Table 1. Crystal data and structure refinement for Complex **1**

Identification code	sg277
Empirical formula	C34 H56 Cl Li2 N3 O4 Sm
Formula weight	770.50
Temperature	173(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 11.307(4) A alpha = 89.778(4) deg. b = 13.137(5) A beta = 81.829(4) deg. c = 17.091(6) A gamma = 66.946(4) deg.
Volume	2308(1) A^3
Z, Calculated density	2, 1.108 Mg/m^3
Absorption coefficient	1.360 mm^-1
F(000)	796
Crystal size	0.20 x 0.20 x 0.04 mm
Theta range for data collection	2.02 to 20.82 deg.
Limiting indices	-11<=h<=11, -13<=k<=13, 0<=l<=17
Reflections collected / unique	17694 / 4811 [R(int) = 0.2535]
Completeness to theta = 20.82	99.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.928070 and 0.546092
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4811 / 0 / 406
Goodness-of-fit on F^2	1.013

Final R indices [I>2sigma(I)]	R1 = 0.0824, wR2 = 0.2028
R indices (all data)	R1 = 0.1264, wR2 = 0.2208
Largest diff. peak and hole	0.997 and -1.296 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for Complex **1**
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Sm	7585(1)	8301(1)	7920(1)	39(1)
Cl	9197(4)	7678(4)	6386(3)	59(2)
Li(1)	7340(30)	8330(20)	5780(20)	55(9)
Li(2)	9510(30)	7650(30)	9595(18)	55(9)
N(1)	5830(12)	8895(13)	6716(9)	45(4)
N(2)	8948(12)	9083(11)	8937(8)	39(4)
N(3)	8787(13)	6682(11)	9047(8)	35(4)
O(1)	7474(13)	9400(13)	5003(8)	81(5)
O(2)	7391(13)	7075(12)	5074(8)	78(5)
O(3)	8872(17)	7958(12)	10769(8)	81(5)
O(4)	11341(14)	6957(11)	9649(10)	90(5)
C(1)	5725(18)	10856(15)	6803(11)	57(6)
C(2)	5437(19)	9856(14)	7175(15)	58(7)
C(3)	4782(17)	9820(20)	7929(12)	64(7)
C(4)	4769(17)	8751(18)	7918(13)	57(6)
C(5)	5366(17)	8207(17)	7213(12)	48(5)
C(6)	5470(20)	7140(17)	6926(11)	65(6)
C(7)	6759(16)	10102(15)	9865(9)	55(6)
C(8)	7665(17)	9919(15)	9077(11)	50(5)
C(9)	7489(19)	10511(14)	8405(12)	55(6)
C(10)	8616(16)	10061(15)	7837(10)	43(5)
C(11)	9513(15)	9214(13)	8185(10)	33(5)
C(12)	10905(17)	8502(16)	7880(11)	66(6)
C(13)	6655(19)	7265(15)	9940(12)	74(7)
C(14)	7540(20)	6775(15)	9201(11)	52(6)
C(15)	7290(20)	6265(17)	8485(14)	68(6)
C(16)	8430(20)	5833(14)	7975(13)	65(7)
C(17)	9370(20)	6090(14)	8302(14)	70(8)
C(18)	10773(16)	5759(15)	7985(11)	60(6)
C(19)	8670(20)	9730(20)	4928(12)	104(9)
C(20)	8740(20)	10130(20)	4119(14)	102(9)
C(21)	7310(20)	10480(20)	3884(14)	116(11)
C(22)	6740(20)	9780(20)	4358(15)	111(10)
C(23)	6510(20)	6930(20)	4640(14)	102(9)
C(24)	7180(20)	6190(30)	3944(15)	163(16)

C(25)	8610(20)	5670(20)	4099(15)	121(11)
C(26)	8590(20)	6200(30)	4869(19)	230(20)
C(27)	9160(30)	8690(20)	11194(15)	111(10)
C(28)	9380(40)	8280(30)	11980(16)	146(13)
C(29)	9080(30)	7420(20)	12039(18)	125(12)
C(30)	8840(40)	7150(20)	11283(17)	162(17)
C(31)	12250(30)	7510(20)	9664(17)	105(9)
C(32)	13430(30)	6750(30)	9700(30)	230(20)
C(33)	13170(40)	5590(30)	9810(40)	300(40)
C(34)	12000(30)	5850(20)	9843(18)	112(10)

Table 3. Bond lengths [A] and angles [deg] for Complex **1**

Sm-Cl	2.891(4)
Sm-N(2)	2.910(14)
Sm-N(3)	2.920(13)
Sm-C(2)	2.944(16)
Sm-C(8)	2.945(18)
Sm-C(17)	2.949(17)
Sm-N(1)	2.953(14)
Sm-C(11)	2.955(17)
Sm-C(15)	2.963(19)
Sm-C(10)	2.964(19)
Sm-C(14)	2.971(17)
Sm-C(9)	2.979(17)
Cl-Li(1)	2.33(3)
Li(1)-O(1)	1.96(3)
Li(1)-O(2)	2.03(3)
Li(1)-N(1)	2.06(3)
Li(2)-O(4)	1.92(3)
Li(2)-O(3)	2.02(3)
Li(2)-N(3)	2.05(4)
Li(2)-N(2)	2.12(3)
N(1)-C(2)	1.37(2)
N(1)-C(5)	1.43(2)
N(2)-C(11)	1.393(18)
N(2)-C(8)	1.42(2)
N(3)-C(14)	1.36(2)
N(3)-C(17)	1.42(2)
O(1)-C(22)	1.45(3)
O(1)-C(19)	1.56(3)
O(2)-C(26)	1.39(2)
O(2)-C(23)	1.39(3)
O(3)-C(27)	1.37(3)
O(3)-C(30)	1.39(3)
O(4)-C(34)	1.41(3)
O(4)-C(31)	1.48(2)
C(1)-C(2)	1.58(2)
C(2)-C(3)	1.40(3)
C(3)-C(4)	1.41(3)
C(4)-C(5)	1.35(2)
C(5)-C(6)	1.44(2)
C(7)-C(8)	1.53(2)
C(8)-C(9)	1.38(2)
C(9)-C(10)	1.41(2)

C(10)-C(11)	1.38(2)
C(11)-C(12)	1.50(2)
C(13)-C(14)	1.47(2)
C(14)-C(15)	1.50(3)
C(15)-C(16)	1.36(3)
C(16)-C(17)	1.41(3)
C(17)-C(18)	1.49(3)
C(19)-C(20)	1.48(3)
C(20)-C(21)	1.62(3)
C(21)-C(22)	1.49(3)
C(23)-C(24)	1.45(3)
C(24)-C(25)	1.55(3)
C(25)-C(26)	1.49(3)
C(27)-C(28)	1.46(3)
C(28)-C(29)	1.31(3)
C(29)-C(30)	1.43(3)
C(31)-C(32)	1.33(3)
C(32)-C(33)	1.67(4)
C(33)-C(34)	1.23(3)

Cl-Sm-N(2)	107.2(3)
Cl-Sm-N(3)	109.2(3)
N(2)-Sm-N(3)	67.4(4)
Cl-Sm-C(2)	89.7(5)
N(2)-Sm-C(2)	121.5(4)
N(3)-Sm-C(2)	156.3(6)
Cl-Sm-C(8)	124.5(4)
N(2)-Sm-C(8)	28.1(4)
N(3)-Sm-C(8)	84.2(5)
C(2)-Sm-C(8)	96.9(5)
Cl-Sm-C(17)	82.8(5)
N(2)-Sm-C(17)	83.7(5)
N(3)-Sm-C(17)	28.1(5)
C(2)-Sm-C(17)	154.8(5)
C(8)-Sm-C(17)	107.2(5)
Cl-Sm-N(1)	72.7(3)
N(2)-Sm-N(1)	145.8(4)
N(3)-Sm-N(1)	146.2(4)
C(2)-Sm-N(1)	26.9(4)
C(8)-Sm-N(1)	123.6(5)
C(17)-Sm-N(1)	129.0(5)
Cl-Sm-C(11)	81.6(3)
N(2)-Sm-C(11)	27.5(4)
N(3)-Sm-C(11)	84.7(4)
C(2)-Sm-C(11)	112.8(5)
C(8)-Sm-C(11)	45.2(4)

C(17)-Sm-C(11)	90.0(5)
N(1)-Sm-C(11)	127.9(5)
Cl-Sm-C(15)	105.9(5)
N(2)-Sm-C(15)	111.9(5)
N(3)-Sm-C(15)	45.9(5)
C(2)-Sm-C(15)	116.3(6)
C(8)-Sm-C(15)	119.3(6)
C(17)-Sm-C(15)	44.5(6)
N(1)-Sm-C(15)	100.5(5)
C(11)-Sm-C(15)	130.2(5)
Cl-Sm-C(10)	80.7(3)
N(2)-Sm-C(10)	45.4(4)
N(3)-Sm-C(10)	110.6(4)
C(2)-Sm-C(10)	85.8(5)
C(8)-Sm-C(10)	45.4(5)
C(17)-Sm-C(10)	116.4(6)
N(1)-Sm-C(10)	103.1(5)
C(11)-Sm-C(10)	27.0(4)
C(15)-Sm-C(10)	156.5(5)
Cl-Sm-C(14)	125.7(4)
N(2)-Sm-C(14)	84.1(5)
N(3)-Sm-C(14)	26.7(4)
C(2)-Sm-C(14)	129.8(7)
C(8)-Sm-C(14)	90.3(6)
C(17)-Sm-C(14)	44.9(6)
N(1)-Sm-C(14)	124.7(6)
C(11)-Sm-C(14)	107.2(6)
C(15)-Sm-C(14)	29.4(5)
C(10)-Sm-C(14)	129.4(6)
Cl-Sm-C(9)	106.3(4)
N(2)-Sm-C(9)	44.9(4)
N(3)-Sm-C(9)	109.8(5)
C(2)-Sm-C(9)	76.7(5)
C(8)-Sm-C(9)	26.9(4)
C(17)-Sm-C(9)	128.5(5)
N(1)-Sm-C(9)	101.4(5)
C(11)-Sm-C(9)	44.2(5)
C(15)-Sm-C(9)	145.1(6)
C(10)-Sm-C(9)	27.4(5)
C(14)-Sm-C(9)	116.9(6)
Li(1)-Cl-Sm	89.8(8)
O(1)-Li(1)-O(2)	101.7(16)
O(1)-Li(1)-N(1)	117.5(15)
O(2)-Li(1)-N(1)	116.1(16)
O(1)-Li(1)-Cl	109.4(14)
O(2)-Li(1)-Cl	107.8(13)

N(1)-Li(1)-Cl	104.0(15)
O(1)-Li(1)-Sm	129.9(14)
O(2)-Li(1)-Sm	127.4(13)
N(1)-Li(1)-Sm	52.7(8)
Cl-Li(1)-Sm	51.3(7)
O(4)-Li(2)-O(3)	97.7(15)
O(4)-Li(2)-N(3)	114.8(17)
O(3)-Li(2)-N(3)	114.7(16)
O(4)-Li(2)-N(2)	114.8(16)
O(3)-Li(2)-N(2)	113.6(16)
N(3)-Li(2)-N(2)	101.9(14)
O(4)-Li(2)-Sm	133.5(14)
O(3)-Li(2)-Sm	128.9(13)
N(3)-Li(2)-Sm	51.0(8)
N(2)-Li(2)-Sm	50.9(8)
C(2)-N(1)-C(5)	103.4(16)
C(2)-N(1)-Li(1)	126.8(17)
C(5)-N(1)-Li(1)	125.3(15)
C(2)-N(1)-Sm	76.2(9)
C(5)-N(1)-Sm	77.1(9)
Li(1)-N(1)-Sm	93.5(10)
C(11)-N(2)-C(8)	107.2(13)
C(11)-N(2)-Li(2)	127.6(14)
C(8)-N(2)-Li(2)	121.9(14)
C(11)-N(2)-Sm	78.1(9)
C(8)-N(2)-Sm	77.3(10)
Li(2)-N(2)-Sm	94.7(10)
C(14)-N(3)-C(17)	108.5(16)
C(14)-N(3)-Li(2)	124.5(16)
C(17)-N(3)-Li(2)	124.1(16)
C(14)-N(3)-Sm	78.8(10)
C(17)-N(3)-Sm	77.1(9)
Li(2)-N(3)-Sm	96.0(9)
C(22)-O(1)-C(19)	112.0(15)
C(22)-O(1)-Li(1)	127.7(18)
C(19)-O(1)-Li(1)	119.1(15)
C(26)-O(2)-C(23)	108.6(18)
C(26)-O(2)-Li(1)	116.5(18)
C(23)-O(2)-Li(1)	134.2(16)
C(27)-O(3)-C(30)	105.6(18)
C(27)-O(3)-Li(2)	121.0(17)
C(30)-O(3)-Li(2)	123.3(19)
C(34)-O(4)-C(31)	106.9(16)
C(34)-O(4)-Li(2)	124.9(17)
C(31)-O(4)-Li(2)	127.1(17)
N(1)-C(2)-C(3)	113.5(19)

N(1)-C(2)-C(1)	118(2)
C(3)-C(2)-C(1)	128(2)
N(1)-C(2)-Sm	76.9(9)
C(3)-C(2)-Sm	79.0(11)
C(1)-C(2)-Sm	113.6(11)
C(2)-C(3)-C(4)	103.2(18)
C(2)-C(3)-Sm	73.7(10)
C(4)-C(3)-Sm	76.1(11)
C(5)-C(4)-C(3)	110.2(19)
C(5)-C(4)-Sm	76.0(11)
C(3)-C(4)-Sm	76.7(11)
C(4)-C(5)-N(1)	109.7(18)
C(4)-C(5)-C(6)	128(2)
N(1)-C(5)-C(6)	121.6(18)
C(4)-C(5)-Sm	77.9(11)
N(1)-C(5)-Sm	75.0(9)
C(6)-C(5)-Sm	117.7(12)
C(9)-C(8)-N(2)	106.8(15)
C(9)-C(8)-C(7)	130.0(17)
N(2)-C(8)-C(7)	123.1(16)
C(9)-C(8)-Sm	77.9(10)
N(2)-C(8)-Sm	74.6(9)
C(7)-C(8)-Sm	116.0(12)
C(8)-C(9)-C(10)	109.8(16)
C(8)-C(9)-Sm	75.2(10)
C(10)-C(9)-Sm	75.7(10)
C(11)-C(10)-C(9)	106.5(15)
C(11)-C(10)-Sm	76.1(11)
C(9)-C(10)-Sm	76.9(10)
C(10)-C(11)-N(2)	109.6(13)
C(10)-C(11)-C(12)	129.9(16)
N(2)-C(11)-C(12)	120.4(15)
C(10)-C(11)-Sm	76.9(11)
N(2)-C(11)-Sm	74.5(9)
C(12)-C(11)-Sm	116.1(11)
N(3)-C(14)-C(13)	124(2)
N(3)-C(14)-C(15)	106.4(15)
C(13)-C(14)-C(15)	129(2)
N(3)-C(14)-Sm	74.6(9)
C(13)-C(14)-Sm	117.0(12)
C(15)-C(14)-Sm	75.0(10)
C(16)-C(15)-C(14)	108(2)
C(16)-C(15)-Sm	78.5(12)
C(14)-C(15)-Sm	75.6(10)
C(15)-C(16)-C(17)	108(2)
C(15)-C(16)-Sm	75.1(11)

C(17)-C(16)-Sm	74.1(10)
C(16)-C(17)-N(3)	109(2)
C(16)-C(17)-C(18)	128(2)
N(3)-C(17)-C(18)	122.4(17)
C(16)-C(17)-Sm	78.5(10)
N(3)-C(17)-Sm	74.8(9)
C(18)-C(17)-Sm	116.4(13)
C(20)-C(19)-O(1)	104(2)
C(19)-C(20)-C(21)	106(2)
C(22)-C(21)-C(20)	105(2)
O(1)-C(22)-C(21)	107(2)
O(2)-C(23)-C(24)	111(2)
C(23)-C(24)-C(25)	103(2)
C(26)-C(25)-C(24)	104.9(18)
O(2)-C(26)-C(25)	108(2)
O(3)-C(27)-C(28)	109(2)
C(29)-C(28)-C(27)	107(3)
C(28)-C(29)-C(30)	109(3)
O(3)-C(30)-C(29)	109(2)
C(32)-C(31)-O(4)	109(2)
C(31)-C(32)-C(33)	103(3)
C(34)-C(33)-C(32)	106(3)
C(33)-C(34)-O(4)	113(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for Complex **1**
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Sm	45(1)	34(1)	35(1)	10(1)	-13(1)	-12(1)
Cl	47(3)	82(4)	36(3)	5(3)	-11(2)	-11(3)
Li(1)	60(20)	27(18)	70(20)	5(17)	-11(17)	-20(15)
Li(2)	70(20)	60(20)	50(20)	34(18)	-29(17)	-35(18)
N(1)	36(9)	49(11)	53(11)	19(10)	-19(7)	-17(8)
N(2)	38(9)	31(9)	46(11)	11(8)	-13(7)	-11(7)
N(3)	49(10)	35(9)	37(10)	5(8)	0(7)	-34(7)
O(1)	66(10)	149(15)	60(10)	61(10)	-35(8)	-68(10)
O(2)	59(10)	102(12)	68(10)	-21(9)	-16(8)	-24(9)
O(3)	191(16)	47(10)	36(9)	5(8)	-14(9)	-80(10)
O(4)	86(11)	35(9)	173(16)	43(10)	-88(11)	-27(8)
C(1)	79(14)	54(14)	50(13)	18(11)	-1(10)	-44(11)
C(2)	60(13)	16(12)	100(20)	-11(13)	-65(13)	0(10)
C(3)	42(12)	90(20)	34(14)	-13(13)	-13(10)	2(12)
C(4)	55(13)	42(15)	59(17)	0(12)	-15(11)	0(11)
C(5)	46(12)	67(15)	46(14)	1(14)	-17(10)	-36(11)
C(6)	100(17)	90(18)	49(14)	17(13)	-28(11)	-79(14)
C(7)	61(13)	62(14)	34(12)	-6(10)	19(10)	-23(10)
C(8)	64(14)	34(12)	45(14)	6(11)	-11(11)	-10(10)
C(9)	73(15)	22(11)	75(16)	3(12)	-54(13)	-11(10)
C(10)	41(12)	69(14)	16(10)	14(10)	-16(9)	-15(11)
C(11)	35(11)	34(11)	23(11)	1(9)	7(9)	-12(9)
C(12)	71(15)	79(16)	66(15)	20(13)	-16(11)	-48(13)
C(13)	93(17)	40(13)	92(19)	11(13)	-24(14)	-28(12)
C(14)	74(16)	52(13)	31(13)	10(11)	24(11)	-36(11)
C(15)	85(18)	55(15)	80(18)	39(14)	-52(15)	-33(13)
C(16)	81(17)	10(11)	78(17)	-3(11)	-25(14)	14(10)
C(17)	110(20)	15(11)	99(19)	11(12)	-94(17)	-15(12)
C(18)	30(12)	55(13)	84(16)	10(12)	1(10)	-9(9)
C(19)	130(20)	150(30)	33(16)	42(16)	7(13)	-65(19)
C(20)	110(20)	110(20)	90(20)	-7(17)	-33(15)	-38(17)
C(21)	100(20)	190(30)	65(18)	80(20)	-18(15)	-70(20)
C(22)	62(17)	180(30)	90(20)	70(20)	-18(15)	-42(17)
C(23)	90(20)	130(20)	68(18)	-18(17)	-28(15)	-21(17)

C(24)	80(20)	300(40)	80(20)	-70(20)	-15(15)	-30(20)
C(25)	110(20)	110(20)	100(20)	-48(17)	-25(16)	18(16)
C(26)	62(19)	320(50)	180(30)	-190(30)	-52(19)	70(20)
C(27)	170(30)	100(20)	70(20)	22(18)	-12(17)	-50(20)
C(28)	290(40)	130(30)	70(20)	30(20)	-80(20)	-110(30)
C(29)	230(40)	70(20)	120(30)	31(18)	-50(20)	-100(20)
C(30)	370(50)	110(30)	100(20)	70(20)	-150(30)	-160(30)
C(31)	90(20)	100(20)	170(30)	65(19)	-104(19)	-65(19)
C(32)	110(30)	140(30)	470(70)	170(40)	-90(40)	-60(20)
C(33)	110(30)	130(30)	690(110)	250(50)	-90(40)	-50(20)
C(34)	90(20)	100(20)	200(30)	70(20)	-110(20)	-55(18)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for Complex 1

	x	y	z	U(eq)
H(1A)	6196	10633	6263	85
H(1B)	6256	11062	7126	85
H(1C)	4903	11491	6790	85
H(3A)	4432	10382	8346	77
H(4A)	4394	8456	8346	69
H(6A)	5114	6793	7353	97
H(6B)	6388	6667	6749	97
H(6C)	4984	7234	6482	97
H(7A)	5917	10700	9825	83
H(7B)	7145	10304	10286	83
H(7C)	6634	9418	9989	83
H(9A)	6722	11129	8336	65
H(10A)	8736	10295	7315	52
H(12A)	11139	8708	7346	99
H(12B)	11022	7722	7860	99
H(12C)	11464	8608	8232	99
H(13A)	7099	7539	10288	110
H(13B)	6402	6702	10205	110
H(13C)	5878	7881	9823	110
H(15A)	6487	6247	8404	81
H(16A)	8571	5431	7486	78
H(18A)	10970	5373	7464	89
H(18B)	11303	5266	8347	89
H(18C)	10970	6422	7937	89
H(19A)	8528	10318	5331	125
H(19B)	9470	9079	4988	125
H(20A)	9396	9537	3743	122
H(20B)	8992	10774	4112	122
H(21A)	6776	11278	4020	139
H(21B)	7356	10332	3310	139
H(22A)	5809	10219	4567	134
H(22B)	6797	9142	4026	134
H(23A)	5934	7653	4475	123
H(23B)	5965	6615	4978	123
H(24A)	7103	6602	3456	195
H(24B)	6830	5611	3898	195
H(25A)	8907	4859	4130	145

H(25B)	9189	5833	3672	145
H(26A)	8742	5656	5283	276
H(26B)	9295	6483	4822	276
H(27A)	8431	9424	11245	133
H(27B)	9948	8764	10917	133
H(28A)	10305	8067	12040	176
H(28B)	8832	8859	12396	176
H(29A)	8290	7585	12439	150
H(29B)	9798	6781	12210	150
H(30A)	9506	6417	11070	195
H(30B)	7975	7103	11337	195
H(31A)	12265	7929	9181	127
H(31B)	11961	8043	10131	127
H(32A)	13789	6916	10155	277
H(32B)	14033	6699	9206	277
H(33A)	13655	5050	9356	363
H(33B)	13465	5242	10302	363
H(34A)	11630	5755	10385	135
H(34B)	11850	5351	9474	135

Table 6. Crystal data and structure refinement for Complex **2**

Identification code	sg060
Empirical formula	C30 H55 I Li2 N5 O1.50 Sm
Formula weight	800.92
Temperature	203(2) K
Wavelength	0.71073 A
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	a = 21.147(1) A alpha = 90 deg. b = 10.1298(5) A beta = 117.247(1) deg. c = 19.766(1) A gamma = 90 deg.
Volume, Z	3764.4(3) A^3, 4
Density (calculated)	1.413 Mg/m^3
Absorption coefficient	2.408 mm^-1
F(000)	1612
Crystal size	0.30 x 0.30 x 0.30 mm
Theta range for data collection	2.06 to 25.00 deg.
Limiting indices	-23<=h<=27, -13<=k<=13, -26<=l<=26
Reflections collected	18778
Independent reflections	6580 [R(int) = 0.0743]
Absorption correction	SADABS empirical
Max. and min. transmission	0.862146 and 0.623697

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6580 / 0 / 352
Goodness-of-fit on F^2	1.030
Final R indices [I>2sigma(I)]	R1 = 0.0422, wR2 = 0.1022
R indices (all data)	R1 = 0.0604, wR2 = 0.1085
Largest diff. peak and hole	1.653 and -1.189 e.A^-3

Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for Complex **2**
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Sm	2773(1)	5471(1)	4826(1)	33(1)
I	2865(1)	7043(1)	6300(1)	51(1)
Li(1)	3810(5)	4900(8)	7076(5)	36(2)
Li(2)	1480(6)	6770(13)	3033(7)	71(3)
N(1)	3804(2)	4086(4)	6144(2)	30(1)
N(2)	1307(2)	5306(5)	3680(3)	47(1)
N(3)	2480(3)	7315(4)	3603(2)	45(1)
N(4)	3438(3)	4113(5)	7845(3)	53(1)
N(5)	4754(3)	5475(5)	8107(3)	49(1)
O(1)	792(3)	7519(7)	2105(3)	97(2)
C(1)	4738(3)	5578(6)	6126(3)	49(2)
C(2)	4184(3)	4520(5)	5778(3)	33(1)
C(3)	3993(3)	3823(5)	5110(3)	38(1)
C(4)	3485(3)	2900(5)	5063(3)	40(1)
C(5)	3390(3)	3069(5)	5707(3)	35(1)
C(6)	2938(3)	2274(6)	5967(3)	48(1)
C(7)	1627(5)	3489(10)	3032(5)	102(3)
C(8)	1528(3)	4151(7)	3675(3)	54(2)
C(9)	1613(3)	3481(7)	4314(4)	64(2)
C(10)	1417(3)	4408(7)	4712(4)	60(2)
C(11)	1225(3)	5524(6)	4257(4)	57(2)
C(12)	920(4)	6784(8)	4424(5)	93(3)
C(13)	3022(5)	5724(6)	3047(4)	71(2)
C(14)	3068(3)	6651(5)	3661(3)	47(1)
C(15)	3664(3)	7001(6)	4312(3)	53(2)
C(16)	3444(3)	7940(6)	4681(3)	53(2)
C(17)	2721(3)	8131(5)	4236(3)	48(1)
C(18)	2236(5)	9101(6)	4329(5)	80(2)
C(19)	2675(5)	4368(9)	7596(6)	113(4)
C(20)	3546(4)	2719(6)	7987(4)	65(2)
C(21)	3838(6)	4921(8)	8516(5)	91(3)
C(22)	4581(5)	4997(9)	8717(4)	82(2)
C(23)	4754(4)	6916(6)	8102(4)	80(2)
C(24)	5447(4)	4992(8)	8251(4)	71(2)
C(31)	856(8)	9596(13)	1639(11)	221(9)
C(32)	1033(7)	8361(16)	1683(8)	175(7)

C(33)	80(6)	7380(16)	1783(11)	241(11)
C(34)	-163(6)	6075(16)	1864(8)	196(7)
O(2)	0	0	5000	195(6)
C(35)	1275(18)	579(27)	5867(18)	296(14)
C(36)	799(20)	412(37)	5518(23)	405(21)

Table 8. Bond lengths [A] and angles [deg] for Complex **2**

Sm-C(2)	2.869(5)
Sm-N(1)	2.882(4)
Sm-N(2)	2.887(4)
Sm-N(3)	2.889(4)
Sm-C(8)	2.900(5)
Sm-C(3)	2.905(5)
Sm-C(14)	2.905(5)
Sm-C(17)	2.918(5)
Sm-C(5)	2.928(5)
Sm-C(11)	2.935(6)
Sm-C(4)	2.937(5)
Sm-C(15)	2.958(6)
I-Li(1)	2.873(9)
Li(1)-N(1)	2.016(9)
Li(1)-N(4)	2.158(9)
Li(1)-N(5)	2.179(10)
Li(2)-O(1)	1.901(12)
Li(2)-N(3)	1.965(13)
Li(2)-N(2)	2.095(13)
N(1)-C(5)	1.372(6)
N(1)-C(2)	1.375(6)
N(2)-C(11)	1.251(8)
N(2)-C(8)	1.262(8)
N(3)-C(14)	1.372(7)
N(3)-C(17)	1.386(7)
N(4)-C(20)	1.437(7)
N(4)-C(19)	1.478(10)
N(4)-C(21)	1.457(9)
N(5)-C(24)	1.443(8)
N(5)-C(23)	1.461(8)
N(5)-C(22)	1.492(8)
O(1)-C(33)	1.347(12)
O(1)-C(32)	1.440(12)
C(1)-C(2)	1.502(7)
C(2)-C(3)	1.384(7)
C(3)-C(4)	1.395(7)
C(4)-C(5)	1.389(7)
C(5)-C(6)	1.509(7)
C(7)-C(8)	1.534(10)
C(8)-C(9)	1.371(9)
C(9)-C(10)	1.404(9)
C(10)-C(11)	1.384(9)

C(11)-C(12)	1.532(10)
C(13)-C(14)	1.502(8)
C(14)-C(15)	1.374(8)
C(15)-C(16)	1.400(8)
C(16)-C(17)	1.385(9)
C(17)-C(18)	1.491(9)
C(21)-C(22)	1.436(11)
C(31)-C(32)	1.30(2)
C(33)-C(34)	1.45(2)
O(2)-C(36)	1.58(4)
O(2)-C(36)#1	1.58(4)
C(35)-C(36)	0.94(4)

C(2)-Sm-N(1)	27.66(12)
C(2)-Sm-N(2)	156.3(2)
N(1)-Sm-N(2)	141.04(13)
C(2)-Sm-N(3)	121.74(14)
N(1)-Sm-N(3)	148.70(12)
N(2)-Sm-N(3)	68.81(14)
C(2)-Sm-C(8)	131.1(2)
N(1)-Sm-C(8)	121.6(2)
N(2)-Sm-C(8)	25.2(2)
N(3)-Sm-C(8)	82.6(2)
C(2)-Sm-C(3)	27.73(14)
N(1)-Sm-C(3)	46.17(12)
N(2)-Sm-C(3)	131.1(2)
N(3)-Sm-C(3)	111.38(14)
C(8)-Sm-C(3)	107.1(2)
C(2)-Sm-C(14)	97.0(2)
N(1)-Sm-C(14)	124.6(2)
N(2)-Sm-C(14)	86.8(2)
N(3)-Sm-C(14)	27.39(14)
C(8)-Sm-C(14)	90.8(2)
C(3)-Sm-C(14)	84.0(2)
C(2)-Sm-C(17)	114.2(2)
N(1)-Sm-C(17)	133.2(2)
N(2)-Sm-C(17)	84.8(2)
N(3)-Sm-C(17)	27.61(14)
C(8)-Sm-C(17)	104.9(2)
C(3)-Sm-C(17)	118.4(2)
C(14)-Sm-C(17)	44.4(2)
C(2)-Sm-C(5)	44.33(14)
N(1)-Sm-C(5)	27.30(12)
N(2)-Sm-C(5)	116.4(2)
N(3)-Sm-C(5)	154.35(14)
C(8)-Sm-C(5)	94.6(2)

C(3)-Sm-C(5)	45.01(14)
C(14)-Sm-C(5)	127.9(2)
C(17)-Sm-C(5)	158.4(2)
C(2)-Sm-C(11)	154.2(2)
N(1)-Sm-C(11)	127.3(2)
N(2)-Sm-C(11)	24.8(2)
N(3)-Sm-C(11)	83.9(2)
C(8)-Sm-C(11)	41.9(2)
C(3)-Sm-C(11)	145.2(2)
C(14)-Sm-C(11)	107.2(2)
C(17)-Sm-C(11)	89.9(2)
C(5)-Sm-C(11)	111.0(2)
C(2)-Sm-C(4)	45.11(14)
N(1)-Sm-C(4)	45.86(13)
N(2)-Sm-C(4)	111.2(2)
N(3)-Sm-C(4)	127.18(14)
C(8)-Sm-C(4)	86.0(2)
C(3)-Sm-C(4)	27.6(2)
C(14)-Sm-C(4)	102.1(2)
C(17)-Sm-C(4)	143.6(2)
C(5)-Sm-C(4)	27.40(13)
C(11)-Sm-C(4)	118.6(2)
C(2)-Sm-C(15)	76.5(2)
N(1)-Sm-C(15)	103.17(14)
N(2)-Sm-C(15)	112.6(2)
N(3)-Sm-C(15)	45.5(2)
C(8)-Sm-C(15)	117.6(2)
C(3)-Sm-C(15)	73.6(2)
C(14)-Sm-C(15)	27.1(2)
C(17)-Sm-C(15)	44.9(2)
C(5)-Sm-C(15)	117.4(2)
C(11)-Sm-C(15)	129.3(2)
C(4)-Sm-C(15)	99.1(2)
Li(1)-I-Sm	81.4(2)
N(1)-Li(1)-N(4)	129.9(4)
N(1)-Li(1)-N(5)	125.7(5)
N(4)-Li(1)-N(5)	85.1(3)
N(1)-Li(1)-I	96.3(3)
N(4)-Li(1)-I	105.5(4)
N(5)-Li(1)-I	114.4(3)
O(1)-Li(2)-N(3)	126.0(7)
O(1)-Li(2)-N(2)	126.9(7)
N(3)-Li(2)-N(2)	106.9(5)
O(1)-Li(2)-Sm	177.7(7)
N(3)-Li(2)-Sm	53.4(3)
N(2)-Li(2)-Sm	53.5(3)

C(5)-N(1)-C(2)	105.6(4)
C(5)-N(1)-Li(1)	128.1(4)
C(2)-N(1)-Li(1)	126.1(4)
C(5)-N(1)-Sm	78.2(3)
C(2)-N(1)-Sm	75.7(3)
Li(1)-N(1)-Sm	108.2(3)
C(11)-N(2)-C(8)	112.1(6)
C(11)-N(2)-Li(2)	124.6(6)
C(8)-N(2)-Li(2)	118.9(6)
C(11)-N(2)-Sm	79.7(3)
C(8)-N(2)-Sm	78.0(3)
Li(2)-N(2)-Sm	90.8(4)
C(14)-N(3)-C(17)	105.8(5)
C(14)-N(3)-Li(2)	127.3(6)
C(17)-N(3)-Li(2)	122.6(6)
C(14)-N(3)-Sm	77.0(3)
C(17)-N(3)-Sm	77.4(3)
Li(2)-N(3)-Sm	93.5(4)
C(20)-N(4)-C(19)	106.8(5)
C(20)-N(4)-C(21)	113.6(6)
C(19)-N(4)-C(21)	107.2(6)
C(20)-N(4)-Li(1)	115.1(4)
C(19)-N(4)-Li(1)	113.3(5)
C(21)-N(4)-Li(1)	100.8(4)
C(24)-N(5)-C(23)	109.7(5)
C(24)-N(5)-C(22)	109.4(6)
C(23)-N(5)-C(22)	109.2(6)
C(24)-N(5)-Li(1)	120.5(4)
C(23)-N(5)-Li(1)	105.3(4)
C(22)-N(5)-Li(1)	102.1(4)
C(33)-O(1)-C(32)	113.9(9)
C(33)-O(1)-Li(2)	127.6(9)
C(32)-O(1)-Li(2)	118.5(7)
N(1)-C(2)-C(3)	110.6(4)
N(1)-C(2)-C(1)	120.6(4)
C(3)-C(2)-C(1)	128.8(5)
N(1)-C(2)-Sm	76.7(3)
C(3)-C(2)-Sm	77.6(3)
C(1)-C(2)-Sm	114.8(3)
C(2)-C(3)-C(4)	106.6(4)
C(2)-C(3)-Sm	74.7(3)
C(4)-C(3)-Sm	77.5(3)
C(5)-C(4)-C(3)	106.6(5)
C(5)-C(4)-Sm	75.9(3)
C(3)-C(4)-Sm	74.9(3)
N(1)-C(5)-C(4)	110.5(4)

N(1)-C(5)-C(6)	120.6(4)
C(4)-C(5)-C(6)	128.8(5)
N(1)-C(5)-Sm	74.5(3)
C(4)-C(5)-Sm	76.7(3)
C(6)-C(5)-Sm	117.8(3)
N(2)-C(8)-C(9)	110.2(6)
N(2)-C(8)-C(7)	127.1(7)
C(9)-C(8)-C(7)	122.5(7)
N(2)-C(8)-Sm	76.9(3)
C(9)-C(8)-Sm	79.4(3)
C(7)-C(8)-Sm	115.7(4)
C(8)-C(9)-C(10)	103.7(6)
C(8)-C(9)-Sm	73.6(3)
C(10)-C(9)-Sm	76.4(4)
C(11)-C(10)-C(9)	104.9(6)
C(11)-C(10)-Sm	74.9(3)
C(9)-C(10)-Sm	76.3(4)
N(2)-C(11)-C(10)	109.1(6)
N(2)-C(11)-C(12)	126.2(7)
C(10)-C(11)-C(12)	124.6(7)
N(2)-C(11)-Sm	75.5(3)
C(10)-C(11)-Sm	78.0(4)
C(12)-C(11)-Sm	115.9(4)
C(15)-C(14)-N(3)	111.1(5)
C(15)-C(14)-C(13)	127.6(6)
N(3)-C(14)-C(13)	121.3(6)
C(15)-C(14)-Sm	78.6(3)
N(3)-C(14)-Sm	75.6(3)
C(13)-C(14)-Sm	115.2(4)
C(14)-C(15)-C(16)	106.4(6)
C(14)-C(15)-Sm	74.3(3)
C(16)-C(15)-Sm	76.2(3)
C(17)-C(16)-C(15)	107.3(5)
C(17)-C(16)-Sm	74.9(3)
C(15)-C(16)-Sm	76.4(3)
N(3)-C(17)-C(16)	109.4(5)
N(3)-C(17)-C(18)	120.9(6)
C(16)-C(17)-C(18)	129.5(6)
N(3)-C(17)-Sm	75.0(3)
C(16)-C(17)-Sm	77.8(3)
C(18)-C(17)-Sm	117.5(4)
C(22)-C(21)-N(4)	112.8(7)
C(21)-C(22)-N(5)	115.9(6)
C(31)-C(32)-O(1)	116(2)
O(1)-C(33)-C(34)	114.7(10)
C(36)-O(2)-C(36)#1	179.999(8)

C(35)-C(36)-O(2)	173(5)

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

Table 9. Anisotropic displacement parameters (A^2 x 10^3) for Complex **2**
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Sm	31(1)	37(1)	27(1)	3(1)	10(1)	3(1)
I	61(1)	51(1)	37(1)	-2(1)	20(1)	14(1)
Li(1)	47(5)	25(4)	36(5)	-6(3)	20(4)	-8(4)
Li(2)	50(7)	89(9)	60(7)	30(6)	13(6)	21(6)
N(1)	31(2)	30(2)	27(2)	0(2)	12(2)	1(2)
N(2)	15(2)	64(4)	45(3)	-13(2)	-1(2)	-5(2)
N(3)	53(3)	36(3)	38(3)	11(2)	15(2)	1(2)
N(4)	76(4)	42(3)	56(3)	-6(2)	44(3)	-12(3)
N(5)	51(3)	51(3)	35(3)	-7(2)	10(2)	-9(2)
O(1)	41(3)	149(5)	73(4)	36(4)	1(3)	12(3)
C(1)	33(3)	68(4)	43(3)	6(3)	14(3)	-9(3)
C(2)	28(3)	35(3)	31(3)	4(2)	10(2)	3(2)
C(3)	35(3)	49(3)	33(3)	6(2)	18(2)	7(2)
C(4)	47(3)	34(3)	36(3)	-5(2)	16(3)	5(2)
C(5)	38(3)	33(3)	30(3)	2(2)	11(2)	5(2)
C(6)	51(4)	45(3)	45(3)	-1(3)	19(3)	-11(3)
C(7)	81(6)	133(8)	100(7)	-57(6)	48(5)	-29(6)
C(8)	28(3)	81(5)	36(3)	-10(3)	1(3)	-25(3)
C(9)	35(4)	59(4)	77(5)	-7(4)	8(3)	-14(3)
C(10)	40(4)	83(5)	58(4)	1(4)	22(3)	-12(3)
C(11)	23(3)	54(4)	74(5)	1(3)	6(3)	-3(3)
C(12)	51(5)	107(7)	109(7)	-14(5)	25(5)	18(4)
C(13)	110(6)	54(4)	71(5)	0(3)	60(5)	0(4)
C(14)	64(4)	37(3)	43(3)	13(3)	27(3)	6(3)
C(15)	44(4)	64(4)	50(4)	24(3)	22(3)	5(3)
C(16)	61(4)	48(4)	41(3)	2(3)	15(3)	-21(3)
C(17)	63(4)	32(3)	47(3)	2(3)	24(3)	-1(3)
C(18)	123(7)	40(4)	97(6)	7(4)	66(6)	16(4)
C(19)	148(9)	92(6)	172(10)	40(6)	138(9)	29(6)
C(20)	103(6)	44(4)	52(4)	7(3)	39(4)	6(4)
C(21)	156(9)	73(5)	73(5)	-23(4)	78(6)	-39(6)
C(22)	91(6)	117(7)	27(3)	-11(4)	19(4)	-19(5)
C(23)	82(5)	46(4)	68(5)	-11(3)	-4(4)	-9(4)
C(24)	54(5)	81(5)	51(4)	-9(4)	0(3)	4(4)

C(31)	140(13)	125(12)	334(26)	52(14)	52(15)	15(10)
C(32)	155(12)	236(17)	154(12)	119(12)	89(10)	57(12)
C(33)	50(7)	187(15)	387(26)	145(16)	13(10)	17(8)
C(34)	61(7)	278(20)	177(14)	68(14)	-6(8)	7(10)

Table 10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for Complex **2**

	x	y	z	U(eq)	
H(1A)	4748(3)	5880(6)	6596(3)	74	
H(1B)	4624(3)	6313(6)	5774(3)	74	
H(1C)	5200(3)	5225(6)	6232(3)	74	
H(3A)	4257(3)	3816(5)	4806(3)	45	
H(4A)	3318(3)	2138(5)	4710(3)	48	
H(6A)	2981(3)	2634(6)	6441(3)	72	
H(6B)	3097(3)	1363(6)	6044(3)	72	
H(6C)	2444(3)	2313(6)	5583(3)	72	
H(7A)	1544(5)	4131(10)	2636(5)	153	
H(7B)	1291(5)	2768(10)	2822(5)	153	
H(7C)	2108(5)	3149(10)	3231(5)	153	
H(9A)	1664(3)	2516(7)	4399(4)	77	
H(10A)	1309(3)	4223(7)	5140(4)	72	
H(12A)	827(4)	7426(8)	4025(5)	140	
H(12B)	1261(4)	7146(8)	4910(5)	140	
H(12C)	481(4)	6578(8)	4444(5)	140	
H(13A)	2533(5)	5669(6)	2654(4)	106	
H(13B)	3185(5)	4855(6)	3263(4)	106	
H(13C)	3319(5)	6049(6)	2827(4)	106	
H(15A)	4162(3)	6800(6)	4429(3)	63	
H(16A)	3763(3)	8511(6)	5107(3)	64	
H(18A)	1757(5)	8981(6)	3923(5)	121	
H(18B)	2396(5)	9990(6)	4307(5)	121	
H(18C)	2240(5)	8963(6)	4816(5)	121	
H(19A)	2577(5)	5302(9)	7490(6)	169	
H(19B)	2555(5)	4107(9)	7995(6)	169	
H(19C)	2391(5)	3863(9)	7139(6)	169	
H(20A)	4041(4)	2506(6)	8146(4)	98	
H(20B)	3247(4)	2237(6)	7526(4)	98	
H(20C)	3422(4)	2473(6)	8386(4)	98	
H(21A)	3638(6)	5814(8)	8423(5)	110	
H(21B)	3785(6)	4552(8)	8946(5)	110	
H(22A)	4790(5)	4117(9)	8876(4)	98	
H(22B)	4812(5)	5585(9)	9157(4)	98	
H(23A)	4286(4)	7237(6)	8002(4)	120	
H(23B)	4870(4)	7231(6)	7709(4)	120	
H(23C)	5105(4)	7239(6)	8594(4)	120	

H(24A)	5442(4)	4035(8)	8246(4)	107
H(24B)	5799(4)	5302(8)	8745(4)	107
H(24C)	5563(4)	5316(8)	7860(4)	107
H(31A)	1032(8)	10065(13)	1331(11)	332
H(31B)	1062(8)	9976(13)	2145(11)	332
H(31C)	342(8)	9670(13)	1407(11)	332
H(32A)	1553(7)	8307(16)	1917(8)	209
H(32B)	848(7)	8011(16)	1165(8)	209
H(33A)	-118(6)	7585(16)	1240(11)	289
H(33B)	-111(6)	8028(16)	2010(11)	289
H(34A)	-678(6)	6066(16)	1633(8)	293
H(34B)	31(6)	5857(16)	2400(8)	293
H(34C)	-2(6)	5429(16)	1614(8)	293

Table 11.. Crystal data and structure refinement for Complex **3**

Identification code	sg321
Empirical formula	C60 H96 N6 Na2 O6 Sm2
Formula weight	1344.11
Temperature	203(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 11.564(2) A alpha = 64.990(3) deg. b = 16.366(3) A beta = 80.609(3) deg. c = 19.305(4) A gamma = 78.348(3) deg.
Volume	3230(1) A^3
Z, Calculated density	2, 1.382 Mg/m^3
Absorption coefficient	1.863 mm^-1
F(000)	1384
Crystal size	0.10 x 0.10 x 0.03 mm
Theta range for data collection	1.17 to 20.81 deg.
Limiting indices	-11<=h<=11, -14<=k<=16, 0<=l<=19
Reflections collected / unique	25553 / 6752 [R(int) = 0.1126]
Completeness to theta = 20.81	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.928078 and 0.670086
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6752 / 901 / 667
Goodness-of-fit on F^2	1.052

Final R indices [I>2sigma(I)] R1 = 0.0488, wR2 = 0.1083

R indices (all data) R1 = 0.0983, wR2 = 0.1229

Largest diff. peak and hole 1.551 and -0.647 e.A^-3

Table 12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for Complex **3**
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Sm(1)	1602(1)	4027(1)	429(1)	34(1)
Sm(2)	3726(1)	9022(1)	5437(1)	31(1)
Na(1)	4205(4)	1845(3)	617(3)	53(1)
Na(2)	2305(4)	6801(3)	5655(3)	50(1)
N(1)	569(7)	5921(6)	-161(5)	33(2)
N(2)	3034(8)	2496(6)	1446(5)	44(2)
N(3)	2737(8)	3246(6)	-463(5)	42(2)
N(4)	3964(7)	10925(6)	4848(5)	32(2)
N(5)	2626(9)	7488(6)	6460(5)	43(2)
N(6)	3493(8)	8256(6)	4540(5)	37(2)
O(1)	6271(8)	1681(9)	603(7)	104(3)
O(2)	4237(9)	296(6)	1299(6)	85(3)
O(3)	2838(9)	5251(6)	6347(5)	78(3)
O(4)	386(9)	6548(8)	5657(7)	96(3)
C(1)	1615(11)	6254(9)	-1487(7)	55(4)
C(2)	1609(10)	5932(7)	-615(7)	33(2)
C(3)	2627(9)	5809(7)	-267(6)	26(2)
C(4)	2124(9)	5653(7)	515(7)	38(2)
C(5)	896(10)	5751(7)	546(7)	35(2)
C(6)	9(10)	5653(9)	1235(7)	52(3)
C(7)	4407(10)	3573(9)	1251(7)	60(4)
C(8)	3261(11)	3206(8)	1555(6)	43(2)
C(9)	2286(11)	3531(9)	1975(6)	49(2)
C(10)	1416(11)	2962(8)	2120(6)	46(2)
C(11)	1913(11)	2345(8)	1801(7)	43(2)
C(12)	1406(12)	1541(8)	1870(7)	63(4)
C(13)	4452(10)	4110(8)	-946(7)	48(3)
C(14)	3853(11)	3326(8)	-799(7)	49(3)
C(15)	4333(11)	2593(9)	-988(7)	58(3)
C(16)	3477(11)	2009(8)	-746(7)	52(2)
C(17)	2498(11)	2435(8)	-431(7)	44(2)
C(18)	1329(10)	2126(8)	-143(7)	53(3)
C(19)	7073(17)	1440(20)	74(13)	190(8)
C(20)	8221(16)	1560(20)	59(13)	173(9)
C(21)	8242(15)	1708(15)	737(14)	134(7)

C(22)	6992(14)	1717(16)	1046(12)	132(6)
C(23)	3703(15)	-328(9)	1189(9)	83(4)
C(24)	3528(15)	-1083(11)	1965(9)	93(5)
C(25)	4493(15)	-1086(10)	2386(10)	98(5)
C(26)	4618(18)	-110(10)	2051(9)	110(5)
C(27)	3479(10)	11219(9)	3531(7)	50(3)
C(28)	3190(10)	10949(7)	4367(7)	36(2)
C(29)	2071(9)	10824(7)	4730(6)	29(2)
C(30)	2216(9)	10628(7)	5539(7)	42(2)
C(31)	3355(10)	10733(8)	5558(7)	36(2)
C(32)	3944(10)	10643(8)	6251(6)	47(3)
C(33)	1542(10)	9121(8)	4054(7)	52(3)
C(34)	2483(11)	8310(8)	4220(7)	45(2)
C(35)	2581(12)	7556(9)	4068(7)	56(3)
C(36)	3643(12)	6999(9)	4298(7)	54(3)
C(37)	4216(11)	7448(8)	4582(7)	43(2)
C(38)	5419(10)	7143(8)	4876(7)	56(3)
C(39)	4616(12)	6539(9)	6876(7)	66(4)
C(40)	3665(11)	7338(8)	6796(7)	47(2)
C(41)	3622(12)	7965(8)	7108(7)	50(3)
C(42)	2465(12)	8518(9)	6969(7)	52(2)
C(43)	1940(11)	8203(8)	6576(6)	43(2)
C(44)	722(10)	8555(9)	6289(8)	61(4)
C(45)	3351(16)	4545(10)	6131(9)	104(6)
C(46)	3252(17)	3659(10)	6775(10)	121(7)
C(47)	2427(16)	3910(11)	7335(9)	103(6)
C(48)	2431(17)	4852(10)	7113(9)	109(6)
C(49)	216(16)	6067(17)	5228(13)	148(7)
C(50)	-960(20)	6540(20)	4916(15)	179(9)
C(51)	-1603(18)	6835(15)	5492(16)	156(8)
C(52)	-725(16)	6784(16)	5949(14)	147(6)
O(5)	3377(11)	6046(14)	2693(12)	261(10)
C(53)	2401(19)	6541(13)	2252(8)	217(11)
C(54)	1349(12)	6249(14)	2710(13)	219(11)
C(55)	1675(15)	5573(13)	3434(10)	209(11)
C(56)	2928(16)	5448(11)	3424(10)	189(9)
O(6)	1130(20)	1307(18)	7310(9)	321(11)
C(57)	1455(16)	1496(16)	7899(15)	284(12)
C(58)	650(20)	1160(17)	8556(10)	237(10)
C(59)	-179(16)	762(15)	8374(12)	231(10)
C(60)	120(20)	853(17)	7604(13)	262(11)

Table 13. Bond lengths [A] and angles [deg] for Complex **3**

Sm(1)-N(3)	2.602(9)
Sm(1)-N(1)#1	2.623(8)
Sm(1)-C(8)	2.839(11)
Sm(1)-N(2)	2.846(9)
Sm(1)-N(1)	2.880(8)
Sm(1)-C(5)	2.868(11)
Sm(1)-C(2)	2.911(10)
Sm(1)-C(9)	2.942(12)
Sm(1)-C(11)	2.910(11)
Sm(1)-C(4)	2.920(10)
Sm(1)-C(10)	2.976(11)
Sm(1)-C(3)	3.046(10)
Sm(2)-N(6)	2.601(9)
Sm(2)-N(4)#2	2.650(8)
Sm(2)-C(43)	2.835(11)
Sm(2)-C(31)	2.850(11)
Sm(2)-N(5)	2.846(9)
Sm(2)-C(30)	2.910(10)
Sm(2)-N(4)	2.884(8)
Sm(2)-C(42)	2.927(11)
Sm(2)-C(40)	2.897(12)
Sm(2)-C(41)	2.942(11)
Sm(2)-C(28)	2.952(11)
Sm(2)-Na(2)	4.121(4)
Na(1)-O(2)	2.307(10)
Na(1)-O(1)	2.347(11)
Na(1)-N(2)	2.385(11)
Na(1)-C(16)	2.781(13)
Na(1)-C(17)	2.793(13)
Na(1)-C(15)	2.799(14)
Na(1)-C(14)	2.806(13)
Na(1)-N(3)	2.832(10)
Na(2)-O(3)	2.317(10)
Na(2)-O(4)	2.337(10)
Na(2)-N(5)	2.377(11)
Na(2)-C(36)	2.742(13)
Na(2)-C(35)	2.766(13)
Na(2)-C(37)	2.809(12)
Na(2)-C(34)	2.837(13)
Na(2)-N(6)	2.866(10)
N(1)-C(5)	1.373(13)
N(1)-C(2)	1.365(13)

N(1)-Sm(1)#1	2.623(8)
N(2)-C(8)	1.345(14)
N(2)-C(11)	1.380(13)
N(3)-C(14)	1.351(13)
N(3)-C(17)	1.384(14)
N(4)-C(28)	1.374(13)
N(4)-C(31)	1.371(13)
N(4)-Sm(2)#2	2.650(8)
N(5)-C(43)	1.355(14)
N(5)-C(40)	1.388(14)
N(6)-C(34)	1.378(14)
N(6)-C(37)	1.391(14)
O(1)-C(22)	1.314(17)
O(1)-C(19)	1.393(19)
O(2)-C(26)	1.422(16)
O(2)-C(23)	1.397(15)
O(3)-C(45)	1.383(15)
O(3)-C(48)	1.385(16)
O(4)-C(52)	1.366(18)
O(4)-C(49)	1.421(18)
C(1)-C(2)	1.536(15)
C(2)-C(3)	1.388(14)
C(3)-C(4)	1.458(15)
C(4)-C(5)	1.391(14)
C(5)-C(6)	1.512(15)
C(7)-C(8)	1.494(15)
C(8)-C(9)	1.427(16)
C(9)-C(10)	1.422(16)
C(10)-C(11)	1.380(16)
C(11)-C(12)	1.494(16)
C(13)-C(14)	1.483(15)
C(14)-C(15)	1.384(16)
C(15)-C(16)	1.401(15)
C(16)-C(17)	1.397(15)
C(17)-C(18)	1.478(15)
C(19)-C(20)	1.37(2)
C(20)-C(21)	1.43(3)
C(21)-C(22)	1.47(2)
C(23)-C(24)	1.499(19)
C(24)-C(25)	1.482(19)
C(25)-C(26)	1.476(19)
C(27)-C(28)	1.481(15)
C(28)-C(29)	1.378(14)
C(29)-C(30)	1.487(15)
C(30)-C(31)	1.371(14)
C(31)-C(32)	1.539(15)

C(33)-C(34)	1.490(16)
C(34)-C(35)	1.365(16)
C(35)-C(36)	1.385(16)
C(36)-C(37)	1.392(16)
C(37)-C(38)	1.498(15)
C(39)-C(40)	1.498(16)
C(40)-C(41)	1.383(16)
C(41)-C(42)	1.451(16)
C(42)-C(43)	1.349(16)
C(43)-C(44)	1.509(16)
C(45)-C(46)	1.469(19)
C(46)-C(47)	1.460(19)
C(47)-C(48)	1.415(19)
C(49)-C(50)	1.51(3)
C(50)-C(51)	1.43(3)
C(51)-C(52)	1.42(3)
O(5)-C(53)	1.4200
O(5)-C(56)	1.4200
C(53)-C(54)	1.4200
C(54)-C(55)	1.4200
C(55)-C(56)	1.4200
O(6)-C(57)	1.4200
O(6)-C(60)	1.4200
C(57)-C(58)	1.4200
C(58)-C(59)	1.4200
C(59)-C(60)	1.4200

N(3)-Sm(1)-N(1)#1	98.7(3)
N(3)-Sm(1)-C(8)	94.9(3)
N(1)#1-Sm(1)-C(8)	143.9(3)
N(3)-Sm(1)-N(2)	77.4(3)
N(1)#1-Sm(1)-N(2)	126.2(3)
C(8)-Sm(1)-N(2)	27.4(3)
N(3)-Sm(1)-N(1)	122.2(3)
N(1)#1-Sm(1)-N(1)	73.8(3)
C(8)-Sm(1)-N(1)	125.0(3)
N(2)-Sm(1)-N(1)	152.2(3)
N(3)-Sm(1)-C(5)	143.6(3)
N(1)#1-Sm(1)-C(5)	89.3(3)
C(8)-Sm(1)-C(5)	99.2(4)
N(2)-Sm(1)-C(5)	125.3(3)
N(1)-Sm(1)-C(5)	27.6(3)
N(3)-Sm(1)-C(2)	99.9(3)
N(1)#1-Sm(1)-C(2)	91.7(3)
C(8)-Sm(1)-C(2)	118.7(3)
N(2)-Sm(1)-C(2)	142.1(3)

N(1)-Sm(1)-C(2)	27.3(3)
C(5)-Sm(1)-C(2)	44.2(3)
N(3)-Sm(1)-C(9)	122.3(3)
N(1)#1-Sm(1)-C(9)	122.8(3)
C(8)-Sm(1)-C(9)	28.5(3)
N(2)-Sm(1)-C(9)	46.5(3)
N(1)-Sm(1)-C(9)	107.8(3)
C(5)-Sm(1)-C(9)	80.2(4)
C(2)-Sm(1)-C(9)	115.4(3)
N(3)-Sm(1)-C(11)	92.7(3)
N(1)#1-Sm(1)-C(11)	101.5(3)
C(8)-Sm(1)-C(11)	44.4(3)
N(2)-Sm(1)-C(11)	27.7(3)
N(1)-Sm(1)-C(11)	145.1(3)
C(5)-Sm(1)-C(11)	120.6(3)
C(2)-Sm(1)-C(11)	160.3(3)
C(9)-Sm(1)-C(11)	44.9(4)
N(3)-Sm(1)-C(4)	126.4(3)
N(1)#1-Sm(1)-C(4)	116.4(3)
C(8)-Sm(1)-C(4)	80.1(3)
N(2)-Sm(1)-C(4)	107.4(3)
N(1)-Sm(1)-C(4)	45.8(3)
C(5)-Sm(1)-C(4)	27.8(3)
C(2)-Sm(1)-C(4)	44.1(3)
C(9)-Sm(1)-C(4)	71.3(3)
C(11)-Sm(1)-C(4)	116.2(3)
N(3)-Sm(1)-C(10)	119.6(3)
N(1)#1-Sm(1)-C(10)	99.1(3)
C(8)-Sm(1)-C(10)	45.7(3)
N(2)-Sm(1)-C(10)	46.2(3)
N(1)-Sm(1)-C(10)	118.3(3)
C(5)-Sm(1)-C(10)	93.7(3)
C(2)-Sm(1)-C(10)	136.6(3)
C(9)-Sm(1)-C(10)	27.8(3)
C(11)-Sm(1)-C(10)	27.1(3)
C(4)-Sm(1)-C(10)	94.6(3)
N(3)-Sm(1)-C(3)	100.3(3)
N(1)#1-Sm(1)-C(3)	117.8(3)
C(8)-Sm(1)-C(3)	92.1(3)
N(2)-Sm(1)-C(3)	115.6(3)
N(1)-Sm(1)-C(3)	46.2(2)
C(5)-Sm(1)-C(3)	46.2(3)
C(2)-Sm(1)-C(3)	26.8(3)
C(9)-Sm(1)-C(3)	94.0(3)
C(11)-Sm(1)-C(3)	135.7(3)
C(4)-Sm(1)-C(3)	28.2(3)

C(10)-Sm(1)-C(3)	120.3(3)
N(6)-Sm(2)-N(4)#2	98.8(3)
N(6)-Sm(2)-C(43)	95.2(3)
N(4)#2-Sm(2)-C(43)	143.8(3)
N(6)-Sm(2)-C(31)	142.9(3)
N(4)#2-Sm(2)-C(31)	90.2(3)
C(43)-Sm(2)-C(31)	98.3(3)
N(6)-Sm(2)-N(5)	77.6(3)
N(4)#2-Sm(2)-N(5)	126.2(3)
C(43)-Sm(2)-N(5)	27.6(3)
C(31)-Sm(2)-N(5)	124.8(3)
N(6)-Sm(2)-C(30)	125.7(3)
N(4)#2-Sm(2)-C(30)	117.1(3)
C(43)-Sm(2)-C(30)	79.3(3)
C(31)-Sm(2)-C(30)	27.5(3)
N(5)-Sm(2)-C(30)	106.8(3)
N(6)-Sm(2)-N(4)	121.8(3)
N(4)#2-Sm(2)-N(4)	74.6(3)
C(43)-Sm(2)-N(4)	124.2(3)
C(31)-Sm(2)-N(4)	27.7(3)
N(5)-Sm(2)-N(4)	151.6(3)
C(30)-Sm(2)-N(4)	45.7(3)
N(6)-Sm(2)-C(42)	121.4(3)
N(4)#2-Sm(2)-C(42)	124.0(3)
C(43)-Sm(2)-C(42)	27.0(3)
C(31)-Sm(2)-C(42)	80.2(4)
N(5)-Sm(2)-C(42)	45.8(3)
C(30)-Sm(2)-C(42)	70.8(4)
N(4)-Sm(2)-C(42)	107.9(3)
N(6)-Sm(2)-C(40)	92.8(3)
N(4)#2-Sm(2)-C(40)	101.1(3)
C(43)-Sm(2)-C(40)	44.9(4)
C(31)-Sm(2)-C(40)	120.8(4)
N(5)-Sm(2)-C(40)	28.0(3)
C(30)-Sm(2)-C(40)	116.3(4)
N(4)-Sm(2)-C(40)	145.3(3)
C(42)-Sm(2)-C(40)	45.6(4)
N(6)-Sm(2)-C(41)	119.9(3)
N(4)#2-Sm(2)-C(41)	99.2(3)
C(43)-Sm(2)-C(41)	45.5(4)
C(31)-Sm(2)-C(41)	93.7(3)
N(5)-Sm(2)-C(41)	46.2(3)
C(30)-Sm(2)-C(41)	94.3(4)
N(4)-Sm(2)-C(41)	118.2(3)
C(42)-Sm(2)-C(41)	28.6(3)
C(40)-Sm(2)-C(41)	27.4(3)

N(6)-Sm(2)-C(28)	98.8(3)
N(4)#2-Sm(2)-C(28)	91.5(3)
C(43)-Sm(2)-C(28)	119.0(3)
C(31)-Sm(2)-C(28)	44.7(3)
N(5)-Sm(2)-C(28)	142.3(3)
C(30)-Sm(2)-C(28)	45.1(3)
N(4)-Sm(2)-C(28)	27.2(3)
C(42)-Sm(2)-C(28)	115.9(4)
C(40)-Sm(2)-C(28)	161.4(3)
C(41)-Sm(2)-C(28)	137.2(3)
N(6)-Sm(2)-Na(2)	43.6(2)
N(4)#2-Sm(2)-Na(2)	121.69(19)
C(43)-Sm(2)-Na(2)	54.4(3)
C(31)-Sm(2)-Na(2)	147.9(2)
N(5)-Sm(2)-Na(2)	34.1(2)
C(30)-Sm(2)-Na(2)	121.2(2)
N(4)-Sm(2)-Na(2)	156.07(19)
C(42)-Sm(2)-Na(2)	78.6(3)
C(40)-Sm(2)-Na(2)	54.2(3)
C(41)-Sm(2)-Na(2)	78.7(3)
C(28)-Sm(2)-Na(2)	129.1(2)
O(2)-Na(1)-O(1)	91.0(4)
O(2)-Na(1)-N(2)	104.2(4)
O(1)-Na(1)-N(2)	117.0(4)
O(2)-Na(1)-C(16)	98.7(4)
O(1)-Na(1)-C(16)	113.1(4)
N(2)-Na(1)-C(16)	123.8(4)
O(2)-Na(1)-C(17)	107.1(4)
O(1)-Na(1)-C(17)	138.5(4)
N(2)-Na(1)-C(17)	94.8(4)
C(16)-Na(1)-C(17)	29.0(3)
O(2)-Na(1)-C(15)	120.0(4)
O(1)-Na(1)-C(15)	91.6(4)
N(2)-Na(1)-C(15)	126.9(4)
C(16)-Na(1)-C(15)	29.1(3)
C(17)-Na(1)-C(15)	47.0(4)
O(2)-Na(1)-C(14)	145.9(4)
O(1)-Na(1)-C(14)	100.0(4)
N(2)-Na(1)-C(14)	99.4(4)
C(16)-Na(1)-C(14)	47.3(4)
C(17)-Na(1)-C(14)	45.9(4)
C(15)-Na(1)-C(14)	28.6(3)
O(2)-Na(1)-N(3)	134.8(4)
O(1)-Na(1)-N(3)	127.1(4)
N(2)-Na(1)-N(3)	81.2(3)
C(16)-Na(1)-N(3)	48.0(3)

C(17)-Na(1)-N(3)	28.5(3)
C(15)-Na(1)-N(3)	47.2(3)
C(14)-Na(1)-N(3)	27.7(3)
O(2)-Na(1)-Sm(1)	132.1(3)
O(1)-Na(1)-Sm(1)	131.5(3)
N(2)-Na(1)-Sm(1)	42.5(2)
C(16)-Na(1)-Sm(1)	85.0(3)
C(17)-Na(1)-Sm(1)	58.4(3)
C(15)-Na(1)-Sm(1)	84.7(3)
C(14)-Na(1)-Sm(1)	58.8(3)
N(3)-Na(1)-Sm(1)	38.87(19)
O(3)-Na(2)-O(4)	89.5(4)
O(3)-Na(2)-N(5)	104.6(4)
O(4)-Na(2)-N(5)	118.5(4)
O(3)-Na(2)-C(36)	99.5(4)
O(4)-Na(2)-C(36)	112.4(4)
N(5)-Na(2)-C(36)	123.0(4)
O(3)-Na(2)-C(35)	120.9(4)
O(4)-Na(2)-C(35)	91.5(4)
N(5)-Na(2)-C(35)	125.7(4)
C(36)-Na(2)-C(35)	29.1(3)
O(3)-Na(2)-C(37)	107.9(4)
O(4)-Na(2)-C(37)	138.2(4)
N(5)-Na(2)-C(37)	94.1(4)
C(36)-Na(2)-C(37)	29.0(3)
C(35)-Na(2)-C(37)	46.9(4)
O(3)-Na(2)-C(34)	146.9(4)
O(4)-Na(2)-C(34)	99.8(4)
N(5)-Na(2)-C(34)	98.8(4)
C(36)-Na(2)-C(34)	47.5(4)
C(35)-Na(2)-C(34)	28.2(3)
C(37)-Na(2)-C(34)	46.5(4)
O(3)-Na(2)-N(6)	135.5(4)
O(4)-Na(2)-N(6)	127.4(4)
N(5)-Na(2)-N(6)	80.8(3)
C(36)-Na(2)-N(6)	47.5(3)
C(35)-Na(2)-N(6)	46.4(3)
C(37)-Na(2)-N(6)	28.4(3)
C(34)-Na(2)-N(6)	28.0(3)
O(3)-Na(2)-Sm(2)	131.6(3)
O(4)-Na(2)-Sm(2)	133.9(3)
N(5)-Na(2)-Sm(2)	42.1(2)
C(36)-Na(2)-Sm(2)	84.0(3)
C(35)-Na(2)-Sm(2)	84.1(3)
C(37)-Na(2)-Sm(2)	57.3(3)
C(34)-Na(2)-Sm(2)	59.1(3)

N(6)-Na(2)-Sm(2)	38.72(18)
C(5)-N(1)-C(2)	105.0(9)
C(5)-N(1)-Sm(1)#1	123.9(7)
C(2)-N(1)-Sm(1)#1	130.6(7)
C(5)-N(1)-Sm(1)	75.7(6)
C(2)-N(1)-Sm(1)	77.6(6)
Sm(1)#1-N(1)-Sm(1)	106.2(3)
C(8)-N(2)-C(11)	105.7(10)
C(8)-N(2)-Na(1)	125.4(8)
C(11)-N(2)-Na(1)	128.0(8)
C(8)-N(2)-Sm(1)	76.0(6)
C(11)-N(2)-Sm(1)	78.7(6)
Na(1)-N(2)-Sm(1)	103.1(3)
C(14)-N(3)-C(17)	106.0(10)
C(14)-N(3)-Sm(1)	126.7(8)
C(17)-N(3)-Sm(1)	123.1(7)
C(14)-N(3)-Na(1)	75.0(7)
C(17)-N(3)-Na(1)	74.2(6)
Sm(1)-N(3)-Na(1)	98.0(3)
C(28)-N(4)-C(31)	107.0(9)
C(28)-N(4)-Sm(2)#2	127.9(7)
C(31)-N(4)-Sm(2)#2	124.5(7)
C(28)-N(4)-Sm(2)	79.2(6)
C(31)-N(4)-Sm(2)	74.8(6)
Sm(2)#2-N(4)-Sm(2)	105.4(3)
C(43)-N(5)-C(40)	105.9(11)
C(43)-N(5)-Na(2)	127.6(9)
C(40)-N(5)-Na(2)	125.6(8)
C(43)-N(5)-Sm(2)	75.8(6)
C(40)-N(5)-Sm(2)	78.0(6)
Na(2)-N(5)-Sm(2)	103.8(3)
C(34)-N(6)-C(37)	107.3(10)
C(34)-N(6)-Sm(2)	127.4(7)
C(37)-N(6)-Sm(2)	120.4(8)
C(34)-N(6)-Na(2)	74.9(6)
C(37)-N(6)-Na(2)	73.6(6)
Sm(2)-N(6)-Na(2)	97.7(3)
C(22)-O(1)-C(19)	101.2(14)
C(22)-O(1)-Na(1)	134.7(11)
C(19)-O(1)-Na(1)	124.0(11)
C(26)-O(2)-C(23)	108.8(11)
C(26)-O(2)-Na(1)	118.4(9)
C(23)-O(2)-Na(1)	131.2(8)
C(45)-O(3)-C(48)	106.4(11)
C(45)-O(3)-Na(2)	132.7(9)
C(48)-O(3)-Na(2)	119.8(9)