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General Considerations. All manipulations were performed under inert atmosphere of argon, nitrogen or hydrogen using either standard Schlenk techniques or a Vacuum Atmospheres glove box. Elemental analyses were preformed by E+R Microanalytical Laboratory. Nuclear magnetic resonance (NMR) spectra were recorded on a Brucker AC-250 MHz or a Varian Unity-300 Fourier transform spectrometer. Infra-red (IR) spectra were recorded on a Perkin-Elmer 1600 series Fourier transform spectrometer. Dry, oxygen-free solvents were employed throughout, which were distilled over sodium benzophenone under an argon atmosphere. $Cp^*_2SmCH(SiMe_3)_2$,[1] N-(1-methylbenzylidene)methylamine,[2] *N*-(1-methyl-*p*-chlorobenzylidene)methylamine,[2] *N*-(1-methyl-*p*-bromobenzylidene)methylamine,[2] 2-phenyl-1-pyrroline[3,4] were prepared according to literature procedures. All other reagents are commercially available and were distilled prior to use.

$Cp^*_2Sm[o\text{-}C_6H_4C{=}NCH_2CH_2CH_2]$ (1). Pentane (25 mL) was added to a Schlenk flask containing 0.310 g (0.53 mmol) of $Cp^*_2SmCH(SiMe_3)_2$. The solution was stirred for 3 h under H_2 (1 atm) atmosphere at 0 °C. A pentane (5 mL) solution of 2-phenyl-1-pyrroline (0.085 g, 0.59 mmol) was then added under Ar atmosphere. The color of the reaction mixture changed to dark-red, and gas evolution was observed. Removal of volatiles after 2 h, was followed by extraction of the resulting residue with pentane (20 mL). Concentration (10 mL) and cooling (- 40 °C) gave the product as yellow crystals (mp 254-255 °C) of **1** (0.21 g, 70 %). Anal. Calcd for $C_{30}H_{40}NSm$: C, 63.6; H, 7.12. Found: C, 63.5; H, 7.25; IR (Nujol, NaCl, cm^{-1}): 1618 m, 1579 s, 1534 m, 1340 m, 1308 m, 1255 w, 1234 w, 1157 m, 1085 m, 1055 s, 961 m, 799 w, 761 m, 722 s, 690 m; ^1H NMR (benzene-d_6, 30 °C): δ -7.02 (s, 3 H, NCH_2), - 1.24 (s, 1 H, *o*-CH), -0.61 (br s, 2 H, CH_2), 1.35 (s, 30 H, C_5Me_5), 3.33 (t, J = 7.2 H, 2 H, CH_2), 6.39 (d, *J* = 7.5 Hz, 1 H, CH), 8.01 (t, *J* = 8.1 , 1 H, CH), 8.80 (d, *J* = 8.1 Hz, 1 H, CH); $^{13}C\{^1H\}$

NMR (benzene-d_6, 22 °C): δ 16.05 (C_5Me_5), 31.51, 46.69, 61.81, 116.36 (C_5Me_5), 127.13, 138.83, 158.11, 195.61.

$Cp^*_2Sm[o\text{-}C_6H_4C(Me)=N(Me)]$ (2). The procedure used for **1** was performed using 0.500 g (0.86 mmol) of $Cp^*_2SmCH(SiMe_3)_2$ and 0.138 g (1.0 mmol) N-(1-methylbenzylidene)methylamine. The product (0.16 g) was isolated as yellow crystals in 33 % yield (mp 242-243 °C). Anal. Calcd for $C_{29}H_{40}NSm$: C, 62.8; H, 7.27. Found: C, 59.1; H, 6.65; IR (Nujol, NaCl, cm^{-1}): 1637 m, 1591 s, 1539 w, 1372 m, 1291 m, 1081 s, 947 m, 799 w, 761 s, 706 m, 692 m; ^1H NMR (benzene-d_6, 22 °C): δ -10.45 (s, 3 H, NCH_3), - 3.27 (s, 1 H, *o*-CH), 1.40 (s, 30 H, C_5Me_5), 2.44 (s, 3 H, $C(CH_3)=NCH_3$), 6.17 (d, J = 7.2 Hz, 1 H, CH), 8.12 (t, J = 8.1 H, 1 H, CH), 9.29 (d, J = 7.2 Hz, 1 H, CH); $^{13}C\{^1H\}$ NMR (benzene-d_6, 22 °C): δ 16.20 (C_5Me_5), 116.63 (C_5Me_5), 127.26, 128.50, 138.78, 165.78, 192.97.

$Cp^*_2Sm[o\text{-}C_6H_4\text{-}p\text{-}Cl\text{-}C(Me)=N(Me)]$ (3). The procedure used for **1** was employed with 0.320 g (0.55 mmol) of $Cp^*_2SmCH(SiMe_3)_2$ and 0.090 g (0.55 mmol) of *N*-(1-methyl-*p*-chlorobenzylidene)methylamine. The product was isolated as orange crystals (mp 242-243 °C) in 47 % yield (0.15 g). Anal. Calcd for $C_{29}H_{39}ClNSm$: C, 59.2; H, 6.68. Found: C, 59.0; H, 6.92; IR (Nujol, NaCl, cm^{-1}): 1598 s, 1525 m, 1290 m, 1238 w, 1146 m, 1088 s, 1009 m, 881 w, 811 m, 767 m, 725 m; ^1H NMR (benzene-d_6, 22 °C): δ -10.52 (s, 3 H, NCH_3), - 3.51 (s, 1 H, *o*-CH), 1.30 (s, 30 H, C_5Me_5), 2.32 (s, 3 H, $C(CH_3)=NCH_3$), 8.09 (d, J = 8.4 , 1 H, CH), 8.85 (d, J = 8.7 Hz, 1 H, CH); $^{13}C\{^1H\}$ NMR (benzene-d_6, 22 °C): δ 16.26 (C_5Me_5), 117.02 (C_5Me_5), 127.38, 128.81, 137.66, 149.14, 195.95.

$Cp^*_2Sm[o\text{-}C_6H_4\text{-}p\text{-}Br\text{-}C(Me)=N(Me)]$ (4). The above procedure was performed using 0.210 g (0.36 mmol) of $Cp^*_2SmCH(SiMe_3)_2$ and 0.077 g (0.36 mmol) of *N*-(1-methyl-*p*-bromobenzylidene)methylamine, to give the product as orange crystals (mp 243-244 °C) of **4** (0.12 g, 53 %). Anal. Calcd for $C_{29}H_{39}BrNSm$: C, 55.0; H, 6.22. Found: C, 51.7; H, 6.02. IR (Nujol, NaCl, cm^{-1}): 1600 s, 1520 m, 1290 m, 1238 w, 1149 m,

1085 s, 1003 m, 884 w, 811 m, 756 m, 723 m. ^{1}H NMR (benzene-d_6, 22 °C): δ -10.38 (s, 3 H, NCH_3), - 3.45 (s, 1 H, *o*-CH), 1.27 (s, 30 H, C_5Me_5), 2.34 (s, 3 H, $C(CH_3)=NCH_3$), 8.23 (d, J = 8.4, 1 H, CH), 8.70 (d, J = 8.1 Hz, 1 H, CH); $^{13}C\{^1H\}$ NMR (toluene-d_8, 22 °C): δ 16.31 (C_5Me_5), 117.00 (C_5Me_5), 130.27, 140.63, 154.73, 192.51, 203.93.

$Cp^*_2Sm[o\text{-}C_6H_4C(H)=N(Me)]$ (5). The above procedure was performed using 0.300 g (0.51 mmol) of $Cp^*_2SmCH(SiMe_3)_2$ and 0.060 g (0.51 mmol) N-(1-methylbenzylideneamine, afforded a yellow powder (80 % pure) in 22 % yield (0.06 g). Attempts to obtain pure **5** failed (by recrystallization from pentane). However, this reaction is observed to proceed cleanly by ^{1}H NMR spectroscopy (in benzene-d_6). IR (Nujol, NaCl, cm^{-1}): 1653 m, 1591 s, 1311 m, 1260 m, 1156 m, 1086 s, 1034 m, 955 m, 796 w, 723 s, 697 m; ^{1}H NMR (benzene-d_6, 22 °C): δ -7.22 (s, 3 H, NCH_3), - 3.94 (s, 1 H, *o*-CH), 1.34 (s, 30 H, C_5Me_5), 6.52 (d, J = 6 Hz, 1 H, CH), 7.00 (s, 1 H, $C(H)=NCH_3$), 8.06 (t, J = 6 H, 1 H, CH), 8.65 (d, J = 7 Hz, 1 H, CH).

References

1. Jeske, G.; Lauke, H.; Mauermann, H.; Swepston, P. N.; Schumann, H.; Marks, T. J. *J. Am. Chem. Soc.* **1985**, *107*, 8091.

2. Evans, D. A.; Domeier, L. A. *Org. Synth., Coll. Vol. VI* , 818.

3. Willoughby, C. A.; Buchwald, S. L. *J. Am. Chem. Soc.* **1994**, *116*, 8952.

4. Haslego, M. L.; Maryanoff, C. A.; Scott, L.; Sorgi, K. L. *Heterocycles* **1993**, *35*, 643.

Experimental

A yellow, irregular shaped crystal was mounted on a thin glass fiber using silicone grease. The crystal, which was mounted from a pool of mineral oil bathed in argon, was then immediately placed under a liquid. N_2 stream on a Siemens P4/PC diffractometer. The radiation used was graphite monachromatized MoKα radiation (λ= 0.71069 Å). The lattice parameters were optimized from a least-squares calculation on 25 carefully centered reflections of high Bragg angle. The data was collected using ω scans with a 1.48° scan range. Three check reflections monitored every 97 reflections showed no systematic variation of intensities. Lattice determination and data collection were carried out using XSCANS Version 2.10b software. All data reduction, including Lorentz and polarization corrections and structure solution and graphics were performed using SHELXTL PC Version 4.2/360 software. The structure refinement was performed using SHELX 93 software[1]. The data were corrected for absorption using the ellipsoid option in the XEMP facility of SHELXTL PC. Data collection parameters are given in Table 1.

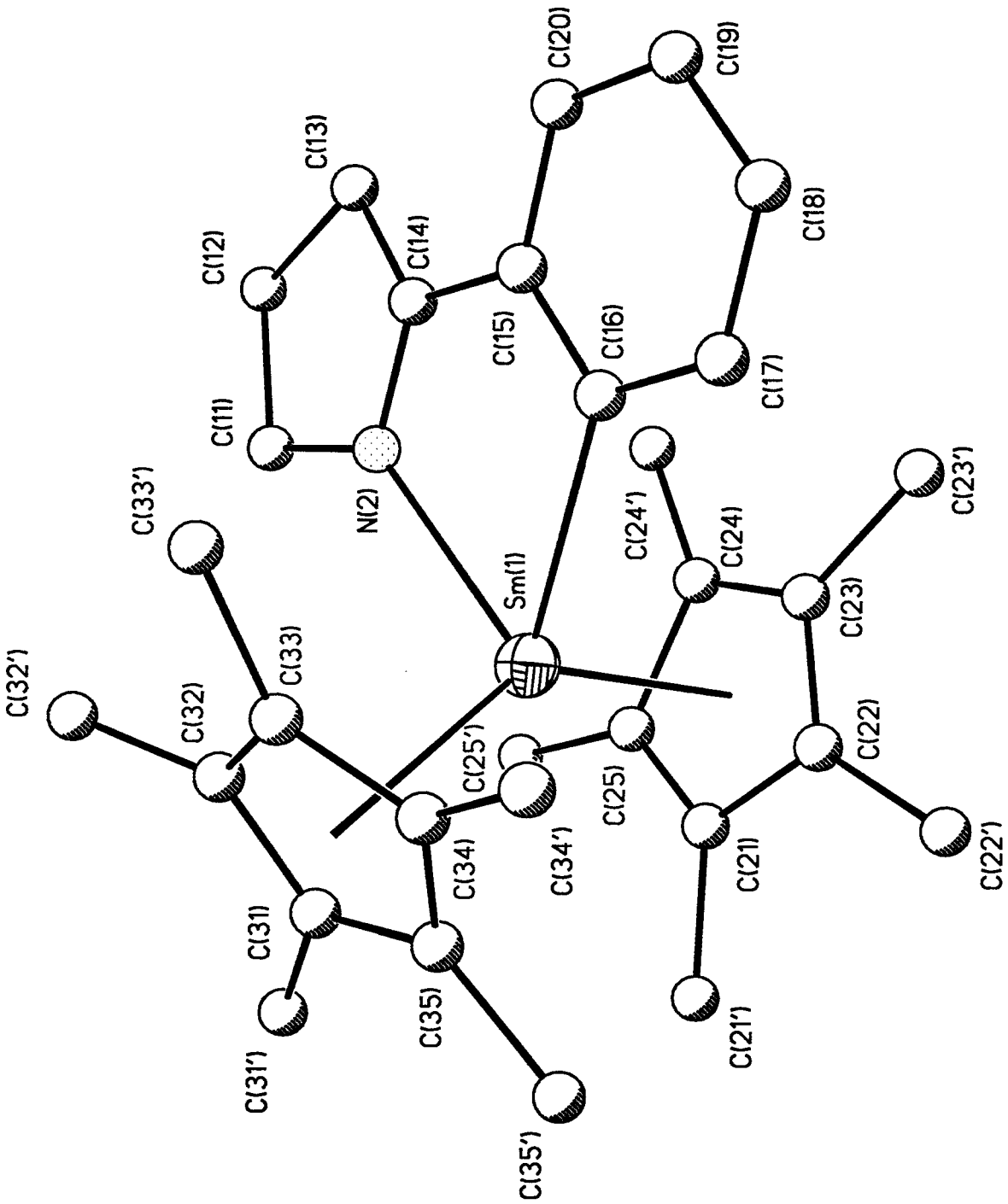
Structure Solution and Refinement

The structure was solved in space group $P\bar{1}$ using Patterson techniques to reveal two samarium atoms in the unit cell. Structure refinement was initiated with these two samarium atoms and several subsequent difference maps revealed the Cp^* and 2-phenylcyclopentaimine (L) ligand atoms. The refinement was plagued by severe disorder. The two Cp^* and L ligands bonded to Sm1 were easily identified and refined. The Cp^* and the L ligands of Sm(2) were more problematic, but using rigid body restraints for the Cp^* ligands allowed the full $Sm(2)(Cp^*)_2L$ molecule to be refined. At this juncture, with only the samarium atoms refined anisotropically, R1= 0.13. It was apparent that the Cp^* ligands of Sm(2) and the L ligands of both Sm1 and Sm2 were disordered. The Cp^* ligands on Sm(2) were each modeled as two one-half occupancy Cp^* ligands and refined using rigid body constraints (1.41 Å for ring C-C bonds and 1.50 Å for ring-methyl C-C bonds). The L ligands of both Sm(1) and Sm(2) were modeled as two one-half occupancy ligands, with the imine of one half-occupancy ligand eclipsing the phenyl of the other half-occupancy ligand. The phenyl rings of all L ligands were refined as rigid hexagons with C-C = 1.39 Å. At this time the SHELXL listing file recommended splitting Sm(2) into two atoms. Subsequent refinements included two one-half occupancy Sm(2) atoms [Sm(2) and Sm(2')]. The final refinement included isotropic thermal parameters on all atoms except for the samarium atoms and converged to R1= 0.0975 and $R2_w$= 0.2493.[2] The four molecular structures resulting from the refinement of the two disordered $Sm(Cp^*)_2L$ molecules are shown in Figures 1-4. Bond distances and angles are listed in Table 3. Attempts to find a tranformation to a higher symmetry monoclinic cell were not successful.

References

1. XSCANS and SHELXTL PC are products of Siemens Analytical X-ray Instruments, Inc., 6300 Enterprise Lane, Madison, Wisconsin 53719. SHELX-93 is a program for crystal structure refinement written by G. M. Sheldrick, (1993), Univ. of Göttingen, Germany.

2. $R1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$ and $R2_w = [\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$. The parameter $w = 1/[\sigma^2(F_o^2) + (0.1177*P)^2 + 72.4471*P]$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C(13)
C(18)
C(12)
C(14)
C(15)
C(16)
C(17)
C(11)
N(2)
C(33')
Sm(1)
C(24')
C(23')
C(24)
C(23)
C(32')
C(33)
C(32)
C(25')
C(25)
C(22)
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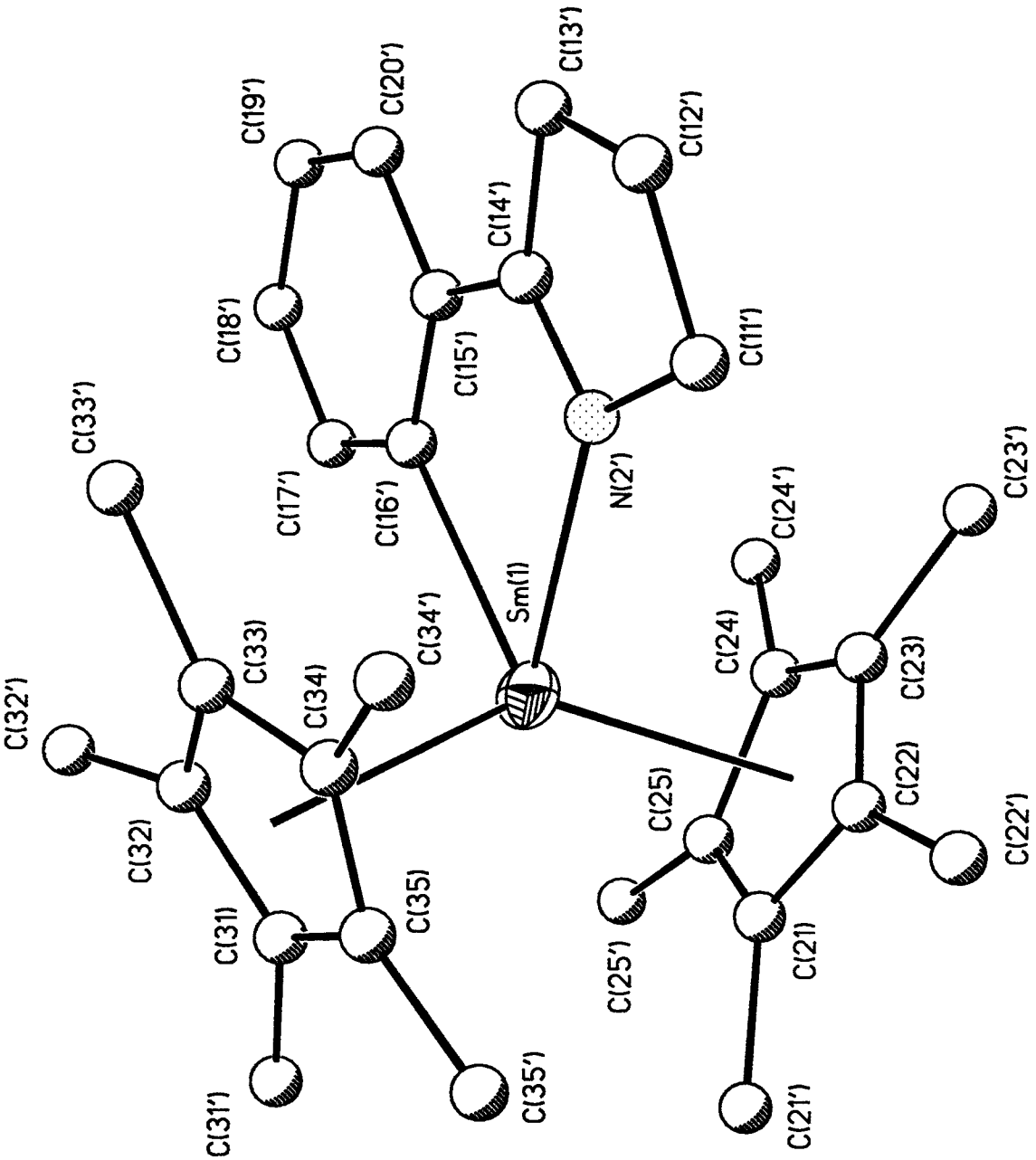
C(21')
C(31')
C(35')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C(34')
Sm(1)
C(24)
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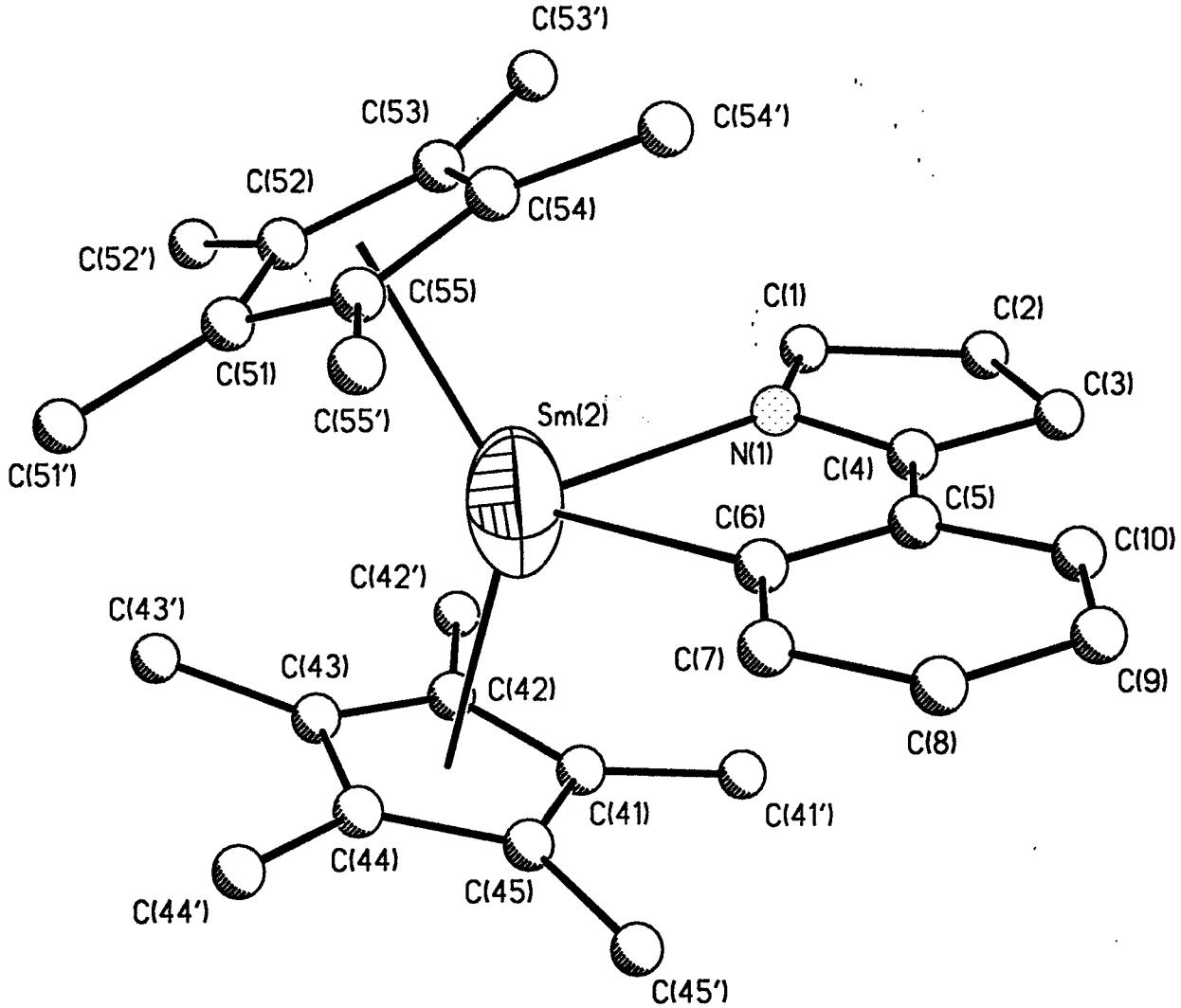

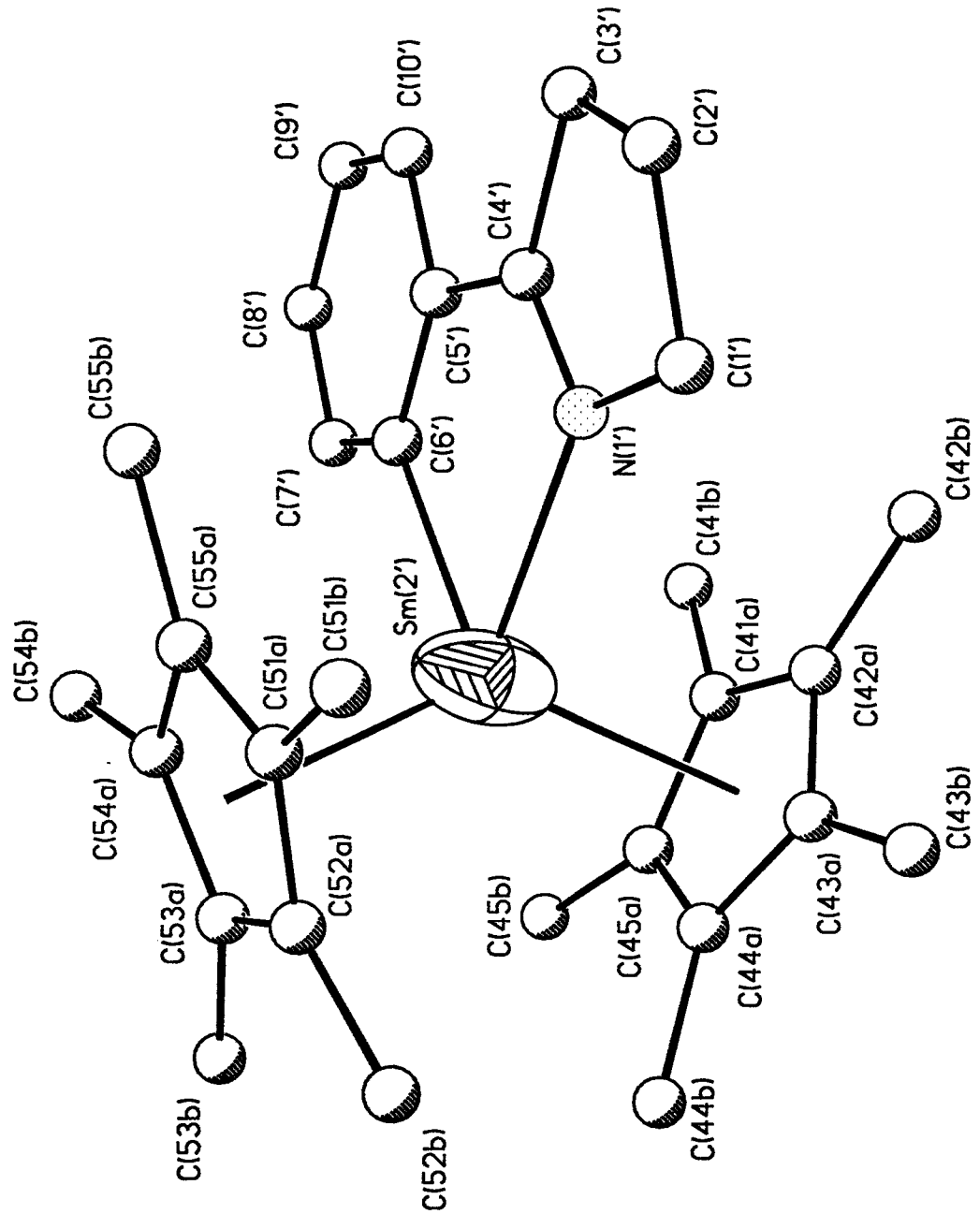
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C(41b)
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Sm(2')
C(54b)
C(51b)
C(41a)
C(51a)
C(42a)
C(54a)
C(43b)
C(52a)
C(53a)
C(45b)
C(45a)
C(44a)
C(43a)
C(53b)
C(44b)
C(52b)

Centroid Information for Sm(Cp*)2(2-phenylcyclopentaimine)

Ce1 = C21 to C25
Ce2 = C31 to C35
Ce3 = C41 to C45
Ce4 = C51 to C55
Ce5 = C41a to C45a
Ce6 = C51a to C55a

Ce1-Sm1-Ce2= 140.1°
Ce3-Sm2-Ce4= 137.7°
Ce5-Sm2'-Ce6= 135.8°

Sm1-Ce1= 2.446 Å
Sm1-Ce2= 2.459 Å
Sm2-Ce3= 2.435 Å
Sm2-Ce4= 2.502 Å
Sm2'-Ce5= 2.538 Å
Sm2'-Ce6= 2.422 Å

Table 1. Crystal data and structure refinement for $Sm(Cp^*)_2$(2-phenylcyclopentaimine).

Empirical formula	$C_{30}H_{37}NSm$
Formula weight	561.96
Temperature	193 K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 11.441(4) Å α = 87.89(2)° b = 15.032(3) Å β = 89.20(2)° c = 15.432(3) Å γ = 81.68(2)°
Volume	2624.2(12) $Å^3$
Z	4
Density (calculated)	1.422 Mg/m^3
Absorption coefficient	2.254 mm^{-1}
Absorption correction	Semi-empirical
Min./Max. Transmission	0.809 / 0.868
F(000)	1144
Crystal size	0.16 x 0.21 x 0.25 mm
θ range for data collection	2.51 to 17.50°
Index ranges	$-1 \le h \le 9$, $-12 \le k \le 12$, $-13 \le \ell \le 13$
Reflections collected	4062
Independent reflections	3312 (R_{int} = 0.0264)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3311 / 0 / 305
Goodness-of-fit on F^2	1.175
Final R indices [$I>2\sigma(I)$]	R1 = 0.0975, wR2 = 0.2493
Final R indices	R1 = 0.0975, wR2 = 0.2493 [4845$F_o>4\sigma(F_o)$]
R indices (all data)	R1 = 0.1214, wR2 = 0.2729
Extinction coefficient	0.027(3)
Largest diff. peak and hole	1.358 and -1.892 $eÅ^{-3}$ (1.1Å from Sm1).

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for Sm(Cp^*)$_2$(2-phenylcyclopentaimine). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Sm(1)	4981(1)	7531(1)	2447(1)	29(1)
Sm(2')	199(10)	7681(8)	7403(8)	98(3)
Sm(2)	-255(11)	7346(8)	7520(9)	115(4)
N(1)	-990(47)	8320(28)	8719(28)	46(15)
C(1)	-1662(48)	9232(33)	8708(34)	38(14)
C(2)	-1605(54)	9584(41)	9666(42)	45(20)
C(3)	-904(48)	8714(33)	10184(43)	44(15)
C(4)	-551(40)	8084(31)	9484(25)	12(11)
C(5)	102(27)	7192(16)	9634(19)	17(12)
C(6)	442(29)	6609(20)	8968(15)	16(12)
C(7)	1114(30)	5779(19)	9149(19)	41(14)
C(8)	1446(30)	5530(18)	9996(22)	47(16)
C(9)	1107(31)	6113(22)	10663(16)	50(16)
C(10)	435(29)	6944(20)	10482(17)	38(13)
N(2)	4263(34)	8582(28)	3630(25)	40(12)
C(11)	3547(45)	9498(34)	3637(33)	49(15)
C(12)	3727(62)	9939(46)	4522(44)	93(22)
C(13)	4468(40)	9042(29)	5071(28)	30(12)
C(14)	4677(39)	8353(30)	4430(30)	29(13)
C(15)	5364(26)	7436(16)	4579(19)	20(12)
C(16)	5672(26)	6854(21)	3907(14)	24(13)
C(17)	6362(26)	6027(18)	4072(15)	12(11)
C(18)	6744(25)	5782(15)	4909(17)	30(12)
C(19)	6437(26)	6363(19)	5582(13)	20(11)
C(20)	5747(27)	7190(17)	5417(16)	38(13)
N(1')	1047(38)	6697(27)	8557(28)	49(12)
C(1')	1822(46)	5781(34)	8543(33)	51(15)
C(2')	1712(45)	5370(34)	9511(37)	46(15)
C(3')	1092(48)	6238(35)	10078(35)	53(16)
C(4')	676(37)	6918(29)	9347(28)	15(12)
C(5')	-92(29)	7749(17)	9497(19)	14(14)
C(6')	-509(33)	8362(21)	8837(15)	21(16)
C(7')	-1155(33)	9186(19)	9038(20)	24(13)
C(8')	-1384(35)	9397(19)	9899(24)	48(26)
C(9')	-967(37)	8784(25)	10559(17)	54(22)
C(10')	-321(31)	7960(22)	10359(17)	42(14)
N(2')	5765(27)	6402(23)	3636(19)	8(9)
C(11')	6540(39)	5520(30)	3661(28)	29(12)
C(12')	6389(49)	5095(37)	4536(35)	59(16)
C(13')	5768(46)	5947(33)	5095(32)	45(14)
C(14')	5439(40)	6632(31)	4434(30)	30(13)
C(15')	4730(29)	7494(19)	4599(21)	27(13)
C(16')	4330(31)	8123(24)	3947(15)	44(16)
C(17')	3628(30)	8921(21)	4156(18)	38(14)
C(18')	3327(30)	9091(18)	5016(21)	65(17)
C(19')	3728(30)	8462(22)	5667(16)	40(14)

C(20')	4429(29)	7664(19)	5459(18)	38(13)
C(21)	6288(21)	8189(16)	1186(15)	39(7)
C(22)	7086(24)	7551(18)	1654(17)	54(8)
C(23)	7256(22)	7880(17)	2450(16)	41(7)
C(24)	6635(27)	8694(21)	2517(19)	67(9)
C(25)	5975(24)	8893(18)	1675(17)	55(8)
C(21')	6000(27)	8167(20)	213(19)	72(9)
C(22')	7665(30)	6633(23)	1278(21)	89(11)
C(23')	8137(33)	7451(24)	3093(24)	100(12)
C(24')	6595(34)	9355(25)	3238(24)	104(12)
C(25')	5202(29)	9813(22)	1448(21)	83(10)
C(31)	3153(20)	7425(15)	1382(14)	35(7)
C(32)	2637(20)	7430(15)	2210(15)	35(7)
C(33)	3049(22)	6654(17)	2607(16)	43(7)
C(34)	3870(23)	6114(17)	2073(16)	47(7)
C(35)	3886(20)	6582(15)	1292(14)	33(6)
C(31')	2843(26)	8133(20)	687(19)	69(9)
C(32')	1703(28)	8141(21)	2553(20)	80(10)
C(33')	2694(31)	6372(23)	3588(22)	89(11)
C(34')	4440(39)	5158(29)	2331(28)	127(14)
C(35')	4509(32)	6229(24)	477(23)	98(11)
C(41)	1483(20)	8371(16)	7473(14)	10(11)
C(42)	858(23)	8597(18)	6698(16)	46(15)
C(43)	1072(26)	7855(19)	6158(18)	72(18)
C(44)	1830(26)	7171(19)	6599(18)	78(19)
C(45)	2085(24)	7489(18)	7411(16)	69(18)
C(41')	1506(32)	8963(24)	8229(21)	63(17)
C(42')	98(37)	9472(26)	6486(24)	113(27)
C(43')	580(41)	7804(28)	5270(27)	130(30)
C(44')	2286(41)	6263(28)	6262(27)	109(25)
C(45')	2858(39)	6980(26)	8091(24)	129(29)
C(41A)	1620(25)	9077(21)	7492(18)	57(16)
C(42A)	2400(26)	8260(20)	7483(18)	59(17)
C(43A)	2348(26)	7899(20)	6657(19)	89(21)
C(44A)	1536(27)	8493(21)	6155(19)	96(23)
C(45A)	1086(26)	9221(21)	6671(19)	72(19)
C(41B)	1398(39)	9686(30)	8243(26)	113(26)
C(42B)	3152(42)	7848(30)	8222(27)	136(31)
C(43B)	3035(41)	7036(30)	6363(28)	100(23)
C(44B)	1208(44)	8371(32)	5234(29)	141(32)
C(45B)	196(42)	10009(32)	6396(28)	119(28)
C(51)	-1318(26)	6206(20)	6438(19)	112(27)
C(52)	-2084(27)	7032(20)	6461(19)	69(18)
C(53)	-2544(27)	7129(21)	7313(19)	46(15)
C(54)	-2062(29)	6362(21)	7818(20)	53(16)
C(55)	-1304(27)	5791(21)	7277(20)	96(23)
C(51')	-637(42)	5833(30)	5659(28)	85(20)
C(52')	-2362(43)	7693(30)	5710(28)	160(37)
C(53')	-3396(43)	7910(31)	7628(28)	140(32)
C(54')	-2311(46)	6184(32)	8763(29)	189(45)
C(55')	-606(44)	4900(32)	7546(29)	124(28)
C(51A)	-867(26)	6292(20)	6836(19)	74(19)
C(52A)	-866(27)	6828(20)	6056(19)	118(27)
C(53A)	-1570(27)	7672(21)	6199(19)	79(20)
C(54A)	-2007(27)	7657(20)	7067(19)	75(19)
C(55A)	-1572(27)	6804(19)	7461(19)	23(12)
C(51B)	-231(42)	5343(29)	6975(27)	118(27)
C(52B)	-228(43)	6551(29)	5222(28)	99(23)
C(53B)	-1812(44)	8449(31)	5544(28)	117(27)

C(54B)	-2794(44)	8415(30)	7496(28)	144(33)
C(55B)	-1817(43)	6496(28)	8381(28)	201(51)

Table 3. Bond lengths [Å] for 1.

Sm(1)-N(2)	2.51(4)	Sm(1)-C(16)	2.53(2)
Sm(1)-N(2')	2.54(3)	Sm(1)-C(16')	2.57(2)
Sm(1)-C(21)	2.68(2)	Sm(1)-C(22)	2.69(3)
Sm(1)-C(23)	2.73(2)	Sm(1)-C(24)	2.76(2)
Sm(1)-C(25)	2.71(3)	Sm(1)-C(31)	2.70(2)
Sm(1)-C(32)	2.74(2)	Sm(1)-C(33)	2.74(2)
Sm(1)-C(34)	2.72(3)	Sm(1)-C(35)	2.75(2)
Sm(2')-Sm(2)	0.789(14)	Sm(2')-N(1')	2.40(4)
Sm(2')-C(6')	2.55(3)	Sm(2')-C(41A)	2.84(3)
Sm(2')-C(42A)	2.79(3)	Sm(2')-C(43A)	2.76(3)
Sm(2')-C(44A)	2.80(3)	Sm(2')-C(45A)	2.85(3)
Sm(2')-C(51A)	2.74(3)	Sm(2')-C(52A)	2.86(3)
Sm(2')-C(53A)	2.77(3)	Sm(2')-C(54A)	2.59(3)
Sm(2')-C(55A)	2.57(3)	Sm(2)-N(1)	2.46(4)
Sm(2)-C(6)	2.54(3)	Sm(2)-C(41)	2.68(3)
Sm(2)-C(42)	2.69(3)	Sm(2)-C(43)	2.73(3)
Sm(2)-C(44)	2.74(3)	Sm(2)-C(45)	2.72(3)
Sm(2)-C(51)	2.84(3)	Sm(2)-C(52)	2.78(3)
Sm(2)-C(53)	2.71(3)	Sm(2)-C(54)	2.74(4)
Sm(2)-C(55)	2.82(3)	N(1)-C(4)	1.31(6)
N(1)-C(1)	1.47(6)	C(1)-C(2)	1.59(8)
C(2)-C(3)	1.62(9)	C(3)-C(4)	1.47(7)
C(4)-C(5)	1.45(6)	N(2)-C(14)	1.34(6)
N(2)-C(11)	1.50(6)	C(11)-C(12)	1.57(8)
C(12)-C(13)	1.69(8)	C(13)-C(14)	1.45(6)
C(14)-C(15)	1.50(5)	N(1')-C(4')	1.32(6)
N(1')-C(1')	1.53(6)	C(1')-C(2')	1.61(7)
C(2')-C(3')	1.66(8)	C(3')-C(4')	1.53(7)
C(4')-C(5')	1.44(5)	N(2')-C(14')	1.32(5)
N(2')-C(11')	1.48(5)	C(11')-C(12')	1.49(7)
C(12')-C(13')	1.64(8)	C(13')-C(14')	1.44(6)
C(14')-C(15')	1.45(5)	C(21)-C(25)	1.33(3)
C(21)-C(22)	1.41(3)	C(21)-C(21')	1.55(4)
C(22)-C(23)	1.37(3)	C(22)-C(22')	1.57(4)
C(23)-C(24)	1.33(4)	C(23)-C(23')	1.49(4)

C(24)-C(25)	1.51(4)	C(24)-C(24')	1.51(4)
C(25)-C(25')	1.56(4)	C(31)-C(32)	1.40(3)
C(31)-C(35)	1.42(3)	C(31)-C(31')	1.49(3)
C(32)-C(33)	1.32(3)	C(32)-C(32')	1.50(4)
C(33)-C(34)	1.42(3)	C(33)-C(33')	1.62(4)
C(34)-C(35)	1.38(3)	C(34)-C(34')	1.53(5)
C(35)-C(35')	1.51(4)		

Table 3. Bond angles [°] for 1.

N(2)-Sm(1)-C(16)	69.5(12)	N(2')-Sm(1)-C(16')	69.4(11)
N(2)-Sm(1)-C(21)	116.2(11)	C(16)-Sm(1)-C(21)	127.5(9)
N(2')-Sm(1)-C(21)	125.4(8)	C(16')-Sm(1)-C(21)	131.3(10)
N(2)-Sm(1)-C(22)	122.3(10)	C(16)-Sm(1)-C(22)	99.5(9)
N(2')-Sm(1)-C(22)	95.0(9)	C(16')-Sm(1)-C(22)	127.8(10)
C(21)-Sm(1)-C(22)	30.4(7)	N(2)-Sm(1)-C(31)	108.4(10)
C(16)-Sm(1)-C(31)	136.3(9)	N(2')-Sm(1)-C(31)	126.9(8)
C(16')-Sm(1)-C(31)	113.4(9)	C(21)-Sm(1)-C(31)	93.5(7)
C(22)-Sm(1)-C(31)	115.3(7)	N(2)-Sm(1)-C(25)	87.8(11)
C(16)-Sm(1)-C(25)	121.3(9)	N(2')-Sm(1)-C(25)	130.0(9)
C(16')-Sm(1)-C(25)	103.8(10)	C(21)-Sm(1)-C(25)	28.5(7)
C(22)-Sm(1)-C(25)	48.6(8)	C(31)-Sm(1)-C(25)	101.8(7)
N(2)-Sm(1)-C(34)	122.0(10)	C(16)-Sm(1)-C(34)	93.3(9)
N(2')-Sm(1)-C(34)	79.1(9)	C(16')-Sm(1)-C(34)	110.6(10)
C(21)-Sm(1)-C(34)	117.6(7)	C(22)-Sm(1)-C(34)	114.8(8)
C(31)-Sm(1)-C(34)	49.2(7)	C(25)-Sm(1)-C(34)	141.7(8)
N(2)-Sm(1)-C(23)	95.6(10)	C(16)-Sm(1)-C(23)	78.8(9)
N(2')-Sm(1)-C(23)	81.8(8)	C(16')-Sm(1)-C(23)	98.6(10)
C(21)-Sm(1)-C(23)	49.2(7)	C(22)-Sm(1)-C(23)	29.2(7)
C(31)-Sm(1)-C(23)	142.4(7)	C(25)-Sm(1)-C(23)	49.4(7)
C(34)-Sm(1)-C(23)	136.3(8)	N(2)-Sm(1)-C(33)	92.5(10)
C(16)-Sm(1)-C(33)	88.9(9)	N(2')-Sm(1)-C(33)	82.4(8)
C(16')-Sm(1)-C(33)	84.1(10)	C(21)-Sm(1)-C(33)	138.8(7)
C(22)-Sm(1)-C(33)	145.0(8)	C(31)-Sm(1)-C(33)	47.5(7)
C(25)-Sm(1)-C(33)	147.5(8)	C(34)-Sm(1)-C(33)	30.3(7)
C(23)-Sm(1)-C(33)	161.8(7)	N(2)-Sm(1)-C(32)	85.0(10)
C(16)-Sm(1)-C(32)	111.2(9)	N(2')-Sm(1)-C(32)	108.9(8)
C(16')-Sm(1)-C(32)	85.3(10)	C(21)-Sm(1)-C(32)	121.2(7)
C(22)-Sm(1)-C(32)	145.1(8)	C(31)-Sm(1)-C(32)	29.8(6)
C(25)-Sm(1)-C(32)	120.1(7)	C(34)-Sm(1)-C(32)	49.3(7)
C(23)-Sm(1)-C(32)	169.3(7)	C(33)-Sm(1)-C(32)	28.0(6)
N(1')-Sm(2')-C(6')	71.7(13)	N(1')-Sm(2')-C(55A)	87.7(12)
C(6')-Sm(2')-C(55A)	88.5(11)	N(1')-Sm(2')-C(54A)	117.1(13)
C(6')-Sm(2')-C(54A)	86.5(11)	C(55A)-Sm(2')-C(54A)	32.0(5)
N(1')-Sm(2')-C(51A)	88.4(12)	C(6')-Sm(2')-C(51A)	117.8(11)

C(55A)-Sm(2')-C(51A)	30.9(5)	C(54A)-Sm(2')-C(51A)	51.1(7)
N(1')-Sm(2')-C(43A)	94.4(13)	C(6')-Sm(2')-C(43A)	122.9(12)
C(55A)-Sm(2')-C(43A)	147.6(11)	C(54A)-Sm(2')-C(43A)	143.4(10)
C(51A)-Sm(2')-C(43A)	116.8(10)	N(1')-Sm(2')-C(53A)	136.3(13)
C(6')-Sm(2')-C(53A)	114.3(11)	C(55A)-Sm(2')-C(53A)	50.9(7)
C(54A)-Sm(2')-C(53A)	30.6(5)	C(51A)-Sm(2')-C(53A)	49.4(7)
C(43A)-Sm(2')-C(53A)	113.1(10)	N(1')-Sm(2')-C(42A)	80.8(12)
C(6')-Sm(2')-C(42A)	93.7(11)	C(55A)-Sm(2')-C(42A)	166.9(10)
C(54A)-Sm(2')-C(42A)	161.0(10)	C(51A)-Sm(2')-C(42A)	141.6(10)
C(43A)-Sm(2')-C(42A)	29.5(4)	C(53A)-Sm(2')-C(42A)	137.9(10)
N(1')-Sm(2')-C(44A)	123.6(13)	C(6')-Sm(2')-C(44A)	124.9(11)
C(55A)-Sm(2')-C(44A)	138.4(10)	C(54A)-Sm(2')-C(44A)	117.3(10)
C(51A)-Sm(2')-C(44A)	115.4(10)	C(43A)-Sm(2')-C(44A)	29.4(4)
C(53A)-Sm(2')-C(44A)	89.7(10)	C(42A)-Sm(2')-C(44A)	48.2(7)
N(1')-Sm(2')-C(41A)	99.8(12)	C(6')-Sm(2')-C(41A)	79.2(10)
C(55A)-Sm(2')-C(41A)	162.6(10)	C(54A)-Sm(2')-C(41A)	133.7(10)
C(51A)-Sm(2')-C(41A)	162.9(10)	C(43A)-Sm(2')-C(41A)	48.1(7)
C(53A)-Sm(2')-C(41A)	123.8(10)	C(42A)-Sm(2')-C(41A)	29.0(4)
C(44A)-Sm(2')-C(41A)	47.7(7)	N(1')-Sm(2')-C(45A)	127.1(12)
C(6')-Sm(2')-C(45A)	97.0(10)	N(1)-Sm(2')-C(45A)	102.5(12)
C(55A)-Sm(2')-C(45A)	144.8(10)	C(54A)-Sm(2')-C(45A)	113.3(10)
C(51A)-Sm(2')-C(45A)	137.7(10)	C(43A)-Sm(2')-C(45A)	48.0(7)
C(53A)-Sm(2')-C(45A)	96.0(10)	C(42A)-Sm(2')-C(45A)	47.7(7)
C(44A)-Sm(2')-C(45A)	28.9(4)	C(41A)-Sm(2')-C(45A)	28.7(4)
N(1')-Sm(2')-C(52A)	115.4(12)	C(6')-Sm(2')-C(52A)	135.1(11)
C(55A)-Sm(2')-C(52A)	49.9(7)	C(54A)-Sm(2')-C(52A)	49.7(7)
C(51A)-Sm(2')-C(52A)	29.4(4)	C(43A)-Sm(2')-C(52A)	101.4(10)
C(53A)-Sm(2')-C(52A)	29.3(4)	C(42A)-Sm(2')-C(52A)	130.9(10)
C(44A)-Sm(2')-C(52A)	89.6(10)	C(41A)-Sm(2')-C(52A)	136.0(9)
C(45A)-Sm(2')-C(52A)	108.5(9)	N(1)-Sm(2)-C(6)	69.6(13)
N(1)-Sm(2)-C(41)	82.8(13)	C(6)-Sm(2)-C(41)	92.0(10)
N(1)-Sm(2)-C(42)	94.5(12)	C(6)-Sm(2)-C(42)	122.3(10)
C(41)-Sm(2)-C(42)	30.4(4)	N(1)-Sm(2)-C(53)	86(2)
C(6)-Sm(2)-C(53)	108.2(10)	C(41)-Sm(2)-C(53)	151.4(10)
C(42)-Sm(2)-C(53)	126.0(10)	N(1)-Sm(2)-C(45)	104(2)
C(6)-Sm(2)-C(45)	79.8(10)	C(41)-Sm(2)-C(45)	30.2(4)
C(42)-Sm(2)-C(45)	49.8(6)	C(53)-Sm(2)-C(45)	169.4(10)
N(1)-Sm(2)-C(43)	124.6(13)	C(6)-Sm(2)-C(43)	128.5(11)
C(41)-Sm(2)-C(43)	49.8(6)	C(42)-Sm(2)-C(43)	30.1(4)

C(53)-Sm(2)-C(43)	121.2(10)	C(45)-Sm(2)-C(43)	49.4(6)
N(1)-Sm(2)-C(54)	89.7(14)	C(6)-Sm(2)-C(54)	81.9(10)
C(41)-Sm(2)-C(54)	171.6(10)	C(42)-Sm(2)-C(54)	155.3(10)
C(53)-Sm(2)-C(54)	30.1(5)	C(45)-Sm(2)-C(54)	151.4(10)
C(43)-Sm(2)-C(54)	138.6(10)	N(1)-Sm(2)-C(44)	132(2)
C(6)-Sm(2)-C(44)	100.7(10)	C(41)-Sm(2)-C(44)	49.6(6)
C(42)-Sm(2)-C(44)	49.5(6)	C(53)-Sm(2)-C(44)	139.5(10)
C(45)-Sm(2)-C(44)	29.9(4)	C(43)-Sm(2)-C(44)	29.8(4)
C(54)-Sm(2)-C(44)	137.1(10)	N(1)-Sm(2)-C(52)	111(2)
C(6)-Sm(2)-C(52)	130.4(10)	C(41)-Sm(2)-C(52)	137.6(9)
C(42)-Sm(2)-C(52)	107.3(9)	C(53)-Sm(2)-C(52)	29.9(5)
C(45)-Sm(2)-C(52)	139.5(10)	C(43)-Sm(2)-C(52)	93.2(10)
C(54)-Sm(2)-C(52)	49.1(7)	C(44)-Sm(2)-C(52)	110.0(10)
N(1)-Sm(2)-C(55)	118.2(13)	C(6)-Sm(2)-C(55)	86.0(10)
C(41)-Sm(2)-C(55)	156.3(10)	C(42)-Sm(2)-C(55)	143.7(10)
C(53)-Sm(2)-C(55)	48.9(7)	C(45)-Sm(2)-C(55)	126.9(10)
C(43)-Sm(2)-C(55)	115.2(10)	C(54)-Sm(2)-C(55)	29.5(5)
C(44)-Sm(2)-C(55)	107.6(10)	C(52)-Sm(2)-C(55)	48.3(7)
N(1)-Sm(2)-C(51)	134(2)	C(6)-Sm(2)-C(51)	114.0(10)
C(41)-Sm(2)-C(51)	139.9(9)	C(42)-Sm(2)-C(51)	115.9(9)
C(53)-Sm(2)-C(51)	48.6(7)	C(45)-Sm(2)-C(51)	122.1(10)
C(43)-Sm(2)-C(51)	90.5(9)	C(54)-Sm(2)-C(51)	48.4(7)
C(44)-Sm(2)-C(51)	94.0(10)	C(52)-Sm(2)-C(51)	29.1(4)
C(55)-Sm(2)-C(51)	29.0(4)	C(4)-N(1)-C(1)	112(4)
C(4)-N(1)-Sm(2)	116(3)	C(1)-N(1)-Sm(2)	131(3)
N(1)-C(1)-C(2)	106(4)	C(1)-C(2)-C(3)	102(4)
C(9')-C(3)-C(7')	146(7)	N(1)-C(4)-C(5)	120(4)
N(1)-C(4)-C(3)	116(4)	C(5)-C(4)-C(3)	123(4)
C(6)-C(5)-C(4)	123(2)	C(10)-C(5)-C(4)	117(2)
C(5)-C(6)-Sm(2)	110(2)	C(7)-C(6)-Sm(2)	130(2)
C(14)-N(2)-C(11)	109(4)	C(14)-N(2)-Sm(1)	117(3)
C(11)-N(2)-Sm(1)	134(3)	N(2)-C(11)-C(12)	109(4)
C(11)-C(12)-C(13)	100(4)	C(14)-C(13)-C(12)	104(4)
C(15')-C(14)-C(13)	125(4)	N(2)-C(14)-C(13)	117(4)
N(2)-C(14)-C(15)	118(4)	C(13)-C(14)-C(15)	125(4)
C(15')-C(15)-C(20)	106(4)	C(16)-C(15)-C(14)	122(3)
C(20)-C(15)-C(14)	118(3)	C(15)-C(16)-Sm(1)	113(2)
C(17)-C(16)-Sm(1)	127(2)	C(4')-N(1')-C(1')	113(4)
C(4')-N(1')-Sm(2')	116(3)	C(1')-N(1')-Sm(2')	131(3)

N(1')-C(1')-C(2')	104(4)	C(1')-C(2')-C(3')	104(4)
C(4')-C(3')-C(2')	101(4)	N(1')-C(4')-C(5')	121(4)
N(1')-C(4')-C(3')	116(4)	C(5')-C(4')-C(3')	123(4)
C(6')-C(5')-C(4')	123(3)	C(10')-C(5')-C(4')	116(3)
C(5')-C(6')-Sm(2')	108(2)	C(7')-C(6')-Sm(2')	132(2)
C(14')-N(2')-C(11')	110(3)	C(11')-N(2')-Sm(1)	135(2)
N(2')-C(11')-C(12')	107(4)	C(11')-C(12')-C(13')	103(4)
C(14')-C(13')-C(12')	103(4)	C(14')-C(13')-C(20)	63(3)
C(16)-C(14')-C(17)	70(3)	N(2')-C(14')-C(13')	115(4)
N(2')-C(14')-C(15')	121(4)	C(13')-C(14')-C(15')	124(4)
C(16')-C(15')-C(14')	124(3)	C(20')-C(15')-C(14')	117(3)
C(15')-C(16')-Sm(1)	111(2)	C(17')-C(16')-Sm(1)	129(2)
C(16')-C(17')-C(13)	92(2)	C(25)-C(21)-C(22)	109(2)
C(25)-C(21)-C(21')	124(2)	C(22)-C(21)-C(21')	126(2)
C(25)-C(21)-Sm(1)	77(2)	C(22)-C(21)-Sm(1)	75.0(14)
C(21')-C(21)-Sm(1)	123(2)	C(23)-C(22)-C(21)	109(2)
C(23)-C(22)-C(22')	128(3)	C(21)-C(22)-C(22')	123(2)
C(23)-C(22)-Sm(1)	77(2)	C(21)-C(22)-Sm(1)	74.6(14)
C(22')-C(22)-Sm(1)	116(2)	C(24)-C(23)-C(22)	110(2)
C(24)-C(23)-C(23')	125(3)	C(22)-C(23)-C(23')	125(3)
C(24)-C(23)-Sm(1)	77(2)	C(22)-C(23)-Sm(1)	74(2)
C(23')-C(23)-Sm(1)	123(2)	C(23)-C(24)-C(25)	106(3)
C(23)-C(24)-C(24')	130(3)	C(25)-C(24)-C(24')	124(3)
C(23)-C(24)-Sm(1)	75(2)	C(25)-C(24)-Sm(1)	72(2)
C(24')-C(24)-Sm(1)	121(2)	C(21)-C(25)-C(24)	106(2)
C(21)-C(25)-C(25')	130(3)	C(24)-C(25)-C(25')	123(3)
C(21)-C(25)-Sm(1)	75(2)	C(24)-C(25)-Sm(1)	76(2)
C(25')-C(25)-Sm(1)	120(2)	C(32)-C(31)-C(35)	108(2)
C(32)-C(31)-C(31')	125(2)	C(35)-C(31)-C(31')	127(2)
C(32)-C(31)-Sm(1)	76.4(13)	C(35)-C(31)-Sm(1)	76.5(13)
C(31')-C(31)-Sm(1)	120(2)	C(33)-C(32)-C(31)	107(2)
C(33)-C(32)-C(32')	126(2)	C(31)-C(32)-C(32')	127(2)
C(33)-C(32)-Sm(1)	76(2)	C(31)-C(32)-Sm(1)	73.8(13)
C(32')-C(32)-Sm(1)	121(2)	C(32)-C(33)-C(34)	112(2)
C(32)-C(33)-C(33')	124(2)	C(34)-C(33)-C(33')	124(2)
C(32)-C(33)-Sm(1)	76.1(14)	C(34)-C(33)-Sm(1)	74.1(14)
C(33')-C(33)-Sm(1)	116(2)	C(35)-C(34)-C(33)	106(2)
C(35)-C(34)-C(34')	130(3)	C(33)-C(34)-C(34')	124(3)
C(35)-C(34)-Sm(1)	76.7(14)	C(33)-C(34)-Sm(1)	75.6(14)

C(34')-C(34)-Sm(1)	120(2)	C(34)-C(35)-C(31)	108(2)
C(34)-C(35)-C(35')	125(2)	C(31)-C(35)-C(35')	127(2)
C(34)-C(35)-Sm(1)	74.2(14)	C(31)-C(35)-Sm(1)	73.2(13)
C(35')-C(35)-Sm(1)	121(2)	C(43)-C(42)-Sm(2)	76.4(9)
C(41)-C(42)-Sm(2)	74.6(9)	C(42')-C(42)-Sm(2)	115.2(10)
C(42)-C(43)-Sm(2)	73.5(9)	C(44)-C(43)-Sm(2)	75.8(10)
C(43')-C(43)-Sm(2)	116.8(9)	C(45)-C(44)-Sm(2)	74.0(9)
C(43)-C(44)-Sm(2)	74.4(10)	C(44')-C(44)-Sm(2)	117.5(9)
C(44)-C(45)-Sm(2)	76.1(9)	C(41)-C(45)-Sm(2)	73.6(10)
C(45')-C(45)-Sm(2)	116.4(10)	C(45A)-C(41A)-Sm(2')	75.9(11)
C(42A)-C(41A)-Sm(2')	73.3(10)	C(41B)-C(41A)-Sm(2')	116.9(10)
C(41A)-C(42A)-Sm(2')	77.7(10)	C(43A)-C(42A)-Sm(2')	74.1(10)
C(42B)-C(42A)-Sm(2')	114.4(11)	C(44A)-C(43A)-Sm(2')	76.8(11)
C(42A)-C(43A)-Sm(2')	76.4(11)	C(43B)-C(43A)-Sm(2')	113.2(10)
C(43A)-C(44A)-Sm(2')	73.8(11)	C(45A)-C(44A)-Sm(2')	77.6(10)
C(44B)-C(44A)-Sm(2')	114.9(10)	C(41A)-C(45A)-Sm(2')	75.4(10)
C(44A)-C(45A)-Sm(2')	73.5(10)	C(45B)-C(45A)-Sm(2')	117.1(10)
C(52)-C(51)-Sm(2)	72.9(10)	C(55)-C(51)-Sm(2)	74.5(11)
C(51')-C(51)-Sm(2)	118.5(10)	C(51B)-C(51)-Sm(2)	82(2)
C(55A)-C(51)-Sm(2)	38.8(11)	C(51)-C(52)-Sm(2)	78.0(10)
C(53)-C(52)-Sm(2)	72.5(11)	C(52')-C(52)-Sm(2)	115.7(11)
C(52A)-C(52)-Sm(2)	66(2)	C(55A)-C(52)-Sm(2)	39.1(12)
C(51A)-C(52)-Sm(2)	50.4(12)	C(54)-C(53)-Sm(2)	75.9(11)
C(52)-C(53)-Sm(2)	77.7(11)	C(53')-C(53)-Sm(2)	112.8(10)
C(53)-C(54)-Sm(2)	74.0(11)	C(55)-C(54)-Sm(2)	78.4(10)
C(54')-C(54)-Sm(2)	113.9(11)	C(54)-C(55)-Sm(2)	72.1(10)
C(51)-C(55)-Sm(2)	76.5(11)	C(55')-C(55)-Sm(2)	117.4(10)
C(52A)-C(51A)-Sm(2')	79.8(10)	C(55A)-C(51A)-Sm(2')	67.9(11)
C(51B)-C(51A)-Sm(2')	118.0(10)	C(52A)-C(53A)-Sm(2')	78.8(10)
C(54A)-C(53A)-Sm(2')	67.7(10)	C(53B)-C(53A)-Sm(2')	119.1(10)
C(55A)-C(54A)-Sm(2')	73.3(11)	C(53A)-C(54A)-Sm(2')	81.7(11)
C(54B)-C(54A)-Sm(2')	111.5(11)	C(51A)-C(55A)-Sm(2')	81.2(11)
C(54A)-C(55A)-Sm(2')	74.7(11)	C(55B)-C(55A)-Sm(2')	110.8(11)

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for $Sm(Cp^*)_2$(2-phenylcyclopentaimine).

	U11	U22	U33	U23	U13	U12
Sm(1)	28(1)	32(1)	29(1)	2(1)	3(1)	-13(1)
Sm(2')	113(8)	107(7)	56(4)	-14(4)	-9(5)	45(5)
Sm(2)	127(9)	131(9)	70(5)	-27(6)	-17(5)	41(5)

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [(ha^*)^2 U_{11} + \ldots + 2hka^*b^* U_{12}]$$