

Full data

Compound 1:

Table 1. Crystal data and structure refinement for [Sm(DippForm)₂(THF)₂].

Identification code	[Sm(DippForm) ₂ (THF) ₂]
Empirical formula	C ₅₈ H ₈₆ N ₄ O ₂ Sm
Formula weight	1021.66
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 12.1023(2) Å alpha = 84.4520(10) deg. b = 12.7993(3) Å beta = 86.800(2) deg. c = 19.6691(5) Å gamma = 63.9530(10) deg.
Volume	2724.19(10) Å ³
Z, Calculated density	2, 1.246 Mg/m ³
Absorption coefficient	1.121 mm ⁻¹
F(000)	1080
Crystal size	0.10 x 0.10 x 0.05 mm
Theta range for data collection	1.04 to 28.28 deg.
Limiting indices	-16<=h<=16, -14<=k<=16, -25<=l<=25
Reflections collected / unique	24871 / 13029 [R(int) = 0.0571]
Completeness to theta = 28.28	96.4 %
Absorption correction	empirical
Max. and min. transmission	0.9461 and 0.8962
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	13029 / 0 / 602
Goodness-of-fit on F ²	1.044
Final R indices [I>2sigma(I)]	R1 = 0.0542, wR2 = 0.0904
R indices (all data)	R1 = 0.0801, wR2 = 0.0989
Largest diff. peak and hole	1.843 and -1.615 e.Å ⁻³

Note: All hydrogen atoms placed in calculated positions (riding model)

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Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for $[\text{Sm}(\text{DippForm})_2(\text{THF})_2]$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U (eq)
Sm(1)	8253(1)	7953(1)	7404(1)	19(1)
O(1)	10155(3)	6944(3)	6648(2)	45(1)
O(2)	9423(2)	9202(2)	7543(1)	35(1)
N(1)	6678(3)	9822(3)	6816(2)	24(1)
N(2)	6691(3)	8152(3)	6478(1)	22(1)
N(3)	7757(3)	6522(3)	8201(1)	20(1)
N(4)	8856(3)	7329(2)	8687(1)	19(1)
C(1)	6246(3)	11048(3)	6722(2)	22(1)
C(2)	6828(3)	11545(3)	6250(2)	25(1)
C(3)	6427(4)	12753(3)	6202(2)	29(1)
C(4)	5500(4)	13447(3)	6618(2)	32(1)
C(5)	4946(4)	12960(3)	7087(2)	30(1)
C(6)	5301(3)	11762(3)	7151(2)	26(1)
C(7)	7892(4)	10795(4)	5796(2)	34(1)
C(8)	8999(4)	11060(5)	5806(3)	56(1)
C(9)	7458(5)	10916(5)	5065(2)	53(1)
C(10)	4697(4)	11246(3)	7695(2)	31(1)
C(11)	5051(4)	11362(5)	8412(2)	48(1)
C(12)	3300(4)	11791(4)	7641(2)	42(1)
C(13)	6228(3)	7604(3)	6051(2)	25(1)
C(14)	5325(4)	7262(3)	6317(2)	28(1)
C(15)	4965(4)	6608(4)	5932(2)	37(1)
C(16)	5442(4)	6334(4)	5287(2)	44(1)
C(17)	6287(4)	6702(4)	5020(2)	42(1)
C(18)	6713(4)	7330(4)	5387(2)	32(1)
C(19)	4728(4)	7628(3)	7011(2)	30(1)
C(20)	4179(4)	6846(4)	7364(2)	38(1)
C(21)	3725(4)	8893(4)	6937(2)	40(1)
C(22)	7682(4)	7680(4)	5072(2)	39(1)
C(23)	8895(5)	6584(5)	4964(3)	69(2)
C(24)	7262(6)	8426(6)	4403(3)	71(2)
C(25)	6293(3)	9293(3)	6407(2)	21(1)
C(26)	7183(3)	5750(3)	8299(2)	22(1)
C(27)	6251(3)	5934(3)	8808(2)	24(1)
C(28)	5732(3)	5150(3)	8888(2)	28(1)
C(29)	6087(4)	4233(3)	8480(2)	30(1)
C(30)	6964(3)	4086(3)	7976(2)	28(1)
C(31)	7522(3)	4844(3)	7868(2)	23(1)
C(32)	5800(3)	6982(3)	9235(2)	26(1)
C(33)	5062(4)	8121(4)	8812(2)	41(1)
C(34)	5069(4)	6893(4)	9876(2)	35(1)
C(35)	8527(3)	4646(3)	7333(2)	27(1)
C(36)	8300(4)	4252(4)	6665(2)	44(1)
C(37)	9771(4)	3772(4)	7629(2)	42(1)
C(38)	9628(3)	7237(3)	9230(2)	18(1)
C(39)	9230(3)	8153(3)	9668(2)	22(1)
C(40)	9971(3)	8055(3)	10207(2)	27(1)
C(41)	11090(4)	7096(4)	10320(2)	30(1)
C(42)	11501(3)	6223(3)	9875(2)	26(1)
C(43)	10790(3)	6278(3)	9325(2)	20(1)
C(44)	7992(3)	9202(3)	9570(2)	24(1)

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C (45)	8022 (4)	10351 (3)	9685 (2)	32 (1)
C (46)	7003 (4)	9045 (4)	10030 (2)	36 (1)
C (47)	11307 (3)	5298 (3)	8842 (2)	23 (1)
C (48)	12533 (4)	5189 (4)	8522 (2)	33 (1)
C (49)	11464 (4)	4137 (3)	9201 (2)	31 (1)
C (50)	8413 (3)	6546 (3)	8711 (2)	19 (1)
C (51)	10913 (4)	5705 (4)	6748 (3)	53 (1)
C (52)	12116 (4)	5478 (4)	6448 (2)	50 (1)
C (53)	11773 (4)	6364 (4)	5822 (2)	47 (1)
C (54)	10689 (4)	7403 (4)	6078 (2)	46 (1)
C (55)	10669 (4)	8597 (4)	7791 (2)	38 (1)
C (56)	10806 (4)	9372 (4)	8284 (2)	41 (1)
C (57)	9914 (5)	10578 (4)	7995 (2)	45 (1)
C (58)	8862 (4)	10370 (4)	7772 (2)	37 (1)

Table 3. Bond lengths [Å] and angles [deg] for [Sm(DippForm)₂(THF)₂].

Sm(1)-N(1)	2.529(3)
Sm(1)-N(3)	2.546(3)
Sm(1)-O(1)	2.560(3)
Sm(1)-O(2)	2.599(3)
Sm(1)-N(2)	2.613(3)
Sm(1)-N(4)	2.617(3)
Sm(1)-C(25)	2.951(4)
Sm(1)-C(50)	2.957(3)
O(1)-C(51)	1.442(5)
O(1)-C(54)	1.465(5)
O(2)-C(55)	1.448(5)
O(2)-C(58)	1.450(5)
N(1)-C(25)	1.323(4)
N(1)-C(1)	1.415(4)
N(2)-C(25)	1.317(4)
N(2)-C(13)	1.422(4)
N(3)-C(50)	1.324(4)
N(3)-C(26)	1.431(4)
N(4)-C(50)	1.324(4)
N(4)-C(38)	1.421(4)
C(1)-C(2)	1.402(5)
C(1)-C(6)	1.408(5)
C(2)-C(3)	1.398(5)
C(2)-C(7)	1.527(5)
C(3)-C(4)	1.371(5)
C(4)-C(5)	1.370(5)
C(5)-C(6)	1.394(5)
C(6)-C(10)	1.522(5)
C(7)-C(8)	1.521(6)
C(7)-C(9)	1.528(6)
C(10)-C(12)	1.525(6)
C(10)-C(11)	1.535(6)
C(13)-C(14)	1.404(5)
C(13)-C(18)	1.413(5)
C(14)-C(15)	1.394(5)
C(14)-C(19)	1.524(5)
C(15)-C(16)	1.375(6)
C(16)-C(17)	1.364(6)
C(17)-C(18)	1.396(6)
C(18)-C(22)	1.512(6)
C(19)-C(20)	1.524(5)
C(19)-C(21)	1.538(6)
C(22)-C(24)	1.518(7)
C(22)-C(23)	1.544(7)
C(26)-C(31)	1.402(5)
C(26)-C(27)	1.419(5)
C(27)-C(28)	1.392(5)
C(27)-C(32)	1.525(5)
C(28)-C(29)	1.381(5)
C(29)-C(30)	1.374(5)
C(30)-C(31)	1.401(5)
C(31)-C(35)	1.513(5)
C(32)-C(33)	1.523(6)
C(32)-C(34)	1.523(5)
C(35)-C(36)	1.531(5)
C(35)-C(37)	1.533(6)
C(38)-C(43)	1.409(5)

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C (38) -C (39)	1.414 (5)
C (39) -C (40)	1.388 (5)
C (39) -C (44)	1.517 (5)
C (40) -C (41)	1.382 (5)
C (41) -C (42)	1.383 (5)
C (42) -C (43)	1.396 (5)
C (43) -C (47)	1.532 (5)
C (44) -C (45)	1.527 (5)
C (44) -C (46)	1.532 (5)
C (47) -C (49)	1.518 (5)
C (47) -C (48)	1.533 (5)
C (51) -C (52)	1.455 (6)
C (52) -C (53)	1.532 (7)
C (53) -C (54)	1.505 (6)
C (55) -C (56)	1.516 (6)
C (56) -C (57)	1.519 (7)
C (57) -C (58)	1.505 (6)

N (1) -Sm (1) -N (3)	125.17 (10)
N (1) -Sm (1) -O (1)	112.24 (10)
N (3) -Sm (1) -O (1)	112.94 (9)
N (1) -Sm (1) -O (2)	83.68 (9)
N (3) -Sm (1) -O (2)	134.07 (9)
O (1) -Sm (1) -O (2)	79.12 (9)
N (1) -Sm (1) -N (2)	52.92 (9)
N (3) -Sm (1) -N (2)	94.15 (9)
O (1) -Sm (1) -N (2)	94.55 (10)
O (2) -Sm (1) -N (2)	130.20 (9)
N (1) -Sm (1) -N (4)	131.96 (9)
N (3) -Sm (1) -N (4)	52.89 (9)
O (1) -Sm (1) -N (4)	109.15 (9)
O (2) -Sm (1) -N (4)	81.18 (9)
N (2) -Sm (1) -N (4)	144.63 (9)
N (1) -Sm (1) -C (25)	26.52 (9)
N (3) -Sm (1) -C (25)	112.49 (9)
O (1) -Sm (1) -C (25)	103.31 (10)
O (2) -Sm (1) -C (25)	106.67 (9)
N (2) -Sm (1) -C (25)	26.49 (9)
N (4) -Sm (1) -C (25)	147.52 (9)
N (1) -Sm (1) -C (50)	136.51 (9)
N (3) -Sm (1) -C (50)	26.52 (9)
O (1) -Sm (1) -C (50)	111.12 (9)
O (2) -Sm (1) -C (50)	107.64 (9)
N (2) -Sm (1) -C (50)	120.36 (9)
N (4) -Sm (1) -C (50)	26.59 (9)
C (25) -Sm (1) -C (50)	134.93 (9)
C (51) -O (1) -C (54)	107.6 (3)
C (51) -O (1) -Sm (1)	121.0 (3)
C (54) -O (1) -Sm (1)	131.5 (2)
C (55) -O (2) -C (58)	109.0 (3)
C (55) -O (2) -Sm (1)	117.3 (2)
C (58) -O (2) -Sm (1)	124.6 (2)
C (25) -N (1) -C (1)	119.3 (3)
C (25) -N (1) -Sm (1)	94.8 (2)
C (1) -N (1) -Sm (1)	145.1 (2)
C (25) -N (2) -C (13)	119.8 (3)
C (25) -N (2) -Sm (1)	91.3 (2)
C (13) -N (2) -Sm (1)	148.7 (2)
C (50) -N (3) -C (26)	117.3 (3)
C (50) -N (3) -Sm (1)	94.3 (2)
C (26) -N (3) -Sm (1)	148.3 (2)

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C (50) -N (4) -C (38)	116.9 (3)
C (50) -N (4) -Sm (1)	91.2 (2)
C (38) -N (4) -Sm (1)	148.5 (2)
C (2) -C (1) -C (6)	119.8 (3)
C (2) -C (1) -N (1)	120.6 (3)
C (6) -C (1) -N (1)	119.3 (3)
C (3) -C (2) -C (1)	119.0 (3)
C (3) -C (2) -C (7)	119.6 (3)
C (1) -C (2) -C (7)	121.4 (3)
C (4) -C (3) -C (2)	120.9 (4)
C (5) -C (4) -C (3)	120.1 (4)
C (4) -C (5) -C (6)	121.2 (3)
C (5) -C (6) -C (1)	118.8 (3)
C (5) -C (6) -C (10)	119.8 (3)
C (1) -C (6) -C (10)	121.3 (3)
C (8) -C (7) -C (2)	113.1 (4)
C (8) -C (7) -C (9)	110.7 (4)
C (2) -C (7) -C (9)	110.3 (3)
C (6) -C (10) -C (12)	113.1 (3)
C (6) -C (10) -C (11)	110.5 (3)
C (12) -C (10) -C (11)	109.8 (3)
C (14) -C (13) -C (18)	119.7 (3)
C (14) -C (13) -N (2)	118.7 (3)
C (18) -C (13) -N (2)	121.5 (3)
C (15) -C (14) -C (13)	119.2 (4)
C (15) -C (14) -C (19)	120.6 (4)
C (13) -C (14) -C (19)	120.2 (3)
C (16) -C (15) -C (14)	121.2 (4)
C (17) -C (16) -C (15)	119.4 (4)
C (16) -C (17) -C (18)	122.2 (4)
C (17) -C (18) -C (13)	118.3 (4)
C (17) -C (18) -C (22)	119.6 (4)
C (13) -C (18) -C (22)	122.1 (4)
C (20) -C (19) -C (14)	114.4 (3)
C (20) -C (19) -C (21)	109.3 (3)
C (14) -C (19) -C (21)	109.7 (3)
C (18) -C (22) -C (24)	111.9 (4)
C (18) -C (22) -C (23)	110.1 (4)
C (24) -C (22) -C (23)	110.5 (4)
N (2) -C (25) -N (1)	120.6 (3)
N (2) -C (25) -Sm (1)	62.25 (19)
N (1) -C (25) -Sm (1)	58.65 (18)
C (31) -C (26) -C (27)	120.9 (3)
C (31) -C (26) -N (3)	118.9 (3)
C (27) -C (26) -N (3)	120.2 (3)
C (28) -C (27) -C (26)	117.9 (3)
C (28) -C (27) -C (32)	121.0 (3)
C (26) -C (27) -C (32)	121.0 (3)
C (29) -C (28) -C (27)	121.6 (3)
C (30) -C (29) -C (28)	119.9 (4)
C (29) -C (30) -C (31)	121.4 (4)
C (30) -C (31) -C (26)	118.2 (3)
C (30) -C (31) -C (35)	121.0 (3)
C (26) -C (31) -C (35)	120.6 (3)
C (33) -C (32) -C (34)	109.6 (3)
C (33) -C (32) -C (27)	111.8 (3)
C (34) -C (32) -C (27)	114.7 (3)
C (31) -C (35) -C (36)	114.2 (3)
C (31) -C (35) -C (37)	109.8 (3)
C (36) -C (35) -C (37)	110.5 (3)
C (43) -C (38) -C (39)	119.8 (3)

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C (43) -C (38) -N (4)	121.5 (3)
C (39) -C (38) -N (4)	118.7 (3)
C (40) -C (39) -C (38)	118.8 (3)
C (40) -C (39) -C (44)	120.4 (3)
C (38) -C (39) -C (44)	120.7 (3)
C (41) -C (40) -C (39)	121.7 (3)
C (40) -C (41) -C (42)	119.4 (4)
C (41) -C (42) -C (43)	121.1 (4)
C (42) -C (43) -C (38)	119.0 (3)
C (42) -C (43) -C (47)	118.7 (3)
C (38) -C (43) -C (47)	122.3 (3)
C (39) -C (44) -C (45)	113.2 (3)
C (39) -C (44) -C (46)	111.1 (3)
C (45) -C (44) -C (46)	110.0 (3)
C (49) -C (47) -C (43)	111.8 (3)
C (49) -C (47) -C (48)	110.2 (3)
C (43) -C (47) -C (48)	110.8 (3)
N (3) -C (50) -N (4)	120.6 (3)
N (3) -C (50) -Sm (1)	59.14 (18)
N (4) -C (50) -Sm (1)	62.25 (18)
O (1) -C (51) -C (52)	107.2 (4)
C (51) -C (52) -C (53)	101.7 (4)
C (54) -C (53) -C (52)	102.8 (3)
O (1) -C (54) -C (53)	106.0 (4)
O (2) -C (55) -C (56)	106.3 (3)
C (55) -C (56) -C (57)	101.8 (3)
C (58) -C (57) -C (56)	102.4 (4)
O (2) -C (58) -C (57)	105.4 (4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{Å}^2 \times 10^3$) for
 [Sm(DippForm)₂(THF)₂].

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^2 U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
Sm(1)	23(1)	14(1)	21(1)	1(1)	-3(1)	-8(1)
O(1)	44(2)	28(2)	57(2)	-1(2)	7(2)	-12(1)
O(2)	38(2)	24(2)	48(2)	1(1)	-11(1)	-19(1)
N(1)	30(2)	13(2)	25(2)	-1(1)	-3(1)	-3(1)
N(2)	29(2)	15(2)	23(2)	-1(1)	-7(1)	-9(1)
N(3)	24(2)	18(2)	20(1)	-2(1)	0(1)	-12(1)
N(4)	21(2)	16(2)	20(1)	-1(1)	-2(1)	-9(1)
C(1)	26(2)	16(2)	23(2)	0(2)	-4(2)	-7(2)
C(2)	25(2)	24(2)	24(2)	1(2)	-2(2)	-7(2)
C(3)	36(2)	22(2)	28(2)	3(2)	-1(2)	-13(2)
C(4)	45(2)	16(2)	35(2)	-4(2)	-2(2)	-13(2)
C(5)	33(2)	18(2)	33(2)	-7(2)	4(2)	-4(2)
C(6)	29(2)	22(2)	26(2)	-4(2)	-1(2)	-10(2)
C(7)	33(2)	25(2)	34(2)	-2(2)	7(2)	-3(2)
C(8)	34(3)	77(4)	52(3)	-21(3)	13(2)	-18(3)
C(9)	51(3)	63(3)	40(3)	-22(2)	13(2)	-19(3)
C(10)	34(2)	21(2)	38(2)	-6(2)	11(2)	-12(2)
C(11)	46(3)	64(3)	36(2)	11(2)	-1(2)	-29(3)
C(12)	38(2)	52(3)	38(2)	-9(2)	7(2)	-22(2)
C(13)	28(2)	16(2)	30(2)	0(2)	-11(2)	-6(2)
C(14)	31(2)	17(2)	35(2)	5(2)	-14(2)	-9(2)
C(15)	39(2)	28(2)	48(3)	1(2)	-16(2)	-17(2)
C(16)	56(3)	34(3)	50(3)	-13(2)	-17(2)	-25(2)
C(17)	49(3)	36(3)	37(2)	-14(2)	-10(2)	-14(2)
C(18)	36(2)	26(2)	31(2)	-7(2)	-7(2)	-8(2)
C(19)	35(2)	25(2)	33(2)	6(2)	-10(2)	-17(2)
C(20)	41(2)	35(2)	43(2)	12(2)	-11(2)	-23(2)
C(21)	40(2)	32(2)	43(2)	3(2)	3(2)	-15(2)
C(22)	46(3)	42(3)	29(2)	-14(2)	4(2)	-19(2)
C(23)	46(3)	63(4)	88(4)	-29(3)	9(3)	-13(3)
C(24)	86(4)	87(5)	53(3)	20(3)	-16(3)	-53(4)
C(25)	21(2)	15(2)	23(2)	1(2)	-2(2)	-4(2)
C(26)	24(2)	17(2)	24(2)	4(2)	-7(2)	-9(2)
C(27)	26(2)	23(2)	24(2)	5(2)	-6(2)	-13(2)
C(28)	28(2)	29(2)	30(2)	6(2)	-4(2)	-16(2)
C(29)	32(2)	27(2)	38(2)	5(2)	-7(2)	-21(2)
C(30)	33(2)	19(2)	36(2)	1(2)	-7(2)	-15(2)
C(31)	26(2)	16(2)	27(2)	4(2)	-6(2)	-10(2)
C(32)	28(2)	25(2)	26(2)	-1(2)	1(2)	-13(2)
C(33)	55(3)	25(2)	37(2)	-4(2)	1(2)	-11(2)
C(34)	34(2)	32(2)	35(2)	-3(2)	6(2)	-10(2)
C(35)	31(2)	18(2)	35(2)	-4(2)	0(2)	-13(2)
C(36)	46(3)	50(3)	43(3)	-18(2)	7(2)	-25(2)
C(37)	30(2)	37(3)	57(3)	-4(2)	0(2)	-13(2)
C(38)	23(2)	19(2)	16(2)	0(1)	2(1)	-13(2)
C(39)	24(2)	19(2)	22(2)	-1(2)	2(2)	-11(2)
C(40)	34(2)	26(2)	24(2)	-7(2)	-2(2)	-14(2)
C(41)	32(2)	35(2)	27(2)	-3(2)	-7(2)	-16(2)
C(42)	23(2)	25(2)	30(2)	2(2)	-5(2)	-9(2)
C(43)	20(2)	20(2)	22(2)	0(2)	2(2)	-10(2)

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C (44)	27 (2)	17 (2)	26 (2)	-5 (2)	-1 (2)	-8 (2)
C (45)	32 (2)	21 (2)	42 (2)	-8 (2)	-1 (2)	-9 (2)
C (46)	30 (2)	28 (2)	49 (3)	-7 (2)	5 (2)	-12 (2)
C (47)	21 (2)	21 (2)	23 (2)	-2 (2)	3 (2)	-6 (2)
C (48)	31 (2)	28 (2)	37 (2)	-5 (2)	9 (2)	-10 (2)
C (49)	38 (2)	22 (2)	33 (2)	-4 (2)	3 (2)	-13 (2)
C (50)	22 (2)	14 (2)	18 (2)	0 (1)	0 (1)	-6 (2)
C (51)	51 (3)	37 (3)	64 (3)	-6 (2)	8 (3)	-12 (2)
C (52)	47 (3)	41 (3)	49 (3)	-7 (2)	5 (2)	-8 (2)
C (53)	40 (3)	60 (3)	43 (3)	-5 (2)	6 (2)	-24 (2)
C (54)	52 (3)	41 (3)	48 (3)	-1 (2)	4 (2)	-23 (2)
C (55)	30 (2)	40 (3)	47 (3)	2 (2)	-4 (2)	-17 (2)
C (56)	38 (2)	60 (3)	35 (2)	-2 (2)	-3 (2)	-31 (2)
C (57)	67 (3)	45 (3)	38 (2)	0 (2)	-7 (2)	-39 (3)
C (58)	52 (3)	28 (2)	34 (2)	0 (2)	-7 (2)	-18 (2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for $[\text{Sm}(\text{DippForm})_2(\text{THF})_2]$.

	x	y	z	U (eq)
H(3)	6804	13099	5877	35
H(4)	5240	14266	6580	38
H(5)	4308	13449	7375	36
H(7)	8163	9962	5975	41
H(8A)	8774	11859	5610	84
H(8B)	9674	10512	5537	84
H(8C)	9261	10979	6279	84
H(9A)	6772	10704	5067	79
H(9B)	8137	10398	4785	79
H(9C)	7185	11725	4875	79
H(10)	5019	10395	7633	38
H(11A)	5950	10998	8447	72
H(11B)	4709	10973	8754	72
H(11C)	4723	12190	8492	72
H(12A)	2959	12626	7703	63
H(12B)	2964	11412	7995	63
H(12C)	3079	11685	7189	63
H(15)	4380	6348	6118	44
H(16)	5184	5892	5029	53
H(17)	6597	6525	4570	50
H(19)	5375	7605	7315	36
H(20A)	3486	6912	7099	57
H(20B)	3889	7089	7824	57
H(20C)	4807	6035	7397	57
H(21A)	3064	8937	6652	59
H(21B)	4080	9401	6721	59
H(21C)	3390	9146	7389	59
H(22)	7839	8150	5398	46
H(23A)	9176	6134	5403	103
H(23B)	9522	6821	4768	103
H(23C)	8759	6103	4651	103
H(24A)	7039	8005	4087	106
H(24B)	7930	8596	4202	106
H(24C)	6545	9159	4489	106
H(25)	5724	9740	6058	25
H(28)	5120	5248	9233	34
H(29)	5725	3705	8548	36
H(30)	7195	3459	7694	33
H(32)	6549	7029	9390	31
H(33A)	5548	8192	8410	62
H(33B)	4862	8779	9090	62
H(33C)	4299	8126	8665	62
H(34A)	4275	6946	9746	53
H(34B)	4931	7532	10157	53
H(34C)	5530	6145	10137	53
H(35)	8571	5405	7221	33
H(36A)	8354	3464	6746	66
H(36B)	8923	4250	6323	66
H(36C)	7480	4791	6497	66
H(37A)	9941	4075	8030	63
H(37B)	10421	3659	7284	63

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H (37C)	9748	3025	7764	63
H (40)	9703	8662	10507	32
H (41)	11572	7036	10699	36
H (42)	12281	5575	9944	32
H (44)	7749	9254	9085	28
H (45A)	8112	10385	10174	48
H (45B)	7255	11004	9525	48
H (45C)	8719	10402	9431	48
H (46A)	6977	8314	9945	54
H (46B)	6200	9700	9929	54
H (46C)	7199	9020	10509	54
H (47)	10708	5502	8465	28
H (48A)	13142	4970	8881	50
H (48B)	12418	5939	8285	50
H (48C)	12824	4589	8195	50
H (49A)	12039	3923	9578	47
H (49B)	11787	3535	8876	47
H (49C)	10665	4206	9382	47
H (50)	8567	5997	9097	22
H (51A)	10546	5276	6523	64
H (51B)	10988	5448	7241	64
H (52A)	12555	4668	6314	60
H (52B)	12631	5622	6766	60
H (53A)	12460	6562	5677	57
H (53B)	11544	6063	5435	57
H (54A)	10957	7967	6233	56
H (54B)	10079	7800	5712	56
H (55A)	11268	8470	7407	46
H (55B)	10812	7831	8027	46
H (56A)	11658	9291	8280	50
H (56B)	10569	9196	8756	50
H (57A)	9645	11146	8348	53
H (57B)	10285	10864	7603	53
H (58A)	8283	10424	8158	45
H (58B)	8410	10950	7396	45

Full data

Compound 2:

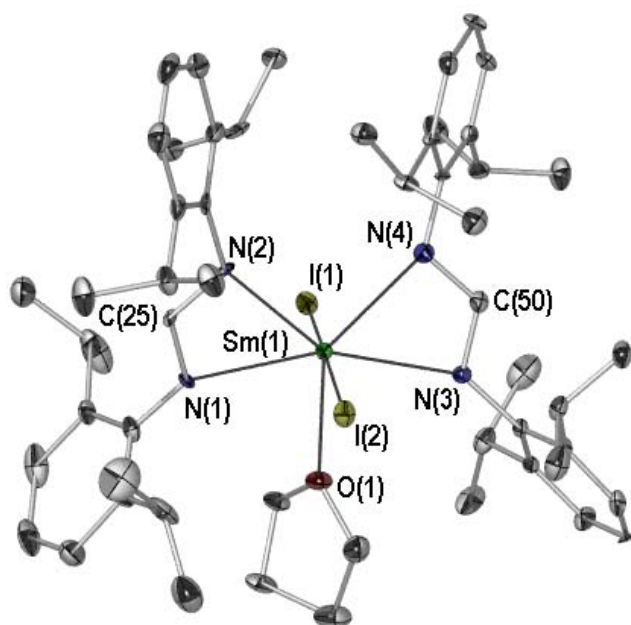


Figure. Molecular structure of the anion of compound **2**, POV-Ray illustration with 40% thermal ellipsoids. All hydrogen atoms omitted for clarity.

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Table 1. Crystal data and structure refinement for
[Na(THF)5][Sm(I)2(DippForm)2(THF)].

Identification code	Na(THF)5][Sm(I)2(DippForm)2(THF)]
Empirical formula	C148 H236 I4 N8 Na2 O12 Sm2
Formula weight	3173.73
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 26.7632(3) Å alpha = 90 deg. b = 14.3697(2) Å beta = 91.7860(10) deg. c = 41.5794(5) Å gamma = 90 deg.
Volume	15982.8(3) Å ³
Z, Calculated density	4, 1.319 Mg/m ³
Absorption coefficient	1.560 mm ⁻¹
F(000)	6536
Crystal size	0.30 x 0.30 x 0.10 mm
Theta range for data collection	1.22 to 28.30 deg.
Limiting indices	-35<=h<=32, -18<=k<=18, -52<=l<=55
Reflections collected / unique	61917 / 30037 [R(int) = 0.0572]
Completeness to theta = 26.00	79.8 %
Absorption correction	empirical
Max. and min. transmission	0.8596 and 0.6518
Refinement method	Full-matrix-block least-squares on F ²
Data / restraints / parameters	30037 / 0 / 1618
Goodness-of-fit on F ²	1.031
Final R indices [I>2sigma(I)]	R1 = 0.0603, wR2 = 0.1742
R indices (all data)	R1 = 0.1324, wR2 = 0.2321
Largest diff. peak and hole	2.369 and -1.989 e.Å ⁻³
Note:	All hydrogen atoms placed in calculated positions (riding model).

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for [Na(THF)₅][Sm(I)₂(DippForm)₂(THF)]. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U (eq)
Sm(1)	3668 (1)	9658 (1)	1425 (1)	17
Sm(2)	8674 (1)	10160 (1)	1416 (1)	16
I (1)	2739 (1)	8516 (1)	1187 (1)	26
I (2)	4569 (1)	10744 (1)	1726 (1)	27
I (3)	7729 (1)	11364 (1)	1264 (1)	23
I (4)	9611 (1)	9054 (1)	1643 (1)	31
Na (1)	4019 (1)	9179 (2)	3764 (1)	27
Na (2)	9073 (1)	10719 (3)	3811 (1)	44
O (1)	3298 (2)	9504 (4)	1964 (2)	29
O (2)	3267 (2)	10000 (4)	3785 (2)	38
O (3)	3747 (2)	8183 (4)	4159 (2)	43
O (4)	4455 (2)	10045 (4)	4156 (2)	37
O (5)	4496 (2)	9946 (4)	3382 (2)	37
O (6)	3867 (2)	8031 (4)	3374 (2)	36
O (7)	8356 (2)	10064 (4)	1974 (1)	28
O (8)	8321 (3)	9946 (5)	3779 (2)	54
O (9)	8868 (3)	11831 (5)	3438 (2)	60
O (10)	8871 (3)	11709 (6)	4221 (2)	78
O (11)	9551 (3)	9796 (4)	4161 (2)	55
O (12)	9542 (3)	10102 (6)	3381 (2)	72
N (1)	3138 (2)	11095 (4)	1458 (2)	17
N (2)	3599 (2)	10899 (4)	1019 (2)	17
N (3)	4107 (2)	8197 (4)	1616 (2)	17
N (4)	4159 (2)	8594 (5)	1081 (2)	22
N (5)	8151 (2)	8699 (4)	1394 (2)	18
N (6)	8570 (2)	9118 (4)	947 (2)	16
N (7)	9105 (2)	11565 (4)	1658 (2)	17
N (8)	9143 (2)	11333 (4)	1107 (2)	18
C (1)	2770 (3)	11550 (5)	1626 (2)	24
C (2)	2896 (3)	11994 (6)	1911 (2)	25
C (3)	2530 (3)	12392 (6)	2109 (3)	40
C (4)	2033 (4)	12338 (7)	2009 (3)	51
C (5)	1897 (3)	11881 (6)	1702 (3)	49
C (6)	2261 (3)	11485 (6)	1515 (2)	25
C (7)	3434 (3)	12157 (7)	2009 (2)	40
C (8)	3542 (4)	12131 (7)	2379 (3)	58
C (9)	3625 (4)	13024 (8)	1861 (3)	65
C (10)	2087 (3)	11020 (6)	1213 (2)	29
C (11)	1658 (3)	10345 (7)	1248 (3)	55
C (12)	1927 (4)	11736 (7)	953 (3)	43
C (13)	3765 (3)	11290 (5)	727 (2)	21
C (14)	3646 (3)	10814 (6)	430 (2)	28
C (15)	3812 (3)	11164 (6)	141 (2)	36
C (16)	4094 (3)	12010 (7)	143 (3)	46
C (17)	4199 (3)	12465 (6)	430 (3)	36
C (18)	4048 (3)	12114 (6)	732 (2)	30
C (19)	3310 (3)	9991 (6)	422 (2)	31
C (20)	3374 (4)	9352 (6)	140 (2)	38
C (21)	2757 (3)	10294 (7)	452 (2)	39

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C (22)	4187 (3)	12639 (5)	1040 (2)	30
C (23)	4757 (3)	12756 (6)	1084 (3)	43
C (24)	3928 (4)	13604 (6)	1052 (3)	49
C (25)	3269 (3)	11388 (5)	1182 (2)	17
C (26)	4271 (3)	7651 (5)	1882 (2)	20
C (27)	3919 (3)	7071 (5)	2034 (2)	20
C (28)	4066 (3)	6560 (6)	2301 (2)	30
C (29)	4550 (3)	6637 (6)	2422 (2)	28
C (30)	4885 (3)	7183 (5)	2273 (2)	24
C (31)	4759 (3)	7698 (5)	2005 (2)	20
C (32)	3385 (3)	6974 (6)	1892 (2)	28
C (33)	2981 (3)	6768 (7)	2131 (2)	42
C (34)	3386 (4)	6218 (7)	1624 (3)	52
C (35)	5165 (3)	8286 (6)	1843 (2)	25
C (36)	5470 (3)	8852 (6)	2086 (3)	41
C (37)	5512 (3)	7675 (6)	1666 (2)	35
C (38)	4303 (3)	8345 (5)	767 (2)	16
C (39)	4652 (3)	8918 (6)	612 (2)	22
C (40)	4789 (3)	8681 (6)	303 (2)	28
C (41)	4596 (3)	7909 (6)	139 (2)	28
C (42)	4258 (3)	7349 (6)	300 (2)	27
C (43)	4101 (3)	7552 (6)	602 (2)	23
C (44)	4897 (3)	9744 (6)	790 (2)	23
C (45)	5062 (3)	10510 (6)	560 (2)	31
C (46)	5329 (3)	9399 (7)	1004 (2)	36
C (47)	3701 (3)	6923 (5)	748 (2)	23
C (48)	3227 (3)	6831 (6)	537 (2)	36
C (49)	3912 (3)	5969 (6)	817 (2)	38
C (50)	4276 (3)	8012 (6)	1324 (2)	20
C (51)	3569 (3)	9452 (7)	2283 (2)	38
C (52)	3173 (4)	9427 (8)	2547 (3)	49
C (53)	2707 (3)	9795 (7)	2354 (2)	39
C (54)	2756 (3)	9441 (6)	2015 (2)	29
C (55)	3215 (4)	10642 (6)	4043 (3)	54
C (56)	2644 (4)	10648 (6)	4119 (3)	51
C (57)	2405 (4)	10462 (7)	3780 (3)	42
C (58)	2774 (4)	9818 (7)	3628 (3)	46
C (59)	3951 (4)	7300 (7)	4200 (3)	64
C (60)	3561 (4)	6681 (6)	4363 (3)	45
C (61)	3235 (4)	7374 (6)	4534 (3)	41
C (62)	3303 (4)	8239 (7)	4346 (3)	59
C (63)	4560 (5)	9876 (7)	4489 (3)	69
C (64)	4558 (5)	10725 (8)	4669 (3)	75
C (65)	4458 (4)	11477 (8)	4417 (3)	55
C (66)	4544 (4)	11015 (6)	4096 (3)	43
C (67)	5031 (4)	10037 (7)	3333 (3)	44
C (68)	5127 (4)	9438 (7)	3050 (3)	51
C (69)	4635 (4)	9581 (7)	2827 (3)	52
C (70)	4261 (4)	9956 (7)	3064 (3)	44
C (71)	4213 (3)	7384 (6)	3254 (2)	32
C (72)	3917 (3)	6488 (6)	3209 (2)	35
C (73)	3393 (3)	6852 (6)	3112 (2)	36
C (74)	3353 (3)	7735 (6)	3303 (2)	37
C (75)	7802 (3)	8120 (5)	1546 (2)	18
C (76)	7973 (3)	7493 (6)	1784 (2)	28
C (77)	7617 (4)	6950 (6)	1940 (2)	40
C (78)	7113 (3)	6999 (6)	1862 (3)	41
C (79)	6949 (3)	7599 (6)	1627 (2)	37
C (80)	7284 (3)	8186 (6)	1468 (2)	30
C (81)	8538 (3)	7389 (6)	1853 (2)	35
C (82)	8696 (4)	7220 (8)	2204 (3)	61

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C (83)	8737 (3)	6609 (7)	1626 (3)	49
C (84)	7075 (3)	8863 (6)	1218 (3)	33
C (85)	6669 (3)	9457 (6)	1373 (3)	50
C (86)	6854 (3)	8382 (6)	913 (2)	39
C (87)	8711 (3)	8899 (6)	628 (2)	23
C (88)	8547 (3)	9509 (6)	371 (2)	23
C (89)	8691 (3)	9290 (6)	65 (2)	30
C (90)	8977 (3)	8513 (6)	-7 (2)	36
C (91)	9136 (3)	7915 (6)	243 (2)	32
C (92)	9010 (3)	8095 (6)	558 (2)	24
C (93)	8199 (3)	10309 (6)	448 (2)	25
C (94)	8197 (4)	11089 (6)	192 (2)	38
C (95)	7658 (3)	9918 (6)	480 (2)	31
C (96)	9188 (3)	7428 (5)	815 (2)	27
C (97)	9750 (3)	7358 (6)	827 (3)	45
C (98)	8975 (4)	6481 (6)	765 (3)	46
C (99)	8265 (3)	8547 (5)	1094 (2)	17
C (100)	9280 (3)	12058 (5)	1932 (2)	19
C (101)	8934 (3)	12545 (5)	2119 (2)	21
C (102)	9107 (3)	13026 (6)	2392 (2)	30
C (103)	9605 (3)	13035 (6)	2482 (2)	31
C (104)	9942 (3)	12571 (6)	2299 (2)	24
C (105)	9785 (3)	12052 (5)	2029 (2)	22
C (106)	8389 (3)	12616 (6)	2003 (2)	25
C (107)	8019 (3)	12548 (6)	2275 (2)	32
C (108)	8292 (4)	13469 (7)	1811 (2)	45
C (109)	10190 (3)	11542 (6)	1832 (2)	22
C (110)	10526 (3)	10931 (6)	2036 (2)	36
C (111)	10496 (3)	12264 (6)	1650 (2)	31
C (112)	9256 (3)	11719 (6)	800 (2)	20
C (113)	9589 (3)	11223 (5)	606 (2)	18
C (114)	9690 (3)	11573 (6)	308 (2)	28
C (115)	9492 (3)	12377 (6)	199 (2)	33
C (116)	9180 (3)	12876 (6)	396 (2)	25
C (117)	9052 (3)	12559 (5)	695 (2)	18
C (118)	9859 (3)	10364 (5)	727 (2)	23
C (119)	10029 (3)	9729 (6)	459 (2)	31
C (120)	10305 (3)	10645 (6)	955 (2)	36
C (121)	8690 (3)	13132 (5)	894 (2)	19
C (122)	8210 (3)	13362 (6)	716 (2)	35
C (123)	8940 (3)	14017 (6)	1019 (2)	38
C (124)	9257 (3)	11832 (5)	1370 (2)	18
C (125)	8650 (4)	9977 (7)	2268 (2)	43
C (126)	8274 (4)	9794 (7)	2520 (3)	53
C (127)	7806 (4)	9468 (7)	2342 (2)	48
C (128)	7833 (3)	10025 (6)	2043 (2)	32
C (129)	8205 (5)	9337 (10)	3565 (4)	128
C (130)	7616 (5)	9280 (9)	3564 (4)	122
C (131)	7475 (5)	9511 (9)	3848 (4)	84
C (132)	7868 (5)	10104 (11)	3943 (3)	92
C (133)	8401 (4)	12072 (8)	3276 (4)	84
C (134)	8412 (3)	13051 (7)	3200 (3)	42
C (135)	8950 (3)	13381 (6)	3276 (3)	40
C (136)	9231 (4)	12459 (7)	3324 (3)	62
C (137)	8666 (5)	11433 (9)	4504 (3)	83
C (138)	8254 (5)	12202 (8)	4567 (3)	80
C (139)	8524 (5)	13031 (10)	4439 (3)	85
C (140)	8782 (6)	12677 (9)	4158 (4)	95
C (141)	9741 (4)	9977 (8)	4468 (3)	56
C (142)	9488 (5)	9224 (9)	4671 (3)	77

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C (143)	9286 (6)	8490 (9)	4408 (4)	104
C (144)	9491 (5)	8812 (7)	4125 (3)	71
C (145)	9353 (5)	9978 (9)	3037 (3)	79
C (146)	9787 (6)	10164 (10)	2851 (4)	120
C (147)	10228 (6)	10002 (17)	3037 (4)	197
C (148)	10082 (5)	9961 (11)	3338 (5)	147

Table 3. Bond lengths [Å] and angles [deg] for
[Na(THF)₅][Sm(I)₂(DippForm)₂(THF)].

Sm(1)-N(2)	2.460(6)
Sm(1)-O(1)	2.486(6)
Sm(1)-N(4)	2.497(7)
Sm(1)-N(1)	2.511(6)
Sm(1)-N(3)	2.522(6)
Sm(1)-C(25)	2.877(7)
Sm(1)-C(50)	2.909(8)
Sm(1)-I(2)	3.1031(7)
Sm(1)-I(1)	3.1143(7)
Sm(2)-N(6)	2.469(6)
Sm(2)-N(8)	2.485(7)
Sm(2)-O(7)	2.498(6)
Sm(2)-N(7)	2.519(6)
Sm(2)-N(5)	2.525(6)
Sm(2)-C(124)	2.874(8)
Sm(2)-C(99)	2.878(8)
Sm(2)-I(4)	3.0904(7)
Sm(2)-I(3)	3.1129(6)
Na(1)-O(3)	2.311(7)
Na(1)-O(4)	2.331(7)
Na(1)-O(2)	2.337(7)
Na(1)-O(6)	2.340(7)
Na(1)-O(5)	2.346(7)
Na(2)-O(9)	2.283(8)
Na(2)-O(10)	2.297(10)
Na(2)-O(8)	2.299(8)
Na(2)-O(11)	2.322(8)
Na(2)-O(12)	2.387(9)
O(1)-C(54)	1.475(9)
O(1)-C(51)	1.494(10)
O(2)-C(55)	1.424(12)
O(2)-C(58)	1.478(11)
O(3)-C(59)	1.390(11)
O(3)-C(62)	1.445(12)
O(4)-C(63)	1.427(12)
O(4)-C(66)	1.437(11)
O(5)-C(70)	1.445(11)
O(5)-C(67)	1.457(11)
O(6)-C(71)	1.414(10)
O(6)-C(74)	1.463(10)
O(7)-C(125)	1.438(10)
O(7)-C(128)	1.439(10)
O(8)-C(129)	1.278(15)
O(8)-C(132)	1.428(14)
O(9)-C(136)	1.416(12)
O(9)-C(133)	1.443(12)
O(10)-C(137)	1.373(15)
O(10)-C(140)	1.434(14)
O(11)-C(141)	1.386(12)
O(11)-C(144)	1.431(12)
O(12)-C(148)	1.478(16)
O(12)-C(145)	1.513(14)
N(1)-C(25)	1.280(10)
N(1)-C(1)	1.389(10)
N(2)-C(25)	1.331(10)
N(2)-C(13)	1.422(10)

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N(3)-C(50)	1.334(10)
N(3)-C(26)	1.414(10)
N(4)-C(50)	1.344(10)
N(4)-C(38)	1.417(10)
N(5)-C(99)	1.313(10)
N(5)-C(75)	1.414(10)
N(6)-C(99)	1.321(10)
N(6)-C(87)	1.425(10)
N(7)-C(124)	1.334(10)
N(7)-C(100)	1.407(10)
N(8)-C(124)	1.337(10)
N(8)-C(112)	1.431(10)
C(1)-C(2)	1.378(12)
C(1)-C(6)	1.428(11)
C(2)-C(3)	1.420(12)
C(2)-C(7)	1.503(11)
C(3)-C(4)	1.383(13)
C(4)-C(5)	1.470(14)
C(5)-C(6)	1.387(13)
C(6)-C(10)	1.484(12)
C(7)-C(9)	1.489(14)
C(7)-C(8)	1.558(14)
C(10)-C(11)	1.513(12)
C(10)-C(12)	1.544(13)
C(13)-C(18)	1.405(12)
C(13)-C(14)	1.440(12)
C(14)-C(15)	1.385(13)
C(14)-C(19)	1.486(12)
C(15)-C(16)	1.432(13)
C(16)-C(17)	1.382(13)
C(17)-C(18)	1.422(13)
C(18)-C(22)	1.525(12)
C(19)-C(20)	1.506(12)
C(19)-C(21)	1.550(12)
C(22)-C(23)	1.541(11)
C(22)-C(24)	1.551(11)
C(26)-C(31)	1.392(11)
C(26)-C(27)	1.420(11)
C(27)-C(28)	1.380(11)
C(27)-C(32)	1.537(11)
C(28)-C(29)	1.379(11)
C(29)-C(30)	1.355(12)
C(30)-C(31)	1.368(11)
C(31)-C(35)	1.548(12)
C(32)-C(33)	1.519(12)
C(32)-C(34)	1.556(13)
C(35)-C(37)	1.490(12)
C(35)-C(36)	1.515(11)
C(38)-C(39)	1.416(11)
C(38)-C(43)	1.428(11)
C(39)-C(40)	1.388(12)
C(39)-C(44)	1.534(11)
C(40)-C(41)	1.393(12)
C(41)-C(42)	1.396(12)
C(42)-C(43)	1.367(12)
C(43)-C(47)	1.540(11)
C(44)-C(46)	1.523(11)
C(44)-C(45)	1.531(11)
C(47)-C(49)	1.506(11)
C(47)-C(48)	1.525(11)
C(51)-C(52)	1.551(14)

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C (52) -C (53)	1.555 (13)
C (53) -C (54)	1.510 (12)
C (55) -C (56)	1.570 (13)
C (56) -C (57)	1.551 (14)
C (57) -C (58)	1.504 (14)
C (59) -C (60)	1.543 (14)
C (60) -C (61)	1.517 (13)
C (61) -C (62)	1.482 (13)
C (63) -C (64)	1.431 (15)
C (64) -C (65)	1.524 (16)
C (65) -C (66)	1.511 (14)
C (67) -C (68)	1.486 (14)
C (68) -C (69)	1.601 (14)
C (69) -C (70)	1.524 (15)
C (71) -C (72)	1.522 (12)
C (72) -C (73)	1.539 (12)
C (73) -C (74)	1.501 (12)
C (75) -C (76)	1.404 (11)
C (75) -C (80)	1.417 (11)
C (76) -C (77)	1.406 (12)
C (76) -C (81)	1.535 (12)
C (77) -C (78)	1.382 (12)
C (78) -C (79)	1.363 (13)
C (79) -C (80)	1.410 (12)
C (80) -C (84)	1.520 (12)
C (81) -C (82)	1.528 (13)
C (81) -C (83)	1.568 (14)
C (84) -C (85)	1.538 (12)
C (84) -C (86)	1.544 (13)
C (87) -C (88)	1.440 (11)
C (87) -C (92)	1.441 (11)
C (88) -C (89)	1.377 (12)
C (88) -C (93)	1.521 (12)
C (89) -C (90)	1.392 (12)
C (90) -C (91)	1.405 (13)
C (91) -C (92)	1.388 (12)
C (92) -C (96)	1.502 (11)
C (93) -C (94)	1.545 (12)
C (93) -C (95)	1.562 (11)
C (96) -C (98)	1.486 (11)
C (96) -C (97)	1.508 (11)
C (100) -C (105)	1.398 (11)
C (100) -C (101)	1.414 (11)
C (101) -C (102)	1.395 (11)
C (101) -C (106)	1.525 (10)
C (102) -C (103)	1.373 (11)
C (103) -C (104)	1.373 (12)
C (104) -C (105)	1.401 (11)
C (105) -C (109)	1.563 (12)
C (106) -C (108)	1.480 (12)
C (106) -C (107)	1.530 (12)
C (109) -C (110)	1.504 (11)
C (109) -C (111)	1.534 (12)
C (112) -C (117)	1.389 (11)
C (112) -C (113)	1.413 (11)
C (113) -C (114)	1.372 (12)
C (113) -C (118)	1.508 (11)
C (114) -C (115)	1.345 (12)
C (115) -C (116)	1.387 (12)
C (116) -C (117)	1.378 (11)
C (117) -C (121)	1.532 (11)

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C (118) -C (119)	1.519 (12)
C (118) -C (120)	1.557 (11)
C (121) -C (122)	1.502 (11)
C (121) -C (123)	1.521 (11)
C (125) -C (126)	1.500 (14)
C (126) -C (127)	1.509 (14)
C (127) -C (128)	1.482 (12)
C (129) -C (130)	1.577 (17)
C (130) -C (131)	1.30 (2)
C (131) -C (132)	1.402 (15)
C (133) -C (134)	1.442 (14)
C (134) -C (135)	1.539 (12)
C (135) -C (136)	1.534 (13)
C (137) -C (138)	1.588 (16)
C (138) -C (139)	1.500 (17)
C (139) -C (140)	1.465 (17)
C (141) -C (142)	1.542 (15)
C (142) -C (143)	1.603 (18)
C (143) -C (144)	1.394 (17)
C (145) -C (146)	1.441 (18)
C (146) -C (147)	1.41 (2)
C (147) -C (148)	1.33 (2)

N (2) -Sm (1) -O (1)	131.3 (2)
N (2) -Sm (1) -N (4)	94.5 (2)
O (1) -Sm (1) -N (4)	133.9 (2)
N (2) -Sm (1) -N (1)	53.9 (2)
O (1) -Sm (1) -N (1)	77.5 (2)
N (4) -Sm (1) -N (1)	147.4 (2)
N (2) -Sm (1) -N (3)	147.5 (2)
O (1) -Sm (1) -N (3)	80.6 (2)
N (4) -Sm (1) -N (3)	54.7 (2)
N (1) -Sm (1) -N (3)	157.9 (2)
N (2) -Sm (1) -C (25)	27.5 (2)
O (1) -Sm (1) -C (25)	103.9 (2)
N (4) -Sm (1) -C (25)	121.5 (2)
N (1) -Sm (1) -C (25)	26.4 (2)
N (3) -Sm (1) -C (25)	173.8 (2)
N (2) -Sm (1) -C (50)	121.4 (2)
O (1) -Sm (1) -C (50)	107.3 (2)
N (4) -Sm (1) -C (50)	27.4 (2)
N (1) -Sm (1) -C (50)	174.7 (2)
N (3) -Sm (1) -C (50)	27.3 (2)
C (25) -Sm (1) -C (50)	148.8 (2)
N (2) -Sm (1) -I (2)	87.34 (15)
O (1) -Sm (1) -I (2)	90.43 (13)
N (4) -Sm (1) -I (2)	97.07 (15)
N (1) -Sm (1) -I (2)	89.90 (15)
N (3) -Sm (1) -I (2)	86.77 (14)
C (25) -Sm (1) -I (2)	89.01 (15)
C (50) -Sm (1) -I (2)	92.08 (15)
N (2) -Sm (1) -I (1)	96.94 (15)
O (1) -Sm (1) -I (1)	84.49 (13)
N (4) -Sm (1) -I (1)	85.62 (15)
N (1) -Sm (1) -I (1)	90.20 (14)
N (3) -Sm (1) -I (1)	91.18 (14)
C (25) -Sm (1) -I (1)	93.40 (15)
C (50) -Sm (1) -I (1)	88.27 (15)
I (2) -Sm (1) -I (1)	174.78 (2)
N (6) -Sm (2) -N (8)	92.8 (2)
N (6) -Sm (2) -O (7)	131.8 (2)

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N (8) -Sm (2) -O (7)	135.3 (2)
N (6) -Sm (2) -N (7)	147.3 (2)
N (8) -Sm (2) -N (7)	55.3 (2)
O (7) -Sm (2) -N (7)	80.7 (2)
N (6) -Sm (2) -N (5)	54.4 (2)
N (8) -Sm (2) -N (5)	146.5 (2)
O (7) -Sm (2) -N (5)	77.5 (2)
N (7) -Sm (2) -N (5)	158.1 (2)
N (6) -Sm (2) -C (124)	120.2 (2)
N (8) -Sm (2) -C (124)	27.7 (2)
O (7) -Sm (2) -C (124)	108.0 (2)
N (7) -Sm (2) -C (124)	27.7 (2)
N (5) -Sm (2) -C (124)	174.1 (2)
N (6) -Sm (2) -C (99)	27.2 (2)
N (8) -Sm (2) -C (99)	119.8 (2)
O (7) -Sm (2) -C (99)	104.6 (2)
N (7) -Sm (2) -C (99)	174.1 (2)
N (5) -Sm (2) -C (99)	27.1 (2)
C (124) -Sm (2) -C (99)	147.4 (2)
N (6) -Sm (2) -I (4)	89.95 (14)
N (8) -Sm (2) -I (4)	95.11 (14)
O (7) -Sm (2) -I (4)	89.16 (13)
N (7) -Sm (2) -I (4)	86.20 (14)
N (5) -Sm (2) -I (4)	91.56 (14)
C (124) -Sm (2) -I (4)	90.78 (14)
C (99) -Sm (2) -I (4)	91.22 (14)
N (6) -Sm (2) -I (3)	96.08 (14)
N (8) -Sm (2) -I (3)	86.45 (14)
O (7) -Sm (2) -I (3)	85.45 (13)
N (7) -Sm (2) -I (3)	89.69 (14)
N (5) -Sm (2) -I (3)	90.47 (14)
C (124) -Sm (2) -I (3)	87.78 (14)
C (99) -Sm (2) -I (3)	93.31 (14)
I (4) -Sm (2) -I (3)	173.69 (2)
O (3) -Na (1) -O (4)	89.8 (3)
O (3) -Na (1) -O (2)	89.8 (3)
O (4) -Na (1) -O (2)	96.7 (3)
O (3) -Na (1) -O (6)	90.2 (3)
O (4) -Na (1) -O (6)	158.7 (3)
O (2) -Na (1) -O (6)	104.5 (3)
O (3) -Na (1) -O (5)	164.2 (3)
O (4) -Na (1) -O (5)	87.2 (3)
O (2) -Na (1) -O (5)	106.0 (3)
O (6) -Na (1) -O (5)	87.0 (3)
O (9) -Na (2) -O (10)	90.8 (3)
O (9) -Na (2) -O (8)	96.2 (3)
O (10) -Na (2) -O (8)	96.7 (3)
O (9) -Na (2) -O (11)	160.3 (3)
O (10) -Na (2) -O (11)	91.5 (3)
O (8) -Na (2) -O (11)	102.9 (3)
O (9) -Na (2) -O (12)	82.6 (3)
O (10) -Na (2) -O (12)	158.0 (4)
O (8) -Na (2) -O (12)	104.8 (3)
O (11) -Na (2) -O (12)	88.0 (3)
C (54) -O (1) -C (51)	108.8 (6)
C (54) -O (1) -Sm (1)	123.7 (5)
C (51) -O (1) -Sm (1)	127.5 (5)
C (55) -O (2) -C (58)	109.9 (7)
C (55) -O (2) -Na (1)	117.4 (5)
C (58) -O (2) -Na (1)	130.7 (6)

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C (59) -O (3) -C (62)	108.1 (7)
C (59) -O (3) -Na (1)	121.5 (6)
C (62) -O (3) -Na (1)	129.1 (6)
C (63) -O (4) -C (66)	107.6 (7)
C (63) -O (4) -Na (1)	131.8 (6)
C (66) -O (4) -Na (1)	118.7 (6)
C (70) -O (5) -C (67)	105.9 (7)
C (70) -O (5) -Na (1)	113.2 (5)
C (67) -O (5) -Na (1)	133.9 (6)
C (71) -O (6) -C (74)	111.1 (6)
C (71) -O (6) -Na (1)	127.4 (5)
C (74) -O (6) -Na (1)	119.2 (5)
C (125) -O (7) -C (128)	109.6 (7)
C (125) -O (7) -Sm (2)	126.9 (6)
C (128) -O (7) -Sm (2)	123.5 (5)
C (129) -O (8) -C (132)	104.4 (10)
C (129) -O (8) -Na (2)	124.4 (9)
C (132) -O (8) -Na (2)	130.5 (7)
C (136) -O (9) -C (133)	106.6 (9)
C (136) -O (9) -Na (2)	121.3 (6)
C (133) -O (9) -Na (2)	132.1 (7)
C (137) -O (10) -C (140)	111.6 (10)
C (137) -O (10) -Na (2)	124.5 (8)
C (140) -O (10) -Na (2)	120.5 (8)
C (141) -O (11) -C (144)	108.6 (8)
C (141) -O (11) -Na (2)	130.5 (6)
C (144) -O (11) -Na (2)	116.2 (7)
C (148) -O (12) -C (145)	99.7 (11)
C (148) -O (12) -Na (2)	132.9 (10)
C (145) -O (12) -Na (2)	125.8 (7)
C (25) -N (1) -C (1)	120.9 (7)
C (25) -N (1) -Sm (1)	93.0 (5)
C (1) -N (1) -Sm (1)	145.5 (6)
C (25) -N (2) -C (13)	117.2 (6)
C (25) -N (2) -Sm (1)	93.9 (5)
C (13) -N (2) -Sm (1)	148.7 (5)
C (50) -N (3) -C (26)	119.6 (7)
C (50) -N (3) -Sm (1)	92.7 (5)
C (26) -N (3) -Sm (1)	146.9 (5)
C (50) -N (4) -C (38)	118.2 (7)
C (50) -N (4) -Sm (1)	93.6 (5)
C (38) -N (4) -Sm (1)	147.8 (5)
C (99) -N (5) -C (75)	120.3 (7)
C (99) -N (5) -Sm (2)	91.6 (5)
C (75) -N (5) -Sm (2)	147.8 (5)
C (99) -N (6) -C (87)	118.6 (7)
C (99) -N (6) -Sm (2)	93.9 (5)
C (87) -N (6) -Sm (2)	147.4 (5)
C (124) -N (7) -C (100)	118.5 (7)
C (124) -N (7) -Sm (2)	91.2 (5)
C (100) -N (7) -Sm (2)	149.7 (5)
C (124) -N (8) -C (112)	118.2 (7)
C (124) -N (8) -Sm (2)	92.6 (5)
C (112) -N (8) -Sm (2)	148.1 (5)
C (2) -C (1) -N (1)	119.5 (7)
C (2) -C (1) -C (6)	121.0 (8)
N (1) -C (1) -C (6)	119.3 (8)
C (1) -C (2) -C (3)	122.0 (8)
C (1) -C (2) -C (7)	120.9 (8)
C (3) -C (2) -C (7)	116.8 (8)

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C (4) -C (3) -C (2)	118.5 (10)
C (3) -C (4) -C (5)	119.7 (9)
C (6) -C (5) -C (4)	120.8 (9)
C (5) -C (6) -C (1)	118.0 (9)
C (5) -C (6) -C (10)	116.9 (8)
C (1) -C (6) -C (10)	125.1 (8)
C (9) -C (7) -C (2)	110.9 (9)
C (9) -C (7) -C (8)	112.0 (8)
C (2) -C (7) -C (8)	114.4 (8)
C (6) -C (10) -C (11)	115.2 (8)
C (6) -C (10) -C (12)	111.4 (7)
C (11) -C (10) -C (12)	107.5 (8)
C (18) -C (13) -N (2)	120.3 (8)
C (18) -C (13) -C (14)	121.1 (8)
N (2) -C (13) -C (14)	118.6 (7)
C (15) -C (14) -C (13)	120.1 (9)
C (15) -C (14) -C (19)	118.8 (9)
C (13) -C (14) -C (19)	120.9 (8)
C (14) -C (15) -C (16)	119.2 (10)
C (17) -C (16) -C (15)	119.9 (10)
C (16) -C (17) -C (18)	122.6 (9)
C (13) -C (18) -C (17)	117.0 (9)
C (13) -C (18) -C (22)	123.1 (8)
C (17) -C (18) -C (22)	119.9 (8)
C (14) -C (19) -C (20)	114.7 (8)
C (14) -C (19) -C (21)	110.6 (7)
C (20) -C (19) -C (21)	111.5 (7)
C (18) -C (22) -C (23)	111.6 (8)
C (18) -C (22) -C (24)	111.8 (8)
C (23) -C (22) -C (24)	109.9 (7)
N (1) -C (25) -N (2)	119.2 (7)
N (1) -C (25) -Sm (1)	60.6 (4)
N (2) -C (25) -Sm (1)	58.6 (4)
C (31) -C (26) -N (3)	121.8 (7)
C (31) -C (26) -C (27)	119.5 (8)
N (3) -C (26) -C (27)	118.6 (7)
C (28) -C (27) -C (26)	119.6 (8)
C (28) -C (27) -C (32)	120.0 (8)
C (26) -C (27) -C (32)	120.3 (8)
C (29) -C (28) -C (27)	119.5 (8)
C (30) -C (29) -C (28)	120.4 (8)
C (29) -C (30) -C (31)	122.4 (8)
C (30) -C (31) -C (26)	118.5 (8)
C (30) -C (31) -C (35)	119.5 (7)
C (26) -C (31) -C (35)	121.9 (8)
C (33) -C (32) -C (27)	116.0 (8)
C (33) -C (32) -C (34)	110.5 (7)
C (27) -C (32) -C (34)	108.4 (7)
C (37) -C (35) -C (36)	108.3 (8)
C (37) -C (35) -C (31)	110.6 (7)
C (36) -C (35) -C (31)	111.9 (8)
C (39) -C (38) -N (4)	118.3 (7)
C (39) -C (38) -C (43)	119.3 (8)
N (4) -C (38) -C (43)	122.3 (8)
C (40) -C (39) -C (38)	118.4 (8)
C (40) -C (39) -C (44)	120.9 (8)
C (38) -C (39) -C (44)	120.6 (8)
C (39) -C (40) -C (41)	122.9 (8)
C (40) -C (41) -C (42)	117.5 (9)
C (43) -C (42) -C (41)	122.5 (8)
C (42) -C (43) -C (38)	119.3 (8)

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C (42) -C (43) -C (47)	118.3 (8)
C (38) -C (43) -C (47)	122.4 (8)
C (46) -C (44) -C (45)	111.7 (7)
C (46) -C (44) -C (39)	109.6 (7)
C (45) -C (44) -C (39)	112.6 (7)
C (49) -C (47) -C (48)	109.3 (7)
C (49) -C (47) -C (43)	110.3 (7)
C (48) -C (47) -C (43)	113.5 (8)
N (3) -C (50) -N (4)	119.0 (7)
N (3) -C (50) -Sm (1)	60.0 (4)
N (4) -C (50) -Sm (1)	59.0 (4)
O (1) -C (51) -C (52)	107.9 (7)
C (51) -C (52) -C (53)	100.4 (8)
C (54) -C (53) -C (52)	106.0 (8)
O (1) -C (54) -C (53)	103.2 (7)
O (2) -C (55) -C (56)	105.8 (7)
C (57) -C (56) -C (55)	101.1 (9)
C (58) -C (57) -C (56)	103.3 (8)
O (2) -C (58) -C (57)	107.1 (8)
O (3) -C (59) -C (60)	108.2 (8)
C (61) -C (60) -C (59)	103.6 (8)
C (62) -C (61) -C (60)	102.8 (8)
O (3) -C (62) -C (61)	110.8 (8)
O (4) -C (63) -C (64)	111.1 (10)
C (63) -C (64) -C (65)	104.3 (10)
C (66) -C (65) -C (64)	105.5 (9)
O (4) -C (66) -C (65)	104.1 (9)
O (5) -C (67) -C (68)	104.8 (8)
C (67) -C (68) -C (69)	102.8 (8)
C (70) -C (69) -C (68)	102.6 (9)
O (5) -C (70) -C (69)	108.1 (8)
O (6) -C (71) -C (72)	104.8 (7)
C (71) -C (72) -C (73)	102.2 (7)
C (74) -C (73) -C (72)	103.2 (7)
O (6) -C (74) -C (73)	105.7 (7)
C (76) -C (75) -N (5)	119.1 (7)
C (76) -C (75) -C (80)	120.0 (8)
N (5) -C (75) -C (80)	120.9 (7)
C (75) -C (76) -C (77)	118.0 (8)
C (75) -C (76) -C (81)	119.5 (8)
C (77) -C (76) -C (81)	122.4 (9)
C (78) -C (77) -C (76)	122.3 (9)
C (79) -C (78) -C (77)	119.4 (9)
C (78) -C (79) -C (80)	121.3 (9)
C (79) -C (80) -C (75)	119.0 (9)
C (79) -C (80) -C (84)	118.6 (8)
C (75) -C (80) -C (84)	122.4 (8)
C (82) -C (81) -C (76)	115.9 (9)
C (82) -C (81) -C (83)	111.8 (8)
C (76) -C (81) -C (83)	107.9 (7)
C (80) -C (84) -C (85)	108.5 (9)
C (80) -C (84) -C (86)	113.5 (7)
C (85) -C (84) -C (86)	109.6 (7)
N (6) -C (87) -C (88)	118.3 (7)
N (6) -C (87) -C (92)	122.0 (8)
C (88) -C (87) -C (92)	119.8 (8)
C (89) -C (88) -C (87)	117.4 (8)
C (89) -C (88) -C (93)	124.0 (8)
C (87) -C (88) -C (93)	118.5 (8)
C (88) -C (89) -C (90)	123.6 (9)
C (89) -C (90) -C (91)	119.2 (9)

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C (92) -C (91) -C (90)	120.5 (9)
C (91) -C (92) -C (87)	119.5 (8)
C (91) -C (92) -C (96)	118.2 (8)
C (87) -C (92) -C (96)	122.3 (8)
C (88) -C (93) -C (94)	113.0 (8)
C (88) -C (93) -C (95)	108.8 (7)
C (94) -C (93) -C (95)	109.6 (7)
C (98) -C (96) -C (92)	111.9 (8)
C (98) -C (96) -C (97)	108.8 (7)
C (92) -C (96) -C (97)	111.1 (7)
N (5) -C (99) -N (6)	120.1 (7)
N (5) -C (99) -Sm (2)	61.3 (4)
N (6) -C (99) -Sm (2)	58.8 (4)
C (105) -C (100) -N (7)	121.7 (7)
C (105) -C (100) -C (101)	119.2 (8)
N (7) -C (100) -C (101)	119.1 (7)
C (102) -C (101) -C (100)	119.1 (8)
C (102) -C (101) -C (106)	120.9 (8)
C (100) -C (101) -C (106)	119.7 (8)
C (103) -C (102) -C (101)	121.5 (9)
C (104) -C (103) -C (102)	119.6 (9)
C (103) -C (104) -C (105)	121.1 (8)
C (100) -C (105) -C (104)	119.5 (8)
C (100) -C (105) -C (109)	122.0 (8)
C (104) -C (105) -C (109)	118.3 (7)
C (108) -C (106) -C (101)	112.0 (7)
C (108) -C (106) -C (107)	110.2 (7)
C (101) -C (106) -C (107)	113.4 (8)
C (110) -C (109) -C (111)	110.8 (7)
C (110) -C (109) -C (105)	112.9 (8)
C (111) -C (109) -C (105)	109.4 (7)
C (117) -C (112) -C (113)	120.5 (8)
C (117) -C (112) -N (8)	121.6 (8)
C (113) -C (112) -N (8)	117.9 (7)
C (114) -C (113) -C (112)	118.5 (8)
C (114) -C (113) -C (118)	119.6 (8)
C (112) -C (113) -C (118)	121.7 (8)
C (115) -C (114) -C (113)	122.1 (9)
C (114) -C (115) -C (116)	118.9 (9)
C (117) -C (116) -C (115)	122.3 (8)
C (116) -C (117) -C (112)	117.6 (8)
C (116) -C (117) -C (121)	119.3 (7)
C (112) -C (117) -C (121)	123.1 (8)
C (113) -C (118) -C (119)	113.6 (8)
C (113) -C (118) -C (120)	110.0 (7)
C (119) -C (118) -C (120)	111.1 (7)
C (122) -C (121) -C (123)	110.2 (7)
C (122) -C (121) -C (117)	113.3 (7)
C (123) -C (121) -C (117)	110.8 (7)
N (7) -C (124) -N (8)	120.9 (7)
N (7) -C (124) -Sm (2)	61.2 (4)
N (8) -C (124) -Sm (2)	59.7 (4)
O (7) -C (125) -C (126)	104.4 (8)
C (125) -C (126) -C (127)	106.0 (9)
C (128) -C (127) -C (126)	100.5 (8)
O (7) -C (128) -C (127)	105.3 (8)
O (8) -C (129) -C (130)	105.1 (11)
C (131) -C (130) -C (129)	107.6 (12)
C (130) -C (131) -C (132)	100.1 (13)
C (131) -C (132) -O (8)	114.2 (12)
C (134) -C (133) -O (9)	108.2 (9)

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C(133)-C(134)-C(135)	106.2(8)
C(136)-C(135)-C(134)	102.3(8)
O(9)-C(136)-C(135)	104.8(8)
O(10)-C(137)-C(138)	103.8(10)
C(139)-C(138)-C(137)	98.6(10)
C(140)-C(139)-C(138)	104.6(12)
O(10)-C(140)-C(139)	105.8(12)
O(11)-C(141)-C(142)	102.6(10)
C(141)-C(142)-C(143)	103.4(11)
C(144)-C(143)-C(142)	103.1(10)
C(143)-C(144)-O(11)	106.5(11)
C(146)-C(145)-O(12)	103.7(12)
C(147)-C(146)-C(145)	110.4(15)
C(148)-C(147)-C(146)	105.1(14)
C(147)-C(148)-O(12)	115.2(14)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{Å}^2 \times 10^3$) for
 $[\text{Na}(\text{THF})_5][\text{Sm}(\text{I})_2(\text{DippForm})_2(\text{THF})]$.

The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^2 U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Sm(1)	16	18	16	1	2	1
Sm(2)	15	17	16	0	1	0
I(1)	20	29	29	-3	0	1
I(2)	20	25	37	-1	-4	-1
I(3)	18	25	26	-1	1	2
I(4)	22	26	45	4	-8	3
Na(1)	26	28	28	-3	5	-7
Na(2)	41	42	50	11	6	-1
O(1)	26	42	18	-1	5	-2
O(2)	34	30	49	-10	0	-2
O(3)	43	39	48	17	7	-2
O(4)	44	34	33	-6	-3	-4
O(5)	34	52	24	1	6	-5
O(6)	33	30	47	-14	13	-6
O(7)	33	36	14	5	5	-1
O(8)	46	49	68	-33	15	-23
O(9)	35	47	99	29	-5	-10
O(10)	78	71	87	-6	26	22
O(11)	95	30	40	10	-8	-5
O(12)	48	121	46	31	7	17
N(1)	20	17	16	-1	6	2
N(2)	22	18	12	9	5	-2
N(3)	18	18	16	3	8	-1
N(4)	20	25	21	0	3	0
N(5)	17	15	22	-1	5	2
N(6)	19	20	11	0	0	-2
N(7)	15	18	19	-4	-1	-1
N(8)	11	18	23	0	4	3
C(1)	21	16	35	-5	4	2
C(2)	28	23	24	-3	13	-1
C(3)	37	44	39	-7	5	7
C(4)	46	42	68	8	33	15
C(5)	24	23	100	2	6	0
C(6)	18	24	32	1	5	4
C(7)	25	54	42	-29	6	2
C(8)	55	53	64	-26	-15	3
C(9)	37	84	73	11	6	-22
C(10)	29	21	37	-3	8	-1
C(11)	20	50	94	-22	3	-8
C(12)	42	42	46	-2	-5	8
C(13)	22	16	24	8	4	10
C(14)	25	34	23	8	4	10
C(15)	36	44	28	5	1	12
C(16)	34	61	43	34	15	18
C(17)	32	31	45	18	7	4
C(18)	23	33	33	13	12	15
C(19)	40	36	17	10	-4	5
C(20)	58	31	23	-10	-4	11

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C (21)	38	45	32	-2	-11	5
C (22)	29	15	46	-2	3	-3
C (23)	28	38	63	-4	13	0
C (24)	43	19	85	4	7	3
C (25)	20	15	17	11	5	3
C (26)	23	17	20	5	5	6
C (27)	21	19	22	6	9	7
C (28)	30	30	30	12	12	4
C (29)	38	39	5	8	0	17
C (30)	17	20	35	4	3	3
C (31)	17	18	25	4	-3	6
C (32)	30	23	32	9	-4	-6
C (33)	29	55	43	26	11	-2
C (34)	50	42	63	10	-16	-22
C (35)	26	19	28	6	-5	2
C (36)	31	33	57	5	-14	-6
C (37)	33	33	38	17	17	10
C (38)	18	22	8	2	2	9
C (39)	23	28	15	5	6	11
C (40)	29	25	30	9	12	6
C (41)	33	35	17	-7	8	7
C (42)	36	25	21	-8	1	7
C (43)	20	26	23	4	3	6
C (44)	22	27	20	-2	11	-5
C (45)	36	29	28	0	5	-3
C (46)	29	45	34	12	4	3
C (47)	35	20	16	2	5	1
C (48)	26	40	43	-14	1	3
C (49)	41	20	54	12	10	2
C (50)	15	21	26	5	4	0
C (51)	40	39	34	-4	-10	4
C (52)	50	65	31	1	6	-17
C (53)	40	47	30	-8	17	-6
C (54)	27	40	20	-1	9	-1
C (55)	41	24	94	5	-6	-3
C (56)	48	16	89	-2	18	-1
C (57)	32	37	56	18	-1	2
C (58)	48	41	50	-3	-2	-1
C (59)	67	60	66	24	29	31
C (60)	41	31	64	5	4	-2
C (61)	38	35	51	12	13	2
C (62)	64	46	72	19	38	17
C (63)	101	49	54	-14	-38	9
C (64)	131	64	29	-15	-9	-1
C (65)	51	63	51	-32	-2	-16
C (66)	28	42	58	-4	0	-20
C (67)	32	53	48	13	1	-9
C (68)	49	40	65	9	32	0
C (69)	74	47	34	4	8	-5
C (70)	45	38	47	6	-3	-11
C (71)	32	32	33	-8	12	-7
C (72)	47	35	23	-6	14	-9
C (73)	31	42	36	-6	8	0
C (74)	40	40	33	-14	9	0
C (75)	30	7	18	-2	-1	-2
C (76)	34	26	26	-1	8	-5
C (77)	63	33	25	16	15	-8
C (78)	32	41	53	7	29	-4
C (79)	30	36	46	14	17	0

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C (80)	26	19	47	-1	7	0
C (81)	42	37	26	20	-13	-7
C (82)	87	66	28	22	-9	-2
C (83)	29	58	60	11	-3	-6
C (84)	13	13	72	-4	5	3
C (85)	31	20	99	-2	10	9
C (86)	35	24	58	9	-7	-3
C (87)	21	33	15	-7	6	-10
C (88)	24	24	22	1	2	-11
C (89)	34	45	12	5	7	-5
C (90)	38	51	18	-13	19	-6
C (91)	32	34	29	-15	6	-12
C (92)	19	27	28	-4	7	-6
C (93)	34	29	11	4	-3	2
C (94)	45	48	21	-2	-1	-2
C (95)	32	42	20	-3	1	-1
C (96)	30	21	31	9	12	1
C (97)	41	41	53	5	7	13
C (98)	72	17	49	-5	7	-3
C (99)	13	13	26	-4	-5	-2
C (100)	20	23	13	-1	0	-2
C (101)	25	15	23	-6	0	-1
C (102)	28	32	29	-4	2	5
C (103)	36	34	24	-17	3	-6
C (104)	24	35	14	-9	-1	-11
C (105)	29	22	16	3	1	-1
C (106)	14	32	28	-7	3	5
C (107)	27	37	33	-16	12	2
C (108)	45	60	31	1	2	14
C (109)	14	32	20	-11	-5	1
C (110)	27	32	48	-5	-15	8
C (111)	10	40	42	-10	2	-4
C (112)	22	26	13	1	5	-12
C (113)	15	24	17	1	8	-3
C (114)	34	29	20	-1	7	0
C (115)	37	46	16	-6	10	-4
C (116)	25	20	29	10	2	0
C (117)	24	12	17	6	1	-3
C (118)	18	23	29	-5	10	-5
C (119)	37	26	31	0	16	6
C (120)	37	32	41	-6	-2	0
C (121)	25	12	22	9	6	2
C (122)	37	34	34	1	7	11
C (123)	45	26	45	-10	19	-3
C (124)	13	11	28	-3	2	-2
C (125)	61	54	13	7	-14	-7
C (126)	97	44	19	16	7	4
C (127)	78	42	26	3	23	-11
C (128)	37	37	24	-2	16	-11
C (129)	93	97	197	-66	34	-10
C (130)	66	60	236	-65	-64	22
C (131)	74	48	132	-21	19	-16
C (132)	64	160	53	-31	14	-28
C (133)	48	55	146	8	-37	-3
C (134)	34	59	34	4	5	6
C (135)	34	29	58	9	14	10
C (136)	44	65	78	23	3	6
C (137)	120	80	47	-33	-27	17
C (138)	65	88	87	-24	27	-18

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C (139)	63	130	61	-28	-5	15
C (140)	118	70	99	-22	50	19
C (141)	66	55	46	17	10	3
C (142)	80	83	69	27	29	25
C (143)	123	67	123	-14	41	-51
C (144)	103	41	69	8	10	-10
C (145)	118	77	41	0	-15	31
C (146)	175	75	117	21	117	4
C (147)	82	402	110	-110	66	-130
C (148)	53	86	298	98	-50	-18

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for [Na(THF) 5] [Sm(I) 2 (DippForm) 2 (THF)] .

	x	y	z	U (eq)
H(3)	2624	12689	2306	48
H(4)	1781	12595	2138	61
H(5)	1557	11857	1631	58
H(7)	3628	11633	1916	48
H(8A)	3390	12676	2480	87
H(8B)	3904	12139	2423	87
H(8C)	3399	11562	2469	87
H(9A)	3536	13028	1630	97
H(9B)	3990	13049	1890	97
H(9C)	3477	13566	1964	97
H(10)	2376	10661	1129	35
H(11A)	1733	9921	1428	82
H(11B)	1611	9986	1049	82
H(11C)	1352	10692	1290	82
H(12A)	1629	12068	1020	65
H(12B)	1853	11413	749	65
H(12C)	2199	12182	923	65
H(15)	3739	10845	-55	43
H(16)	4208	12260	-53	55
H(17)	4380	13033	426	43
H(19)	3396	9619	619	37
H(20A)	3291	9687	-60	57
H(20B)	3152	8814	159	57
H(20C)	3722	9139	136	57
H(21A)	2721	10650	651	58
H(21B)	2543	9742	456	58
H(21C)	2658	10683	267	58
H(22)	4068	12264	1225	36
H(23A)	4913	12144	1114	64
H(23B)	4832	13143	1274	64
H(23C)	4889	13056	893	64
H(24A)	4036	13930	1249	73
H(24B)	3565	13521	1049	73
H(24C)	4021	13972	864	73
H(25)	3132	11947	1095	21
H(28)	3836	6159	2401	36
H(29)	4650	6304	2610	33
H(30)	5218	7209	2357	29
H(32)	3296	7578	1785	34
H(33A)	3017	6126	2207	63
H(33B)	2652	6849	2026	63
H(33C)	3016	7196	2313	63
H(34A)	3463	5611	1720	78
H(34B)	3638	6373	1467	78
H(34C)	3055	6193	1515	78
H(35)	4998	8722	1686	30
H(36A)	5682	8434	2217	61
H(36B)	5245	9195	2224	61
H(36C)	5682	9292	1972	61
H(37A)	5737	8060	1540	52

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H (37B)	5319	7264	1521	52
H (37C)	5710	7299	1820	52
H (40)	5025	9062	199	33
H (41)	4690	7769	-74	34
H (42)	4131	6806	195	33
H (44)	4641	10019	932	27
H (45A)	5141	11076	683	47
H (45B)	4792	10640	402	47
H (45C)	5360	10304	449	47
H (46A)	5599	9176	870	54
H (46B)	5214	8890	1140	54
H (46C)	5453	9910	1141	54
H (47)	3606	7203	958	28
H (48A)	3106	7452	477	55
H (48B)	2971	6505	657	55
H (48C)	3301	6478	343	55
H (49A)	4057	5719	621	57
H (49B)	3645	5556	886	57
H (49C)	4172	6012	987	57
H (50)	4475	7477	1289	25
H (51A)	3789	10001	2314	45
H (51B)	3779	8885	2295	45
H (52A)	3265	9840	2730	58
H (52B)	3119	8787	2628	58
H (53A)	2396	9558	2448	46
H (53B)	2699	10484	2357	46
H (54A)	2637	8791	1994	34
H (54B)	2565	9836	1859	34
H (55A)	3326	11271	3979	64
H (55B)	3417	10442	4234	64
H (56A)	2560	10151	4272	61
H (56B)	2538	11257	4205	61
H (57A)	2074	10163	3795	50
H (57B)	2368	11047	3655	50
H (58A)	2675	9161	3661	56
H (58B)	2786	9937	3394	56
H (59A)	4261	7334	4336	76
H (59B)	4035	7033	3989	76
H (60A)	3364	6319	4201	55
H (60B)	3725	6246	4518	55
H (61A)	2880	7174	4527	49
H (61B)	3348	7456	4761	49
H (62A)	3008	8339	4201	71
H (62B)	3331	8776	4495	71
H (63A)	4891	9574	4516	83
H (63B)	4306	9447	4573	83
H (64A)	4885	10826	4782	90
H (64B)	4292	10718	4829	90
H (65A)	4111	11707	4427	66
H (65B)	4690	12007	4450	66
H (66A)	4309	11258	3928	51
H (66B)	4891	11118	4028	51
H (67A)	5226	9820	3525	53
H (67B)	5120	10692	3289	53
H (68A)	5169	8778	3114	61
H (68B)	5430	9644	2939	61
H (69A)	4693	10033	2653	62
H (69B)	4519	8985	2732	62
H (70A)	4162	10599	3004	52
H (70B)	3957	9563	3060	52
H (71A)	4497	7293	3409	38

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H (71B)	4344	7600	3047	38
H (72A)	3911	6124	3411	42
H (72B)	4056	6096	3038	42
H (73A)	3365	6978	2878	43
H (73B)	3131	6402	3170	43
H (74A)	3170	8216	3176	45
H (74B)	3174	7622	3504	45
H (77)	7728	6535	2106	48
H (78)	6882	6617	1970	50
H (79)	6603	7624	1570	45
H (81)	8697	7985	1787	42
H (82A)	8609	7764	2334	91
H (82B)	9058	7118	2221	91
H (82C)	8522	6670	2285	91
H (83A)	8589	6010	1684	73
H (83B)	9101	6570	1651	73
H (83C)	8644	6759	1403	73
H (84)	7351	9285	1152	39
H (85A)	6377	9068	1413	75
H (85B)	6572	9966	1227	75
H (85C)	6801	9714	1577	75
H (86A)	7116	8020	811	58
H (86B)	6725	8855	762	58
H (86C)	6582	7967	973	58
H (89)	8589	9691	-107	37
H (90)	9064	8389	-223	43
H (91)	9332	7383	196	38
H (93)	8310	10582	660	30
H (94A)	8530	11367	185	57
H (94B)	7954	11567	248	57
H (94C)	8104	10826	-19	57
H (95A)	7555	9599	280	46
H (95B)	7427	10432	520	46
H (95C)	7652	9477	660	46
H (96)	9078	7666	1027	33
H (97A)	9867	7185	614	67
H (97B)	9855	6884	985	67
H (97C)	9894	7961	890	67
H (98A)	8610	6511	771	69
H (98B)	9103	6066	936	69
H (98C)	9073	6242	556	69
H (99)	8127	8026	982	21
H (102)	8875	13355	2518	36
H (103)	9714	13361	2670	38
H (104)	10288	12602	2356	29
H (106)	8322	12075	1857	30
H (10A)	8069	13075	2422	48
H (10B)	8074	11965	2393	48
H (10C)	7677	12562	2185	48
H (10D)	8359	14018	1946	68
H (10E)	7943	13476	1734	68
H (10F)	8512	13477	1627	68
H (109)	10013	11138	1668	27
H (11D)	10753	10587	1899	54
H (11E)	10323	10490	2156	54
H (11F)	10722	11317	2188	54
H (11G)	10702	12624	1804	46
H (11H)	10269	12684	1531	46
H (11I)	10712	11945	1499	46
H (114)	9908	11235	174	33
H (115)	9564	12600	-10	39

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H(116)	9052	13457	323	30
H(118)	9618	10003	857	28
H(11J)	9746	9594	312	46
H(11K)	10157	9146	553	46
H(11L)	10294	10036	342	46
H(12D)	10458	10084	1049	55
H(12E)	10184	11043	1127	55
H(12F)	10554	10984	833	55
H(12I)	8604	12749	1086	23
H(12G)	8277	13795	540	53
H(12H)	7977	13650	863	53
H(12I)	8061	12790	627	53
H(12J)	9238	13856	1151	57
H(12K)	8706	14365	1150	57
H(12L)	9039	14401	837	57
H(124)	9449	12385	1352	21
H(12M)	8838	10557	2315	51
H(12N)	8889	9454	2254	51
H(12O)	8207	10369	2643	64
H(12P)	8398	9309	2672	64
H(12Q)	7817	8792	2297	58
H(12R)	7502	9614	2462	58
H(12S)	7640	9724	1865	39
H(12T)	7698	10658	2076	39
H(12U)	8355	8727	3621	154
H(12V)	8322	9531	3352	154
H(13A)	7469	9710	3400	147
H(13B)	7504	8640	3511	147
H(13C)	7454	8963	3992	101
H(13D)	7150	9840	3840	101
H(13E)	7935	10028	4177	111
H(13F)	7761	10756	3905	111
H(13G)	8357	11703	3076	101
H(13H)	8119	11934	3416	101
H(13I)	8172	13395	3333	51
H(13J)	8322	13155	2970	51
H(13K)	9084	13742	3095	48
H(13L)	8968	13766	3474	48
H(13M)	9366	12238	3119	75
H(13N)	9511	12530	3484	75
H(13O)	8921	11419	4681	100
H(13P)	8512	10809	4482	100
H(13Q)	7938	12077	4445	96
H(13R)	8187	12268	4799	96
H(13S)	8286	13530	4375	102
H(13T)	8766	13280	4602	102
H(14A)	8572	12757	3960	114
H(14B)	9102	13011	4131	114
H(14C)	9649	10610	4540	67
H(14D)	10109	9913	4480	67
H(14E)	9210	9489	4793	92
H(14F)	9731	8931	4824	92
H(14G)	9403	7853	4460	124
H(14H)	8916	8492	4392	124
H(14I)	9266	8670	3938	85
H(14J)	9818	8512	4091	85
H(14K)	9230	9337	2999	95
H(14L)	9081	10423	2983	95
H(14M)	9783	9758	2658	144
H(14N)	9780	10819	2777	144
H(14O)	10386	9410	2973	236

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H (14P)	10470	10515	3009	236
H (14Q)	10268	10439	3465	176
H (14R)	10177	9346	3428	176

Full data

Compound 3:

Table 1. Crystal data and structure refinement for [Sm(DippForm)₃].5/2C₇H₈.

Identification code	Sm(DippForm) ₃].5/2C ₇ H ₈
Empirical formula	C _{92.50} H ₁₂₅ N ₆ Sm
Formula weight	1471.34
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 13.1662(2) Å alpha = 90 deg. b = 37.9133(8) Å beta = 96.1070(10) deg. c = 16.4994(3) Å gamma = 90 deg.
Volume	8189.3(3) Å ³
Z, Calculated density	4, 1.193 Mg/m ³
Absorption coefficient	0.765 mm ⁻¹
F(000)	3136
Crystal size	0.20 x 0.20 x 0.10 mm
Theta range for data collection	1.65 to 28.37 deg.
Limiting indices	-17<=h<=16, -45<=k<=50, -22<=l<=20
Reflections collected / unique	44716 / 18160 [R(int) = 0.1993]
Completeness to theta = 26.00	92.0 %
Absorption correction	empirical
Max. and min. transmission	0.9274 and 0.8621
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	18160 / 0 / 939
Goodness-of-fit on F ²	0.956
Final R indices [I>2sigma(I)]	R1 = 0.0938, wR2 = 0.1435
R indices (all data)	R1 = 0.2713, wR2 = 0.2011
Largest diff. peak and hole	1.200 and -1.646 e.Å ⁻³

Note: All hydrogen atoms placed in calculated positions (riding model).

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Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for $[\text{Sm}(\text{DippForm})_3] \cdot 5/2\text{C}_7\text{H}_8$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U (eq)
Sm(1)	7695 (1)	1438 (1)	8934 (1)	23 (1)
N(1)	8494 (4)	2002 (2)	8648 (3)	19 (2)
N(2)	6877 (4)	2015 (2)	9090 (4)	24 (2)
N(3)	8384 (4)	1043 (2)	7943 (4)	22 (2)
N(4)	6701 (4)	1210 (2)	7691 (4)	22 (2)
N(5)	8715 (4)	1279 (2)	10224 (4)	23 (2)
N(6)	7038 (4)	1103 (2)	10043 (4)	21 (2)
C(1)	9278 (6)	2226 (2)	8364 (5)	26 (2)
C(2)	10255 (6)	2222 (2)	8808 (5)	31 (2)
C(3)	10984 (6)	2458 (3)	8563 (5)	37 (3)
C(4)	10776 (6)	2689 (3)	7928 (6)	43 (3)
C(5)	9827 (6)	2688 (2)	7487 (5)	39 (3)
C(6)	9053 (6)	2455 (2)	7696 (5)	28 (2)
C(7)	10493 (5)	2000 (2)	9545 (5)	25 (2)
C(8)	11618 (5)	1904 (2)	9730 (5)	37 (3)
C(9)	10141 (6)	2179 (3)	10301 (5)	41 (3)
C(10)	8024 (6)	2467 (3)	7169 (5)	35 (2)
C(11)	8134 (6)	2433 (3)	6269 (5)	51 (3)
C(12)	7432 (6)	2813 (2)	7286 (5)	46 (3)
C(13)	6095 (6)	2260 (2)	9288 (5)	28 (2)
C(14)	5113 (6)	2215 (3)	8866 (5)	29 (2)
C(15)	4350 (6)	2457 (3)	9033 (5)	38 (3)
C(16)	4560 (7)	2728 (3)	9579 (6)	48 (3)
C(17)	5516 (7)	2761 (3)	9992 (5)	43 (3)
C(18)	6299 (6)	2527 (2)	9881 (5)	30 (2)
C(19)	4879 (5)	1942 (3)	8210 (5)	35 (3)
C(20)	3758 (5)	1838 (3)	8067 (5)	41 (3)
C(21)	5244 (5)	2077 (2)	7401 (5)	39 (3)
C(22)	7338 (6)	2577 (3)	10373 (5)	41 (3)
C(23)	7233 (7)	2600 (3)	11284 (5)	59 (3)
C(24)	7901 (7)	2909 (3)	10137 (6)	62 (3)
C(25)	7688 (6)	2185 (2)	8837 (4)	26 (2)
C(26)	9201 (5)	830 (3)	7645 (5)	26 (2)
C(27)	10075 (6)	1014 (3)	7438 (5)	32 (2)
C(28)	10842 (6)	806 (3)	7152 (5)	38 (3)
C(29)	10776 (7)	452 (3)	7068 (6)	52 (3)
C(30)	9907 (7)	280 (3)	7258 (6)	52 (3)
C(31)	9121 (6)	466 (3)	7560 (5)	36 (2)
C(32)	10171 (6)	1409 (3)	7475 (5)	33 (2)
C(33)	11259 (5)	1550 (2)	7541 (5)	42 (3)
C(34)	9557 (6)	1581 (3)	6736 (6)	47 (3)
C(35)	8194 (6)	250 (3)	7786 (6)	41 (3)
C(36)	8514 (7)	-79 (3)	8284 (6)	65 (3)
C(37)	7507 (7)	133 (3)	7046 (6)	60 (3)
C(38)	5774 (6)	1169 (2)	7145 (5)	26 (2)
C(39)	4907 (6)	1029 (2)	7453 (5)	29 (2)
C(40)	4016 (6)	999 (2)	6928 (6)	40 (3)
C(41)	3956 (7)	1101 (3)	6124 (5)	52 (3)
C(42)	4815 (6)	1241 (3)	5831 (5)	42 (3)
C(43)	5728 (6)	1281 (2)	6342 (5)	28 (2)
C(44)	4968 (6)	885 (3)	8307 (5)	31 (2)

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C (45)	3931 (5)	866 (2)	8658 (5)	36 (2)
C (46)	5452 (6)	521 (3)	8374 (6)	56 (3)
C (47)	6613 (6)	1445 (3)	5952 (5)	32 (2)
C (48)	6307 (7)	1778 (3)	5463 (5)	61 (3)
C (49)	7103 (6)	1187 (3)	5386 (5)	48 (3)
C (50)	7507 (6)	1025 (2)	7480 (5)	25 (2)
C (51)	9651 (6)	1272 (2)	10787 (5)	31 (2)
C (52)	10521 (6)	1108 (2)	10524 (5)	26 (2)
C (53)	11399 (6)	1094 (3)	11072 (6)	41 (3)
C (54)	11423 (7)	1240 (3)	11849 (6)	54 (3)
C (55)	10566 (6)	1405 (3)	12063 (5)	52 (3)
C (56)	9675 (6)	1430 (3)	11561 (5)	37 (2)
C (57)	10492 (5)	938 (3)	9713 (5)	35 (3)
C (58)	11532 (5)	906 (3)	9380 (5)	48 (3)
C (59)	10031 (6)	570 (3)	9732 (5)	43 (3)
C (60)	8772 (6)	1618 (3)	11856 (5)	37 (2)
C (61)	9083 (7)	1976 (3)	12243 (6)	70 (4)
C (62)	8275 (6)	1405 (3)	12501 (5)	61 (3)
C (63)	6273 (5)	912 (2)	10415 (4)	23 (2)
C (64)	5371 (5)	1094 (3)	10587 (5)	29 (2)
C (65)	4636 (6)	906 (3)	10980 (5)	34 (2)
C (66)	4774 (6)	557 (3)	11202 (5)	38 (2)
C (67)	5643 (6)	383 (3)	11029 (5)	37 (2)
C (68)	6391 (6)	556 (3)	10620 (5)	32 (2)
C (69)	5222 (5)	1481 (2)	10407 (5)	26 (2)
C (70)	4114 (5)	1603 (2)	10341 (5)	38 (3)
C (71)	5866 (6)	1706 (2)	11034 (5)	38 (2)
C (72)	7323 (6)	330 (3)	10469 (5)	36 (3)
C (73)	7033 (6)	-9 (3)	10023 (6)	50 (3)
C (74)	8029 (6)	249 (3)	11247 (5)	51 (3)
C (75)	7924 (5)	1113 (2)	10498 (5)	25 (2)
C (76)	3795 (10)	-771 (4)	6853 (7)	114 (5)
C (77)	4787 (10)	-952 (5)	6660 (7)	76 (4)
C (78)	4892 (11)	-1324 (4)	6682 (6)	79 (4)
C (79)	5800 (12)	-1475 (4)	6507 (6)	83 (4)
C (80)	6599 (10)	-1277 (4)	6309 (7)	83 (4)
C (81)	6481 (10)	-905 (4)	6274 (7)	80 (4)
C (82)	5584 (11)	-749 (4)	6452 (6)	81 (4)
C (83A)	-1340 (30)	-1023 (14)	5070 (30)	360 (40)
C (83B)	1450 (30)	-203 (13)	5140 (20)	170 (30)
C (84)	-630 (40)	-810 (20)	5322 (15)	770 (90)
C (85)	340 (20)	-695 (9)	5077 (15)	200 (13)
C (87)	963 (15)	-510 (5)	6359 (13)	159 (7)
C (88)	50 (20)	-725 (7)	6593 (16)	222 (15)
C (89)	-510 (30)	-872 (12)	5810 (40)	470 (50)
C (90)	3301 (19)	149 (8)	6079 (18)	153 (15)
C (91)	4188 (14)	91 (5)	5485 (10)	116 (6)
C (92)	5076 (15)	265 (5)	5560 (10)	121 (6)
C (93)	5889 (13)	184 (4)	5084 (11)	118 (6)
C (94)	1010 (30)	-455 (10)	5504 (15)	235 (15)

Table 3. Bond lengths [Å] and angles [deg] for
[Sm(DippForm)3].5/2C7H8.

Sm(1)-N(1)	2.448(6)
Sm(1)-N(6)	2.460(6)
Sm(1)-N(3)	2.462(6)
Sm(1)-N(2)	2.463(7)
Sm(1)-N(5)	2.467(6)
Sm(1)-N(4)	2.469(6)
Sm(1)-C(25)	2.833(9)
Sm(1)-C(75)	2.848(8)
Sm(1)-C(50)	2.854(9)
N(1)-C(25)	1.331(8)
N(1)-C(1)	1.452(9)
N(2)-C(25)	1.351(8)
N(2)-C(13)	1.449(9)
N(3)-C(50)	1.317(9)
N(3)-C(26)	1.470(9)
N(4)-C(50)	1.349(9)
N(4)-C(38)	1.446(9)
N(5)-C(75)	1.337(8)
N(5)-C(51)	1.464(9)
N(6)-C(75)	1.319(8)
N(6)-C(63)	1.432(9)
C(1)-C(6)	1.410(11)
C(1)-C(2)	1.411(10)
C(2)-C(3)	1.402(11)
C(2)-C(7)	1.485(11)
C(3)-C(4)	1.371(11)
C(4)-C(5)	1.377(11)
C(5)-C(6)	1.420(10)
C(6)-C(10)	1.530(10)
C(7)-C(8)	1.525(9)
C(7)-C(9)	1.535(10)
C(10)-C(11)	1.513(10)
C(10)-C(12)	1.547(11)
C(13)-C(14)	1.412(10)
C(13)-C(18)	1.412(11)
C(14)-C(15)	1.409(11)
C(14)-C(19)	1.506(11)
C(15)-C(16)	1.374(12)
C(16)-C(17)	1.372(11)
C(17)-C(18)	1.387(11)
C(18)-C(22)	1.527(11)
C(19)-C(20)	1.522(9)
C(19)-C(21)	1.553(10)
C(22)-C(23)	1.525(11)
C(22)-C(24)	1.533(11)
C(26)-C(31)	1.391(11)
C(26)-C(27)	1.417(10)
C(27)-C(28)	1.402(10)
C(27)-C(32)	1.504(12)
C(28)-C(29)	1.351(12)
C(29)-C(30)	1.381(11)
C(30)-C(31)	1.388(11)
C(31)-C(35)	1.549(11)
C(32)-C(33)	1.523(10)
C(32)-C(34)	1.535(11)
C(35)-C(37)	1.507(11)

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C (35) -C (36)	1.528 (12)
C (38) -C (43)	1.386 (10)
C (38) -C (39)	1.402 (10)
C (39) -C (40)	1.387 (10)
C (39) -C (44)	1.507 (10)
C (40) -C (41)	1.376 (11)
C (41) -C (42)	1.382 (11)
C (42) -C (43)	1.401 (10)
C (43) -C (47)	1.524 (10)
C (44) -C (46)	1.516 (12)
C (44) -C (45)	1.541 (9)
C (47) -C (48)	1.528 (12)
C (47) -C (49)	1.542 (11)
C (51) -C (56)	1.407 (11)
C (51) -C (52)	1.413 (10)
C (52) -C (53)	1.390 (10)
C (52) -C (57)	1.481 (11)
C (53) -C (54)	1.394 (12)
C (54) -C (55)	1.370 (12)
C (55) -C (56)	1.366 (10)
C (56) -C (60)	1.512 (11)
C (57) -C (59)	1.523 (11)
C (57) -C (58)	1.533 (9)
C (60) -C (61)	1.537 (12)
C (60) -C (62)	1.537 (11)
C (63) -C (68)	1.397 (11)
C (63) -C (64)	1.428 (10)
C (64) -C (65)	1.414 (10)
C (64) -C (69)	1.504 (11)
C (65) -C (66)	1.381 (11)
C (66) -C (67)	1.376 (10)
C (67) -C (68)	1.413 (10)
C (68) -C (72)	1.537 (11)
C (69) -C (70)	1.524 (9)
C (69) -C (71)	1.526 (10)
C (72) -C (73)	1.512 (12)
C (72) -C (74)	1.535 (11)
C (76) -C (77)	1.539 (15)
C (77) -C (82)	1.376 (15)
C (77) -C (78)	1.415 (16)
C (78) -C (79)	1.384 (15)
C (79) -C (80)	1.359 (15)
C (80) -C (81)	1.421 (15)
C (81) -C (82)	1.380 (14)
C (83A) -C (84)	1.27 (6)
C (83B) -C (94)	1.30 (4)
C (84) -C (89)	0.83 (7)
C (84) -C (85)	1.45 (5)
C (85) -C (94)	1.41 (3)
C (87) -C (94)	1.43 (2)
C (87) -C (88)	1.53 (2)
C (88) -C (89)	1.53 (4)
C (90) -C (91)	1.62 (2)
C (91) -C (92)	1.337 (18)
C (91) -C (93) #1	1.399 (18)
C (92) -C (93)	1.427 (17)
C (93) -C (91) #1	1.399 (18)
N (1) -Sm (1) -N (6)	141.9 (2)
N (1) -Sm (1) -N (3)	101.9 (2)
N (6) -Sm (1) -N (3)	111.3 (2)

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N (1) -Sm (1) -N (2)	56.45 (18)
N (6) -Sm (1) -N (2)	100.9 (2)
N (3) -Sm (1) -N (2)	143.7 (2)
N (1) -Sm (1) -N (5)	100.1 (2)
N (6) -Sm (1) -N (5)	55.53 (19)
N (3) -Sm (1) -N (5)	102.6 (2)
N (2) -Sm (1) -N (5)	109.4 (2)
N (1) -Sm (1) -N (4)	110.2 (2)
N (6) -Sm (1) -N (4)	103.8 (2)
N (3) -Sm (1) -N (4)	55.62 (19)
N (2) -Sm (1) -N (4)	101.4 (2)
N (5) -Sm (1) -N (4)	145.3 (2)
N (1) -Sm (1) -C (25)	28.00 (17)
N (6) -Sm (1) -C (25)	124.0 (2)
N (3) -Sm (1) -C (25)	124.7 (2)
N (2) -Sm (1) -C (25)	28.46 (17)
N (5) -Sm (1) -C (25)	107.0 (2)
N (4) -Sm (1) -C (25)	107.7 (2)
N (1) -Sm (1) -C (75)	123.2 (2)
N (6) -Sm (1) -C (75)	27.55 (17)
N (3) -Sm (1) -C (75)	109.1 (2)
N (2) -Sm (1) -C (75)	107.2 (2)
N (5) -Sm (1) -C (75)	27.98 (18)
N (4) -Sm (1) -C (75)	126.6 (2)
C (25) -Sm (1) -C (75)	118.9 (2)
N (1) -Sm (1) -C (50)	108.5 (2)
N (6) -Sm (1) -C (50)	109.6 (2)
N (3) -Sm (1) -C (50)	27.44 (19)
N (2) -Sm (1) -C (50)	125.1 (2)
N (5) -Sm (1) -C (50)	125.5 (2)
N (4) -Sm (1) -C (50)	28.18 (19)
C (25) -Sm (1) -C (50)	120.0 (2)
C (75) -Sm (1) -C (50)	121.0 (2)
C (25) -N (1) -C (1)	112.5 (7)
C (25) -N (1) -Sm (1)	92.3 (5)
C (1) -N (1) -Sm (1)	155.0 (5)
C (25) -N (2) -C (13)	111.7 (7)
C (25) -N (2) -Sm (1)	91.2 (5)
C (13) -N (2) -Sm (1)	157.1 (5)
C (50) -N (3) -C (26)	113.9 (7)
C (50) -N (3) -Sm (1)	93.1 (5)
C (26) -N (3) -Sm (1)	152.9 (5)
C (50) -N (4) -C (38)	114.7 (7)
C (50) -N (4) -Sm (1)	92.0 (5)
C (38) -N (4) -Sm (1)	153.2 (5)
C (75) -N (5) -C (51)	114.2 (7)
C (75) -N (5) -Sm (1)	92.1 (5)
C (51) -N (5) -Sm (1)	153.7 (5)
C (75) -N (6) -C (63)	112.9 (6)
C (75) -N (6) -Sm (1)	92.9 (4)
C (63) -N (6) -Sm (1)	154.2 (5)
C (6) -C (1) -C (2)	121.0 (8)
C (6) -C (1) -N (1)	121.0 (7)
C (2) -C (1) -N (1)	117.8 (7)
C (3) -C (2) -C (1)	117.3 (8)
C (3) -C (2) -C (7)	120.3 (7)
C (1) -C (2) -C (7)	122.2 (8)
C (4) -C (3) -C (2)	122.7 (8)
C (3) -C (4) -C (5)	120.0 (8)

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C (4) -C (5) -C (6)	120.4 (8)
C (1) -C (6) -C (5)	118.5 (7)
C (1) -C (6) -C (10)	124.2 (8)
C (5) -C (6) -C (10)	117.2 (8)
C (2) -C (7) -C (8)	114.6 (6)
C (2) -C (7) -C (9)	111.1 (7)
C (8) -C (7) -C (9)	108.4 (6)
C (11) -C (10) -C (6)	112.5 (6)
C (11) -C (10) -C (12)	107.3 (7)
C (6) -C (10) -C (12)	112.5 (7)
C (14) -C (13) -C (18)	121.6 (8)

C (14) -C (13) -N (2)	116.6 (8)
C (18) -C (13) -N (2)	121.8 (7)
C (15) -C (14) -C (13)	117.4 (9)
C (15) -C (14) -C (19)	119.5 (7)
C (13) -C (14) -C (19)	122.9 (8)
C (16) -C (15) -C (14)	121.0 (9)
C (17) -C (16) -C (15)	120.3 (9)
C (16) -C (17) -C (18)	122.1 (9)
C (17) -C (18) -C (13)	117.4 (8)
C (17) -C (18) -C (22)	119.1 (8)
C (13) -C (18) -C (22)	123.5 (8)
C (14) -C (19) -C (20)	114.3 (7)
C (14) -C (19) -C (21)	109.4 (7)
C (20) -C (19) -C (21)	109.6 (7)
C (23) -C (22) -C (18)	111.2 (7)
C (23) -C (22) -C (24)	107.4 (8)
C (18) -C (22) -C (24)	113.5 (8)
N (1) -C (25) -N (2)	120.1 (8)
N (1) -C (25) -Sm (1)	59.7 (4)
N (2) -C (25) -Sm (1)	60.4 (4)
C (31) -C (26) -C (27)	121.1 (8)
C (31) -C (26) -N (3)	121.9 (7)
C (27) -C (26) -N (3)	117.0 (8)
C (28) -C (27) -C (26)	116.0 (9)
C (28) -C (27) -C (32)	120.8 (8)
C (26) -C (27) -C (32)	123.1 (8)
C (29) -C (28) -C (27)	123.4 (9)
C (28) -C (29) -C (30)	119.5 (9)
C (29) -C (30) -C (31)	120.5 (10)
C (30) -C (31) -C (26)	119.3 (8)
C (30) -C (31) -C (35)	117.0 (9)
C (26) -C (31) -C (35)	123.6 (8)
C (27) -C (32) -C (33)	115.4 (7)
C (27) -C (32) -C (34)	110.9 (7)
C (33) -C (32) -C (34)	108.6 (7)
C (37) -C (35) -C (36)	107.6 (8)
C (37) -C (35) -C (31)	112.4 (8)
C (36) -C (35) -C (31)	112.4 (8)
C (43) -C (38) -C (39)	120.5 (7)
C (43) -C (38) -N (4)	120.7 (7)
C (39) -C (38) -N (4)	118.7 (7)
C (40) -C (39) -C (38)	118.2 (8)
C (40) -C (39) -C (44)	120.8 (7)
C (38) -C (39) -C (44)	120.8 (7)
C (41) -C (40) -C (39)	122.5 (8)
C (40) -C (41) -C (42)	118.7 (8)
C (41) -C (42) -C (43)	120.8 (8)
C (38) -C (43) -C (42)	119.4 (7)

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C (38) -C (43) -C (47)	124.8 (7)
C (42) -C (43) -C (47)	115.8 (7)
C (39) -C (44) -C (46)	112.3 (7)
C (39) -C (44) -C (45)	114.0 (7)
C (46) -C (44) -C (45)	108.2 (7)
C (43) -C (47) -C (48)	113.0 (7)
C (43) -C (47) -C (49)	112.6 (8)
C (48) -C (47) -C (49)	107.9 (7)
N (3) -C (50) -N (4)	119.3 (8)
N (3) -C (50) -Sm (1)	59.5 (4)
N (4) -C (50) -Sm (1)	59.8 (4)
C (56) -C (51) -C (52)	121.7 (7)
C (56) -C (51) -N (5)	120.3 (7)
C (52) -C (51) -N (5)	117.9 (7)
C (53) -C (52) -C (51)	117.6 (8)
C (53) -C (52) -C (57)	120.7 (8)
C (51) -C (52) -C (57)	121.7 (7)
C (52) -C (53) -C (54)	121.2 (8)
C (55) -C (54) -C (53)	118.7 (9)
C (56) -C (55) -C (54)	123.6 (9)
C (55) -C (56) -C (51)	117.1 (8)
C (55) -C (56) -C (60)	119.5 (8)
C (51) -C (56) -C (60)	123.4 (7)
C (52) -C (57) -C (59)	110.5 (7)
C (52) -C (57) -C (58)	114.9 (7)
C (59) -C (57) -C (58)	107.9 (7)
C (56) -C (60) -C (61)	111.6 (7)
C (56) -C (60) -C (62)	112.4 (8)
C (61) -C (60) -C (62)	106.9 (7)
C (68) -C (63) -C (64)	119.6 (7)
C (68) -C (63) -N (6)	121.8 (7)
C (64) -C (63) -N (6)	118.6 (8)
C (65) -C (64) -C (63)	118.1 (9)
C (65) -C (64) -C (69)	120.0 (7)
C (63) -C (64) -C (69)	121.8 (7)
C (66) -C (65) -C (64)	121.8 (8)
C (67) -C (66) -C (65)	119.6 (8)
C (66) -C (67) -C (68)	121.0 (9)
C (63) -C (68) -C (67)	119.9 (8)
C (63) -C (68) -C (72)	124.7 (7)
C (67) -C (68) -C (72)	115.4 (8)
C (64) -C (69) -C (70)	114.5 (7)
C (64) -C (69) -C (71)	111.1 (7)
C (70) -C (69) -C (71)	109.7 (7)
C (73) -C (72) -C (74)	109.5 (8)
C (73) -C (72) -C (68)	112.8 (7)
C (74) -C (72) -C (68)	113.6 (7)
N (6) -C (75) -N (5)	119.5 (7)
N (6) -C (75) -Sm (1)	59.6 (4)
N (5) -C (75) -Sm (1)	59.9 (4)
C (82) -C (77) -C (78)	119.3 (13)
C (82) -C (77) -C (76)	119.2 (16)
C (78) -C (77) -C (76)	121.5 (14)
C (79) -C (78) -C (77)	119.3 (13)
C (80) -C (79) -C (78)	122.0 (15)
C (79) -C (80) -C (81)	118.3 (14)
C (82) -C (81) -C (80)	120.6 (14)
C (77) -C (82) -C (81)	120.4 (14)
C (89) -C (84) -C (83A)	102 (8)
C (89) -C (84) -C (85)	106 (6)
C (83A) -C (84) -C (85)	138 (4)

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C (94) -C (85) -C (84)	126 (3)
C (94) -C (87) -C (88)	116 (2)
C (87) -C (88) -C (89)	107 (3)
C (84) -C (89) -C (88)	138 (8)
C (92) -C (91) -C (93) #1	115.5 (17)
C (92) -C (91) -C (90)	123.8 (19)
C (93) #1 -C (91) -C (90)	120 (2)
C (91) -C (92) -C (93)	122.9 (17)
C (91) #1 -C (93) -C (92)	121.6 (16)
C (83B) -C (94) -C (85)	122 (3)
C (83B) -C (94) -C (87)	129 (4)
C (85) -C (94) -C (87)	108 (3)

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

Table 4. Anisotropic displacement parameters ($\text{Å}^2 \times 10^3$) for
 [Sm(DippForm)₃].5/2C₇H₈.

The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Sm(1)	21(1)	28(1)	22(1)	1(1)	6(1)	-1(1)
N(1)	15(3)	19(5)	24(4)	4(3)	9(3)	2(3)
N(2)	14(3)	29(5)	28(4)	7(3)	6(3)	-3(3)
N(3)	23(4)	19(5)	25(4)	-1(3)	2(3)	-3(3)
N(4)	23(4)	15(4)	30(4)	1(3)	7(3)	2(3)
N(5)	27(4)	11(4)	33(4)	4(3)	5(3)	3(3)
N(6)	13(3)	19(5)	30(4)	-3(3)	2(3)	-2(3)
C(1)	31(5)	13(6)	35(5)	1(4)	8(4)	-2(4)
C(2)	22(5)	36(7)	34(5)	-8(5)	4(4)	9(5)
C(3)	24(5)	54(8)	34(6)	0(5)	9(4)	-8(5)
C(4)	39(6)	38(8)	57(7)	1(6)	24(5)	-15(5)
C(5)	31(5)	45(8)	41(6)	19(5)	4(4)	-4(5)
C(6)	24(5)	30(7)	31(5)	-5(4)	11(4)	6(4)
C(7)	17(4)	27(6)	30(5)	10(4)	-3(4)	2(4)
C(8)	16(4)	46(8)	48(6)	1(5)	3(4)	-5(4)
C(9)	31(5)	60(8)	32(6)	3(5)	0(4)	-8(5)
C(10)	33(5)	40(7)	34(6)	0(5)	13(4)	-1(5)
C(11)	45(6)	76(9)	33(6)	-1(6)	6(4)	11(6)
C(12)	37(5)	44(8)	57(7)	17(5)	10(5)	14(5)
C(13)	22(5)	36(7)	30(5)	1(4)	15(4)	8(4)
C(14)	25(5)	41(7)	22(5)	12(4)	6(4)	2(5)
C(15)	30(5)	49(8)	39(6)	-2(5)	16(4)	8(5)
C(16)	51(7)	48(9)	49(7)	10(6)	19(5)	24(6)
C(17)	55(6)	33(7)	45(6)	-10(5)	22(5)	8(6)
C(18)	34(5)	24(6)	37(6)	-1(4)	22(4)	2(5)
C(19)	16(4)	46(8)	43(6)	-6(5)	-1(4)	2(5)
C(20)	20(5)	52(8)	51(6)	7(5)	-2(4)	1(5)
C(21)	27(5)	42(8)	48(6)	4(5)	5(4)	-2(5)
C(22)	43(6)	40(8)	43(6)	-12(5)	22(5)	-4(5)
C(23)	98(8)	55(9)	24(6)	-7(5)	5(5)	2(7)
C(24)	63(7)	48(9)	78(8)	-26(7)	19(6)	-21(6)
C(25)	27(4)	26(6)	26(5)	-5(4)	4(4)	4(5)
C(26)	14(4)	27(7)	37(5)	-1(4)	1(4)	-6(4)
C(27)	30(5)	34(7)	32(5)	1(5)	5(4)	9(5)
C(28)	41(5)	20(7)	57(6)	7(5)	25(5)	12(5)
C(29)	49(6)	37(8)	76(8)	-4(6)	33(6)	22(6)
C(30)	57(6)	30(7)	76(8)	-9(6)	34(6)	18(6)
C(31)	40(6)	34(7)	37(6)	-6(5)	9(4)	-11(5)
C(32)	32(5)	29(7)	42(6)	-8(5)	17(4)	0(5)
C(33)	24(5)	54(8)	51(6)	1(5)	11(4)	-4(5)
C(34)	34(5)	46(8)	60(7)	6(6)	5(5)	-11(5)
C(35)	44(6)	20(7)	61(7)	-2(5)	18(5)	-2(5)
C(36)	66(7)	51(9)	80(9)	3(7)	12(6)	-10(6)
C(37)	63(7)	52(9)	64(8)	-9(6)	0(6)	-15(6)
C(38)	25(5)	27(6)	25(5)	-1(4)	0(4)	-9(4)
C(39)	22(5)	34(7)	31(5)	7(4)	1(4)	-7(4)
C(40)	23(5)	42(8)	54(7)	2(5)	7(4)	-12(5)
C(41)	39(6)	86(10)	30(6)	-1(6)	-10(4)	-12(6)
C(42)	40(6)	51(8)	34(6)	2(5)	1(5)	4(5)
C(43)	23(5)	32(7)	31(5)	1(4)	9(4)	3(4)

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C (44)	24 (5)	39 (7)	31 (5)	5 (5)	4 (4)	4 (5)
C (45)	24 (5)	35 (7)	48 (6)	19 (5)	3 (4)	-6 (4)
C (46)	45 (6)	72 (10)	51 (7)	16 (6)	8 (5)	-2 (6)
C (47)	39 (5)	32 (6)	24 (5)	0 (5)	-1 (4)	-5 (5)
C (48)	71 (7)	79 (10)	36 (6)	4 (6)	9 (5)	-13 (7)
C (49)	54 (6)	75 (9)	17 (5)	5 (5)	12 (4)	-3 (6)
C (50)	39 (5)	15 (5)	19 (4)	3 (4)	1 (4)	-6 (4)
C (51)	25 (5)	27 (7)	39 (6)	2 (4)	-2 (4)	-14 (4)
C (52)	22 (5)	27 (6)	29 (5)	5 (4)	-1 (4)	-3 (4)
C (53)	23 (5)	51 (8)	48 (7)	10 (6)	-1 (4)	2 (5)
C (54)	37 (6)	71 (10)	51 (7)	14 (6)	-14 (5)	-13 (6)
C (55)	37 (5)	80 (10)	39 (6)	0 (6)	0 (4)	-8 (6)
C (56)	29 (5)	57 (8)	25 (5)	-6 (6)	-4 (4)	-19 (6)
C (57)	18 (5)	51 (8)	35 (6)	-4 (5)	1 (4)	6 (5)
C (58)	28 (5)	51 (8)	67 (7)	-2 (6)	10 (5)	7 (5)
C (59)	35 (5)	43 (8)	54 (7)	-14 (5)	13 (4)	0 (5)
C (60)	42 (5)	36 (7)	33 (6)	-11 (5)	7 (4)	-8 (5)
C (61)	72 (7)	87 (11)	56 (7)	-34 (7)	29 (6)	-16 (7)
C (62)	59 (6)	76 (10)	51 (7)	-18 (7)	21 (5)	-11 (7)
C (63)	23 (5)	28 (6)	18 (5)	1 (4)	6 (3)	-10 (4)
C (64)	17 (4)	40 (7)	31 (5)	-3 (5)	4 (4)	-8 (5)
C (65)	30 (5)	38 (7)	37 (6)	0 (5)	13 (4)	-1 (5)
C (66)	40 (5)	34 (7)	41 (6)	9 (5)	14 (4)	-7 (5)
C (67)	39 (5)	36 (7)	37 (6)	10 (5)	0 (4)	-3 (5)
C (68)	25 (5)	37 (7)	34 (5)	8 (5)	8 (4)	-7 (5)
C (69)	23 (4)	19 (6)	38 (5)	6 (4)	9 (4)	-5 (5)
C (70)	30 (5)	49 (8)	37 (6)	-1 (5)	18 (4)	14 (5)
C (71)	38 (5)	31 (7)	46 (6)	-5 (5)	15 (4)	2 (5)
C (72)	28 (5)	41 (8)	42 (6)	5 (5)	16 (4)	-2 (5)
C (73)	56 (6)	36 (8)	61 (7)	4 (6)	9 (5)	-1 (6)
C (74)	45 (6)	49 (8)	60 (7)	13 (6)	9 (5)	3 (6)
C (75)	27 (5)	36 (7)	16 (5)	-4 (4)	14 (4)	-7 (4)
C (76)	126 (11)	130 (16)	92 (11)	-31 (10)	33 (9)	-2 (11)
C (77)	84 (10)	103 (14)	42 (7)	-14 (8)	5 (6)	-9 (11)
C (78)	106 (11)	88 (14)	42 (7)	10 (7)	12 (7)	-25 (10)
C (79)	105 (10)	89 (13)	49 (7)	1 (8)	-15 (7)	13 (11)
C (80)	70 (9)	93 (15)	77 (9)	13 (9)	-29 (7)	-22 (9)
C (81)	89 (10)	71 (13)	77 (10)	-8 (8)	1 (7)	-14 (9)
C (82)	98 (10)	90 (13)	57 (8)	-11 (8)	14 (7)	-22 (10)
C (83A)	260 (50)	470 (90)	300 (60)	70 (50)	-190 (40)	-190 (50)
C (83B)	230 (50)	200 (60)	110 (40)	70 (40)	130 (40)	110 (40)
C (84)	310 (50)	2000 (300)	35 (15)	-170 (50)	80 (20)	-350 (80)
C (85)	160 (20)	290 (40)	150 (20)	-110 (20)	17 (17)	0 (20)
C (87)	200 (19)	150 (20)	125 (18)	-29 (14)	10 (14)	50 (16)
C (88)	250 (30)	190 (30)	260 (30)	160 (20)	180 (20)	140 (20)
C (89)	220 (40)	340 (50)	770 (110)	140 (60)	-310 (60)	-50 (30)
C (90)	110 (20)	180 (40)	180 (30)	-60 (30)	70 (20)	30 (20)
C (91)	120 (14)	90 (16)	127 (15)	-35 (11)	-33 (11)	-11 (11)
C (92)	101 (12)	132 (19)	123 (14)	-23 (12)	-20 (11)	32 (14)
C (93)	141 (15)	64 (13)	136 (15)	-27 (11)	-45 (12)	-10 (11)
C (94)	370 (40)	270 (40)	97 (19)	-40 (20)	140 (20)	-20 (30)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for [Sm(DippForm)₃].5/2C₇H₈.

	x	y	z	U (eq)
H(3)	11649	2457	8849	44
H(4)	11286	2849	7792	52
H(5)	9689	2845	7040	47
H(7)	10101	1775	9456	30
H(8A)	11859	1792	9250	55
H(8B)	11702	1740	10191	55
H(8C)	12017	2118	9867	55
H(9A)	10487	2407	10388	62
H(9B)	10309	2029	10779	62
H(9C)	9400	2217	10218	62
H(10)	7600	2266	7331	42
H(11A)	8530	2632	6093	77
H(11B)	7456	2432	5961	77
H(11C)	8488	2212	6171	77
H(12A)	7333	2841	7863	69
H(12B)	6765	2803	6961	69
H(12C)	7822	3013	7110	69
H(15)	3679	2433	8764	46
H(16)	4042	2893	9671	58
H(17)	5646	2950	10366	52
H(19)	5281	1725	8378	42
H(20A)	3521	1762	8583	62
H(20B)	3677	1643	7674	62
H(20C)	3353	2040	7852	62
H(21A)	4914	2303	7253	59
H(21B)	5061	1905	6968	59
H(21C)	5987	2109	7473	59
H(22)	7772	2368	10279	49
H(23A)	6819	2807	11390	89
H(23B)	7912	2623	11586	89
H(23C)	6901	2386	11459	89
H(24A)	8027	2894	9564	93
H(24B)	8555	2929	10480	93
H(24C)	7483	3118	10219	93
H(25)	7684	2434	8793	32
H(28)	11440	920	7009	45
H(29)	11322	322	6881	63
H(30)	9847	32	7181	63
H(32)	9861	1489	7971	40
H(33A)	11680	1422	7970	64
H(33B)	11256	1802	7677	64
H(33C)	11540	1518	7020	64
H(34A)	9828	1502	6235	70
H(34B)	9615	1838	6780	70
H(34C)	8838	1512	6720	70
H(35)	7785	404	8123	49
H(36A)	7910	-189	8476	98
H(36B)	8996	-13	8753	98
H(36C)	8843	-247	7943	98
H(37A)	7896	-15	6702	90

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H (37B)	7244	340	6737	90
H (37C)	6935	-3	7219	90
H (40)	3425	904	7131	47
H (41)	3337	1076	5777	63
H (42)	4786	1310	5276	50
H (44)	5417	1046	8665	37
H (45A)	3597	1097	8607	54
H (45B)	4039	799	9234	54
H (45C)	3497	689	8356	54
H (46A)	5067	361	7990	84
H (46B)	5442	432	8930	84
H (46C)	6160	536	8244	84
H (47)	7149	1513	6401	38
H (48A)	5797	1718	5008	92
H (48B)	6911	1879	5252	92
H (48C)	6017	1950	5817	92
H (49A)	6580	1102	4964	72
H (49B)	7399	987	5705	72
H (49C)	7641	1309	5127	72
H (50)	7443	884	7001	30
H (53)	11994	983	10913	49
H (54)	12022	1224	12224	65
H (55)	10594	1509	12589	63
H (57)	10038	1083	9319	42
H (58A)	11845	1140	9363	72
H (58B)	11437	807	8829	72
H (58C)	11977	751	9735	72
H (59A)	10430	428	10148	65
H (59B)	10043	459	9198	65
H (59C)	9324	588	9863	65
H (60)	8250	1660	11380	44
H (61A)	8483	2090	12434	105
H (61B)	9359	2127	11837	105
H (61C)	9605	1940	12705	105
H (62A)	8004	1184	12260	92
H (62B)	7718	1542	12694	92
H (62C)	8788	1353	12961	92
H (65)	4030	1024	11096	41
H (66)	4273	437	11472	45
H (67)	5741	143	11186	45
H (69)	5476	1526	9867	31
H (70A)	3704	1460	9934	57
H (70B)	4076	1852	10176	57
H (70C)	3850	1577	10871	57
H (71A)	6586	1638	11044	57
H (71B)	5640	1668	11574	57
H (71C)	5787	1955	10885	57
H (72)	7732	471	10108	43
H (73A)	6723	-171	10389	76
H (73B)	7646	-118	9844	76
H (73C)	6544	41	9548	76
H (74A)	7662	103	11611	77
H (74B)	8243	470	11522	77
H (74C)	8632	121	11105	77
H (75)	7999	1002	11018	30
H (76A)	3824	-520	6718	172
H (76B)	3719	-798	7434	172
H (76C)	3211	-880	6529	172
H (78)	4344	-1468	6815	94
H (79)	5868	-1724	6525	99
H (80)	7220	-1385	6197	99

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H (81)	7024	-762	6126	95
H (82)	5516	-499	6430	98
H (83A)	-1913	-994	5403	535
H (83B)	-1090	-1266	5120	535
H (83C)	-1576	-972	4501	535
H (83D)	1504	-270	4572	261
H (83E)	2134	-161	5418	261
H (83F)	1042	13	5152	261
H (85)	539	-789	4584	240
H (87)	1467	-419	6758	190
H (88)	-127	-761	7129	267
H (89)	-803	-1095	5897	562
H (90A)	2716	-2	5900	230
H (90B)	3086	397	6056	230
H (90C)	3564	89	6639	230
H (92)	5169	451	5947	145
H (93)	6497	321	5154	141

Full data

Compound 4:

Table 1. Crystal data and structure refinement for [Sm(F)(DippForm)₂(THF)].

Identification code	Sm(F)(DippForm) ₂ (THF)]
Empirical formula	C ₅₄ H ₇₈ F N ₄ O Sm
Formula weight	968.55
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 20.4714(2) Å alpha = 90 deg. b = 12.1996(2) Å beta = 110.0650(10) deg. c = 21.6593(3) Å gamma = 90 deg.
Volume	5080.93(12) Å ³
Z, Calculated density	4, 1.266 Mg/m ³
Absorption coefficient	1.199 mm ⁻¹
F(000)	2036
Crystal size	0.30 x 0.20 x 0.20 mm
Theta range for data collection	3.28 to 28.24 deg.
Limiting indices	-27<=h<=25, -11<=k<=16, -28<=l<=19
Reflections collected / unique	32459 / 12173 [R(int) = 0.0518]
Completeness to theta = 28.24	96.9 %
Absorption correction	empirical
Max. and min. transmission	0.7954 and 0.7149
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	12173 / 0 / 566
Goodness-of-fit on F ²	1.044
Final R indices [I>2sigma(I)]	R1 = 0.0605, wR2 = 0.1572
R indices (all data)	R1 = 0.0674, wR2 = 0.1654
Largest diff. peak and hole	3.806 and -5.153 e.Å ⁻³

Note: All hydrogen atoms placed in calculated positions (riding model).

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for $[\text{Sm}(\text{F}(\text{DippForm})_2(\text{THF}))]$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U (eq)
Sm(1)	5687(1)	6010(1)	2647(1)	18(1)
F(1)	6691(1)	5446(2)	2776(1)	33(1)
O(1)	6217(1)	7789(2)	2571(1)	29(1)
N(1)	4850(1)	4719(2)	1939(1)	21(1)
N(2)	5101(1)	6251(2)	1459(1)	20(1)
N(3)	5177(1)	7004(2)	3351(1)	20(1)
N(4)	5551(1)	5248(2)	3644(1)	20(1)
C(1)	4524(2)	3672(3)	1881(2)	22(1)
C(2)	4921(2)	2761(3)	2200(2)	25(1)
C(3)	4598(2)	1747(3)	2157(2)	31(1)
C(4)	3893(2)	1627(3)	1813(2)	34(1)
C(5)	3503(2)	2522(3)	1509(2)	33(1)
C(6)	3801(2)	3554(3)	1541(2)	26(1)
C(7)	5701(2)	2878(3)	2563(2)	32(1)
C(8)	5993(2)	2035(3)	3116(2)	40(1)
C(9)	6096(2)	2821(4)	2088(2)	44(1)
C(10)	3348(2)	4534(3)	1261(2)	36(1)
C(11)	3171(3)	5114(4)	1800(3)	67(2)
C(12)	2682(2)	4265(5)	696(2)	49(1)
C(13)	5215(2)	6743(2)	907(2)	21(1)
C(14)	4806(2)	7643(3)	595(2)	25(1)
C(15)	4919(2)	8121(3)	54(2)	32(1)
C(16)	5432(2)	7730(3)	-174(2)	33(1)
C(17)	5847(2)	6871(3)	149(2)	29(1)
C(18)	5759(2)	6376(3)	696(2)	23(1)
C(19)	4226(2)	8070(3)	828(2)	26(1)
C(20)	4136(2)	9311(3)	761(2)	39(1)
C(21)	3543(2)	7487(3)	472(2)	33(1)
C(22)	6255(2)	5461(3)	1048(2)	25(1)
C(23)	7015(2)	5840(3)	1274(2)	35(1)
C(24)	6158(2)	4439(3)	616(2)	34(1)
C(25)	4857(2)	5223(2)	1402(2)	21(1)
C(26)	4977(2)	8039(3)	3532(2)	23(1)
C(27)	4282(2)	8391(3)	3237(2)	32(1)
C(28)	4094(2)	9420(4)	3414(2)	47(1)
C(29)	4576(2)	10076(3)	3860(3)	48(1)
C(30)	5256(2)	9751(3)	4128(2)	41(1)
C(31)	5473(2)	8727(3)	3965(2)	28(1)
C(32)	3732(2)	7681(3)	2758(2)	38(1)
C(33)	3310(3)	8323(4)	2138(2)	52(1)
C(34)	3241(3)	7208(4)	3078(3)	57(1)
C(35)	6239(2)	8428(3)	4251(2)	29(1)
C(36)	6699(2)	9311(4)	4115(2)	39(1)
C(37)	6456(2)	8197(3)	4984(2)	37(1)
C(38)	5626(2)	4333(3)	4072(2)	21(1)
C(39)	6297(2)	3929(2)	4419(2)	24(1)
C(40)	6369(2)	3055(3)	4850(2)	29(1)
C(41)	5797(2)	2569(3)	4936(2)	30(1)
C(42)	5137(2)	2938(3)	4568(2)	27(1)
C(43)	5035(2)	3813(3)	4128(2)	23(1)
C(44)	6931(2)	4452(3)	4324(2)	29(1)

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C (45)	7571 (2)	3704 (4)	4506 (2)	39 (1)
C (46)	7128 (2)	5528 (3)	4698 (3)	45 (1)
C (47)	4296 (2)	4148 (3)	3723 (2)	25 (1)
C (48)	3864 (2)	3170 (3)	3353 (2)	32 (1)
C (49)	3931 (2)	4694 (3)	4153 (2)	34 (1)
C (50)	5288 (2)	6173 (2)	3773 (2)	20 (1)
C (51)	5803 (2)	8744 (3)	2270 (2)	36 (1)
C (52)	6279 (3)	9475 (4)	2050 (3)	55 (1)
C (53)	6867 (3)	8742 (4)	2041 (3)	54 (1)
C (54)	6934 (2)	7958 (3)	2605 (2)	35 (1)

Table 3. Bond lengths [Å] and angles [deg] for
[Sm(F) (DippForm) 2 (THF)] .

Sm(1)-F(1)	2.093(2)
Sm(1)-N(1)	2.443(3)
Sm(1)-N(3)	2.446(3)
Sm(1)-N(4)	2.454(3)
Sm(1)-N(2)	2.454(3)
Sm(1)-O(1)	2.457(2)
Sm(1)-C(25)	2.817(3)
Sm(1)-C(50)	2.833(3)
O(1)-C(51)	1.457(5)
O(1)-C(54)	1.457(4)
N(1)-C(25)	1.320(4)
N(1)-C(1)	1.426(4)
N(2)-C(25)	1.340(4)
N(2)-C(13)	1.426(4)
N(3)-C(50)	1.332(4)
N(3)-C(26)	1.423(4)
N(4)-C(50)	1.321(4)
N(4)-C(38)	1.424(4)
C(1)-C(2)	1.410(5)
C(1)-C(6)	1.416(4)
C(2)-C(3)	1.391(5)
C(2)-C(7)	1.525(5)
C(3)-C(4)	1.386(6)
C(4)-C(5)	1.379(6)
C(5)-C(6)	1.391(5)
C(6)-C(10)	1.508(5)
C(7)-C(9)	1.513(6)
C(7)-C(8)	1.535(5)
C(10)-C(11)	1.511(7)
C(10)-C(12)	1.522(6)
C(13)-C(14)	1.406(4)
C(13)-C(18)	1.413(4)
C(14)-C(15)	1.397(5)
C(14)-C(19)	1.532(5)
C(15)-C(16)	1.388(6)
C(16)-C(17)	1.379(5)
C(17)-C(18)	1.397(5)
C(18)-C(22)	1.526(5)
C(19)-C(21)	1.522(5)
C(19)-C(20)	1.527(5)
C(22)-C(24)	1.531(5)
C(22)-C(23)	1.533(5)
C(26)-C(31)	1.401(5)
C(26)-C(27)	1.412(5)
C(27)-C(28)	1.404(5)
C(27)-C(32)	1.514(5)
C(28)-C(29)	1.376(6)
C(29)-C(30)	1.371(6)
C(30)-C(31)	1.410(5)
C(31)-C(35)	1.520(5)
C(32)-C(34)	1.519(7)
C(32)-C(33)	1.538(6)
C(35)-C(37)	1.521(6)
C(35)-C(36)	1.525(5)
C(38)-C(43)	1.408(5)
C(38)-C(39)	1.411(5)

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C (39) -C (40)	1.391 (5)
C (39) -C (44)	1.522 (5)
C (40) -C (41)	1.381 (5)
C (41) -C (42)	1.387 (5)
C (42) -C (43)	1.398 (5)
C (43) -C (47)	1.521 (5)
C (44) -C (46)	1.522 (5)
C (44) -C (45)	1.532 (5)
C (47) -C (49)	1.532 (5)
C (47) -C (48)	1.536 (5)
C (51) -C (52)	1.515 (6)
C (52) -C (53)	1.504 (7)
C (53) -C (54)	1.522 (6)

F (1) -Sm (1) -N (1)	108.51 (9)
F (1) -Sm (1) -N (3)	133.59 (9)
N (1) -Sm (1) -N (3)	110.68 (9)
F (1) -Sm (1) -N (4)	99.23 (8)
N (1) -Sm (1) -N (4)	92.35 (9)
N (3) -Sm (1) -N (4)	55.75 (8)
F (1) -Sm (1) -N (2)	106.53 (9)
N (1) -Sm (1) -N (2)	55.55 (9)
N (3) -Sm (1) -N (2)	115.71 (9)
N (4) -Sm (1) -N (2)	143.67 (9)
F (1) -Sm (1) -O (1)	82.16 (8)
N (1) -Sm (1) -O (1)	139.35 (9)
N (3) -Sm (1) -O (1)	84.05 (8)
N (4) -Sm (1) -O (1)	125.41 (8)
N (2) -Sm (1) -O (1)	83.82 (9)
F (1) -Sm (1) -C (25)	105.01 (9)
N (1) -Sm (1) -C (25)	27.92 (9)
N (3) -Sm (1) -C (25)	121.24 (9)
N (4) -Sm (1) -C (25)	119.99 (9)
N (2) -Sm (1) -C (25)	28.41 (9)
O (1) -Sm (1) -C (25)	111.87 (9)
F (1) -Sm (1) -C (50)	117.89 (9)
N (1) -Sm (1) -C (50)	103.78 (9)
N (3) -Sm (1) -C (50)	28.01 (9)
N (4) -Sm (1) -C (50)	27.77 (8)
N (2) -Sm (1) -C (50)	135.41 (9)
O (1) -Sm (1) -C (50)	105.05 (8)
C (25) -Sm (1) -C (50)	126.18 (9)
C (51) -O (1) -C (54)	109.4 (3)
C (51) -O (1) -Sm (1)	122.2 (2)
C (54) -O (1) -Sm (1)	125.5 (2)
C (25) -N (1) -C (1)	119.1 (3)
C (25) -N (1) -Sm (1)	92.01 (18)
C (1) -N (1) -Sm (1)	147.0 (2)
C (25) -N (2) -C (13)	118.6 (3)
C (25) -N (2) -Sm (1)	91.00 (19)
C (13) -N (2) -Sm (1)	140.1 (2)
C (50) -N (3) -C (26)	119.0 (3)
C (50) -N (3) -Sm (1)	92.37 (19)
C (26) -N (3) -Sm (1)	146.7 (2)
C (50) -N (4) -C (38)	119.5 (3)
C (50) -N (4) -Sm (1)	92.29 (19)
C (38) -N (4) -Sm (1)	148.2 (2)
C (2) -C (1) -C (6)	119.9 (3)
C (2) -C (1) -N (1)	119.3 (3)
C (6) -C (1) -N (1)	120.7 (3)
C (3) -C (2) -C (1)	119.2 (3)

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C (3) -C (2) -C (7)	120.5 (3)
C (1) -C (2) -C (7)	120.3 (3)
C (4) -C (3) -C (2)	120.9 (3)
C (5) -C (4) -C (3)	120.0 (3)
C (4) -C (5) -C (6)	121.3 (3)
C (5) -C (6) -C (1)	118.7 (3)
C (5) -C (6) -C (10)	119.9 (3)
C (1) -C (6) -C (10)	121.2 (3)
C (9) -C (7) -C (2)	110.7 (3)
C (9) -C (7) -C (8)	110.0 (3)
C (2) -C (7) -C (8)	113.5 (3)
C (6) -C (10) -C (11)	109.7 (3)
C (6) -C (10) -C (12)	114.2 (3)
C (11) -C (10) -C (12)	109.7 (4)
C (14) -C (13) -C (18)	119.7 (3)
C (14) -C (13) -N (2)	119.4 (3)
C (18) -C (13) -N (2)	120.8 (3)
C (15) -C (14) -C (13)	119.2 (3)
C (15) -C (14) -C (19)	120.3 (3)
C (13) -C (14) -C (19)	120.5 (3)
C (16) -C (15) -C (14)	121.2 (3)
C (17) -C (16) -C (15)	119.5 (3)
C (16) -C (17) -C (18)	121.4 (3)
C (17) -C (18) -C (13)	119.0 (3)
C (17) -C (18) -C (22)	118.8 (3)
C (13) -C (18) -C (22)	122.2 (3)
C (21) -C (19) -C (20)	110.8 (3)
C (21) -C (19) -C (14)	110.9 (3)
C (20) -C (19) -C (14)	112.9 (3)
C (18) -C (22) -C (24)	111.5 (3)
C (18) -C (22) -C (23)	111.6 (3)
C (24) -C (22) -C (23)	110.3 (3)
N (1) -C (25) -N (2)	118.1 (3)
N (1) -C (25) -Sm (1)	60.06 (16)
N (2) -C (25) -Sm (1)	60.59 (17)
C (31) -C (26) -C (27)	120.4 (3)
C (31) -C (26) -N (3)	120.4 (3)
C (27) -C (26) -N (3)	119.1 (3)
C (28) -C (27) -C (26)	118.5 (3)
C (28) -C (27) -C (32)	119.3 (3)
C (26) -C (27) -C (32)	122.2 (3)
C (29) -C (28) -C (27)	121.0 (4)
C (28) -C (29) -C (30)	120.5 (4)
C (29) -C (30) -C (31)	120.8 (4)
C (26) -C (31) -C (30)	118.7 (3)
C (26) -C (31) -C (35)	122.6 (3)
C (30) -C (31) -C (35)	118.7 (3)
C (27) -C (32) -C (34)	110.9 (4)
C (27) -C (32) -C (33)	111.8 (4)
C (34) -C (32) -C (33)	109.3 (4)
C (31) -C (35) -C (37)	111.2 (3)
C (31) -C (35) -C (36)	111.8 (3)
C (37) -C (35) -C (36)	110.7 (3)
C (43) -C (38) -C (39)	120.4 (3)
C (43) -C (38) -N (4)	120.4 (3)
C (39) -C (38) -N (4)	119.2 (3)
C (40) -C (39) -C (38)	119.0 (3)
C (40) -C (39) -C (44)	120.9 (3)
C (38) -C (39) -C (44)	120.1 (3)
C (41) -C (40) -C (39)	121.4 (3)

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C (40) -C (41) -C (42)	119.1 (3)
C (41) -C (42) -C (43)	121.9 (3)
C (42) -C (43) -C (38)	118.1 (3)
C (42) -C (43) -C (47)	119.0 (3)
C (38) -C (43) -C (47)	122.9 (3)
C (46) -C (44) -C (39)	111.8 (3)
C (46) -C (44) -C (45)	109.3 (3)
C (39) -C (44) -C (45)	114.0 (3)
C (43) -C (47) -C (49)	111.2 (3)
C (43) -C (47) -C (48)	111.9 (3)
C (49) -C (47) -C (48)	110.0 (3)
N (4) -C (50) -N (3)	119.5 (3)
N (4) -C (50) -Sm (1)	59.94 (17)
N (3) -C (50) -Sm (1)	59.62 (17)
O (1) -C (51) -C (52)	105.8 (3)
C (53) -C (52) -C (51)	104.9 (4)
C (52) -C (53) -C (54)	102.5 (4)
O (1) -C (54) -C (53)	103.6 (3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{Å}^2 \times 10^3$) for
 [Sm(F) (DippForm)₂ (THF)].

The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^2 U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Sm(1)	18(1)	16(1)	18(1)	-2(1)	3(1)	-2(1)
F(1)	27(1)	36(1)	35(1)	4(1)	10(1)	6(1)
O(1)	27(1)	23(1)	35(1)	-2(1)	10(1)	-6(1)
N(1)	22(1)	17(1)	20(1)	0(1)	3(1)	-2(1)
N(2)	20(1)	14(1)	23(1)	0(1)	5(1)	0(1)
N(3)	21(1)	15(1)	22(1)	-1(1)	5(1)	1(1)
N(4)	21(1)	16(1)	21(1)	-1(1)	5(1)	0(1)
C(1)	27(2)	16(1)	21(2)	-4(1)	6(1)	-6(1)
C(2)	32(2)	19(1)	23(2)	-1(1)	7(1)	2(1)
C(3)	44(2)	18(2)	33(2)	-1(1)	14(2)	0(1)
C(4)	46(2)	22(2)	37(2)	-7(1)	16(2)	-13(2)
C(5)	31(2)	32(2)	32(2)	-5(2)	5(2)	-13(2)
C(6)	26(2)	27(2)	23(2)	0(1)	4(1)	-5(1)
C(7)	32(2)	18(2)	39(2)	2(1)	5(2)	4(1)
C(8)	45(2)	27(2)	33(2)	-1(2)	-6(2)	9(2)
C(9)	37(2)	35(2)	58(3)	8(2)	15(2)	8(2)
C(10)	25(2)	29(2)	42(2)	12(2)	-4(2)	-7(1)
C(11)	84(4)	40(2)	48(3)	-16(2)	-16(3)	30(3)
C(12)	39(2)	67(3)	31(2)	-2(2)	0(2)	8(2)
C(13)	25(2)	16(1)	19(1)	-2(1)	4(1)	-4(1)
C(14)	28(2)	21(2)	22(2)	-2(1)	4(1)	-3(1)
C(15)	39(2)	24(2)	29(2)	8(1)	8(2)	3(1)
C(16)	43(2)	31(2)	25(2)	5(1)	12(2)	-5(2)
C(17)	32(2)	30(2)	26(2)	-1(1)	11(1)	-3(1)
C(18)	27(2)	18(1)	20(2)	-2(1)	5(1)	-3(1)
C(19)	29(2)	21(2)	26(2)	-1(1)	4(1)	4(1)
C(20)	44(2)	24(2)	44(2)	-1(2)	10(2)	7(2)
C(21)	29(2)	31(2)	36(2)	-2(2)	7(2)	3(1)
C(22)	26(2)	25(2)	22(2)	-2(1)	6(1)	2(1)
C(23)	25(2)	34(2)	39(2)	-8(2)	5(2)	1(1)
C(24)	41(2)	25(2)	32(2)	-4(1)	6(2)	3(2)
C(25)	20(1)	19(1)	20(1)	-4(1)	1(1)	2(1)
C(26)	27(2)	17(1)	26(2)	-2(1)	8(1)	0(1)
C(27)	26(2)	25(2)	37(2)	-7(1)	3(2)	5(1)
C(28)	37(2)	34(2)	61(3)	-11(2)	4(2)	17(2)
C(29)	49(2)	25(2)	63(3)	-16(2)	11(2)	10(2)
C(30)	40(2)	21(2)	56(3)	-15(2)	9(2)	-3(2)
C(31)	29(2)	18(1)	38(2)	-6(1)	11(2)	-2(1)
C(32)	27(2)	36(2)	41(2)	-12(2)	1(2)	6(2)
C(33)	52(3)	63(3)	34(2)	2(2)	6(2)	-1(2)
C(34)	72(3)	44(3)	45(3)	3(2)	8(2)	-24(2)
C(35)	27(2)	23(2)	35(2)	-9(1)	9(1)	-7(1)
C(36)	38(2)	46(2)	29(2)	-3(2)	8(2)	-18(2)
C(37)	33(2)	36(2)	43(2)	9(2)	14(2)	1(2)
C(38)	28(2)	14(1)	17(1)	-3(1)	4(1)	2(1)
C(39)	26(2)	20(2)	21(2)	-2(1)	3(1)	1(1)
C(40)	34(2)	24(2)	22(2)	0(1)	1(1)	4(1)
C(41)	42(2)	18(2)	24(2)	1(1)	5(1)	1(1)
C(42)	35(2)	21(2)	24(2)	-2(1)	9(1)	-6(1)
C(43)	26(2)	18(1)	22(2)	-2(1)	4(1)	1(1)

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C (44)	25 (2)	29 (2)	31 (2)	2 (1)	6 (1)	4 (1)
C (45)	30 (2)	39 (2)	41 (2)	-1 (2)	5 (2)	7 (2)
C (46)	31 (2)	34 (2)	66 (3)	-7 (2)	14 (2)	-4 (2)
C (47)	24 (2)	22 (2)	26 (2)	2 (1)	6 (1)	-1 (1)
C (48)	29 (2)	34 (2)	31 (2)	-4 (2)	8 (1)	-7 (1)
C (49)	33 (2)	27 (2)	44 (2)	-4 (2)	15 (2)	2 (1)
C (50)	21 (2)	17 (1)	20 (2)	-1 (1)	4 (1)	-3 (1)
C (51)	37 (2)	25 (2)	37 (2)	0 (2)	3 (2)	-2 (2)
C (52)	69 (3)	32 (2)	67 (3)	14 (2)	27 (3)	0 (2)
C (53)	70 (3)	38 (2)	71 (4)	5 (2)	48 (3)	-7 (2)
C (54)	31 (2)	33 (2)	44 (2)	-4 (2)	16 (2)	-9 (2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for [Sm(F)(DippForm)₂(THF)].

	x	y	z	U (eq)
H(3)	4864	1128	2365	38
H(4)	3679	930	1786	41
H(5)	3020	2431	1274	40
H(7)	5782	3622	2769	38
H(8A)	5972	1302	2925	60
H(8B)	5717	2048	3406	60
H(8C)	6478	2217	3369	60
H(9A)	6032	2095	1882	66
H(9B)	6592	2946	2327	66
H(9C)	5921	3383	1749	66
H(10)	3623	5054	1090	44
H(11A)	2844	4667	1932	101
H(11B)	2959	5825	1638	101
H(11C)	3597	5227	2179	101
H(12A)	2788	3763	390	73
H(12B)	2480	4941	465	73
H(12C)	2349	3917	870	73
H(15)	4641	8725	-161	38
H(16)	5496	8052	-548	40
H(17)	6202	6611	-5	35
H(19)	4360	7889	1305	32
H(20A)	4581	9670	993	58
H(20B)	3790	9547	953	58
H(20C)	3978	9514	295	58
H(21A)	3408	7617	-1	50
H(21B)	3181	7769	631	50
H(21C)	3600	6698	559	50
H(22)	6144	5256	1448	30
H(23A)	7152	5978	890	52
H(23B)	7314	5270	1547	52
H(23C)	7065	6516	1531	52
H(24A)	5670	4208	472	51
H(24B)	6453	3847	868	51
H(24C)	6287	4606	230	51
H(25)	4692	4868	987	25
H(28)	3628	9667	3223	56
H(29)	4436	10761	3983	58
H(30)	5585	10220	4427	49
H(32)	3971	7059	2622	45
H(33A)	3005	8848	2249	78
H(33B)	3027	7811	1804	78
H(33C)	3628	8717	1966	78
H(34A)	3501	6732	3444	86
H(34B)	2877	6781	2754	86
H(34C)	3026	7806	3243	86
H(35)	6309	7739	4031	34
H(36A)	6559	9435	3640	58
H(36B)	7186	9073	4285	58
H(36C)	6649	9994	4333	58
H(37A)	6348	8834	5208	56
H(37B)	6957	8051	5161	56

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H (37C)	6202	7556	5056	56
H (40)	6820	2787	5090	34
H (41)	5854	1989	5243	35
H (42)	4743	2587	4617	32
H (44)	6802	4628	3846	35
H (45A)	7925	4035	4355	58
H (45B)	7437	2987	4296	58
H (45C)	7759	3611	4985	58
H (46A)	6721	6012	4579	67
H (46B)	7501	5883	4584	67
H (46C)	7288	5383	5172	67
H (47)	4322	4696	3389	30
H (48A)	4103	2822	3081	47
H (48B)	3405	3426	3071	47
H (48C)	3810	2636	3670	47
H (49A)	3880	4162	4472	51
H (49B)	3470	4952	3875	51
H (49C)	4209	5317	4386	51
H (50)	5180	6245	4164	24
H (51A)	5639	9130	2592	43
H (51B)	5393	8523	1890	43
H (52A)	6032	9778	1607	67
H (52B)	6455	10090	2361	67
H (53A)	7300	9164	2118	64
H (53B)	6750	8345	1618	64
H (54A)	7150	7258	2546	42
H (54B)	7216	8285	3032	42
