Supporting Information:

Thorium Metallocene Cation Chemistry: Synthesis and Characterization of the Bent $[(C_5Me_5)_2Th(C_6H_5)(THF)][BPh_4]$ and the Parallel Ring $[(C_5Me_5)_2Th(NCR)_5][BPh_4]_2$ (R = Me, Ph) Complexes

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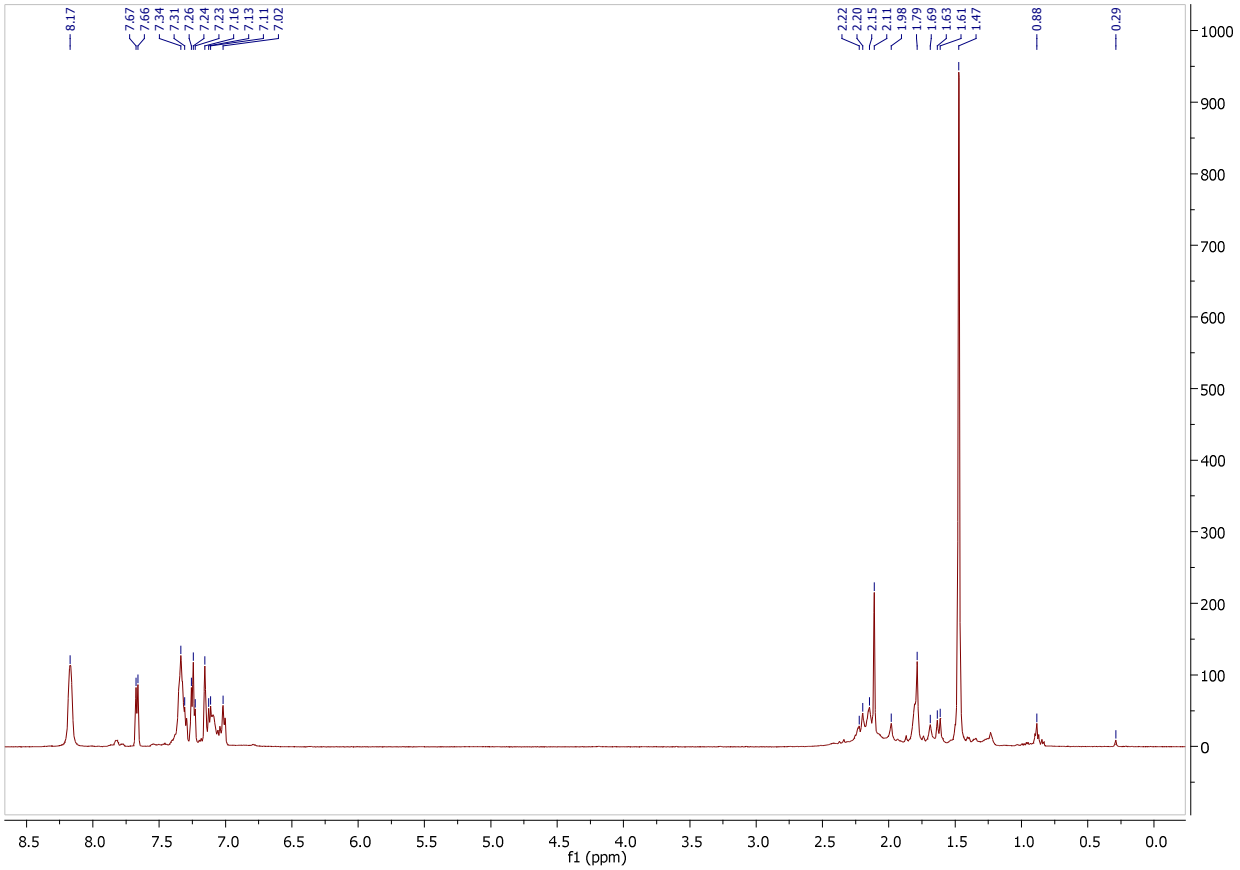
NMR SPECTRUM OF CRUDE $[(C_5ME_5)_2TH(C_6H_5)(THF)][BPH_4]$



X-RAY CRYSTAL STRUCTURES AND CRYSTALLOGRAPHIC DISCUSSIONS

Table S1. Metrical Parameter Comparison of $[(C_5Me_5)_2Th(C_6H_5)(THF)][BPh_4]$, 1.

	1*	$[Li(DME)_3][Th(C_6H_5)_6]$[1]	$[Li(12\text{-}c\text{-}4)(THF)][Th(C_6H_5)_6]$[1]	$[(C_5Me_5)_2Th(CH_3)(THF)]\{^tBuCH_2CH[B(C_6F_5)_2]_2H\}$[2]
Th–Cent (Å)	2.507 2.507 2.516 2.507	-	-	2.482 2.491
Th–Cent avg (Å)	2.509	-	-	2.486
Th–C_{ispo} avg (Å)	2.412(5)	2.589(3)	2.603(3)	-
Th–C_{ipso}–C_{ortho} (°)	48	4	37	-
Th–O (Å)	2.476(3)	-	-	2.455(4)
Cent–Th–Cent (°)	135.6 137.1	-	-	137.1

*Structure shows two independent Units

The crystal structure of **1** contains two independent $[(C_5Me_5)_2Th(C_6H_5)(THF)][BPh_4]$ units which display similar metrical parameters. In unit 1, the 2.507 Å Th–(ring centroid) distances are equivalent, as are the 135.6º (ring centroid)–Th–(ring centroid) angles. In unit 2, the Th–(ring centroid) distances are 2.516 and 2.507 Å, and the (ring centroid)–Th–(ring centroid) angle is 137.1º. The 2.412(5) Å ave Th–$C_{ipso}(C_6H_5)$ bond length in **1** is shorter than the 2.589(3) and 2.603(3) average values for $[Li(DME)_3]_2[Th(C_6H_5)_6]$ and $[Li(THF)(12\text{-crown-}4)]_2[Th(C_6H_5)_6]$, respectively, and is likely due to the less-crowded nature of **1**.

As with $[Li(THF)(12\text{-crown-}4)]_2[Th(C_6H_5)_6]$,[1] the crystal structure of **1** shows the presence of Th···H–C_{ortho} agostic interactions; the phenyl group is tipped to the side such that the difference between the Th–C_{ipso}–C_{ortho} bond angles [in the case of **1** this is (Th1–C21–C22) –

(Th1–C21–C26)] is 48º, which is even larger than the 37º maximum value in [Li(THF)(12-crown-4)]$_2$[Th(C_6H_5)$_6$]. These values are much greater than the 4º difference in [Li(DME)$_3$]$_2$[Th(C_6H_5)$_6$], which does not contain agostic interactions in the solid state.[1]

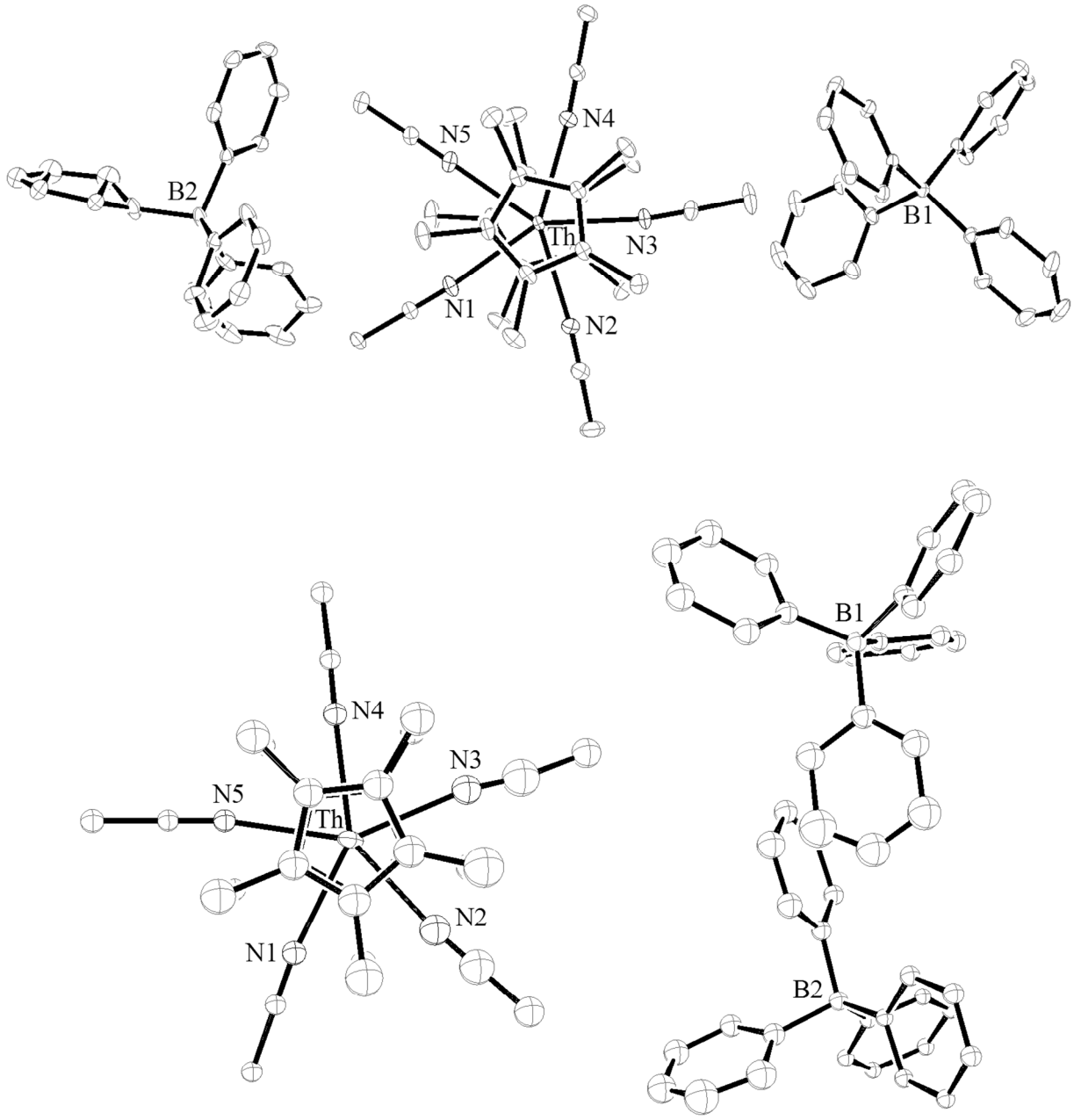


Figure S1. Thermal ellipsoid plots of **2-RT** and **2-cold** showing different spatial arrangements when crystallized at room temperature [**2-RT**, top] and −15 ºC [**2-cold**, bottom]. Thermal ellipsoids are drawn at the 25% probability level and hydrogen atoms and co-crystallized solvent omitted for clarity.

Table S2. Comparison of Selected Bond Distances (Å) and Angles (º) for $[(C_5Me_5)_2Th(NCMe)_5][BPh_4]_2$, **2-RT**, $[(C_5Me_5)_2Th(NCPh)_5][BPh_4]_2$, **3** and Other Selected Compounds.

Complex	**M–(Cnt) (avg) (Å)**	**M–N (ave) (Å)**	**Cnt–M–Cnt (avg) (º)**
$[(C_5Me_5)_2Th(NCMe)_5][BPh_4]_2$, **2-RT**	2.598	2.592(3)	179.1
$[(C_5Me_5)_2Th(NCPh)_5][BPh_4]_2$, **3**	2.602	2.580(2)	178.4
$[(C_5Me_5)_2U(NCMe)_5][BPh_4]_2$[3–4]	2.574[a]	2.550(3)[a]	178.6
$[(C_5Me_5)_3Th(THF)][BPh_4]$[5]	2.620	--	118.0
$[(C_5Me_5)_2Th(C_6H_5)(THF)][BPh_4]$, **1**	2.509	--	136.4
$(C_5Me_5)_2ThMe_2$[6]	2.518	--	133.9

[a] Adjusted for the 0.04 Å difference in atomic radii for 12-coordinate Th^{4+} vs U^{4+} [7]

X-RAY CRYSTALLOGRAPHY INFORMATION

Table S3. X-ray Data and Collection Parameters for $[(C_5Me_5)_2Th(C_6H_5)(THF)][BPh_4]$, **1**, $[(C_5Me_5)_2Th(NCMe)_5][BPh_4]_2$, **2-RT** and **2-cold**, and $[(C_5Me_5)_2Th(NCPh)_5][BPh_4]_2$, **3**.

Compound	**1**	**2-RT**	**2-cold**	**3**
Empirical Formula	$C_{54}H_{63}BOTh \cdot 2.5(C_7H_8)$	$C_{87}H_{101}B_2N_8Th$	$C_{78}H_{85}B_2N_5Th$	$C_{103}H_{95}B_2N_5Th$
Temperature (K)	88(2)	133(2)	133(2)	88(2)
Crystal System	Triclinic	Triclinic	Monoclinic	Triclinic
Space Group	$P\bar{1}$	$P\bar{1}$	$P2_1/n$	$P\bar{1}$
***a* (Å)**	15.7795(11)	9.3728(4)	13.7878(9)	9.4734(4)
***b* (Å)**	17.1913(12)	18.0456(7)	18.1632(11)	20.0458(9)
***c* (Å)**	23.3021(16)	24.2143(10)	34.707(2)	26.0053(11)
α (deg)	84.3575(9)	92.6310(5)	90	98.7599(6)
β (deg)	81.1822(9)	100.7768(5)	97.4515(8)	91.6509(6)
γ (deg)	72.3591(8)	104.2950(5)	90	101.1373(6)
Volume (Å^3)	5943.7(7)	3880.5(3)	8618.3(9)	4780.3(4)
Z	4	2	4	2
ρ_{calcd} (Mg/m^3)	1.342	1.294	1.037	1.151
μ (mm^{-1})	2.551	1.971	1.767	1.605
R1[a] ($I > 2.0\sigma(I)$)	0.0429	0.0330	0.0340	0.0349
wR2 (all data)	0.1076	0.0779	0.0835	0.0801

[a]Definitions: $R1 = \Sigma||F_o| - |F_c||/ \Sigma |F_o|$, $wR2 = [\Sigma w(F_o^2 - F_c^2)^2/ \Sigma w(F_o^2)^2]^{1/2}$.

Goof = S = $[\Sigma[w(F_o^2-F_c^2)^2] / (n-p)]^{1/2}$ where n is the number of reflections and p is the total number of parameters refined.

X-ray Data Collection, Structure Solution and Refinement for $[(C_5Me_5)_2Th(C_6H_5)(THF)][BPh_4]$, 1. A colorless crystal of approximate dimensions 0.110 x 0.145 x 0.219 mm was mounted on a glass fiber and transferred to a Bruker SMART APEX II diffractometer. The APEX2[8] program package was used to determine the unit-cell parameters and for data collection (120 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT[9] and SADABS[10] to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL[11] program. There were no systematic absences nor any diffraction symmetry other than the Friedel condition. The centrosymmetric triclinic space group $P\bar{1}$ was assigned and later determined to be correct. The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors[12] for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model. There were two molecules of the formula-unit present (Z = 4). There were also two and one-half molecules of toluene solvent present per formula-unit. The half-molecule solvents were located about inversion centers. At convergence, wR2 = 0.1076 and Goof = 1.035 for 1337 variables refined against 25960 data (0.78Å), R1 = 0.0429 for those 19492 data with $I > 2.0\sigma(I)$.

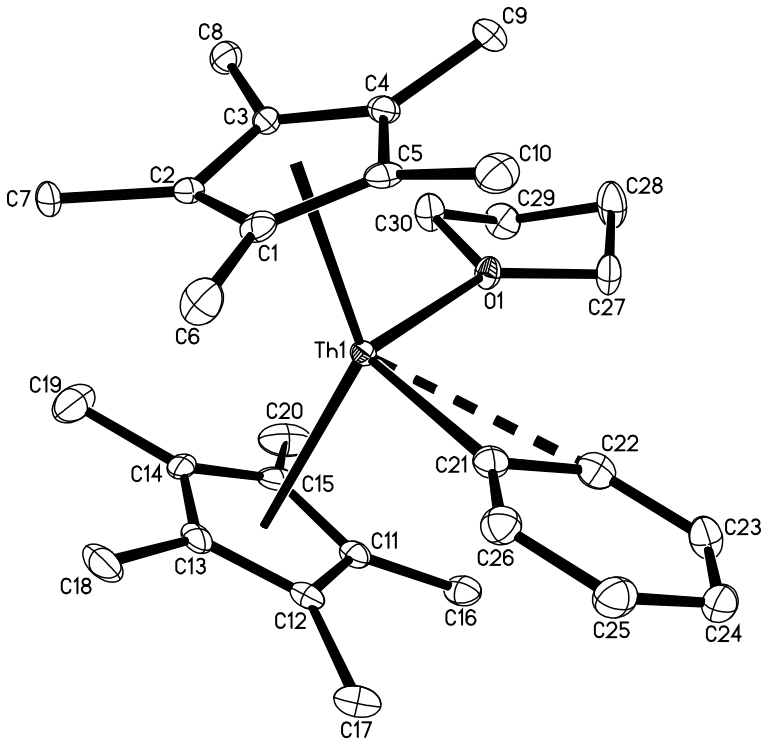


Figure S2. Thermal ellipsoid plot of cationic portion in $[(C_5Me_5)_2Th(C_6H_5)(THF)][BPh_4]$, **1**, only one of the two independent units are shown. Ellipsoids are drawn at the 50% probability level with hydrogens, BPh_4 anion and lattice solvent omitted for clarity.

Table S4. Crystal data and structure refinement for $[(C_5Me_5)_2Th(C_6H_5)(THF)][BPh_4]$, **1**.

Identification code	rrl12 (Ryan Langeslay)	
Empirical formula	$C_{54}\ H_{63}\ B\ O\ Th \bullet 2.5(C_7H_8)$	
Formula weight	1201.22	
Temperature	88(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 15.7795(11) Å	α = 84.3575(9)°.
	b = 17.1913(12) Å	β = 81.1822(9)°.
	c = 23.3021(16) Å	γ = 72.3591(8)°.
Volume	5943.7(7) $Å^3$	
Z	4	
Density (calculated)	1.342 Mg/m^3	
Absorption coefficient	2.551 mm^{-1}	
F(000)	2460	
Crystal color	colorless	
Crystal size	0.219 x 0.145 x 0.110 mm^3	
Theta range for data collection	1.245 to 27.103°	
Index ranges	$-20 \le h \le 20, -21 \le k \le 22, -29 \le l \le 28$	
Reflections collected	58798	
Independent reflections	25960 [R(int) = 0.0369]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.5880	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	25960 / 0 / 1337	
Goodness-of-fit on F^2	1.035	
Final R indices [I>2sigma(I) = 19492 data]	R1 = 0.0429, wR2 = 0.0979	
R indices (all data, 0.78Å)	R1 = 0.0674, wR2 = 0.1076	
Largest diff. peak and hole	4.572 and −0.886 e.$Å^{-3}$	

Table S5. Bond lengths [Å] and angles [°] for $[(C_5Me_5)_2Th(C_6H_5)(THF)][BPh_4]$, **1**.

Th(1)-Cnt1	2.507	C(14)-C(15)	1.396(7)
Th(1)-Cnt2	2.507	C(14)-C(19)	1.528(7)
Th(1)-C(21)	2.408(5)	C(15)-C(20)	1.511(7)
Th(1)-O(1)	2.476(3)	C(21)-C(22)	1.396(7)
Th(1)-C(14)	2.770(5)	C(21)-C(26)	1.404(7)
Th(1)-C(15)	2.771(5)	C(22)-C(23)	1.401(7)
Th(1)-C(5)	2.774(5)	C(23)-C(24)	1.367(7)
Th(1)-C(1)	2.775(5)	C(24)-C(25)	1.399(7)
Th(1)-C(11)	2.775(5)	C(25)-C(26)	1.373(7)
Th(1)-C(4)	2.778(5)	C(27)-C(28)	1.524(7)
Th(1)-C(13)	2.782(5)	C(28)-C(29)	1.509(7)
Th(1)-C(2)	2.787(5)	C(29)-C(30)	1.499(6)
Th(1)-C(3)	2.795(5)	Th(2)-Cnt3	2.516
Th(1)-C(12)	2.803(5)	Th(2)-Cnt4	2.505
Th(1)-C(22)	2.960(5)	Th(2)-C(51)	2.416(5)
O(1)-C(30)	1.471(5)	Th(2)-O(2)	2.470(3)
O(1)-C(27)	1.486(5)	Th(2)-C(42)	2.771(5)
C(1)-C(5)	1.409(7)	Th(2)-C(45)	2.775(5)
C(1)-C(2)	1.419(6)	Th(2)-C(32)	2.776(5)
C(1)-C(6)	1.517(6)	Th(2)-C(31)	2.778(5)
C(2)-C(3)	1.414(6)	Th(2)-C(43)	2.784(5)
C(2)-C(7)	1.518(6)	Th(2)-C(41)	2.787(4)
C(3)-C(4)	1.414(6)	Th(2)-C(44)	2.788(5)
C(3)-C(8)	1.509(6)	Th(2)-C(34)	2.790(5)
C(4)-C(5)	1.437(6)	Th(2)-C(33)	2.798(5)
C(4)-C(9)	1.512(6)	Th(2)-C(35)	2.802(5)
C(5)-C(10)	1.498(7)	O(2)-C(57)	1.468(6)
C(11)-C(15)	1.420(7)	O(2)-C(60)	1.487(5)
C(11)-C(12)	1.429(6)	C(31)-C(35)	1.421(7)
C(11)-C(16)	1.502(7)	C(31)-C(32)	1.424(7)
C(12)-C(13)	1.403(7)	C(31)-C(36)	1.498(7)
C(12)-C(17)	1.512(7)	C(32)-C(33)	1.420(7)
C(13)-C(14)	1.415(7)	C(32)-C(37)	1.508(7)
C(13)-C(18)	1.513(7)	C(33)-C(34)	1.406(7)

C(33)-C(38)	1.505(7)	C(69)-C(70)	1.375(8)
C(34)-C(35)	1.398(7)	C(70)-C(71)	1.390(8)
C(34)-C(39)	1.510(7)	C(71)-C(72)	1.400(7)
C(35)-C(40)	1.503(7)	C(73)-C(74)	1.392(7)
C(41)-C(42)	1.422(6)	C(73)-C(78)	1.412(6)
C(41)-C(45)	1.428(6)	C(74)-C(75)	1.409(7)
C(41)-C(46)	1.492(6)	C(75)-C(76)	1.383(7)
C(42)-C(43)	1.406(7)	C(76)-C(77)	1.386(7)
C(42)-C(47)	1.514(6)	C(77)-C(78)	1.387(7)
C(43)-C(44)	1.426(6)	C(79)-C(80)	1.403(6)
C(43)-C(48)	1.509(6)	C(79)-C(84)	1.406(6)
C(44)-C(45)	1.417(6)	C(80)-C(81)	1.396(7)
C(44)-C(49)	1.509(6)	C(81)-C(82)	1.376(7)
C(45)-C(50)	1.508(6)	C(82)-C(83)	1.386(7)
C(51)-C(56)	1.396(7)	C(83)-C(84)	1.389(7)
C(51)-C(52)	1.406(7)	B(2)-C(97)	1.637(8)
C(52)-C(53)	1.387(7)	B(2)-C(91)	1.640(7)
C(53)-C(54)	1.386(7)	B(2)-C(85)	1.645(7)
C(54)-C(55)	1.383(7)	B(2)-C(103)	1.659(7)
C(55)-C(56)	1.387(7)	C(85)-C(86)	1.400(7)
C(57)-C(58)	1.505(7)	C(85)-C(90)	1.402(7)
C(58)-C(59)	1.507(7)	C(86)-C(87)	1.394(7)
C(59)-C(60)	1.523(6)	C(87)-C(88)	1.378(7)
B(1)-C(73)	1.632(7)	C(88)-C(89)	1.381(7)
B(1)-C(79)	1.637(7)	C(89)-C(90)	1.397(7)
B(1)-C(67)	1.650(7)	C(91)-C(92)	1.400(6)
B(1)-C(61)	1.653(7)	C(91)-C(96)	1.405(6)
C(61)-C(62)	1.398(7)	C(92)-C(93)	1.398(7)
C(61)-C(66)	1.402(7)	C(93)-C(94)	1.375(7)
C(62)-C(63)	1.403(7)	C(94)-C(95)	1.392(7)
C(63)-C(64)	1.382(8)	C(95)-C(96)	1.396(7)
C(64)-C(65)	1.383(7)	C(97)-C(98)	1.397(7)
C(65)-C(66)	1.405(6)	C(97)-C(102)	1.402(7)
C(67)-C(68)	1.399(7)	C(98)-C(99)	1.394(8)
C(67)-C(72)	1.409(7)	C(99)-C(100)	1.357(9)
C(68)-C(69)	1.394(7)	C(100)-C(101)	1.377(9)

C(101)-C(102)	1.406(8)	C(138)-C(140)#1	1.383(11)
C(103)-C(104)	1.405(7)	C(138)-C(139)	1.460(11)
C(103)-C(108)	1.408(7)	C(139)-C(140)	1.288(11)
C(104)-C(105)	1.401(7)	C(140)-C(138)#1	1.383(11)
C(105)-C(106)	1.358(8)	C(142)-C(143)	1.57(2)
C(106)-C(107)	1.387(7)	C(143)-C(145)#2	1.447(14)
C(107)-C(108)	1.394(6)	C(143)-C(144)	1.511(14)
C(109)-C(114)	1.413(12)	C(144)-C(145)	1.263(12)
C(109)-C(115)	1.438(11)	C(145)-C(143)#2	1.447(14)
C(109)-C(110)	1.446(11)	Cnt1-Th(1)-C(21)	100.9
C(110)-C(111)	1.365(10)	Cnt1-Th(1)-C(22)	115.6
C(111)-C(112)	1.394(11)	Cnt1-Th(1)-O(1)	103.2
C(112)-C(113)	1.400(10)	Cnt2-Th(1)-C(21)	98.5
C(113)-C(114)	1.319(11)	Cnt2-Th(1)-C(22)	99.7
C(116)-C(117)	1.382(8)	Cnt2-Th(1)-O(1)	107.4
C(116)-C(121)	1.409(8)	Cnt1-Th(1)-Cnt2	135.6
C(116)-C(122)	1.497(8)	Cnt3-Th(2)-C(51)	97.8
C(117)-C(118)	1.363(9)	Cnt3-Th(2)-C(52)	100.4
C(118)-C(119)	1.369(9)	Cnt3-Th(2)-O(2)	108.8
C(119)-C(120)	1.372(9)	Cnt4-Th(2)-C(51)	99.7
C(120)-C(121)	1.347(8)	Cnt4-Th(2)-C(52)	113.1
C(123)-C(129)	1.379(11)	Cnt4-Th(2)-O(2)	102.6
C(123)-C(128)	1.387(10)	Cnt3-Th(2)-Cnt4	137.1
C(123)-C(124)	1.442(11)	C(21)-Th(1)-O(1)	109.20(13)
C(124)-C(125)	1.343(12)	C(21)-Th(1)-C(14)	119.83(16)
C(125)-C(126)	1.362(12)	O(1)-Th(1)-C(14)	109.24(14)
C(126)-C(127)	1.459(13)	C(21)-Th(1)-C(15)	117.55(15)
C(127)-C(128)	1.340(11)	O(1)-Th(1)-C(15)	84.40(13)
C(130)-C(131)	1.382(8)	C(14)-Th(1)-C(15)	29.18(15)
C(130)-C(135)	1.391(8)	C(21)-Th(1)-C(5)	76.54(15)
C(130)-C(136)	1.497(8)	O(1)-Th(1)-C(5)	102.93(13)
C(131)-C(132)	1.369(8)	C(14)-Th(1)-C(5)	134.38(15)
C(132)-C(133)	1.349(9)	C(15)-Th(1)-C(5)	161.44(15)
C(133)-C(134)	1.368(10)	C(21)-Th(1)-C(1)	84.32(15)
C(134)-C(135)	1.361(9)	O(1)-Th(1)-C(1)	127.69(13)
C(137)-C(138)	1.320(18)	C(14)-Th(1)-C(1)	105.81(15)

C(15)-Th(1)-C(1)	134.75(15)	C(5)-Th(1)-C(3)	48.93(13)
C(5)-Th(1)-C(1)	29.41(14)	C(1)-Th(1)-C(3)	48.62(13)
C(21)-Th(1)-C(11)	88.38(15)	C(11)-Th(1)-C(3)	145.24(14)
O(1)-Th(1)-C(11)	88.72(12)	C(4)-Th(1)-C(3)	29.39(13)
C(14)-Th(1)-C(11)	48.65(14)	C(13)-Th(1)-C(3)	115.27(14)
C(15)-Th(1)-C(11)	29.66(14)	C(2)-Th(1)-C(3)	29.35(12)
C(5)-Th(1)-C(11)	163.28(13)	C(21)-Th(1)-C(12)	73.01(15)
C(1)-Th(1)-C(11)	143.22(14)	O(1)-Th(1)-C(12)	117.51(12)
C(21)-Th(1)-C(4)	101.24(15)	C(14)-Th(1)-C(12)	48.50(14)
O(1)-Th(1)-C(4)	78.94(12)	C(15)-Th(1)-C(12)	48.64(14)
C(14)-Th(1)-C(4)	130.29(14)	C(5)-Th(1)-C(12)	135.32(14)
C(15)-Th(1)-C(4)	141.00(14)	C(1)-Th(1)-C(12)	114.79(14)
C(5)-Th(1)-C(4)	29.99(13)	C(11)-Th(1)-C(12)	29.67(13)
C(1)-Th(1)-C(4)	48.75(13)	C(4)-Th(1)-C(12)	163.50(13)
C(11)-Th(1)-C(4)	166.28(14)	C(13)-Th(1)-C(12)	29.10(14)
C(21)-Th(1)-C(13)	91.70(16)	C(2)-Th(1)-C(12)	118.78(14)
O(1)-Th(1)-C(13)	132.45(13)	C(3)-Th(1)-C(12)	144.38(14)
C(14)-Th(1)-C(13)	29.54(15)	C(21)-Th(1)-C(22)	27.80(14)
C(15)-Th(1)-C(13)	48.37(15)	O(1)-Th(1)-C(22)	82.53(12)
C(5)-Th(1)-C(13)	123.67(14)	C(14)-Th(1)-C(22)	125.28(14)
C(1)-Th(1)-C(13)	95.63(14)	C(15)-Th(1)-C(22)	108.26(15)
C(11)-Th(1)-C(13)	48.52(14)	C(5)-Th(1)-C(22)	89.74(14)
C(4)-Th(1)-C(13)	139.53(14)	C(1)-Th(1)-C(22)	107.06(14)
C(21)-Th(1)-C(2)	113.67(15)	C(11)-Th(1)-C(22)	79.80(14)
O(1)-Th(1)-C(2)	116.21(12)	C(4)-Th(1)-C(22)	104.22(14)
C(14)-Th(1)-C(2)	87.59(14)	C(13)-Th(1)-C(22)	104.77(15)
C(15)-Th(1)-C(2)	112.69(15)	C(2)-Th(1)-C(22)	136.06(14)
C(5)-Th(1)-C(2)	48.76(14)	C(3)-Th(1)-C(22)	133.55(14)
C(1)-Th(1)-C(2)	29.55(13)	C(12)-Th(1)-C(22)	78.11(14)
C(11)-Th(1)-C(2)	135.76(14)	C(30)-O(1)-C(27)	107.6(3)
C(4)-Th(1)-C(2)	48.55(13)	C(30)-O(1)-Th(1)	116.3(2)
C(13)-Th(1)-C(2)	91.10(14)	C(27)-O(1)-Th(1)	136.1(3)
C(21)-Th(1)-C(3)	125.46(15)	C(5)-C(1)-C(2)	108.6(4)
O(1)-Th(1)-C(3)	87.05(12)	C(5)-C(1)-C(6)	125.7(4)
C(14)-Th(1)-C(3)	100.92(14)	C(2)-C(1)-C(6)	125.4(4)
C(15)-Th(1)-C(3)	115.59(14)	C(5)-C(1)-Th(1)	75.3(3)

C(2)-C(1)-Th(1)	75.7(3)	C(11)-C(12)-Th(1)	74.1(3)
C(6)-C(1)-Th(1)	120.4(3)	C(17)-C(12)-Th(1)	124.0(3)
C(3)-C(2)-C(1)	108.1(4)	C(12)-C(13)-C(14)	108.6(4)
C(3)-C(2)-C(7)	124.3(4)	C(12)-C(13)-C(18)	124.3(5)
C(1)-C(2)-C(7)	125.9(4)	C(14)-C(13)-C(18)	127.0(5)
C(3)-C(2)-Th(1)	75.6(3)	C(12)-C(13)-Th(1)	76.3(3)
C(1)-C(2)-Th(1)	74.7(3)	C(14)-C(13)-Th(1)	74.7(3)
C(7)-C(2)-Th(1)	127.6(3)	C(18)-C(13)-Th(1)	119.3(3)
C(4)-C(3)-C(2)	108.0(4)	C(15)-C(14)-C(13)	108.1(4)
C(4)-C(3)-C(8)	126.5(4)	C(15)-C(14)-C(19)	125.0(5)
C(2)-C(3)-C(8)	124.9(4)	C(13)-C(14)-C(19)	126.3(5)
C(4)-C(3)-Th(1)	74.6(3)	C(15)-C(14)-Th(1)	75.5(3)
C(2)-C(3)-Th(1)	75.0(3)	C(13)-C(14)-Th(1)	75.7(3)
C(8)-C(3)-Th(1)	123.6(3)	C(19)-C(14)-Th(1)	121.6(3)
C(3)-C(4)-C(5)	108.0(4)	C(14)-C(15)-C(11)	108.4(4)
C(3)-C(4)-C(9)	128.2(4)	C(14)-C(15)-C(20)	126.4(5)
C(5)-C(4)-C(9)	123.4(4)	C(11)-C(15)-C(20)	124.3(5)
C(3)-C(4)-Th(1)	76.0(3)	C(14)-C(15)-Th(1)	75.4(3)
C(5)-C(4)-Th(1)	74.9(3)	C(11)-C(15)-Th(1)	75.3(3)
C(9)-C(4)-Th(1)	120.8(3)	C(20)-C(15)-Th(1)	124.1(3)
C(1)-C(5)-C(4)	107.3(4)	C(22)-C(21)-C(26)	115.1(4)
C(1)-C(5)-C(10)	127.4(4)	C(22)-C(21)-Th(1)	98.6(3)
C(4)-C(5)-C(10)	124.8(5)	C(26)-C(21)-Th(1)	146.2(4)
C(1)-C(5)-Th(1)	75.3(3)	C(21)-C(22)-C(23)	123.0(5)
C(4)-C(5)-Th(1)	75.1(3)	C(21)-C(22)-Th(1)	53.6(3)
C(10)-C(5)-Th(1)	121.9(3)	C(23)-C(22)-Th(1)	175.1(4)
C(15)-C(11)-C(12)	107.4(4)	C(24)-C(23)-C(22)	119.6(5)
C(15)-C(11)-C(16)	125.9(4)	C(23)-C(24)-C(25)	119.3(5)
C(12)-C(11)-C(16)	126.6(4)	C(26)-C(25)-C(24)	120.1(5)
C(15)-C(11)-Th(1)	75.0(3)	C(25)-C(26)-C(21)	122.8(5)
C(12)-C(11)-Th(1)	76.2(3)	O(1)-C(27)-C(28)	104.7(4)
C(16)-C(11)-Th(1)	117.0(3)	C(29)-C(28)-C(27)	102.7(4)
C(13)-C(12)-C(11)	107.5(4)	C(30)-C(29)-C(28)	100.9(4)
C(13)-C(12)-C(17)	126.6(4)	O(1)-C(30)-C(29)	104.7(4)
C(11)-C(12)-C(17)	125.3(4)	C(51)-Th(2)-O(2)	107.85(13)
C(13)-C(12)-Th(1)	74.6(3)	C(51)-Th(2)-C(42)	82.74(16)

O(2)-Th(2)-C(42)	126.47(12)	C(42)-Th(2)-C(34)	99.39(15)
C(51)-Th(2)-C(45)	124.61(16)	C(45)-Th(2)-C(34)	124.04(15)
O(2)-Th(2)-C(45)	87.41(12)	C(32)-Th(2)-C(34)	48.51(14)
C(42)-Th(2)-C(45)	48.82(13)	C(31)-Th(2)-C(34)	48.59(14)
C(51)-Th(2)-C(32)	121.87(16)	C(43)-Th(2)-C(34)	125.67(14)
O(2)-Th(2)-C(32)	91.08(13)	C(41)-Th(2)-C(34)	98.24(15)
C(42)-Th(2)-C(32)	128.31(15)	C(44)-Th(2)-C(34)	146.11(15)
C(45)-Th(2)-C(32)	110.27(14)	C(51)-Th(2)-C(33)	112.27(16)
C(51)-Th(2)-C(31)	96.33(16)	O(2)-Th(2)-C(33)	120.01(13)
O(2)-Th(2)-C(31)	84.89(12)	C(42)-Th(2)-C(33)	101.56(15)
C(42)-Th(2)-C(31)	147.53(14)	C(45)-Th(2)-C(33)	103.53(14)
C(45)-Th(2)-C(31)	138.66(14)	C(32)-Th(2)-C(33)	29.51(14)
C(32)-Th(2)-C(31)	29.71(14)	C(31)-Th(2)-C(33)	48.68(14)
C(51)-Th(2)-C(43)	75.88(15)	C(43)-Th(2)-C(33)	130.73(14)
O(2)-Th(2)-C(43)	100.79(12)	C(41)-Th(2)-C(33)	86.34(14)
C(42)-Th(2)-C(43)	29.33(14)	C(44)-Th(2)-C(33)	132.46(14)
C(45)-Th(2)-C(43)	48.78(14)	C(34)-Th(2)-C(33)	29.15(15)
C(32)-Th(2)-C(43)	154.58(15)	C(51)-Th(2)-C(35)	73.55(16)
C(31)-Th(2)-C(43)	171.43(14)	O(2)-Th(2)-C(35)	109.40(13)
C(51)-Th(2)-C(41)	112.09(15)	C(42)-Th(2)-C(35)	123.69(14)
O(2)-Th(2)-C(41)	117.11(12)	C(45)-Th(2)-C(35)	151.15(14)
C(42)-Th(2)-C(41)	29.65(13)	C(32)-Th(2)-C(35)	48.39(14)
C(45)-Th(2)-C(41)	29.75(13)	C(31)-Th(2)-C(35)	29.49(14)
C(32)-Th(2)-C(41)	105.80(15)	C(43)-Th(2)-C(35)	142.16(14)
C(31)-Th(2)-C(41)	133.96(14)	C(41)-Th(2)-C(35)	127.18(14)
C(43)-Th(2)-C(41)	48.78(14)	C(44)-Th(2)-C(35)	171.67(14)
C(51)-Th(2)-C(44)	100.66(15)	C(34)-Th(2)-C(35)	28.94(15)
O(2)-Th(2)-C(44)	77.88(12)	C(33)-Th(2)-C(35)	47.90(15)
C(42)-Th(2)-C(44)	48.68(13)	C(57)-O(2)-C(60)	108.6(3)
C(45)-Th(2)-C(44)	29.50(13)	C(57)-O(2)-Th(2)	116.0(3)
C(32)-Th(2)-C(44)	137.34(14)	C(60)-O(2)-Th(2)	135.1(2)
C(31)-Th(2)-C(44)	158.78(14)	C(35)-C(31)-C(32)	107.0(4)
C(43)-Th(2)-C(44)	29.65(14)	C(35)-C(31)-C(36)	125.5(5)
C(41)-Th(2)-C(44)	48.87(13)	C(32)-C(31)-C(36)	127.4(5)
C(51)-Th(2)-C(34)	83.13(16)	C(35)-C(31)-Th(2)	76.2(3)
O(2)-Th(2)-C(34)	133.43(13)	C(32)-C(31)-Th(2)	75.0(3)

C(36)-C(31)-Th(2)	117.5(3)	C(47)-C(42)-Th(2)	121.0(3)
C(33)-C(32)-C(31)	107.8(4)	C(42)-C(43)-C(44)	108.0(4)
C(33)-C(32)-C(37)	124.2(5)	C(42)-C(43)-C(48)	127.5(4)
C(31)-C(32)-C(37)	127.0(5)	C(44)-C(43)-C(48)	124.1(4)
C(33)-C(32)-Th(2)	76.1(3)	C(42)-C(43)-Th(2)	74.8(3)
C(31)-C(32)-Th(2)	75.2(3)	C(44)-C(43)-Th(2)	75.4(3)
C(37)-C(32)-Th(2)	123.5(3)	C(48)-C(43)-Th(2)	121.7(3)
C(34)-C(33)-C(32)	108.0(4)	C(45)-C(44)-C(43)	107.7(4)
C(34)-C(33)-C(38)	126.2(5)	C(45)-C(44)-C(49)	126.2(4)
C(32)-C(33)-C(38)	124.6(5)	C(43)-C(44)-C(49)	125.6(4)
C(34)-C(33)-Th(2)	75.1(3)	C(45)-C(44)-Th(2)	74.7(3)
C(32)-C(33)-Th(2)	74.4(3)	C(43)-C(44)-Th(2)	75.0(3)
C(38)-C(33)-Th(2)	126.4(4)	C(49)-C(44)-Th(2)	122.6(3)
C(35)-C(34)-C(33)	108.4(4)	C(44)-C(45)-C(41)	108.4(4)
C(35)-C(34)-C(39)	125.4(5)	C(44)-C(45)-C(50)	127.1(4)
C(33)-C(34)-C(39)	126.0(5)	C(41)-C(45)-C(50)	124.1(4)
C(35)-C(34)-Th(2)	76.0(3)	C(44)-C(45)-Th(2)	75.8(3)
C(33)-C(34)-Th(2)	75.7(3)	C(41)-C(45)-Th(2)	75.6(3)
C(39)-C(34)-Th(2)	119.3(3)	C(50)-C(45)-Th(2)	121.2(3)
C(34)-C(35)-C(31)	108.8(4)	C(56)-C(51)-C(52)	115.8(4)
C(34)-C(35)-C(40)	126.3(5)	C(56)-C(51)-Th(2)	145.7(4)
C(31)-C(35)-C(40)	124.4(5)	C(52)-C(51)-Th(2)	98.5(3)
C(34)-C(35)-Th(2)	75.0(3)	C(53)-C(52)-C(51)	123.2(5)
C(31)-C(35)-Th(2)	74.3(3)	C(53)-C(52)-Th(2)	176.8(4)
C(40)-C(35)-Th(2)	123.3(4)	C(51)-C(52)-Th(2)	53.6(3)
C(42)-C(41)-C(45)	107.1(4)	C(54)-C(53)-C(52)	118.9(5)
C(42)-C(41)-C(46)	126.7(4)	C(55)-C(54)-C(53)	119.5(5)
C(45)-C(41)-C(46)	124.8(4)	C(54)-C(55)-C(56)	120.7(5)
C(42)-C(41)-Th(2)	74.5(3)	C(55)-C(56)-C(51)	121.8(5)
C(45)-C(41)-Th(2)	74.6(3)	O(2)-C(57)-C(58)	105.2(4)
C(46)-C(41)-Th(2)	127.0(3)	C(57)-C(58)-C(59)	102.3(4)
C(43)-C(42)-C(41)	108.8(4)	C(58)-C(59)-C(60)	102.6(4)
C(43)-C(42)-C(47)	125.9(4)	O(2)-C(60)-C(59)	104.2(4)
C(41)-C(42)-C(47)	124.8(4)	C(73)-B(1)-C(79)	103.5(4)
C(43)-C(42)-Th(2)	75.8(3)	C(73)-B(1)-C(67)	110.8(4)
C(41)-C(42)-Th(2)	75.8(3)	C(79)-B(1)-C(67)	113.5(4)

C(73)-B(1)-C(61)	112.1(4)	C(97)-B(2)-C(85)	112.9(4)
C(79)-B(1)-C(61)	113.0(4)	C(91)-B(2)-C(85)	112.2(4)
C(67)-B(1)-C(61)	104.3(4)	C(97)-B(2)-C(103)	111.0(4)
C(62)-C(61)-C(66)	115.6(4)	C(91)-B(2)-C(103)	111.9(4)
C(62)-C(61)-B(1)	122.5(4)	C(85)-B(2)-C(103)	104.0(4)
C(66)-C(61)-B(1)	121.7(4)	C(86)-C(85)-C(90)	115.0(4)
C(61)-C(62)-C(63)	122.0(5)	C(86)-C(85)-B(2)	124.0(4)
C(64)-C(63)-C(62)	121.0(5)	C(90)-C(85)-B(2)	120.8(5)
C(63)-C(64)-C(65)	118.5(5)	C(87)-C(86)-C(85)	123.1(5)
C(64)-C(65)-C(66)	120.3(5)	C(88)-C(87)-C(86)	120.0(5)
C(61)-C(66)-C(65)	122.6(5)	C(87)-C(88)-C(89)	119.0(5)
C(68)-C(67)-C(72)	115.2(4)	C(88)-C(89)-C(90)	120.4(5)
C(68)-C(67)-B(1)	121.6(4)	C(89)-C(90)-C(85)	122.5(5)
C(72)-C(67)-B(1)	123.0(4)	C(92)-C(91)-C(96)	114.0(5)
C(69)-C(68)-C(67)	123.1(5)	C(92)-C(91)-B(2)	122.7(4)
C(70)-C(69)-C(68)	120.2(5)	C(96)-C(91)-B(2)	123.1(4)
C(69)-C(70)-C(71)	119.0(5)	C(93)-C(92)-C(91)	124.0(4)
C(70)-C(71)-C(72)	120.3(5)	C(94)-C(93)-C(92)	119.5(5)
C(71)-C(72)-C(67)	122.1(5)	C(93)-C(94)-C(95)	119.2(5)
C(74)-C(73)-C(78)	114.7(5)	C(94)-C(95)-C(96)	119.8(5)
C(74)-C(73)-B(1)	124.1(4)	C(95)-C(96)-C(91)	123.3(5)
C(78)-C(73)-B(1)	121.0(4)	C(98)-C(97)-C(102)	113.6(5)
C(73)-C(74)-C(75)	122.9(5)	C(98)-C(97)-B(2)	122.8(5)
C(76)-C(75)-C(74)	119.7(5)	C(102)-C(97)-B(2)	123.4(5)
C(75)-C(76)-C(77)	119.6(5)	C(99)-C(98)-C(97)	124.0(6)
C(76)-C(77)-C(78)	119.3(5)	C(100)-C(99)-C(98)	120.7(6)
C(77)-C(78)-C(73)	123.8(5)	C(99)-C(100)-C(101)	118.1(6)
C(80)-C(79)-C(84)	114.6(4)	C(100)-C(101)-C(102)	121.0(5)
C(80)-C(79)-B(1)	122.7(4)	C(97)-C(102)-C(101)	122.5(5)
C(84)-C(79)-B(1)	122.5(4)	C(104)-C(103)-C(108)	115.3(4)
C(81)-C(80)-C(79)	122.8(4)	C(104)-C(103)-B(2)	121.3(4)
C(82)-C(81)-C(80)	120.7(5)	C(108)-C(103)-B(2)	123.2(4)
C(81)-C(82)-C(83)	118.6(5)	C(105)-C(104)-C(103)	122.2(5)
C(82)-C(83)-C(84)	120.3(4)	C(106)-C(105)-C(104)	120.6(5)
C(83)-C(84)-C(79)	123.1(4)	C(105)-C(106)-C(107)	119.5(5)
C(97)-B(2)-C(91)	105.1(4)	C(106)-C(107)-C(108)	120.1(5)

C(107)-C(108)-C(103)	122.2(5)	C(125)-C(126)-C(127)	116.7(10)
C(114)-C(109)-C(115)	122.0(9)	C(128)-C(127)-C(126)	123.0(9)
C(114)-C(109)-C(110)	119.5(7)	C(127)-C(128)-C(123)	118.6(9)
C(115)-C(109)-C(110)	118.4(10)	C(131)-C(130)-C(135)	117.8(6)
C(111)-C(110)-C(109)	116.3(9)	C(131)-C(130)-C(136)	120.7(6)
C(110)-C(111)-C(112)	122.5(8)	C(135)-C(130)-C(136)	121.5(6)
C(111)-C(112)-C(113)	120.2(7)	C(132)-C(131)-C(130)	120.8(6)
C(114)-C(113)-C(112)	119.2(9)	C(133)-C(132)-C(131)	120.8(6)
C(113)-C(114)-C(109)	122.3(9)	C(132)-C(133)-C(134)	119.1(6)
C(117)-C(116)-C(121)	116.7(6)	C(135)-C(134)-C(133)	121.3(7)
C(117)-C(116)-C(122)	122.1(6)	C(134)-C(135)-C(130)	120.0(6)
C(121)-C(116)-C(122)	121.2(6)	C(137)-C(138)-C(140)#1	121.5(12)
C(118)-C(117)-C(116)	121.4(6)	C(137)-C(138)-C(139)	123.6(11)
C(117)-C(118)-C(119)	120.9(6)	C(140)#1-C(138)-C(139)	114.8(8)
C(118)-C(119)-C(120)	118.7(6)	C(140)-C(139)-C(138)	120.6(9)
C(121)-C(120)-C(119)	121.1(6)	C(139)-C(140)-C(138)#1	124.6(9)
C(120)-C(121)-C(116)	121.2(6)	C(145)#2-C(143)-C(144)	106.6(10)
C(129)-C(123)-C(128)	120.0(10)	C(145)#2-C(143)-C(142)	118.2(12)
C(129)-C(123)-C(124)	120.7(8)	C(144)-C(143)-C(142)	135.0(13)
C(128)-C(123)-C(124)	119.2(9)	C(145)-C(144)-C(143)	132.4(11)
C(125)-C(124)-C(123)	120.5(8)	C(144)-C(145)-C(143)#2	120.9(11)
C(124)-C(125)-C(126)	122.0(11)		

Symmetry transformations used to generate equivalent atoms:

#1 -x-2,-y,-z+1 #2 -x,-y-1,-z+2

X-ray Data Collection, Structure Solution and Refinement for $[(C_5Me_5)_2Th(NCMe)_5][BPh_4]_2$, 2-RT. A colorless crystal of approximate dimensions 0.086 x 0.321 x 0.429 mm was mounted on a glass fiber and transferred to a Bruker SMART APEX II diffractometer. The APEX2[13] program package was used to determine the unit-cell parameters and for data collection (30 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT[14] and SADABS[15] to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL[16] program. There were no systematic absences nor any diffraction symmetry other than the Friedel condition. The centrosymmetric triclinic space group $P\bar{1}$ was assigned and later determined to be correct.

The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors[12] for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model. There were three molecules of acetonitrile solvent and one-half molecule of hexane solvent present. The hexane was located about an inversion center. The solvents were refined using isotropic thermal parameters due to high thermal motion. Carbon atoms C(58), C(59) and C(60) were disordered and included using multiple components, partial site-occupancy-factors and isotropic thermal parameters.

At convergence, wR2 = 0.0779 and Goof = 1.071 for 842 variables refined against 19278 data (0.73Å), R1 = 0.0330 for those 17901 data with $I > 2.0\sigma(I)$.

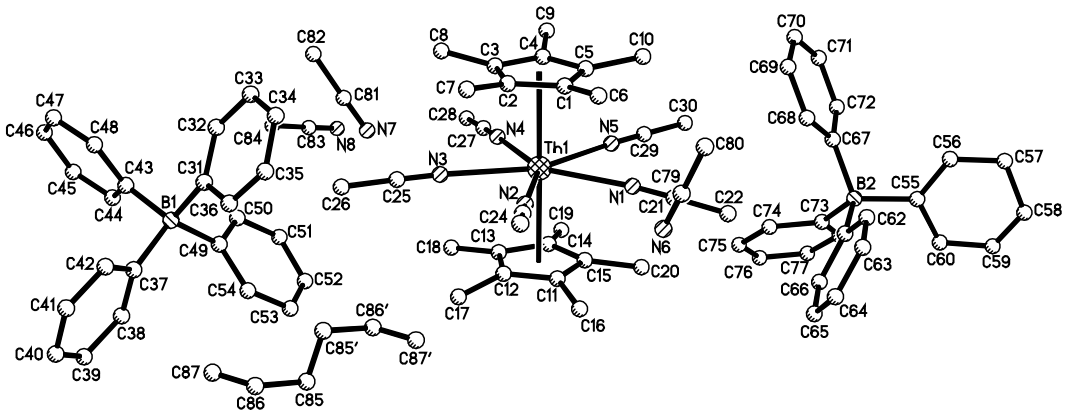


Figure S3. Thermal ellipsoid plot of $[(C_5Me_5)_2Th(NCMe)_5][BPh_4]_2$, **2-RT**, shown at the 50% probability level with hydrogens omitted for clarity.

Table S6. Crystal data and structure refinement for $[(C_5Me_5)_2Th(NCMe)_5][BPh_4]_2$, **2-RT**.

Identification code	rrl55 (Ryan Langeslay)	
Empirical formula	$C_{87}\ H_{101}\ B_2\ N_8\ Th$	
Formula weight	1512.41	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 9.3728(4) Å	α = 92.6310(5)°.
	b = 18.0456(7) Å	β = 100.7768(5)°.
	c = 24.2143(10) Å	γ = 104.2950(5)°.
Volume	3880.5(3) $Å^3$	
Z	2	
Density (calculated)	1.294 Mg/m^3	
Absorption coefficient	1.971 mm^{-1}	
F(000)	1558	
Crystal color	colorless	
Crystal size	0.429 x 0.321 x 0.086 mm^3	
Theta range for data collection	1.518 to 29.181°	
Index ranges	$-12 \le h \le 12, -24 \le k \le 24, -32 \le l \le 31$	
Reflections collected	48846	
Independent reflections	19278 [R(int) = 0.0198]	
Completeness to theta = 25.500°	99.8 %	
Absorption correction	Numerical	
Max. and min. transmission	0.6410 and 0.4064	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	19278 / 0 / 842	
Goodness-of-fit on F^2	1.071	
Final R indices [I>2sigma(I) = 17901 data]	R1 = 0.0330, wR2 = 0.0764	
R indices (all data, 0.73Å)	R1 = 0.0370, wR2 = 0.0779	
Largest diff. peak and hole	2.517 and −0.859 $e.Å^{-3}$	

Table S7. Bond lengths [Å] and angles [°] for $[(C_5Me_5)_2Th(NCMe)_5][BPh_4]_2$, **2-RT.**

Th(1)-Cnt1	2.601	C(11)-C(16)	1.518(5)
Th(1)-Cnt2	2.594	C(12)-C(13)	1.410(4)
Th(1)-N(3)	2.555(2)	C(12)-C(17)	1.509(4)
Th(1)-N(4)	2.584(3)	C(13)-C(14)	1.421(4)
Th(1)-N(1)	2.604(3)	C(13)-C(18)	1.502(4)
Th(1)-N(5)	2.605(3)	C(14)-C(15)	1.411(5)
Th(1)-N(2)	2.610(3)	C(14)-C(19)	1.505(4)
Th(1)-C(14)	2.855(3)	C(15)-C(20)	1.507(5)
Th(1)-C(5)	2.856(3)	C(21)-C(22)	1.450(5)
Th(1)-C(11)	2.857(3)	C(23)-C(24)	1.453(5)
Th(1)-C(12)	2.860(3)	C(25)-C(26)	1.443(5)
Th(1)-C(15)	2.860(3)	C(27)-C(28)	1.464(5)
Th(1)-C(4)	2.861(3)	C(29)-C(30)	1.447(4)
Th(1)-C(13)	2.861(3)	B(1)-C(37)	1.640(4)
Th(1)-C(1)	2.863(3)	B(1)-C(43)	1.645(4)
Th(1)-C(3)	2.873(3)	B(1)-C(31)	1.646(4)
Th(1)-C(2)	2.881(3)	B(1)-C(49)	1.648(5)
N(1)-C(21)	1.134(4)	C(31)-C(32)	1.402(4)
N(2)-C(23)	1.139(4)	C(31)-C(36)	1.402(4)
N(3)-C(25)	1.129(4)	C(32)-C(33)	1.396(5)
N(4)-C(27)	1.133(4)	C(33)-C(34)	1.383(5)
N(5)-C(29)	1.136(4)	C(34)-C(35)	1.383(5)
C(1)-C(2)	1.416(4)	C(35)-C(36)	1.398(5)
C(1)-C(5)	1.421(4)	C(37)-C(42)	1.400(4)
C(1)-C(6)	1.507(5)	C(37)-C(38)	1.403(4)
C(2)-C(3)	1.417(4)	C(38)-C(39)	1.394(5)
C(2)-C(7)	1.510(4)	C(39)-C(40)	1.380(5)
C(3)-C(4)	1.415(4)	C(40)-C(41)	1.379(5)
C(3)-C(8)	1.505(4)	C(41)-C(42)	1.396(4)
C(4)-C(5)	1.415(5)	C(43)-C(48)	1.395(5)
C(4)-C(9)	1.507(4)	C(43)-C(44)	1.408(5)
C(5)-C(10)	1.509(4)	C(44)-C(45)	1.382(6)
C(11)-C(12)	1.407(4)	C(45)-C(46)	1.366(8)
C(11)-C(15)	1.413(5)	C(46)-C(47)	1.397(8)

C(47)-C(48)	1.390(5)	C(63)-C(64)	1.386(7)
C(49)-C(50)	1.407(5)	C(64)-C(65)	1.383(7)
C(49)-C(54)	1.412(5)	C(65)-C(66)	1.399(5)
C(50)-C(51)	1.412(6)	C(67)-C(68)	1.387(5)
C(51)-C(52)	1.374(7)	C(67)-C(72)	1.397(5)
C(52)-C(53)	1.372(7)	C(68)-C(69)	1.399(5)
C(53)-C(54)	1.400(5)	C(69)-C(70)	1.360(6)
B(2)-C(73)	1.639(6)	C(70)-C(71)	1.378(6)
B(2)-C(55)	1.644(5)	C(71)-C(72)	1.391(5)
B(2)-C(67)	1.651(5)	C(73)-C(74)	1.399(5)
B(2)-C(61)	1.652(5)	C(73)-C(78)	1.409(5)
C(55)-C(60B)	1.331(16)	C(74)-C(75)	1.404(5)
C(55)-C(56)	1.384(6)	C(75)-C(76)	1.359(6)
C(55)-C(60)	1.479(7)	C(76)-C(77)	1.328(8)
C(56)-C(57)	1.402(5)	C(77)-C(78)	1.425(7)
C(57)-C(58B)	1.146(11)	N(6)-C(79)	1.138(5)
C(57)-C(58)	1.612(13)	C(79)-C(80)	1.448(5)
C(57)-C(59B)	2.007(18)	N(7)-C(81)	1.122(6)
C(58)-C(59)	1.263(14)	C(81)-C(82)	1.453(8)
C(59)-C(60)	1.388(8)	N(8)-C(83)	1.144(8)
C(58B)-C(59B)	1.26(2)	C(83)-C(84)	1.416(8)
C(59B)-C(60B)	1.43(2)	C(85)-C(85)#1	1.320(15)
C(61)-C(62)	1.395(5)	C(85)-C(86)	1.491(14)
C(61)-C(66)	1.402(4)	C(86)-C(87)	1.195(13)
C(62)-C(63)	1.378(6)		

Cnt1-Th(1)-N(1)	90.7	Cnt1-Th(1)-Cnt2	179.1
Cnt1-Th(1)-N(2)	88.3	N(3)-Th(1)-N(4)	75.11(9)
Cnt1-Th(1)-N(3)	89.6	N(3)-Th(1)-N(1)	143.08(9)
Cnt1-Th(1)-N(4)	90.6	N(4)-Th(1)-N(1)	141.80(9)
Cnt1-Th(1)-N(5)	90.5	N(3)-Th(1)-N(5)	146.81(9)
Cnt2-Th(1)-N(1)	89.4	N(4)-Th(1)-N(5)	71.69(9)
Cnt2-Th(1)-N(2)	90.9	N(1)-Th(1)-N(5)	70.12(9)
Cnt2-Th(1)-N(3)	89.8	N(3)-Th(1)-N(2)	71.82(9)
Cnt2-Th(1)-N(4)	89.8	N(4)-Th(1)-N(2)	146.92(9)
Cnt2-Th(1)-N(5)	90.4	N(1)-Th(1)-N(2)	71.29(9)

N(5)-Th(1)-N(2)	141.36(9)	N(3)-Th(1)-C(4)	95.84(8)
N(3)-Th(1)-C(14)	99.35(9)	N(4)-Th(1)-C(4)	69.16(9)
N(4)-Th(1)-C(14)	70.42(8)	N(1)-Th(1)-C(4)	99.72(9)
N(1)-Th(1)-C(14)	95.25(9)	N(5)-Th(1)-C(4)	72.15(8)
N(5)-Th(1)-C(14)	69.85(8)	N(2)-Th(1)-C(4)	113.21(8)
N(2)-Th(1)-C(14)	115.73(8)	C(14)-Th(1)-C(4)	131.06(9)
N(3)-Th(1)-C(5)	114.45(8)	C(5)-Th(1)-C(4)	28.66(10)
N(4)-Th(1)-C(5)	95.50(9)	C(11)-Th(1)-C(4)	168.93(9)
N(1)-Th(1)-C(5)	71.85(9)	C(12)-Th(1)-C(4)	161.74(9)
N(5)-Th(1)-C(5)	69.06(8)	C(15)-Th(1)-C(4)	143.21(9)
N(2)-Th(1)-C(5)	97.27(9)	N(3)-Th(1)-C(13)	71.24(8)
C(14)-Th(1)-C(5)	138.90(9)	N(4)-Th(1)-C(13)	69.50(8)
N(3)-Th(1)-C(11)	95.21(9)	N(1)-Th(1)-C(13)	114.24(8)
N(4)-Th(1)-C(11)	114.59(9)	N(5)-Th(1)-C(13)	97.03(8)
N(1)-Th(1)-C(11)	70.76(9)	N(2)-Th(1)-C(13)	100.11(8)
N(5)-Th(1)-C(11)	98.71(9)	C(14)-Th(1)-C(13)	28.78(9)
N(2)-Th(1)-C(11)	69.83(8)	C(5)-Th(1)-C(13)	162.61(9)
C(14)-Th(1)-C(11)	47.13(9)	C(11)-Th(1)-C(13)	47.04(9)
C(5)-Th(1)-C(11)	142.60(9)	C(12)-Th(1)-C(13)	28.54(9)
N(3)-Th(1)-C(12)	68.74(8)	C(15)-Th(1)-C(13)	47.16(9)
N(4)-Th(1)-C(12)	96.55(9)	C(4)-Th(1)-C(13)	138.59(9)
N(1)-Th(1)-C(12)	98.53(9)	N(3)-Th(1)-C(1)	98.26(8)
N(5)-Th(1)-C(12)	115.20(8)	N(4)-Th(1)-C(1)	115.42(8)
N(2)-Th(1)-C(12)	72.30(8)	N(1)-Th(1)-C(1)	69.77(9)
C(14)-Th(1)-C(12)	47.20(8)	N(5)-Th(1)-C(1)	95.58(8)
C(5)-Th(1)-C(12)	167.95(9)	N(2)-Th(1)-C(1)	69.28(8)
C(11)-Th(1)-C(12)	28.51(9)	C(14)-Th(1)-C(1)	162.37(9)
N(3)-Th(1)-C(15)	114.56(8)	C(5)-Th(1)-C(1)	28.78(9)
N(4)-Th(1)-C(15)	98.03(9)	C(11)-Th(1)-C(1)	129.98(9)
N(1)-Th(1)-C(15)	68.55(9)	C(12)-Th(1)-C(1)	141.58(9)
N(5)-Th(1)-C(15)	71.08(9)	C(15)-Th(1)-C(1)	138.31(9)
N(2)-Th(1)-C(15)	96.34(9)	C(4)-Th(1)-C(1)	47.30(9)
C(14)-Th(1)-C(15)	28.59(10)	C(13)-Th(1)-C(1)	167.37(9)
C(5)-Th(1)-C(15)	130.96(9)	N(3)-Th(1)-C(3)	69.00(8)
C(11)-Th(1)-C(15)	28.61(9)	N(4)-Th(1)-C(3)	72.42(8)
C(12)-Th(1)-C(15)	47.09(9)	N(1)-Th(1)-C(3)	115.45(9)

N(5)-Th(1)-C(3)	100.14(8)	C(1)-C(2)-C(7)	125.7(3)
N(2)-Th(1)-C(3)	94.68(8)	C(3)-C(2)-C(7)	125.2(3)
C(14)-Th(1)-C(3)	142.80(9)	C(1)-C(2)-Th(1)	75.02(15)
C(5)-Th(1)-C(3)	47.11(9)	C(3)-C(2)-Th(1)	75.42(15)
C(11)-Th(1)-C(3)	161.14(9)	C(7)-C(2)-Th(1)	124.33(19)
C(12)-Th(1)-C(3)	137.74(9)	C(4)-C(3)-C(2)	108.0(3)
C(15)-Th(1)-C(3)	168.98(9)	C(4)-C(3)-C(8)	125.5(3)
C(4)-Th(1)-C(3)	28.56(8)	C(2)-C(3)-C(8)	125.8(3)
C(13)-Th(1)-C(3)	130.30(9)	C(4)-C(3)-Th(1)	75.25(16)
C(1)-Th(1)-C(3)	47.17(9)	C(2)-C(3)-Th(1)	76.06(16)
N(3)-Th(1)-C(2)	70.65(8)	C(8)-C(3)-Th(1)	122.48(19)
N(4)-Th(1)-C(2)	100.39(8)	C(3)-C(4)-C(5)	108.0(3)
N(1)-Th(1)-C(2)	96.48(9)	C(3)-C(4)-C(9)	125.1(3)
N(5)-Th(1)-C(2)	115.01(8)	C(5)-C(4)-C(9)	126.0(3)
N(2)-Th(1)-C(2)	67.84(8)	C(3)-C(4)-Th(1)	76.19(15)
C(14)-Th(1)-C(2)	168.26(9)	C(5)-C(4)-Th(1)	75.45(16)
C(5)-Th(1)-C(2)	47.04(8)	C(9)-C(4)-Th(1)	122.84(19)
C(11)-Th(1)-C(2)	137.65(9)	C(4)-C(5)-C(1)	108.1(3)
C(12)-Th(1)-C(2)	129.76(8)	C(4)-C(5)-C(10)	125.2(3)
C(15)-Th(1)-C(2)	161.58(10)	C(1)-C(5)-C(10)	125.9(3)
C(4)-Th(1)-C(2)	47.02(8)	C(4)-C(5)-Th(1)	75.89(16)
C(13)-Th(1)-C(2)	141.89(8)	C(1)-C(5)-Th(1)	75.90(15)
C(1)-Th(1)-C(2)	28.53(8)	C(10)-C(5)-Th(1)	122.4(2)
C(3)-Th(1)-C(2)	28.52(9)	C(12)-C(11)-C(15)	108.3(3)
C(21)-N(1)-Th(1)	175.4(3)	C(12)-C(11)-C(16)	123.4(3)
C(23)-N(2)-Th(1)	169.1(2)	C(15)-C(11)-C(16)	127.5(3)
C(25)-N(3)-Th(1)	172.1(3)	C(12)-C(11)-Th(1)	75.87(15)
C(27)-N(4)-Th(1)	171.5(2)	C(15)-C(11)-Th(1)	75.84(16)
C(29)-N(5)-Th(1)	175.0(3)	C(16)-C(11)-Th(1)	122.7(2)
C(2)-C(1)-C(5)	107.6(3)	C(11)-C(12)-C(13)	108.1(3)
C(2)-C(1)-C(6)	126.5(3)	C(11)-C(12)-C(17)	125.9(3)
C(5)-C(1)-C(6)	125.0(3)	C(13)-C(12)-C(17)	125.1(3)
C(2)-C(1)-Th(1)	76.45(16)	C(11)-C(12)-Th(1)	75.62(16)
C(5)-C(1)-Th(1)	75.32(16)	C(13)-C(12)-Th(1)	75.78(15)
C(6)-C(1)-Th(1)	122.50(19)	C(17)-C(12)-Th(1)	123.13(19)
C(1)-C(2)-C(3)	108.2(3)	C(12)-C(13)-C(14)	107.8(3)

C(12)-C(13)-C(18)	126.7(3)	C(42)-C(37)-C(38)	114.7(3)
C(14)-C(13)-C(18)	124.7(3)	C(42)-C(37)-B(1)	123.6(3)
C(12)-C(13)-Th(1)	75.67(16)	C(38)-C(37)-B(1)	121.2(3)
C(14)-C(13)-Th(1)	75.36(16)	C(39)-C(38)-C(37)	123.4(3)
C(18)-C(13)-Th(1)	122.6(2)	C(40)-C(39)-C(38)	120.0(3)
C(15)-C(14)-C(13)	107.9(3)	C(41)-C(40)-C(39)	118.7(3)
C(15)-C(14)-C(19)	124.6(3)	C(40)-C(41)-C(42)	120.8(3)
C(13)-C(14)-C(19)	126.7(3)	C(41)-C(42)-C(37)	122.5(3)
C(15)-C(14)-Th(1)	75.91(17)	C(48)-C(43)-C(44)	115.7(3)
C(13)-C(14)-Th(1)	75.86(16)	C(48)-C(43)-B(1)	121.6(3)
C(19)-C(14)-Th(1)	122.5(2)	C(44)-C(43)-B(1)	122.4(3)
C(14)-C(15)-C(11)	107.9(3)	C(45)-C(44)-C(43)	122.3(5)
C(14)-C(15)-C(20)	126.0(4)	C(46)-C(45)-C(44)	120.1(5)
C(11)-C(15)-C(20)	125.1(4)	C(45)-C(46)-C(47)	120.1(4)
C(14)-C(15)-Th(1)	75.49(16)	C(48)-C(47)-C(46)	119.0(5)
C(11)-C(15)-Th(1)	75.55(16)	C(47)-C(48)-C(43)	122.8(4)
C(20)-C(15)-Th(1)	124.1(2)	C(50)-C(49)-C(54)	115.5(3)
N(1)-C(21)-C(22)	178.3(4)	C(50)-C(49)-B(1)	123.2(3)
N(2)-C(23)-C(24)	177.9(3)	C(54)-C(49)-B(1)	121.0(3)
N(3)-C(25)-C(26)	178.7(5)	C(49)-C(50)-C(51)	121.4(4)
N(4)-C(27)-C(28)	178.6(4)	C(52)-C(51)-C(50)	120.9(4)
N(5)-C(29)-C(30)	179.5(4)	C(53)-C(52)-C(51)	119.3(4)
C(37)-B(1)-C(43)	102.9(2)	C(52)-C(53)-C(54)	120.4(4)
C(37)-B(1)-C(31)	114.4(2)	C(53)-C(54)-C(49)	122.4(4)
C(43)-B(1)-C(31)	111.4(3)	C(73)-B(2)-C(55)	113.7(3)
C(37)-B(1)-C(49)	111.0(3)	C(73)-B(2)-C(67)	105.0(3)
C(43)-B(1)-C(49)	113.7(3)	C(55)-B(2)-C(67)	110.8(3)
C(31)-B(1)-C(49)	103.7(2)	C(73)-B(2)-C(61)	110.4(3)
C(32)-C(31)-C(36)	114.8(3)	C(55)-B(2)-C(61)	105.0(3)
C(32)-C(31)-B(1)	121.9(3)	C(67)-B(2)-C(61)	112.1(3)
C(36)-C(31)-B(1)	122.8(3)	C(60B)-C(55)-C(56)	98.4(8)
C(33)-C(32)-C(31)	123.3(3)	C(56)-C(55)-C(60)	117.5(4)
C(34)-C(33)-C(32)	119.8(3)	C(60B)-C(55)-B(2)	128.5(8)
C(35)-C(34)-C(33)	119.1(3)	C(56)-C(55)-B(2)	123.4(4)
C(34)-C(35)-C(36)	120.2(3)	C(60)-C(55)-B(2)	119.0(4)
C(35)-C(36)-C(31)	122.8(3)	C(55)-C(56)-C(57)	123.7(4)

C(58B)-C(57)-C(56)	128.9(8)	C(68)-C(67)-B(2)	126.4(3)
C(56)-C(57)-C(58)	113.6(5)	C(72)-C(67)-B(2)	119.3(3)
C(58B)-C(57)-C(59B)	35.2(7)	C(67)-C(68)-C(69)	123.3(4)
C(56)-C(57)-C(59B)	93.8(6)	C(70)-C(69)-C(68)	120.4(4)
C(59)-C(58)-C(57)	121.1(7)	C(69)-C(70)-C(71)	118.7(3)
C(58)-C(59)-C(60)	122.8(7)	C(70)-C(71)-C(72)	120.2(4)
C(59)-C(60)-C(55)	120.7(6)	C(71)-C(72)-C(67)	123.2(4)
C(57)-C(58B)-C(59B)	113.1(10)	C(74)-C(73)-C(78)	112.7(4)
C(58B)-C(59B)-C(60B)	119.6(15)	C(74)-C(73)-B(2)	118.6(3)
C(58B)-C(59B)-C(57)	31.7(6)	C(78)-C(73)-B(2)	128.6(4)
C(60B)-C(59B)-C(57)	87.9(11)	C(73)-C(74)-C(75)	124.6(3)
C(55)-C(60B)-C(59B)	127.3(15)	C(76)-C(75)-C(74)	119.7(5)
C(62)-C(61)-C(66)	115.2(3)	C(77)-C(76)-C(75)	119.1(5)
C(62)-C(61)-B(2)	120.0(3)	C(76)-C(77)-C(78)	121.9(4)
C(66)-C(61)-B(2)	124.6(3)	C(73)-C(78)-C(77)	121.9(4)
C(63)-C(62)-C(61)	123.4(4)	N(6)-C(79)-C(80)	179.3(4)
C(62)-C(63)-C(64)	120.0(4)	N(7)-C(81)-C(82)	177.3(6)
C(65)-C(64)-C(63)	119.1(4)	N(8)-C(83)-C(84)	178.6(8)
C(64)-C(65)-C(66)	119.8(4)	C(85)#1-C(85)-C(86)	95.3(11)
C(65)-C(66)-C(61)	122.5(4)	C(87)-C(86)-C(85)	111.3(12)
C(68)-C(67)-C(72)	114.2(3)		

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+1

X-ray Data Collection, Structure Solution and Refinement for $[(C_5Me_5)_2Th(NCMe)_5][BPh_4]_2$, 2- cold. A colorless crystal of approximate dimensions 0.162 x 0.384 x 0.769 mm was mounted on a glass fiber and transferred to a Bruker SMART APEX II diffractometer. The APEX2[13] program package was used to determine the unit-cell parameters and for data collection (15 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT[14] and SADABS[15] to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL[16] program. The diffraction symmetry was 2/*m* and the systematic absences were consistent with the monoclinic space group $P2_1/n$ that was later determined to be correct.

The structure was solved by dual space methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors[5] for neutral atoms were used throughout the analysis.

Hydrogen atoms were included using a riding model. Several atoms were disordered and included using multiple components with partial site-occupancy-factors.

Least-squares analysis yielded wR2 = 0.0835 and Goof = 1.026 for 937 variables refined against 16407 data (0.82 Å), R1 = 0.0340 for those 12445 data with $I > 2.0\sigma(I)$.

There were several high residuals present in the final difference-Fourier map. It was not possible to determine the nature of the residuals although it was probable that diethylether and/or acetonitrile solvent was present. The SQUEEZE[17] routine in the PLATON[18] program package was used to account for the electrons in the solvent accessible voids.

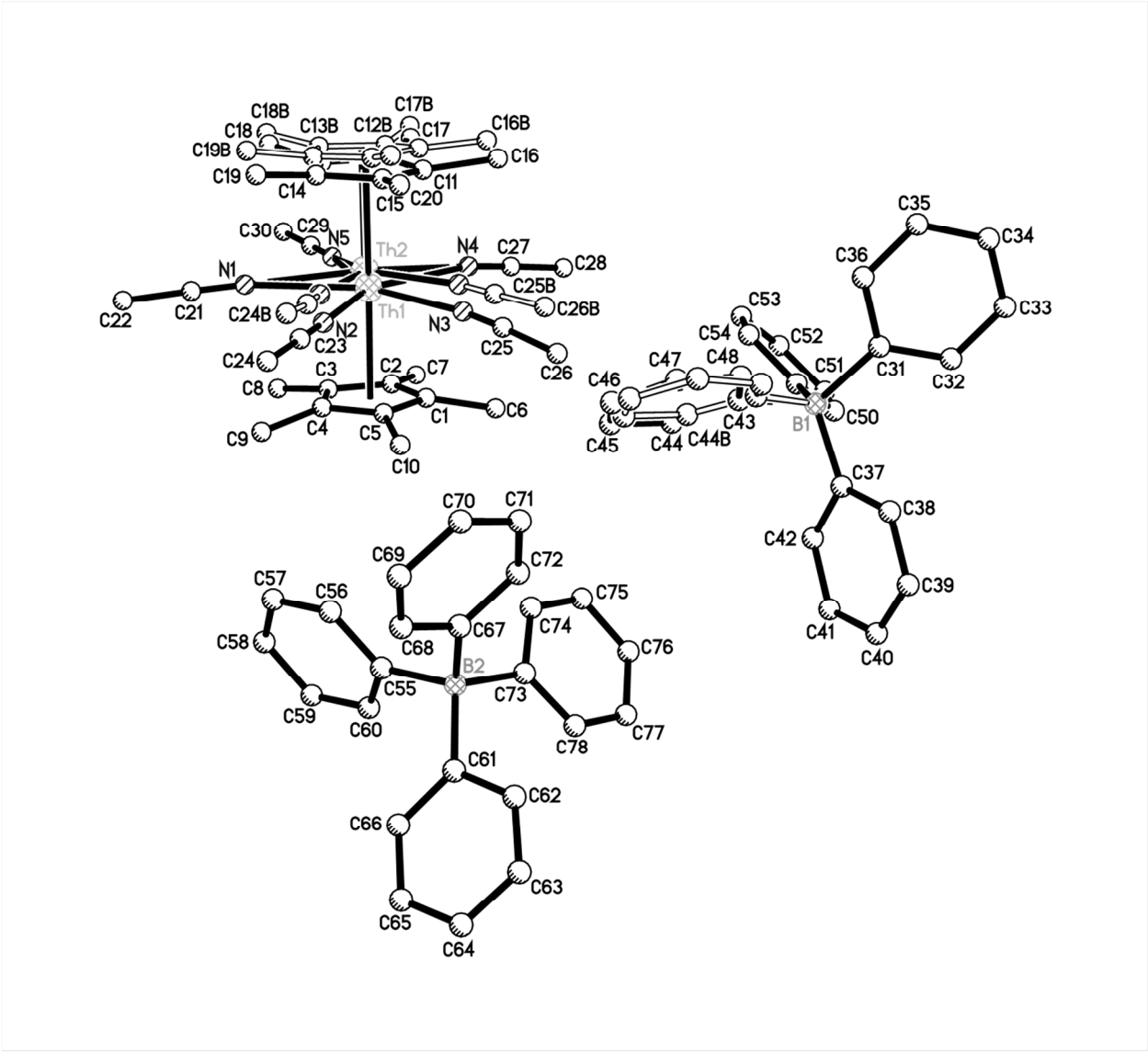


Figure S4. The thermal ellipsoid plot of $[(C_5Me_5)_2Th(NCMe)_5][BPh_4]_2$, **2-cold**, shown at the 30% p5robability level with hydrogens omitted for clarity.

Table S8. Crystal data and structure refinement for $[(C_5Me_5)_2Th(NCMe)_5][BPh_4]_2$, **2-cold**.

.

Identification code	rrl47 (Ryan Langeslay)	
Empirical formula	$C_{78}\ H_{85}\ B_2\ N_5\ Th$	
Formula weight	1346.17	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 13.7878(9) Å	α = 90°.
	b = 18.1632(11) Å	β = 97.4515(8)°.
	c = 34.707(2) Å	γ = 90°.
Volume	8618.3(9) $Å^3$	
Z	4	
Density (calculated)	1.037 Mg/m^3	
Absorption coefficient	1.767 mm^{-1}	
F(000)	2752	
Crystal color	colorless	
Crystal size	0.769 x 0.384 x 0.162 mm^3	
Theta range for data collection	1.183 to 25.719°	
Index ranges	$-16 \le h \le 16, -22 \le k \le 22, -42 \le l \le 42$	
Reflections collected	88084	
Independent reflections	16407 [R(int) = 0.0520]	
Completeness to theta = 25.500°	100.0 %	
Absorption correction	Numerical	
Max. and min. transmission	0.8267 and 0.4850	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	16407 / 0 / 937	
Goodness-of-fit on F^2	1.026	
Final R indices [I>2sigma(I) = 12445 data]	R1 = 0.0340, wR2 = 0.0760	
R indices (all data, 0.82 Å)	R1 = 0.0546, wR2 = 0.0835	
Largest diff. peak and hole	0.586 and −0.423 e.$Å^{-3}$	

Table S9. Bond lengths [Å] and angles [°] for $[(C_5Me_5)_2Th(NCMe)_5][BPh_4]_2$, **2-cold.**

Th(1)-Cnt1	2.479	Th(2)-C(14B)	2.80(2)
Th(1)-Cnt2	2.562	Th(2)-C(15)	2.811(18)
Th(2)-Cnt1	2.778	Th(2)-C(13B)	2.83(2)
Th(2)-Cnt3	2.560	Th(2)-C(15B)	2.840(19)
Th(1)-N(3)	2.610(7)	Th(2)-C(11B)	2.88(2)
Th(1)-N(2)	2.613(7)	Th(2)-C(2)	2.950(3)
Th(1)-N(1)	2.632(3)	Th(2)-C(3)	2.953(3)
Th(1)-N(4)	2.634(3)	Th(2)-C(1)	3.052(4)
Th(1)-C(5)	2.709(4)	Th(2)-C(4)	3.056(4)
Th(1)-N(5)	2.727(4)	Th(2)-C(5)	3.124(4)
Th(1)-C(1)	2.736(3)	C(1)-C(2)	1.406(5)
Th(1)-C(4)	2.740(4)	C(1)-C(5)	1.421(4)
Th(1)-C(11)	2.79(2)	C(1)-C(6)	1.510(4)
Th(1)-C(12)	2.793(17)	C(2)-C(3)	1.419(4)
Th(1)-C(2)	2.795(3)	C(2)-C(7)	1.501(4)
Th(1)-C(3)	2.798(3)	C(3)-C(4)	1.414(5)
Th(1)-C(13)	2.818(16)	C(3)-C(8)	1.506(5)
Th(1)-C(14)	2.863(16)	C(4)-C(5)	1.419(5)
Th(1)-C(15)	2.881(17)	C(4)-C(9)	1.512(4)
Th(1)-C(15B)	3.01(2)	C(5)-C(10)	1.505(5)
Th(1)-C(14B)	3.06(3)	C(11)-C(12)	1.35(4)
Th(1)-C(11B)	3.13(2)	C(11)-C(15)	1.44(3)
Th(1)-C(12B)	3.19(2)	C(11)-C(16)	1.59(3)
Th(1)-C(13B)	3.23(2)	C(12)-C(13)	1.39(3)
Th(2)-N(5)	2.386(4)	C(12)-C(17)	1.500(14)
Th(2)-C(12)	2.426(17)	C(13)-C(14)	1.414(17)
Th(2)-C(13)	2.454(16)	C(13)-C(18)	1.50(3)
Th(2)-N(4)	2.537(3)	C(14)-C(19)	1.45(3)
Th(2)-N(1)	2.557(3)	C(14)-C(15)	1.47(3)
Th(2)-C(11)	2.60(2)	C(15)-C(20)	1.51(2)
Th(2)-N(3B)	2.615(6)	C(11B)-C(15B)	1.42(3)
Th(2)-N(2B)	2.621(7)	C(11B)-C(12B)	1.44(4)
Th(2)-C(14)	2.686(17)	C(11B)-C(16B)	1.45(3)
Th(2)-C(12B)	2.80(2)	C(12B)-C(13B)	1.45(3)

C(12B)-C(17B)	1.494(14)	C(41)-C(42)	1.388(5)
C(13B)-C(14B)	1.408(17)	C(43)-C(44)	1.409(17)
C(13B)-C(18B)	1.48(3)	C(43)-C(48)	1.43(2)
C(14B)-C(15B)	1.36(3)	C(44)-C(45)	1.35(3)
C(14B)-C(19B)	1.59(3)	C(45)-C(46)	1.38(2)
C(15B)-C(20B)	1.53(2)	C(46)-C(47)	1.37(4)
N(1)-C(21)	1.140(4)	C(47)-C(48)	1.38(3)
N(4)-C(27)	1.135(4)	C(43B)-C(48B)	1.32(3)
N(5)-C(29)	1.138(4)	C(43B)-C(44B)	1.42(2)
C(21)-C(22)	1.448(4)	C(44B)-C(45B)	1.48(4)
N(2)-C(23)	1.104(10)	C(45B)-C(46B)	1.40(3)
C(23)-C(24)	1.449(15)	C(46B)-C(47B)	1.34(6)
N(3)-C(25)	1.124(10)	C(47B)-C(48B)	1.45(5)
C(25)-C(26)	1.457(13)	C(49)-C(54)	1.395(5)
N(2B)-C(23B)	1.175(9)	C(49)-C(50)	1.398(5)
C(23B)-C(24B)	1.486(11)	C(50)-C(51)	1.398(5)
N(3B)-C(25B)	1.107(11)	C(51)-C(52)	1.358(6)
C(25B)-C(26B)	1.568(16)	C(52)-C(53)	1.364(7)
C(27)-C(28)	1.443(4)	C(53)-C(54)	1.428(7)
C(29)-C(30)	1.450(5)	B(2)-C(61)	1.644(5)
B(1)-C(37)	1.640(5)	B(2)-C(73)	1.645(5)
B(1)-C(43)	1.642(7)	B(2)-C(55)	1.649(5)
B(1)-C(49)	1.647(6)	B(2)-C(67)	1.649(5)
B(1)-C(31)	1.655(5)	C(55)-C(60)	1.391(5)
B(1)-C(43B)	1.689(11)	C(55)-C(56)	1.401(5)
C(31)-C(32)	1.389(5)	C(56)-C(57)	1.388(6)
C(31)-C(36)	1.406(5)	C(57)-C(58)	1.360(7)
C(32)-C(33)	1.395(5)	C(58)-C(59)	1.371(6)
C(33)-C(34)	1.374(6)	C(59)-C(60)	1.388(5)
C(34)-C(35)	1.371(6)	C(61)-C(66)	1.399(4)
C(35)-C(36)	1.387(5)	C(61)-C(62)	1.405(4)
C(37)-C(38)	1.393(4)	C(62)-C(63)	1.380(4)
C(37)-C(42)	1.401(5)	C(63)-C(64)	1.391(4)
C(38)-C(39)	1.394(5)	C(64)-C(65)	1.372(4)
C(39)-C(40)	1.380(5)	C(65)-C(66)	1.393(4)
C(40)-C(41)	1.371(5)	C(67)-C(68)	1.396(4)

C(67)-C(72)	1.400(4)	C(73)-C(74)	1.403(5)
C(68)-C(69)	1.385(4)	C(74)-C(75)	1.388(6)
C(69)-C(70)	1.388(4)	C(75)-C(76)	1.371(6)
C(70)-C(71)	1.384(5)	C(76)-C(77)	1.379(5)
C(71)-C(72)	1.380(5)	C(77)-C(78)	1.391(4)
C(73)-C(78)	1.386(5)		

Cnt1-Th(1)-N(1)	91.0	N(2)-Th(1)-C(5)	67.85(19)
Cnt1-Th(1)-N(2)	89.4	N(1)-Th(1)-C(5)	98.48(10)
Cnt1-Th(1)-N(3)	89.5	N(4)-Th(1)-C(5)	99.88(10)
Cnt1-Th(1)-N(4)	90.6	N(3)-Th(1)-N(5)	149.19(14)
Cnt1-Th(1)-N(5)	89.1	N(2)-Th(1)-N(5)	141.89(15)
Cnt2-Th(1)-N(1)	88.3	N(1)-Th(1)-N(5)	68.94(9)
Cnt2-Th(1)-N(2)	91.5	N(4)-Th(1)-N(5)	72.51(9)
Cnt2-Th(1)-N(3)	91.8	C(5)-Th(1)-N(5)	115.46(10)
Cnt2-Th(1)-N(4)	89.2	N(3)-Th(1)-C(1)	69.19(16)
Cnt2-Th(1)-N(5)	89.6	N(2)-Th(1)-C(1)	96.67(19)
Cnt1-Th(1)-Cnt2	178.6	N(1)-Th(1)-C(1)	117.01(9)
Cnt1-Th(2)-N(1)	86.1	N(4)-Th(1)-C(1)	70.66(9)
Cnt1-Th(2)-N(2B)	88.2	C(5)-Th(1)-C(1)	30.24(9)
Cnt1-Th(2)-N(3B)	87.9	N(5)-Th(1)-C(1)	98.41(10)
Cnt1-Th(2)-N(4)	86.2	N(3)-Th(1)-C(4)	96.78(18)
Cnt1-Th(2)-N(5)	89.8	N(2)-Th(1)-C(4)	69.15(18)
Cnt3-Th(2)-N(1)	94.9	N(1)-Th(1)-C(4)	69.89(10)
Cnt3-Th(2)-N(2B)	90.3	N(4)-Th(1)-C(4)	116.64(10)
Cnt3-Th(2)-N(3B)	90.0	C(5)-Th(1)-C(4)	30.18(10)
Cnt3-Th(2)-N(4)	93.8	N(5)-Th(1)-C(4)	95.30(10)
Cnt3-Th(2)-N(5)	92.5	C(1)-Th(1)-C(4)	49.43(9)
Cnt2-Th(2)-Cnt3	177.7	N(3)-Th(1)-C(11)	72.9(6)
N(3)-Th(1)-N(2)	68.86(19)	N(2)-Th(1)-C(11)	99.8(6)
N(3)-Th(1)-N(1)	141.86(15)	N(1)-Th(1)-C(11)	113.6(5)
N(2)-Th(1)-N(1)	73.02(16)	N(4)-Th(1)-C(11)	68.9(6)
N(3)-Th(1)-N(4)	76.72(15)	C(5)-Th(1)-C(11)	140.9(5)
N(2)-Th(1)-N(4)	145.58(16)	N(5)-Th(1)-C(11)	97.3(6)
N(1)-Th(1)-N(4)	141.39(10)	C(1)-Th(1)-C(11)	129.3(5)
N(3)-Th(1)-C(5)	68.00(18)	C(4)-Th(1)-C(11)	167.4(6)

N(3)-Th(1)-C(12)	100.2(5)	C(1)-Th(1)-C(13)	164.3(4)
N(2)-Th(1)-C(12)	116.1(4)	C(4)-Th(1)-C(13)	137.8(3)
N(1)-Th(1)-C(12)	95.6(4)	C(11)-Th(1)-C(13)	47.7(6)
N(4)-Th(1)-C(12)	69.1(4)	C(12)-Th(1)-C(13)	28.7(5)
C(5)-Th(1)-C(12)	165.9(5)	C(2)-Th(1)-C(13)	138.5(4)
N(5)-Th(1)-C(12)	70.5(5)	C(3)-Th(1)-C(13)	127.9(4)
C(1)-Th(1)-C(12)	139.7(4)	N(3)-Th(1)-C(14)	98.3(5)
C(4)-Th(1)-C(12)	163.0(5)	N(2)-Th(1)-C(14)	71.6(4)
C(11)-Th(1)-C(12)	27.9(7)	N(1)-Th(1)-C(14)	68.3(4)
N(3)-Th(1)-C(2)	97.68(16)	N(4)-Th(1)-C(14)	114.3(4)
N(2)-Th(1)-C(2)	114.93(19)	C(5)-Th(1)-C(14)	139.4(4)
N(1)-Th(1)-C(2)	98.92(9)	N(5)-Th(1)-C(14)	96.0(4)
N(4)-Th(1)-C(2)	69.30(9)	C(1)-Th(1)-C(14)	165.6(4)
C(5)-Th(1)-C(2)	49.22(10)	C(4)-Th(1)-C(14)	128.9(4)
N(5)-Th(1)-C(2)	69.85(9)	C(11)-Th(1)-C(14)	48.2(6)
C(1)-Th(1)-C(2)	29.44(10)	C(12)-Th(1)-C(14)	47.1(4)
C(4)-Th(1)-C(2)	48.90(9)	C(2)-Th(1)-C(14)	164.1(4)
C(11)-Th(1)-C(2)	138.2(6)	C(3)-Th(1)-C(14)	139.1(4)
C(12)-Th(1)-C(2)	129.0(4)	C(13)-Th(1)-C(14)	28.8(3)
N(3)-Th(1)-C(3)	114.94(17)	N(3)-Th(1)-C(15)	70.6(4)
N(2)-Th(1)-C(3)	97.80(17)	N(2)-Th(1)-C(15)	71.6(5)
N(1)-Th(1)-C(3)	70.77(9)	N(1)-Th(1)-C(15)	96.8(3)
N(4)-Th(1)-C(3)	96.85(9)	N(4)-Th(1)-C(15)	97.0(4)
C(5)-Th(1)-C(3)	49.19(10)	C(5)-Th(1)-C(15)	129.7(4)
N(5)-Th(1)-C(3)	67.78(9)	N(5)-Th(1)-C(15)	114.7(4)
C(1)-Th(1)-C(3)	48.77(10)	C(1)-Th(1)-C(15)	139.6(4)
C(4)-Th(1)-C(3)	29.55(10)	C(4)-Th(1)-C(15)	140.7(4)
C(11)-Th(1)-C(3)	162.4(6)	C(11)-Th(1)-C(15)	29.4(7)
C(12)-Th(1)-C(3)	138.3(5)	C(12)-Th(1)-C(15)	47.0(5)
C(2)-Th(1)-C(3)	29.39(8)	C(2)-Th(1)-C(15)	164.1(4)
N(3)-Th(1)-C(13)	117.1(4)	C(3)-Th(1)-C(15)	166.0(4)
N(2)-Th(1)-C(13)	99.1(5)	C(13)-Th(1)-C(15)	48.1(4)
N(1)-Th(1)-C(13)	67.9(3)	C(14)-Th(1)-C(15)	29.6(5)
N(4)-Th(1)-C(13)	96.1(4)	N(1)-Th(1)-C(15B)	91.7(4)
C(5)-Th(1)-C(13)	164.0(4)	N(4)-Th(1)-C(15B)	94.1(4)
N(5)-Th(1)-C(13)	68.7(4)	C(5)-Th(1)-C(15B)	142.3(4)

N(5)-Th(1)-C(15B)	102.1(4)	N(4)-Th(1)-C(13B)	90.3(3)
C(1)-Th(1)-C(15B)	149.3(4)	C(5)-Th(1)-C(13B)	167.4(3)
C(4)-Th(1)-C(15B)	148.2(4)	N(5)-Th(1)-C(13B)	60.6(3)
C(2)-Th(1)-C(15B)	162.9(4)	C(1)-Th(1)-C(13B)	155.8(3)
C(3)-Th(1)-C(15B)	161.9(4)	C(4)-Th(1)-C(13B)	137.6(3)
N(1)-Th(1)-C(14B)	67.5(4)	C(2)-Th(1)-C(13B)	130.1(3)
N(4)-Th(1)-C(14B)	107.1(4)	C(3)-Th(1)-C(13B)	122.6(3)
C(5)-Th(1)-C(14B)	150.4(4)	C(15B)-Th(1)-C(13B)	42.7(4)
N(5)-Th(1)-C(14B)	84.8(4)	C(14B)-Th(1)-C(13B)	25.7(4)
C(1)-Th(1)-C(14B)	175.1(4)	C(11B)-Th(1)-C(13B)	42.7(6)
C(4)-Th(1)-C(14B)	134.2(4)	C(12B)-Th(1)-C(13B)	26.0(5)
C(2)-Th(1)-C(14B)	154.4(4)	N(5)-Th(2)-C(12)	83.0(5)
C(3)-Th(1)-C(14B)	136.1(4)	N(5)-Th(2)-C(13)	80.6(5)
C(15B)-Th(1)-C(14B)	25.8(5)	C(12)-Th(2)-C(13)	33.1(6)
N(1)-Th(1)-C(11B)	108.7(5)	N(5)-Th(2)-N(4)	80.14(10)
N(4)-Th(1)-C(11B)	68.0(4)	C(12)-Th(2)-N(4)	76.7(5)
C(5)-Th(1)-C(11B)	148.8(5)	C(13)-Th(2)-N(4)	108.7(4)
N(5)-Th(1)-C(11B)	89.1(6)	N(5)-Th(2)-N(1)	75.64(10)
C(1)-Th(1)-C(11B)	133.3(5)	C(12)-Th(2)-N(1)	107.5(5)
C(4)-Th(1)-C(11B)	174.4(5)	C(13)-Th(2)-N(1)	74.9(3)
C(2)-Th(1)-C(11B)	136.3(5)	N(4)-Th(2)-N(1)	154.58(11)
C(3)-Th(1)-C(11B)	155.7(6)	N(5)-Th(2)-C(11)	112.1(6)
C(15B)-Th(1)-C(11B)	26.6(6)	C(12)-Th(2)-C(11)	30.8(8)
C(14B)-Th(1)-C(11B)	42.7(6)	C(13)-Th(2)-C(11)	53.2(6)
N(1)-Th(1)-C(12B)	94.1(4)	N(4)-Th(2)-C(11)	73.4(6)
N(4)-Th(1)-C(12B)	65.8(3)	N(1)-Th(2)-C(11)	123.2(5)
C(5)-Th(1)-C(12B)	165.6(3)	N(5)-Th(2)-N(3B)	149.25(16)
N(5)-Th(1)-C(12B)	63.0(4)	N(4)-Th(2)-N(3B)	69.11(15)
C(1)-Th(1)-C(12B)	136.0(3)	N(1)-Th(2)-N(3B)	134.67(16)
C(4)-Th(1)-C(12B)	157.1(4)	N(5)-Th(2)-N(2B)	141.73(16)
C(2)-Th(1)-C(12B)	121.9(3)	N(4)-Th(2)-N(2B)	137.74(16)
C(3)-Th(1)-C(12B)	130.7(4)	N(1)-Th(2)-N(2B)	66.10(15)
C(15B)-Th(1)-C(12B)	43.4(4)	N(3B)-Th(2)-N(2B)	68.84(19)
C(14B)-Th(1)-C(12B)	42.6(4)	N(5)-Th(2)-C(14)	109.8(5)
C(11B)-Th(1)-C(12B)	26.4(7)	C(12)-Th(2)-C(14)	52.2(5)
N(1)-Th(1)-C(13B)	68.9(3)	C(13)-Th(2)-C(14)	31.5(4)

N(4)-Th(2)-C(14)	124.3(4)	N(5)-Th(2)-C(11B)	102.5(6)
N(1)-Th(2)-C(14)	72.2(4)	N(4)-Th(2)-C(11B)	73.4(5)
C(11)-Th(2)-C(14)	51.8(7)	N(1)-Th(2)-C(11B)	119.2(5)
N(5)-Th(2)-C(12B)	73.6(4)	N(3B)-Th(2)-C(11B)	69.7(6)
N(4)-Th(2)-C(12B)	73.6(4)	N(2B)-Th(2)-C(11B)	95.8(6)
N(1)-Th(2)-C(12B)	106.2(4)	C(12B)-Th(2)-C(11B)	29.4(7)
N(3B)-Th(2)-C(12B)	97.4(5)	C(14B)-Th(2)-C(11B)	46.8(6)
N(2B)-Th(2)-C(12B)	116.0(4)	C(13B)-Th(2)-C(11B)	48.0(6)
N(5)-Th(2)-C(14B)	97.6(5)	C(15B)-Th(2)-C(11B)	28.7(7)
N(4)-Th(2)-C(14B)	118.5(4)	N(5)-Th(2)-C(2)	71.78(10)
N(1)-Th(2)-C(14B)	72.8(4)	C(12)-Th(2)-C(2)	139.3(5)
N(3B)-Th(2)-C(14B)	97.4(5)	C(13)-Th(2)-C(2)	152.4(5)
N(2B)-Th(2)-C(14B)	71.3(5)	N(4)-Th(2)-C(2)	68.05(9)
C(12B)-Th(2)-C(14B)	48.1(5)	N(1)-Th(2)-C(2)	96.76(9)
N(5)-Th(2)-C(15)	130.5(4)	C(11)-Th(2)-C(2)	139.9(5)
C(12)-Th(2)-C(15)	50.6(5)	N(3B)-Th(2)-C(2)	95.53(16)
C(13)-Th(2)-C(15)	51.8(4)	N(2B)-Th(2)-C(2)	112.20(18)
N(4)-Th(2)-C(15)	101.1(4)	C(14)-Th(2)-C(2)	167.5(4)
N(1)-Th(2)-C(15)	100.4(4)	C(12B)-Th(2)-C(2)	131.6(4)
C(11)-Th(2)-C(15)	30.5(7)	C(14B)-Th(2)-C(2)	167.0(4)
C(14)-Th(2)-C(15)	30.9(6)	C(15)-Th(2)-C(2)	154.7(4)
N(5)-Th(2)-C(13B)	70.7(4)	C(13B)-Th(2)-C(2)	142.3(4)
N(4)-Th(2)-C(13B)	102.3(4)	C(15B)-Th(2)-C(2)	164.9(5)
N(1)-Th(2)-C(13B)	76.9(4)	C(11B)-Th(2)-C(2)	141.5(5)
N(3B)-Th(2)-C(13B)	115.5(4)	N(5)-Th(2)-C(3)	69.56(10)
N(2B)-Th(2)-C(13B)	99.2(4)	C(12)-Th(2)-C(3)	152.4(5)
C(12B)-Th(2)-C(13B)	29.8(6)	C(13)-Th(2)-C(3)	137.7(4)
C(14B)-Th(2)-C(13B)	29.0(4)	N(4)-Th(2)-C(3)	95.23(9)
N(5)-Th(2)-C(15B)	117.1(5)	N(1)-Th(2)-C(3)	69.23(9)
N(4)-Th(2)-C(15B)	100.5(4)	C(11)-Th(2)-C(3)	167.6(5)
N(1)-Th(2)-C(15B)	97.4(4)	N(3B)-Th(2)-C(3)	111.84(17)
N(3B)-Th(2)-C(15B)	70.6(5)	N(2B)-Th(2)-C(3)	96.32(17)
N(2B)-Th(2)-C(15B)	69.2(5)	C(14)-Th(2)-C(3)	140.2(4)
C(12B)-Th(2)-C(15B)	48.1(5)	C(12B)-Th(2)-C(3)	142.8(4)
C(14B)-Th(2)-C(15B)	27.9(6)	C(14B)-Th(2)-C(3)	141.9(4)
C(13B)-Th(2)-C(15B)	47.5(5)	C(15)-Th(2)-C(3)	155.9(4)

C(13B)-Th(2)-C(3)	132.6(4)	C(2)-Th(2)-C(4)	44.81(9)
C(15B)-Th(2)-C(3)	163.8(4)	C(3)-Th(2)-C(4)	27.14(9)
C(11B)-Th(2)-C(3)	167.4(5)	C(1)-Th(2)-C(4)	44.03(8)
C(2)-Th(2)-C(3)	27.81(8)	N(5)-Th(2)-C(5)	112.38(10)
N(5)-Th(2)-C(1)	98.28(10)	C(12)-Th(2)-C(5)	159.3(5)
C(12)-Th(2)-C(1)	142.5(5)	C(13)-Th(2)-C(5)	157.6(5)
C(13)-Th(2)-C(1)	175.5(4)	N(4)-Th(2)-C(5)	91.92(10)
N(4)-Th(2)-C(1)	66.79(9)	N(1)-Th(2)-C(5)	90.26(10)
N(1)-Th(2)-C(1)	109.07(10)	C(11)-Th(2)-C(5)	129.4(6)
C(11)-Th(2)-C(1)	123.9(5)	N(3B)-Th(2)-C(5)	69.52(17)
N(3B)-Th(2)-C(1)	69.68(16)	N(2B)-Th(2)-C(5)	69.58(18)
N(2B)-Th(2)-C(1)	94.62(18)	C(14)-Th(2)-C(5)	128.0(4)
C(14)-Th(2)-C(1)	150.9(5)	C(12B)-Th(2)-C(5)	163.5(4)
C(12B)-Th(2)-C(1)	140.4(4)	C(14B)-Th(2)-C(5)	140.8(5)
C(14B)-Th(2)-C(1)	163.9(5)	C(15)-Th(2)-C(5)	117.0(4)
C(15)-Th(2)-C(1)	128.1(4)	C(13B)-Th(2)-C(5)	165.8(4)
C(13B)-Th(2)-C(1)	166.2(4)	C(15B)-Th(2)-C(5)	130.3(5)
C(15B)-Th(2)-C(1)	140.2(5)	C(11B)-Th(2)-C(5)	139.2(6)
C(11B)-Th(2)-C(1)	130.7(5)	C(2)-Th(2)-C(5)	44.25(9)
C(2)-Th(2)-C(1)	27.03(9)	C(3)-Th(2)-C(5)	44.24(9)
C(3)-Th(2)-C(1)	44.70(9)	C(1)-Th(2)-C(5)	26.56(8)
N(5)-Th(2)-C(4)	95.09(11)	C(4)-Th(2)-C(5)	26.52(9)
C(12)-Th(2)-C(4)	173.3(5)	C(2)-C(1)-C(5)	108.4(3)
C(13)-Th(2)-C(4)	140.3(4)	C(2)-C(1)-C(6)	126.0(3)
N(4)-Th(2)-C(4)	109.36(10)	C(5)-C(1)-C(6)	124.6(3)
N(1)-Th(2)-C(4)	65.82(10)	C(2)-C(1)-Th(1)	77.61(19)
C(11)-Th(2)-C(4)	152.5(6)	C(5)-C(1)-Th(1)	73.8(2)
N(3B)-Th(2)-C(4)	94.67(18)	C(6)-C(1)-Th(1)	123.8(2)
N(2B)-Th(2)-C(4)	70.23(17)	C(2)-C(1)-Th(2)	72.46(19)
C(14)-Th(2)-C(4)	123.2(4)	C(5)-C(1)-Th(2)	79.5(2)
C(12B)-Th(2)-C(4)	167.8(4)	C(6)-C(1)-Th(2)	123.3(2)
C(14B)-Th(2)-C(4)	131.9(4)	C(1)-C(2)-C(3)	108.0(3)
C(15)-Th(2)-C(4)	128.9(4)	C(1)-C(2)-C(7)	126.5(3)
C(13B)-Th(2)-C(4)	142.5(4)	C(3)-C(2)-C(7)	124.9(3)
C(15B)-Th(2)-C(4)	139.4(5)	C(1)-C(2)-Th(1)	72.96(18)
C(11B)-Th(2)-C(4)	162.4(6)	C(3)-C(2)-Th(1)	75.42(17)

C(7)-C(2)-Th(1)	124.8(2)	C(16)-C(11)-Th(1)	123.8(10)
C(1)-C(2)-Th(2)	80.51(18)	C(11)-C(12)-C(13)	111.6(15)
C(3)-C(2)-Th(2)	76.19(18)	C(11)-C(12)-C(17)	123.1(19)
C(7)-C(2)-Th(2)	117.2(2)	C(13)-C(12)-C(17)	125.0(17)
C(4)-C(3)-C(2)	108.0(3)	C(11)-C(12)-Th(1)	75.9(9)
C(4)-C(3)-C(8)	125.6(3)	C(13)-C(12)-Th(1)	76.6(8)
C(2)-C(3)-C(8)	125.5(3)	C(17)-C(12)-Th(1)	120.1(11)
C(4)-C(3)-Th(1)	72.97(19)	C(12)-C(13)-C(14)	107.2(15)
C(2)-C(3)-Th(1)	75.19(17)	C(12)-C(13)-C(18)	126.1(16)
C(8)-C(3)-Th(1)	126.3(2)	C(14)-C(13)-C(18)	125.6(16)
C(4)-C(3)-Th(2)	80.50(19)	C(12)-C(13)-Th(1)	74.6(9)
C(2)-C(3)-Th(2)	75.99(17)	C(14)-C(13)-Th(1)	77.3(8)
C(8)-C(3)-Th(2)	118.8(2)	C(18)-C(13)-Th(1)	123.4(13)
C(3)-C(4)-C(5)	108.1(3)	C(13)-C(14)-C(19)	126.5(18)
C(3)-C(4)-C(9)	125.4(3)	C(13)-C(14)-C(15)	107.3(15)
C(5)-C(4)-C(9)	125.0(3)	C(19)-C(14)-C(15)	125.5(15)
C(3)-C(4)-Th(1)	77.47(19)	C(13)-C(14)-Th(1)	73.8(8)
C(5)-C(4)-Th(1)	73.7(2)	C(19)-C(14)-Th(1)	123.3(11)
C(9)-C(4)-Th(1)	126.0(3)	C(15)-C(14)-Th(1)	75.9(9)
C(3)-C(4)-Th(2)	72.36(19)	C(11)-C(15)-C(14)	105.2(16)
C(5)-C(4)-Th(2)	79.4(2)	C(11)-C(15)-C(20)	130.7(19)
C(9)-C(4)-Th(2)	125.4(3)	C(14)-C(15)-C(20)	123.8(16)
C(4)-C(5)-C(1)	107.5(3)	C(11)-C(15)-Th(1)	71.8(12)
C(4)-C(5)-C(10)	124.9(3)	C(14)-C(15)-Th(1)	74.5(9)
C(1)-C(5)-C(10)	126.3(3)	C(20)-C(15)-Th(1)	122.8(9)
C(4)-C(5)-Th(1)	76.1(2)	C(15B)-C(11B)-C(12B)	107.0(19)
C(1)-C(5)-Th(1)	75.9(2)	C(15B)-C(11B)-C(16B)	128(2)
C(10)-C(5)-Th(1)	124.2(3)	C(12B)-C(11B)-C(16B)	125(2)
C(4)-C(5)-Th(2)	74.1(2)	C(15B)-C(11B)-Th(2)	74.1(10)
C(1)-C(5)-Th(2)	73.9(2)	C(12B)-C(11B)-Th(2)	72.0(10)
C(10)-C(5)-Th(2)	127.9(3)	C(16B)-C(11B)-Th(2)	121.4(11)
C(12)-C(11)-C(15)	109(2)	C(11B)-C(12B)-C(13B)	107.0(14)
C(12)-C(11)-C(16)	128(2)	C(11B)-C(12B)-C(17B)	127.8(16)
C(15)-C(11)-C(16)	121(2)	C(13B)-C(12B)-C(17B)	123.1(16)
C(12)-C(11)-Th(1)	76.2(13)	C(11B)-C(12B)-Th(2)	78.5(8)
C(15)-C(11)-Th(1)	78.8(11)	C(13B)-C(12B)-Th(2)	76.4(8)

C(17B)-C(12B)-Th(2)	124.2(11)	C(37)-B(1)-C(43)	105.2(3)
C(14B)-C(13B)-C(12B)	105.8(16)	C(37)-B(1)-C(49)	111.7(3)
C(14B)-C(13B)-C(18B)	125.2(18)	C(43)-B(1)-C(49)	106.0(5)
C(12B)-C(13B)-C(18B)	128.6(15)	C(37)-B(1)-C(31)	112.1(3)
C(14B)-C(13B)-Th(2)	74.2(10)	C(43)-B(1)-C(31)	118.0(4)
C(12B)-C(13B)-Th(2)	73.8(9)	C(49)-B(1)-C(31)	103.6(3)
C(18B)-C(13B)-Th(2)	122.3(14)	C(37)-B(1)-C(43B)	102.3(4)
C(15B)-C(14B)-C(13B)	111.2(18)	C(49)-B(1)-C(43B)	124.1(6)
C(15B)-C(14B)-C(19B)	122.1(17)	C(31)-B(1)-C(43B)	102.8(6)
C(13B)-C(14B)-C(19B)	125.1(17)	C(32)-C(31)-C(36)	115.5(3)
C(15B)-C(14B)-Th(2)	77.8(12)	C(32)-C(31)-B(1)	122.8(3)
C(13B)-C(14B)-Th(2)	76.8(10)	C(36)-C(31)-B(1)	121.2(3)
C(19B)-C(14B)-Th(2)	124.4(12)	C(31)-C(32)-C(33)	122.6(4)
C(14B)-C(15B)-C(11B)	108.7(16)	C(34)-C(33)-C(32)	120.3(4)
C(14B)-C(15B)-C(20B)	129.5(19)	C(35)-C(34)-C(33)	118.7(4)
C(11B)-C(15B)-C(20B)	121(2)	C(34)-C(35)-C(36)	121.1(4)
C(14B)-C(15B)-Th(2)	74.3(12)	C(35)-C(36)-C(31)	121.8(4)
C(11B)-C(15B)-Th(2)	77.2(11)	C(38)-C(37)-C(42)	114.4(3)
C(20B)-C(15B)-Th(2)	124.4(11)	C(38)-C(37)-B(1)	123.2(3)
C(21)-N(1)-Th(2)	177.9(3)	C(42)-C(37)-B(1)	122.0(3)
C(21)-N(1)-Th(1)	168.5(3)	C(37)-C(38)-C(39)	123.3(3)
C(27)-N(4)-Th(2)	174.0(3)	C(40)-C(39)-C(38)	119.7(4)
C(27)-N(4)-Th(1)	169.7(3)	C(41)-C(40)-C(39)	119.1(3)
C(29)-N(5)-Th(2)	170.1(3)	C(40)-C(41)-C(42)	120.2(4)
C(29)-N(5)-Th(1)	172.1(3)	C(41)-C(42)-C(37)	123.2(4)
N(1)-C(21)-C(22)	178.4(4)	C(44)-C(43)-C(48)	115.1(11)
C(23)-N(2)-Th(1)	176.4(7)	C(44)-C(43)-B(1)	127.9(10)
N(2)-C(23)-C(24)	179.0(12)	C(48)-C(43)-B(1)	116.7(9)
C(25)-N(3)-Th(1)	173.9(7)	C(45)-C(44)-C(43)	124.9(14)
N(3)-C(25)-C(26)	174.6(9)	C(44)-C(45)-C(46)	118.1(14)
C(23B)-N(2B)-Th(2)	170.5(6)	C(47)-C(46)-C(45)	120.6(14)
N(2B)-C(23B)-C(24B)	175.8(9)	C(46)-C(47)-C(48)	121.6(15)
C(25B)-N(3B)-Th(2)	171.1(7)	C(47)-C(48)-C(43)	119.6(15)
N(3B)-C(25B)-C(26B)	177.2(11)	C(48B)-C(43B)-C(44B)	116.3(19)
N(4)-C(27)-C(28)	179.1(4)	C(48B)-C(43B)-B(1)	134.9(14)
N(5)-C(29)-C(30)	178.7(4)	C(44B)-C(43B)-B(1)	108.3(14)

C(43B)-C(44B)-C(45B)	118.2(19)	C(59)-C(60)-C(55)	123.2(4)
C(46B)-C(45B)-C(44B)	122(2)	C(66)-C(61)-C(62)	114.7(3)
C(47B)-C(46B)-C(45B)	117(3)	C(66)-C(61)-B(2)	126.1(3)
C(46B)-C(47B)-C(48B)	120(3)	C(62)-C(61)-B(2)	119.2(3)
C(43B)-C(48B)-C(47B)	125(3)	C(63)-C(62)-C(61)	123.3(3)
C(54)-C(49)-C(50)	114.4(4)	C(62)-C(63)-C(64)	120.1(3)
C(54)-C(49)-B(1)	123.6(4)	C(65)-C(64)-C(63)	118.6(3)
C(50)-C(49)-B(1)	121.6(3)	C(64)-C(65)-C(66)	120.7(3)
C(49)-C(50)-C(51)	124.1(4)	C(65)-C(66)-C(61)	122.6(3)
C(52)-C(51)-C(50)	119.8(5)	C(68)-C(67)-C(72)	114.8(3)
C(51)-C(52)-C(53)	119.4(5)	C(68)-C(67)-B(2)	120.2(3)
C(52)-C(53)-C(54)	120.7(4)	C(72)-C(67)-B(2)	125.0(3)
C(49)-C(54)-C(53)	121.6(4)	C(69)-C(68)-C(67)	123.6(3)
C(61)-B(2)-C(73)	110.8(3)	C(68)-C(69)-C(70)	119.8(3)
C(61)-B(2)-C(55)	111.1(3)	C(71)-C(70)-C(69)	118.3(3)
C(73)-B(2)-C(55)	105.4(3)	C(72)-C(71)-C(70)	120.9(3)
C(61)-B(2)-C(67)	106.8(3)	C(71)-C(72)-C(67)	122.6(3)
C(73)-B(2)-C(67)	112.3(3)	C(78)-C(73)-C(74)	114.9(3)
C(55)-B(2)-C(67)	110.5(3)	C(78)-C(73)-B(2)	125.2(3)
C(60)-C(55)-C(56)	114.8(4)	C(74)-C(73)-B(2)	119.8(3)
C(60)-C(55)-B(2)	120.5(3)	C(75)-C(74)-C(73)	122.5(4)
C(56)-C(55)-B(2)	124.6(3)	C(76)-C(75)-C(74)	120.6(4)
C(57)-C(56)-C(55)	122.0(4)	C(75)-C(76)-C(77)	118.7(4)
C(58)-C(57)-C(56)	121.0(5)	C(76)-C(77)-C(78)	120.1(4)
C(57)-C(58)-C(59)	119.2(4)	C(73)-C(78)-C(77)	123.2(3)
C(58)-C(59)-C(60)	119.8(4)		

X-ray Data Collection, Structure Solution and Refinement for $[(C_5Me_5)_2Th(NCPh)_5][BPh_4]_2$, 3. A yellow crystal of approximate dimensions 0.070 x 0.222 x 0.442 mm was mounted on a glass fiber and transferred to a Bruker SMART APEX II diffractometer. The APEX2[13] program package was used to determine the unit-cell parameters and for data collection (40 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT[14] and SADABS[15] to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL[16] program. There were no systematic absences nor any diffraction symmetry other than the Friedel condition. The centrosymmetric triclinic space group $P\bar{1}$ was assigned and later determined to be correct.

The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors[12] for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model.

At convergence, wR2 = 0.0801 and Goof = 1.081 for 1010 variables refined against 23753 data (0.73Å), R1 = 0.0349 for those 21209 data with $I > 2.0\sigma(I)$.

There were several high residuals present in the final difference-Fourier map. Three tertahydrofuran solvent molecules were identified. Refinement of the solvents resulted in poor geometries and higher-than-acceptable thermal parameters. Restrained refinement did not produce a better model. It was decided to complete the refinement using the SQUEEZE[17] routine to account for the solvent contributions.

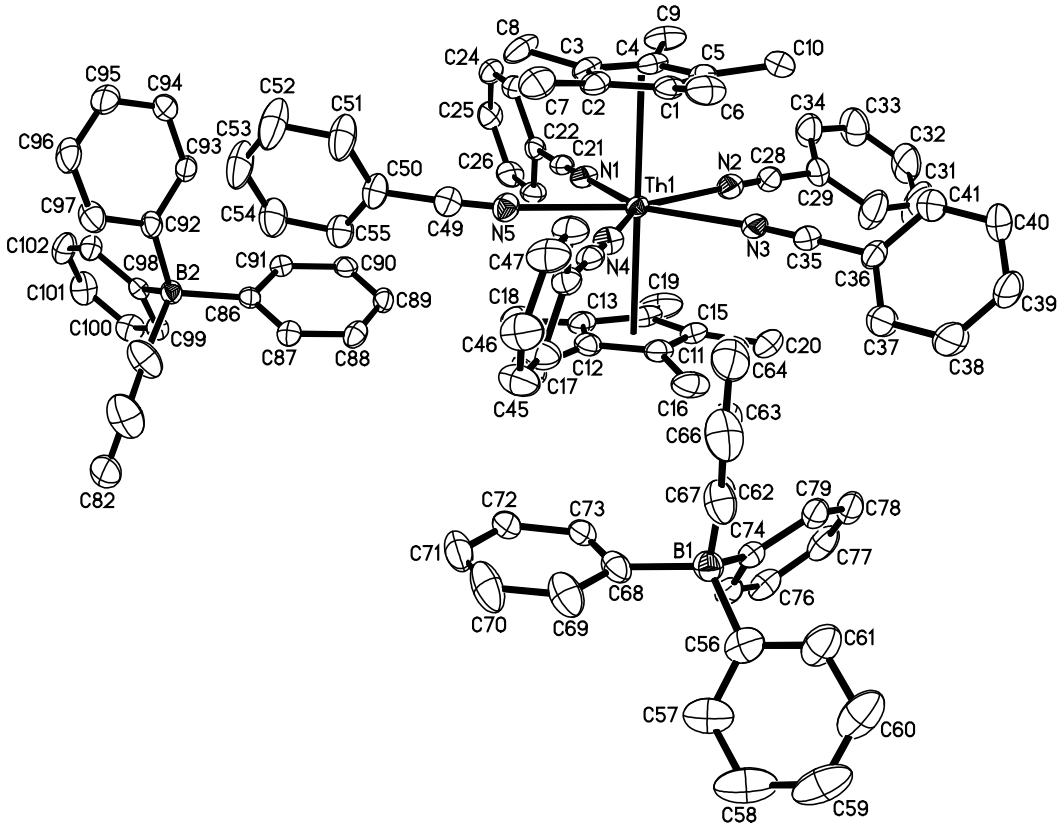


Figure S5. Thermal ellipsoid plot of $[(C_5Me_5)_2Th(NCPh)_5][BPh_4]_2$, **3**, shown at the 50% probability level with hydrogens omitted for clarity.

Table S10. Crystal data and structure refinement for $[(C_5Me_5)_2Th(NCPh)_5][BPh_4]_2$, **3**.

Identification code	rrl53 (Ryan Langeslay)	
Empirical formula	$C_{103}\ H_{95}\ B_2\ N_5\ Th$	
Formula weight	1656.49	
Temperature	88(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 9.4734(4) Å	α = 98.7599(6)°.
	b = 20.0458(9) Å	β = 91.6509(6)°.
	c = 26.0053(11) Å	γ = 101.1373(6)°.
Volume	4780.3(4) Å^3	
Z	2	
Density (calculated)	1.151 Mg/m^3	
Absorption coefficient	1.605 mm^{-1}	
F(000)	1696	
Crystal color	yellow	
Crystal size	0.442 x 0.222 x 0.070 mm^3	
Theta range for data collection	1.587 to 29.207°	
Index ranges	$-13 \le h \le 12$, $-26 \le k \le 26$, $-35 \le l \le 34$	
Reflections collected	60333	
Independent reflections	23753 [R(int) = 0.0265]	
Completeness to theta = 25.500°	99.8 %	
Absorption correction	Numerical	
Max. and min. transmission	0.9201 and 0.6393	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	23753 / 0 / 1010	
Goodness-of-fit on F^2	1.081	
Final R indices [I>2sigma(I) = 21209 data]	R1 = 0.0349, wR2 = 0.0779	
R indices (all data, 0.73Å)	R1 = 0.0421, wR2 = 0.0801	
Largest diff. peak and hole	2.499 and −1.175 e.Å^{-3}	

Table S11. Bond lengths [Å] and angles [°] for $[(C_5Me_5)_2Th(NCPh)_5][BPh_4]_2$, **3**.

Th(1)-Cnt1	2.603	C(11)-C(16)	1.508(4)
Th(1)-Cnt2	2.601	C(12)-C(13)	1.417(4)
Th(1)-N(2)	2.567(2)	C(12)-C(17)	1.504(4)
Th(1)-N(3)	2.569(2)	C(13)-C(14)	1.411(4)
Th(1)-N(5)	2.572(2)	C(13)-C(18)	1.509(4)
Th(1)-N(4)	2.592(2)	C(14)-C(15)	1.419(4)
Th(1)-N(1)	2.599(2)	C(14)-C(19)	1.496(4)
Th(1)-C(11)	2.850(2)	C(15)-C(20)	1.509(4)
Th(1)-C(12)	2.852(2)	C(21)-C(22)	1.439(3)
Th(1)-C(3)	2.863(2)	C(22)-C(23)	1.394(3)
Th(1)-C(1)	2.867(3)	C(22)-C(27)	1.396(3)
Th(1)-C(5)	2.868(3)	C(23)-C(24)	1.380(4)
Th(1)-C(2)	2.869(3)	C(24)-C(25)	1.385(4)
Th(1)-C(15)	2.869(2)	C(25)-C(26)	1.383(4)
Th(1)-C(13)	2.872(3)	C(26)-C(27)	1.387(4)
Th(1)-C(4)	2.873(3)	C(28)-C(29)	1.431(4)
Th(1)-C(14)	2.883(3)	C(29)-C(34)	1.378(4)
N(1)-C(21)	1.143(3)	C(29)-C(30)	1.386(4)
N(2)-C(28)	1.140(3)	C(30)-C(31)	1.379(5)
N(3)-C(35)	1.145(3)	C(31)-C(32)	1.373(6)
N(4)-C(42)	1.139(3)	C(32)-C(33)	1.351(5)
N(5)-C(49)	1.137(3)	C(33)-C(34)	1.390(5)
C(1)-C(5)	1.412(4)	C(35)-C(36)	1.431(4)
C(1)-C(2)	1.414(4)	C(36)-C(37)	1.376(4)
C(1)-C(6)	1.505(4)	C(36)-C(41)	1.388(4)
C(2)-C(3)	1.426(4)	C(37)-C(38)	1.391(4)
C(2)-C(7)	1.508(4)	C(38)-C(39)	1.362(5)
C(3)-C(4)	1.412(4)	C(39)-C(40)	1.376(5)
C(3)-C(8)	1.510(4)	C(40)-C(41)	1.379(4)
C(4)-C(5)	1.421(4)	C(42)-C(43)	1.442(4)
C(4)-C(9)	1.504(4)	C(43)-C(48)	1.391(4)
C(5)-C(10)	1.505(4)	C(43)-C(44)	1.393(4)
C(11)-C(15)	1.410(4)	C(44)-C(45)	1.384(4)
C(11)-C(12)	1.411(4)	C(45)-C(46)	1.373(4)

C(46)-C(47)	1.378(4)	C(75)-C(76)	1.387(4)
C(47)-C(48)	1.387(4)	C(76)-C(77)	1.378(4)
C(49)-C(50)	1.436(4)	C(77)-C(78)	1.385(4)
C(50)-C(51)	1.388(4)	C(78)-C(79)	1.390(4)
C(50)-C(55)	1.394(4)	B(2)-C(92)	1.644(4)
C(51)-C(52)	1.385(5)	B(2)-C(98)	1.648(4)
C(52)-C(53)	1.384(5)	B(2)-C(80)	1.652(4)
C(53)-C(54)	1.378(5)	B(2)-C(86)	1.661(4)
C(54)-C(55)	1.377(4)	C(80)-C(81)	1.394(4)
B(1)-C(74)	1.646(4)	C(80)-C(85)	1.398(4)
B(1)-C(56)	1.648(4)	C(81)-C(82)	1.397(4)
B(1)-C(62)	1.653(4)	C(82)-C(83)	1.371(5)
B(1)-C(68)	1.656(4)	C(83)-C(84)	1.372(5)
C(56)-C(57)	1.388(5)	C(84)-C(85)	1.389(5)
C(56)-C(61)	1.402(5)	C(86)-C(87)	1.403(4)
C(57)-C(58)	1.406(5)	C(86)-C(91)	1.406(4)
C(58)-C(59)	1.381(6)	C(87)-C(88)	1.395(4)
C(59)-C(60)	1.365(6)	C(88)-C(89)	1.379(4)
C(60)-C(61)	1.411(5)	C(89)-C(90)	1.383(4)
C(62)-C(63)	1.396(4)	C(90)-C(91)	1.393(4)
C(62)-C(67)	1.397(4)	C(92)-C(93)	1.387(4)
C(63)-C(64)	1.392(4)	C(92)-C(97)	1.406(4)
C(64)-C(65)	1.378(5)	C(93)-C(94)	1.391(4)
C(65)-C(66)	1.381(5)	C(94)-C(95)	1.382(4)
C(66)-C(67)	1.403(5)	C(95)-C(96)	1.382(5)
C(68)-C(73)	1.392(4)	C(96)-C(97)	1.388(4)
C(68)-C(69)	1.408(4)	C(98)-C(103)	1.404(4)
C(69)-C(70)	1.399(5)	C(98)-C(99)	1.407(4)
C(70)-C(71)	1.377(5)	C(99)-C(100)	1.386(4)
C(71)-C(72)	1.379(5)	C(100)-C(101)	1.390(4)
C(72)-C(73)	1.403(4)	C(101)-C(102)	1.373(4)
C(74)-C(75)	1.401(4)	C(102)-C(103)	1.392(4)
C(74)-C(79)	1.404(4)		

Cnt1-Th(1)-N(1)	89.9	Cnt1-Th(1)-N(3)	90.0
Cnt1-Th(1)-N(2)	89.4	Cnt1-Th(1)-N(4)	90.6

Cnt1-Th(1)-N(5)	90.1	N(3)-Th(1)-C(1)	69.90(7)
Cnt2-Th(1)-N(1)	88.7	N(5)-Th(1)-C(1)	97.84(8)
Cnt2-Th(1)-N(2)	89.5	N(4)-Th(1)-C(1)	71.11(7)
Cnt2-Th(1)-N(3)	90.7	N(1)-Th(1)-C(1)	114.66(7)
Cnt2-Th(1)-N(4)	91.0	C(11)-Th(1)-C(1)	131.68(7)
Cnt2-Th(1)-N(5)	90.2	C(12)-Th(1)-C(1)	142.09(8)
Cnt1-Th(1)-Cnt2	178.4	C(3)-Th(1)-C(1)	47.11(7)
N(2)-Th(1)-N(3)	72.90(7)	N(2)-Th(1)-C(5)	69.60(8)
N(2)-Th(1)-N(5)	143.29(7)	N(3)-Th(1)-C(5)	70.41(7)
N(3)-Th(1)-N(5)	143.81(7)	N(5)-Th(1)-C(5)	114.85(8)
N(2)-Th(1)-N(4)	145.37(7)	N(4)-Th(1)-C(5)	98.52(8)
N(3)-Th(1)-N(4)	72.47(7)	N(1)-Th(1)-C(5)	97.04(7)
N(5)-Th(1)-N(4)	71.34(7)	C(11)-Th(1)-C(5)	141.26(7)
N(2)-Th(1)-N(1)	71.30(7)	C(12)-Th(1)-C(5)	166.85(8)
N(3)-Th(1)-N(1)	144.20(7)	C(3)-Th(1)-C(5)	47.07(8)
N(5)-Th(1)-N(1)	71.99(7)	C(1)-Th(1)-C(5)	28.50(8)
N(4)-Th(1)-N(1)	143.33(7)	N(2)-Th(1)-C(2)	114.34(8)
N(2)-Th(1)-C(11)	97.53(8)	N(3)-Th(1)-C(2)	96.98(7)
N(3)-Th(1)-C(11)	70.87(7)	N(5)-Th(1)-C(2)	70.41(7)
N(5)-Th(1)-C(11)	97.40(8)	N(4)-Th(1)-C(2)	70.16(7)
N(4)-Th(1)-C(11)	71.02(7)	N(1)-Th(1)-C(2)	97.79(7)
N(1)-Th(1)-C(11)	113.66(7)	C(11)-Th(1)-C(2)	141.18(8)
N(2)-Th(1)-C(12)	114.38(7)	C(12)-Th(1)-C(2)	131.25(8)
N(3)-Th(1)-C(12)	98.28(7)	C(3)-Th(1)-C(2)	28.81(8)
N(5)-Th(1)-C(12)	70.10(7)	C(1)-Th(1)-C(2)	28.54(8)
N(4)-Th(1)-C(12)	70.98(7)	C(5)-Th(1)-C(2)	47.09(8)
N(1)-Th(1)-C(12)	96.10(7)	N(2)-Th(1)-C(15)	70.08(7)
C(11)-Th(1)-C(12)	28.66(7)	N(3)-Th(1)-C(15)	70.73(7)
N(2)-Th(1)-C(3)	96.90(8)	N(5)-Th(1)-C(15)	114.94(7)
N(3)-Th(1)-C(3)	114.87(7)	N(4)-Th(1)-C(15)	98.29(8)
N(5)-Th(1)-C(3)	70.00(8)	N(1)-Th(1)-C(15)	96.59(7)
N(4)-Th(1)-C(3)	97.46(8)	C(11)-Th(1)-C(15)	28.54(8)
N(1)-Th(1)-C(3)	70.14(7)	C(12)-Th(1)-C(15)	47.07(8)
C(11)-Th(1)-C(3)	165.51(8)	C(3)-Th(1)-C(15)	164.25(8)
C(12)-Th(1)-C(3)	140.07(8)	C(1)-Th(1)-C(15)	140.61(8)
N(2)-Th(1)-C(1)	96.85(8)	C(5)-Th(1)-C(15)	130.19(8)

C(2)-Th(1)-C(15)	165.61(8)	C(2)-Th(1)-C(14)	165.03(8)
N(2)-Th(1)-C(13)	96.40(8)	C(15)-Th(1)-C(14)	28.56(8)
N(3)-Th(1)-C(13)	115.52(7)	C(13)-Th(1)-C(14)	28.38(8)
N(5)-Th(1)-C(13)	70.51(8)	C(4)-Th(1)-C(14)	128.96(8)
N(4)-Th(1)-C(13)	98.36(8)	C(21)-N(1)-Th(1)	179.5(2)
N(1)-Th(1)-C(13)	68.75(7)	C(28)-N(2)-Th(1)	178.5(2)
C(11)-Th(1)-C(13)	47.16(7)	C(35)-N(3)-Th(1)	176.2(2)
C(12)-Th(1)-C(13)	28.67(7)	C(42)-N(4)-Th(1)	175.5(2)
C(3)-Th(1)-C(13)	129.59(7)	C(49)-N(5)-Th(1)	172.3(2)
C(1)-Th(1)-C(13)	166.69(8)	C(5)-C(1)-C(2)	108.4(2)
C(5)-Th(1)-C(13)	163.12(8)	C(5)-C(1)-C(6)	125.0(3)
C(2)-Th(1)-C(13)	140.89(8)	C(2)-C(1)-C(6)	125.5(3)
C(15)-Th(1)-C(13)	47.00(8)	C(5)-C(1)-Th(1)	75.77(15)
N(2)-Th(1)-C(4)	69.63(7)	C(2)-C(1)-Th(1)	75.80(14)
N(3)-Th(1)-C(4)	97.93(7)	C(6)-C(1)-Th(1)	123.96(17)
N(5)-Th(1)-C(4)	97.13(8)	C(1)-C(2)-C(3)	107.5(2)
N(4)-Th(1)-C(4)	115.40(7)	C(1)-C(2)-C(7)	125.3(3)
N(1)-Th(1)-C(4)	69.75(7)	C(3)-C(2)-C(7)	126.5(3)
C(11)-Th(1)-C(4)	165.40(8)	C(1)-C(2)-Th(1)	75.66(15)
C(12)-Th(1)-C(4)	163.74(8)	C(3)-C(2)-Th(1)	75.36(14)
C(3)-Th(1)-C(4)	28.50(8)	C(7)-C(2)-Th(1)	122.37(18)
C(1)-Th(1)-C(4)	47.08(8)	C(4)-C(3)-C(2)	108.2(2)
C(5)-Th(1)-C(4)	28.66(8)	C(4)-C(3)-C(8)	125.8(3)
C(2)-Th(1)-C(4)	47.21(8)	C(2)-C(3)-C(8)	125.0(3)
C(15)-Th(1)-C(4)	139.70(8)	C(4)-C(3)-Th(1)	76.13(14)
C(13)-Th(1)-C(4)	138.50(8)	C(2)-C(3)-Th(1)	75.83(14)
N(2)-Th(1)-C(14)	69.48(8)	C(8)-C(3)-Th(1)	123.33(18)
N(3)-Th(1)-C(14)	97.96(8)	C(3)-C(4)-C(5)	107.8(2)
N(5)-Th(1)-C(14)	97.74(8)	C(3)-C(4)-C(9)	125.2(3)
N(4)-Th(1)-C(14)	115.62(7)	C(5)-C(4)-C(9)	126.1(3)
N(1)-Th(1)-C(14)	69.18(7)	C(3)-C(4)-Th(1)	75.37(15)
C(11)-Th(1)-C(14)	47.02(8)	C(5)-C(4)-Th(1)	75.47(15)
C(12)-Th(1)-C(14)	46.97(8)	C(9)-C(4)-Th(1)	123.69(18)
C(3)-Th(1)-C(14)	139.33(8)	C(1)-C(5)-C(4)	108.1(2)
C(1)-Th(1)-C(14)	164.35(9)	C(1)-C(5)-C(10)	126.7(3)
C(5)-Th(1)-C(14)	139.07(9)	C(4)-C(5)-C(10)	124.4(3)

C(1)-C(5)-Th(1)	75.74(15)	C(27)-C(22)-C(21)	120.7(2)
C(4)-C(5)-Th(1)	75.87(15)	C(24)-C(23)-C(22)	119.6(2)
C(10)-C(5)-Th(1)	122.67(18)	C(23)-C(24)-C(25)	119.6(2)
C(15)-C(11)-C(12)	108.2(2)	C(26)-C(25)-C(24)	121.0(3)
C(15)-C(11)-C(16)	125.9(3)	C(25)-C(26)-C(27)	120.2(3)
C(12)-C(11)-C(16)	125.1(3)	C(26)-C(27)-C(22)	118.7(2)
C(15)-C(11)-Th(1)	76.49(14)	N(2)-C(28)-C(29)	178.5(3)
C(12)-C(11)-Th(1)	75.77(14)	C(34)-C(29)-C(30)	120.8(3)
C(16)-C(11)-Th(1)	122.50(18)	C(34)-C(29)-C(28)	121.3(3)
C(11)-C(12)-C(13)	108.0(2)	C(30)-C(29)-C(28)	117.9(3)
C(11)-C(12)-C(17)	125.8(3)	C(31)-C(30)-C(29)	118.5(4)
C(13)-C(12)-C(17)	125.2(3)	C(32)-C(31)-C(30)	120.5(4)
C(11)-C(12)-Th(1)	75.57(14)	C(33)-C(32)-C(31)	121.0(3)
C(13)-C(12)-Th(1)	76.45(15)	C(32)-C(33)-C(34)	119.9(3)
C(17)-C(12)-Th(1)	122.73(18)	C(29)-C(34)-C(33)	119.3(3)
C(14)-C(13)-C(12)	107.9(2)	N(3)-C(35)-C(36)	179.1(3)
C(14)-C(13)-C(18)	125.7(3)	C(37)-C(36)-C(41)	121.1(3)
C(12)-C(13)-C(18)	125.5(3)	C(37)-C(36)-C(35)	118.9(3)
C(14)-C(13)-Th(1)	76.22(15)	C(41)-C(36)-C(35)	119.9(3)
C(12)-C(13)-Th(1)	74.89(14)	C(36)-C(37)-C(38)	119.0(3)
C(18)-C(13)-Th(1)	123.71(18)	C(39)-C(38)-C(37)	120.0(3)
C(13)-C(14)-C(15)	108.0(2)	C(38)-C(39)-C(40)	121.0(3)
C(13)-C(14)-C(19)	125.5(3)	C(39)-C(40)-C(41)	120.0(3)
C(15)-C(14)-C(19)	125.6(3)	C(40)-C(41)-C(36)	118.8(3)
C(13)-C(14)-Th(1)	75.40(15)	N(4)-C(42)-C(43)	179.4(3)
C(15)-C(14)-Th(1)	75.19(15)	C(48)-C(43)-C(44)	121.2(3)
C(19)-C(14)-Th(1)	124.18(18)	C(48)-C(43)-C(42)	119.9(2)
C(11)-C(15)-C(14)	107.9(2)	C(44)-C(43)-C(42)	118.8(2)
C(11)-C(15)-C(20)	124.8(3)	C(45)-C(44)-C(43)	118.7(3)
C(14)-C(15)-C(20)	126.5(3)	C(46)-C(45)-C(44)	120.6(3)
C(11)-C(15)-Th(1)	74.97(15)	C(45)-C(46)-C(47)	120.5(3)
C(14)-C(15)-Th(1)	76.25(14)	C(46)-C(47)-C(48)	120.4(3)
C(20)-C(15)-Th(1)	123.24(19)	C(47)-C(48)-C(43)	118.6(3)
N(1)-C(21)-C(22)	178.4(3)	N(5)-C(49)-C(50)	176.2(3)
C(23)-C(22)-C(27)	120.9(2)	C(51)-C(50)-C(55)	121.3(3)
C(23)-C(22)-C(21)	118.3(2)	C(51)-C(50)-C(49)	119.6(3)

C(55)-C(50)-C(49)	119.0(3)	C(75)-C(74)-C(79)	115.2(3)
C(52)-C(51)-C(50)	119.0(3)	C(75)-C(74)-B(1)	121.6(2)
C(53)-C(52)-C(51)	119.6(3)	C(79)-C(74)-B(1)	122.9(2)
C(54)-C(53)-C(52)	121.1(3)	C(76)-C(75)-C(74)	122.5(3)
C(55)-C(54)-C(53)	120.1(3)	C(77)-C(76)-C(75)	120.3(3)
C(54)-C(55)-C(50)	118.8(3)	C(76)-C(77)-C(78)	119.4(3)
C(74)-B(1)-C(56)	104.9(2)	C(77)-C(78)-C(79)	119.7(3)
C(74)-B(1)-C(62)	112.5(2)	C(78)-C(79)-C(74)	122.8(3)
C(56)-B(1)-C(62)	110.4(2)	C(92)-B(2)-C(98)	106.4(2)
C(74)-B(1)-C(68)	112.0(2)	C(92)-B(2)-C(80)	111.2(2)
C(56)-B(1)-C(68)	114.5(2)	C(98)-B(2)-C(80)	110.9(2)
C(62)-B(1)-C(68)	102.8(2)	C(92)-B(2)-C(86)	110.2(2)
C(57)-C(56)-C(61)	116.4(3)	C(98)-B(2)-C(86)	109.9(2)
C(57)-C(56)-B(1)	124.9(3)	C(80)-B(2)-C(86)	108.3(2)
C(61)-C(56)-B(1)	118.6(3)	C(81)-C(80)-C(85)	114.2(3)
C(56)-C(57)-C(58)	122.0(4)	C(81)-C(80)-B(2)	123.5(2)
C(59)-C(58)-C(57)	119.8(4)	C(85)-C(80)-B(2)	122.2(3)
C(60)-C(59)-C(58)	120.1(4)	C(80)-C(81)-C(82)	123.1(3)
C(59)-C(60)-C(61)	119.7(4)	C(83)-C(82)-C(81)	120.8(3)
C(56)-C(61)-C(60)	121.9(4)	C(82)-C(83)-C(84)	117.9(3)
C(63)-C(62)-C(67)	115.8(3)	C(83)-C(84)-C(85)	121.1(3)
C(63)-C(62)-B(1)	122.3(2)	C(84)-C(85)-C(80)	123.0(3)
C(67)-C(62)-B(1)	121.5(3)	C(87)-C(86)-C(91)	114.8(2)
C(64)-C(63)-C(62)	123.2(3)	C(87)-C(86)-B(2)	123.0(2)
C(65)-C(64)-C(63)	119.5(3)	C(91)-C(86)-B(2)	122.2(2)
C(64)-C(65)-C(66)	119.4(3)	C(88)-C(87)-C(86)	122.8(2)
C(65)-C(66)-C(67)	120.5(3)	C(89)-C(88)-C(87)	120.6(3)
C(62)-C(67)-C(66)	121.6(3)	C(88)-C(89)-C(90)	118.4(2)
C(73)-C(68)-C(69)	114.4(3)	C(89)-C(90)-C(91)	120.7(2)
C(73)-C(68)-B(1)	123.6(3)	C(90)-C(91)-C(86)	122.6(2)
C(69)-C(68)-B(1)	121.3(3)	C(93)-C(92)-C(97)	114.9(3)
C(70)-C(69)-C(68)	122.8(3)	C(93)-C(92)-B(2)	122.4(2)
C(71)-C(70)-C(69)	120.6(3)	C(97)-C(92)-B(2)	122.2(2)
C(70)-C(71)-C(72)	118.5(3)	C(92)-C(93)-C(94)	123.4(3)
C(71)-C(72)-C(73)	120.3(3)	C(95)-C(94)-C(93)	120.2(3)
C(68)-C(73)-C(72)	123.4(3)	C(96)-C(95)-C(94)	118.3(3)

C(95)-C(96)-C(97)	120.6(3)	C(100)-C(99)-C(98)	122.9(3)
C(96)-C(97)-C(92)	122.6(3)	C(99)-C(100)-C(101)	120.4(3)
C(103)-C(98)-C(99)	114.4(2)	C(102)-C(101)-C(100)	118.6(3)
C(103)-C(98)-B(2)	123.8(2)	C(101)-C(102)-C(103)	120.5(3)
C(99)-C(98)-B(2)	121.8(2)	C(102)-C(103)-C(98)	123.1(3)

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