Supporting Information

Experimental Section

General Comments. Unless otherwise noted, reactions and manipulations were performed at 20 °C in a recirculating Vacuum Atmospheres Model HE-553-2 inert atmosphere (He or N_2) drybox with a MO-40-2 Dri-Train, or using standard Schlenk and high vacuum line techniques. Glassware was dried a minimum of 12 h at 150 °C before use. Reagents were purchased from commercial suppliers and used without further purification unless otherwise noted. Celite (Aldrich) and alumina (Brockman I, Aldrich) were dried in vacuo at 250 °C for 48 h prior to use. Toluene (Fisher), hexanes (Fisher), diethyl ether (Fisher), and tetrahydrofuran (Fisher) were passed through a column of activated alumina (A2, 12 x 32, Purifry) under nitrogen or argon pressure and sparged with N_2 prior to use.[1] Deuterated solvents (Cambridge Isotope Laboratories) were purified by storage over activated 4Å sieves or sodium metal and degassed by three freeze-pump-thaw cycles prior to use. All other reagents were ACS reagent grade and used as received.

Melting point data (°C) were obtained in sealed capillary tubes and are uncorrected. Nuclear magnetic resonance spectra were recorded on a Varian Unity Inova 300 MHz spectrometer. ^{1}H NMR spectra are referenced to the residual protio signal for the respective deuterated solvent. Infrared spectroscopy was performed on a Nicolet

Magna-IR 560 FTIR Spectrometer E. S. P. instrument using mineral oil mulls on KBr plates. Elemental analysis and mass spectrometry were performed at the University of California, Berkeley Micro-Mass Facility.

ansa-Cyclopentadienyl-amido ligands and the corresponding dilihtio salts, $Li_2[C_5Me_4Si(Me)_2NPh]$ and $Li_2[C_5Me_4Si(Me)_2N$-*t*-Bu] were prepared by literature methods.[2]

1 (a) Pangborn, A. B.; Giardellop, M. A.; Grubbs, R. H.; Rosen, R. K.; Timmers, F. J. *Organometallics* **1996**, *15*, 1518-1520. (b) Alaimo, P. J.; Peters, D. W.; Arnold, J. Bergman, R. G. *J. Chem. Ed.* **2001**, *78*, 64.

2 Alt, H. G.; Fottinger, K.; Milius, W. *Journal of Organometallic Chemistry* **1999**, *572*, 21-30.

Synthesis of $(C_5Me_4Si(Me)_2NPhThCl_2)_4$ (1). A 125 mL Erlenmeyer flask was charged with the solids, $Li_2[C_5Me_4Si(Me)_2NPh]$ (0.277 g, 0.978 mmol) and $ThCl_4$ (0.400 g, 1.07 mmol), and a magnetic stirbar. Diethyl ether (25 mL) was added and the reaction vessel was stoppered. The reaction mixture was allowed to stir for 4 d at ambient temperature - producing a cloudy very lightly yellow tinged solution. Stirring was stopped and the precipitates allowed to settle for 2 h. The reaction mixture was then filtered through a Celite pad over a coarse 15 mL filter frit. The precipitates were washed with diethyl ether (5 x 10 mL portions). These washings were combined with the original filtered solution and the volatiles were removed in vacuo. The majority of the residual

solid materials were dissolved in toluene (25 mL) and this solution was filtered through a plug of glass fiber filter. The volatiles were removed in vacuo to yield $(C_5Me_4Si(Me)_2NPhThCl_2)_4 \bullet C_7H_8$ (**1**$\bullet C_7H_8$). Crude yield: 0.501 g, 0.210 mmol, 21.5% based upon $Li_2[C_5Me_4Si(Me)_2NPh]$. The solid material, **1**, was collected in a 20 mL scintillation vial and dissolved in minimum volume of toluene (15 mL), and crystallized over 2 d at –35 °C. The microcrystalline solid material was collected on a fine porosity 15 mL filter frit and washed with cold hexanes (2 x 10 mL portions) and residual volatiles removed in vacuo. Yield of **1**$\bullet C_7H_8$; 0.314 g, 0.132 mmol, 13.5%. ^{1}H NMR (C_6D_6, 300 MHz, 21 °C): δ 7.28 (t, J = 7.8 Hz, 8H, meta N-Ph), 7.12 (d, J = 7.2 Hz, 2H, ortho C_7H_8), 7.04 (t, J = 6.9 Hz, 1H para C_7H_8), 6.99 (d, J = 7.3 Hz, 8H, ortho N-Ph), 6.91 (t, J = 7.1 Hz, 4H, para N-Ph), 2.11 (s, 3H, methyl C_7H_8), 2.05 (s, 12H, $H_3CC_5(Me)_3$), 1.92 (s, 12H, $H_3CC_5(Me)_3$), 1.88 (s, 12H, $H_3CC_5(Me)_3$), 1.62 (s, 12H, $H_3CC_5(Me)_3$), 0.49 (s, 12H, H_3CSi), 0.37 (s, 12H, H_3CSi). IR (mineral oil mull, KBr plates, cm^{-1}) 1587 (s), 1326 (w), 1294 (m), 1244 (s, br), 1168 (m), 1102 (s), 1068 (m), 1026 (m), 997 (w), 892 (s, br), 835 (s, br), 780 (s, br), 727 (m), 697 (s, sh), 608 (w, sh). Mp > 250 °C. Anal. Calcd for $C_{75}H_{100}Si_4N_4Th_4Cl_8$: C, 37.82%; H, 4.23%; N, 2.35%. Found: C, 37.70; H, 4.38% N, 2.28%.

Synthesis of $\{Li(Et_2O)_4[C_5Me_4Si(Me)_2N$-*t*-$BuThCl_3]\}_2$ (2). A 125 mL Erlenmeyer flask was charged with the solids, $Li_2[C_5Me_4Si(Me)_2N$-*t*-Bu] (0.313 g, 1.19

mmol) and $ThCl_4$ (0.468 g, 1.25 mmol), and a magnetic stirbar. Diethyl ether (25 mL) was added and the reaction vessel was stoppered. The reaction mixture was allowed to stir for 4 d at ambient temperature producing a cloudy yellowish solution. Stirring was stopped and the precipitates allowed to settle for 2 h. The reaction mixture was then filtered through a Celite pad over a coarse 15 mL filter frit. The precipitates were washed with diethyl ether (4 x 10 mL portions). These washings were combined with the original filtered solution and the volatiles were removed in vacuo. The residual solid materials were dissolved in a minimal amount of diethyl ether (3 mL). The concentrated solution was transferred to a 20 mL scintillation vial and crystals were allowed to form at –35 °C. The crystals were isolated on a fine filter frit, washed with cold hexanes (2 x 10 mL portions) and allowed to dry under a constant stream of nitrogen to yield light yellow $Li_2(OEt_2)_4(C_5Me_4Si(Me)_2N\text{-}t\text{-}BuThCl_3)_2$ (**2**). If solid **2** is subjected to dynamic vacuum for 12 h, one equivalent of diethyl ether is lost from each lithium center to form $Li_2(OEt_2)_2(C_5Me_4Si(Me)_2N\text{-}t\text{-}BuThCl_3)_2$ (**2** – $2OEt_2$) Yield: 0.344 g, 0.514 mmol, 43% based upon $Li_2[C_5Me_4Si(Me)_2N\text{-}t\text{-}Bu]$. ^1H NMR (C_6D_6, 300 MHz, 21 °C): δ 3.27 (q, J = 7.4 Hz, 4H, $O(CH_2CH_3)_2$), 2.53 (s, br, 6H, $C_5(CH_3)_2(CH_3)_2$), 2.30 (s, 6H, $C_5(CH_3)_2(CH_3)_2$), 1.48 (s, 9H, $NC(CH_3)_3$), 1.07 (t, J = 7.5 Hz, 6H, $O(CH_2CH_3)_2$), 0.63 (s, 6H, $Si(CH_3)_2$). IR (mineral oil mull, KBr plates, cm^{-1}) 1595 (w), 1405 (s, sh), 1293 (s), 1259 (w, br), 1044 (w,br), 910 (w), 853 (s, br). Mp > 250 °C. Anal. Calcd for $C_{19}H_{37}SiNThCl_3LiO$: C, 34.12%; H, 5.58%; N, 2.09%. Found: C, 33.38; H, 5.03% N, 2.06%.

Crystallography Section

Experimental

Colorless, irregular shaped crystals of **1** and **2** were mounted onto glass fibers using a spot of silicone grease. Due to air sensitivity, the crystals were mounted from a pool of mineral oil under argon gas flow. In turn, the crystals were placed on a Bruker P4/CCD diffractometer, and cooled to 203 K using a Bruker LT-2 temperature device. The instrument was equipped with a sealed, graphite monochromatized MoKα X-ray source (λ= 0.71073 Å). A hemisphere of data was collected using φ scans, with 30 second frame exposures and 0.3° frame widths. Data collection and initial indexing and cell refinement were handled using SMART[1] software. Frame integration, including Lorentz-polarization corrections, and final cell parameter calculations were carried out using SAINT[2] software. The data were corrected for absorption using the SADABS[3] program. Decay of reflection intensity was monitored *via* analysis of redundant frames. The structure was solved using Direct methods and difference Fourier techniques. A solvent hexane molecule was found in the difference map for **1**. All hydrogen atom positions were idealized, and rode on the atom they were attached to. The final refinement included anisotropic temperature factors on all non-hydrogen atoms. Atom C(6) of **1** was restrained to approximate isotropic refinement, with a standard deviation of 0.04 Å^2, using the ISOR facility in SHELXTL[4]. Structure solution, refinement, graphics, and creation of publication materials were performed using SHELXTL NT[4]. Additional details of data collection and structure refinement are listed in Table 1.

References

1. SMART-NT 4, **1996**, Bruker AXS, Inc., Madison, Wisconsin 53719.
2. SAINT-NT 5.050, **1998**, Bruker AXS, Inc., Madison, Wisconsin 53719.
3. SADABS, first release, George Sheldrick, University of Göttingen, Germany.
4. SHELXTL NT Version 5.10, **1997**, Bruker AXS, Inc., Madison, Wisconsin 53719.

Crystallography data for 1.

Table 1. Crystal data and structure refinement for $C_5Me_4Si(Me)_2NPhThCl_2$.hexane (**1**).

Identification code	ccd514
Empirical formula	$C_{74}\ H_{106}\ Cl_8\ N_4\ Si_4\ Th_4$
Formula weight	2375.75
Temperature	203(2) K
Wavelength	0.71073 Å

Crystal system	tetragonal	
Space group	P 41212	
Unit cell dimensions	a = 16.521(3) Å	α= 90°.
	b = 16.521(3) Å	β= 90°.
	c = 31.814(9) Å	γ = 90°.
Volume	8683(3) $Å_3$	
Z	4	
Density (calculated)	1.817 Mg/m_3	
Absorption coefficient	7.171 mm^{-1}	
F(000)	4520	
Crystal size	0.33 x 0.25 x 0.25 mm_3	
Theta range for data collection	1.39 to 25.35°.	
Index ranges	-19<=h<=19, -19<=k<=18, -36<=l<=38	
Reflections collected	56640	
Independent reflections	7954 [R(int) = 0.0848]	
Max. and min. transmission	0.2673 and 0.2007	
Refinement method	Full-matrix least-squares on F_2	
Data / restraints / parameters	7954 / 6 / 425	
Goodness-of-fit on F_2	1.592	
Final R indices [I>2sigma(I)]	R1 = 0.0695, wR2 = 0.0942	
R indices (all data)	R1 = 0.0784, wR2 = 0.0956	
Absolute structure parameter	0.019(11)	
Largest diff. peak and hole	2.153 and -1.423 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $C_5Me_4Si(Me)_2NPhThCl_2$.hexane (**1**). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Th(1)	5245(1)	3165(1)	377(1)	26(1)
Th(2)	6938(1)	4936(1)	430(1)	29(1)
Si(1)	4327(2)	1680(2)	865(1)	40(1)
Si(2)	8872(2)	5308(3)	302(1)	45(1)
Cl(1)	3886(2)	3886(2)	0	41(1)
Cl(2)	6284(2)	6284(2)	0	43(1)
Cl(3)	5354(2)	4685(2)	775(1)	34(1)
Cl(4)	6133(2)	4121(2)	-220(1)	34(1)
Cl(5)	6862(2)	3284(2)	687(1)	37(1)
N(1)	4650(6)	2669(6)	966(3)	34(2)
N(2)	8064(6)	4846(5)	42(3)	33(2)
C(1)	5696(8)	1592(7)	292(4)	32(3)
C(2)	5893(7)	1925(8)	-111(4)	38(3)
C(3)	5179(8)	2112(7)	-317(4)	37(3)
C(4)	4511(7)	1905(7)	-48(4)	34(3)
C(5)	4839(8)	1604(7)	338(4)	40(3)
C(6)	6314(8)	1277(8)	610(5)	55(4)
C(7)	6733(7)	1968(8)	-285(4)	49(4)
C(8)	5096(8)	2452(8)	-746(4)	53(4)
C(9)	3624(7)	1920(8)	-181(4)	46(4)
C(10)	4682(9)	939(8)	1257(4)	52(4)
C(11)	3202(8)	1628(9)	865(4)	57(4)
C(12)	4562(7)	3041(8)	1368(3)	35(3)
C(13)	5153(10)	2979(11)	1664(5)	83(6)
C(14)	5088(12)	3349(11)	2047(4)	80(6)
C(16)	3801(13)	3796(14)	1876(7)	108(8)
C(17)	3867(10)	3432(10)	1476(5)	69(5)
C(18)	8000(8)	4926(8)	1084(4)	40(3)
C(19)	7302(8)	5186(9)	1281(4)	41(3)
C(20)	7114(7)	5947(9)	1135(4)	38(4)
C(15)	4412(14)	3744(11)	2145(5)	86(6)
C(21)	7700(8)	6198(9)	836(4)	44(4)
C(22)	8275(8)	5540(8)	782(4)	35(3)

C(23)	8471(9)	4153(8)	1187(4)	52(4)
C(24)	6887(9)	4732(10)	1633(4)	65(5)
C(25)	6443(8)	6493(10)	1315(5)	66(5)
C(26)	7745(8)	7032(8)	643(4)	52(4)
C(27)	9739(8)	4638(10)	367(5)	72(5)
C(28)	9280(9)	6197(9)	19(6)	76(5)
C(29)	8188(8)	4525(8)	-364(4)	41(3)
C(30)	8026(10)	4959(10)	-731(5)	66(5)
C(31)	8109(12)	4635(12)	-1108(5)	78(6)
C(32)	8384(13)	3922(15)	-1191(6)	102(8)
C(33)	8555(16)	3483(14)	-833(7)	124(9)
C(34)	8479(12)	3774(10)	-418(7)	92(6)
C(35)	3813(14)	5975(15)	2289(7)	134(9)
C(36)	6331(18)	4268(16)	-1945(6)	149(11)
C(37)	6099(15)	4062(12)	-1522(6)	129(9)

Table 3. Bond lengths [Å] and angles [°] for $C_5Me_4Si(Me)_2NPhThCl_2$.hexane (1).

Th(1)-N(1)	2.268(9)
Th(1)-C(5)	2.668(12)
Th(1)-C(1)	2.716(12)
Th(1)-C(4)	2.762(12)
Th(1)-C(2)	2.784(11)
Th(1)-Cl(1)	2.8109(13)
Th(1)-C(3)	2.814(12)
Th(1)-Cl(3)	2.819(3)
Th(1)-Cl(5)	2.854(3)
Th(1)-Cl(4)	2.874(3)
Th(1)-Si(1)	3.274(4)
Th(1)-Th(2)	4.0522(9)
Th(2)-N(2)	2.238(9)
Th(2)-C(22)	2.669(12)
Th(2)-C(18)	2.720(13)
Th(2)-C(21)	2.757(13)
Th(2)-C(19)	2.804(12)
Th(2)-Cl(4)	2.805(3)
Th(2)-C(20)	2.810(12)
Th(2)-Cl(2)	2.8285(14)
Th(2)-Cl(5)	2.852(3)
Th(2)-Cl(3)	2.869(3)
Th(2)-Si(2)	3.279(4)
Si(1)-N(1)	1.749(10)
Si(1)-C(10)	1.844(13)
Si(1)-C(11)	1.860(13)
Si(1)-C(5)	1.880(14)
Si(2)-N(2)	1.747(10)
Si(2)-C(27)	1.822(16)
Si(2)-C(28)	1.848(15)
Si(2)-C(22)	1.859(14)
Cl(1)-Th(1)#1	2.8109(13)
Cl(2)-Th(2)#1	2.8285(14)
N(1)-C(12)	1.427(14)
N(2)-C(29)	1.411(15)
C(1)-C(5)	1.423(17)
C(1)-C(2)	1.432(16)

C(1)-C(6)	1.529(15)
C(2)-C(3)	1.386(16)
C(2)-C(7)	1.496(16)
C(3)-C(4)	1.439(18)
C(3)-C(8)	1.482(18)
C(4)-C(5)	1.433(18)
C(4)-C(9)	1.524(15)
C(12)-C(13)	1.359(18)
C(12)-C(17)	1.363(18)
C(13)-C(14)	1.37(2)
C(14)-C(15)	1.33(2)
C(16)-C(15)	1.32(2)
C(16)-C(17)	1.41(2)
C(18)-C(19)	1.382(18)
C(18)-C(22)	1.469(18)
C(18)-C(23)	1.531(18)
C(19)-C(20)	1.377(18)
C(19)-C(24)	1.511(17)
C(20)-C(21)	1.418(18)
C(20)-C(25)	1.540(18)
C(21)-C(22)	1.454(18)
C(21)-C(26)	1.511(18)
C(29)-C(34)	1.342(19)
C(29)-C(30)	1.40(2)
C(30)-C(31)	1.32(2)
C(31)-C(32)	1.29(2)
C(32)-C(33)	1.38(3)
C(33)-C(34)	1.41(3)
C(35)-C(35)#2	1.43(4)
C(35)-C(36)#1	1.45(3)
C(36)-C(37)	1.44(2)
C(36)-C(35)#1	1.45(3)

N(1)-Th(1)-C(5)	65.2(4)
N(1)-Th(1)-C(1)	81.7(4)
C(5)-Th(1)-C(1)	30.6(4)
N(1)-Th(1)-C(4)	86.7(4)
C(5)-Th(1)-C(4)	30.5(4)
C(1)-Th(1)-C(4)	49.6(4)

N(1)-Th(1)-C(2)	111.2(4)
C(5)-Th(1)-C(2)	50.2(4)
C(1)-Th(1)-C(2)	30.1(3)
C(4)-Th(1)-C(2)	48.8(4)
N(1)-Th(1)-Cl(1)	99.2(3)
C(5)-Th(1)-Cl(1)	100.9(3)
C(1)-Th(1)-Cl(1)	125.6(3)
C(4)-Th(1)-Cl(1)	76.1(3)
C(2)-Th(1)-Cl(1)	112.4(3)
N(1)-Th(1)-C(3)	114.1(4)
C(5)-Th(1)-C(3)	49.9(4)
C(1)-Th(1)-C(3)	48.8(3)
C(4)-Th(1)-C(3)	29.9(4)
C(2)-Th(1)-C(3)	28.7(3)
Cl(1)-Th(1)-C(3)	84.0(2)
N(1)-Th(1)-Cl(3)	88.8(3)
C(5)-Th(1)-Cl(3)	153.9(3)
C(1)-Th(1)-Cl(3)	151.6(3)
C(4)-Th(1)-Cl(3)	156.8(3)
C(2)-Th(1)-Cl(3)	151.8(3)
Cl(1)-Th(1)-Cl(3)	82.25(9)
C(3)-Th(1)-Cl(3)	154.9(3)
N(1)-Th(1)-Cl(5)	98.4(2)
C(5)-Th(1)-Cl(5)	108.5(3)
C(1)-Th(1)-Cl(5)	81.0(3)
C(4)-Th(1)-Cl(5)	129.2(3)
C(2)-Th(1)-Cl(5)	83.3(3)
Cl(1)-Th(1)-Cl(5)	149.98(11)
C(3)-Th(1)-Cl(5)	110.5(3)
Cl(3)-Th(1)-Cl(5)	73.97(8)
N(1)-Th(1)-Cl(4)	165.0(2)
C(5)-Th(1)-Cl(4)	129.0(3)
C(1)-Th(1)-Cl(4)	108.6(3)
C(4)-Th(1)-Cl(4)	108.3(3)
C(2)-Th(1)-Cl(4)	80.7(3)
Cl(1)-Th(1)-Cl(4)	83.84(10)
C(3)-Th(1)-Cl(4)	80.8(3)
Cl(3)-Th(1)-Cl(4)	77.00(9)
Cl(5)-Th(1)-Cl(4)	73.29(9)

N(1)-Th(1)-Si(1)	30.4(3)
C(5)-Th(1)-Si(1)	35.1(3)
C(1)-Th(1)-Si(1)	57.2(3)
C(4)-Th(1)-Si(1)	57.6(3)
C(2)-Th(1)-Si(1)	83.8(3)
Cl(1)-Th(1)-Si(1)	98.59(11)
C(3)-Th(1)-Si(1)	83.7(3)
Cl(3)-Th(1)-Si(1)	118.97(10)
Cl(5)-Th(1)-Si(1)	108.79(9)
Cl(4)-Th(1)-Si(1)	164.01(10)
N(1)-Th(1)-Th(2)	121.7(2)
C(5)-Th(1)-Th(2)	150.9(3)
C(1)-Th(1)-Th(2)	120.4(3)
C(4)-Th(1)-Th(2)	150.2(3)
C(2)-Th(1)-Th(2)	106.8(3)
Cl(1)-Th(1)-Th(2)	105.27(9)
C(3)-Th(1)-Th(2)	120.4(3)
Cl(3)-Th(1)-Th(2)	45.07(6)
Cl(5)-Th(1)-Th(2)	44.73(6)
Cl(4)-Th(1)-Th(2)	43.81(6)
Si(1)-Th(1)-Th(2)	147.26(7)
N(2)-Th(2)-C(22)	64.5(4)
N(2)-Th(2)-C(18)	83.4(4)
C(22)-Th(2)-C(18)	31.6(4)
N(2)-Th(2)-C(21)	86.0(4)
C(22)-Th(2)-C(21)	31.0(4)
C(18)-Th(2)-C(21)	49.6(4)
N(2)-Th(2)-C(19)	111.4(4)
C(22)-Th(2)-C(19)	50.4(4)
C(18)-Th(2)-C(19)	28.9(4)
C(21)-Th(2)-C(19)	48.6(4)
N(2)-Th(2)-Cl(4)	87.4(2)
C(22)-Th(2)-Cl(4)	151.8(3)
C(18)-Th(2)-Cl(4)	150.1(3)
C(21)-Th(2)-Cl(4)	157.7(3)
C(19)-Th(2)-Cl(4)	152.2(3)
N(2)-Th(2)-C(20)	113.2(3)
C(22)-Th(2)-C(20)	50.1(4)
C(18)-Th(2)-C(20)	47.8(4)

C(21)-Th(2)-C(20)	29.5(4)
C(19)-Th(2)-C(20)	28.4(4)
Cl(4)-Th(2)-C(20)	157.4(3)
N(2)-Th(2)-Cl(2)	95.9(3)
C(22)-Th(2)-Cl(2)	103.0(3)
C(18)-Th(2)-Cl(2)	128.4(3)
C(21)-Th(2)-Cl(2)	78.8(3)
C(19)-Th(2)-Cl(2)	115.7(3)
Cl(4)-Th(2)-Cl(2)	80.80(10)
C(20)-Th(2)-Cl(2)	87.6(3)
N(2)-Th(2)-Cl(5)	97.5(2)
C(22)-Th(2)-Cl(5)	105.9(3)
C(18)-Th(2)-Cl(5)	78.7(3)
C(21)-Th(2)-Cl(5)	127.6(3)
C(19)-Th(2)-Cl(5)	82.8(3)
Cl(4)-Th(2)-Cl(5)	74.36(9)
C(20)-Th(2)-Cl(5)	110.2(3)
Cl(2)-Th(2)-Cl(5)	151.08(11)
N(2)-Th(2)-Cl(3)	163.7(2)
C(22)-Th(2)-Cl(3)	130.4(3)
C(18)-Th(2)-Cl(3)	107.2(3)
C(21)-Th(2)-Cl(3)	110.3(3)
C(19)-Th(2)-Cl(3)	81.2(3)
Cl(4)-Th(2)-Cl(3)	77.30(9)
C(20)-Th(2)-Cl(3)	82.8(3)
Cl(2)-Th(2)-Cl(3)	87.16(9)
Cl(5)-Th(2)-Cl(3)	73.26(9)
N(2)-Th(2)-Si(2)	30.0(2)
C(22)-Th(2)-Si(2)	34.5(3)
C(18)-Th(2)-Si(2)	57.9(3)
C(21)-Th(2)-Si(2)	58.1(3)
C(19)-Th(2)-Si(2)	83.3(3)
Cl(4)-Th(2)-Si(2)	117.40(9)
C(20)-Th(2)-Si(2)	83.5(3)
Cl(2)-Th(2)-Si(2)	99.45(11)
Cl(5)-Th(2)-Si(2)	104.96(10)
Cl(3)-Th(2)-Si(2)	164.55(9)
N(2)-Th(2)-Th(1)	120.2(2)
C(22)-Th(2)-Th(1)	149.2(3)

C(18)-Th(2)-Th(1)	118.2(3)
C(21)-Th(2)-Th(1)	151.8(3)
C(19)-Th(2)-Th(1)	107.1(3)
Cl(4)-Th(2)-Th(1)	45.17(6)
C(20)-Th(2)-Th(1)	122.3(3)
Cl(2)-Th(2)-Th(1)	106.56(9)
Cl(5)-Th(2)-Th(1)	44.78(6)
Cl(3)-Th(2)-Th(1)	44.07(6)
Si(2)-Th(2)-Th(1)	143.41(8)
N(1)-Si(1)-C(10)	113.5(6)
N(1)-Si(1)-C(11)	110.4(6)
C(10)-Si(1)-C(11)	106.7(7)
N(1)-Si(1)-C(5)	95.1(5)
C(10)-Si(1)-C(5)	114.5(6)
C(11)-Si(1)-C(5)	116.6(6)
N(1)-Si(1)-Th(1)	41.1(3)
C(10)-Si(1)-Th(1)	132.1(5)
C(11)-Si(1)-Th(1)	119.8(5)
C(5)-Si(1)-Th(1)	54.6(4)
N(2)-Si(2)-C(27)	112.9(6)
N(2)-Si(2)-C(28)	113.3(7)
C(27)-Si(2)-C(28)	104.5(7)
N(2)-Si(2)-C(22)	94.2(5)
C(27)-Si(2)-C(22)	116.7(7)
C(28)-Si(2)-C(22)	115.4(7)
N(2)-Si(2)-Th(2)	39.8(3)
C(27)-Si(2)-Th(2)	129.6(5)
C(28)-Si(2)-Th(2)	124.4(6)
C(22)-Si(2)-Th(2)	54.5(4)
Th(1)-Cl(1)-Th(1)#1	149.22(17)
Th(2)-Cl(2)-Th(2)#1	146.67(17)
Th(1)-Cl(3)-Th(2)	90.86(8)
Th(2)-Cl(4)-Th(1)	91.02(8)
Th(2)-Cl(5)-Th(1)	90.50(8)
C(12)-N(1)-Si(1)	122.5(8)
C(12)-N(1)-Th(1)	129.0(7)
Si(1)-N(1)-Th(1)	108.5(5)
C(29)-N(2)-Si(2)	119.1(8)
C(29)-N(2)-Th(2)	130.6(8)

Si(2)-N(2)-Th(2)	110.2(5)
C(5)-C(1)-C(2)	108.3(11)
C(5)-C(1)-C(6)	126.9(12)
C(2)-C(1)-C(6)	124.8(12)
C(5)-C(1)-Th(1)	72.8(7)
C(2)-C(1)-Th(1)	77.5(7)
C(6)-C(1)-Th(1)	116.3(8)
C(3)-C(2)-C(1)	108.4(11)
C(3)-C(2)-C(7)	127.1(13)
C(1)-C(2)-C(7)	124.1(12)
C(3)-C(2)-Th(1)	76.9(7)
C(1)-C(2)-Th(1)	72.3(7)
C(7)-C(2)-Th(1)	121.9(9)
C(2)-C(3)-C(4)	108.5(12)
C(2)-C(3)-C(8)	126.8(13)
C(4)-C(3)-C(8)	124.6(12)
C(2)-C(3)-Th(1)	74.5(7)
C(4)-C(3)-Th(1)	73.1(7)
C(8)-C(3)-Th(1)	119.5(8)
C(5)-C(4)-C(3)	107.6(11)
C(5)-C(4)-C(9)	127.4(13)
C(3)-C(4)-C(9)	124.6(12)
C(5)-C(4)-Th(1)	71.1(7)
C(3)-C(4)-Th(1)	77.1(7)
C(9)-C(4)-Th(1)	123.1(8)
C(1)-C(5)-C(4)	107.0(12)
C(1)-C(5)-Si(1)	122.8(9)
C(4)-C(5)-Si(1)	124.7(10)
C(1)-C(5)-Th(1)	76.6(7)
C(4)-C(5)-Th(1)	78.4(7)
Si(1)-C(5)-Th(1)	90.4(5)
C(13)-C(12)-C(17)	117.8(13)
C(13)-C(12)-N(1)	121.1(13)
C(17)-C(12)-N(1)	121.1(12)
C(12)-C(13)-C(14)	121.8(16)
C(15)-C(14)-C(13)	119.6(17)
C(15)-C(16)-C(17)	119.7(18)
C(12)-C(17)-C(16)	119.7(15)
C(19)-C(18)-C(22)	109.9(12)

C(19)-C(18)-C(23)	125.9(13)
C(22)-C(18)-C(23)	124.0(13)
C(19)-C(18)-Th(2)	78.9(7)
C(22)-C(18)-Th(2)	72.3(7)
C(23)-C(18)-Th(2)	119.8(8)
C(20)-C(19)-C(18)	108.6(12)
C(20)-C(19)-C(24)	127.0(13)
C(18)-C(19)-C(24)	124.1(14)
C(20)-C(19)-Th(2)	76.0(7)
C(18)-C(19)-Th(2)	72.2(7)
C(24)-C(19)-Th(2)	123.0(8)
C(19)-C(20)-C(21)	109.9(12)
C(19)-C(20)-C(25)	124.8(13)
C(21)-C(20)-C(25)	124.7(14)
C(19)-C(20)-Th(2)	75.6(7)
C(21)-C(20)-Th(2)	73.2(7)
C(25)-C(20)-Th(2)	124.9(8)
C(16)-C(15)-C(14)	121.3(17)
C(20)-C(21)-C(22)	107.9(13)
C(20)-C(21)-C(26)	125.0(13)
C(22)-C(21)-C(26)	127.0(13)
C(20)-C(21)-Th(2)	77.3(8)
C(22)-C(21)-Th(2)	71.2(8)
C(26)-C(21)-Th(2)	121.4(8)
C(21)-C(22)-C(18)	103.7(12)
C(21)-C(22)-Si(2)	126.7(11)
C(18)-C(22)-Si(2)	124.0(10)
C(21)-C(22)-Th(2)	77.8(7)
C(18)-C(22)-Th(2)	76.1(7)
Si(2)-C(22)-Th(2)	91.0(5)
C(34)-C(29)-C(30)	115.9(15)
C(34)-C(29)-N(2)	121.1(15)
C(30)-C(29)-N(2)	123.0(13)
C(31)-C(30)-C(29)	122.1(17)
C(32)-C(31)-C(30)	126(2)
C(31)-C(32)-C(33)	112.5(16)
C(32)-C(33)-C(34)	125.2(19)
C(29)-C(34)-C(33)	117.8(18)
C(35)#2-C(35)-C(36)#1	119(3)

C(37)-C(36)-C(35)#1	118(2)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $C_5Me_4Si(Me)_2NPhThCl_2$.hexane (**1**). 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}
Th(1)	26(1)	26(1)	28(1)	0(1)	-2(1)	0(1)
Th(2)	26(1)	32(1)	29(1)	-2(1)	-2(1)	-4(1)
Si(1)	43(2)	40(2)	36(2)	12(2)	-6(2)	-5(2)
Si(2)	32(2)	64(3)	39(2)	-14(2)	4(2)	-9(2)
Cl(1)	31(2)	31(2)	60(3)	10(2)	-10(2)	5(2)
Cl(2)	43(2)	43(2)	45(3)	12(2)	-12(2)	-5(2)
Cl(3)	35(2)	31(2)	36(2)	-5(1)	4(1)	0(1)
Cl(4)	37(2)	45(2)	21(2)	-1(1)	-1(1)	-9(1)
Cl(5)	32(2)	33(2)	45(2)	0(2)	-10(2)	2(2)
N(1)	32(6)	46(7)	25(6)	3(5)	-9(5)	-4(5)
N(2)	41(6)	34(6)	24(6)	-9(5)	5(5)	-4(5)
C(1)	59(9)	26(7)	11(7)	-4(5)	-11(6)	5(6)
C(2)	27(7)	45(9)	43(8)	-19(7)	-1(6)	15(6)
C(3)	45(8)	31(7)	36(8)	-14(6)	-10(7)	13(6)
C(4)	44(8)	18(6)	41(8)	-2(6)	-16(7)	2(6)
C(5)	51(9)	39(8)	31(8)	-2(6)	-20(7)	-1(7)
C(6)	47(9)	30(7)	88(12)	10(7)	-41(8)	17(7)
C(7)	46(9)	40(8)	61(10)	-18(7)	5(7)	10(7)
C(8)	57(10)	61(10)	39(9)	-22(7)	-18(7)	14(8)
C(9)	38(8)	44(9)	57(9)	-6(7)	-14(6)	-15(7)
C(10)	71(11)	57(10)	28(8)	15(7)	-17(8)	-11(8)
C(11)	44(9)	83(12)	44(9)	17(8)	5(7)	-13(8)
C(12)	44(8)	49(8)	12(6)	11(6)	1(5)	-8(7)
C(13)	68(12)	101(16)	80(13)	-30(11)	-13(10)	23(10)
C(14)	125(17)	98(14)	18(8)	-12(8)	-16(9)	-8(12)
C(16)	88(16)	160(20)	79(15)	-35(15)	3(13)	43(14)
C(17)	79(12)	90(13)	39(10)	-15(9)	-11(9)	38(10)
C(18)	47(9)	40(8)	34(8)	-2(6)	-15(7)	6(7)
C(19)	43(8)	51(9)	28(7)	-9(7)	-11(6)	1(7)
C(20)	21(7)	57(10)	37(9)	-19(7)	1(6)	-12(7)
C(15)	134(19)	85(14)	40(11)	-31(10)	2(12)	-6(13)
C(21)	37(8)	54(10)	41(9)	-10(7)	-17(7)	4(7)
C(22)	26(8)	52(9)	29(8)	-7(6)	-8(6)	-7(7)

C(23)	59(10)	54(10)	41(10)	-2(7)	-22(8)	2(8)
C(24)	57(10)	117(14)	22(7)	-1(8)	1(7)	-12(10)
C(25)	42(10)	89(13)	68(12)	-29(10)	-3(8)	6(9)
C(26)	43(9)	51(10)	63(11)	-13(8)	-5(7)	-4(7)
C(27)	35(8)	120(14)	60(11)	-21(11)	0(8)	1(9)
C(28)	68(11)	80(12)	82(13)	-9(11)	44(11)	-37(9)
C(29)	37(8)	54(9)	33(8)	-2(7)	11(7)	-3(7)
C(30)	89(13)	72(12)	36(9)	-12(8)	0(9)	-9(11)
C(31)	91(14)	100(15)	42(11)	-11(10)	23(10)	-42(13)
C(32)	117(18)	160(20)	29(11)	-56(13)	14(11)	-7(16)
C(33)	210(30)	94(18)	72(16)	-46(14)	40(17)	31(16)
C(34)	119(17)	60(12)	97(16)	15(12)	3(14)	39(11)
C(35)	90(20)	150(30)	150(30)	-41(19)	-1(16)	1(16)
C(36)	240(30)	170(30)	38(13)	-7(15)	-20(17)	-40(20)
C(37)	210(30)	84(18)	95(18)	-10(14)	-3(18)	14(16)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $C_5Me_4Si(Me)_2NPhThCl_2$.hexane (**1**).

	x	y	z	U(eq)
H(6A)	6037	1083	856	82
H(6B)	6675	1706	688	82
H(6C)	6618	842	487	82
H(7A)	7114	1808	-73	74
H(7B)	6847	2512	-373	74
H(7C)	6778	1611	-522	74
H(8A)	4533	2518	-812	79
H(8B)	5340	2090	-946	79
H(8C)	5363	2968	-759	79
H(9A)	3292	1750	50	70
H(9B)	3546	1560	-414	70
H(9C)	3477	2460	-262	70
H(10A)	5263	949	1268	78
H(10B)	4503	408	1178	78
H(10C)	4466	1076	1528	78
H(11A)	2991	2002	662	86
H(11B)	3002	1767	1139	86
H(11C)	3033	1089	794	86
H(13)	5614	2677	1604	99
H(14)	5514	3324	2238	96
H(16)	3332	4072	1950	130
H(17)	3437	3458	1288	83
H(15)	4367	3989	2407	104
H(23A)	8929	4108	1003	77
H(23B)	8125	3691	1150	77
H(23C)	8655	4174	1473	77
H(24A)	7145	4217	1672	98
H(24B)	6328	4651	1563	98
H(24C)	6925	5040	1888	98
H(25A)	6423	6990	1159	99
H(25B)	6557	6609	1605	99
H(25C)	5931	6222	1294	99
H(26A)	8193	7055	451	79

H(26B)	7819	7428	860	79
H(26C)	7252	7143	494	79
H(27A)	9571	4152	507	107
H(27B)	10146	4906	531	107
H(27C)	9957	4504	96	107
H(28A)	8855	6583	-25	115
H(28B)	9495	6028	-247	115
H(28C)	9703	6440	184	115
H(30)	7854	5493	-709	79
H(31)	7954	4952	-1336	93
H(32)	8458	3725	-1463	122
H(33)	8735	2954	-868	149
H(34)	8626	3456	-189	110
H(35A)	3248	6113	2248	161
H(35B)	3855	5391	2264	161
H(36A)	6914	4215	-1965	179
H(36B)	6203	4835	-1989	179
H(37A)	6396	4391	-1327	194
H(37B)	6217	3501	-1471	194
H(37C)	5530	4155	-1486	194

Crystallography data for 2.

Table 1. Crystal data and structure refinement for $C_5Me_4Si(Me)_2N$-t-Bu (2).

Identification code	ccd531	
Empirical formula	$C_{46}\ H_{94}\ Cl_6\ Li_2\ N_2\ O_4\ Si_2\ Th_2$	
Formula weight	1486.07	
Temperature	203(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	P 1bar	
Unit cell dimensions	a = 11.261(3) Å	_= 84.364(4)°.
	b = 13.431(3) Å	_= 76.713(4)°.
	c = 22.979(5) Å	_ = 74.913(4)°.
Volume	3263.1(12) $Å^3$	
Z	2	
Density (calculated)	1.512 Mg/m^3	
Absorption coefficient	4.870 mm^{-1}	
F(000)	1464	
Crystal size	0.12 x 0.08 x 0.04 mm^3	
Theta range for data collection	1.57 to 25.35°.	
Index ranges	-13<=h<=13, -16<=k<=16, -27<=l<=27	
Reflections collected	21281	
Independent reflections	10985 [R(int) = 0.0265]	
Max. and min. transmission	0.8290 and 0.5926	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10985 / 1 / 467	
Goodness-of-fit on F^2	1.315	
Final R indices [I>2sigma(I)]	R1 = 0.0486, wR2 = 0.1116	
R indices (all data)	R1 = 0.0657, wR2 = 0.1158	
Largest diff. peak and hole	2.142 and -1.080 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $C_5Me_4Si(Me)_2N$-t-Bu (2). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Th(1)	4858(1)	4269(1)	4131(1)	32(1)
Th(2)	82(1)	8947(1)	885(1)	37(1)
Cl(1)	4281(2)	6344(2)	3794(1)	56(1)
Cl(2)	3437(2)	5147(2)	5248(1)	45(1)
Cl(3)	4956(2)	2533(2)	4887(1)	55(1)
Cl(4)	779(3)	10612(2)	1191(1)	68(1)
Cl(5)	1560(2)	9490(2)	-248(1)	48(1)
Cl(6)	-142(3)	7505(2)	167(1)	60(1)
Si(1)	4088(2)	3198(2)	3089(1)	45(1)
Si(2)	829(3)	7207(2)	1932(1)	59(1)
N(1)	3344(6)	3914(5)	3709(3)	42(2)
N(2)	1597(7)	7754(5)	1295(3)	50(2)
C(1)	5711(7)	3311(6)	3076(3)	35(2)
C(2)	6539(8)	2687(6)	3437(3)	38(2)
C(3)	7347(7)	3258(6)	3547(3)	39(2)
C(4)	7070(7)	4241(6)	3248(4)	41(2)
C(5)	6069(7)	4269(6)	2946(3)	36(2)
C(6)	6647(9)	1538(6)	3625(4)	56(2)
C(7)	8398(9)	2871(8)	3876(4)	61(3)
C(8)	7749(8)	5078(7)	3202(4)	54(2)
C(9)	5546(9)	5118(6)	2542(3)	47(2)
C(10)	3933(10)	1836(8)	3164(6)	83(4)
C(11)	3655(11)	3694(10)	2348(4)	82(4)
C(12)	1954(8)	4133(8)	3962(4)	56(2)
C(13)	1654(11)	3431(12)	4493(7)	124(6)
C(14)	1209(10)	4126(12)	3478(6)	104(5)
C(15)	1466(10)	5269(10)	4175(6)	94(4)
C(16)	-770(8)	8077(6)	1947(3)	41(2)
C(17)	-1091(8)	9147(7)	2069(4)	48(2)
C(18)	-2067(9)	9676(7)	1796(4)	56(2)
C(19)	-2406(8)	8924(9)	1510(4)	57(3)

C(20)	-1654(9)	7952(7)	1613(4)	50(2)
C(21)	-496(10)	9612(8)	2474(4)	67(3)
C(22)	-2720(11)	10811(8)	1823(5)	81(3)
C(23)	-3538(10)	9176(11)	1208(5)	95(4)
C(24)	-1882(12)	6968(9)	1454(5)	85(4)
C(25)	843(12)	5813(8)	1862(7)	107(5)
C(26)	1361(13)	7247(12)	2635(5)	117(6)
C(27)	2986(9)	7425(9)	1043(5)	69(3)
C(28)	3691(12)	6640(17)	1420(8)	216(13)
C(29)	3207(12)	6980(11)	422(6)	112(5)
C(30)	3514(11)	8372(12)	946(7)	117(5)
C(31)	7647(15)	164(11)	5462(7)	115(5)
C(32)	6676(13)	-106(10)	5298(6)	109(5)
C(33)	8540(30)	1480(20)	5828(12)	228(12)
C(34)	9030(20)	1900(20)	5406(12)	234(13)
C(35)	4320(15)	1512(12)	7018(7)	120(5)
C(36)	5507(14)	1291(11)	7184(7)	122(5)
C(37)	3321(13)	1411(10)	6200(7)	102(4)
C(38)	2315(14)	2298(11)	6259(7)	124(5)
C(39)	2498(19)	13611(15)	620(9)	152(7)
C(40)	1960(20)	14243(18)	302(10)	204(10)
C(41)	3390(20)	11692(18)	464(11)	196(9)
C(42)	3900(30)	11480(20)	949(12)	256(13)
C(43)	-1738(15)	13948(12)	1086(8)	120(5)
C(44)	-2687(14)	13475(11)	1138(7)	120(5)
C(45)	-920(13)	13221(11)	1943(7)	106(4)
C(46)	250(13)	12828(10)	2143(6)	106(4)
Li(1)	5639(16)	2173(13)	5783(8)	63(4)
Li(2)	618(17)	12287(13)	785(9)	68(5)
O(1)	7333(7)	1211(6)	5659(3)	77(2)
O(2)	4401(7)	1520(6)	6380(4)	83(2)
O(3)	2265(7)	12568(6)	698(4)	79(2)
O(4)	-689(8)	13255(6)	1305(4)	88(2)

Table 3. Bond lengths [Å] and angles [°] for $C_5Me_4Si(Me)_2N$-t-Bu (**2**).

Th(1)-N(1)	2.312(6)
Th(1)-C(1)	2.712(7)
Th(1)-C(5)	2.750(8)
Th(1)-Cl(3)	2.761(2)
Th(1)-Cl(1)	2.767(2)
Th(1)-C(2)	2.797(7)
Th(1)-C(4)	2.823(8)
Th(1)-C(3)	2.854(7)
Th(1)-Cl(2)	2.874(2)
Th(1)-Cl(2)#1	2.933(2)
Th(1)-Si(1)	3.292(2)
Th(2)-N(2)	2.320(7)
Th(2)-C(16)	2.681(8)
Th(2)-C(17)	2.744(9)
Th(2)-Cl(4)	2.756(2)
Th(2)-Cl(6)	2.758(2)
Th(2)-C(20)	2.797(8)
Th(2)-C(18)	2.835(9)
Th(2)-C(19)	2.845(8)
Th(2)-Cl(5)	2.889(2)
Th(2)-Cl(5)#2	2.932(2)
Th(2)-Si(2)	3.279(3)
Cl(1)-Li(1)#1	2.331(17)
Cl(2)-Th(1)#1	2.933(2)
Cl(3)-Li(1)	2.325(18)
Cl(4)-Li(2)	2.328(18)
Cl(5)-Th(2)#2	2.932(2)
Cl(6)-Li(2)#2	2.344(19)
Si(1)-N(1)	1.721(7)
Si(1)-C(1)	1.867(8)
Si(1)-C(10)	1.870(10)
Si(1)-C(11)	1.889(10)
Si(2)-N(2)	1.722(8)
Si(2)-C(26)	1.858(11)

Si(2)-C(16)	1.868(8)
Si(2)-C(25)	1.891(11)
N(1)-C(12)	1.501(10)
N(2)-C(27)	1.500(12)
C(1)-C(5)	1.430(10)
C(1)-C(2)	1.440(11)
C(2)-C(3)	1.408(11)
C(2)-C(6)	1.543(11)
C(3)-C(4)	1.420(11)
C(3)-C(7)	1.503(11)
C(4)-C(5)	1.444(11)
C(4)-C(8)	1.498(11)
C(5)-C(9)	1.485(11)
C(12)-C(13)	1.499(15)
C(12)-C(14)	1.540(13)
C(12)-C(15)	1.568(14)
C(16)-C(17)	1.427(11)
C(16)-C(20)	1.440(12)
C(17)-C(18)	1.389(12)
C(17)-C(21)	1.524(12)
C(18)-C(19)	1.430(14)
C(18)-C(22)	1.511(13)
C(19)-C(20)	1.390(13)
C(19)-C(23)	1.535(13)
C(20)-C(24)	1.503(12)
C(27)-C(28)	1.480(16)
C(27)-C(30)	1.516(17)
C(27)-C(29)	1.544(16)
C(31)-C(32)	1.375(17)
C(31)-O(1)	1.450(15)
C(33)-C(34)	1.18(3)
C(33)-O(1)	1.62(3)
C(35)-C(36)	1.423(18)
C(35)-O(2)	1.448(16)
C(37)-C(38)	1.407(17)
C(37)-O(2)	1.416(14)

C(39)-C(40)	1.20(2)
C(39)-O(3)	1.477(19)
C(41)-C(42)	1.34(2)
C(41)-O(3)	1.52(2)
C(43)-C(44)	1.356(18)
C(43)-O(4)	1.458(15)
C(45)-O(4)	1.425(15)
C(45)-C(46)	1.448(17)
Li(1)-O(1)	1.983(18)
Li(1)-O(2)	2.03(2)
Li(1)-Cl(1)#1	2.331(16)
Li(2)-O(4)	1.95(2)
Li(2)-O(3)	1.95(2)
Li(2)-Cl(6)#2	2.344(19)

N(1)-Th(1)-C(1)	64.0(2)
N(1)-Th(1)-C(5)	80.6(2)
C(1)-Th(1)-C(5)	30.4(2)
N(1)-Th(1)-Cl(3)	92.71(17)
C(1)-Th(1)-Cl(3)	98.18(17)
C(5)-Th(1)-Cl(3)	124.54(16)
N(1)-Th(1)-Cl(1)	93.62(17)
C(1)-Th(1)-Cl(1)	103.81(17)
C(5)-Th(1)-Cl(1)	77.61(17)
Cl(3)-Th(1)-Cl(1)	157.71(7)
N(1)-Th(1)-C(2)	85.4(2)
C(1)-Th(1)-C(2)	30.2(2)
C(5)-Th(1)-C(2)	49.0(2)
Cl(3)-Th(1)-C(2)	75.74(17)
Cl(1)-Th(1)-C(2)	126.07(17)
N(1)-Th(1)-C(4)	109.8(2)
C(1)-Th(1)-C(4)	49.7(2)
C(5)-Th(1)-C(4)	30.0(2)
Cl(3)-Th(1)-C(4)	114.85(18)
Cl(1)-Th(1)-C(4)	82.87(18)
C(2)-Th(1)-C(4)	48.1(2)

N(1)-Th(1)-C(3)	112.1(2)
C(1)-Th(1)-C(3)	49.3(2)
C(5)-Th(1)-C(3)	48.7(2)
Cl(3)-Th(1)-C(3)	85.91(18)
Cl(1)-Th(1)-C(3)	111.27(18)
C(2)-Th(1)-C(3)	28.8(2)
C(4)-Th(1)-C(3)	29.0(2)
N(1)-Th(1)-Cl(2)	103.27(17)
C(1)-Th(1)-Cl(2)	166.89(17)
C(5)-Th(1)-Cl(2)	156.70(17)
Cl(3)-Th(1)-Cl(2)	78.54(7)
Cl(1)-Th(1)-Cl(2)	79.21(7)
C(2)-Th(1)-Cl(2)	153.22(17)
C(4)-Th(1)-Cl(2)	143.11(16)
C(3)-Th(1)-Cl(2)	141.92(16)
N(1)-Th(1)-Cl(2)#1	174.05(16)
C(1)-Th(1)-Cl(2)#1	121.83(17)
C(5)-Th(1)-Cl(2)#1	104.02(16)
Cl(3)-Th(1)-Cl(2)#1	87.70(7)
Cl(1)-Th(1)-Cl(2)#1	83.87(7)
C(2)-Th(1)-Cl(2)#1	100.44(18)
C(4)-Th(1)-Cl(2)#1	75.27(16)
C(3)-Th(1)-Cl(2)#1	73.88(16)
Cl(2)-Th(1)-Cl(2)#1	70.98(6)
N(1)-Th(1)-Si(1)	29.70(16)
C(1)-Th(1)-Si(1)	34.55(17)
C(5)-Th(1)-Si(1)	56.46(16)
Cl(3)-Th(1)-Si(1)	93.26(7)
Cl(1)-Th(1)-Si(1)	102.73(7)
C(2)-Th(1)-Si(1)	57.09(18)
C(4)-Th(1)-Si(1)	82.84(16)
C(3)-Th(1)-Si(1)	82.48(16)
Cl(2)-Th(1)-Si(1)	132.47(6)
Cl(2)#1-Th(1)-Si(1)	156.22(6)
N(2)-Th(2)-C(16)	64.6(2)
N(2)-Th(2)-C(17)	81.6(3)

C(16)-Th(2)-C(17)	30.5(2)
N(2)-Th(2)-Cl(4)	93.34(18)
C(16)-Th(2)-Cl(4)	103.33(18)
C(17)-Th(2)-Cl(4)	77.32(19)
N(2)-Th(2)-Cl(6)	92.32(18)
C(16)-Th(2)-Cl(6)	97.90(18)
C(17)-Th(2)-Cl(6)	124.13(18)
Cl(4)-Th(2)-Cl(6)	158.43(8)
N(2)-Th(2)-C(20)	86.0(3)
C(16)-Th(2)-C(20)	30.4(2)
C(17)-Th(2)-C(20)	48.8(2)
Cl(4)-Th(2)-C(20)	125.69(18)
Cl(6)-Th(2)-C(20)	75.46(18)
N(2)-Th(2)-C(18)	109.7(3)
C(16)-Th(2)-C(18)	49.3(2)
C(17)-Th(2)-C(18)	28.8(3)
Cl(4)-Th(2)-C(18)	82.1(2)
Cl(6)-Th(2)-C(18)	115.3(2)
C(20)-Th(2)-C(18)	48.2(3)
N(2)-Th(2)-C(19)	112.2(3)
C(16)-Th(2)-C(19)	48.8(3)
C(17)-Th(2)-C(19)	47.7(3)
Cl(4)-Th(2)-C(19)	110.7(2)
Cl(6)-Th(2)-C(19)	86.2(2)
C(20)-Th(2)-C(19)	28.5(3)
C(18)-Th(2)-C(19)	29.2(3)
N(2)-Th(2)-Cl(5)	101.48(19)
C(16)-Th(2)-Cl(5)	165.81(18)
C(17)-Th(2)-Cl(5)	156.35(18)
Cl(4)-Th(2)-Cl(5)	79.09(7)
Cl(6)-Th(2)-Cl(5)	79.39(7)
C(20)-Th(2)-Cl(5)	154.02(18)
C(18)-Th(2)-Cl(5)	144.28(19)
C(19)-Th(2)-Cl(5)	143.79(19)
N(2)-Th(2)-Cl(5)#2	172.58(18)
C(16)-Th(2)-Cl(5)#2	122.80(18)

C(17)-Th(2)-Cl(5)#2	104.54(19)
Cl(4)-Th(2)-Cl(5)#2	84.13(7)
Cl(6)-Th(2)-Cl(5)#2	87.61(7)
C(20)-Th(2)-Cl(5)#2	101.1(2)
C(18)-Th(2)-Cl(5)#2	76.88(19)
C(19)-Th(2)-Cl(5)#2	75.2(2)
Cl(5)-Th(2)-Cl(5)#2	71.21(7)
N(2)-Th(2)-Si(2)	30.06(19)
C(16)-Th(2)-Si(2)	34.74(18)
C(17)-Th(2)-Si(2)	57.0(2)
Cl(4)-Th(2)-Si(2)	102.29(8)
Cl(6)-Th(2)-Si(2)	92.94(8)
C(20)-Th(2)-Si(2)	57.4(2)
C(18)-Th(2)-Si(2)	82.48(19)
C(19)-Th(2)-Si(2)	82.3(2)
Cl(5)-Th(2)-Si(2)	131.13(7)
Cl(5)#2-Th(2)-Si(2)	157.36(7)
Li(1)#1-Cl(1)-Th(1)	133.2(4)
Th(1)-Cl(2)-Th(1)#1	109.02(6)
Li(1)-Cl(3)-Th(1)	129.8(4)
Li(2)-Cl(4)-Th(2)	132.6(5)
Th(2)-Cl(5)-Th(2)#2	108.79(7)
Li(2)#2-Cl(6)-Th(2)	130.0(4)
N(1)-Si(1)-C(1)	96.8(3)
N(1)-Si(1)-C(10)	114.7(4)
C(1)-Si(1)-C(10)	113.6(4)
N(1)-Si(1)-C(11)	118.4(5)
C(1)-Si(1)-C(11)	109.6(4)
C(10)-Si(1)-C(11)	104.1(6)
N(1)-Si(1)-Th(1)	41.7(2)
C(1)-Si(1)-Th(1)	55.5(2)
C(10)-Si(1)-Th(1)	122.6(4)
C(11)-Si(1)-Th(1)	133.3(4)
N(2)-Si(2)-C(26)	117.0(6)
N(2)-Si(2)-C(16)	96.9(4)
C(26)-Si(2)-C(16)	111.6(5)

N(2)-Si(2)-C(25)	114.0(5)
C(26)-Si(2)-C(25)	105.8(7)
C(16)-Si(2)-C(25)	111.6(5)
N(2)-Si(2)-Th(2)	42.4(2)
C(26)-Si(2)-Th(2)	133.6(5)
C(16)-Si(2)-Th(2)	54.9(2)
C(25)-Si(2)-Th(2)	120.6(5)
C(12)-N(1)-Si(1)	123.8(5)
C(12)-N(1)-Th(1)	127.2(5)
Si(1)-N(1)-Th(1)	108.6(3)
C(27)-N(2)-Si(2)	124.3(6)
C(27)-N(2)-Th(2)	128.0(6)
Si(2)-N(2)-Th(2)	107.5(3)
C(5)-C(1)-C(2)	106.4(7)
C(5)-C(1)-Si(1)	122.4(6)
C(2)-C(1)-Si(1)	125.2(6)
C(5)-C(1)-Th(1)	76.3(4)
C(2)-C(1)-Th(1)	78.1(4)
Si(1)-C(1)-Th(1)	90.0(3)
C(3)-C(2)-C(1)	109.3(7)
C(3)-C(2)-C(6)	124.0(8)
C(1)-C(2)-C(6)	126.4(7)
C(3)-C(2)-Th(1)	77.8(4)
C(1)-C(2)-Th(1)	71.6(4)
C(6)-C(2)-Th(1)	122.0(5)
C(2)-C(3)-C(4)	108.3(7)
C(2)-C(3)-C(7)	126.3(8)
C(4)-C(3)-C(7)	125.3(8)
C(2)-C(3)-Th(1)	73.3(4)
C(4)-C(3)-Th(1)	74.3(4)
C(7)-C(3)-Th(1)	122.4(5)
C(3)-C(4)-C(5)	107.6(7)
C(3)-C(4)-C(8)	127.2(8)
C(5)-C(4)-C(8)	125.0(8)
C(3)-C(4)-Th(1)	76.7(5)
C(5)-C(4)-Th(1)	72.2(4)

C(8)-C(4)-Th(1)	120.7(5)
C(1)-C(5)-C(4)	108.3(7)
C(1)-C(5)-C(9)	125.5(7)
C(4)-C(5)-C(9)	126.1(7)
C(1)-C(5)-Th(1)	73.4(4)
C(4)-C(5)-Th(1)	77.8(4)
C(9)-C(5)-Th(1)	117.8(5)
C(13)-C(12)-N(1)	111.3(8)
C(13)-C(12)-C(14)	113.1(10)
N(1)-C(12)-C(14)	111.8(8)
C(13)-C(12)-C(15)	107.5(10)
N(1)-C(12)-C(15)	109.4(7)
C(14)-C(12)-C(15)	103.2(9)
C(17)-C(16)-C(20)	106.0(7)
C(17)-C(16)-Si(2)	123.6(6)
C(20)-C(16)-Si(2)	125.6(6)
C(17)-C(16)-Th(2)	77.2(5)
C(20)-C(16)-Th(2)	79.3(5)
Si(2)-C(16)-Th(2)	90.4(3)
C(18)-C(17)-C(16)	109.9(8)
C(18)-C(17)-C(21)	125.7(9)
C(16)-C(17)-C(21)	124.2(8)
C(18)-C(17)-Th(2)	79.3(5)
C(16)-C(17)-Th(2)	72.3(5)
C(21)-C(17)-Th(2)	118.2(6)
C(17)-C(18)-C(19)	106.7(8)
C(17)-C(18)-C(22)	127.6(10)
C(19)-C(18)-C(22)	125.5(10)
C(17)-C(18)-Th(2)	71.9(5)
C(19)-C(18)-Th(2)	75.8(5)
C(22)-C(18)-Th(2)	120.7(6)
C(20)-C(19)-C(18)	109.3(8)
C(20)-C(19)-C(23)	127.0(10)
C(18)-C(19)-C(23)	123.2(10)
C(20)-C(19)-Th(2)	73.8(5)
C(18)-C(19)-Th(2)	75.0(5)

C(23)-C(19)-Th(2)	123.4(6)
C(19)-C(20)-C(16)	107.8(8)
C(19)-C(20)-C(24)	123.3(9)
C(16)-C(20)-C(24)	128.5(9)
C(19)-C(20)-Th(2)	77.7(5)
C(16)-C(20)-Th(2)	70.4(5)
C(24)-C(20)-Th(2)	123.4(6)
C(28)-C(27)-N(2)	114.3(10)
C(28)-C(27)-C(30)	109.6(13)
N(2)-C(27)-C(30)	108.6(9)
C(28)-C(27)-C(29)	108.2(13)
N(2)-C(27)-C(29)	109.0(9)
C(30)-C(27)-C(29)	106.8(11)
C(32)-C(31)-O(1)	114.0(12)
C(34)-C(33)-O(1)	107(3)
C(36)-C(35)-O(2)	114.2(13)
C(38)-C(37)-O(2)	114.7(12)
C(40)-C(39)-O(3)	119(2)
C(42)-C(41)-O(3)	99(2)
C(44)-C(43)-O(4)	110.1(13)
O(4)-C(45)-C(46)	110.2(12)
O(1)-Li(1)-O(2)	109.5(9)
O(1)-Li(1)-Cl(3)	110.5(8)
O(2)-Li(1)-Cl(3)	108.8(8)
O(1)-Li(1)-Cl(1)#1	108.6(8)
O(2)-Li(1)-Cl(1)#1	107.0(8)
Cl(3)-Li(1)-Cl(1)#1	112.5(7)
O(4)-Li(2)-O(3)	111.7(9)
O(4)-Li(2)-Cl(4)	110.2(9)
O(3)-Li(2)-Cl(4)	106.6(8)
O(4)-Li(2)-Cl(6)#2	108.0(8)
O(3)-Li(2)-Cl(6)#2	107.3(9)
Cl(4)-Li(2)-Cl(6)#2	113.1(7)
C(31)-O(1)-C(33)	110.9(12)
C(31)-O(1)-Li(1)	125.7(9)
C(33)-O(1)-Li(1)	123.2(12)

C(37)-O(2)-C(35)	116.3(11)
C(37)-O(2)-Li(1)	118.1(9)
C(35)-O(2)-Li(1)	121.8(9)
C(39)-O(3)-C(41)	115.7(14)
C(39)-O(3)-Li(2)	124.4(10)
C(41)-O(3)-Li(2)	115.7(11)
C(45)-O(4)-C(43)	111.3(10)
C(45)-O(4)-Li(2)	125.7(10)
C(43)-O(4)-Li(2)	121.5(10)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $C_5Me_4Si(Me)_2N$-t-Bu (**2**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Th(1)	36(1)	38(1)	24(1)	-5(1)	-3(1)	-12(1)
Th(2)	46(1)	44(1)	24(1)	3(1)	-4(1)	-20(1)
Cl(1)	83(2)	38(1)	44(1)	-4(1)	-11(1)	-11(1)
Cl(2)	40(1)	66(1)	32(1)	-15(1)	0(1)	-19(1)
Cl(3)	86(2)	48(1)	34(1)	2(1)	-7(1)	-27(1)
Cl(4)	105(2)	70(2)	47(2)	2(1)	-17(1)	-52(2)
Cl(5)	46(1)	58(1)	33(1)	8(1)	0(1)	-14(1)
Cl(6)	89(2)	55(1)	40(1)	-8(1)	-2(1)	-34(1)
Si(1)	49(1)	54(1)	39(2)	-9(1)	-8(1)	-23(1)
Si(2)	66(2)	60(2)	44(2)	11(1)	-8(1)	-11(1)
N(1)	34(4)	53(4)	36(4)	0(3)	-4(3)	-13(3)
N(2)	50(4)	58(4)	41(5)	3(3)	-6(4)	-16(3)
C(1)	45(5)	37(4)	22(4)	-10(3)	3(3)	-14(3)
C(2)	47(5)	39(4)	19(4)	-5(3)	9(4)	-5(4)
C(3)	34(4)	56(5)	21(5)	-4(4)	-3(3)	-5(4)
C(4)	36(4)	50(5)	37(5)	-13(4)	2(4)	-13(4)
C(5)	35(4)	47(5)	24(5)	-4(3)	2(3)	-11(3)
C(6)	76(7)	38(5)	43(6)	-3(4)	-3(5)	-1(4)
C(7)	49(6)	79(7)	50(6)	-7(5)	-11(5)	-3(5)
C(8)	46(5)	74(6)	46(6)	-5(5)	3(4)	-31(5)
C(9)	71(6)	48(5)	20(5)	7(3)	-6(4)	-16(4)
C(10)	72(7)	68(7)	114(10)	-29(7)	5(7)	-39(6)
C(11)	82(8)	141(11)	40(7)	1(6)	-25(6)	-46(7)
C(12)	34(5)	88(7)	48(6)	-18(5)	0(4)	-22(5)
C(13)	55(8)	159(14)	129(14)	47(11)	19(8)	-32(8)
C(14)	45(7)	188(14)	94(10)	-27(9)	-20(7)	-40(8)
C(15)	44(6)	132(11)	97(10)	-40(8)	-18(6)	7(6)
C(16)	47(5)	52(5)	20(5)	7(3)	-1(4)	-12(4)
C(17)	54(5)	56(5)	35(5)	2(4)	-3(4)	-22(4)
C(18)	57(6)	64(6)	33(6)	9(4)	8(5)	-10(5)
C(19)	38(5)	112(9)	25(5)	17(5)	1(4)	-36(5)

C(20)	65(6)	64(6)	22(5)	3(4)	7(4)	-34(5)
C(21)	105(8)	83(7)	20(5)	-12(4)	2(5)	-45(6)
C(22)	80(8)	70(7)	71(8)	-4(6)	-1(6)	5(6)
C(23)	66(7)	171(13)	63(8)	45(8)	-25(6)	-64(8)
C(24)	125(10)	102(9)	46(7)	4(6)	5(7)	-82(8)
C(25)	97(10)	55(7)	149(14)	21(8)	6(9)	-19(6)
C(26)	105(10)	189(15)	28(7)	10(7)	-19(7)	13(10)
C(27)	51(6)	84(8)	67(8)	11(6)	-9(5)	-18(5)
C(28)	50(8)	360(30)	141(17)	145(18)	5(9)	35(12)
C(29)	72(9)	140(13)	109(12)	-40(10)	-2(8)	-4(8)
C(30)	56(8)	158(14)	139(15)	-22(11)	1(8)	-44(8)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $C_5Me_4Si(Me)_2N$-t-Bu (2).

	x	y	z	U(eq)
H(6A)	6002	1312	3504	85
H(6B)	6548	1451	4052	85
H(6C)	7458	1136	3436	85
H(7A)	8805	3414	3885	92
H(7B)	8997	2296	3675	92
H(7C)	8062	2658	4278	92
H(8A)	7359	5660	2976	81
H(8B)	8613	4826	3005	81
H(8C)	7711	5282	3596	81
H(9A)	5938	5677	2530	71
H(9B)	4655	5356	2688	71
H(9C)	5708	4870	2147	71
H(10A)	3080	1831	3168	124
H(10B)	4152	1520	3530	124
H(10C)	4487	1458	2832	124
H(11A)	2823	3632	2354	123
H(11B)	4244	3298	2032	123
H(11C)	3680	4406	2281	123
H(13A)	2141	3469	4780	185
H(13B)	1856	2735	4368	185
H(13C)	774	3639	4674	185
H(14A)	1428	4596	3153	156
H(14B)	324	4335	3647	156
H(14C)	1413	3443	3333	156
H(15A)	1617	5740	3840	140
H(15B)	1904	5358	4472	140
H(15C)	580	5406	4345	140
H(21A)	157	9086	2606	101
H(21B)	-1127	9890	2815	101
H(21C)	-144	10152	2257	101

H(22A)	-3356	10963	1589	122
H(22B)	-2116	11211	1666	122
H(22C)	-3105	10980	2231	122
H(23A)	-3879	9910	1192	142
H(23B)	-4170	8847	1433	142
H(23C)	-3271	8930	809	142
H(24A)	-1259	6390	1567	127
H(24B)	-1827	6976	1030	127
H(24C)	-2705	6909	1663	127
H(25A)	1675	5388	1856	161
H(25B)	599	5742	1498	161
H(25C)	263	5601	2197	161
H(26A)	2184	6794	2612	175
H(26B)	782	7029	2968	175
H(26C)	1393	7939	2689	175
H(28A)	3369	6035	1473	324
H(28B)	3594	6914	1804	324
H(28C)	4566	6463	1229	324
H(29A)	2747	7475	173	167
H(29B)	2922	6357	467	167
H(29C)	4088	6831	242	167
H(30A)	3069	8873	694	175
H(30B)	4391	8180	758	175
H(30C)	3417	8662	1325	175
H(31A)	8357	83	5124	138
H(31B)	7908	-308	5782	138
H(32A)	6946	-809	5180	163
H(32B)	6434	338	4970	163
H(32C)	5971	-35	5631	163
H(33A)	8265	1916	6168	273
H(33B)	9117	846	5930	273
H(34A)	9731	2094	5497	351
H(34B)	8441	2510	5300	351
H(34C)	9328	1450	5077	351
H(35A)	3830	2181	7165	144
H(35B)	3873	1001	7213	144

H(36A)	5380	1314	7611	183
H(36B)	5956	1795	6995	183
H(36C)	5986	617	7058	183
H(37A)	3561	1223	5785	123
H(37B)	3032	847	6436	123
H(38A)	1632	2166	6120	186
H(38B)	2588	2862	6025	186
H(38C)	2039	2472	6672	186
H(39A)	2293	13892	1014	183
H(39B)	3394	13532	469	183
H(40A)	2192	14881	302	306
H(40B)	1066	14350	447	306
H(40C)	2185	14003	-98	306
H(41A)	3134	11109	359	235
H(41B)	3959	11916	122	235
H(42A)	4624	10907	874	384
H(42B)	3288	11298	1283	384
H(42C)	4136	12070	1039	384
H(43A)	-2038	14568	1315	144
H(43B)	-1458	14147	670	144
H(44A)	-3370	13937	990	180
H(44B)	-2974	13291	1551	180
H(44C)	-2390	12865	910	180
H(45A)	-1486	12779	2105	127
H(45B)	-1320	13908	2087	127
H(46A)	83	12811	2572	159
H(46B)	806	13270	1984	159
H(46C)	637	12143	2005	159