Electronic Supplementary Information

Cyclopentadienyl capped thorium(IV) porphyrinoid complex

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Materials & General Methods

All reagents and solvents were purchased from commercial supplies and used without further purification. Anhydrous tetrahydrofuran (100 mL Sure/Seal™) was stored over activated molecular sieves then filtered through dried basic aluminum oxide before use. High-resolution mass spectra (HRMS) were measured using an Ion Spec Fourier Transform mass spectrometer (9.4 T). Proton and carbon NMR spectra were recorded using a Varian 400 spectrometer at room temperature and chemical shifts are reported in ppm using TMS or solvent residual signals as internal reference standards. All NMR spectroscopic solvents were purchased from Cambridge Isotope Laboratories. UV-Vis spectra were recorded from 250 to 800 nm using a Varian Cary 5000 spectrophotometer at room temperature. Unless otherwise indicated, a cell length of 10 mm was used for all UV-Vis spectra studies.

Dipyriamethyrin was synthesized as previously reported.[1]

Th(IV)[dipyriamethyrin]Cl_2 (**1**). In an inert atmosphere glove box, a borosilicate scintillation vial was charged with dipyriamethyrin (45 mg, 0.06 mmol) and sodium bis(trimethyl)silylamide (NaHMDS, 21.3 mg, 0.11 mmol, 2.1 equiv.). The solids were dissolved in anhydrous THF (3 mL) and stirred at ambient temperature for 20 minutes. The solution immediately turned purple. The mixture was concentrated under reduced pressure. Drying was continued for 0.5 to 1 h after the bulk of the THF had been removed. This yielded a purple solid with green metallic luster. To this solid, $ThCl_4(DME)_2$ (30.6 mg, 0.06 mmol, 1 equiv.) and anhydrous THF (3 mL) were added. The reaction was stirred at ambient temperature overnight, at which point the solution turned from purple to red-purple yielding a bronze-coloured precipitate, which was washed (3 x 7.5 mL) with anhydrous THF: hexanes (1:19, v/v). The resulting solid was taken up in anhydrous THF (20 mL) and cooled to -35° C and held at that temperature for 30 min. The solution was decanted to remove any additional salt that had precipitated. Removing the volatiles

from the decanted THF solution under reduced pressure yielded the product in the form of a powder (62.1 mg, 91% yield). Crystalline material (43 mg, 63%) was obtained by allowing the solution to concentrate to ca. 1 mL then removing the remaining THF: hexanes mixture by decanting with a glass pipette. Single crystals suitable for X-ray diffraction were obtained by slow evaporation of a solution in anhydrous THF: hexanes (1:1, v/v, 10 mL) over one to three days.

Th(IV)[dipyriamethyrin][F][Cp] (**2**).

In an inert atmosphere glove box, a borosilicate scintillation vial was charged with a Teflon-coated magnetic stir bar, Th(IV)[dipyriamethyrin]Cl_2 (**1**) (20 mg, 0.025 mmol), and sodium cyclopentadienyl (4.6 mg, 0.052 mmol, 2.1 equiv.). The solids were stirred in anhydrous THF (3 mL) at ambient temperature for 18 h. The reaction mixture was concentrated under reduced pressure and the resulting solids washed (3 x 7.5 mL) with anhydrous THF: hexanes (1:20, v/v) by vigorously shaking to yield a purple solid. The solid was taken up in THF (20 mL), cooled to -35° C for 30 min, and the solution was decanted to remove any additional salt that had precipitated to yield complex **2** as a purple solid with metallic luster (20.4 mg, 93% yield) (Figure S1). Single crystals suitable for X-ray diffraction analyses were obtained by slow evaporation of the complex **2** in 5 mL of a THF: hexanes (1:10, v/v) mixture. The original solid material was used for the UV-vis and ^{1}H NMR spectroscopic analyses. ^{1}H NMR (400 MHz, THF-d_8) δ 7.83-7.61 (m, 2H), 7.51-7.34 (m, 14H), 6.50 (s, 1H), 6.40 (s, 1H), 5.79 (s, 3H), 2.79-2.62 (m, 14H), 1.05 (t, J= 7.5Hz, 6H) 0.78-0.62 (m, 12H).

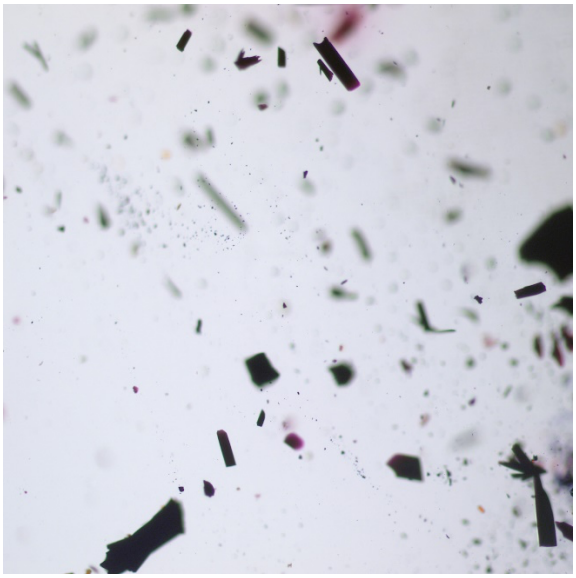

Figure S1 – Pictures of the single crystals of complex **2** used for X-ray diffraction studies.

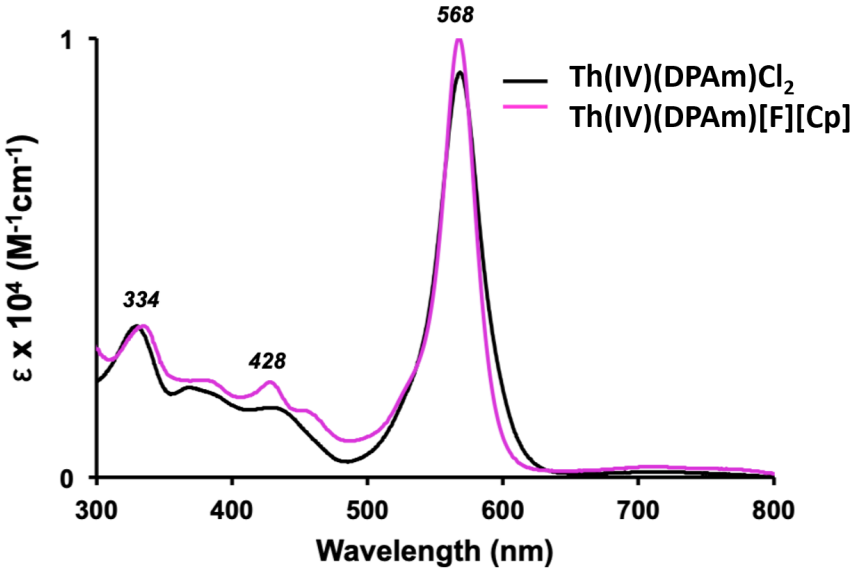

Figure S2 – Overlaid UV-vis spectra of the Th(IV)-dipyriamethyrinCl_2 with the Th(IV)-dipyriamethyrin[F][Cp] complex.

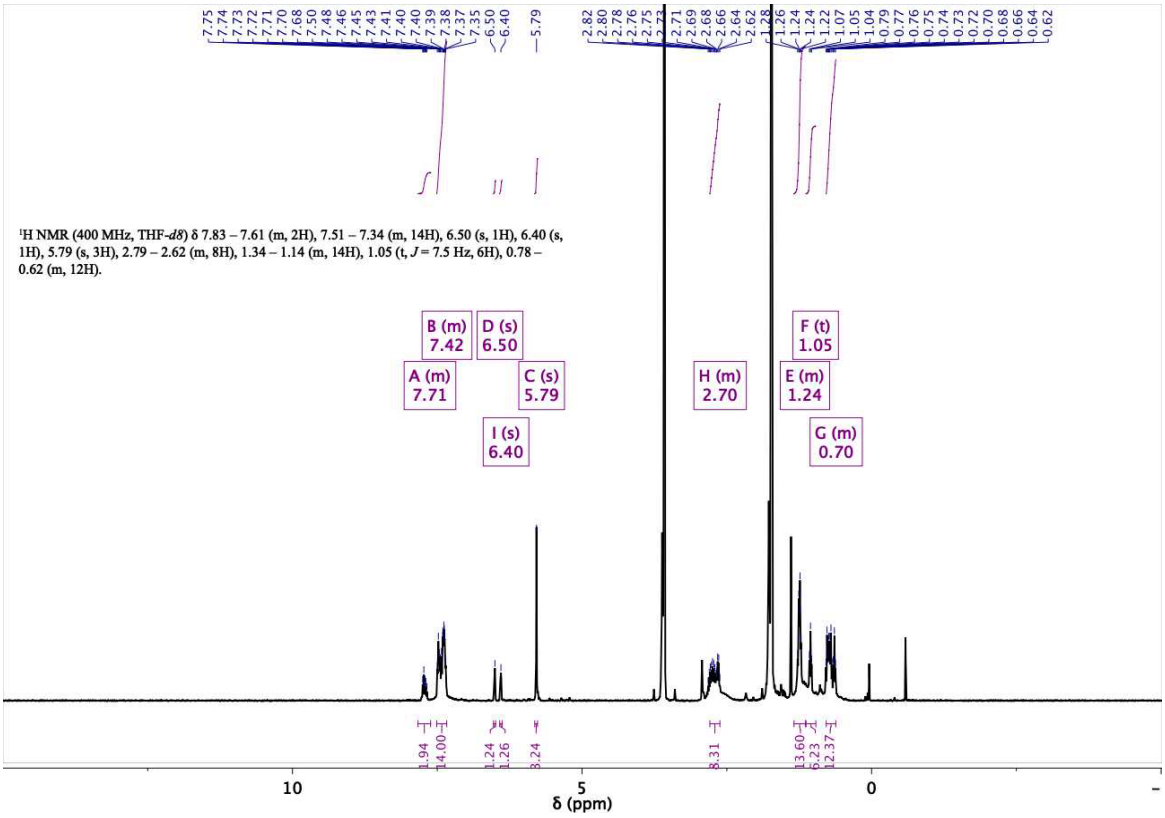

Figure S3: ^{1}H NMR spectrum of complex **2** in THF-d_8.

Th(IV)[dipyriamethyrin][benzoate]$_2$ (**4**)

In an inert atmosphere glove box, a borosilicate scintillation vial was charged with a Teflon coated magnetic stir bar, Th(IV)[dipyriamethyrin]Cl_2 (**3**) (20 mg, 0.025 mmol), and silver benzoate (5.8 mg, 0.052 mmol, 2.1 equiv.). The solids were dissolved in anhydrous THF (3 mL) and stirred at ambient temperature for 18 h. The reaction mixture was filtered through a pipette filter and concentrated under reduced pressure and the resulting solids washed (3 x 7.5 mL) with anhydrous THF: hexanes (1:20, v/v) by vigorously shaking to yield a purple solid. The solid was taken up in THF (20 mL), cooled to -35° C for 30 min, and the solution was decanted to remove any additional salt that had precipitated. This yielded complex **4** as a purple solid with green metallic luster (20.4 mg, 93% yield). Single crystals suitable for X-ray diffraction analyses were obtained by slow evaporation of the complex **4** in 5 mL of a THF: toluene (1:5, v/v) mixture.

Sodium Cyclopentadienide

Under an inert atmosphere, 400 mL of diglyme and 2.29g of sodium (0.1 mole) were added to a 1000 mL round bottom flask. The flask was set reflux (162° C) and 4.62g of dicyclopentadiene was slowly added to the reaction solution. When the hydrogen gas generation stopped, the reactions was deemed complete. The solution was cooled, filtered and washed with hexanes.

Computational Calculations - Experimental

Density functional theory calculations were carried out using the PBE0 hybrid functional as implemented in the Gaussian 16 quantum chemistry code. 60-electron Stuttgart-Bonn relativistic pseudopotentials were used for Th together with (14s 13p 10d 8f 6g)/[10s 9p 5d 4f 3g] segmented valence basis sets. Dunning's cc-pVTZ basis sets were employed for N, C ,O, F, and Cl, and cc-pVDZ for H. Spin-unrestricted calculations were performed. The ultrafine integration grid was employed, as were the default geometry and SCF convergence criteria. No symmetry constraints were imposed. Basis set superposition errors were calculated using the counterpoise correction for the complexation energies.

Geometries of the Relaxed Structures:

Complex 2

```
Th -0.0230000000 -0.0010000000 -0.6150000000
F 0.0240000000 0.0620000000 1.4800000000
N -2.8070000000 -0.3600000000 -0.6320000000
N -0.9680000000 -2.5430000000 0.0400000000
N 1.7240000000 -2.1100000000 -0.2340000000
N 2.7530000000 0.3390000000 -0.7830000000
N 0.9340000000 2.5580000000 -0.1640000000
N -1.7530000000 2.1130000000 -0.2880000000
C -3.4670000000 0.7070000000 -1.1410000000
C -4.5660000000 0.3330000000 -1.9910000000
C -4.6180000000 -1.0660000000 -1.9410000000
C -3.5590000000 -1.4690000000 -1.0260000000
C -3.3930000000 -2.7050000000 -0.3610000000
C -2.2270000000 -3.0450000000 0.3730000000
C -2.1200000000 -4.0290000000 1.4360000000
C -0.7550000000 -4.1760000000 1.6910000000
C -0.0940000000 -3.2880000000 0.7680000000
C 1.3170000000 -3.2240000000 0.4300000000
C 2.1950000000 -4.3060000000 0.6770000000
H 1.8270000000 -5.2030000000 1.1820000000
C 3.5100000000 -4.2400000000 0.2170000000
H 4.2040000000 -5.0760000000 0.3890000000
C 3.9330000000 -3.0950000000 -0.4620000000
H 4.9700000000 -2.9850000000 -0.7960000000
C 3.0140000000 -2.0400000000 -0.6540000000
C 3.4150000000 -0.7600000000 -1.2120000000
C 4.4770000000 -0.4500000000 -2.1360000000
C 4.4930000000 0.9470000000 -2.2280000000
C 3.4650000000 1.4170000000 -1.3100000000
C 3.3250000000 2.7030000000 -0.7370000000
C 2.2060000000 3.0920000000 0.0450000000
C 2.1560000000 4.1550000000 1.0350000000
C 0.8080000000 4.3110000000 1.3670000000
C 0.0990000000 3.3520000000 0.5590000000
C -1.3260000000 3.2630000000 0.2950000000
C -2.2010000000 4.3560000000 0.5110000000
H -1.8220000000 5.2790000000 0.9590000000
C -3.5260000000 4.2660000000 0.0830000000
H -4.2150000000 5.1110000000 0.2260000000
C -3.9630000000 3.0880000000 -0.5270000000
H -5.0060000000 2.9650000000 -0.8380000000
C -3.0520000000 2.0200000000 -0.6760000000
C -5.4500000000 1.2330000000 -2.8190000000
H -5.5550000000 0.7980000000 -3.8360000000
H -4.9520000000 2.2130000000 -2.9700000000
C -6.8580000000 1.4490000000 -2.2320000000
H -7.4640000000 2.1160000000 -2.8790000000
H -6.8170000000 1.9020000000 -1.2190000000
H -7.3990000000 0.4870000000 -2.1290000000
C -5.4850000000 -1.9280000000 -2.8260000000
H -6.2390000000 -1.2800000000 -3.3190000000
H -6.0620000000 -2.6650000000 -2.2350000000
C -4.6830000000 -2.6730000000 -3.9090000000
H -4.1300000000 -1.9650000000 -4.5600000000
H -5.3560000000 -3.2770000000 -4.5510000000
H -3.9400000000 -3.3600000000 -3.4560000000
C -4.5150000000 -3.6880000000 -0.3790000000
C -4.3200000000 -4.9820000000 -0.9100000000
```

H -3.3320000000 -5.2480000000 -1.3140000000
C -5.3680000000 -5.9130000000 -0.9230000000
H -5.2050000000 -6.9130000000 -1.3520000000
C -6.6200000000 -5.5730000000 -0.3850000000
H -7.4390000000 -6.3080000000 -0.3850000000
C -6.8230000000 -4.2920000000 0.1540000000
H -7.7990000000 -4.0230000000 0.5840000000
C -5.7830000000 -3.3520000000 0.1460000000
H -5.9380000000 -2.3450000000 0.5600000000
C -3.2160000000 -4.6120000000 2.2950000000
H -2.7970000000 -5.4550000000 2.8830000000
H -4.0270000000 -5.0480000000 1.6830000000
C -3.8130000000 -3.5760000000 3.2660000000
H -4.2750000000 -2.7320000000 2.7160000000
H -3.0320000000 -3.1480000000 3.9270000000
H -4.5940000000 -4.0370000000 3.9060000000
C -0.1500000000 -5.0300000000 2.7800000000
H -0.7470000000 -4.8920000000 3.7070000000
H 0.8640000000 -4.6600000000 3.0330000000
C -0.0960000000 -6.5350000000 2.4560000000
H 0.5060000000 -6.7430000000 1.5470000000
H -1.1100000000 -6.9390000000 2.2630000000
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H 7.3770000000 -2.2660000000 -2.9400000000
H 6.7680000000 -1.9130000000 -1.2900000000
C 5.2900000000 1.7330000000 -3.2400000000
H 6.0130000000 1.0480000000 -3.7280000000
H 5.9010000000 2.5210000000 -2.7570000000
C 4.4040000000 2.3790000000 -4.3220000000
H 5.0250000000 2.9040000000 -5.0770000000
H 3.7100000000 3.1220000000 -3.8800000000
H 3.7900000000 1.6190000000 -4.8460000000
C 4.4300000000 3.6910000000 -0.9050000000
C 5.7320000000 3.4120000000 -0.4350000000
H 5.9290000000 2.4430000000 0.0470000000
C 6.7560000000 4.3610000000 -0.5650000000
H 7.7610000000 4.1370000000 -0.1770000000
C 6.5010000000 5.5930000000 -1.1900000000
H 7.3060000000 6.3340000000 -1.2990000000
C 5.2130000000 5.8760000000 -1.6750000000
H 5.0080000000 6.8370000000 -2.1690000000
C 4.1820000000 4.9370000000 -1.5220000000
H 3.1670000000 5.1610000000 -1.8830000000
C 3.2980000000 4.8110000000 1.7720000000
H 2.9080000000 5.6930000000 2.3190000000
H 4.0620000000 5.2050000000 1.0750000000
C 3.9710000000 3.8580000000 2.7770000000
H 4.7870000000 4.3730000000 3.3260000000
H 4.4070000000 2.9770000000 2.2640000000
H 3.2410000000 3.4770000000 3.5200000000
C 0.2640000000 5.2450000000 2.4200000000
H 0.9180000000 5.1850000000 3.3170000000
H -0.7290000000 4.8910000000 2.7650000000
C 0.1730000000 6.7200000000 1.9830000000
H 1.1690000000 7.1130000000 1.6950000000
H -0.2220000000 7.3570000000 2.8010000000
H -0.4860000000 6.8510000000 1.0990000000
C -0.8560000000 0.9160000000 -3.1990000000

H -1.5430000000 1.7700000000 -3.1990000000
C -1.2260000000 -0.4580000000 -3.1930000000
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C -0.0340000000 -1.2360000000 -3.2210000000
H 0.0190000000 -2.3310000000 -3.2230000000
C 1.0710000000 -0.3390000000 -3.2750000000
H 2.1260000000 -0.6190000000 -3.3420000000
C 0.5670000000 0.9910000000 -3.2490000000
H 1.1660000000 1.9070000000 -3.2740000000

Complex 3

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Cl 0.0310000000 0.0720000000 2.0030000000
N -2.8000000000 -0.3610000000 -0.6610000000
N -0.9660000000 -2.5390000000 0.0140000000
N 1.7210000000 -2.1080000000 -0.2680000000
N 2.7450000000 0.3380000000 -0.8090000000
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C 0.1640000000 6.7030000000 1.9840000000
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C -0.8560000000 0.9110000000 -3.1880000000
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C -1.2240000000 -0.4650000000 -3.1820000000
H -2.2440000000 -0.8590000000 -3.1760000000
C -0.0310000000 -1.2400000000 -3.2070000000
H 0.0240000000 -2.3350000000 -3.2080000000
C 1.0720000000 -0.3410000000 -3.2630000000
H 2.1280000000 -0.6180000000 -3.3330000000
C 0.5660000000 0.9880000000 -3.2370000000
H 1.1640000000 1.9060000000 -3.2620000000

Structural Information and Single Crystal X-ray Experimental

Crystallographic Material for Complex **2**.

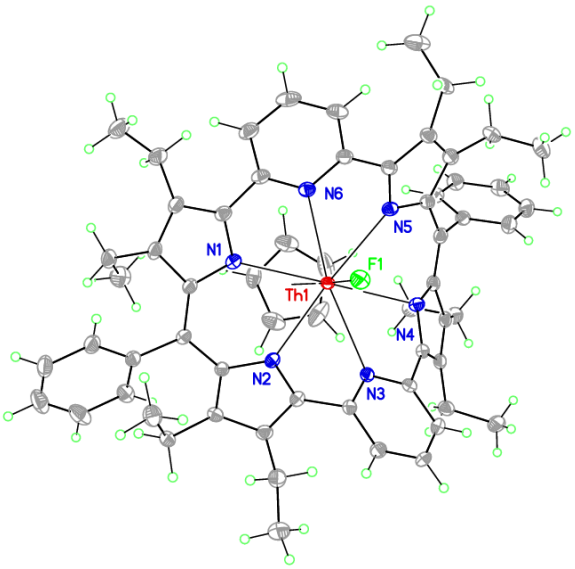

Figure S4. View of the Th ion complex in **2** showing the heteroatom labeling scheme. Displacement ellipsoids are scaled to the 50% probability level. CCDC no. 2288552.

X-ray experimental for $[(C_{56}H_{56}N_6)Th(C_5H_5)]^{1+}\ F^{1-}$ (**2**): Crystals grew as black prisms by slow evaporation from hexanes/THF (20:1). The data crystal was separated from a cluster of crystals and had approximate dimensions; 0.20 x 0.077 x 0.071 mm. The data were collected on an Agilent Technologies SuperNova Dual Source diffractometer using a μ-focus Cu Kα radiation source (λ = 1.5418 Å) with collimating mirror monochromators. A total of 1835 frames of data were collected using ω-scans with a scan range of 1° and a counting time of 3 seconds per frame for frames collected with a detector offset of +/- 41.6° and 10 seconds per frame with frames collected with a detector offset of 112.0°. The data was collected at 100 K using an Oxford Cryostream low temperature device. Data collection, unit cell refinement and data reduction were performed using Rigaku Oxford Diffraction's CrysAlisPro V 1.171.41.70a.[2] The structure was solved by direct methods using SHELXT 2 and refined by full-matrix least-squares on F2 with anisotropic

displacement parameters for the non-H atoms using SHELXL-2018/3.[4] Structure analysis was aided by use of the programs PLATON 4 and OLEX2.[5,6] The hydrogen atoms on the carbon atoms were calculated in ideal positions with isotropic displacement parameters set to 1.2xUeq of the attached atom (1.5xUeq for methyl hydrogen atoms).
The function, ∑w(|Fo|2 - |Fc|2)2, was minimized, where w = 1/[(σ (Fo))2 + (0.0529*P)2 + (9.5167*P)] and P = (|Fo|2 + 2|Fc|2)/3. Rw(F2) refined to 0.0828, with R(F) equal to 0.0307 and a goodness of fit, S, = 1.06. Definitions used for calculating R(F), Rw(F2) and the goodness of fit, S, are given below.[7] The data were checked for secondary extinction effects but no correction was necessary. Neutral atom scattering factors and values used to calculate the linear absorption coefficient are from the International Tables for X-ray Crystallography (1992).[8] All figures were generated using SHELXTL/PC.[9]

Crystallographic Material for Complex **4**.

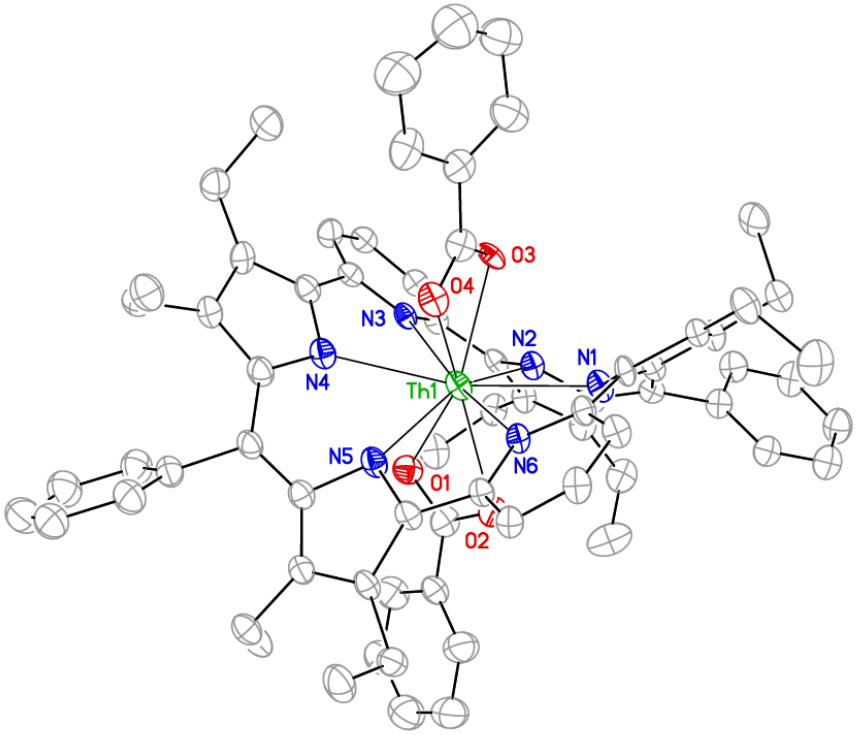

Figure S5. View of the Th complex in **4** showing the heteroatom labeling scheme. Displacement ellipsoids are scaled to the 30% probability level. CCDC no. 2288553

X-ray Experimental for $(C_{56}H_{56}N_6)Th(C_7H_5O_2)_2$ (**4**): Crystals grew as long, thin black needles by slow evaporation from THF. The data crystal was cut from a longer crystal and had approximate dimensions; 0.20 x 0.039 x 0.031 mm. The data were collected on an Agilent Technologies SuperNova Dual Source diffractometer using a μ-focus Cu Kα radiation source (λ = 1.5418 Å) with collimating mirror monochromators. A total of 964 frames of data were collected using ω-scans with a scan range of 1° and a counting time of 29.5 seconds per frame for frames collected with a detector offset of - 42.4° and 97.5 seconds per frame with frames collected with a detector offset of 106.6°. The data were collected at

100 K using an Oxford Cryostream low temperature device. Details of crystal data, data collection and structure refinement are listed in Table 1. Data collection, unit cell refinement and data reduction were performed using Rigaku Oxford Diffraction's CrysAlisPro V 1.171.40.53.[1] The structure was solved by direct methods using SHELXT[2] and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for the non-H atoms using SHELXL-2016/6.[3] Structure analysis was aided by use of the programs PLATON[4], OLEX2[5] and WinGX.[6] The hydrogen atoms on the carbon atoms were calculated in ideal positions with isotropic displacement parameters set to 1.2xUeq of the attached atom (1.5xUeq for methyl hydrogen atoms).

Two molecules of what appeared to be THF were disordered. The contributions to the scattering factors due to this solvent molecule were removed by use of the utility SQUEEZE[7] in PLATON. PLATON was used as incorporated in WinGX.

The function, $\Sigma w(|F_O|^2 - |F_C|^2)^2$, was minimized, where $w = 1/[(s(F_O))^2 + (0.0745*P)^2]$ and $P = (|F_O|^2 + 2|F_C|^2)/3$. $R_w(F^2)$ refined to 0.278, with R(F) equal to 0.1056 and a goodness of fit, S, = 1.06. Definitions used for calculating R(F), $R_w(F^2)$ and the goodness of fit, S, are given below.[8] The data were checked for secondary extinction effects but no correction was necessary. Neutral atom scattering factors and values used to calculate the linear absorption coefficient are from the International Tables for X-ray Crystallography (1992).[9] All figures were generated using SHELXTL/PC.[10]

Putative structure of complex **3**

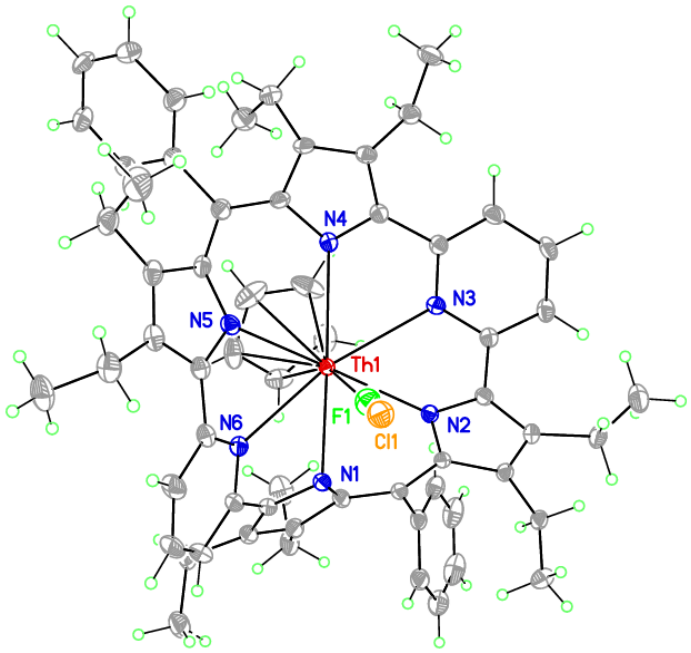

Figure S6. View of the Th ion complex in **3** showing the heteroatom labeling scheme. Displacement ellipsoids are scaled to the 50% probability level. There is a mix of the F ion and Cl ion salt in the data crystal. The site occupancy for Cl ion is approximately 6%. CCDC no. 2288552.

Crystal data and structure refinement for complex **2**.

Empirical formula	C61 H61 F N6 Th	
Formula weight	1129.19	
Temperature	100(2) K	
Wavelength	1.54184 Å	
Crystal system	monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 16.63492(9) Å	α= 90°.
	b = 11.85014(7) Å	β= 90.9154(5)°.
	c = 24.83906(14) Å	γ = 90°.
Volume	4895.80(5) $Å^3$	
Z	4	
Density (calculated)	1.532 Mg/m^3	
Absorption coefficient	10.218 mm^{-1}	
F(000)	2272	
Crystal size	0.200 x 0.077 x 0.071 mm^3	
Theta range for data collection	3.559 to 75.779°.	
Index ranges	-19<=h<=20, -14<=k<=12, -31<=l<=28	
Reflections collected	51244	
Independent reflections	10134 [R(int) = 0.0337]	
Completeness to theta = 67.684°	100.0 %	
Absorption correction	Gaussian and multi-scan	
Max. and min. transmission	1.00 and 0.421	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10134 / 0 / 630	
Goodness-of-fit on F^2	1.062	
Final R indices [I>2sigma(I)]	R1 = 0.0307, wR2 = 0.0819	
R indices (all data)	R1 = 0.0315, wR2 = 0.0828	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.579 and -0.952 $e.Å^{-3}$	

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)
For complex **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Th1	7596(1)	6222(1)	7674(1)	13(1)
F1	8597(2)	6809(2)	8217(1)	37(1)
N1	6528(2)	6240(2)	8517(1)	17(1)
N2	7594(2)	4396(2)	8360(1)	15(1)
N3	8711(2)	4543(2)	7592(1)	15(1)
N4	8595(2)	6145(2)	6774(1)	17(1)
N5	7879(2)	8172(2)	7124(1)	17(1)
N6	7053(2)	8214(2)	8038(1)	18(1)
C1	6100(2)	7185(3)	8524(1)	18(1)
C2	5268(2)	7010(3)	8626(1)	22(1)
C3	5189(2)	5864(3)	8709(1)	21(1)
C4	5993(2)	5392(3)	8666(1)	17(1)
C5	6278(2)	4323(3)	8809(1)	16(1)
C6	7079(2)	3959(3)	8744(1)	15(1)
C7	7504(2)	3156(3)	9080(1)	16(1)
C8	8290(2)	3136(3)	8901(1)	18(1)
C9	8305(2)	3861(3)	8445(1)	16(1)
C10	8914(2)	3928(3)	8032(1)	16(1)
C11	9632(2)	3302(3)	8048(1)	20(1)
C12	10116(2)	3264(3)	7602(1)	21(1)
C13	9877(2)	3832(3)	7144(2)	22(1)
C14	9179(2)	4470(3)	7156(1)	16(1)
C15	8891(2)	5118(3)	6693(1)	16(1)
C16	8865(2)	4780(3)	6141(1)	18(1)
C17	8534(2)	5675(3)	5863(1)	18(1)
C18	8401(2)	6562(3)	6262(1)	17(1)
C19	8216(2)	7687(3)	6185(1)	19(1)
C20	8112(2)	8474(3)	6611(1)	18(1)
C21	8270(2)	9664(3)	6590(1)	21(1)
C22	8160(2)	10074(3)	7101(1)	21(1)
C23	7879(2)	9148(3)	7412(1)	18(1)

C24	7452(2)	9176(3)	7914(1)	19(1)
C25	7372(2)	10152(3)	8231(2)	26(1)
C26	6824(2)	10156(3)	8644(2)	30(1)
C27	6359(2)	9216(3)	8734(1)	26(1)
C28	6509(2)	8250(3)	8429(1)	19(1)
C29	4615(2)	7892(3)	8574(2)	29(1)
C30	4302(3)	8371(4)	9104(2)	40(1)
C31	4383(2)	5286(3)	8753(2)	28(1)
C32	4132(2)	4706(4)	8230(2)	36(1)
C33	5718(2)	3529(3)	9080(1)	20(1)
C34	5497(2)	2529(3)	8829(2)	24(1)
C35	4990(2)	1765(4)	9082(2)	34(1)
C36	4708(2)	2019(4)	9589(2)	39(1)
C37	4919(2)	3013(4)	9842(2)	35(1)
C38	5423(2)	3775(3)	9590(2)	25(1)
C39	7254(2)	2540(3)	9582(1)	19(1)
C40	7385(2)	3240(3)	10092(1)	25(1)
C41	8969(2)	2516(3)	9182(1)	23(1)
C42	9104(3)	1309(3)	8996(2)	33(1)
C43	9081(2)	3643(3)	5914(2)	23(1)
C44	9878(3)	3615(3)	5613(2)	30(1)
C45	8270(2)	5604(3)	5279(1)	24(1)
C46	7368(2)	5373(3)	5226(2)	29(1)
C47	8115(2)	8114(3)	5620(1)	19(1)
C48	8766(2)	8257(3)	5279(1)	26(1)
C49	8648(2)	8653(3)	4757(2)	29(1)
C50	7889(3)	8868(3)	4565(2)	28(1)
C51	7233(2)	8714(3)	4895(2)	25(1)
C52	7346(2)	8367(3)	5426(1)	21(1)
C53	8550(2)	10389(3)	6132(2)	27(1)
C54	9465(3)	10448(4)	6090(2)	42(1)
C55	8299(2)	11288(3)	7261(2)	27(1)
C56	7547(3)	12027(3)	7193(2)	37(1)
C57	6109(2)	6491(3)	7089(2)	32(1)
C58	5955(2)	5577(3)	7422(1)	27(1)
C59	6433(2)	4665(3)	7258(2)	32(1)

C60	6865(2)	5036(4)	6809(2)	37(1)
C61	6657(3)	6151(4)	6708(2)	40(1)

Bond lengths [Å] and angles [°] for complex **2**.

Th1-F1	2.235(3)	C7-C8	1.389(4)
Th1-N6	2.690(3)	C7-C39	1.509(4)
Th1-N3	2.728(3)	C8-C9	1.421(4)
Th1-N5	2.731(3)	C8-C41	1.510(4)
Th1-N2	2.752(3)	C9-C10	1.456(4)
Th1-N1	2.767(3)	C10-C11	1.406(4)
Th1-N4	2.809(3)	C11-C12	1.380(5)
Th1-C60	2.826(4)	C11-H11	0.95
Th1-C61	2.845(4)	C12-C13	1.376(5)
Th1-C59	2.856(4)	C12-H12	0.95
Th1-C57	2.868(4)	C13-C14	1.387(5)
Th1-C58	2.895(3)	C13-H13	0.95
N1-C1	1.328(4)	C14-C15	1.456(4)
N1-C4	1.397(4)	C15-C16	1.429(4)
N2-C9	1.355(4)	C16-C17	1.375(5)
N2-C6	1.393(4)	C16-C43	1.507(4)
N3-C14	1.348(4)	C17-C18	1.464(4)
N3-C10	1.351(4)	C17-C45	1.512(4)
N4-C15	1.329(4)	C18-C19	1.381(5)
N4-C18	1.397(4)	C19-C20	1.422(5)
N5-C23	1.360(4)	C19-C47	1.498(4)
N5-C20	1.384(4)	C20-C21	1.436(5)
N6-C28	1.339(4)	C21-C22	1.374(5)
N6-C24	1.356(4)	C21-C53	1.506(5)
C1-C2	1.428(5)	C22-C23	1.426(5)
C1-C28	1.454(5)	C22-C55	1.510(4)
C2-C3	1.379(5)	C23-C24	1.445(5)
C2-C29	1.511(5)	C24-C25	1.407(5)
C3-C4	1.455(4)	C25-C26	1.382(5)
C3-C31	1.511(5)	C25-H25	0.95
C4-C5	1.397(4)	C26-C27	1.377(6)
C5-C6	1.413(4)	C26-H26	0.95
C5-C33	1.492(4)	C27-C28	1.396(5)
C6-C7	1.442(4)	C27-H27	0.95

C29-C30	1.534(6)	C43-H43A	0.99
C29-H29A	0.99	C43-H43B	0.99
C29-H29B	0.99	C44-H44A	0.98
C30-H30A	0.98	C44-H44B	0.98
C30-H30B	0.98	C44-H44C	0.98
C30-H30C	0.98	C45-C46	1.528(5)
C31-C32	1.522(6)	C45-H45A	0.99
C31-H31A	0.99	C45-H45B	0.99
C31-H31B	0.99	C46-H46A	0.98
C32-H32A	0.98	C46-H46B	0.98
C32-H32B	0.98	C46-H46C	0.98
C32-H32C	0.98	C47-C52	1.392(5)
C33-C34	1.386(5)	C47-C48	1.397(5)
C33-C38	1.398(5)	C48-C49	1.389(5)
C34-C35	1.393(5)	C48-H48	0.95
C34-H34	0.95	C49-C50	1.367(6)
C35-C36	1.384(7)	C49-H49	0.95
C35-H35	0.95	C50-C51	1.388(6)
C36-C37	1.378(7)	C50-H50	0.95
C36-H36	0.95	C51-C52	1.391(5)
C37-C38	1.387(5)	C51-H51	0.95
C37-H37	0.95	C52-H52	0.95
C38-H38	0.95	C53-C54	1.529(5)
C39-C40	1.528(5)	C53-H53A	0.99
C39-H39A	0.99	C53-H53B	0.99
C39-H39B	0.99	C54-H54A	0.98
C40-H40A	0.98	C54-H54B	0.98
C40-H40B	0.98	C54-H54C	0.98
C40-H40C	0.98	C55-C56	1.533(5)
C41-C42	1.521(5)	C55-H55A	0.99
C41-H41A	0.99	C55-H55B	0.99
C41-H41B	0.99	C56-H56A	0.98
C42-H42A	0.98	C56-H56B	0.98
C42-H42B	0.98	C56-H56C	0.98
C42-H42C	0.98	C57-C61	1.385(7)
C43-C44	1.531(5)	C57-C58	1.388(6)

C57-H57	0.95	C59-H59	0.95
C58-C59	1.406(6)	C60-C61	1.387(7)
C58-H58	0.95	C60-H60	0.95
C59-C60	1.406(6)	C61-H61	0.95

F1-Th1-N6	77.03(8)	N5-Th1-C61	72.46(10)
F1-Th1-N3	76.81(8)	N2-Th1-C61	119.50(10)
N6-Th1-N3	153.82(8)	N1-Th1-C61	106.74(11)
F1-Th1-N5	84.61(8)	N4-Th1-C61	69.58(11)
N6-Th1-N5	59.11(8)	C60-Th1-C61	28.32(14)
N3-Th1-N5	117.18(8)	F1-Th1-C59	155.95(10)
F1-Th1-N2	83.13(8)	N6-Th1-C59	117.34(10)
N6-Th1-N2	118.60(8)	N3-Th1-C59	87.66(10)
N3-Th1-N2	58.74(8)	N5-Th1-C59	119.09(10)
N5-Th1-N2	167.70(8)	N2-Th1-C59	73.08(10)
F1-Th1-N1	91.29(9)	N1-Th1-C59	80.78(11)
N6-Th1-N1	61.05(8)	N4-Th1-C59	95.53(11)
N3-Th1-N1	120.48(8)	C60-Th1-C59	28.65(13)
N5-Th1-N1	119.37(8)	C61-Th1-C59	46.77(12)
N2-Th1-N1	62.03(8)	F1-Th1-C57	154.03(10)
F1-Th1-N4	92.62(8)	N6-Th1-C57	77.33(10)
N6-Th1-N4	120.14(8)	N3-Th1-C57	128.67(10)
N3-Th1-N4	60.37(8)	N5-Th1-C57	78.81(10)
N5-Th1-N4	61.29(8)	N2-Th1-C57	113.02(10)
N2-Th1-N4	118.26(7)	N1-Th1-C57	79.83(11)
N1-Th1-N4	176.08(8)	N4-Th1-C57	96.69(11)
F1-Th1-C60	156.94(10)	C60-Th1-C57	46.56(12)
N6-Th1-C60	123.28(11)	C61-Th1-C57	28.05(14)
N3-Th1-C60	82.26(10)	C59-Th1-C57	46.67(11)
N5-Th1-C60	96.60(12)	F1-Th1-C58	154.62(9)
N2-Th1-C60	94.29(12)	N6-Th1-C58	89.05(10)
N1-Th1-C60	107.79(10)	N3-Th1-C58	115.54(10)
N4-Th1-C60	68.36(10)	N5-Th1-C58	106.50(10)
F1-Th1-C61	155.70(10)	N2-Th1-C58	85.19(10)
N6-Th1-C61	97.24(12)	N1-Th1-C58	63.34(9)
N3-Th1-C61	106.26(12)	N4-Th1-C58	112.75(9)

C60-Th1-C58	46.45(10)	C6-C5-C33	117.1(3)
C61-Th1-C58	46.02(11)	N2-C6-C5	123.8(3)
C59-Th1-C58	28.31(11)	N2-C6-C7	110.0(3)
C57-Th1-C58	27.87(12)	C5-C6-C7	126.1(3)
C1-N1-C4	105.0(3)	C8-C7-C6	106.2(3)
C1-N1-Th1	111.5(2)	C8-C7-C39	122.0(3)
C4-N1-Th1	127.9(2)	C6-C7-C39	131.2(3)
C9-N2-C6	105.2(3)	C7-C8-C9	105.9(3)
C9-N2-Th1	117.1(2)	C7-C8-C41	124.1(3)
C6-N2-Th1	136.34(19)	C9-C8-C41	129.8(3)
C14-N3-C10	118.4(3)	N2-C9-C8	112.4(3)
C14-N3-Th1	120.6(2)	N2-C9-C10	118.6(3)
C10-N3-Th1	119.6(2)	C8-C9-C10	128.0(3)
C15-N4-C18	105.5(3)	N3-C10-C11	120.6(3)
C15-N4-Th1	112.0(2)	N3-C10-C9	115.5(3)
C18-N4-Th1	125.6(2)	C11-C10-C9	123.5(3)
C23-N5-C20	105.5(3)	C12-C11-C10	120.1(3)
C23-N5-Th1	117.0(2)	C12-C11-H11	120.0
C20-N5-Th1	137.1(2)	C10-C11-H11	120.0
C28-N6-C24	118.5(3)	C13-C12-C11	118.9(3)
C28-N6-Th1	120.4(2)	C13-C12-H12	120.5
C24-N6-Th1	119.5(2)	C11-C12-H12	120.5
N1-C1-C2	113.7(3)	C12-C13-C14	118.7(3)
N1-C1-C28	118.5(3)	C12-C13-H13	120.7
C2-C1-C28	127.8(3)	C14-C13-H13	120.7
C3-C2-C1	105.3(3)	N3-C14-C13	123.2(3)
C3-C2-C29	128.6(3)	N3-C14-C15	114.4(3)
C1-C2-C29	125.6(3)	C13-C14-C15	122.4(3)
C2-C3-C4	106.1(3)	N4-C15-C16	113.3(3)
C2-C3-C31	122.9(3)	N4-C15-C14	118.8(3)
C4-C3-C31	130.4(3)	C16-C15-C14	127.9(3)
C5-C4-N1	120.2(3)	C17-C16-C15	105.8(3)
C5-C4-C3	129.7(3)	C17-C16-C43	126.7(3)
N1-C4-C3	109.5(3)	C15-C16-C43	127.3(3)
C4-C5-C6	124.4(3)	C16-C17-C18	106.1(3)
C4-C5-C33	118.4(3)	C16-C17-C45	123.1(3)

C18-C17-C45	130.2(3)	C30-C29-H29A	108.3
C19-C18-N4	121.1(3)	C2-C29-H29B	108.3
C19-C18-C17	129.4(3)	C30-C29-H29B	108.3
N4-C18-C17	109.1(3)	H29A-C29-H29B	107.4
C18-C19-C20	124.0(3)	C29-C30-H30A	109.5
C18-C19-C47	118.5(3)	C29-C30-H30B	109.5
C20-C19-C47	117.5(3)	H30A-C30-H30B	109.5
N5-C20-C19	123.7(3)	C29-C30-H30C	109.5
N5-C20-C21	110.0(3)	H30A-C30-H30C	109.5
C19-C20-C21	126.3(3)	H30B-C30-H30C	109.5
C22-C21-C20	106.7(3)	C3-C31-C32	112.0(3)
C22-C21-C53	122.9(3)	C3-C31-H31A	109.2
C20-C21-C53	130.4(3)	C32-C31-H31A	109.2
C21-C22-C23	106.1(3)	C3-C31-H31B	109.2
C21-C22-C55	124.0(3)	C32-C31-H31B	109.2
C23-C22-C55	129.8(3)	H31A-C31-H31B	107.9
N5-C23-C22	111.5(3)	C31-C32-H32A	109.5
N5-C23-C24	118.6(3)	C31-C32-H32B	109.5
C22-C23-C24	128.3(3)	H32A-C32-H32B	109.5
N6-C24-C25	120.8(3)	C31-C32-H32C	109.5
N6-C24-C23	115.2(3)	H32A-C32-H32C	109.5
C25-C24-C23	123.7(3)	H32B-C32-H32C	109.5
C26-C25-C24	119.2(3)	C34-C33-C38	119.4(3)
C26-C25-H25	120.4	C34-C33-C5	120.0(3)
C24-C25-H25	120.4	C38-C33-C5	120.6(3)
C27-C26-C25	119.7(3)	C33-C34-C35	120.7(4)
C27-C26-H26	120.1	C33-C34-H34	119.6
C25-C26-H26	120.1	C35-C34-H34	119.6
C26-C27-C28	118.0(3)	C36-C35-C34	119.0(4)
C26-C27-H27	121.0	C36-C35-H35	120.5
C28-C27-H27	121.0	C34-C35-H35	120.5
N6-C28-C27	123.2(3)	C37-C36-C35	120.9(4)
N6-C28-C1	114.4(3)	C37-C36-H36	119.6
C27-C28-C1	122.4(3)	C35-C36-H36	119.6
C2-C29-C30	115.9(3)	C36-C37-C38	120.2(4)
C2-C29-H29A	108.3	C36-C37-H37	119.9

C38-C37-H37	119.9	H44A-C44-H44B	109.5
C37-C38-C33	119.7(4)	C43-C44-H44C	109.5
C37-C38-H38	120.1	H44A-C44-H44C	109.5
C33-C38-H38	120.1	H44B-C44-H44C	109.5
C7-C39-C40	112.6(3)	C17-C45-C46	111.2(3)
C7-C39-H39A	109.1	C17-C45-H45A	109.4
C40-C39-H39A	109.1	C46-C45-H45A	109.4
C7-C39-H39B	109.1	C17-C45-H45B	109.4
C40-C39-H39B	109.1	C46-C45-H45B	109.4
H39A-C39-H39B	107.8	H45A-C45-H45B	108.0
C39-C40-H40A	109.5	C45-C46-H46A	109.5
C39-C40-H40B	109.5	C45-C46-H46B	109.5
H40A-C40-H40B	109.5	H46A-C46-H46B	109.5
C39-C40-H40C	109.5	C45-C46-H46C	109.5
H40A-C40-H40C	109.5	H46A-C46-H46C	109.5
H40B-C40-H40C	109.5	H46B-C46-H46C	109.5
C8-C41-C42	115.5(3)	C52-C47-C48	118.8(3)
C8-C41-H41A	108.4	C52-C47-C19	119.1(3)
C42-C41-H41A	108.4	C48-C47-C19	122.2(3)
C8-C41-H41B	108.4	C49-C48-C47	120.5(3)
C42-C41-H41B	108.4	C49-C48-H48	119.8
H41A-C41-H41B	107.5	C47-C48-H48	119.8
C41-C42-H42A	109.5	C50-C49-C48	120.3(4)
C41-C42-H42B	109.5	C50-C49-H49	119.8
H42A-C42-H42B	109.5	C48-C49-H49	119.8
C41-C42-H42C	109.5	C49-C50-C51	120.0(3)
H42A-C42-H42C	109.5	C49-C50-H50	120.0
H42B-C42-H42C	109.5	C51-C50-H50	120.0
C16-C43-C44	114.5(3)	C50-C51-C52	120.1(3)
C16-C43-H43A	108.6	C50-C51-H51	119.9
C44-C43-H43A	108.6	C52-C51-H51	119.9
C16-C43-H43B	108.6	C51-C52-C47	120.1(3)
C44-C43-H43B	108.6	C51-C52-H52	119.9
H43A-C43-H43B	107.6	C47-C52-H52	119.9
C43-C44-H44A	109.5	C21-C53-C54	113.4(3)
C43-C44-H44B	109.5	C21-C53-H53A	108.9

C54-C53-H53A	108.9	C58-C57-H57	126.0
C21-C53-H53B	108.9	Th1-C57-H57	114.1
C54-C53-H53B	108.9	C57-C58-C59	108.4(3)
H53A-C53-H53B	107.7	C57-C58-Th1	75.0(2)
C53-C54-H54A	109.5	C59-C58-Th1	74.3(2)
C53-C54-H54B	109.5	C57-C58-H58	125.8
H54A-C54-H54B	109.5	C59-C58-H58	125.8
C53-C54-H54C	109.5	Th1-C58-H58	116.9
H54A-C54-H54C	109.5	C60-C59-C58	106.7(4)
H54B-C54-H54C	109.5	C60-C59-Th1	74.5(2)
C22-C55-C56	113.2(3)	C58-C59-Th1	77.4(2)
C22-C55-H55A	108.9	C60-C59-H59	126.6
C56-C55-H55A	108.9	C58-C59-H59	126.6
C22-C55-H55B	108.9	Th1-C59-H59	114.0
C56-C55-H55B	108.9	C61-C60-C59	108.2(4)
H55A-C55-H55B	107.7	C61-C60-Th1	76.6(2)
C55-C56-H56A	109.5	C59-C60-Th1	76.8(2)
C55-C56-H56B	109.5	C61-C60-H60	125.9
H56A-C56-H56B	109.5	C59-C60-H60	125.9
C55-C56-H56C	109.5	Th1-C60-H60	113.1
H56A-C56-H56C	109.5	C57-C61-C60	108.6(4)
H56B-C56-H56C	109.5	C57-C61-Th1	76.9(2)
C61-C57-C58	108.1(4)	C60-C61-Th1	75.1(2)
C61-C57-Th1	75.1(2)	C57-C61-H61	125.7
C58-C57-Th1	77.1(2)	C60-C61-H61	125.7
C61-C57-H57	126.0	Th1-C61-H61	114.5

Anisotropic displacement parameters ($Å^2 x\ 10^3$) for complex **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Th1	15(1)	11(1)	14(1)	0(1)	1(1)	1(1)
F1	41(1)	26(1)	43(1)	8(1)	16(1)	6(1)
N1	16(1)	17(2)	16(1)	-1(1)	0(1)	2(1)
N2	12(1)	17(1)	15(1)	-1(1)	-2(1)	1(1)
N3	15(1)	14(1)	16(1)	-1(1)	2(1)	-1(1)
N4	18(1)	16(1)	17(1)	0(1)	0(1)	3(1)
N5	18(1)	15(1)	18(1)	-3(1)	-1(1)	1(1)
N6	19(1)	17(1)	17(1)	1(1)	-1(1)	2(1)
C1	22(2)	19(2)	15(1)	-1(1)	1(1)	5(1)
C2	20(2)	26(2)	19(2)	3(1)	4(1)	6(1)
C3	15(1)	28(2)	20(2)	5(1)	3(1)	5(1)
C4	14(1)	19(2)	19(1)	1(1)	2(1)	3(1)
C5	15(1)	18(2)	14(1)	-1(1)	0(1)	3(1)
C6	17(1)	14(1)	13(1)	0(1)	2(1)	1(1)
C7	19(1)	14(1)	15(1)	1(1)	0(1)	0(1)
C8	18(1)	17(1)	18(1)	2(1)	-1(1)	3(1)
C9	15(2)	17(2)	16(2)	-1(1)	1(1)	1(1)
C10	14(1)	15(1)	19(2)	1(1)	1(1)	-1(1)
C11	15(1)	21(2)	25(2)	4(1)	-2(1)	2(1)
C12	14(1)	20(2)	30(2)	2(1)	3(1)	5(1)
C13	19(2)	22(2)	25(2)	1(1)	7(1)	2(1)
C14	18(1)	12(1)	19(1)	1(1)	1(1)	-1(1)
C15	15(1)	15(1)	19(2)	1(1)	2(1)	0(1)
C16	17(1)	18(2)	18(1)	0(1)	4(1)	-2(1)
C17	19(1)	21(2)	14(1)	0(1)	5(1)	-1(1)
C18	18(1)	20(2)	14(1)	2(1)	3(1)	-1(1)
C19	14(1)	22(2)	21(2)	2(1)	1(1)	1(1)
C20	16(1)	17(2)	21(2)	5(1)	0(1)	2(1)
C21	16(1)	21(2)	26(2)	4(1)	-2(1)	1(1)
C22	17(1)	16(2)	29(2)	1(1)	-3(1)	-1(1)
C23	18(1)	15(2)	22(2)	0(1)	-1(1)	0(1)

C24	19(1)	15(2)	23(2)	-1(1)	-1(1)	1(1)
C25	33(2)	15(2)	30(2)	-7(1)	-1(2)	-1(1)
C26	43(2)	20(2)	27(2)	-11(1)	-1(2)	8(2)
C27	30(2)	24(2)	22(2)	-6(1)	5(1)	7(1)
C28	24(2)	18(2)	16(1)	-2(1)	-1(1)	5(1)
C29	25(2)	29(2)	32(2)	8(2)	4(1)	11(2)
C30	38(2)	41(2)	42(2)	9(2)	12(2)	21(2)
C31	14(2)	33(2)	37(2)	12(2)	4(1)	4(1)
C32	20(2)	35(2)	54(3)	0(2)	-5(2)	-5(2)
C33	15(1)	22(2)	23(2)	5(1)	1(1)	3(1)
C34	20(2)	26(2)	27(2)	5(1)	-3(1)	-2(1)
C35	29(2)	29(2)	45(2)	14(2)	-10(2)	-9(2)
C36	21(2)	46(2)	50(2)	26(2)	1(2)	-6(2)
C37	23(2)	46(2)	36(2)	19(2)	12(2)	9(2)
C38	20(2)	30(2)	26(2)	7(1)	5(1)	6(1)
C39	20(1)	18(2)	18(2)	5(1)	2(1)	2(1)
C40	28(2)	29(2)	19(2)	2(1)	1(1)	-2(1)
C41	18(2)	29(2)	23(2)	9(1)	-1(1)	4(1)
C42	29(2)	29(2)	43(2)	8(2)	1(2)	8(1)
C43	29(2)	17(2)	23(2)	-2(1)	6(1)	0(1)
C44	36(2)	24(2)	31(2)	-3(2)	14(2)	6(2)
C45	28(2)	26(2)	18(2)	-1(1)	2(1)	2(1)
C46	31(2)	34(2)	24(2)	-7(2)	-5(1)	2(2)
C47	22(2)	19(2)	18(2)	3(1)	2(1)	2(1)
C48	21(2)	32(2)	25(2)	7(1)	2(1)	2(1)
C49	30(2)	32(2)	25(2)	5(1)	9(2)	2(1)
C50	42(2)	26(2)	15(2)	6(1)	1(2)	3(1)
C51	25(2)	27(2)	23(2)	7(1)	-4(1)	1(1)
C52	20(2)	21(2)	21(2)	1(1)	3(1)	2(1)
C53	31(2)	18(2)	33(2)	8(1)	4(2)	0(1)
C54	38(2)	30(2)	57(3)	15(2)	15(2)	-5(2)
C55	30(2)	15(2)	35(2)	0(1)	-3(2)	-6(1)
C56	42(2)	18(2)	51(2)	-2(2)	-9(2)	3(2)
C57	28(2)	24(2)	45(2)	3(2)	-17(2)	1(2)
C58	18(2)	42(2)	21(2)	-6(2)	1(1)	-8(2)
C59	34(2)	22(2)	41(2)	-1(2)	-16(2)	-7(2)

C60	18(2)	55(3)	37(2)	-28(2)	-2(1)	0(2)
C61	33(2)	61(3)	25(2)	12(2)	-5(2)	-20(2)

Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for complex **2**.

	x	y	z	U(eq)
H11	9784	2906	8366	24
H12	10606	2851	7612	25
H13	10185	3788	6825	26
H25	7689	10801	8162	31
H26	6769	10805	8865	36
H27	5948	9224	8995	31
H29A	4156	7558	8372	34
H29B	4823	8525	8357	34
H30A	3890	8942	9027	60
H30B	4747	8718	9308	60
H30C	4069	7761	9318	60
H31A	3971	5851	8849	34
H31B	4412	4719	9046	34
H32A	4110	5262	7939	55
H32B	3601	4362	8272	55
H32C	4525	4119	8144	55
H34	5693	2362	8481	29
H35	4840	1080	8909	41
H36	4365	1501	9765	47
H37	4719	3177	10189	42
H38	5566	4462	9765	30
H39A	7566	1830	9614	23
H39B	6678	2337	9549	23
H40A	7045	3915	10075	38
H40B	7951	3466	10121	38
H40C	7243	2789	10408	38
H41A	8862	2506	9573	28
H41B	9472	2947	9130	28
H42A	9199	1303	8608	50
H42B	8627	855	9074	50
H42C	9571	992	9188	50

H43A	8645	3397	5665	28
H43B	9111	3091	6213	28
H44A	9867	4185	5327	45
H44B	9953	2866	5454	45
H44C	10322	3776	5865	45
H45A	8570	4992	5099	29
H45B	8398	6322	5096	29
H46A	7212	5348	4844	44
H46B	7070	5975	5405	44
H46C	7244	4647	5394	44
H48	9294	8083	5405	31
H49	9097	8774	4533	34
H50	7811	9124	4206	33
H51	6705	8845	4758	30
H52	6898	8304	5657	25
H53A	8338	11163	6179	33
H53B	8324	10088	5790	33
H54A	9609	10936	5788	62
H54B	9680	9689	6031	62
H54C	9694	10756	6425	62
H55A	8734	11605	7040	32
H55B	8481	11313	7642	32
H56A	7356	11993	6819	56
H56B	7680	12808	7288	56
H56C	7125	11750	7431	56
H57	5879	7221	7118	39
H58	5589	5570	7711	33
H59	6459	3939	7419	39
H60	7236	4600	6610	44
H61	6857	6605	6425	48

Torsion angles [°] for complex **2**.

C4-N1-C1-C2	-5.3(4)
Th1-N1-C1-C2	136.9(2)
C4-N1-C1-C28	174.9(3)
Th1-N1-C1-C28	-42.9(3)
N1-C1-C2-C3	2.6(4)
C28-C1-C2-C3	-177.6(3)
N1-C1-C2-C29	-170.2(3)
C28-C1-C2-C29	9.6(6)
C1-C2-C3-C4	1.3(4)
C29-C2-C3-C4	173.7(3)
C1-C2-C3-C31	-171.1(3)
C29-C2-C3-C31	1.3(6)
C1-N1-C4-C5	-166.7(3)
Th1-N1-C4-C5	59.7(4)
C1-N1-C4-C3	5.9(4)
Th1-N1-C4-C3	-127.8(3)
C2-C3-C4-C5	167.1(3)
C31-C3-C4-C5	-21.3(6)
C2-C3-C4-N1	-4.5(4)
C31-C3-C4-N1	167.1(3)
N1-C4-C5-C6	-9.5(5)
C3-C4-C5-C6	179.6(3)
N1-C4-C5-C33	166.6(3)
C3-C4-C5-C33	-4.3(5)
C9-N2-C6-C5	177.5(3)
Th1-N2-C6-C5	12.1(5)
C9-N2-C6-C7	1.6(3)
Th1-N2-C6-C7	-163.8(2)
C4-C5-C6-N2	-26.0(5)
C33-C5-C6-N2	157.9(3)
C4-C5-C6-C7	149.3(3)
C33-C5-C6-C7	-26.8(5)
N2-C6-C7-C8	1.4(4)
C5-C6-C7-C8	-174.4(3)
N2-C6-C7-C39	173.1(3)

C5-C6-C7-C39	-2.7(6)
C6-C7-C8-C9	-3.7(3)
C39-C7-C8-C9	-176.3(3)
C6-C7-C8-C41	172.2(3)
C39-C7-C8-C41	-0.4(5)
C6-N2-C9-C8	-4.1(4)
Th1-N2-C9-C8	164.7(2)
C6-N2-C9-C10	165.5(3)
Th1-N2-C9-C10	-25.7(4)
C7-C8-C9-N2	5.0(4)
C41-C8-C9-N2	-170.6(3)
C7-C8-C9-C10	-163.4(3)
C41-C8-C9-C10	21.0(6)
C14-N3-C10-C11	5.2(4)
Th1-N3-C10-C11	-161.2(2)
C14-N3-C10-C9	-167.9(3)
Th1-N3-C10-C9	25.6(4)
N2-C9-C10-N3	0.7(4)
C8-C9-C10-N3	168.4(3)
N2-C9-C10-C11	-172.3(3)
C8-C9-C10-C11	-4.5(5)
N3-C10-C11-C12	-3.4(5)
C9-C10-C11-C12	169.1(3)
C10-C11-C12-C13	-0.9(5)
C11-C12-C13-C14	3.2(5)
C10-N3-C14-C13	-2.9(5)
Th1-N3-C14-C13	163.5(2)
C10-N3-C14-C15	177.1(3)
Th1-N3-C14-C15	-16.6(3)
C12-C13-C14-N3	-1.4(5)
C12-C13-C14-C15	178.6(3)
C18-N4-C15-C16	-3.5(4)
Th1-N4-C15-C16	136.3(2)
C18-N4-C15-C14	177.8(3)
Th1-N4-C15-C14	-42.4(3)
N3-C14-C15-N4	41.2(4)

C13-C14-C15-N4	-138.8(3)
N3-C14-C15-C16	-137.2(3)
C13-C14-C15-C16	42.8(5)
N4-C15-C16-C17	0.6(4)
C14-C15-C16-C17	179.1(3)
N4-C15-C16-C43	-174.3(3)
C14-C15-C16-C43	4.2(5)
C15-C16-C17-C18	2.5(3)
C43-C16-C17-C18	177.4(3)
C15-C16-C17-C45	-169.6(3)
C43-C16-C17-C45	5.3(5)
C15-N4-C18-C19	-168.0(3)
Th1-N4-C18-C19	59.4(4)
C15-N4-C18-C17	5.0(4)
Th1-N4-C18-C17	-127.6(2)
C16-C17-C18-C19	167.5(3)
C45-C17-C18-C19	-21.2(6)
C16-C17-C18-N4	-4.8(4)
C45-C17-C18-N4	166.6(3)
N4-C18-C19-C20	-7.7(5)
C17-C18-C19-C20	-179.1(3)
N4-C18-C19-C47	172.4(3)
C17-C18-C19-C47	1.0(5)
C23-N5-C20-C19	177.7(3)
Th1-N5-C20-C19	5.3(5)
C23-N5-C20-C21	0.9(3)
Th1-N5-C20-C21	-171.6(2)
C18-C19-C20-N5	-25.8(5)
C47-C19-C20-N5	154.1(3)
C18-C19-C20-C21	150.5(3)
C47-C19-C20-C21	-29.6(5)
N5-C20-C21-C22	2.2(4)
C19-C20-C21-C22	-174.5(3)
N5-C20-C21-C53	178.8(3)
C19-C20-C21-C53	2.1(6)
C20-C21-C22-C23	-4.2(4)

C53-C21-C22-C23	178.8(3)
C20-C21-C22-C55	177.4(3)
C53-C21-C22-C55	0.5(5)
C20-N5-C23-C22	-3.7(4)
Th1-N5-C23-C22	170.6(2)
C20-N5-C23-C24	162.8(3)
Th1-N5-C23-C24	-22.9(4)
C21-C22-C23-N5	5.1(4)
C55-C22-C23-N5	-176.7(3)
C21-C22-C23-C24	-159.8(3)
C55-C22-C23-C24	18.4(6)
C28-N6-C24-C25	7.6(5)
Th1-N6-C24-C25	-158.0(3)
C28-N6-C24-C23	-165.8(3)
Th1-N6-C24-C23	28.5(4)
N5-C23-C24-N6	-2.9(5)
C22-C23-C24-N6	161.0(3)
N5-C23-C24-C25	-176.2(3)
C22-C23-C24-C25	-12.2(6)
N6-C24-C25-C26	-5.7(5)
C23-C24-C25-C26	167.2(3)
C24-C25-C26-C27	-1.0(6)
C25-C26-C27-C28	5.4(6)
C24-N6-C28-C27	-3.0(5)
Th1-N6-C28-C27	162.5(3)
C24-N6-C28-C1	178.6(3)
Th1-N6-C28-C1	-15.8(4)
C26-C27-C28-N6	-3.5(5)
C26-C27-C28-C1	174.7(3)
N1-C1-C28-N6	41.3(4)
C2-C1-C28-N6	-138.5(3)
N1-C1-C28-C27	-137.1(3)
C2-C1-C28-C27	43.1(5)
C3-C2-C29-C30	84.1(5)
C1-C2-C29-C30	-104.9(4)
C2-C3-C31-C32	100.2(4)

C4-C3-C31-C32	-70.2(5)
C4-C5-C33-C34	116.2(4)
C6-C5-C33-C34	-67.4(4)
C4-C5-C33-C38	-64.8(4)
C6-C5-C33-C38	111.6(4)
C38-C33-C34-C35	-0.5(5)
C5-C33-C34-C35	178.5(3)
C33-C34-C35-C36	0.0(5)
C34-C35-C36-C37	0.4(6)
C35-C36-C37-C38	-0.3(6)
C36-C37-C38-C33	-0.2(6)
C34-C33-C38-C37	0.6(5)
C5-C33-C38-C37	-178.4(3)
C8-C7-C39-C40	86.3(4)
C6-C7-C39-C40	-84.3(4)
C7-C8-C41-C42	91.2(4)
C9-C8-C41-C42	-93.9(4)
C17-C16-C43-C44	79.4(5)
C15-C16-C43-C44	-106.8(4)
C16-C17-C45-C46	96.8(4)
C18-C17-C45-C46	-73.3(5)
C18-C19-C47-C52	107.2(4)
C20-C19-C47-C52	-72.7(4)
C18-C19-C47-C48	-72.3(4)
C20-C19-C47-C48	107.8(4)
C52-C47-C48-C49	0.4(6)
C19-C47-C48-C49	179.9(3)
C47-C48-C49-C50	-2.3(6)
C48-C49-C50-C51	1.3(6)
C49-C50-C51-C52	1.7(6)
C50-C51-C52-C47	-3.6(5)
C48-C47-C52-C51	2.5(5)
C19-C47-C52-C51	-177.0(3)
C22-C21-C53-C54	88.4(4)
C20-C21-C53-C54	-87.8(5)
C21-C22-C55-C56	90.1(5)

C23-C22-C55-C56	-87.9(5)	
C61-C57-C58-C59	2.0(4)	
Th1-C57-C58-C59	-67.4(3)	
C61-C57-C58-Th1	69.3(3)	
C57-C58-C59-C60	-1.5(4)	
Th1-C58-C59-C60	-69.3(3)	
C57-C58-C59-Th1	67.8(3)	
C58-C59-C60-C61	0.5(4)	
Th1-C59-C60-C61	-70.9(3)	
C58-C59-C60-Th1	71.3(3)	
C58-C57-C61-C60	-1.7(5)	
Th1-C57-C61-C60	69.1(3)	
C58-C57-C61-Th1	-70.8(3)	
C59-C60-C61-C57	0.7(5)	
Th1-C60-C61-C57	-70.3(3)	
C59-C60-C61-Th1		71.0(3)

Crystal data and structure refinement for complex **4**.

Identification code	shelx	
Empirical formula	C70 H66 N6 O4 Th	
Formula weight	1287.32	
Temperature	100(2) K	
Wavelength	1.54184 Å	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 14.3363(14) Å	α= 92.393(6)°.
	b = 14.7285(10) Å	β= 90.934(7)°.
	c = 17.9046(13) Å	γ = 117.483(9)°.
Volume	3348.3(5) $Å^3$	
Z	2	
Density (calculated)	1.277 Mg/m^3	
Absorption coefficient	7.561 mm^{-1}	
F(000)	1300	
Crystal size	0.200 x 0.039 x 0.031 mm^3	
Theta range for data collection	3.388 to 68.408°.	
Index ranges	-17<=h<=11, -15<=k<=17, -20<=l<=21	
Reflections collected	18270	
Independent reflections	11816 [R(int) = 0.1482]	
Completeness to theta = 67.684°	96.5 %	
Absorption correction	Gaussian and multi-scan	
Max. and min. transmission	1.00 and 0.441	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11816 / 1323 / 738	
Goodness-of-fit on F^2	1.057	
Final R indices [I>2sigma(I)]	R1 = 0.1053, wR2 = 0.2406	
R indices (all data)	R1 = 0.1438, wR2 = 0.2783	
Extinction coefficient	n/a	
Largest diff. peak and hole	4.637 and -3.328 $e.Å^{-3}$	

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

	x	y	z	U(eq)
Th1	4276(1)	5384(1)	2492(1)	39(1)
O1	3615(10)	6620(9)	2114(8)	52(3)
O2	2649(8)	5461(9)	2868(7)	44(2)
O3	5174(9)	4423(8)	1965(6)	40(2)
O4	5757(9)	5189(8)	3067(6)	42(2)
N1	2913(11)	3435(10)	2619(7)	41(3)
N2	3142(10)	4478(9)	1291(7)	38(2)
N3	5021(10)	6076(9)	1168(7)	35(2)
N4	5963(11)	7122(10)	2366(8)	45(3)
N5	4860(11)	6595(10)	3725(8)	44(3)
N6	3779(10)	4571(9)	3808(7)	34(2)
C1	3143(12)	2972(10)	3154(8)	36(3)
C2	2779(12)	1883(11)	2989(9)	38(3)
C3	2200(13)	1703(11)	2317(9)	41(3)
C4	2289(12)	2678(11)	2099(8)	35(3)
C5	1709(12)	2861(12)	1544(9)	39(3)
C6	2035(13)	3780(13)	1203(9)	44(3)
C7	1511(14)	4127(14)	663(10)	51(3)
C8	2319(14)	4924(13)	317(10)	48(3)
C9	3273(12)	5088(11)	702(8)	35(2)
C10	4364(13)	5783(12)	556(9)	42(3)
C11	4739(13)	6047(12)	-160(9)	42(3)
C12	5806(14)	6613(13)	-238(10)	46(3)
C13	6489(14)	6918(14)	392(10)	49(3)
C14	6055(13)	6655(12)	1105(10)	41(3)
C15	6611(13)	7152(12)	1802(9)	43(3)
C16	7687(13)	7840(12)	1979(9)	44(3)
C17	7677(14)	8350(12)	2664(10)	46(3)
C18	6600(14)	7915(13)	2857(10)	47(3)
C19	6153(13)	8258(12)	3446(10)	45(3)
C20	5252(13)	7701(12)	3806(9)	42(3)

C21	4680(13)	7924(12)	4337(10)	45(3)
C22	4077(13)	7021(12)	4690(9)	41(3)
C23	4245(13)	6245(12)	4307(8)	39(3)
C24	3873(11)	5163(11)	4431(8)	35(3)
C25	3716(12)	4784(12)	5158(9)	38(3)
C26	3522(12)	3788(12)	5207(9)	41(3)
C27	3392(13)	3165(12)	4594(9)	43(3)
C28	3504(12)	3589(11)	3886(9)	37(3)
C29	2890(15)	1133(13)	3432(11)	53(4)
C30	1857(18)	462(18)	3845(13)	74(6)
C31	1755(14)	683(13)	1874(10)	50(4)
C32	2580(16)	721(15)	1291(12)	61(5)
C33	665(13)	1979(13)	1262(10)	45(3)
C34	-126(14)	1476(14)	1757(11)	50(3)
C35	-1077(16)	681(16)	1486(12)	60(4)
C36	-1245(17)	372(17)	719(13)	66(4)
C37	-453(15)	853(16)	231(12)	62(4)
C38	513(15)	1651(15)	504(11)	55(4)
C39	363(15)	3801(18)	614(13)	66(4)
C40	60(20)	4220(30)	1251(17)	100(8)
C41	2185(15)	5560(14)	-263(11)	55(4)
C42	2484(18)	6651(15)	36(13)	66(5)
C43	8625(15)	7964(15)	1537(12)	58(4)
C44	8706(17)	6959(16)	1405(12)	61(5)
C45	8654(14)	9106(14)	3123(10)	49(4)
C46	8860(17)	8653(16)	3813(12)	63(5)
C47	6738(14)	9406(13)	3649(12)	53(3)
C48	6895(16)	10084(16)	3072(14)	66(4)
C49	7441(19)	11147(18)	3216(16)	77(5)
C50	7830(20)	11500(20)	3933(16)	80(5)
C51	7703(17)	10888(18)	4480(14)	71(5)
C52	7141(16)	9788(17)	4340(13)	67(4)
C53	4632(15)	8922(13)	4497(10)	49(4)
C54	4075(17)	9128(16)	3842(13)	64(5)
C55	3359(14)	6876(13)	5328(10)	48(3)
C56	4043(18)	7396(15)	6056(12)	66(5)

C57	2832(15)	6250(14)	2552(11)	51(3)
C58	2135(14)	6746(14)	2620(11)	50(3)
C59	1497(18)	6524(19)	3179(16)	77(5)
C60	850(20)	7010(20)	3268(17)	83(5)
C61	980(20)	7800(20)	2778(18)	89(6)
C62	1650(19)	8011(19)	2281(16)	77(5)
C63	2262(18)	7509(17)	2140(14)	67(4)
C64	5836(14)	4682(14)	2521(10)	46(3)
C65	6689(14)	4342(14)	2522(11)	52(3)
C66	7555(16)	4859(18)	3015(14)	68(4)
C67	8410(20)	4610(20)	3066(18)	95(6)
C68	8170(20)	3760(30)	2610(19)	100(7)
C69	7470(20)	3300(20)	2086(17)	87(6)
C70	6590(20)	3532(19)	2068(14)	75(5)

Bond lengths [Å] and angles [°] for complex **4**.

Th1-O4	2.483(10)	C5-C33	1.52(2)
Th1-O3	2.482(10)	C6-C7	1.46(2)
Th1-O2	2.489(11)	C7-C8	1.39(3)
Th1-O1	2.519(12)	C7-C39	1.49(3)
Th1-N2	2.587(12)	C8-C9	1.43(2)
Th1-N4	2.609(14)	C8-C41	1.49(2)
Th1-N6	2.645(12)	C9-C10	1.46(2)
Th1-N5	2.644(13)	C10-C11	1.40(2)
Th1-N1	2.646(13)	C11-C12	1.38(2)
Th1-N3	2.660(13)	C11-H11	0.95
O1-C57	1.29(2)	C12-C13	1.40(2)
O2-C57	1.23(2)	C12-H12	0.95
O3-C64	1.28(2)	C13-C14	1.42(2)
O4-C64	1.24(2)	C13-H13	0.95
N1-C1	1.320(19)	C14-C15	1.44(2)
N1-C4	1.370(19)	C15-C16	1.42(2)
N2-C9	1.37(2)	C16-C17	1.41(2)
N2-C6	1.44(2)	C16-C43	1.51(3)
N3-C14	1.34(2)	C17-C18	1.43(3)
N3-C10	1.35(2)	C17-C45	1.52(2)
N4-C18	1.37(2)	C18-C19	1.43(2)
N4-C15	1.37(2)	C19-C20	1.36(3)
N5-C23	1.34(2)	C19-C47	1.52(2)
N5-C20	1.46(2)	C20-C21	1.39(2)
N6-C28	1.33(2)	C21-C22	1.39(2)
N6-C24	1.352(19)	C21-C53	1.52(2)
C1-C2	1.46(2)	C22-C23	1.42(2)
C1-C28	1.50(2)	C22-C55	1.51(2)
C2-C3	1.40(2)	C23-C24	1.46(2)
C2-C29	1.45(2)	C24-C25	1.42(2)
C3-C4	1.45(2)	C25-C26	1.37(2)
C3-C31	1.51(2)	C25-H25	0.95
C4-C5	1.40(2)	C26-C27	1.35(2)
C5-C6	1.38(2)	C26-H26	0.95

C27-C28	1.42(2)	C42-H42C	0.98
C27-H27	0.95	C43-C44	1.55(3)
C29-C30	1.57(3)	C43-H43A	0.99
C29-H29A	0.99	C43-H43B	0.99
C29-H29B	0.99	C44-H44A	0.98
C30-H30A	0.98	C44-H44B	0.98
C30-H30B	0.98	C44-H44C	0.98
C30-H30C	0.98	C45-C46	1.52(3)
C31-C32	1.57(3)	C45-H45A	0.99
C31-H31A	0.99	C45-H45B	0.99
C31-H31B	0.99	C46-H46A	0.98
C32-H32A	0.98	C46-H46B	0.98
C32-H32B	0.98	C46-H46C	0.98
C32-H32C	0.98	C47-C52	1.34(3)
C33-C34	1.39(3)	C47-C48	1.42(3)
C33-C38	1.40(3)	C48-C49	1.40(3)
C34-C35	1.39(3)	C48-H48	0.95
C34-H34	0.95	C49-C50	1.37(4)
C35-C36	1.41(3)	C49-H49	0.95
C35-H35	0.95	C50-C51	1.32(4)
C36-C37	1.38(3)	C50-H50	0.95
C36-H36	0.95	C51-C52	1.45(3)
C37-C38	1.40(3)	C51-H51	0.95
C37-H37	0.95	C52-H52	0.95
C38-H38	0.95	C53-C54	1.53(3)
C39-C40	1.44(4)	C53-H53A	0.99
C39-H39A	0.99	C53-H53B	0.99
C39-H39B	0.99	C54-H54A	0.98
C40-H40A	0.98	C54-H54B	0.98
C40-H40B	0.98	C54-H54C	0.98
C40-H40C	0.98	C55-C56	1.56(3)
C41-C42	1.53(3)	C55-H55A	0.99
C41-H41A	0.99	C55-H55B	0.99
C41-H41B	0.99	C56-H56A	0.98
C42-H42A	0.98	C56-H56B	0.98
C42-H42B	0.98	C56-H56C	0.98

C57-C58	1.49(3)	C64-C65	1.52(3)
C58-C59	1.31(3)	C65-C70	1.37(3)
C58-C63	1.39(3)	C65-C66	1.39(3)
C59-C60	1.42(3)	C66-C67	1.43(4)
C59-H59	0.95	C66-H66	0.95
C60-C61	1.43(4)	C67-C68	1.37(4)
C60-H60	0.95	C67-H67	0.95
C61-C62	1.26(4)	C68-C69	1.28(4)
C61-H61	0.95	C68-H68	0.95
C62-C63	1.40(3)	C69-C70	1.45(4)
C62-H62	0.95	C69-H69	0.95
C63-H63	0.95	C70-H70	0.95

O4-Th1-O3	52.1(3)	O2-Th1-N5	75.7(4)
O4-Th1-O2	139.4(4)	O1-Th1-N5	81.7(4)
O3-Th1-O2	150.9(4)	N2-Th1-N5	156.3(4)
O4-Th1-O1	146.0(4)	N4-Th1-N5	65.9(4)
O3-Th1-O1	140.5(4)	N6-Th1-N5	60.5(4)
O2-Th1-O1	51.5(4)	O4-Th1-N1	93.4(4)
O4-Th1-N2	129.2(4)	O3-Th1-N1	75.7(4)
O3-Th1-N2	77.5(4)	O2-Th1-N1	76.8(4)
O2-Th1-N2	82.6(4)	O1-Th1-N1	119.3(4)
O1-Th1-N2	77.4(4)	N2-Th1-N1	65.4(4)
O4-Th1-N4	73.6(4)	N4-Th1-N1	165.5(4)
O3-Th1-N4	91.0(4)	N6-Th1-N1	58.0(4)
O2-Th1-N4	117.3(4)	N5-Th1-N1	117.4(4)
O1-Th1-N4	74.8(4)	O4-Th1-N3	101.6(4)
N2-Th1-N4	117.9(4)	O3-Th1-N3	70.3(4)
O4-Th1-N6	69.1(4)	O2-Th1-N3	117.4(4)
O3-Th1-N6	100.2(4)	O1-Th1-N3	71.0(4)
O2-Th1-N6	72.5(4)	N2-Th1-N3	60.8(4)
O1-Th1-N6	118.8(4)	N4-Th1-N3	57.9(4)
N2-Th1-N6	121.6(4)	N6-Th1-N3	169.9(4)
N4-Th1-N6	120.5(4)	N5-Th1-N3	121.9(4)
O4-Th1-N5	74.5(4)	N1-Th1-N3	120.7(4)
O3-Th1-N5	126.2(4)	C57-O1-Th1	93.0(10)

C57-O2-Th1	96.0(11)	C5-C6-N2	115.4(14)
C64-O3-Th1	93.7(10)	C5-C6-C7	132.2(16)
C64-O4-Th1	94.6(9)	N2-C6-C7	111.5(14)
C1-N1-C4	106.2(12)	C8-C7-C6	105.2(15)
C1-N1-Th1	115.4(10)	C8-C7-C39	128.7(17)
C4-N1-Th1	131.8(10)	C6-C7-C39	125.3(17)
C9-N2-C6	101.0(12)	C7-C8-C9	105.8(15)
C9-N2-Th1	116.0(9)	C7-C8-C41	125.8(17)
C6-N2-Th1	129.7(10)	C9-C8-C41	127.9(16)
C14-N3-C10	120.4(14)	N2-C9-C8	115.1(14)
C14-N3-Th1	119.6(10)	N2-C9-C10	114.7(13)
C10-N3-Th1	119.9(10)	C8-C9-C10	130.2(15)
C18-N4-C15	104.1(14)	N3-C10-C11	121.7(14)
C18-N4-Th1	134.5(11)	N3-C10-C9	114.2(14)
C15-N4-Th1	116.4(10)	C11-C10-C9	123.8(14)
C23-N5-C20	103.7(13)	C12-C11-C10	118.7(15)
C23-N5-Th1	116.1(10)	C12-C11-H11	120.6
C20-N5-Th1	129.0(10)	C10-C11-H11	120.6
C28-N6-C24	118.0(13)	C11-C12-C13	119.9(17)
C28-N6-Th1	121.1(10)	C11-C12-H12	120.0
C24-N6-Th1	120.7(9)	C13-C12-H12	120.0
N1-C1-C2	114.1(13)	C12-C13-C14	118.5(16)
N1-C1-C28	114.3(12)	C12-C13-H13	120.7
C2-C1-C28	129.9(13)	C14-C13-H13	120.7
C3-C2-C29	127.4(14)	N3-C14-C13	120.7(14)
C3-C2-C1	102.4(13)	N3-C14-C15	113.9(15)
C29-C2-C1	129.9(15)	C13-C14-C15	124.0(15)
C2-C3-C4	107.7(13)	N4-C15-C16	112.8(14)
C2-C3-C31	122.0(14)	N4-C15-C14	113.7(15)
C4-C3-C31	129.5(15)	C16-C15-C14	132.1(16)
N1-C4-C5	121.2(13)	C15-C16-C17	104.6(15)
N1-C4-C3	109.3(12)	C15-C16-C43	127.0(16)
C5-C4-C3	128.5(14)	C17-C16-C43	128.4(16)
C6-C5-C4	124.9(14)	C18-C17-C16	105.8(14)
C6-C5-C33	116.8(14)	C18-C17-C45	128.8(16)
C4-C5-C33	118.3(14)	C16-C17-C45	125.0(16)

N4-C18-C17	111.9(15)	C2-C29-H29B	109.3
N4-C18-C19	120.2(15)	C30-C29-H29B	109.3
C17-C18-C19	127.8(15)	H29A-C29-H29B	107.9
C20-C19-C18	128.1(15)	C29-C30-H30A	109.5
C20-C19-C47	117.1(16)	C29-C30-H30B	109.5
C18-C19-C47	114.6(16)	H30A-C30-H30B	109.5
C19-C20-C21	135.1(15)	C29-C30-H30C	109.5
C19-C20-N5	114.7(15)	H30A-C30-H30C	109.5
C21-C20-N5	109.4(14)	H30B-C30-H30C	109.5
C20-C21-C22	106.9(14)	C3-C31-C32	108.8(15)
C20-C21-C53	128.8(16)	C3-C31-H31A	109.9
C22-C21-C53	124.2(16)	C32-C31-H31A	109.9
C21-C22-C23	106.1(15)	C3-C31-H31B	109.9
C21-C22-C55	127.4(15)	C32-C31-H31B	109.9
C23-C22-C55	126.4(15)	H31A-C31-H31B	108.3
N5-C23-C22	112.4(14)	C31-C32-H32A	109.5
N5-C23-C24	115.4(14)	C31-C32-H32B	109.5
C22-C23-C24	132.2(15)	H32A-C32-H32B	109.5
N6-C24-C25	122.8(14)	C31-C32-H32C	109.5
N6-C24-C23	114.7(13)	H32A-C32-H32C	109.5
C25-C24-C23	122.2(13)	H32B-C32-H32C	109.5
C26-C25-C24	116.4(14)	C34-C33-C38	120.0(17)
C26-C25-H25	121.8	C34-C33-C5	120.3(16)
C24-C25-H25	121.8	C38-C33-C5	119.8(17)
C27-C26-C25	122.3(15)	C33-C34-C35	119.3(18)
C27-C26-H26	118.9	C33-C34-H34	120.3
C25-C26-H26	118.9	C35-C34-H34	120.3
C26-C27-C28	117.6(15)	C34-C35-C36	121(2)
C26-C27-H27	121.2	C34-C35-H35	119.6
C28-C27-H27	121.2	C36-C35-H35	119.6
N6-C28-C27	122.6(14)	C37-C36-C35	120(2)
N6-C28-C1	111.9(13)	C37-C36-H36	120.1
C27-C28-C1	124.5(13)	C35-C36-H36	120.1
C2-C29-C30	111.8(16)	C36-C37-C38	119(2)
C2-C29-H29A	109.3	C36-C37-H37	120.3
C30-C29-H29A	109.3	C38-C37-H37	120.3

C37-C38-C33	121(2)	C43-C44-H44C	109.5
C37-C38-H38	119.7	H44A-C44-H44C	109.5
C33-C38-H38	119.7	H44B-C44-H44C	109.5
C40-C39-C7	110.3(19)	C46-C45-C17	112.9(16)
C40-C39-H39A	109.6	C46-C45-H45A	109.0
C7-C39-H39A	109.6	C17-C45-H45A	109.0
C40-C39-H39B	109.6	C46-C45-H45B	109.0
C7-C39-H39B	109.6	C17-C45-H45B	109.0
H39A-C39-H39B	108.1	H45A-C45-H45B	107.8
C39-C40-H40A	109.5	C45-C46-H46A	109.5
C39-C40-H40B	109.5	C45-C46-H46B	109.5
H40A-C40-H40B	109.5	H46A-C46-H46B	109.5
C39-C40-H40C	109.5	C45-C46-H46C	109.5
H40A-C40-H40C	109.5	H46A-C46-H46C	109.5
H40B-C40-H40C	109.5	H46B-C46-H46C	109.5
C8-C41-C42	112.7(16)	C52-C47-C48	119.4(19)
C8-C41-H41A	109.1	C52-C47-C19	123(2)
C42-C41-H41A	109.1	C48-C47-C19	117.9(18)
C8-C41-H41B	109.1	C49-C48-C47	121(2)
C42-C41-H41B	109.1	C49-C48-H48	119.5
H41A-C41-H41B	107.8	C47-C48-H48	119.5
C41-C42-H42A	109.5	C50-C49-C48	118(3)
C41-C42-H42B	109.5	C50-C49-H49	121.2
H42A-C42-H42B	109.5	C48-C49-H49	121.2
C41-C42-H42C	109.5	C51-C50-C49	123(2)
H42A-C42-H42C	109.5	C51-C50-H50	118.7
H42B-C42-H42C	109.5	C49-C50-H50	118.7
C16-C43-C44	113.8(17)	C50-C51-C52	120(2)
C16-C43-H43A	108.8	C50-C51-H51	119.8
C44-C43-H43A	108.8	C52-C51-H51	119.8
C16-C43-H43B	108.8	C47-C52-C51	119(2)
C44-C43-H43B	108.8	C47-C52-H52	120.5
H43A-C43-H43B	107.7	C51-C52-H52	120.5
C43-C44-H44A	109.5	C21-C53-C54	109.8(14)
C43-C44-H44B	109.5	C21-C53-H53A	109.7
H44A-C44-H44B	109.5	C54-C53-H53A	109.7

C21-C53-H53B	109.7	C61-C60-H60	120.9
C54-C53-H53B	109.7	C62-C61-C60	118(3)
H53A-C53-H53B	108.2	C62-C61-H61	120.9
C53-C54-H54A	109.5	C60-C61-H61	120.9
C53-C54-H54B	109.5	C61-C62-C63	126(3)
H54A-C54-H54B	109.5	C61-C62-H62	117.1
C53-C54-H54C	109.5	C63-C62-H62	117.1
H54A-C54-H54C	109.5	C58-C63-C62	116(2)
H54B-C54-H54C	109.5	C58-C63-H63	122.1
C22-C55-C56	108.7(15)	C62-C63-H63	122.1
C22-C55-H55A	109.9	O4-C64-O3	119.5(16)
C56-C55-H55A	109.9	O4-C64-C65	120.4(15)
C22-C55-H55B	109.9	O3-C64-C65	120.1(17)
C56-C55-H55B	109.9	C70-C65-C66	121(2)
H55A-C55-H55B	108.3	C70-C65-C64	121.0(19)
C55-C56-H56A	109.5	C66-C65-C64	118.1(19)
C55-C56-H56B	109.5	C65-C66-C67	123(3)
H56A-C56-H56B	109.5	C65-C66-H66	118.4
C55-C56-H56C	109.5	C67-C66-H66	118.4
H56A-C56-H56C	109.5	C68-C67-C66	109(3)
H56B-C56-H56C	109.5	C68-C67-H67	125.5
O2-C57-O1	118.8(17)	C66-C67-H67	125.5
O2-C57-C58	121.9(18)	C69-C68-C67	132(3)
O1-C57-C58	119.2(16)	C69-C68-H68	114.0
C59-C58-C63	122(2)	C67-C68-H68	114.0
C59-C58-C57	119(2)	C68-C69-C70	116(3)
C63-C58-C57	118.9(19)	C68-C69-H69	121.8
C58-C59-C60	120(3)	C70-C69-H69	121.8
C58-C59-H59	120.1	C65-C70-C69	117(2)
C60-C59-H59	120.1	C65-C70-H70	121.6
C59-C60-C61	118(3)	C69-C70-H70	121.6
C59-C60-H60	120.9		

Anisotropic displacement parameters ($Å^2$ x 10^3) for complex **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Th1	60(1)	34(1)	24(1)	1(1)	-5(1)	23(1)
O1	63(5)	50(5)	53(6)	13(4)	8(4)	32(5)
O2	42(5)	48(5)	44(5)	12(4)	-4(4)	22(4)
O3	62(5)	35(4)	29(4)	-10(4)	-3(4)	29(4)
O4	62(5)	45(5)	21(4)	10(3)	-10(4)	26(4)
N1	62(6)	34(4)	28(4)	10(3)	-6(4)	23(4)
N2	51(5)	36(5)	24(4)	6(4)	1(4)	17(4)
N3	50(4)	28(5)	26(4)	4(4)	0(3)	17(4)
N4	58(5)	40(5)	29(5)	0(4)	0(4)	17(4)
N5	62(6)	35(4)	30(5)	0(4)	5(4)	17(4)
N6	48(6)	29(4)	20(4)	5(3)	0(4)	12(4)
C1	47(6)	23(4)	31(5)	6(4)	-2(5)	12(4)
C2	43(6)	31(5)	36(5)	1(4)	-2(5)	15(5)
C3	48(7)	30(5)	38(5)	4(4)	-6(5)	13(5)
C4	47(6)	31(5)	25(5)	3(4)	2(4)	17(4)
C5	46(5)	43(5)	31(6)	4(4)	-1(4)	23(4)
C6	54(5)	44(5)	33(6)	4(4)	-4(5)	21(4)
C7	60(5)	49(7)	42(7)	12(5)	-5(5)	22(5)
C8	58(5)	41(6)	41(7)	9(5)	-9(5)	20(5)
C9	54(5)	32(5)	21(5)	-2(4)	-4(4)	21(4)
C10	51(5)	38(6)	32(5)	3(5)	-1(4)	17(5)
C11	53(5)	42(6)	31(5)	2(5)	-4(5)	23(5)
C12	57(6)	45(7)	40(6)	4(5)	4(5)	25(5)
C13	52(6)	46(7)	41(5)	5(5)	6(4)	15(5)
C14	50(5)	36(6)	39(5)	3(4)	1(4)	22(4)
C15	55(5)	36(6)	37(5)	1(4)	2(4)	21(4)
C16	53(5)	36(6)	32(5)	11(4)	3(4)	11(4)
C17	54(5)	36(6)	43(6)	3(5)	-2(4)	15(5)
C18	54(5)	42(6)	39(6)	-6(5)	-1(4)	18(5)
C19	53(6)	39(5)	37(6)	-7(4)	2(5)	17(4)
C20	51(6)	38(5)	35(6)	0(4)	-1(4)	19(4)

C21	50(7)	34(5)	47(7)	-1(5)	3(5)	16(5)
C22	52(6)	32(5)	33(5)	-6(4)	-4(4)	16(5)
C23	58(7)	36(4)	20(5)	-1(4)	1(4)	19(5)
C24	41(6)	34(4)	26(4)	0(4)	-5(5)	15(5)
C25	45(7)	38(5)	25(5)	1(4)	-4(5)	13(5)
C26	47(7)	41(5)	27(5)	3(4)	-14(5)	13(5)
C27	50(7)	40(6)	36(5)	2(4)	-7(5)	19(5)
C28	40(6)	32(4)	36(5)	-1(4)	-8(5)	14(5)
C29	70(7)	43(6)	50(7)	7(5)	-8(6)	30(6)
C30	91(11)	72(11)	49(10)	18(8)	2(8)	28(9)
C31	62(7)	40(6)	44(7)	1(5)	-3(5)	22(6)
C32	72(10)	52(9)	47(9)	-16(7)	-4(7)	21(8)
C33	48(5)	47(6)	36(5)	5(5)	-7(4)	18(4)
C34	55(6)	52(7)	42(6)	11(5)	-1(5)	23(5)
C35	59(7)	60(7)	53(6)	9(6)	-3(6)	20(5)
C36	68(7)	60(8)	56(6)	2(6)	-3(6)	18(6)
C37	63(7)	66(8)	44(7)	5(6)	-12(5)	18(5)
C38	60(7)	54(7)	43(6)	-4(5)	-10(5)	21(5)
C39	61(6)	72(9)	65(8)	19(7)	-7(6)	30(6)
C40	82(12)	151(18)	80(12)	14(12)	10(10)	65(13)
C41	56(7)	54(7)	53(7)	16(5)	-10(6)	23(6)
C42	85(12)	58(8)	61(11)	25(7)	-10(9)	38(8)
C43	57(7)	56(7)	50(8)	0(6)	6(6)	16(6)
C44	72(10)	63(9)	42(9)	-10(8)	-10(8)	27(8)
C45	53(6)	51(7)	43(6)	-4(5)	1(5)	24(5)
C46	74(11)	58(10)	50(8)	-1(7)	-5(8)	26(9)
C47	55(7)	41(5)	57(6)	-1(4)	4(6)	18(5)
C48	70(8)	55(6)	72(8)	11(5)	4(7)	26(6)
C49	87(9)	64(6)	80(7)	11(6)	7(7)	33(6)
C50	91(10)	70(8)	83(7)	0(6)	6(7)	42(7)
C51	72(9)	69(7)	65(7)	-9(6)	0(7)	28(6)
C52	68(8)	62(6)	60(7)	-13(6)	0(6)	24(6)
C53	63(8)	41(6)	47(7)	4(5)	-1(6)	28(6)
C54	84(11)	56(9)	63(10)	-12(8)	-19(9)	44(9)
C55	55(7)	46(7)	45(6)	4(5)	6(5)	25(6)
C56	87(11)	49(9)	49(8)	-5(7)	4(8)	20(9)

C57	58(7)	53(6)	45(7)	16(5)	3(5)	26(5)
C58	59(7)	46(6)	45(7)	-6(5)	-3(5)	24(5)
C59	83(9)	76(9)	82(9)	15(7)	26(7)	43(7)
C60	87(9)	82(9)	92(10)	6(7)	21(7)	49(7)
C61	97(10)	82(9)	99(10)	4(7)	6(7)	51(8)
C62	91(9)	75(9)	82(9)	6(7)	-7(6)	51(7)
C63	81(9)	64(8)	67(8)	12(6)	-1(6)	42(7)
C64	54(6)	54(7)	30(5)	14(4)	0(4)	23(5)
C65	59(6)	54(6)	46(7)	23(5)	6(5)	27(5)
C66	61(7)	66(8)	67(8)	24(6)	-5(6)	20(6)
C67	90(9)	105(10)	98(10)	16(7)	-6(7)	52(8)
C68	104(10)	104(10)	100(10)	18(7)	2(7)	53(8)
C69	96(9)	91(10)	86(9)	13(7)	14(7)	54(7)
C70	94(8)	73(8)	67(9)	13(6)	12(7)	46(7)

Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for complex **4**.

	x	y	z	U(eq)
H11	4266	5841	-584	50
H12	6077	6795	-720	56
H13	7228	7294	344	59
H25	3745	5198	5587	46
H26	3477	3525	5688	49
H27	3232	2468	4637	51
H29A	3479	1491	3806	64
H29B	3064	681	3101	64
H30A	1258	174	3484	111
H30B	1745	889	4231	111
H30C	1925	-96	4079	111
H31A	1087	546	1610	60
H31B	1609	125	2215	60
H32A	2677	1237	930	91
H32B	2323	48	1027	91
H32C	3253	902	1553	91
H34	-16	1676	2275	60
H35	-1622	339	1822	72
H36	-1904	-167	539	79
H37	-560	646	-286	75
H38	1069	1971	172	66
H39A	186	4037	148	79
H39B	-33	3043	596	79
H40A	-707	3945	1239	150
H40B	388	4971	1235	150
H40C	293	4040	1713	150
H41A	1442	5226	-451	66
H41B	2627	5591	-690	66
H42A	2396	7038	-367	98
H42B	3219	6986	222	98
H42C	2028	6627	445	98

H43A	9275	8479	1807	70
H43B	8582	8231	1046	70
H44A	9322	7092	1111	92
H44B	8069	6447	1132	92
H44C	8777	6703	1887	92
H45A	9272	9336	2805	59
H45B	8568	9715	3278	59
H46A	8891	8019	3667	94
H46B	8291	8502	4160	94
H46C	9531	9145	4059	94
H48	6626	9814	2580	79
H49	7541	11605	2831	93
H50	8200	12224	4040	96
H51	7984	11169	4968	85
H52	7058	9343	4731	80
H53A	5354	9493	4575	59
H53B	4247	8878	4960	59
H54A	4448	9154	3383	96
H54B	4068	9784	3941	96
H54C	3350	8577	3782	96
H55A	2913	6135	5393	57
H55B	2893	7188	5222	57
H56A	4456	8134	5997	98
H56B	4520	7101	6148	98
H56C	3585	7280	6480	98
H59	1469	6038	3522	92
H60	340	6818	3644	100
H61	568	8153	2825	106
H62	1751	8558	1975	93
H63	2733	7681	1742	81
H66	7583	5405	3332	81
H67	9032	4975	3369	114
H68	8617	3452	2697	120
H69	7517	2829	1728	104
H70	5981	3142	1757	90

Torsion angles [°] for complex **4**.

C4-N1-C1-C2	6(2)	C5-C6-C7-C39	32(3)
Th1-N1-C1-C2	-148.9(11)	N2-C6-C7-C39	-159.3(18)
C4-N1-C1-C28	-160.4(14)	C6-C7-C8-C9	-5(2)
Th1-N1-C1-C28	44.5(17)	C39-C7-C8-C9	164.6(19)
N1-C1-C2-C3	-6(2)	C6-C7-C8-C41	-177.6(18)
C28-C1-C2-C3	158.3(17)	C39-C7-C8-C41	-8(3)
N1-C1-C2-C29	179.5(18)	C6-N2-C9-C8	8.4(17)
C28-C1-C2-C29	-16(3)	Th1-N2-C9-C8	-136.5(12)
C29-C2-C3-C4	177.7(17)	C6-N2-C9-C10	-170.2(13)
C1-C2-C3-C4	2.7(18)	Th1-N2-C9-C10	44.9(16)
C29-C2-C3-C31	-12(3)	C7-C8-C9-N2	-2(2)
C1-C2-C3-C31	173.2(16)	C41-C8-C9-N2	170.0(18)
C1-N1-C4-C5	165.4(15)	C7-C8-C9-C10	176.2(16)
Th1-N1-C4-C5	-45(2)	C41-C8-C9-C10	-12(3)
C1-N1-C4-C3	-4.0(19)	C14-N3-C10-C11	2(2)
Th1-N1-C4-C3	145.2(12)	Th1-N3-C10-C11	-173.6(12)
C2-C3-C4-N1	1(2)	C14-N3-C10-C9	175.3(13)
C31-C3-C4-N1	-168.9(17)	Th1-N3-C10-C9	0.0(17)
C2-C3-C4-C5	-167.9(16)	N2-C9-C10-N3	-29.0(19)
C31-C3-C4-C5	23(3)	C8-C9-C10-N3	152.7(16)
N1-C4-C5-C6	35(3)	N2-C9-C10-C11	144.5(16)
C3-C4-C5-C6	-158.2(18)	C8-C9-C10-C11	-34(3)
N1-C4-C5-C33	-148.4(15)	N3-C10-C11-C12	1(2)
C3-C4-C5-C33	19(3)	C9-C10-C11-C12	-172.3(15)
C4-C5-C6-N2	17(2)	C10-C11-C12-C13	-1(2)
C33-C5-C6-N2	-160.1(14)	C11-C12-C13-C14	-2(3)
C4-C5-C6-C7	-174.8(18)	C10-N3-C14-C13	-4(2)
C33-C5-C6-C7	8(3)	Th1-N3-C14-C13	171.4(12)
C9-N2-C6-C5	159.0(15)	C10-N3-C14-C15	162.8(14)
Th1-N2-C6-C5	-63.2(19)	Th1-N3-C14-C15	-21.9(17)
C9-N2-C6-C7	-11.7(18)	C12-C13-C14-N3	4(2)
Th1-N2-C6-C7	126.1(13)	C12-C13-C14-C15	-161.4(16)
C5-C6-C7-C8	-158(2)	C18-N4-C15-C16	9.6(19)
N2-C6-C7-C8	11(2)	Th1-N4-C15-C16	-149.1(11)

C18-N4-C15-C14	-158.4(14)	C19-C20-C21-C53	26(3)
Th1-N4-C15-C14	42.9(17)	N5-C20-C21-C53	-165.8(16)
N3-C14-C15-N4	-13(2)	C20-C21-C22-C23	-4.9(19)
C13-C14-C15-N4	153.1(16)	C53-C21-C22-C23	171.8(15)
N3-C14-C15-C16	-178.2(16)	C20-C21-C22-C55	177.2(16)
C13-C14-C15-C16	-12(3)	C53-C21-C22-C55	-6(3)
N4-C15-C16-C17	-6.9(19)	C20-N5-C23-C22	9.4(18)
C14-C15-C16-C17	158.2(18)	Th1-N5-C23-C22	-137.9(11)
N4-C15-C16-C43	171.4(17)	C20-N5-C23-C24	-170.8(13)
C14-C15-C16-C43	-23(3)	Th1-N5-C23-C24	41.9(17)
C15-C16-C17-C18	1.3(18)	C21-C22-C23-N5	-3(2)
C43-C16-C17-C18	-177.0(18)	C55-C22-C23-N5	174.7(15)
C15-C16-C17-C45	174.6(16)	C21-C22-C23-C24	177.0(17)
C43-C16-C17-C45	-4(3)	C55-C22-C23-C24	-5(3)
C15-N4-C18-C17	-8.6(19)	C28-N6-C24-C25	2(2)
Th1-N4-C18-C17	144.3(14)	Th1-N6-C24-C25	-173.6(11)
C15-N4-C18-C19	167.4(17)	C28-N6-C24-C23	176.1(14)
Th1-N4-C18-C19	-40(3)	Th1-N6-C24-C23	0.8(18)
C16-C17-C18-N4	5(2)	N5-C23-C24-N6	-28(2)
C45-C17-C18-N4	-168.4(17)	C22-C23-C24-N6	151.5(17)
C16-C17-C18-C19	-171.0(18)	N5-C23-C24-C25	146.2(15)
C45-C17-C18-C19	16(3)	C22-C23-C24-C25	-34(3)
N4-C18-C19-C20	30(3)	N6-C24-C25-C26	4(2)
C17-C18-C19-C20	-155.0(19)	C23-C24-C25-C26	-170.3(15)
N4-C18-C19-C47	-146.1(17)	C24-C25-C26-C27	-6(2)
C17-C18-C19-C47	29(3)	C25-C26-C27-C28	2(3)
C18-C19-C20-C21	-174.2(19)	C24-N6-C28-C27	-5(2)
C47-C19-C20-C21	1(3)	Th1-N6-C28-C27	170.0(12)
C18-C19-C20-N5	18(3)	C24-N6-C28-C1	164.2(13)
C47-C19-C20-N5	-166.4(15)	Th1-N6-C28-C1	-20.5(17)
C23-N5-C20-C19	158.6(16)	C26-C27-C28-N6	3(2)
Th1-N5-C20-C19	-60(2)	C26-C27-C28-C1	-164.8(15)
C23-N5-C20-C21	-12.4(18)	N1-C1-C28-N6	-16(2)
Th1-N5-C20-C21	129.0(13)	C2-C1-C28-N6	179.9(16)
C19-C20-C21-C22	-158(2)	N1-C1-C28-C27	153.2(16)
N5-C20-C21-C22	10.7(19)	C2-C1-C28-C27	-11(3)

C3-C2-C29-C30	-73(2)	C20-C21-C53-C54	68(2)
C1-C2-C29-C30	101(2)	C22-C21-C53-C54	-108(2)
C2-C3-C31-C32	-92(2)	C21-C22-C55-C56	-72(2)
C4-C3-C31-C32	76(2)	C23-C22-C55-C56	110.3(19)
C6-C5-C33-C34	-125.1(18)	Th1-O2-C57-O1	8.5(19)
C4-C5-C33-C34	58(2)	Th1-O2-C57-C58	-175.7(16)
C6-C5-C33-C38	57(2)	Th1-O1-C57-O2	-8.3(19)
C4-C5-C33-C38	-120.3(18)	Th1-O1-C57-C58	175.8(15)
C38-C33-C34-C35	-3(3)	O2-C57-C58-C59	19(3)
C5-C33-C34-C35	179.3(16)	O1-C57-C58-C59	-165(2)
C33-C34-C35-C36	1(3)	O2-C57-C58-C63	-167.6(19)
C34-C35-C36-C37	1(3)	O1-C57-C58-C63	8(3)
C35-C36-C37-C38	0(3)	C63-C58-C59-C60	5(4)
C36-C37-C38-C33	-2(3)	C57-C58-C59-C60	178(2)
C34-C33-C38-C37	4(3)	C58-C59-C60-C61	-5(4)
C5-C33-C38-C37	-178.6(17)	C59-C60-C61-C62	1(4)
C8-C7-C39-C40	-98(3)	C60-C61-C62-C63	3(5)
C6-C7-C39-C40	70(3)	C59-C58-C63-C62	-1(3)
C7-C8-C41-C42	108(2)	C57-C58-C63-C62	-174.2(19)
C9-C8-C41-C42	-63(3)	C61-C62-C63-C58	-3(4)
C15-C16-C43-C44	-56(2)	Th1-O4-C64-O3	-4.2(17)
C17-C16-C43-C44	121.7(19)	Th1-O4-C64-C65	177.8(14)
C18-C17-C45-C46	67(2)	Th1-O3-C64-O4	4.2(17)
C16-C17-C45-C46	-105(2)	Th1-O3-C64-C65	-177.7(14)
C20-C19-C47-C52	62(3)	O4-C64-C65-C70	158.3(19)
C18-C19-C47-C52	-122(2)	O3-C64-C65-C70	-20(3)
C20-C19-C47-C48	-121(2)	O4-C64-C65-C66	-20(3)
C18-C19-C47-C48	56(2)	O3-C64-C65-C66	162.2(17)
C52-C47-C48-C49	-2(3)	C70-C65-C66-C67	2(3)
C19-C47-C48-C49	-179(2)	C64-C65-C66-C67	-180(2)
C47-C48-C49-C50	1(4)	C65-C66-C67-C68	-5(4)
C48-C49-C50-C51	0(4)	C66-C67-C68-C69	14(5)
C49-C50-C51-C52	0(4)	C67-C68-C69-C70	-17(6)
C48-C47-C52-C51	2(3)	C66-C65-C70-C69	-5(3)
C19-C47-C52-C51	178.8(19)	C64-C65-C70-C69	177(2)
C50-C51-C52-C47	-1(4)	C68-C69-C70-C65	11(4)

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