SUPPLEMENTARY INFORMATION

Anti-Bimetallic Complexes of Divalent Lanthanides with Silylated Pentalene and Cyclooctatetraenyl Bridging Ligands as Molecular Models for Lanthanide-based Polymers

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	1	**2**	**3.toluene**	**4.toluene**	**5.hexane**	**6.toluene**	**7**
formula	$C_{54}H_{92}Eu_2O_2Si_2$	$C_{54}H_{92}O_2Si_2Yb_2$	$C_{53}H_{86}Eu_2Si_2$	$C_{53}H_{86}Si_2Yb_2$	$C_{71}H_{108}O_2Si_2Sm_2$	$C_{63}H_{86}Si_2Sm_2$	$C_{36}H_{63}Si_2Sm$
fw	1133.38	1175.54	1083.32	1125.48	1218.34	1112.1	702.39
crystal system	Monoclinic	Monoclinic	Orthorhombic	Monoclinic	Monoclinic	Orthorhombic	Monoclinic
space group	$P2_1/n$ (No.14)	$P2_1/n$ (No.14)	Pnmm (No.59)	$P2_1/m$ (No.11)	$P2_1$ (No.4)	Pnmm (No.59)	$P2_1/m$ (No.11)
a (Å)	12.2667(3)	12.0652(4)	7.8251(4)	8.2612(1)	12.9282(3)	7.8240(2)	8.5333(3)
b (Å)	17.0031(5)	16.9479(5)	17.3663(9)	17.4200(4)	14.3909(5)	17.3596(5)	22.5383(6)
c (Å)	13.3634(4)	13.3213(4)	18.6689(7)	17.7584(3)	18.0915(5)	18.6606(4)	9.7450(3)
β (°)	90.668(2)	92.640(2)	90.000	94.206(1)	93.106(2)	90.000	100.809 (1)
volume ($Å^3$)	2787.04(14)	2721.05(15)	2537.0(2)	2548.73(8)	3360.95(17)	2534.51(11)	1840.96(10)
Z	2	2	2	2	2	2	2
Calc. density (Mg/m^3)	1.35	1.44	1.42	1.47	1.20	1.46	1.27
abs. coeff. (mm^{-1})	2.31	3.50	2.53	3.73	1.80	2.38	1.68
R1 [I > 2σ(I)]	0.047	0.045	0.048	0.036	0.055	0.034	0.026
wR2 [I > 2σ(I)]	0.097	0.093	0.095	0.086	0.132	0.085	0.054
R1 (all data)	0.057	0.066	0.080	0.048	0.092	0.047	0.034
wR2 (all data)	0.101	0.101	0.108	0.089	0.142	0.092	0.056

Summary of Crystallographic data for complexes **1** – **7**.

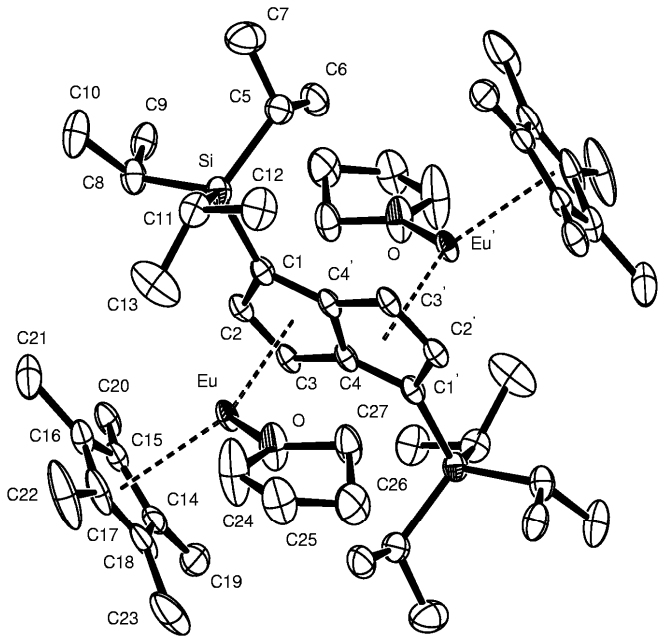

Table 1. Crystal data and structure refinement for **[EuCp*(THF)]$_2$($C_8H_4^{1,4\text{-SiiPr3}}$) (1)**

Identification code	oct1105	
Empirical formula	C54 H92 Eu2 O2 Si2	
Formula weight	1133.38	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$ (No.14)	
Unit cell dimensions	a = 12.2667(3) Å	α= 90°.
	b = 17.0031(5) Å	β= 90.668(2)°.
	c = 13.3634(4) Å	γ = 90°.
Volume	2787.04(14) Å^3	
Z	2	
Density (calculated)	1.35 Mg/m^3	
Absorption coefficient	2.31 mm^{-1}	
F(000)	1172	
Crystal size	0.30 x 0.25 x 0.20 mm^3	
Theta range for data collection	3.53 to 26.05°.	
Index ranges	-14<=h<=15, -20<=k<=20, -16<=l<=16	
Reflections collected	35094	
Independent reflections	5468 [R(int) = 0.044]	

Reflections with I>2sigma(I)	4676
Completeness to theta = 26.05°	99.3 %
Tmax. and Tmin.	0.644 and 0.481
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5468 / 0 / 276
Goodness-of-fit on F^2	1.187
Final R indices [I>2sigma(I)]	R1 = 0.047, wR2 = 0.097
R indices (all data)	R1 = 0.057, wR2 = 0.101
Largest diff. peak and hole	2.03 and -0.92 e.$Å^{-3}$ (near Eu)

Isomorphous with aqnalagous Yb complex

Data collection KappaCCD , Program package WinGX , Abs correction MULTISCAN

Refinement using SHELXL-97 , Drawing using ORTEP-3 for Windows

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for oct1105. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Eu	3830(1)	6183(1)	4062(1)	56(1)
Si	6560(1)	5237(1)	2799(1)	60(1)
O	4652(5)	7355(3)	4999(4)	107(2)
C(1)	5474(4)	5056(3)	3715(4)	53(1)
C(2)	4424(4)	4686(3)	3528(4)	53(1)
C(3)	3840(4)	4575(3)	4387(4)	51(1)
C(4)	4505(4)	4856(3)	5219(4)	51(1)
C(5)	7809(6)	4647(5)	3161(5)	80(2)
C(6)	7558(7)	3794(5)	3460(6)	102(3)
C(7)	8727(7)	4688(7)	2398(7)	126(4)
C(8)	5982(6)	4965(4)	1522(5)	74(2)
C(9)	5905(6)	4070(4)	1344(5)	83(2)
C(10)	6568(7)	5350(5)	629(5)	107(3)
C(11)	6970(6)	6317(4)	2749(5)	77(2)
C(12)	7651(7)	6604(5)	3650(6)	104(3)
C(13)	5979(7)	6848(5)	2631(9)	141(4)
C(14)	1626(6)	6197(5)	3535(5)	79(2)
C(15)	2137(5)	5902(3)	2683(4)	58(2)
C(16)	2724(6)	6510(4)	2238(5)	71(2)
C(17)	2562(8)	7189(4)	2822(7)	103(3)
C(18)	1901(8)	6997(5)	3613(7)	107(4)
C(19)	851(6)	5729(7)	4191(6)	123(4)
C(20)	1978(6)	5095(3)	2248(5)	74(2)
C(21)	3289(7)	6478(6)	1240(6)	113(3)
C(22)	2973(11)	8006(5)	2524(9)	192(7)
C(23)	1441(12)	7573(7)	4384(8)	222(9)
C(24)	4667(12)	8165(5)	4711(8)	174(6)
C(25)	4940(9)	8635(5)	5497(7)	119(3)
C(26)	4924(8)	8085(5)	6395(7)	116(3)
C(27)	5187(8)	7347(4)	5982(5)	99(3)

Table 3. Bond lengths [Å] and angles [°] for oct1105.

Eu-M(1)	2.477(5)
Eu-M(2)	2.502(6)
Eu-O	2.555(4)
Eu-C(2)	2.744(5)
Eu-C(3)	2.768(5)
Eu-C(14)	2.785(6)
Eu-C(15)	2.801(5)
Eu-C(18)	2.800(6)
Eu-C(1)	2.824(5)
Eu-C(16)	2.830(5)
Eu-C(17)	2.833(6)
Eu-C(4)	2.853(5)
Eu-C(4)’	2.859(5)
Si-C(1)	1.846(6)
Si-C(5)	1.889(7)
Si-C(8)	1.898(6)
Si-C(11)	1.906(7)
O-C(24)	1.430(9)
O-C(27)	1.462(8)
C(1)-C(4)’	1.433(7)
C(1)-C(2)	1.453(7)
C(2)-C(3)	1.373(8)
C(3)-C(4)	1.452(7)
C(4)-C(1)’	1.433(7)
C(4)-C(4)’	1.440(11)
C(5)-C(7)	1.530(11)
C(5)-C(6)	1.536(11)
C(8)-C(9)	1.543(9)
C(8)-C(10)	1.545(9)
C(11)-C(13)	1.522(11)
C(11)-C(12)	1.536(9)
C(14)-C(15)	1.399(9)
C(14)-C(18)	1.405(11)
C(14)-C(19)	1.525(11)
C(15)-C(16)	1.396(9)
C(15)-C(20)	1.503(7)

C(16)-C(17)	1.408(10)
C(16)-C(21)	1.512(10)
C(17)-C(18)	1.379(13)
C(17)-C(22)	1.533(11)
C(18)-C(23)	1.535(11)
C(24)-C(25)	1.358(11)
C(25)-C(26)	1.522(12)
C(26)-C(27)	1.410(10)

M(1)-Eu-M(2)	131.5(2)
M(1)-Eu-O	117.1(2)
M(2)-Eu-O	111.3(2)
C(1)-Si-C(5)	109.4(3)
C(1)-Si-C(8)	106.9(3)
C(5)-Si-C(8)	113.2(3)
C(1)-Si-C(11)	112.1(3)
C(5)-Si-C(11)	107.9(3)
C(8)-Si-C(11)	107.4(3)
C(24)-O-C(27)	104.1(5)
C(24)-O-Eu	128.7(4)
C(27)-O-Eu	127.2(4)
C(4)'-C(1)-C(2)	102.9(5)
C(4)'-C(1)-Si	129.6(4)
C(2)-C(1)-Si	127.1(4)
C(3)-C(2)-C(1)	112.7(5)
C(2)-C(3)-C(4)	107.5(5)
C(1)'-C(4)-C(4)'	111.2(5)
C(1)'-C(4)-C(3)	143.1(5)
C(4)'-C(4)-C(3)	105.7(6)
C(7)-C(5)-C(6)	111.6(7)
C(7)-C(5)-Si	113.9(6)
C(6)-C(5)-Si	113.8(5)
C(9)-C(8)-C(10)	109.1(6)
C(9)-C(8)-Si	113.6(4)
C(10)-C(8)-Si	114.8(4)
C(13)-C(11)-C(12)	108.6(7)
C(13)-C(11)-Si	111.4(5)
C(12)-C(11)-Si	114.8(5)

C(15)-C(14)-C(18)	107.3(8)
C(15)-C(14)-C(19)	124.8(7)
C(18)-C(14)-C(19)	127.8(8)
C(16)-C(15)-C(14)	108.6(6)
C(16)-C(15)-C(20)	125.2(6)
C(14)-C(15)-C(20)	125.8(7)
C(15)-C(16)-C(17)	107.1(7)
C(15)-C(16)-C(21)	126.3(6)
C(17)-C(16)-C(21)	126.0(8)
C(18)-C(17)-C(16)	108.5(7)
C(18)-C(17)-C(22)	127.8(10)
C(16)-C(17)-C(22)	123.4(10)
C(17)-C(18)-C(14)	108.4(7)
C(17)-C(18)-C(23)	125.9(11)
C(14)-C(18)-C(23)	125.4(12)
C(25)-C(24)-O	111.3(7)
C(24)-C(25)-C(26)	104.0(7)
C(27)-C(26)-C(25)	103.4(7)
C(26)-C(27)-O	104.0(6)

Symmetry transformations used to generate equivalent atoms: ‘ -x+1,-y+1,-z+1

M(1) and M(2) are the centroids of the C(1),C(2),C(3),C(4),C(4)’ and C(14) to C(19) rings

Least-squares planes (x,y,z in crystal coordinates) and deviations from them
(* indicates atom used to define plane)

- 5.0496 (0.0299) x + 15.4026 (0.0177) y - 1.2681 (0.0259) z = 4.5449 (0.0228)

*	0.0071 (0.0034)	C1_a
*	-0.0087 (0.0031)	C2_a
*	0.0067 (0.0033)	C3_a
*	-0.0018 (0.0038)	C4_a
*	-0.0032 (0.0040)	C4_$1a
	2.5295 (0.0019)	Eu

Rms deviation of fitted atoms = 0.0061

9.7882 (0.0233) x - 4.0314 (0.0488) y + 7.2803 (0.0347) z = 1.6676 (0.0350)

Angle to previous plane (with approximate esd) = 53.24 (0.24)

*	-0.0002 (0.0036)	C14_a
*	-0.0020 (0.0034)	C15_a
*	0.0034 (0.0037)	C16_a
*	-0.0036 (0.0042)	C17_a
*	0.0024 (0.0041)	C18_a
	-0.0938 (0.0114)	C19_a
	-0.1485 (0.0097)	C20_a
	-0.1570 (0.0119)	C21_a
	-0.1470 (0.0130)	C22_a
	-0.1189 (0.0124)	C23_a
	2.5454 (0.0024)	Eu

Rms deviation of fitted atoms = 0.0026

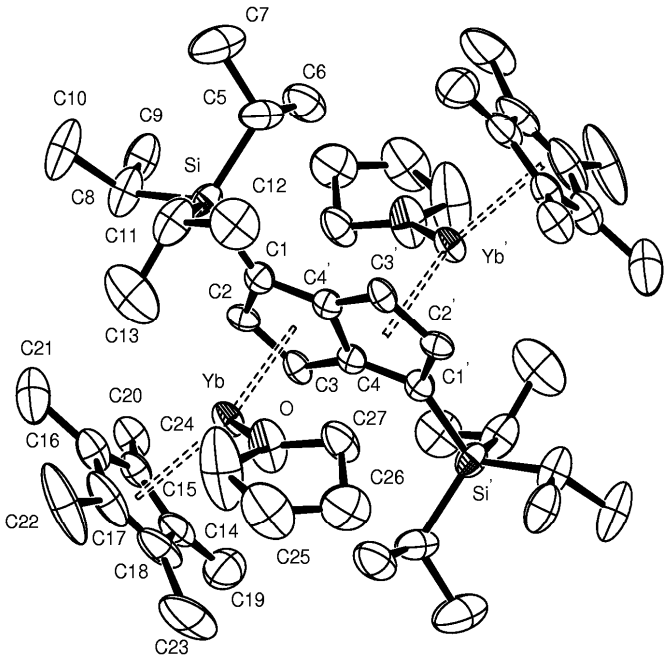

Table 1. Crystal data and structure refinement for **[YbCp*(THF)]$_2$($C_8H_4^{1,4\text{-SiiPr3}}$) (2)**.

Identification code	aug1405	
Empirical formula	C54 H92 O2 Si2 Yb2	
Formula weight	1175.54	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$ (No.14)	
Unit cell dimensions	a = 12.0652(4) Å	α= 90°.
	b = 16.9479(5) Å	β= 92.640(2)°.
	c = 13.3213(4) Å	γ = 90°.
Volume	2721.05(15) Å^3	
Z	2	
Density (calculated)	1.44 Mg/m^3	
Absorption coefficient	3.50 mm^{-1}	
F(000)	1200	
Crystal size	0.1 x 0.1 x 0.1 mm^3	
Theta range for data collection	3.59 to 26.01°.	
Index ranges	-14<=h<=14, -20<=k<=20, -16<=l<=16	
Reflections collected	33563	
Independent reflections	5336 [R(int) = 0.065]	

Reflections with I>2sigma(I)	4160
Completeness to theta = 26.01°	99.5 %
Tmax. and Tmin.	0.873 and 0.781
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5336 / 0 / 276
Goodness-of-fit on F^2	1.024
Final R indices [I>2sigma(I)]	R1 = 0.045, wR2 = 0.093
R indices (all data)	R1 = 0.066, wR2 = 0.101
Largest diff. peak and hole	4.35 and -1.10 e.$Å^{-3}$ (near Yb)

Data collection KappaCCD , Program package WinGX , Abs correction MULTISCAN

Refinement using SHELXL-97 , Drawing using ORTEP-3 for Windows

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for aug1405. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Yb	3885(1)	6179(1)	3980(1)	35(1)
Si	6584(2)	5230(1)	2834(1)	38(1)
O	4708(5)	7235(3)	4983(4)	62(2)
C(1)	5474(5)	5065(3)	3719(4)	32(1)
C(2)	4388(5)	4746(3)	3483(5)	32(1)
C(3)	3776(5)	4642(3)	4343(4)	31(1)
C(4)	4478(5)	4869(3)	5199(4)	30(1)
C(5)	7844(6)	4623(5)	3217(6)	53(2)
C(6)	7572(7)	3779(5)	3527(6)	65(2)
C(7)	8748(7)	4622(7)	2437(7)	87(3)
C(8)	5999(7)	4965(5)	1530(5)	54(2)
C(9)	5857(7)	4077(5)	1356(5)	58(2)
C(10)	6631(9)	5331(6)	658(6)	80(3)
C(11)	7030(6)	6310(4)	2809(5)	53(2)
C(12)	7630(7)	6596(5)	3779(7)	69(2)
C(13)	6055(8)	6841(5)	2549(9)	92(3)
C(14)	1704(6)	6264(4)	3499(5)	49(2)
C(15)	2166(5)	5942(3)	2640(5)	37(2)
C(16)	2802(6)	6532(4)	2194(5)	48(2)
C(17)	2727(8)	7221(4)	2775(7)	70(3)
C(18)	2045(7)	7056(5)	3578(7)	64(2)
C(19)	885(7)	5835(6)	4130(6)	77(3)
C(20)	1914(6)	5136(4)	2203(5)	45(2)
C(21)	3300(7)	6483(6)	1185(6)	76(3)
C(22)	3154(10)	8031(5)	2470(8)	119(5)
C(23)	1657(10)	7649(6)	4346(8)	124(5)
C(24)	4810(12)	8051(5)	4690(8)	119(5)
C(25)	4877(9)	8538(5)	5592(8)	87(3)
C(26)	4861(8)	7956(5)	6449(7)	75(3)
C(27)	5199(6)	7207(4)	5985(5)	54(2)

Table 3. Bond lengths [Å] and angles [°] for aug1405.

Yb-O	2.420(4)
Yb-M(2)	2.427(7)
Yb-M(1)	2.439(7)
Yb-C(2)	2.596(6)
Yb-C(3)	2.654(6)
Yb-C(14)	2.683(7)
Yb-C(15)	2.704(6)
Yb-C(18)	2.704(7)
Yb-C(1)	2.725(6)
Yb-C(17)	2.727(7)
Yb-C(16)	2.727(7)
Yb-C(4)	2.823(6)
Yb-C(4)’	2.838(6)
Si-C(1)	1.846(6)
Si-C(5)	1.886(7)
Si-C(8)	1.899(7)
Si-C(11)	1.908(7)
O-C(27)	1.436(8)
O-C(24)	1.443(9)
C(1)-C(2)	1.439(8)
C(1)-C(4)’	1.444(8)
C(2)-C(3)	1.401(8)
C(3)-C(4)	1.441(8)
C(4)-C(4)’	1.457(11)
C(5)-C(6)	1.529(11)
C(5)-C(7)	1.540(11)
C(8)-C(9)	1.532(10)
C(8)-C(10)	1.549(10)
C(11)-C(13)	1.508(12)
C(11)-C(12)	1.530(10)
C(14)-C(15)	1.406(9)
C(14)-C(18)	1.407(11)
C(14)-C(19)	1.513(12)
C(15)-C(16)	1.409(10)
C(15)-C(20)	1.510(9)
C(16)-C(17)	1.407(11)

C(16)-C(21)	1.499(11)
C(17)-C(18)	1.407(13)
C(17)-C(22)	1.528(12)
C(18)-C(23)	1.524(11)
C(24)-C(25)	1.457(13)
C(25)-C(26)	1.509(13)
C(26)-C(27)	1.476(10)

O-Yb-M(2)	113.1(2)
O-Yb-M(1)	114.0(2)
M(2)-Yb-M(1)	132.8(2)
C(1)-Si-C(5)	110.2(3)
C(1)-Si-C(8)	107.4(3)
C(5)-Si-C(8)	112.3(4)
C(1)-Si-C(11)	111.6(3)
C(5)-Si-C(11)	107.7(4)
C(8)-Si-C(11)	107.7(3)
C(27)-O-C(24)	104.3(6)
C(27)-O-Yb	129.1(4)
C(24)-O-Yb	126.6(5)
C(2)-C(1)-C(4)’	103.9(5)
C(2)-C(1)-Si	126.7(4)
C(4)’-C(1)-Si	129.0(4)
C(3)-C(2)-C(1)	112.2(5)
C(2)-C(3)-C(4)	107.5(5)
C(3)-C(4)-C(1)’	143.6(5)
C(3)-C(4)-C(4)’	106.2(6)
C(1)’-C(4)-C(4)’	110.1(6)
C(6)-C(5)-C(7)	110.4(7)
C(6)-C(5)-Si	113.8(5)
C(7)-C(5)-Si	113.9(6)
C(9)-C(8)-C(10)	109.6(6)
C(9)-C(8)-Si	113.9(5)
C(10)-C(8)-Si	114.6(5)
C(13)-C(11)-C(12)	109.8(7)
C(13)-C(11)-Si	111.1(5)
C(12)-C(11)-Si	114.3(5)
C(15)-C(14)-C(18)	107.8(7)

C(15)-C(14)-C(19)	124.0(7)
C(18)-C(14)-C(19)	127.8(8)
C(14)-C(15)-C(16)	108.2(6)
C(14)-C(15)-C(20)	125.8(6)
C(16)-C(15)-C(20)	125.7(6)
C(17)-C(16)-C(15)	107.8(7)
C(17)-C(16)-C(21)	125.3(8)
C(15)-C(16)-C(21)	126.0(7)
C(18)-C(17)-C(16)	108.0(7)
C(18)-C(17)-C(22)	126.6(9)
C(16)-C(17)-C(22)	124.6(10)
C(14)-C(18)-C(17)	108.2(7)
C(14)-C(18)-C(23)	125.6(10)
C(17)-C(18)-C(23)	126.0(9)
O-C(24)-C(25)	108.7(8)
C(24)-C(25)-C(26)	104.6(7)
C(27)-C(26)-C(25)	103.4(7)
O-C(27)-C(26)	104.5(6)

Symmetry transformations used to generate equivalent atoms:

‘ -x+1,-y+1,-z+1

```
 Least-squares planes (x,y,z in crystal coordinates) and deviations
from them
 (* indicates atom used to define plane)

 - 4.2663 (0.0352) x + 15.7928 (0.0180) y - 0.8661 (0.0293) z =
5.3336 (0.0256)

 *    0.0083 (0.0039)  C1_a
 *   -0.0118 (0.0035)  C2_a
 *    0.0103 (0.0038)  C3_a
 *   -0.0046 (0.0045)  C4_a
 *   -0.0022 (0.0046)  C4_$1a
      2.4228 (0.0025)  Yb

 Rms deviation of fitted atoms =   0.0083


  9.4069 (0.0266) x - 4.8322 (0.0558) y + 6.9405 (0.0396) z = 1.0011
(0.0412)

 Angle to previous plane (with approximate esd) = 54.07 ( 0.28 )

 *    0.0038 (0.0040)  C14_a
 *   -0.0030 (0.0040)  C15_a
 *    0.0012 (0.0043)  C16_a
 *    0.0012 (0.0045)  C17_a
 *   -0.0031 (0.0044)  C18_a
     -0.1220 (0.0126)  C19_a
     -0.1536 (0.0113)  C20_a
     -0.2068 (0.0130)  C21_a
     -0.2009 (0.0138)  C22_a
     -0.1224 (0.0137)  C23_a
      2.4295 (0.0028)  Yb

 Rms deviation of fitted atoms =   0.0027
```

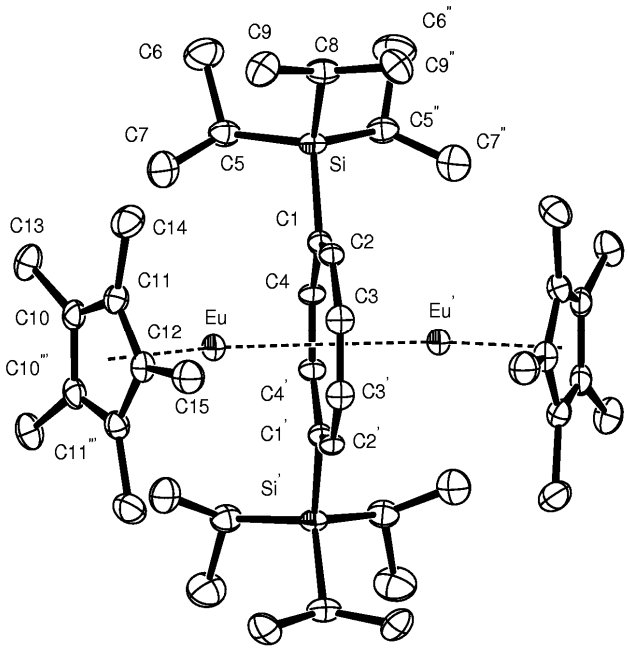

Table 1. Crystal data and structure refinement for **[EuCp*]$_2$(COT$^{1,4\text{-SiiPr3}}$) (3).toluene**.

Identification code	nov106	
Empirical formula	C46 H78 Eu2 Si2 . (C7 H8)	
Formula weight	1083.32	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pnmm (No.59)	
Unit cell dimensions	a = 7.8251(4) Å	α= 90°.
	b = 17.3663(9) Å	β= 90°.
	c = 18.6689(7) Å	γ = 90°.
Volume	2537.0(2) Å^3	
Z	2	
Density (calculated)	1.42 Mg/m^3	
Absorption coefficient	2.53 mm^{-1}	
F(000)	1116	
Crystal size	0.10 x 0.05 x 0.05 mm^3	
Theta range for data collection	3.48 to 26.03°.	
Index ranges	-6<=h<=9, -21<=k<=21, -22<=l<=17	
Reflections collected	8380	
Independent reflections	2635 [R(int) = 0.080]	

Reflections with I>2sigma(I)	1926
Completeness to theta = 26.03°	98.9 %
Tmax. and Tmin.	0.9797 and 0.8803
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2635 / 6 / 142
Goodness-of-fit on F^2	1.017
Final R indices [I>2sigma(I)]	R1 = 0.048, wR2 = 0.095
R indices (all data)	R1 = 0.080, wR2 = 0.108
Largest diff. peak and hole	1.33 and -0.89 e.$Å^{-3}$ (near solvate)

The complex lies on a site of mm symmetry.

The toluene solvate molecule is disordered across a site of mm symmetry and was included as a rigid body C6 ring with two alterative methyl sites, SADI restraints , isotropic C atoms, and H atoms omitted.

Data collection KappaCCD , Program package WinGX , Abs correction MULTISCAN

Refinement using SHELXL-97 , Drawing using ORTEP-3 for Windows

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for nov106. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Eu	1048(1)	2500	6350(1)	22(1)
Si	3058(3)	4506(1)	7500	22(1)
C(1)	2028(9)	3521(4)	7500	20(2)
C(2)	203(9)	3497(4)	7500	19(2)
C(3)	-1051(8)	2895(4)	7500	22(2)
C(4)	3245(9)	2906(3)	7500	20(2)
C(5)	4499(7)	4564(3)	6678(3)	30(1)
C(6)	5152(9)	5384(3)	6507(3)	53(2)
C(7)	3685(7)	4235(3)	5998(3)	39(2)
C(8)	1504(10)	5346(4)	7500	31(2)
C(9)	413(7)	5435(3)	6823(3)	35(1)
C(10)	620(6)	2913(3)	4917(2)	26(1)
C(11)	-874(6)	3157(3)	5263(2)	24(1)
C(12)	-1794(9)	2500	5476(3)	22(2)
C(13)	1935(7)	3392(3)	4523(3)	34(1)
C(14)	-1473(7)	3984(3)	5352(3)	37(2)
C(15)	-3537(9)	2500	5826(4)	34(2)
C(1S)	4447(11)	7500	7500	59(2)a
C(2S)	3065(12)	7500(20)	7032(2)	59(2)a
C(3S)	1408(11)	7500(40)	7301(5)	59(2)a
C(4S)	1133(11)	7500(50)	8036(6)	59(2)a
C(5S)	2516(13)	7500(40)	8504(3)	59(2)a
C(6S)	4173(12)	7500(19)	8235(1)	59(2)a
C(7S)	6220(30)	7500	7321(17)	59(2)b
C(7T)	3480(50)	7500	6281(12)	59(2)b

occupancy: a 0.25 , b 0.125

Table 3. Bond lengths [Å] and angles [°] for nov106.

Eu-M(1)	2.147(4)
Eu-M(2)	2.505(4)
Eu-C(12)	2.759(7)
Eu-C(11)	2.772(5)
Eu-C(3)	2.788(4)
Eu-C(10)	2.791(4)
Eu-C(2)	2.836(4)
Eu-C(4)	2.839(5)
Si-C(1)	1.891(7)
Si-C(8)	1.900(7)
Si-C(5)	1.907(5)
C(1)-C(2)	1.429(9)
C(1)-C(4)	1.432(9)
C(2)-C(3)	1.434(9)
C(3)-C(3)’	1.372(13)
C(4)-C(4)’	1.409(12)
C(5)-C(7)	1.530(7)
C(5)-C(6)	1.546(7)
C(8)-C(9)	1.532(6)
C(8)-C(9)”	1.532(6)
C(10)-C(11)	1.401(7)
C(10)-C(10)’	1.433(10)
C(10)-C(13)	1.514(7)
C(11)-C(12)	1.406(6)
C(11)-C(14)	1.520(7)
C(12)-C(11)’	1.406(6)
C(12)-C(15)	1.512(10)

M(1)-Eu-M(2)	153.12(2)
C(1)-Si-C(8)	115.0(3)
C(1)-Si-C(5)	107.45(19)
C(8)-Si-C(5)	109.8(2)
C(5)-Si-C(5)”	107.2(3)
C(2)-C(1)-C(4)	130.0(6)
C(2)-C(1)-Si	116.9(5)
C(4)-C(1)-Si	113.1(5)

C(1)-C(2)-C(3)	134.9(6)
C(3)'-C(3)-C(2)	136.8(4)
C(4)'-C(4)-C(1)	138.3(4)
C(7)-C(5)-C(6)	108.1(4)
C(7)-C(5)-Si	113.7(4)
C(6)-C(5)-Si	114.2(4)
C(9)-C(8)-C(9)"	111.1(6)
C(9)-C(8)-Si	115.7(3)
C(9)"-C(8)-Si	115.7(3)
C(11)-C(10)-C(10)'	107.6(3)
C(11)-C(10)-C(13)	128.6(5)
C(10)'-C(10)-C(13)	123.4(3)
C(10)-C(11)-C(12)	108.2(4)
C(10)-C(11)-C(14)	126.4(4)
C(12)-C(11)-C(14)	125.3(5)
C(11)-C(12)-C(11)'	108.4(6)
C(11)-C(12)-C(15)	125.7(3)
C(11)'-C(12)-C(15)	125.7(3)
Eu-M(1)-Eu"	177.54(2)

M(1) and M(2) are the centroids of the C8 and C5 rings.

Symmetry transformations used to generate equivalent atoms: ' x,-y+1/2,z " x,y,-z+3/2

```
 Least-squares planes (x,y,z in crystal coordinates) and deviations
from them
 (* indicates atom used to define plane)

  0.0000 (0.0000) x - 0.0000 (0.0000) y + 18.6689 (0.0010) z =
14.0017 (0.0007)

 *    0.0000 (0.0000)  C1_a
 *    0.0000 (0.0000)  C2_a
 *    0.0000 (0.0000)  C3_a
 *    0.0000 (0.0000)  C4_a
 *    0.0000 (0.0000)  C1_$1a
 *    0.0000 (0.0000)  C2_$1a
 *    0.0000 (0.0000)  C3_$1a
 *    0.0000 (0.0000)  C4_$1a
     -2.1467 (0.0003)  Eu

 Rms deviation of fitted atoms =   0.0000


  3.7788 (0.0228) x - 0.0004 (0.0026) y + 16.3478 (0.0300) z = 8.2726
(0.0168)

 Angle to previous plane (with approximate esd) = 28.88 ( 0.15 )

 *   -0.0008 (0.0004)  C10_a
 *    0.0002 (0.0039)  C11_a
 *    0.0006 (0.0039)  C12_a
 *   -0.0006 (0.0019)  C10_$1a
 *    0.0005 (0.0023)  C11_$1a
      2.5042 (0.0029)  Eu
     -0.1484 (0.0096)  C13_a
     -0.0807 (0.0069)  C14_a
     -0.0856 (0.0120)  C15_a

 Rms deviation of fitted atoms =   0.0006
```

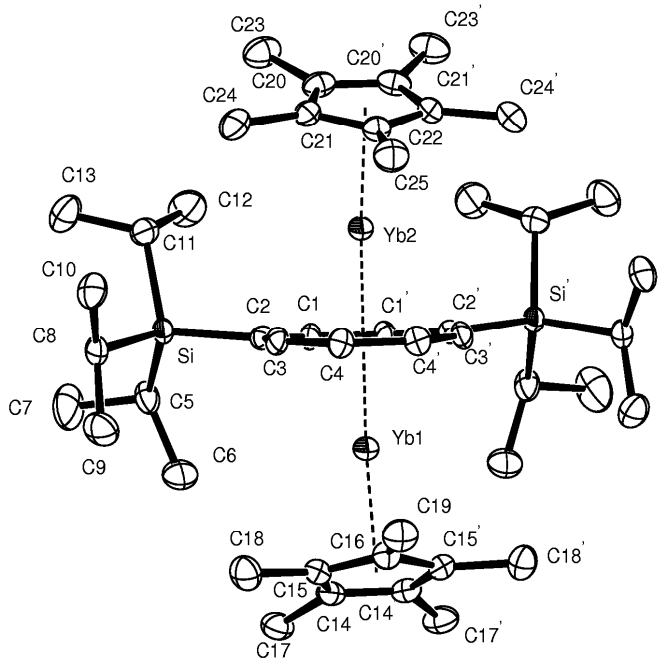

Table 1. Crystal data and structure refinement for **[YbCp*]$_2$(COT$^{1,4\text{-SiiPr3}}$) (4).toluene**.

Identification code	nov806	
Empirical formula	C53 H86 Si2 Yb2	
Formula weight	1125.48	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/m$ (No.11)	
Unit cell dimensions	a = 8.2612(1) Å	α= 90°.
	b = 17.4200(4) Å	β= 94.206(1)°.
	c = 17.7584(3) Å	γ = 90°.
Volume	2548.73(8) Å^3	
Z	2	
Density (calculated)	1.47 Mg/m^3	
Absorption coefficient	3.73 mm^{-1}	
F(000)	1144	
Crystal size	0.15 x 0.15 x 0.1 mm^3	
Theta range for data collection	3.40 to 26.03°.	
Index ranges	-10<=h<=10, -21<=k<=21, -21<=l<=21	
Reflections collected	41532	
Independent reflections	5174 [R(int) = 0.059]	

Reflections with I>2sigma(I)	4396
Completeness to theta = 26.03°	99.6 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5174 / 0 / 289
Goodness-of-fit on F^2	1.351
Final R indices [I>2sigma(I)]	R1 = 0.036, wR2 = 0.086
R indices (all data)	R1 = 0.048, wR2 = 0.089
Largest diff. peak and hole	2.44 and -0.95 e.$Å^{-3}$ (near Yb)

Data collection KappaCCD , Program package WinGX , Abs correction MULTISCAN

Refinement using SHELXL-97 , Drawing using ORTEP-3 for Windows

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for nov806. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Yb(1)	785(1)	7500	3586(1)	22(1)
Yb(2)	1025(1)	7500	1389(1)	21(1)
Si	2743(2)	5481(1)	2484(1)	21(1)
C(1)	2980(7)	7092(3)	2606(3)	21(1)
C(2)	1814(7)	6483(3)	2516(3)	21(1)
C(3)	83(7)	6509(4)	2425(3)	23(1)
C(4)	-1124(7)	7093(3)	2376(3)	24(1)
C(5)	4386(8)	5409(4)	3284(4)	30(2)
C(6)	3868(9)	5715(5)	4039(4)	40(2)
C(7)	5098(11)	4595(5)	3409(5)	61(3)
C(8)	1231(8)	4664(4)	2550(3)	27(1)
C(9)	316(9)	4639(4)	3262(4)	41(2)
C(10)	21(8)	4553(4)	1860(4)	34(2)
C(11)	3665(8)	5363(4)	1539(3)	28(1)
C(12)	5030(9)	5926(5)	1409(4)	47(2)
C(13)	4246(9)	4546(4)	1372(4)	44(2)
C(14)	731(7)	7093(4)	5030(3)	25(1)
C(15)	-764(7)	6838(4)	4675(3)	25(1)
C(16)	-1683(10)	7500	4455(5)	26(2)
C(17)	2017(8)	6611(4)	5454(4)	35(2)
C(18)	-1378(9)	6026(4)	4605(4)	37(2)
C(19)	-3409(11)	7500	4110(5)	35(2)
C(20)	1289(7)	7094(4)	-46(3)	28(1)
C(21)	-261(7)	6844(4)	147(3)	25(1)
C(22)	-1204(10)	7500	262(5)	24(2)
C(23)	2617(8)	6591(5)	-308(4)	41(2)
C(24)	-840(9)	6029(4)	203(4)	35(2)
C(25)	-2970(11)	7500	420(5)	35(2)
C(1S)	3859(13)	2500	2490(6)	39(2)
C(2S)	3310(15)	2500	3200(6)	45(3)
C(3S)	1699(18)	2500	3306(8)	57(3)
C(4S)	542(16)	2500	2670(10)	68(4)
C(5S)	1132(19)	2500	1970(9)	67(4)

C(6S)	2800(18)	2500	1892(7)	53(3)
C(7S)	5737(19)	2500	2400(10)	86(5)

Table 3. Bond lengths [Å] and angles [°] for nov806.

Yb(1)-M(1)	1.976(6)
Yb(1)-M(2)	2.369(6)
Yb(1)…Yb(2)	3.9200(5)
Yb(1)-C(16)	2.646(9)
Yb(1)-C(15)	2.660(6)
Yb(1)-C(14)	2.664(6)
Yb(1)-C(4)	2.665(6)
Yb(1)-C(1)	2.699(6)
Yb(1)-C(3)	2.718(6)
Yb(1)-C(2)	2.776(6)
Yb(2)-M(1)	1.945(6)
Yb(2)-M(3)	2.358(6)
Yb(2)-C(22)	2.618(8)
Yb(2)-C(21)	2.638(6)
Yb(2)-C(20)	2.668(6)
Yb(2)-C(3)	2.679(6)
Yb(2)-C(4)	2.679(6)
Yb(2)-C(1)	2.696(6)
Yb(2)-C(2)	2.715(6)
Si-C(5)	1.896(6)
Si-C(8)	1.902(6)
Si-C(11)	1.904(6)
Si-C(2)	1.910(6)
C(1)-C(1)’	1.420(11)
C(1)-C(2)	1.435(8)
C(2)-C(3)	1.428(8)
C(3)-C(4)	1.423(8)
C(4)-C(4)’	1.417(12)
C(5)-C(6)	1.533(9)
C(5)-C(7)	1.545(10)
C(8)-C(9)	1.521(9)
C(8)-C(10)	1.536(8)
C(11)-C(12)	1.524(9)
C(11)-C(13)	1.537(9)
C(14)-C(15)	1.416(8)
C(14)-C(14)’	1.419(13)

C(14)-C(17)	1.511(8)
C(15)-C(16)	1.420(8)
C(15)-C(18)	1.505(9)
C(16)-C(15)’	1.420(8)
C(16)-C(19)	1.510(12)
C(20)-C(20)’	1.413(14)
C(20)-C(21)	1.418(9)
C(20)-C(23)	1.505(9)
C(21)-C(22)	1.406(8)
C(21)-C(24)	1.504(9)
C(22)-C(21)’	1.406(8)
C(22)-C(25)	1.506(12)

M(1)-Yb(1)-M(2)	160.5(2)
M(1)-Yb(2)-M(3)	160.5(2)
C(5)-Si-C(8)	110.0(3)
C(5)-Si-C(11)	110.1(3)
C(8)-Si-C(11)	106.3(3)
C(5)-Si-C(2)	107.8(3)
C(8)-Si-C(2)	114.5(3)
C(11)-Si-C(2)	108.2(3)
C(1)’-C(1)-C(2)	137.7(3)
C(3)-C(2)-C(1)	130.4(6)
C(3)-C(2)-Si	115.3(4)
C(1)-C(2)-Si	114.3(4)
C(4)-C(3)-C(2)	136.1(6)
C(4)’-C(4)-C(3)	135.7(3)
C(6)-C(5)-C(7)	108.8(6)
C(6)-C(5)-Si	113.7(5)
C(7)-C(5)-Si	114.3(5)
C(9)-C(8)-C(10)	109.0(5)
C(9)-C(8)-Si	116.3(5)
C(10)-C(8)-Si	116.0(4)
C(12)-C(11)-C(13)	108.8(6)
C(12)-C(11)-Si	114.3(5)
C(13)-C(11)-Si	114.9(5)
C(15)-C(14)-C(14)’	108.3(4)
C(15)-C(14)-C(17)	127.3(6)

C(14)'-C(14)-C(17)	123.7(4)
C(14)-C(15)-C(16)	107.4(6)
C(14)-C(15)-C(18)	127.5(6)
C(16)-C(15)-C(18)	124.8(6)
C(15)'-C(16)-C(15)	108.7(8)
C(15)'-C(16)-C(19)	125.6(4)
C(15)-C(16)-C(19)	125.6(4)
C(20)'-C(20)-C(21)	107.9(4)
C(20)'-C(20)-C(23)	125.7(4)
C(21)-C(20)-C(23)	125.9(6)
C(22)-C(21)-C(20)	107.8(6)
C(22)-C(21)-C(24)	125.1(6)
C(20)-C(21)-C(24)	127.1(6)
C(21)'-C(22)-C(21)	108.6(8)
C(21)'-C(22)-C(25)	125.6(4)
C(21)-C(22)-C(25)	125.6(4)
Yb(2)-M(1)-Yb(1)	178.4(2)

Symmetry transformations used to generate equivalent atoms: ' x,-y+3/2,z

M(1) is the centroid of the C8 ring

M(2) and M(3) are the centroids of the Cp* rings

```
 Least-squares planes (x,y,z in crystal coordinates) and deviations
from them
 (* indicates atom used to define plane)

 - 3.8663 (0.0310) x + 0.0000 (0.0005) y + 16.2608 (0.0303) z =
7.8963 (0.0140)

 *   -0.0005 (0.0016)  C14_a
 *    0.0013 (0.0043)  C15_a
 *   -0.0016 (0.0053)  C16_a
 *   -0.0005 (0.0016)  C14_$1a
 *    0.0013 (0.0043)  C15_$1a
     -2.3693 (0.0036)  Yb1
      0.1928 (0.0119)  C17_a
      0.1240 (0.0089)  C18_a
      0.1046 (0.0154)  C19_a

 Rms deviation of fitted atoms =   0.0011


 - 0.9842 (0.0168) x - 0.0000 (0.0001) y + 17.7396 (0.0017) z =
4.3080 (0.0035)

 Angle to previous plane (with approximate esd) = 21.06 ( 0.22 )

 *    0.0213 (0.0032)  C1_a
 *   -0.0238 (0.0045)  C2_a
 *   -0.0146 (0.0047)  C3_a
 *    0.0171 (0.0033)  C4_a
 *    0.0213 (0.0032)  C1_$1a
 *   -0.0238 (0.0045)  C2_$1a
 *   -0.0146 (0.0047)  C3_$1a
 *    0.0171 (0.0033)  C4_$1a
      1.9753 (0.0029)  Yb1
     -1.9446 (0.0028)  Yb2
     -0.1718 (0.0044)  Si_a

 Rms deviation of fitted atoms =   0.0195


  2.0788 (0.0345) x - 0.0000 (0.0002) y + 16.8130 (0.0247) z = 0.1915
(0.0035)

 Angle to previous plane (with approximate esd) = 21.42 ( 0.17 )

 *   -0.0003 (0.0016)  C20_a
 *    0.0007 (0.0042)  C21_a
 *   -0.0009 (0.0052)  C22_a
 *   -0.0003 (0.0016)  C20_$1a
 *    0.0007 (0.0042)  C21_$1a
      2.3571 (0.0036)  Yb2

 Rms deviation of fitted atoms =   0.0006
```

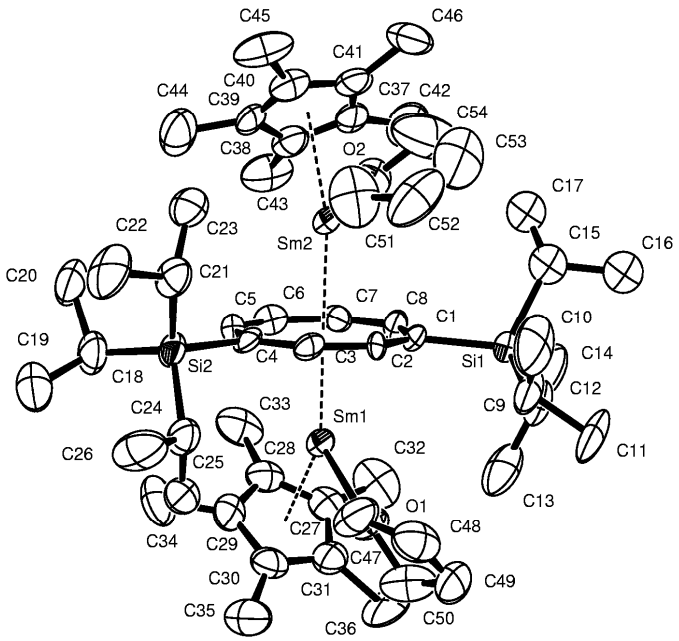

Table 1. Crystal data and structure refinement for **[SmCp*(THF)]$_2$(COT$^{1,4\text{-SiiPr3}}$) (5).hexane**.

Identification code	jun505	
Empirical formula	C65 H94 O2 Si2 Sm2 . (C6 H14)	
Formula weight	1218.34	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1$ (No.4)	
Unit cell dimensions	a = 12.9282(3) Å	α= 90°.
	b = 14.3909(5) Å	β= 93.106(2)°.
	c = 18.0915(5) Å	γ = 90°.
Volume	3360.95(17) Å^3	
Z	2	
Density (calculated)	1.20 Mg/m^3	
Absorption coefficient	1.80 mm^{-1}	
F(000)	1272	
Crystal size	0.10 x 0.10 x 0.05 mm^3	
Theta range for data collection	3.40 to 26.05°.	
Index ranges	-15<=h<=15, -17<=k<=17, -22<=l<=22	
Reflections collected	51794	
Independent reflections	13142 [R(int) = 0.083]	

Reflections with I>2sigma(I)	9422
Completeness to theta = 26.05°	99.6 %
Tmax. and Tmin.	0.897 and 0.778
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	13142 / 15 / 573
Goodness-of-fit on F^2	1.059
Final R indices [I>2sigma(I)]	R1 = 0.055, wR2 = 0.132
R indices (all data)	R1 = 0.092, wR2 = 0.149
Absolute structure parameter	-0.026(19)
Largest diff. peak and hole	1.12 and -0.56 e.$Å^{-3}$ (near Sm2)

One iPr group (C(15)) is disordered and was refined with isotropic C atoms. The poorly defined hexane solvate was included with isotropic C atoms and 1,2 SADI restraints.

Data collection KappaCCD , Program package WinGX , Abs correction MULTISCAN
Refinement using SHELXL-97 , Drawing using ORTEP-3 for Windows

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for jun505. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Sm(1)	1459(1)	7172(12)	1516(1)	37(1)
Sm(2)	3465(1)	7233(12)	3594(1)	36(1)
Si(1)	64(2)	7646(13)	3605(1)	50(1)
Si(2)	4386(2)	8803(13)	1577(1)	45(1)
O(1)	305(5)	8697(14)	1223(4)	59(2)
O(2)	3458(5)	8795(14)	4358(4)	65(2)
C(1)	1283(6)	7464(14)	3094(5)	33(3)
C(2)	1794(7)	8257(14)	2845(5)	30(2)
C(3)	2665(7)	8484(15)	2431(5)	35(2)
C(4)	3443(7)	8018(15)	2065(6)	34(3)
C(5)	3622(6)	7030(15)	1994(4)	40(3)
C(6)	3137(9)	6229(15)	2247(6)	45(3)
C(7)	2270(9)	6027(15)	2669(6)	41(3)
C(8)	1525(8)	6520(15)	3023(6)	39(3)
C(9)	-459(7)	8860(15)	3429(6)	65(3)
C(10)	25(10)	9623(17)	3936(8)	115(6)
C(11)	-1651(7)	8994(16)	3443(7)	85(4)
C(12)	-992(7)	6828(15)	3237(7)	68(3)
C(13)	-1159(8)	6923(15)	2404(7)	89(4)
C(14)	-948(10)	5778(16)	3445(11)	127(7)
C(18)	5287(8)	8103(15)	981(6)	64(3)
C(19)	5752(9)	8621(16)	361(7)	90(4)
C(20)	6167(8)	7602(15)	1444(7)	82(4)
C(21)	5111(7)	9544(14)	2305(6)	56(3)
C(22)	6012(9)	10131(16)	2011(8)	97(5)
C(23)	5501(8)	9004(15)	2975(6)	67(3)
C(24)	3539(7)	9604(14)	942(6)	53(2)
C(25)	2956(8)	9078(15)	348(5)	61(3)
C(26)	4049(10)	10473(15)	641(8)	97(5)
C(27)	563(8)	5541(14)	829(5)	52(3)
C(28)	1630(8)	5492(14)	686(5)	52(3)
C(29)	1840(7)	6228(14)	194(5)	50(2)
C(30)	909(8)	6712(14)	33(5)	55(3)

C(31)	115(8)	6278(15)	422(5)	57(3)
C(32)	21(11)	4844(15)	1282(7)	85(4)
C(33)	2338(10)	4740(14)	914(6)	72(3)
C(34)	2888(9)	6407(15)	-136(6)	82(4)
C(35)	784(9)	7512(15)	-515(6)	83(4)
C(36)	-1046(8)	6486(16)	346(7)	87(4)
C(37)	3937(8)	5687(15)	4587(6)	56(3)
C(38)	4485(7)	5517(15)	3958(6)	52(3)
C(39)	5271(7)	6244(15)	3959(6)	56(3)
C(40)	5155(8)	6816(14)	4560(6)	58(3)
C(41)	4332(8)	6475(15)	4976(6)	56(3)
C(42)	3084(9)	5092(16)	4849(8)	91(5)
C(43)	4407(10)	4705(15)	3465(7)	78(4)
C(44)	6085(9)	6330(16)	3386(7)	90(4)
C(45)	5894(10)	7647(15)	4770(8)	93(5)
C(46)	4059(10)	6786(16)	5746(5)	90(5)
C(47)	653(9)	9598(16)	1289(8)	80(4)
C(48)	-233(10)	10181(15)	1492(6)	79(4)
C(49)	-1162(9)	9618(16)	1305(7)	85(4)
C(50)	-737(10)	8802(16)	940(8)	95(4)
C(51)	3625(13)	9743(16)	4149(9)	108(5)
C(52)	2931(11)	10347(16)	4558(10)	111(5)
C(53)	2692(14)	9776(18)	5134(10)	126(6)
C(54)	3180(17)	8896(19)	5081(9)	150(7)
C(15)	246(13)	7190(20)	4598(9)	63(5)a
C(16)	-785(13)	7180(20)	5003(9)	70(5)a
C(17)	943(15)	6680(20)	4904(11)	67(6)a
C(1S)	1560(30)	6950(30)	-2780(20)	360(20)
C(2S)	1820(30)	7980(30)	-2770(20)	260(16)
C(3S)	2850(20)	7930(20)	-2301(18)	255(15)
C(4S)	3040(20)	8920(20)	-2032(16)	230(12)
C(5S)	4170(30)	8760(30)	-1760(20)	330(20)
C(6S)	4130(30)	9760(30)	-1475(18)	291(17)
C(15A)	364(17)	7730(20)	4657(12)	47(6)b
C(16A)	-580(20)	7840(30)	5103(15)	71(9)b
C(17A)	1190(16)	7340(20)	5003(11)	57(7)b

Occupancy : a , b

Table 3. Bond lengths [Å] and angles [°] for jun505.

Sm(1)-M(1)	2.220(10)
Sm(1)-M(2)	2.581(10)
Sm(1)-O(1)	2.690(7)
Sm(1)-C(7)	2.816(10)
Sm(1)-C(30)	2.818(9)
Sm(1)-C(29)	2.817(9)
Sm(1)-C(6)	2.826(11)
Sm(1)-C(28)	2.862(10)
Sm(1)-C(31)	2.867(9)
Sm(1)-C(27)	2.870(9)
Sm(1)-C(8)	2.879(11)
Sm(1)-C(2)	2.880(9)
Sm(1)-C(5)	2.890(8)
Sm(1)-C(1)	2.906(9)
Sm(1)-C(3)	2.909(10)
Sm(1)-C(4)	2.962(10)
Sm(2)-M(1)	2.235(10)
Sm(2)-M(3)	2.580(10)
Sm(2)-O(2)	2.638(8)
Sm(2)-C(39)	2.784(9)
Sm(2)-C(40)	2.788(9)
Sm(2)-C(7)	2.814(10)
Sm(2)-C(6)	2.845(12)
Sm(2)-C(8)	2.852(11)
Sm(2)-C(38)	2.860(10)
Sm(2)-C(2)	2.891(9)
Sm(2)-C(41)	2.897(9)
Sm(2)-C(37)	2.903(9)
Sm(2)-C(3)	2.916(9)
Sm(2)-C(5)	2.929(8)
Sm(2)-C(1)	2.935(8)
Sm(2)-C(4)	2.988(10)
Si(1)-C(1)	1.888(9)
Si(1)-C(9)	1.894(12)
Si(1)-C(12)	1.895(11)
Si(1)-C(15)	1.916(18)

Si(1)-C(15A)	1.92(2)
Si(2)-C(21)	1.901(10)
Si(2)-C(4)	1.912(10)
Si(2)-C(18)	1.917(11)
Si(2)-C(24)	1.926(9)
O(1)-C(47)	1.376(14)
O(1)-C(50)	1.423(13)
O(2)-C(54)	1.383(19)
O(2)-C(51)	1.436(16)
C(1)-C(8)	1.401(15)
C(1)-C(2)	1.406(13)
C(2)-C(3)	1.424(12)
C(3)-C(4)	1.405(14)
C(4)-C(5)	1.448(17)
C(5)-C(6)	1.401(16)
C(6)-C(7)	1.419(15)
C(7)-C(8)	1.381(15)
C(9)-C(10)	1.542(15)
C(9)-C(11)	1.554(12)
C(12)-C(13)	1.517(15)
C(12)-C(14)	1.558(17)
C(18)-C(19)	1.499(14)
C(18)-C(20)	1.553(14)
C(21)-C(23)	1.504(13)
C(21)-C(22)	1.557(14)
C(24)-C(25)	1.486(13)
C(24)-C(26)	1.528(14)
C(27)-C(31)	1.399(15)
C(27)-C(28)	1.419(14)
C(27)-C(32)	1.495(15)
C(28)-C(29)	1.420(14)
C(28)-C(33)	1.462(14)
C(29)-C(30)	1.407(13)
C(29)-C(34)	1.531(14)
C(30)-C(31)	1.420(15)
C(30)-C(35)	1.523(15)
C(31)-C(36)	1.530(14)
C(37)-C(38)	1.394(15)

C(37)-C(41)	1.416(16)
C(37)-C(42)	1.494(15)
C(38)-C(39)	1.458(15)
C(38)-C(43)	1.470(15)
C(39)-C(40)	1.378(15)
C(39)-C(44)	1.522(14)
C(40)-C(41)	1.423(15)
C(40)-C(45)	1.565(15)
C(41)-C(46)	1.522(14)
C(47)-C(48)	1.481(17)
C(48)-C(49)	1.473(17)
C(49)-C(50)	1.469(18)
C(51)-C(52)	1.476(19)
C(52)-C(53)	1.37(2)
C(53)-C(54)	1.42(2)
C(15)-C(17)	1.26(3)
C(15)-C(16)	1.55(2)
C(1S)-C(2S)	1.53(2)
C(2S)-C(3S)	1.55(2)
C(3S)-C(4S)	1.53(2)
C(4S)-C(5S)	1.53(2)
C(5S)-C(6S)	1.53(2)
C(15A)-C(17A)	1.33(3)
C(15A)-C(16A)	1.50(3)

M(1)-Sm(1)-M(2)	140.3(3)
M(1)-Sm(1)-O(1)	114.6(3)
M(2)-Sm(1)-O(1)	105.1(3)
M(1)-Sm(2)-M(3)	142.0(3)
M(1)-Sm(2)-O(2)	114.4(3)
M(3)-Sm(2)-O(2)	103.6(3)
C(1)-Si(1)-C(9)	110.2(5)
C(1)-Si(1)-C(12)	110.3(4)
C(9)-Si(1)-C(12)	105.6(5)
C(1)-Si(1)-C(15)	110.4(6)
C(9)-Si(1)-C(15)	119.8(9)
C(12)-Si(1)-C(15)	99.6(8)
C(1)-Si(1)-C(15A)	111.3(7)

C(9)-Si(1)-C(15A)	99.3(9)
C(12)-Si(1)-C(15A)	119.1(9)
C(21)-Si(2)-C(4)	108.3(4)
C(21)-Si(2)-C(18)	113.1(5)
C(4)-Si(2)-C(18)	111.8(5)
C(21)-Si(2)-C(24)	108.7(5)
C(4)-Si(2)-C(24)	105.8(4)
C(18)-Si(2)-C(24)	108.8(5)
C(47)-O(1)-C(50)	103.3(9)
C(47)-O(1)-Sm(1)	125.2(6)
C(50)-O(1)-Sm(1)	131.4(8)
C(54)-O(2)-C(51)	101.5(12)
C(54)-O(2)-Sm(2)	126.4(11)
C(51)-O(2)-Sm(2)	131.8(7)
C(8)-C(1)-C(2)	130.3(9)
C(8)-C(1)-Si(1)	112.1(6)
C(2)-C(1)-Si(1)	117.6(7)
C(1)-C(2)-C(3)	139.0(10)
C(4)-C(3)-C(2)	138.2(12)
C(3)-C(4)-C(5)	129.3(10)
C(3)-C(4)-Si(2)	115.2(9)
C(5)-C(4)-Si(2)	115.5(7)
C(6)-C(5)-C(4)	134.6(9)
C(5)-C(6)-C(7)	136.5(11)
C(8)-C(7)-C(6)	137.3(12)
C(7)-C(8)-C(1)	134.9(11)
C(10)-C(9)-C(11)	105.8(9)
C(10)-C(9)-Si(1)	115.3(8)
C(11)-C(9)-Si(1)	117.2(8)
C(13)-C(12)-C(14)	109.1(12)
C(13)-C(12)-Si(1)	110.7(7)
C(14)-C(12)-Si(1)	120.1(8)
C(19)-C(18)-C(20)	108.8(8)
C(19)-C(18)-Si(2)	116.2(8)
C(20)-C(18)-Si(2)	113.0(8)
C(23)-C(21)-C(22)	109.4(9)
C(23)-C(21)-Si(2)	113.6(7)
C(22)-C(21)-Si(2)	114.7(8)

C(25)-C(24)-C(26)	111.8(9)
C(25)-C(24)-Si(2)	112.0(7)
C(26)-C(24)-Si(2)	117.4(7)
C(31)-C(27)-C(28)	108.7(9)
C(31)-C(27)-C(32)	127.2(11)
C(28)-C(27)-C(32)	123.8(11)
C(27)-C(28)-C(29)	107.3(9)
C(27)-C(28)-C(33)	125.8(11)
C(29)-C(28)-C(33)	126.3(10)
C(30)-C(29)-C(28)	108.0(9)
C(30)-C(29)-C(34)	127.0(10)
C(28)-C(29)-C(34)	124.9(10)
C(29)-C(30)-C(31)	108.2(9)
C(29)-C(30)-C(35)	124.6(10)
C(31)-C(30)-C(35)	127.0(10)
C(27)-C(31)-C(30)	107.7(9)
C(27)-C(31)-C(36)	124.9(11)
C(30)-C(31)-C(36)	127.0(11)
C(38)-C(37)-C(41)	111.1(10)
C(38)-C(37)-C(42)	125.1(13)
C(41)-C(37)-C(42)	123.7(12)
C(37)-C(38)-C(39)	105.0(10)
C(37)-C(38)-C(43)	127.8(11)
C(39)-C(38)-C(43)	126.6(10)
C(40)-C(39)-C(38)	108.9(9)
C(40)-C(39)-C(44)	126.7(11)
C(38)-C(39)-C(44)	124.4(11)
C(39)-C(40)-C(41)	109.1(10)
C(39)-C(40)-C(45)	123.8(11)
C(41)-C(40)-C(45)	126.8(11)
C(37)-C(41)-C(40)	105.8(9)
C(37)-C(41)-C(46)	126.5(11)
C(40)-C(41)-C(46)	126.8(11)
O(1)-C(47)-C(48)	107.5(10)
C(49)-C(48)-C(47)	105.3(10)
C(50)-C(49)-C(48)	102.9(10)
O(1)-C(50)-C(49)	107.0(10)
O(2)-C(51)-C(52)	108.8(13)

C(53)-C(52)-C(51)	101.3(14)
C(52)-C(53)-C(54)	111.3(17)
O(2)-C(54)-C(53)	107.2(16)
C(17)-C(15)-C(16)	113.6(18)
C(17)-C(15)-Si(1)	131.0(15)
C(16)-C(15)-Si(1)	112.3(13)
C(17A)-C(15A)-C(16A)	116(2)
C(17A)-C(15A)-Si(1)	123.7(17)
C(16A)-C(15A)-Si(1)	114.4(16)
Sm(1)-M(1)-Sm(2)	175.8(3)

M(1) is the centroid of the C(1) to C(8) ring

M(2) is the centroid of the C(27) to C(31) ring

M(3) is the centroid of the C(37) to C(41) ring

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 Least-squares planes (x,y,z in crystal coordinates) and deviations
from them
 (* indicates atom used to define plane)

  2.1367 (0.0601) x + 8.7566 (0.0547) y + 13.8594 (0.0553) z = 6.1136
(0.0325)

 *    0.0081 (0.0060)  C27
 *   -0.0063 (0.0059)  C28
 *    0.0021 (0.0059)  C29
 *    0.0028 (0.0059)  C30
 *   -0.0068 (0.0060)  C31
      2.5796 (0.0041)  Sm1
     -0.0905 (0.0179)  C32
     -0.1960 (0.0168)  C33
     -0.0739 (0.0172)  C34
     -0.0820 (0.0180)  C35
     -0.1779 (0.0177)  C36

 Rms deviation of fitted atoms =   0.0057


  6.9961 (0.0213) x + 0.3259 (0.0289) y + 14.6553 (0.0208) z = 5.6938
(0.0209)

 Angle to previous plane (with approximate esd) = 40.91 ( 0.31 )

 *   -0.0190 (0.0077)  C1
 *   -0.0003 (0.0078)  C2
 *    0.0102 (0.0068)  C3
 *    0.0022 (0.0085)  C4
 *   -0.0086 (0.0070)  C5
 *   -0.0024 (0.0089)  C6
 *    0.0026 (0.0077)  C7
 *    0.0153 (0.0091)  C8
     -2.2176 (0.0023)  Sm1
      2.2339 (0.0023)  Sm2
     -0.1171 (0.0081)  Si1
     -0.0275 (0.0082)  Si2

 Rms deviation of fitted atoms =   0.0100


  7.8765 (0.0482) x - 8.3570 (0.0561) y + 9.1576 (0.0738) z = 2.5508
(0.0629)

 Angle to previous plane (with approximate esd) = 39.60 ( 0.35 )

 *   -0.0020 (0.0060)  C37
 *   -0.0040 (0.0059)  C38
 *    0.0089 (0.0060)  C39
 *   -0.0102 (0.0060)  C40
 *    0.0074 (0.0058)  C41
     -2.5747 (0.0041)  Sm2
      0.0638 (0.0178)  C42
      0.1614 (0.0176)  C43
      0.0525 (0.0179)  C44
      0.0688 (0.0172)  C45
      0.2367 (0.0173)  C46
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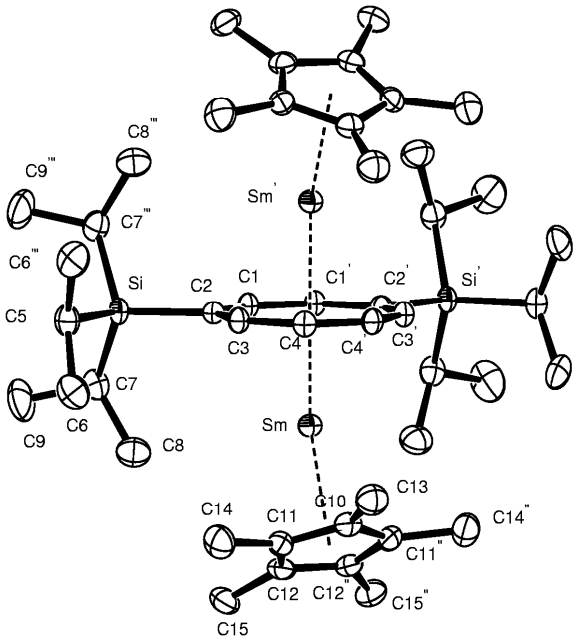

Table 1. Crystal data and structure refinement for **[SmCp*]$_2$(COT$^{1,4\text{-SiiPr3}}$). toluene**

Identification code	jun105	
Empirical formula	C46 H78 Si2 Sm2 . (C7 H8)	
Formula weight	1112.10	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pnmm (No.59)	
Unit cell dimensions	a = 7.8240(2) Å	α= 90°.
	b = 17.3596(5) Å	β= 90°.
	c = 18.6606(4) Å	γ = 90°.
Volume	2534.51(11) Å^3	
Z	2	
Density (calculated)	1.46 Mg/m^3	
Absorption coefficient	2.38 mm^{-1}	
F(000)	1144	
Crystal size	0.15 x 0.10 x 0.10 mm^3	
Theta range for data collection	3.40 to 26.02°.	
Index ranges	-9<=h<=9, -21<=k<=21, -23<=l<=23	
Reflections collected	32966	

Independent reflections	2653 [R(int) = 0.073]
Reflections with I>2sigma(I)	2181
Completeness to theta = 26.02°	99.7 %
Tmax. and Tmin.	0.789 and 0.704
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2653 / 16 / 146
Goodness-of-fit on F^2	1.074
Final R indices [I>2sigma(I)]	R1 = 0.034, wR2 = 0.085
R indices (all data)	R1 = 0.047, wR2 = 0.092
Largest diff. peak and hole	1.93 and -0.79 e.$Å^{-3}$ (near disordered solvate)

The toluene solvate was approximated by a disordered model with isotropic C atoms and H atoms omitted.

Data collection KappaCCD , Program package WinGX , Abs correction MULTISCAN
Refinement using SHELXL-97 , Drawing using ORTEP-3 for Windows

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for jun105. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Sm	1063(1)	2500	6348(1)	22(1)
Si	3063(2)	4506(1)	7500	21(1)
C(1)	3266(8)	2909(3)	7500	19(1)
C(2)	2026(8)	3519(3)	7500	20(1)
C(3)	223(8)	3496(3)	7500	21(1)
C(4)	-1051(8)	2907(3)	7500	20(1)
C(5)	1507(9)	5347(4)	7500	30(2)
C(6)	414(7)	5432(3)	6829(3)	39(1)
C(7)	4487(6)	4573(3)	6676(3)	30(1)
C(8)	3687(7)	4236(3)	6003(3)	40(1)
C(9)	5160(9)	5381(3)	6508(3)	56(2)
C(10)	-1802(9)	2500	5481(3)	26(1)
C(11)	-880(6)	3159(3)	5261(2)	25(1)
C(12)	623(6)	2911(3)	4910(2)	27(1)
C(13)	-3535(9)	2500	5828(4)	38(2)
C(14)	-1458(7)	3980(3)	5347(3)	38(1)
C(15)	1925(7)	3393(3)	4528(2)	34(1)
C(1S)	4528(16)	7500	7500	48(3)
C(2S)	4460(20)	7500	6805(8)	107(9)
C(3S)	3005(19)	7500	6448(9)	165(8)
C(4S)	1570(19)	7500	6834(6)	52(4)
C(5S)	1480(20)	7500	7500	114(7)
C(6S)	2999(19)	7500	7934(8)	42(4)

Table 3. Bond lengths [Å] and angles [°] for jun105.

Sm-M(1)	2.151(4)
Sm-M(2)	2.510(4)
Sm-C(10)	2.764(7)
Sm-C(11)	2.781(4)
Sm-C(12)	2.797(4)
Sm-C(4)	2.803(4)
Sm-C(3)	2.836(4)
Sm-C(1)	2.846(4)
Sm-C(2)	2.884(4)
Si-C(2)	1.896(6)
Si-C(5)	1.901(7)
Si-C(7)	1.902(5)
C(1)-C(1)'	1.419(11)
C(1)-C(2)	1.436(8)
C(2)-C(3)	1.411(9)
C(3)-C(4)	1.427(8)
C(4)-C(4)'	1.412(12)
C(5)-C(6)	1.524(6)
C(7)-C(8)	1.520(7)
C(7)-C(9)	1.531(7)
C(10)-C(11)	1.414(6)
C(10)-C(13)	1.502(10)
C(11)-C(12)	1.414(6)
C(11)-C(14)	1.503(7)
C(12)-C(12)"	1.426(9)
C(12)-C(15)	1.499(7)
M(1)-Sm-M(2)	152.7(2)
Sm'-M(1)-Sm	177.8(2)
C(2)-Si-C(5)	114.8(3)
C(2)-Si-C(7)	107.81(18)
C(5)-Si-C(7)	109.15(19)
C(7)'"-Si-C(7)	107.8(3)
C(1)'-C(1)-C(2)	137.5(3)
C(3)-C(2)-C(1)	130.9(6)
C(3)-C(2)-Si	117.0(4)

C(1)-C(2)-Si	112.2(4)
C(2)-C(3)-C(4)	135.9(6)
C(4)'-C(4)-C(3)	135.7(3)
C(6)-C(5)-C(6)'"	110.5(6)
C(6)-C(5)-Si	115.8(3)
C(8)-C(7)-C(9)	109.0(5)
C(8)-C(7)-Si	113.8(3)
C(9)-C(7)-Si	115.0(4)
C(11)-C(10)-C(11)"	108.1(6)
C(11)-C(10)-C(13)	125.8(3)
C(12)-C(11)-C(10)	108.2(4)
C(12)-C(11)-C(14)	126.1(4)
C(10)-C(11)-C(14)	125.6(4)
C(11)-C(12)-C(12)"	107.8(3)
C(11)-C(12)-C(15)	127.9(4)
C(12)"-C(12)-C(15)	124.0(3)

Symmetry transformations used to generate equivalent atoms:

" x,-y+1/2,z ' x,-y+1/2,-z+3/2 '" x,y,-z+3/2

```
 Least-squares planes (x,y,z in crystal coordinates) and deviations
from them
 (* indicates atom used to define plane)

  0.0000 (0.0000) x - 0.0000 (0.0000) y + 18.6606 (0.0005) z =
13.9955 (0.0004)

 *    0.0000 (0.0000)  C1_a
 *    0.0000 (0.0000)  C2_a
 *    0.0000 (0.0000)  C3_a
 *    0.0000 (0.0000)  C4_a
 *    0.0000 (0.0000)  C1_$1a
 *    0.0000 (0.0000)  C2_$1a
 *    0.0000 (0.0000)  C3_$1a
 *    0.0000 (0.0000)  C4_$1a
     -2.1504 (0.0003)  Sm

 Rms deviation of fitted atoms =   0.0000


  3.8246 (0.0221) x - 0.0000 (0.0002) y + 16.2791 (0.0296) z = 8.2298
(0.0166)

 Angle to previous plane (with approximate esd) = 29.26 ( 0.15 )

 *    0.0029 (0.0040)  C10_a
 *   -0.0023 (0.0032)  C11_a
 *    0.0009 (0.0012)  C12_a
 *   -0.0023 (0.0032)  C11_$2a
 *    0.0009 (0.0012)  C12_$2a
      2.5099 (0.0028)  Sm
     -0.0944 (0.0118)  C13_a
     -0.0829 (0.0070)  C14_a
     -0.1219 (0.0093)  C15_a

 Rms deviation of fitted atoms =   0.0020
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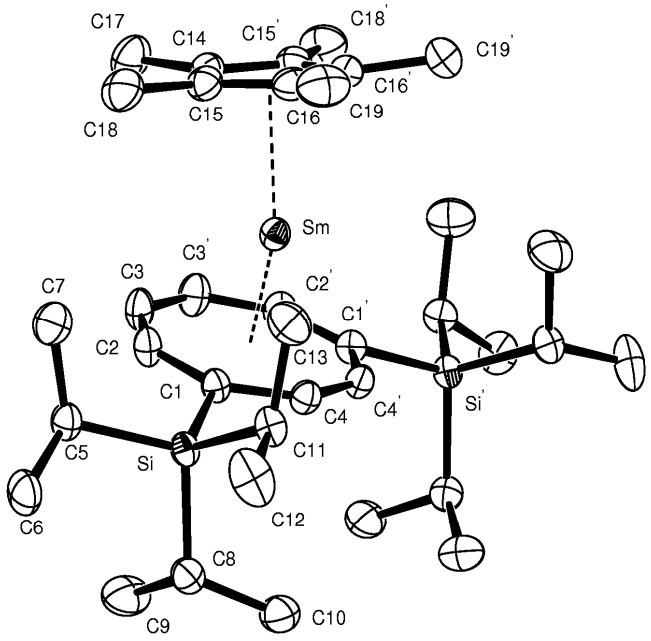

Table 1. Crystal data and structure refinement for **Sm(COT$^{1,4\text{-SiiPr3}}$)(Cp*) (7)**.

Identification code	jun1606	
Empirical formula	C36 H63 Si2 Sm	
Formula weight	702.39	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/m$ (No.11)	
Unit cell dimensions	a = 8.5333(3) Å	α= 90°.
	b = 22.5383(6) Å	β= 100.809(1)°.
	c = 9.7450(3) Å	γ = 90°.
Volume	1840.96(10) Å^3	
Z	2	
Density (calculated)	1.27 Mg/m^3	
Absorption coefficient	1.68 mm^{-1}	
F(000)	738	
Crystal size	0.28 x 0.25 x 0.18 mm^3	
Theta range for data collection	3.43 to 26.01°.	
Index ranges	-10<=h<=10, -27<=k<=27, -11<=l<=12	
Reflections collected	25206	
Independent reflections	3712 [R(int) = 0.056]	

Reflections with I>2sigma(I)	3345
Completeness to theta = 26.01°	99.7 %
Tmax. and Tmin.	0.7137 and 0.6792
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3712 / 0 / 184
Goodness-of-fit on F^2	1.095
Final R indices [I>2sigma(I)]	R1 = 0.026, wR2 = 0.054
R indices (all data)	R1 = 0.034, wR2 = 0.056
Largest diff. peak and hole	0.48 and -0.90 e.$Å^{-3}$

The molecule lies on a crystallographic mirror plane.

Data collection KappaCCD , Program package WinGX , Abs correction MULTISCAN

Refinement using SHELXL-97 , Drawing using ORTEP-3 for Windows

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for jun1606. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Sm	148(1)	2500	3720(1)	23(1)
Si	-2537(1)	4021(1)	1727(1)	22(1)
C(1)	-1471(3)	3281(1)	1943(3)	23(1)
C(2)	113(3)	3259(1)	1687(3)	28(1)
C(3)	1222(3)	2812(1)	1527(3)	31(1)
C(4)	-2528(3)	2813(1)	2161(3)	24(1)
C(5)	-1072(3)	4650(1)	1657(3)	28(1)
C(6)	-1861(3)	5229(1)	1035(3)	38(1)
C(7)	32(4)	4784(1)	3047(3)	45(1)
C(8)	-3930(3)	4001(1)	-40(3)	28(1)
C(9)	-3004(4)	3885(2)	-1212(3)	49(1)
C(10)	-5324(3)	3562(1)	-145(3)	39(1)
C(11)	-3785(3)	4118(1)	3134(3)	28(1)
C(12)	-4702(4)	4706(1)	3039(3)	48(1)
C(13)	-2865(4)	4017(2)	4611(3)	47(1)
C(14)	3099(4)	2500	5294(4)	29(1)
C(15)	2343(3)	3009(1)	5715(3)	30(1)
C(16)	1122(3)	2814(1)	6409(3)	31(1)
C(17)	4550(5)	2500	4616(5)	46(1)
C(18)	2830(4)	3643(1)	5529(3)	45(1)
C(19)	113(4)	3195(2)	7180(3)	47(1)

Table 3. Bond lengths [Å] and angles [°] for jun1606.

Sm-M(1)	1.843(2)
Sm-M(2)	2.407(2)
Sm-C(3)	2.577(3)
Sm-C(4)	2.592(2)
Sm-C(2)	2.614(3)
Sm-C(1)	2.665(2)
Sm-C(15)	2.691(3)
Sm-C(16)	2.691(3)
Sm-C(14)	2.691(4)
Si-C(1)	1.893(2)
Si-C(11)	1.900(2)
Si-C(8)	1.901(3)
Si-C(5)	1.901(2)
C(1)-C(2)	1.420(3)
C(1)-C(4)	1.429(3)
C(2)-C(3)	1.412(3)
C(3)-C(3)’	1.406(5)
C(4)-C(4)’	1.410(5)
C(5)-C(7)	1.528(4)
C(5)-C(6)	1.539(4)
C(8)-C(9)	1.529(4)
C(8)-C(10)	1.537(4)
C(11)-C(13)	1.522(4)
C(11)-C(12)	1.534(4)
C(14)-C(15)	1.415(3)
C(14)-C(17)	1.509(5)
C(15)-C(16)	1.415(4)
C(15)-C(18)	1.508(4)
C(16)-C(16)’	1.414(5)
C(16)-C(19)	1.512(4)
M(1)-Sm-M(2)	161.4(1)
C(1)-Si-C(11)	110.14(11)
C(1)-Si-C(8)	106.68(11)
C(11)-Si-C(8)	108.43(11)
C(1)-Si-C(5)	110.87(11)

C(11)-Si-C(5)	113.64(11)
C(8)-Si-C(5)	106.76(11)
C(2)-C(1)-C(4)	130.5(2)
C(2)-C(1)-Si	117.60(17)
C(4)-C(1)-Si	111.28(16)
C(3)-C(2)-C(1)	136.3(2)
C(3)'-C(3)-C(2)	135.57(14)
C(4)'-C(4)-C(1)	137.54(13)
C(7)-C(5)-C(6)	109.4(2)
C(7)-C(5)-Si	114.57(18)
C(6)-C(5)-Si	113.87(17)
C(9)-C(8)-C(10)	109.9(2)
C(9)-C(8)-Si	110.94(18)
C(10)-C(8)-Si	114.82(18)
C(13)-C(11)-C(12)	110.8(2)
C(13)-C(11)-Si	113.90(19)
C(12)-C(11)-Si	113.89(18)
C(15)'-C(14)-C(15)	108.5(3)
C(15)'-C(14)-C(17)	125.69(16)
C(15)-C(14)-C(17)	125.69(16)
C(16)-C(15)-C(14)	107.6(2)
C(16)-C(15)-C(18)	126.7(2)
C(14)-C(15)-C(18)	125.6(2)
C(16)'-C(16)-C(15)	108.17(15)
C(16)'-C(16)-C(19)	124.64(17)
C(15)-C(16)-C(19)	126.8(3)

Symmetry transformations used to generate equivalent atoms: ' x,-y+1/2,z

M(1) and M(2) are the centroids of the cot and Cp* rings

Least-squares planes (x,y,z in crystal coordinates) and deviations from them
 (* indicates atom used to define plane)

  1.5273 (0.0084) x - 0.0000 (0.0001) y + 9.0904 (0.0035) z = 1.5614 (0.0018)

 *   -0.0194 (0.0020) C1_a
 *   -0.0106 (0.0022) C2_a
 *   0.0130 (0.0015) C3_a
 *   0.0169 (0.0014) C4_a
 *   -0.0194 (0.0020) C1_$1a
 *   -0.0106 (0.0022) C2_$1a
 *   0.0130 (0.0015) C3_$1a
 *   0.0169 (0.0014) C4_$1a
      1.8427 (0.0013) Sm
     -0.3791 (0.0020) Si_a

 Rms deviation of fitted atoms =   0.0153

  4.2008 (0.0141) x + 0.0000 (0.0002) y + 7.4322 (0.0120) z = 5.2337 (0.0045)

 Angle to previous plane (with approximate esd) = 19.18 (0.16)

 *   0.0024 (0.0023) C14_a
 *   -0.0019 (0.0019) C15_a
 *   0.0007 (0.0007) C16_a
 *   -0.0019 (0.0019) C15_$1a
 *   0.0007 (0.0007) C16_$1a
     -2.4069 (0.0016) Sm
      0.1084 (0.0071) C17_a
      0.0644 (0.0038) C18_a
      0.1504 (0.0055) C19_a

 Rms deviation of fitted atoms =   0.0017