4)	6187(3)	30.4(15)
C014	5709(4)	9891(4)	6423(3)	39.2(17)
C015	4504(4)	10297(4)	7681(4)	44.2(19)
C016	6663(4)	2379(5)	7334(4)	53(2)
C017	6487(3)	9912(4)	8307(3)	39.9(17)
C018	7329(3)	8732(5)	8861(4)	46.0(19)
O1A	3915(3)	5411(3)	7263(14)	33.2(11)
C1A	3280(5)	5855(7)	7143(8)	39(2)
C2A	3400(10)	6820(7)	7025(14)	49(3)
C3A	3067(11)	5751(17)	7740(10)	54(3)
C4A	2749(10)	5474(17)	6519(10)	64(3)
O1B	3912(2)	5411(3)	7247(6)	33.2(11)
C1B	3281(3)	5892(4)	7019(4)	39(2)
C2B	3446(5)	6806(5)	7329(6)	49(3)
C3B	2770(5)	5429(7)	7241(6)	54(3)
C4B	3018(5)	5969(8)	6261(4)	64(3)
O7A	4905(7)	6833(3)	6340(3)	25.5(10)
C25A	4882(5)	6310(5)	5766(3)	32.0(19)
C26A	4875(7)	5347(5)	5975(5)	33(3)
C27A	5503(6)	6484(8)	5598(6)	52(3)
C28A	4247(7)	6508(9)	5165(6)	58(4)
O7B	4891(10)	6831(3)	6336(4)	25.5(10)
C25B	4747(6)	6316(6)	5729(4)	32.0(19)
C26B	5096(9)	5429(6)	5952(7)	33(3)
C27B	5030(10)	6775(10)	5257(6)	52(3)
C28B	3995(7)	6168(14)	5386(9)	58(4)

Table S17. Anisotropic Displacement Parameters ($Å^2×10^3$) for 2-Sm. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sm1	20.57(14)	17.77(14)	19.20(14)	0.63(15)	6.55(11)	-0.23(15)
Si1	23.3(9)	21.9(9)	22.9(8)	-0.3(7)	7.1(7)	-3.6(7)
Si2	23.8(9)	21.5(9)	24.9(8)	3.8(7)	10.9(8)	3.0(7)
Si3	21.6(9)	20.8(9)	19.2(8)	1.6(7)	6.4(7)	-1.5(7)
Si4	23.4(9)	18.9(8)	21.5(8)	0.9(7)	8.6(7)	-0.4(7)

O2	52(3)	64(4)	26(2)	-17(2)	14(2)	-35(3)
O3	24(2)	39(3)	28(2)	9(2)	8.8(19)	-8(2)
O4	19(2)	20(2)	30(2)	2.1(18)	7.2(19)	-2.0(18)
O5	32(3)	22(2)	43(3)	1(2)	17(2)	7(2)
O6	31(3)	37(3)	25(2)	10(2)	10(2)	5(2)
O8	21(2)	36(3)	29(2)	15(2)	2.4(19)	4(2)
O9	29(2)	28(2)	22(2)	4.6(18)	11.7(19)	-2.9(19)
O10	27(2)	23(2)	17.0(19)	4.6(17)	9.5(18)	2.1(18)
O11	23(2)	21(2)	26(2)	-3.4(18)	5.2(19)	-6.0(18)
O12	32(2)	18(2)	30(2)	-2.0(18)	14(2)	4.3(18)
N1	23(3)	16(2)	27(3)	1(2)	9(2)	2(2)
N2	20(3)	23(3)	19(2)	2(2)	4(2)	-1(2)
C00K	38(4)	32(4)	18(3)	5(3)	7(3)	-5(3)
C00L	23(3)	33(4)	24(3)	2(3)	2(3)	-5(3)
C00N	16(3)	40(4)	41(4)	10(3)	13(3)	1(3)
C00O	47(4)	28(4)	35(4)	-2(3)	23(3)	-1(3)
C00P	39(4)	20(3)	45(4)	1(3)	26(4)	5(3)
C00Q	35(4)	30(4)	27(3)	3(3)	14(3)	-9(3)
C00R	49(4)	32(4)	28(3)	7(3)	15(3)	-13(4)
C00S	26(3)	34(4)	30(3)	12(3)	0(3)	7(3)
C00T	40(4)	25(4)	49(4)	2(3)	18(4)	2(3)
C00U	41(4)	21(3)	39(4)	-4(3)	19(3)	0(3)
C00V	42(4)	43(4)	31(3)	13(3)	16(3)	5(4)
C00W	33(4)	28(4)	38(4)	4(3)	10(3)	0(3)
C00X	32(4)	39(5)	83(6)	18(4)	20(4)	0(3)
C00Y	40(4)	44(5)	35(4)	-19(3)	8(3)	-21(4)
C01A	85(6)	36(4)	33(4)	4(3)	32(4)	2(4)
C01B	44(4)	43(5)	42(4)	13(3)	25(4)	-8(3)
C01C	38(4)	59(5)	37(4)	14(4)	10(4)	-2(4)
C01D	54(5)	37(5)	52(5)	-2(4)	11(4)	2(4)
C01E	80(6)	25(4)	41(4)	-6(3)	18(4)	-5(4)
C01F	64(5)	51(5)	28(3)	16(4)	6(4)	6(4)
C01G	29(4)	86(7)	51(5)	18(5)	7(4)	-3(4)
C01H	27(4)	60(6)	69(6)	16(5)	1(4)	1(4)
C01I	66(6)	45(5)	59(5)	24(4)	24(5)	5(4)
C01J	68(6)	66(6)	34(4)	18(4)	7(4)	9(5)
C01K	47(5)	53(5)	70(6)	-12(4)	39(5)	1(4)
C01L	55(5)	53(5)	36(4)	-17(4)	11(4)	-27(4)
C01M	59(5)	43(5)	62(5)	-7(4)	40(5)	9(4)
C01N	54(5)	89(7)	45(5)	0(5)	21(4)	-35(5)
C01O	61(6)	46(6)	122(9)	-19(6)	2(6)	-3(5)
C01P	94(8)	105(9)	32(4)	-4(5)	9(5)	-44(7)

C01Q	62(6)	88(7)	63(6)	-45(5)	25(5)	-40(5)
C01R	44(5)	128(9)	66(6)	59(6)	21(5)	32(6)
C010	29(4)	39(4)	54(4)	-1(4)	16(3)	7(3)
C011	63(5)	38(4)	42(4)	-4(3)	30(4)	8(4)
C012	34(4)	30(4)	32(3)	9(3)	17(3)	-1(3)
C014	38(4)	28(4)	44(4)	5(3)	6(3)	-3(3)
C015	46(5)	29(4)	53(5)	6(4)	13(4)	10(3)
C016	47(5)	37(4)	94(6)	-4(4)	47(5)	11(4)
C017	39(4)	28(4)	45(4)	3(3)	7(4)	-8(3)
C018	29(4)	45(5)	54(4)	7(4)	2(3)	-11(4)
O1A	15(2)	26(3)	56(3)	8(2)	9(2)	0.0(19)
C1A	15(3)	28(4)	66(6)	9(4)	5(4)	-5(3)
C2A	41(4)	46(4)	57(5)	-1(3)	13(3)	7(3)
C3A	44(4)	55(4)	65(4)	6(3)	22(3)	6(3)
C4A	34(6)	70(9)	64(7)	18(6)	-8(5)	7(6)
O1B	15(2)	26(3)	56(3)	8(2)	9(2)	0.0(19)
C1B	15(3)	28(4)	66(6)	9(4)	5(4)	-5(3)
C2B	41(4)	46(4)	57(5)	-1(3)	13(3)	7(3)
C3B	44(4)	55(4)	65(4)	6(3)	22(3)	6(3)
C4B	34(6)	70(9)	64(7)	18(6)	-8(5)	7(6)
O7A	36(3)	22(2)	18(2)	-2.2(17)	8.5(19)	-1.3(19)
C25A	47(6)	28(4)	20(3)	-5(3)	12(4)	2(4)
C26A	44(10)	28(4)	29(4)	-2(3)	17(5)	-4(5)
C27A	94(11)	33(7)	37(7)	-7(5)	34(7)	-7(7)
C28A	77(11)	43(9)	34(7)	-4(6)	-3(6)	6(7)
O7B	36(3)	22(2)	18(2)	-2.2(17)	8.5(19)	-1.3(19)
C25B	47(6)	28(4)	20(3)	-5(3)	12(4)	2(4)
C26B	44(10)	28(4)	29(4)	-2(3)	17(5)	-4(5)
C27B	94(11)	33(7)	37(7)	-7(5)	34(7)	-7(7)
C28B	77(11)	43(9)	34(7)	-4(6)	-3(6)	6(7)

Table S18. Bond Lengths for 2-Sm.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Sm1	Si1	3.3196(18)	C00L	C01L	1.523(9)
Sm1	Si2	3.3012(18)	C00L	C017	1.530(8)
Sm1	Si3	3.2999(17)	C00L	C018	1.516(9)
Sm1	Si4	3.3214(18)	C00N	C00X	1.503(9)
Sm1	O4	2.544(4)	C00N	C01G	1.493(9)
Sm1	O10	2.541(4)	C00N	C01K	1.543(9)
Sm1	N1	2.716(5)	C00O	C00Q	1.513(8)

Sm1	N2	2.707(5)	C00P	C01M	1.525(9)
Sm1	O1A	2.545(4)	C00P	C010	1.534(9)
Sm1	O1B	2.545(4)	C00P	C015	1.529(9)
Sm1	O7A	2.531(4)	C00Q	C01E	1.516(9)
Sm1	O7B	2.531(4)	C00Q	C01N	1.526(9)
Si1	O2	1.627(4)	C00S	C01D	1.525(9)
Si1	O3	1.625(4)	C00S	C01F	1.541(9)
Si1	N1	1.637(5)	C00S	C01H	1.515(9)
Si1	O1A	1.685(5)	C00T	C00U	1.535(9)
Si1	O1B	1.685(5)	C00U	C011	1.525(9)
Si2	O4	1.687(4)	C00U	C016	1.543(9)
Si2	O5	1.634(4)	C00V	C01I	1.502(10)
Si2	O6	1.642(4)	C00V	C01J	1.517(10)
Si2	N1	1.641(5)	C00V	C01R	1.517(10)
Si3	O8	1.636(4)	C00W	C012	1.512(8)
Si3	O9	1.635(4)	C00Y	C01O	1.493(11)
Si3	N2	1.640(5)	C00Y	C01P	1.519(10)
Si3	O7A	1.699(4)	C00Y	C01Q	1.523(10)
Si3	O7B	1.699(4)	C01B	C012	1.523(8)
Si4	O10	1.696(4)	C012	C014	1.531(9)
Si4	O11	1.640(4)	O1A	C1A	1.452(8)
Si4	O12	1.633(4)	C1A	C2A	1.516(5)
Si4	N2	1.637(5)	C1A	C3A	1.516(5)
O2	C00Y	1.439(7)	C1A	C4A	1.516(5)
O3	C00Q	1.436(7)	O1B	C1B	1.452(7)
O4	C00N	1.456(7)	C1B	C2B	1.516(5)
O5	C00U	1.430(7)	C1B	C3B	1.516(5)
O6	C00V	1.451(7)	C1B	C4B	1.515(5)
O8	C00S	1.438(7)	O7A	C25A	1.447(7)
O9	C012	1.442(7)	C25A	C26A	1.523(5)
O10	C00K	1.453(6)	C25A	C27A	1.522(5)
O11	C00L	1.451(7)	C25A	C28A	1.522(5)
O12	C00P	1.431(7)	O7B	C25B	1.447(7)
C00K	C00R	1.517(8)	C25B	C26B	1.522(5)
C00K	C01A	1.494(9)	C25B	C27B	1.522(5)
C00K	C01C	1.545(9)	C25B	C28B	1.522(5)

Table S19. Bond Angles for 2-Sm.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
Si1	Sm1	Si4	150.04(4)	C00N	O4	Si2	134.0(4)

Si2	Sm1	Si1	59.03(4)	C00U	O5	Si2	135.2(4)
Si2	Sm1	Si4	131.73(4)	C00V	O6	Si2	138.3(4)
Si3	Sm1	Si1	130.74(4)	C00S	O8	Si3	137.5(4)
Si3	Sm1	Si2	147.64(4)	C012	O9	Si3	136.1(4)
Si3	Sm1	Si4	58.96(4)	Si4	O10	Sm1	101.37(16)
O4	Sm1	Si1	87.01(9)	C00K	O10	Sm1	123.5(3)
O4	Sm1	Si2	30.15(9)	C00K	O10	Si4	132.3(4)
O4	Sm1	Si3	121.14(9)	C00L	O11	Si4	137.7(4)
O4	Sm1	Si4	112.57(9)	C00P	O12	Si4	136.4(4)
O4	Sm1	N1	58.46(14)	Si1	N1	Sm1	96.2(2)
O4	Sm1	N2	121.36(13)	Si1	N1	Si2	168.4(3)
O4	Sm1	O1A	116.64(15)	Si2	N1	Sm1	95.3(2)
O4	Sm1	O1B	116.72(13)	Si3	N2	Sm1	95.6(2)
O10	Sm1	Si1	124.50(9)	Si4	N2	Sm1	96.6(2)
O10	Sm1	Si2	111.82(9)	Si4	N2	Si3	167.7(3)
O10	Sm1	Si3	87.74(9)	O10	C00K	C00R	105.5(5)
O10	Sm1	Si4	30.05(9)	O10	C00K	C01A	111.1(5)
O10	Sm1	O4	106.82(13)	O10	C00K	C01C	109.1(5)
O10	Sm1	N1	122.26(13)	C00R	C00K	C01C	107.3(6)
O10	Sm1	N2	58.48(13)	C01A	C00K	C00R	111.2(6)
O10	Sm1	O1A	108.6(5)	C01A	C00K	C01C	112.3(6)
O10	Sm1	O1B	109.1(2)	O11	C00L	C01L	110.5(5)
N1	Sm1	Si1	29.36(11)	O11	C00L	C017	109.6(5)
N1	Sm1	Si2	29.67(11)	O11	C00L	C018	104.8(5)
N1	Sm1	Si3	149.66(10)	C01L	C00L	C017	110.1(6)
N1	Sm1	Si4	151.38(10)	C018	C00L	C01L	111.1(6)
N2	Sm1	Si1	150.61(10)	C018	C00L	C017	110.5(6)
N2	Sm1	Si2	150.32(11)	O4	C00N	C00X	105.9(5)
N2	Sm1	Si3	29.64(10)	O4	C00N	C01G	112.4(5)
N2	Sm1	Si4	29.32(10)	O4	C00N	C01K	109.0(6)
N2	Sm1	N1	179.23(14)	C00X	C00N	C01K	108.7(6)
O1A	Sm1	Si1	29.83(10)	C01G	C00N	C00X	113.1(7)
O1A	Sm1	Si2	87.6(2)	C01G	C00N	C01K	107.7(6)
O1A	Sm1	Si3	111.1(4)	O12	C00P	C01M	106.2(6)
O1A	Sm1	Si4	124.3(3)	O12	C00P	C010	110.6(5)
O1A	Sm1	N1	58.28(19)	O12	C00P	C015	107.9(5)
O1A	Sm1	N2	121.84(19)	C01M	C00P	C010	110.6(6)
O1B	Sm1	Si1	29.83(10)	C01M	C00P	C015	110.7(6)
O1B	Sm1	Si2	87.79(12)	C015	C00P	C010	110.7(6)
O1B	Sm1	Si3	110.62(18)	O3	C00Q	C00O	111.4(5)
O1B	Sm1	Si4	124.58(14)	O3	C00Q	C01E	108.0(5)
O1B	Sm1	N1	58.41(15)	O3	C00Q	C01N	105.3(5)

O1B	Sm1	N2	121.70(15)	C00O	C00Q	C01E	111.4(6)
O7A	Sm1	Si1	110.4(2)	C00O	C00Q	C01N	110.3(6)
O7A	Sm1	Si2	121.25(16)	C01E	C00Q	C01N	110.3(6)
O7A	Sm1	Si3	30.40(9)	O8	C00S	C01D	110.4(5)
O7A	Sm1	Si4	87.76(13)	O8	C00S	C01F	110.9(5)
O7A	Sm1	O4	103.3(3)	O8	C00S	C01H	105.0(5)
O7A	Sm1	O10	117.48(14)	C01D	C00S	C01F	109.8(6)
O7A	Sm1	N1	120.24(14)	C01H	C00S	C01D	110.5(6)
O7A	Sm1	N2	59.01(14)	C01H	C00S	C01F	110.2(6)
O7B	Sm1	Si1	110.0(3)	O5	C00U	C00T	108.8(5)
O7B	Sm1	Si2	121.5(2)	O5	C00U	C011	111.4(5)
O7B	Sm1	Si3	30.40(10)	O5	C00U	C016	105.8(6)
O7B	Sm1	Si4	87.95(16)	C00T	C00U	C016	109.8(5)
O7B	Sm1	O4	103.8(4)	C011	C00U	C00T	110.2(6)
O7B	Sm1	O10	117.61(15)	C011	C00U	C016	110.7(6)
O7B	Sm1	N1	120.11(15)	O6	C00V	C01I	110.3(6)
O7B	Sm1	N2	59.14(15)	O6	C00V	C01J	104.7(6)
O2	Si1	Sm1	110.94(18)	O6	C00V	C01R	110.1(5)
O2	Si1	N1	116.2(3)	C01I	C00V	C01J	110.2(6)
O2	Si1	O1A	104.5(9)	C01I	C00V	C01R	110.7(7)
O2	Si1	O1B	103.5(4)	C01J	C00V	C01R	110.8(7)
O3	Si1	Sm1	141.02(17)	O2	C00Y	C01O	111.0(6)
O3	Si1	O2	104.6(2)	O2	C00Y	C01P	104.3(6)
O3	Si1	N1	121.4(2)	O2	C00Y	C01Q	111.4(6)
O3	Si1	O1A	107.4(6)	C01O	C00Y	C01P	112.0(8)
O3	Si1	O1B	108.0(3)	C01O	C00Y	C01Q	109.4(7)
N1	Si1	Sm1	54.44(16)	C01P	C00Y	C01Q	108.6(7)
N1	Si1	O1A	101.2(3)	O9	C012	C00W	111.1(5)
N1	Si1	O1B	101.4(3)	O9	C012	C01B	106.1(5)
O1A	Si1	Sm1	48.72(15)	O9	C012	C014	107.6(5)
O1B	Si1	Sm1	48.71(15)	C00W	C012	C01B	111.0(5)
O4	Si2	Sm1	49.26(14)	C00W	C012	C014	111.3(6)
O5	Si2	Sm1	145.22(17)	C01B	C012	C014	109.6(5)
O5	Si2	O4	108.4(2)	Si1	O1A	Sm1	101.5(2)
O5	Si2	O6	105.0(2)	C1A	O1A	Sm1	124.5(5)
O5	Si2	N1	122.1(2)	C1A	O1A	Si1	134.0(6)
O6	Si2	Sm1	106.19(17)	O1A	C1A	C2A	105.5(6)
O6	Si2	O4	103.3(2)	O1A	C1A	C3A	110.8(6)
N1	Si2	Sm1	55.02(17)	O1A	C1A	C4A	109.6(6)
N1	Si2	O4	101.3(2)	C3A	C1A	C2A	111.2(8)
N1	Si2	O6	115.1(2)	C4A	C1A	C2A	109.7(8)
O8	Si3	Sm1	108.70(16)	C4A	C1A	C3A	110.0(8)

O8	Si3	N2	115.4(2)	Si1	O1B	Sm1	101.46(19)
O8	Si3	O7A	103.5(5)	C1B	O1B	Sm1	121.3(3)
O8	Si3	O7B	102.5(7)	C1B	O1B	Si1	136.0(4)
O9	Si3	Sm1	142.93(16)	O1B	C1B	C2B	105.6(5)
O9	Si3	O8	104.8(2)	O1B	C1B	C3B	110.7(6)
O9	Si3	N2	122.0(2)	O1B	C1B	C4B	109.6(6)
O9	Si3	O7A	108.0(3)	C3B	C1B	C2B	111.2(7)
O9	Si3	O7B	108.6(4)	C4B	C1B	C2B	109.6(7)
N2	Si3	Sm1	54.73(17)	C4B	C1B	C3B	110.1(7)
N2	Si3	O7A	101.4(3)	Si3	O7A	Sm1	100.68(17)
N2	Si3	O7B	101.7(3)	C25A	O7A	Sm1	124.8(4)
O7A	Si3	Sm1	48.92(13)	C25A	O7A	Si3	134.4(4)
O7B	Si3	Sm1	48.92(14)	O7A	C25A	C26A	105.7(5)
O10	Si4	Sm1	48.58(13)	O7A	C25A	C27A	110.2(6)
O11	Si4	Sm1	110.47(16)	O7A	C25A	C28A	110.7(6)
O11	Si4	O10	104.2(2)	C27A	C25A	C26A	109.8(7)
O12	Si4	Sm1	142.53(17)	C28A	C25A	C26A	109.6(7)
O12	Si4	O10	108.8(2)	C28A	C25A	C27A	110.8(8)
O12	Si4	O11	103.8(2)	Si3	O7B	Sm1	100.69(18)
O12	Si4	N2	121.9(2)	C25B	O7B	Sm1	125.1(4)
N2	Si4	Sm1	54.07(17)	C25B	O7B	Si3	132.3(6)
N2	Si4	O10	100.7(2)	O7B	C25B	C26B	105.7(5)
N2	Si4	O11	115.9(2)	O7B	C25B	C27B	110.2(6)
C00Y	O2	Si1	139.1(4)	O7B	C25B	C28B	110.7(6)
C00Q	O3	Si1	134.8(4)	C27B	C25B	C26B	109.8(7)
Si2	O4	Sm1	100.60(18)	C28B	C25B	C26B	109.6(7)
C00N	O4	Sm1	124.7(3)	C28B	C25B	C27B	110.8(8)

Table S20. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 2-Sm.

Atom	*x*	*y*	*z*	U(eq)
H00A	4671.57	4197.77	8771.14	52
H00B	4345.94	3791.92	9272.21	52
H00C	3994.32	4609.96	8798.71	52
H00D	4517.55	6272.89	8871.99	54
H00E	5094.79	5934.48	9544.1	54
H00F	5138.58	5722.31	8828.97	54
H00G	5769.26	1827.74	7853.06	56
H00H	5423.4	1656.6	7063	56
H00I	5125.14	2391.16	7415.74	56

H00J	6265.72	8406.28	7121.41	51
H00K	6781.14	8807.85	6812.28	51
H00L	6416.96	7883.13	6542.09	51
H00M	6300.17	6617	7231.95	77
H00N	7072.08	6764.1	7688.8	77
H00O	6511.03	6818.53	8016.12	77
H01A	5424.04	8258.61	9519.05	73
H01B	5275.08	7504.04	9971.04	73
H01C	4694.29	7822.9	9294.59	73
H01D	5958.92	8414.85	5372.71	60
H01E	6316.6	9355.91	5591.19	60
H01F	5524.67	9305.77	5188.66	60
H01G	6243.69	6320.19	9190.18	69
H01H	6244.16	6605.35	9910.24	69
H01I	6399.29	7324.96	9437.37	69
H01J	3639.95	9684.91	6330.69	75
H01K	3431.49	10087.49	5590.76	75
H01L	4194.27	9818.53	6001.73	75
H01M	3935.19	2154.9	7976.64	75
H01N	4271.65	2270.36	8773.36	75
H01O	4640.64	2650.48	8301.3	75
H01P	4162.77	8824.92	5020.62	76
H01Q	3407.84	9151.08	4640.33	76
H01R	3571.08	8114.43	4741.95	76
H01S	7130.42	5598.8	8846.26	86
H01T	7679.83	5577.25	8503.1	86
H01U	7288.54	4690.58	8547.44	86
H01V	2798.96	7847.51	5338.87	85
H01W	2558.33	8856.91	5202.95	85
H01X	2816.18	8469.57	5950.3	85
H01Y	5535.69	3036.45	9274.84	84
H	6208.91	2503.78	9676.42	84
HA	5965.07	2605.18	8878.73	84
H01Z	6654.49	4777.4	10055.19	89
HB	6546.75	3868.74	10387.87	89
HC	5912.46	4422.33	9916.96	89
H01	6962.98	4447.24	7365.48	78
HD	7339.25	5329.11	7280.92	78
HE	6563.09	5189.16	6836.55	78
H0AA	6122.62	9508.68	9357.91	74
HF	6891.13	9811.89	9643.86	74
HG	6698.66	8805.48	9726.39	74

H1AA	4340.39	9476.81	9070.61	75
HH	3981.14	10333.32	8652.43	75
HI	4778.98	10312.09	9018.93	75
H2AA	2935.02	3847.58	8314.91	92
HJ	3208.68	2972.93	8752.18	92
HK	2882.48	2908.75	7951.48	92
H3AA	4223.51	2469.44	6239.29	128
HL	3507.17	1992.97	5991.11	128
HM	3846.08	2320.06	6752.14	128
H4AA	3155.67	4178.43	5280.46	121
HN	3076.27	3156.18	5066.64	121
HO	3802.6	3605.8	5337.62	121
H5AA	2812.95	3217.51	6617.9	106
HP	2505.22	2801.19	5880.52	106
HQ	2522.55	3853.54	5978.24	106
H6AA	7097.89	3227.28	9045.12	119
HR	7318.35	3175.74	9843.52	119
HS	7347.81	4101.17	9490.27	119
H7AA	3895.92	8713.45	7382.14	61
HT	3431.09	9300.25	7659.16	61
HU	3833.58	8472.31	8084.84	61
H8AA	5237.01	3530.32	6588.41	67
HV	5535.36	2775.29	6252.45	67
HW	5948.89	3669.17	6518.98	67
H9AA	5346.42	10195.01	6068.55	59
HX	6127	10223.82	6524.67	59
HY	5598.11	9850.42	6827.49	59
H0BA	4858.3	10711.56	7934.3	66
HZ	4077.11	10614.38	7493.7	66
H5BA	4615.35	10034.86	7316.29	66
H1BA	6956.72	2830.73	7260.35	80
H6BA	6576.37	1915.06	6992.44	80
H7BA	6880.48	2116.84	7780.58	80
H2BA	6519.99	9754.88	7876.06	60
H8BA	6810.16	10381.33	8521.34	60
H9BA	6032.56	10121.85	8231.85	60
H3BA	7414.11	8202.03	9144.15	69
H0CA	7668.73	9182.11	9078.46	69
H1CA	7348.69	8578.32	8424.09	69
H2AB	3793.01	7036.25	7397.62	74
H2AC	3006.36	7170.16	6998.87	74
H2AD	3478.65	6876.62	6604.21	74

H3AB	3101.22	5126.12	7874.21	81
H3AC	2602.01	5949.49	7617.5	81
H3AD	3359	6108.83	8114.43	81
H4AB	2947.71	5341.29	6184.53	95
H4AC	2386.32	5906.34	6334.46	95
H4AD	2567.99	4928.78	6636.19	95
H2BB	3627.59	6753.42	7819.56	74
H2BC	3037.34	7167.08	7189.93	74
H2BD	3778.02	7089.43	7179.72	74
H3BB	2689.26	4830.07	7050.84	81
H3BC	2350.18	5764.6	7084.85	81
H3BD	2941.58	5391.28	7732.19	81
H4BA	3245.66	6459.12	6130.84	95
H4BB	2535.07	6083.16	6094.04	95
H4BC	3104.68	5415.22	6067.49	95
H26A	5282.09	5221.69	6364.65	49
H26B	4858.15	4957.94	5602.85	49
H26C	4480.58	5241.45	6093.04	49
H27A	5513.08	7109.75	5478.55	78
H27B	5489.2	6111.55	5218.31	78
H27C	5904.7	6344.09	5988.32	78
H28A	3855.61	6432.48	5292.81	86
H28B	4214.46	6100.66	4797.99	86
H28C	4262.1	7119.99	5016.91	86
H26D	5576.66	5528.04	6191.11	49
H26E	5028.29	5056.46	5557.94	49
H26F	4907.91	5133.09	6250.84	49
H27D	4761.65	7301.81	5064.16	78
H27E	5017.05	6367.17	4896.65	78
H27F	5494.93	6951.82	5508.06	78
H28D	3825.65	5857.54	5693.3	86
H28E	3908.28	5810.19	4980.86	86
H28F	3768.72	6741.47	5262.89	86

Table S21. Atomic Occupancy for 2-Sm.

Atom	***Occupancy***	**Atom**	***Occupancy***	**Atom**	***Occupancy***
O1A	0.270(8)	C1A	0.270(8)	C2A	0.270(8)
H2AB	0.270(8)	H2AC	0.270(8)	H2AD	0.270(8)
C3A	0.270(8)	H3AB	0.270(8)	H3AC	0.270(8)
H3AD	0.270(8)	C4A	0.270(8)	H4AB	0.270(8)

H4AC	0.270(8)	H4AD	0.270(8)	O1B	0.730(8)
C1B	0.730(8)	C2B	0.730(8)	H2BB	0.730(8)
H2BC	0.730(8)	H2BD	0.730(8)	C3B	0.730(8)
H3BB	0.730(8)	H3BC	0.730(8)	H3BD	0.730(8)
C4B	0.730(8)	H4BA	0.730(8)	H4BB	0.730(8)
H4BC	0.730(8)	O7A	0.582(9)	C25A	0.582(9)
C26A	0.582(9)	H26A	0.582(9)	H26B	0.582(9)
H26C	0.582(9)	C27A	0.582(9)	H27A	0.582(9)
H27B	0.582(9)	H27C	0.582(9)	C28A	0.582(9)
H28A	0.582(9)	H28B	0.582(9)	H28C	0.582(9)
O7B	0.418(9)	C25B	0.418(9)	C26B	0.418(9)
H26D	0.418(9)	H26E	0.418(9)	H26F	0.418(9)
C27B	0.418(9)	H27D	0.418(9)	H27E	0.418(9)
H27F	0.418(9)	C28B	0.418(9)	H28D	0.418(9)
H28E	0.418(9)	H28F	0.418(9)		

Table S22. Crystal data and structure refinement for 2-Eu.

Identification code	2-Eu
Empirical formula	$C_{32}H_{72}Eu_{0.67}N_{1.33}O_8Si_{2.67}$
Formula weight	779.79
Temperature/K	102.5
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	21.372(3)
b/Å	15.061(2)
c/Å	21.461(3)
α/°	90
β/°	111.428(5)
γ/°	90
Volume/Å^3	6430.3(16)
Z	6
ρ_{calc}g/cm^3	1.208
μ/mm^{-1}	1.100
F(000)	2500.0
Crystal size/mm^3	0.26 × 0.258 × 0.154
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.604 to 58.26
Index ranges	-29 ≤ h ≤ 29, -20 ≤ k ≤ 20, -29 ≤ l ≤ 29
Reflections collected	169239
Independent reflections	17268 [R_{int} = 0.0794, R_{sigma} = 0.0383]
Data/restraints/parameters	17268/29/684
Goodness-of-fit on F^2	1.034
Final R indexes [I>=2σ (I)]	R_1 = 0.0321, wR_2 = 0.0673
Final R indexes [all data]	R_1 = 0.0431, wR_2 = 0.0728
Largest diff. peak/hole / e Å^{-3}	0.89/-0.74

Table S23. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 2-Eu. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Eu1	7475.5(2)	6202.2(2)	5025.3(2)	13.78(3)
Si1	8088.7(3)	8238.2(4)	5371.0(3)	15.45(11)
Si2	6470.4(3)	7924.0(4)	4816.1(3)	15.96(11)
Si4	7285.2(3)	4347.9(4)	4148.2(3)	17.15(11)
Si3	8000.5(3)	4289.4(4)	5776.6(3)	16.96(11)
O1	8434.3(7)	7284.8(9)	5235.8(7)	17.5(3)
O5	6041.0(7)	8487.6(10)	5172.3(7)	22.1(3)
O11	7631.4(8)	3779.3(10)	3712.8(7)	24.7(3)

O6	6078.1(8)	8086.6(11)	4013.8(7)	25.6(3)
O9	7818.7(8)	3454.4(10)	6167.9(7)	24.9(3)
O8	8825.2(8)	4335.1(11)	6075.0(8)	26.3(3)
O12	6500.6(8)	4036.2(13)	3849.9(9)	35.8(4)
O10A	7293(6)	5424.2(14)	3927.1(16)	24.1(4)
C37A	7187(4)	5877(4)	3298(2)	25.2(7)
C38A	6534(5)	5559(8)	2769(5)	53.4(11)
C39A	7777(5)	5732(9)	3075(5)	59(4)
C40A	7129(8)	6850(3)	3453(5)	48.2(12)
O10B	7246(2)	5425.0(11)	3919.7(9)	24.1(4)
O2	8435.9(7)	8382.3(10)	6183.0(7)	21.3(3)
O3	8374.2(8)	9065.6(10)	5061.3(7)	22.5(3)
O4A	6323(3)	6818.2(15)	4823(9)	14.9(12)
O4B	6359.3(16)	6835.3(11)	4950(4)	14.9(12)
O7	7780.5(7)	5238.7(9)	6059.9(7)	18.0(3)
N1	7289.7(8)	7979.2(11)	5082.4(8)	16.8(3)
N2	7643.1(9)	4417.6(11)	4963.8(8)	18.2(3)
C25	7827.2(12)	5546.4(15)	6718.6(10)	25.0(5)
C1	9126.4(11)	7004.6(15)	5383.4(11)	24.0(4)
C21	5621.3(12)	8726.5(16)	3592.4(11)	28.3(5)
C41	8286.2(12)	3426.3(15)	3835.6(12)	26.0(5)
C42	8825.1(12)	4070.0(16)	4244.5(13)	29.7(5)
C20	6709.0(12)	8461.6(16)	6371.4(11)	28.4(5)
C2	9082.7(12)	6156.0(15)	4993.3(13)	29.9(5)
C9	8151.7(13)	9567.0(15)	4449.4(12)	28.2(5)
C5	8756.5(11)	9087.6(15)	6636.3(11)	25.5(5)
C33	7292.0(13)	2802.3(15)	5998.3(12)	28.7(5)
C26	7691.0(17)	6524.1(17)	6645.6(12)	41.3(7)
C17	6183.0(12)	8955.2(15)	5794.5(11)	24.9(5)
C45	6099.1(13)	3335.0(18)	3449.2(13)	35.6(6)
C29	9379.9(12)	3748.9(17)	6381.8(12)	30.5(5)
C37B	6999.3(15)	5890.5(18)	3282.1(12)	25.2(7)
C22	5921.4(16)	9650.0(19)	3739.0(15)	44.1(7)
C27	7271.1(15)	5090.4(19)	6902.8(13)	38.8(6)
C32	9298.6(16)	2899(2)	5989.2(17)	50.8(8)
C11	7786.9(15)	8973.5(17)	3854.2(12)	37.7(6)
C44	8338.2(15)	2546.5(17)	4190.2(17)	46.9(7)
C24	5526.0(16)	8447(2)	2882.6(12)	46.5(7)
C3	9514.7(13)	7703.6(18)	5185.2(15)	39.9(6)
C10	8781.7(15)	9962.6(19)	4386.7(15)	43.7(7)
C8	8860.0(16)	8729.6(19)	7329.4(12)	41.6(7)
C19	5524.9(13)	9002.0(19)	5910.3(13)	37.2(6)

C6	9431.0(13)	9323(2)	6585.6(15)	45.1(7)
C48	6322(2)	2456(2)	3785.0(18)	66.7(10)
C30	9458.4(18)	3555(3)	7100.9(15)	63.0(10)
C46	6139.6(17)	3323(2)	2753.0(15)	55.5(9)
C43	8327.9(16)	3296(2)	3150.6(15)	53.8(9)
C31	9998.5(14)	4252(2)	6374.6(17)	52.0(8)
C47	5383.9(16)	3561(3)	3379(2)	68.5(11)
C38B	6237.6(18)	5940(3)	3033(2)	53.4(11)
C39B	7238(3)	5437(3)	2777.3(16)	45.3(11)
C40B	7299(3)	6814(2)	3445(2)	48.2(12)
C13A	5701(11)	6342(17)	4721(8)	21.8(14)
C13B	5782(6)	6282(9)	4896(4)	21.8(14)
C14A	5267(4)	6753(5)	5028(5)	42.5(10)
C14B	5613(2)	6472(3)	5520(3)	42.5(10)
C15A	5406(4)	6159(6)	3986(4)	44.6(10)
C15B	5164(2)	6507(3)	4268(2)	44.6(10)
C16A	5955(7)	5424(10)	5072(6)	26.9(11)
C16B	5985(4)	5335(5)	4875(3)	26.9(11)
C18	6422.1(14)	9882.6(16)	5713.1(13)	33.6(6)
C4	9441.8(13)	6787(2)	6134.8(13)	38.1(6)
C34	6610.2(14)	3227.3(18)	5644.3(15)	39.9(6)
C23	4950.6(13)	8700.4(19)	3687.8(14)	40.0(6)
C28	8492.6(14)	5328(2)	7247.9(13)	43.3(7)
C36	7429.8(14)	2104.0(16)	5549.4(13)	34.7(6)
C12	7695.3(14)	10302.9(16)	4521.9(13)	36.4(6)
C7	8308.0(14)	9903.9(17)	6493.3(13)	35.9(6)
C35	7337.5(17)	2386.8(18)	6660.5(14)	44.1(7)

Table S24. Anisotropic Displacement Parameters ($Å^2×10^3$) for 2-Eu. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Eu1	14.55(5)	12.39(5)	13.18(5)	-0.32(4)	3.61(3)	0.85(4)
Si1	15.6(3)	13.8(3)	16.6(2)	-0.4(2)	5.4(2)	0.0(2)
Si2	14.6(3)	16.3(3)	15.6(2)	-0.4(2)	3.8(2)	2.7(2)
Si4	18.4(3)	15.9(3)	16.4(3)	-3.6(2)	5.4(2)	-0.8(2)
Si3	20.4(3)	15.8(3)	15.5(3)	2.7(2)	7.6(2)	3.4(2)
O1	13.5(7)	15.6(7)	23.3(7)	-0.9(6)	6.5(6)	1.8(5)
O5	18.9(7)	24.8(8)	21.7(7)	-5.2(6)	6.2(6)	3.3(6)
O11	24.0(8)	28.3(8)	20.9(7)	-6.4(6)	7.2(6)	3.7(7)

O6	24.1(8)	31.4(9)	17.3(7)	0.9(6)	3.0(6)	12.6(7)
O9	36.7(9)	18.2(7)	22.6(7)	4.2(6)	14.1(7)	0.7(7)
O8	21.2(8)	29.2(9)	27.4(8)	9.5(7)	7.5(6)	7.9(7)
O12	23.3(8)	44.3(11)	38.7(10)	-24.7(8)	10.2(7)	-10.1(8)
O10A	35.0(10)	19.7(7)	14.6(6)	0.4(6)	5.6(6)	4.6(6)
C37A	30.3(16)	23.6(10)	16.1(9)	2.4(8)	2.1(10)	7.5(11)
C38A	49(2)	54(3)	39(2)	9.4(18)	-4.9(17)	17.5(19)
C39A	81(11)	74(10)	37(7)	11(6)	38(7)	8(8)
C40A	82(4)	31.4(15)	26.1(14)	6.6(12)	13.9(18)	0.3(17)
O10B	35.0(10)	19.7(7)	14.6(6)	0.4(6)	5.6(6)	4.6(6)
O2	22.5(7)	19.9(8)	18.0(7)	-4.4(6)	3.2(6)	-2.6(6)
O3	23.5(8)	18.0(7)	27.4(8)	2.6(6)	10.8(6)	-2.1(6)
O4A	12.7(7)	18.0(7)	12(4)	-3.7(7)	2.2(12)	-2.5(6)
O4B	12.7(7)	18.0(7)	12(4)	-3.7(7)	2.2(12)	-2.5(6)
O7	22.5(7)	18.3(7)	13.1(6)	0.3(5)	6.3(6)	1.9(6)
N1	17.2(8)	15.5(8)	17.0(8)	0.4(6)	5.3(6)	1.1(7)
N2	21.3(9)	16.2(8)	17.4(8)	-0.7(7)	7.5(7)	-0.4(7)
C25	34.4(12)	26.5(12)	13.3(9)	-1.5(8)	7.8(9)	6.4(10)
C1	15.6(10)	23.0(11)	32.9(12)	-4.8(9)	8.3(9)	2.5(8)
C21	29.6(12)	28.3(12)	19.8(10)	3.9(9)	0.7(9)	10.1(10)
C41	25.3(11)	23.2(11)	33.5(12)	-8.5(9)	15.4(10)	1.5(9)
C42	27.0(12)	25.9(12)	41.1(14)	-8.8(10)	18.2(11)	-2.5(10)
C20	34.4(13)	29.3(12)	20.5(10)	-1.1(9)	8.7(9)	8.7(10)
C2	21.3(11)	25.6(12)	43.5(14)	-8.4(10)	12.7(10)	0.7(9)
C9	39.7(14)	20.6(11)	27.7(11)	4.8(9)	16.3(10)	-3.1(10)
C5	25.5(11)	23.6(11)	22.7(10)	-10.6(9)	3.2(9)	-1.7(9)
C33	40.9(14)	17.3(11)	35.6(13)	3.6(9)	23.2(11)	-1.9(10)
C26	76(2)	27.1(13)	23.4(12)	-1.1(10)	21.0(13)	8.1(13)
C17	28.4(11)	24.6(11)	22.4(10)	-4.7(9)	10.1(9)	6.3(9)
C45	26.3(12)	40.5(15)	38.5(14)	-20.3(12)	10.0(11)	-15.6(11)
C29	26.2(12)	37.3(14)	26.5(11)	8.2(10)	8.1(9)	15.8(10)
C37B	30.3(16)	23.6(10)	16.1(9)	2.4(8)	2.1(10)	7.5(11)
C22	48.1(17)	34.4(15)	42.6(16)	6.7(12)	7.7(13)	1.3(13)
C27	47.0(16)	42.4(16)	33.8(13)	-1.6(12)	23.0(12)	-4.4(13)
C32	48.4(18)	38.4(16)	62(2)	3.8(14)	15.2(15)	16.6(14)
C11	59.6(18)	29.7(13)	25.6(12)	2.2(10)	17.6(12)	-7.1(12)
C44	37.0(15)	20.5(13)	81(2)	1.6(14)	18.7(15)	1.9(11)
C24	55.7(18)	52.9(18)	21.6(12)	4.9(12)	3.2(12)	18.1(15)
C3	27.9(13)	34.5(14)	62.9(18)	2.2(13)	23.3(13)	0.6(11)
C10	53.8(18)	34.1(15)	53.5(17)	8.2(13)	31.9(15)	-9.8(13)
C8	50.9(17)	42.5(16)	21.3(11)	-8.5(11)	1.1(11)	5.2(13)
C19	34.9(14)	45.1(16)	37.2(14)	-4.3(12)	20.0(11)	11.9(12)

C6	29.3(14)	48.8(18)	53.8(17)	-24.0(14)	11.1(12)	-15.8(13)
C48	78(3)	46(2)	61(2)	-8.3(17)	7.5(19)	-22.6(18)
C30	59(2)	95(3)	34.7(15)	30.3(17)	16.8(15)	45(2)
C46	52.5(19)	68(2)	44.5(17)	-31.6(16)	16.2(14)	-27.6(17)
C43	48.2(18)	77(2)	43.4(16)	-28.3(16)	25.3(14)	2.5(16)
C31	27.7(14)	57(2)	66(2)	9.3(16)	10.7(14)	12.7(14)
C47	30.6(16)	91(3)	79(3)	-48(2)	14.3(16)	-16.8(17)
C38B	49(2)	54(3)	39(2)	9.4(18)	-4.9(17)	17.5(19)
C39B	79(3)	37(2)	21.4(17)	7.5(15)	20.3(19)	12(2)
C40B	82(4)	31.4(15)	26.1(14)	6.6(12)	13.9(18)	0.3(17)
C13A	9(3)	20(2)	29(5)	5(4)	-1(3)	-1(2)
C13B	9(3)	20(2)	29(5)	5(4)	-1(3)	-1(2)
C14A	42(2)	37(2)	63(3)	-13(2)	37(2)	-15.2(18)
C14B	42(2)	37(2)	63(3)	-13(2)	37(2)	-15.2(18)
C15A	21.9(19)	45(2)	54(3)	6.5(19)	-2.4(16)	-7.3(16)
C15B	21.9(19)	45(2)	54(3)	6.5(19)	-2.4(16)	-7.3(16)
C16A	20.4(14)	22(2)	45(4)	-6(3)	19(3)	-3.1(14)
C16B	20.4(14)	22(2)	45(4)	-6(3)	19(3)	-3.1(14)
C18	39.8(14)	22.5(12)	32.9(13)	-3.9(10)	6.6(11)	6.1(11)
C4	30.4(13)	46.1(16)	33.3(13)	0.3(12)	6.2(11)	13.8(12)
C34	37.6(15)	31.9(14)	57.7(17)	2.0(13)	26.2(13)	-4.4(12)
C23	25.9(12)	43.0(16)	42.4(15)	4.7(12)	2.1(11)	16.1(12)
C28	40.2(15)	63(2)	23.9(12)	-2.5(12)	8.7(11)	5.7(14)
C36	49.3(16)	20.5(12)	40.1(14)	-1.8(10)	23.0(12)	-2.7(11)
C12	46.4(16)	21.5(12)	38.8(14)	6.4(10)	12.5(12)	4.6(11)
C7	40.7(15)	25.7(12)	35.6(13)	-11.1(10)	7.3(11)	3.3(11)
C35	71(2)	30.2(14)	46.4(16)	7.9(12)	39.3(16)	-1.4(14)

Table S25. Bond Lengths for 2-Eu.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Eu1	Si1	3.3106(7)	O3	C9	1.437(3)
Eu1	Si2	3.2917(7)	O4A	C13A	1.46(2)
Eu1	Si4	3.3088(7)	O4B	C13B	1.458(13)
Eu1	Si3	3.2918(7)	O7	C25	1.456(2)
Eu1	O1	2.5268(14)	C25	C26	1.498(3)
Eu1	O10A	2.531(2)	C25	C27	1.544(3)
Eu1	O10B	2.5279(16)	C25	C28	1.497(3)
Eu1	O4A	2.518(4)	C1	C2	1.512(3)
Eu1	O4B	2.518(2)	C1	C3	1.495(3)
Eu1	O7	2.5306(14)	C1	C4	1.539(3)

Eu1	N1	2.7149(17)	C21	C22	1.516(4)
Eu1	N2	2.7211(18)	C21	C24	1.521(3)
Si1	O1	1.6877(15)	C21	C23	1.521(4)
Si1	O2	1.6400(15)	C41	C42	1.516(3)
Si1	O3	1.6319(16)	C41	C44	1.512(4)
Si1	N1	1.6368(18)	C41	C43	1.518(3)
Si2	O5	1.6307(15)	C20	C17	1.527(3)
Si2	O6	1.6349(15)	C9	C11	1.520(3)
Si2	O4A	1.6961(19)	C9	C10	1.522(4)
Si2	O4B	1.6961(19)	C9	C12	1.521(3)
Si2	N1	1.6334(18)	C5	C8	1.521(3)
Si4	O11	1.6307(16)	C5	C6	1.527(4)
Si4	O12	1.6302(17)	C5	C7	1.520(3)
Si4	O10A	1.691(2)	C33	C34	1.517(4)
Si4	O10B	1.6879(17)	C33	C36	1.526(3)
Si4	N2	1.6375(17)	C33	C35	1.523(3)
Si3	O9	1.6361(16)	C17	C19	1.517(3)
Si3	O8	1.6421(17)	C17	C18	1.519(3)
Si3	O7	1.6864(15)	C45	C48	1.499(4)
Si3	N2	1.6401(17)	C45	C46	1.528(4)
O1	C1	1.457(2)	C45	C47	1.519(4)
O5	C17	1.441(3)	C29	C32	1.507(4)
O11	C41	1.429(3)	C29	C30	1.519(4)
O6	C21	1.433(3)	C29	C31	1.529(4)
O9	C33	1.437(3)	C37B	C38B	1.518(4)
O8	C29	1.431(3)	C37B	C39B	1.517(3)
O12	C45	1.433(3)	C37B	C40B	1.518(3)
O10A	C37A	1.456(3)	C13A	C14A	1.45(3)
C37A	C38A	1.519(3)	C13A	C15A	1.495(19)
C37A	C39A	1.517(3)	C13A	C16A	1.57(3)
C37A	C40A	1.518(3)	C13B	C14B	1.538(13)
O10B	C37B	1.454(3)	C13B	C15B	1.542(8)
O2	C5	1.434(3)	C13B	C16B	1.495(15)

Table S26. Bond Angles for 2-Eu.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
Si2	Eu1	Si1	59.075(17)	O10A	C37A	C39A	111.1(3)
Si2	Eu1	Si4	130.458(16)	O10A	C37A	C40A	104.3(3)
Si2	Eu1	Si3	147.661(15)	C39A	C37A	C38A	111.3(4)
Si4	Eu1	Si1	149.948(15)	C39A	C37A	C40A	110.6(4)

Si3	Eu1	Si1	131.651(16)	C40A	C37A	C38A	110.0(4)
Si3	Eu1	Si4	59.273(17)	Si4	O10B	Eu1	101.55(7)
O1	Eu1	Si1	29.95(3)	C37B	O10B	Eu1	122.63(14)
O1	Eu1	Si2	87.84(3)	C37B	O10B	Si4	134.36(16)
O1	Eu1	Si4	124.71(3)	C5	O2	Si1	137.50(14)
O1	Eu1	Si3	111.59(3)	C9	O3	Si1	136.50(14)
O1	Eu1	O10A	107.7(2)	Si2	O4A	Eu1	100.94(15)
O1	Eu1	O10B	109.46(9)	C13A	O4A	Eu1	128.8(10)
O1	Eu1	O7	106.32(5)	C13A	O4A	Si2	130.2(10)
O1	Eu1	N1	58.56(5)	Si2	O4B	Eu1	100.90(11)
O1	Eu1	N2	122.24(5)	C13B	O4B	Eu1	122.8(5)
O10A	Eu1	Si1	123.45(11)	C13B	O4B	Si2	134.9(5)
O10A	Eu1	Si2	111.51(19)	Si3	O7	Eu1	100.72(6)
O10A	Eu1	Si4	30.07(5)	C25	O7	Eu1	125.01(12)
O10A	Eu1	Si3	87.71(9)	C25	O7	Si3	133.69(13)
O10A	Eu1	N1	121.53(8)	Si1	N1	Eu1	95.88(7)
O10A	Eu1	N2	58.39(8)	Si2	N1	Eu1	95.15(7)
O10B	Eu1	Si1	124.36(5)	Si2	N1	Si1	168.91(12)
O10B	Eu1	Si2	110.10(7)	Si4	N2	Eu1	95.55(8)
O10B	Eu1	Si4	29.99(4)	Si4	N2	Si3	169.56(12)
O10B	Eu1	Si3	88.22(5)	Si3	N2	Eu1	94.77(7)
O10B	Eu1	O7	117.23(5)	O7	C25	C26	105.63(17)
O10B	Eu1	N1	121.16(5)	O7	C25	C27	108.71(19)
O10B	Eu1	N2	58.73(5)	O7	C25	C28	112.08(19)
O4A	Eu1	Si1	88.84(11)	C26	C25	C27	109.0(2)
O4A	Eu1	Si2	30.39(5)	C28	C25	C26	112.9(2)
O4A	Eu1	Si4	107.7(3)	C28	C25	C27	108.3(2)
O4A	Eu1	Si3	122.96(18)	O1	C1	C2	105.78(17)
O4A	Eu1	O1	118.14(7)	O1	C1	C3	111.04(19)
O4A	Eu1	O7	106.6(3)	O1	C1	C4	108.11(18)
O4A	Eu1	N1	59.63(9)	C2	C1	C4	108.3(2)
O4A	Eu1	N2	119.57(9)	C3	C1	C2	111.5(2)
O4B	Eu1	Si1	87.24(6)	C3	C1	C4	111.9(2)
O4B	Eu1	Si2	30.40(4)	O6	C21	C22	110.3(2)
O4B	Eu1	Si4	111.48(13)	O6	C21	C24	104.91(19)
O4B	Eu1	Si3	120.54(10)	O6	C21	C23	110.8(2)
O4B	Eu1	O1	117.03(6)	C22	C21	C24	110.7(2)
O4B	Eu1	O7	102.00(17)	C22	C21	C23	110.1(2)
O4B	Eu1	N1	58.60(6)	C24	C21	C23	109.9(2)
O4B	Eu1	N2	120.61(6)	O11	C41	C42	110.77(18)
O7	Eu1	Si1	112.36(3)	O11	C41	C44	107.81(19)
O7	Eu1	Si2	121.16(3)	O11	C41	C43	105.6(2)

O7	Eu1	Si4	87.36(3)	C42	C41	C43	110.0(2)
O7	Eu1	Si3	30.22(3)	C44	C41	C42	111.6(2)
O7	Eu1	O10A	117.01(7)	C44	C41	C43	110.8(2)
O7	Eu1	N1	121.38(5)	O3	C9	C11	110.84(19)
O7	Eu1	N2	58.66(5)	O3	C9	C10	106.2(2)
N1	Eu1	Si1	29.46(4)	O3	C9	C12	107.45(19)
N1	Eu1	Si2	29.62(4)	C11	C9	C10	110.8(2)
N1	Eu1	Si4	150.24(4)	C11	C9	C12	111.3(2)
N1	Eu1	Si3	150.44(4)	C12	C9	C10	110.2(2)
N1	Eu1	N2	179.20(5)	O2	C5	C8	105.29(19)
N2	Eu1	Si1	151.33(4)	O2	C5	C6	110.69(19)
N2	Eu1	Si2	149.59(4)	O2	C5	C7	110.63(18)
N2	Eu1	Si4	29.51(4)	C8	C5	C6	110.4(2)
N2	Eu1	Si3	29.77(4)	C7	C5	C8	109.9(2)
O2	Si1	O1	103.81(8)	C7	C5	C6	109.9(2)
O3	Si1	O1	109.11(8)	O9	C33	C34	111.02(19)
O3	Si1	O2	103.91(8)	O9	C33	C36	108.48(19)
O3	Si1	N1	121.44(8)	O9	C33	C35	105.5(2)
N1	Si1	O1	101.17(8)	C34	C33	C36	110.3(2)
N1	Si1	O2	115.99(8)	C34	C33	C35	111.3(2)
O5	Si2	O6	104.82(8)	C35	C33	C36	110.2(2)
O5	Si2	O4A	111.6(4)	O5	C17	C20	110.91(17)
O5	Si2	O4B	106.6(2)	O5	C17	C19	106.30(19)
O5	Si2	N1	121.62(9)	O5	C17	C18	107.98(18)
O6	Si2	O4A	97.5(6)	C19	C17	C20	110.0(2)
O6	Si2	O4B	105.9(3)	C19	C17	C18	110.3(2)
N1	Si2	O6	115.63(9)	C18	C17	C20	111.2(2)
N1	Si2	O4A	103.07(19)	O12	C45	C48	110.3(2)
N1	Si2	O4B	100.86(12)	O12	C45	C46	111.1(2)
O11	Si4	O10A	106.8(3)	O12	C45	C47	104.7(2)
O11	Si4	O10B	108.83(11)	C48	C45	C46	109.7(3)
O11	Si4	N2	120.91(9)	C48	C45	C47	112.2(3)
O12	Si4	O11	103.92(9)	C47	C45	C46	108.7(3)
O12	Si4	O10A	106.2(4)	O8	C29	C32	111.1(2)
O12	Si4	O10B	103.18(16)	O8	C29	C30	110.6(2)
O12	Si4	N2	116.74(9)	O8	C29	C31	105.3(2)
N2	Si4	O10A	100.95(15)	C32	C29	C30	110.6(3)
N2	Si4	O10B	101.72(9)	C32	C29	C31	109.8(2)
O9	Si3	O8	104.74(8)	C30	C29	C31	109.3(3)
O9	Si3	O7	108.46(8)	O10B	C37B	C38B	109.2(3)
O9	Si3	N2	122.06(9)	O10B	C37B	C39B	110.7(2)
O8	Si3	O7	102.99(8)	O10B	C37B	C40B	104.3(2)

N2	Si3	O8	115.24(9)	C39B C37B C38B	111.6(3)
N2	Si3	O7	101.59(8)	C39B C37B C40B	110.7(3)
Si1	O1	Eu1	101.68(6)	C40B C37B C38B	110.1(3)
C1	O1	Eu1	122.98(12)	O4A C13A C15A	104.9(15)
C1	O1	Si1	133.01(13)	O4A C13A C16A	103.0(14)
C17	O5	Si2	136.47(14)	C14A C13A O4A	114.8(18)
C41	O11	Si4	135.12(14)	C14A C13A C15A	117.6(14)
C21	O6	Si2	137.24(14)	C14A C13A C16A	108.9(13)
C33	O9	Si3	134.94(14)	C15A C13A C16A	106.4(17)
C29	O8	Si3	138.09(16)	O4B C13B C14B	106.6(8)
C45	O12	Si4	138.82(16)	O4B C13B C15B	112.0(7)
Si4	O10A	Eu1	101.33(10)	O4B C13B C16B	107.6(9)
C37A	O10A	Eu1	124.5(3)	C14B C13B C15B	108.7(8)
C37A	O10A	Si4	134.1(3)	C16B C13B C14B	111.6(6)
O10A	C37A	C38A	109.5(3)	C16B C13B C15B	110.4(8)

Table S27. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 2-Eu.

Atom	*x*	*y*	*z*	U(eq)
H38A	6617.96	5018.31	2557.91	80
H38B	6354.65	6021.29	2429.46	80
H38C	6206.92	5430.72	2980.3	80
H39A	8184.45	5983.62	3409.25	89
H39B	7686.2	6025.14	2643.29	89
H39C	7839.97	5094.42	3029.59	89
H40A	6702.71	6950.79	3514.7	72
H40B	7144.1	7215.16	3080.12	72
H40C	7503.41	7013	3862.74	72
H42A	8769	4637.17	4006.36	45
H42B	9269.42	3823.85	4311.29	45
H42C	8785.11	4165.25	4680.16	45
H20A	6542.09	7866.79	6412.26	43
H20B	6796.21	8790.06	6788.91	43
H20C	7126.3	8411.28	6283.09	43
H2A	8845.64	5702.97	5150.29	45
H2B	9536.85	5946.27	5060.67	45
H2C	8837.15	6268.87	4516.12	45
H26A	8054.22	6821.98	6550.86	62
H26B	7666.66	6759.61	7061.82	62
H26C	7263.12	6630.37	6276.36	62

H22A	6005.78	9802.61	4206.67	66
H22B	5606.94	10079.59	3443.86	66
H22C	6345.53	9664.98	3661.3	66
H27A	6831.64	5218.22	6557.15	58
H27B	7282.16	5316.14	7334.98	58
H27C	7346.54	4447.39	6933.19	58
H32A	8894.34	2587.33	5984.75	76
H32B	9692.9	2520.39	6198.71	76
H32C	9255.55	3036.14	5529.02	76
H11A	8093.32	8509.44	3818.11	57
H11B	7633.6	9330.01	3443.87	57
H11C	7398.52	8698.33	3916.97	57
H44A	8274.66	2639.64	4615.17	70
H44B	8782.77	2287.16	4277.52	70
H44C	7990.74	2142.34	3907.74	70
H24A	5960.3	8461.71	2825.29	70
H24B	5213.66	8856.9	2563.74	70
H24C	5342.69	7843.83	2801.26	70
H3A	9304.61	7815.41	4703.27	60
H3B	9977.99	7500.99	5291.34	60
H3C	9516.1	8252.34	5431.05	60
H10A	9026.46	10307.11	4789.74	66
H10B	8654.35	10351.76	3994	66
H10C	9069.76	9483.46	4336.08	66
H8A	8423.07	8584.83	7355.33	62
H8B	9085.22	9179.86	7666.47	62
H8C	9138.33	8193.3	7413.2	62
H19A	5185.67	9300.12	5530.2	56
H19B	5591.27	9336.55	6321.2	56
H19C	5372.53	8399.63	5954.15	56
H6A	9724.83	8801.02	6697.3	68
H6B	9642.08	9805.19	6898.66	68
H6C	9359.09	9514.78	6128.11	68
H48A	6804.56	2380.02	3886.35	100
H48B	6074.04	1978.1	3486.77	100
H48C	6232.83	2434.99	4201.48	100
H30A	9527.05	4112.84	7352.28	95
H30B	9846.95	3165.68	7306.45	95
H30C	9051.84	3261.52	7108.1	95
H46A	5987.15	3895.13	2532.8	83
H46B	5852.18	2847.6	2486.01	83
H46C	6605.45	3217.34	2793.81	83

H43A	7952.25	2924.12	2875.11	81
H43B	8753.54	3004.6	3200.18	81
H43C	8304.72	3874.18	2934.13	81
H31A	9942.65	4394.89	5911.82	78
H31B	10399.16	3881.75	6575.18	78
H31C	10050.26	4802.56	6632.32	78
H47A	5348.25	3553.53	3821.8	103
H47B	5074.14	3122.91	3089.5	103
H47C	5267.92	4153.75	3181.78	103
H38D	6051.36	5338.49	2985.21	80
H38E	6068.1	6241.82	2598.94	80
H38F	6101.65	6272.61	3355.87	80
H39D	7728.86	5388.44	2962.63	68
H39E	7098.84	5788.42	2364.4	68
H39F	7039.43	4843.01	2678.72	68
H40D	7171.38	7075.32	3799.73	72
H40E	7128.58	7187.1	3043.68	72
H40F	7789.62	6776.19	3596.25	72
H14A	5526.59	6868.92	5501.83	64
H14B	4893.19	6352.72	4988.42	64
H14C	5090.71	7313.54	4799.72	64
H14D	6011.31	6367.83	5923.53	64
H14E	5248.56	6078.97	5523.45	64
H14F	5469.99	7092.14	5512.39	64
H15A	5309.74	6722.31	3740.42	67
H15B	4988.68	5820.37	3882.16	67
H15C	5726.73	5815.24	3854.09	67
H15D	5010.55	7109.63	4308.8	67
H15E	4801.98	6083.41	4226.2	67
H15F	5284.63	6469.45	3870.31	67
H16A	6262.11	5153.43	4881.35	40
H16B	5570.06	5029.76	4999.66	40
H16C	6191.44	5517.22	5553.19	40
H16D	6088.42	5235.97	4471.37	40
H16E	5615	4944.21	4866.17	40
H16F	6382.86	5204.55	5272.07	40
H18A	6821.24	9840.92	5592.36	50
H18B	6534.54	10208.49	6135.26	50
H18C	6064.62	10196.74	5359.15	50
H4A	9416.73	7309.83	6396.1	57
H4B	9913.23	6616.87	6248.49	57
H4C	9196.18	6293.93	6238.38	57

H34A	6530.55	3680.14	5934.72	60
H34B	6259.37	2771.94	5541.7	60
H34C	6600.36	3504.29	5227.57	60
H23A	4750.64	8109.03	3570.83	60
H23B	4647.71	9145.07	3397.93	60
H23C	5021.25	8830.13	4156.15	60
H28A	8541.49	4682.04	7295.98	65
H28B	8517.75	5589.67	7674.48	65
H28C	8854.1	5569.58	7119.63	65
H36A	7442.13	2389.04	5143.57	52
H36B	7072.46	1656.16	5426.34	52
H36C	7863.22	1818.28	5789.96	52
H12A	7326.52	10042.61	4629.15	55
H12B	7510.96	10634.1	4100.83	55
H12C	7954.4	10705.92	4882.26	55
H7A	8218.08	10107.02	6034.82	54
H7B	8533.94	10376.89	6808.85	54
H7C	7882.87	9754.1	6543.86	54
H35A	7782.1	2117.89	6877.34	66
H35B	6990.61	1928.94	6577.49	66
H35C	7269.09	2846.28	6952.65	66

Table S28. Atomic Occupancy for 2-Eu.

Atom	***Occupancy***	**Atom**	***Occupancy***	**Atom**	***Occupancy***
O10A	0.257(5)	C37A	0.257(5)	C38A	0.257(5)
H38A	0.257(5)	H38B	0.257(5)	H38C	0.257(5)
C39A	0.257(5)	H39A	0.257(5)	H39B	0.257(5)
H39C	0.257(5)	C40A	0.257(5)	H40A	0.257(5)
H40B	0.257(5)	H40C	0.257(5)	O10B	0.743(5)
O4A	0.370(4)	O4B	0.630(4)	C37B	0.743(5)
C38B	0.743(5)	H38D	0.743(5)	H38E	0.743(5)
H38F	0.743(5)	C39B	0.743(5)	H39D	0.743(5)
H39E	0.743(5)	H39F	0.743(5)	C40B	0.743(5)
H40D	0.743(5)	H40E	0.743(5)	H40F	0.743(5)
C13A	0.370(4)	C13B	0.630(4)	C14A	0.370(4)
H14A	0.370(4)	H14B	0.370(4)	H14C	0.370(4)
C14B	0.630(4)	H14D	0.630(4)	H14E	0.630(4)
H14F	0.630(4)	C15A	0.370(4)	H15A	0.370(4)
H15B	0.370(4)	H15C	0.370(4)	C15B	0.630(4)
H15D	0.630(4)	H15E	0.630(4)	H15F	0.630(4)

C16A	0.370(4)	H16A	0.370(4)	H16B	0.370(4)
H16C	0.370(4)	C16B	0.630(4)	H16D	0.630(4)
H16E	0.630(4)	H16F	0.630(4)		

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