C(52)-O(4)-C(49)	104.9(13)
C(52)-O(4)-Na(2)	136.8(11)
C(49)-O(4)-Na(2)	118.3(10)
N(1)-C(2)-C(3)	115.7(10)
N(1)-C(2)-C(1)	121.0(10)
C(3)-C(2)-C(1)	122.1(10)
N(1)-C(2)-Sm(1)	75.1(6)
C(3)-C(2)-Sm(1)	82.0(6)
C(1)-C(2)-Sm(1)	121.9(8)
C(2)-C(3)-C(4)	100.5(9)
C(2)-C(3)-Sm(1)	71.2(6)
C(4)-C(3)-Sm(1)	71.1(6)
C(5)-C(4)-C(3)	109.3(10)
C(5)-C(4)-Sm(1)	74.0(6)
C(3)-C(4)-Sm(1)	80.7(6)
N(1)-C(5)-C(4)	109.4(10)
N(1)-C(5)-C(6)	122.7(10)
C(4)-C(5)-C(6)	127.9(11)
N(1)-C(5)-Sm(1)	76.7(6)
C(4)-C(5)-Sm(1)	78.2(6)
C(6)-C(5)-Sm(1)	110.0(7)
N(2)-C(8)-C(9)	111.3(11)
N(2)-C(8)-C(7)	121.5(11)
C(9)-C(8)-C(7)	127.2(12)
N(2)-C(8)-Sm(1)	76.6(6)
C(9)-C(8)-Sm(1)	79.7(7)
C(7)-C(8)-Sm(1)	110.8(7)
C(8)-C(9)-C(10)	105.2(12)
C(8)-C(9)-Sm(1)	71.8(7)
C(10)-C(9)-Sm(1)	77.4(7)
C(11)-C(10)-C(9)	105.8(11)
C(11)-C(10)-Sm(1)	73.8(7)
C(9)-C(10)-Sm(1)	74.8(6)
N(2)-C(11)-C(10)	112.0(11)
N(2)-C(11)-C(12)	121.0(11)
C(10)-C(11)-C(12)	126.7(12)
N(2)-C(11)-Sm(1)	73.6(6)
C(10)-C(11)-Sm(1)	79.1(7)
C(12)-C(11)-Sm(1)	119.2(8)
N(3)-C(14)-C(15)	111.0(11)
N(3)-C(14)-C(13)	123.2(11)
C(15)-C(14)-C(13)	125.7(11)
N(3)-C(14)-Na(1)	77.2(6)
C(15)-C(14)-Na(1)	75.5(8)
C(13)-C(14)-Na(1)	115.2(8)
C(14)-C(15)-C(16)	107.1(11)

C(14)-C(15)-Na(1)	76.0(7)
C(16)-C(15)-Na(1)	74.7(7)
C(17)-C(16)-C(15)	105.6(12)
C(17)-C(16)-Na(1)	75.9(7)
C(15)-C(16)-Na(1)	76.2(8)
N(3)-C(17)-C(16)	110.3(11)
N(3)-C(17)-C(18)	122.7(11)
C(16)-C(17)-C(18)	126.9(11)
N(3)-C(17)-Na(1)	77.4(6)
C(16)-C(17)-Na(1)	75.0(7)
C(18)-C(17)-Na(1)	117.7(8)
C(20)-C(19)-O(1)	115.1(19)
C(19)-C(20)-C(21)	104.5(17)
C(22)-C(21)-C(20)	102.1(16)
O(1)-C(22)-C(21)	114.7(17)
O(2)-C(23)-C(24)	106.2(12)
C(23)-C(24)-C(25)	104.1(13)
C(26)-C(25)-C(24)	101.6(13)
O(2)-C(26)-C(25)	108.4(13)
N(4)-C(28)-C(29)	112.1(11)
N(4)-C(28)-C(27)	123.6(10)
C(29)-C(28)-C(27)	123.6(11)
N(4)-C(28)-Sm(2)	73.6(6)
C(29)-C(28)-Sm(2)	81.4(6)
C(27)-C(28)-Sm(2)	120.0(8)
C(28)-C(29)-C(30)	103.4(9)
C(31)-C(30)-C(29)	106.8(10)
C(31)-C(30)-Sm(2)	73.8(6)
C(29)-C(30)-Sm(2)	81.5(6)
C(30)-C(31)-N(4)	110.3(11)
C(30)-C(31)-C(32)	127.8(11)
N(4)-C(31)-C(32)	121.9(10)
C(30)-C(31)-Sm(2)	78.7(7)
N(4)-C(31)-Sm(2)	77.6(6)
C(32)-C(31)-Sm(2)	110.1(7)
N(6)-C(34)-C(35)	108.2(11)
N(6)-C(34)-C(33)	121.4(11)
C(35)-C(34)-C(33)	130.3(12)
N(6)-C(34)-Na(2)	77.2(6)
C(35)-C(34)-Na(2)	73.0(7)
C(33)-C(34)-Na(2)	118.9(8)
C(36)-C(35)-C(34)	109.7(12)
C(36)-C(35)-Na(2)	74.5(7)
C(34)-C(35)-Na(2)	78.8(8)
C(35)-C(36)-C(37)	106.0(12)
C(35)-C(36)-Na(2)	76.4(7)

C(37)-C(36)-Na(2)	78.2(7)
C(36)-C(37)-N(6)	108.7(12)
C(36)-C(37)-C(38)	126.9(12)
N(6)-C(37)-C(38)	124.4(11)
C(36)-C(37)-Na(2)	72.8(7)
N(6)-C(37)-Na(2)	78.1(6)
C(38)-C(37)-Na(2)	116.4(8)
C(41)-C(40)-N(5)	110.2(11)
C(41)-C(40)-C(39)	126.1(12)
N(5)-C(40)-C(39)	123.4(12)
C(41)-C(40)-Sm(2)	78.1(7)
N(5)-C(40)-Sm(2)	74.0(6)
C(39)-C(40)-Sm(2)	120.1(8)
C(40)-C(41)-C(42)	105.4(11)
C(40)-C(41)-Sm(2)	74.5(7)
C(42)-C(41)-Sm(2)	75.1(6)
C(43)-C(42)-C(41)	105.9(12)
C(43)-C(42)-Sm(2)	72.7(7)
C(41)-C(42)-Sm(2)	76.3(6)
C(42)-C(43)-N(5)	112.6(13)
C(42)-C(43)-C(44)	126.8(12)
N(5)-C(43)-C(44)	120.6(12)
C(42)-C(43)-Sm(2)	80.3(7)
N(5)-C(43)-Sm(2)	76.7(6)
C(44)-C(43)-Sm(2)	111.8(7)
O(3)-C(45)-C(46)	110.7(13)
C(47)-C(46)-C(45)	102.6(13)
C(46)-C(47)-C(48)	105.9(14)
O(3)-C(48)-C(47)	110.2(13)
C(50)-C(49)-O(4)	102.7(18)
C(49)-C(50)-C(51)	104(2)
C(52)-C(51)-C(50)	105(2)
C(51)-C(52)-O(4)	111(2)
C(53)-O(5)-C(56)	108.0
C(54)-C(53)-O(5)	108.0
C(53)-C(54)-C(55)	108.0
C(54)-C(55)-C(56)	108.0
C(55)-C(56)-O(5)	108.0
C(57)-O(6)-C(60)	108.0
O(6)-C(57)-C(58)	108.0
C(59)-C(58)-C(57)	108.0
C(58)-C(59)-C(60)	108.0
O(6)-C(60)-C(59)	108.0

Symmetry transformations used to generate equivalent atoms:

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

Table 14. Anisotropic displacement parameters (A^2 x 10^3) for Complex **3**
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(1)	30(1)	34(1)	34(1)	-9(1)	-3(1)	-6(1)
Sm(2)	28(1)	32(1)	31(1)	-10(1)	-4(1)	-5(1)
Na(1)	45(3)	46(3)	65(3)	-20(2)	-13(2)	2(2)
Na(2)	51(3)	47(3)	54(3)	-21(2)	0(2)	-17(2)
N(1)	19(4)	36(4)	38(4)	-9(4)	-4(3)	-6(4)
N(2)	48(5)	37(4)	39(4)	-7(3)	-15(4)	-1(3)
N(3)	44(5)	41(4)	39(4)	-14(4)	-2(4)	-4(3)
N(4)	18(5)	37(4)	41(4)	-16(4)	-7(4)	-1(4)
N(5)	52(6)	37(4)	37(4)	-10(4)	2(4)	-13(4)
N(6)	36(5)	42(4)	37(4)	-19(4)	-2(4)	-4(3)
O(1)	39(5)	177(10)	129(9)	-101(8)	-16(4)	7(5)
O(2)	130(9)	47(4)	78(6)	-15(4)	-50(6)	-1(5)
O(3)	116(8)	45(4)	66(5)	-25(4)	15(5)	-14(5)
O(4)	60(5)	145(9)	129(9)	-92(7)	22(5)	-54(5)
C(1)	36(8)	70(9)	43(5)	-6(6)	1(6)	-11(7)
C(2)	23(5)	27(4)	44(4)	-9(4)	-2(4)	-7(5)
C(3)	8(4)	23(4)	43(5)	-10(4)	-6(4)	3(4)
C(4)	24(5)	37(4)	52(5)	-13(4)	-12(4)	-5(5)
C(5)	25(5)	36(4)	42(5)	-14(4)	1(4)	-5(5)
C(6)	49(8)	63(9)	54(7)	-35(7)	2(6)	-11(7)
C(7)	44(7)	68(9)	63(10)	-17(8)	-25(6)	-4(6)
C(8)	50(6)	39(5)	31(6)	0(4)	-13(4)	-10(4)
C(9)	66(7)	44(5)	33(5)	-11(4)	-10(5)	-8(5)
C(10)	46(6)	52(6)	31(4)	-5(4)	-12(5)	-6(5)
C(11)	47(6)	39(4)	34(6)	-3(3)	-15(5)	-6(5)
C(12)	76(10)	56(7)	53(9)	-8(6)	-10(7)	-28(7)
C(13)	34(8)	56(7)	48(8)	-19(6)	-1(6)	-3(6)
C(14)	53(6)	49(6)	45(5)	-20(4)	11(5)	-16(5)
C(15)	50(6)	60(7)	63(5)	-30(6)	14(5)	-13(5)
C(16)	60(7)	46(6)	50(6)	-20(5)	6(5)	-11(5)
C(17)	46(5)	45(6)	38(6)	-14(5)	-4(4)	-7(5)
C(18)	50(6)	36(8)	70(10)	-17(7)	-14(6)	1(6)
C(19)	67(8)	390(20)	166(16)	-187(16)	-25(11)	24(16)
C(20)	49(9)	290(20)	145(17)	-86(16)	-4(11)	33(14)

C(21)	52(8)	154(16)	211(19)	-86(16)	-38(11)	5(11)
C(22)	58(8)	224(18)	156(15)	-126(14)	-29(9)	20(12)
C(23)	125(13)	50(8)	82(9)	-27(7)	-32(9)	-9(8)
C(24)	117(13)	86(10)	79(10)	-29(8)	-6(9)	-31(9)
C(25)	118(14)	58(8)	94(11)	2(8)	-41(9)	-8(10)
C(26)	196(16)	68(8)	71(9)	-15(7)	-57(10)	-24(10)
C(27)	42(8)	55(8)	41(5)	-5(6)	-14(6)	-2(7)
C(28)	23(6)	30(4)	48(4)	-8(4)	-18(4)	10(5)
C(29)	9(5)	25(5)	58(6)	-16(5)	-5(4)	-10(4)
C(30)	17(5)	40(4)	69(6)	-25(5)	4(4)	-1(5)
C(31)	19(6)	39(4)	51(5)	-24(5)	-2(5)	3(5)
C(32)	40(8)	64(9)	43(7)	-29(7)	5(6)	-11(7)
C(33)	43(8)	57(7)	62(9)	-23(6)	-26(7)	-4(5)
C(34)	42(6)	50(6)	48(5)	-22(4)	-5(5)	-11(4)
C(35)	59(7)	69(7)	57(5)	-37(6)	-8(5)	-16(5)
C(36)	69(7)	48(6)	54(6)	-29(6)	-3(5)	-10(5)
C(37)	47(5)	39(6)	48(7)	-22(5)	2(4)	-8(4)
C(38)	45(6)	52(8)	59(9)	-17(7)	2(6)	-2(6)
C(39)	82(10)	62(7)	44(8)	-16(6)	-26(7)	12(7)
C(40)	56(7)	40(4)	36(6)	-5(3)	-7(5)	-6(5)
C(41)	63(7)	51(6)	31(4)	-8(4)	-3(5)	-21(5)
C(42)	71(7)	48(6)	36(5)	-18(4)	10(5)	-14(5)
C(43)	48(5)	47(5)	26(6)	-9(5)	10(4)	-11(4)
C(44)	44(6)	59(9)	69(10)	-19(8)	16(6)	-20(6)
C(45)	149(14)	59(7)	75(9)	-20(7)	29(9)	2(10)
C(46)	175(16)	53(7)	100(12)	-19(7)	35(11)	1(10)
C(47)	141(14)	67(8)	71(10)	-10(7)	25(9)	-16(10)
C(48)	169(15)	67(7)	70(8)	-23(6)	36(10)	-22(10)
C(49)	94(11)	240(20)	183(17)	-151(14)	3(11)	-59(11)
C(50)	153(17)	230(20)	180(19)	-80(15)	-68(14)	-44(15)
C(51)	91(10)	113(14)	290(20)	-98(15)	-60(13)	-5(11)
C(52)	69(8)	201(17)	235(18)	-150(15)	12(11)	-37(13)
O(5)	162(13)	320(20)	199(18)	-31(15)	23(11)	-21(15)
C(53)	190(20)	260(20)	160(17)	-48(15)	-11(14)	-42(19)
C(54)	168(14)	240(20)	230(20)	-45(19)	-49(15)	-70(17)
C(55)	171(16)	170(20)	250(20)	-14(16)	-11(14)	-98(17)
C(56)	187(17)	190(20)	194(18)	-35(14)	-54(14)	-99(16)
O(6)	260(20)	540(30)	251(19)	-240(20)	63(15)	-146(19)
C(57)	210(20)	430(30)	320(30)	-220(20)	19(18)	-155(19)
C(58)	200(20)	390(30)	240(20)	-230(20)	-15(16)	-79(19)
C(59)	190(20)	360(30)	240(20)	-200(20)	24(16)	-109(17)
C(60)	230(20)	440(30)	260(20)	-250(20)	-14(18)	-100(20)

Table 15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for Complex **3**

	x	y	z	U(eq)
H(1A)	825	6287	-1614	83
H(1B)	2163	5825	-1653	83
H(1C)	1862	6852	-1743	83
H(3A)	3420	5822	-476	32
H(4A)	2561	5509	932	46
H(6A)	-785	5742	1087	78
H(6B)	65	6106	1423	78
H(6C)	179	5048	1635	78
H(7A)	4907	3221	988	90
H(7B)	4805	3530	1673	90
H(7C)	4254	4206	895	90
H(9A)	2230	4016	2124	58
H(10A)	658	2998	2380	55
H(12A)	1955	1210	1608	94
H(12B)	659	1748	1638	94
H(12C)	1276	1144	2407	94
H(13A)	3934	4522	-747	71
H(13B)	4634	4431	-1494	71
H(13C)	5181	3892	-693	71
H(15A)	5091	2503	-1233	69
H(16A)	3547	1449	-787	63
H(18A)	821	2542	56	80
H(18B)	1429	1519	263	80
H(18C)	969	2116	-559	80
H(19A)	7064	799	189	228
H(19B)	6801	1804	-439	228
H(20A)	8431	2087	-403	207
H(20B)	8776	1017	69	207
H(21A)	8757	1214	1098	161
H(21B)	8508	2291	612	161
H(22A)	6936	1197	1543	159
H(22B)	6723	2274	1137	159
H(23A)	4213	-565	837	100
H(23B)	2939	-38	974	100
H(24A)	3597	-1668	1924	112
H(24B)	2750	-962	2221	112
H(25A)	4267	-1307	2940	118

H(25B)	5226	-1459	2292	118
H(26A)	4136	191	2368	132
H(26B)	5448	-42	2031	132
H(27A)	4316	11266	3404	76
H(27B)	3016	11804	3256	76
H(27C)	3292	10764	3387	76
H(29A)	1380	10855	4516	35
H(30A)	1638	10464	5956	51
H(32A)	3391	10461	6706	71
H(32B)	4165	11225	6157	71
H(32C)	4647	10186	6329	71
H(33A)	1753	9545	4226	78
H(33B)	794	8929	4322	78
H(33C)	1465	9417	3506	78
H(35A)	2014	7432	3842	68
H(36A)	3920	6433	4269	65
H(38A)	5740	6551	4869	83
H(38B)	5356	7100	5397	83
H(38C)	5941	7581	4552	83
H(39A)	4413	6192	6623	99
H(39B)	4685	6154	7415	99
H(39C)	5365	6755	6640	99
H(41A)	4217	8021	7358	60
H(42A)	2147	8999	7121	62
H(44A)	576	8213	6015	91
H(44B)	677	9195	5947	91
H(44C)	131	8482	6721	91
H(45A)	4189	4596	5958	125
H(45B)	2956	4588	5702	125
H(46A)	2935	3254	6622	146
H(46B)	4022	3360	6978	146
H(47A)	2685	3558	7853	124
H(47B)	1629	3795	7330	124
H(48A)	1627	5148	7196	131
H(48B)	2943	4934	7429	131
H(49A)	847	6117	4812	177
H(49B)	188	5421	5556	177
H(50A)	-1377	6123	4841	215
H(50B)	-860	7064	4426	215
H(51A)	-2014	7461	5258	187
H(51B)	-2188	6434	5801	187
H(52A)	-873	6331	6473	176
H(52B)	-776	7376	5974	176
H(53A)	2372	7197	2100	260
H(53B)	2482	6427	1786	260
H(54A)	931	5996	2461	263

H(54B)	821	6766	2776	263
H(55A)	1411	4999	3529	251
H(55B)	1302	5769	3843	251
H(56A)	3259	4814	3514	227
H(56B)	3149	5584	3828	227
H(57A)	1424	2155	7729	341
H(57B)	2265	1199	8021	341
H(58A)	1074	703	8990	284
H(58B)	233	1658	8699	284
H(59A)	-985	1072	8430	277
H(59B)	-145	116	8721	277
H(60A)	293	250	7586	314
H(60B)	-547	1206	7294	314

Table 16. Crystal data and structure refinement for Complex **4**

Identification code	sg308
Empirical formula	C32 H52 Cl2 Li2 N4 O2 Yb2
Formula weight	955.64
Temperature	203(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 11.475(2) A alpha = 90 deg. b = 11.541(2) A beta = 109.508(3) deg. c = 15.711(3) A gamma = 90 deg.
Volume	1961.3(6) A^3
Z, Calculated density	2, 1.618 Mg/m^3
Absorption coefficient	4.905 mm^-1
F(000)	936
Crystal size	0.20 x 0.20 x 0.01 mm
Theta range for data collection	1.88 to 23.25 deg.
Limiting indices	-12<=h<=12, 0<=k<=12, 0<=l<=17
Reflections collected / unique	15360 / 2804 [R(int) = 0.1429]
Completeness to theta = 23.25	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.862139 and 0.216347
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2804 / 0 / 199
Goodness-of-fit on F^2	1.022

Final R indices [I>2sigma(I)] R1 = 0.0536, wR2 = 0.1214

R indices (all data) R1 = 0.0771, wR2 = 0.1262

Largest diff. peak and hole 2.281 and -1.553 e.A^-3

Table 17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for Complex **4**
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Yb	9896(1)	3330(1)	10138(1)	46(1)
Cl	9359(3)	5246(2)	10933(2)	55(1)
Li	7014(17)	5033(19)	8460(15)	53(6)
N(1)	7531(9)	3421(9)	8948(6)	43(3)
N(2)	12221(9)	3406(10)	11375(7)	45(3)
O(1)	5424(8)	5007(8)	7610(7)	72(3)
C(1)	6786(14)	3358(14)	10261(10)	75(5)
C(2)	7470(12)	2855(11)	9702(11)	60(4)
C(3)	8036(12)	1748(12)	9775(12)	73(5)
C(4)	8449(15)	1681(15)	9043(14)	86(5)
C(5)	8117(12)	2665(11)	8542(12)	58(4)
C(6)	8219(15)	2955(14)	7654(11)	87(6)
C(7)	11319(13)	3411(13)	12632(9)	69(4)
C(8)	11506(11)	2877(12)	11827(9)	48(4)
C(9)	11123(13)	1814(12)	11465(13)	75(5)
C(10)	11614(13)	1635(11)	10750(12)	71(5)
C(11)	12311(12)	2635(12)	10737(11)	58(4)
C(12)	13117(14)	2875(13)	10190(12)	79(5)
C(13)	4520(15)	4168(13)	7654(13)	87(6)
C(14)	3783(18)	4562(18)	8177(14)	116(7)
C(15)	5003(16)	5881(14)	6901(15)	98(6)
C(16)	5100(20)	5480(20)	6031(17)	145(9)

Table 18. Bond lengths [A] and angles [deg] for Complex 4

Yb-Cl#1	2.688(3)
Yb-C(2)	2.691(13)
Yb-Cl	2.711(3)
Yb-C(3)	2.721(12)
Yb-C(9)	2.725(14)
Yb-C(10)	2.716(13)
Yb-C(11)	2.733(13)
Yb-C(8)	2.730(12)
Yb-N(1)	2.735(10)
Yb-N(2)	2.728(9)
Yb-C(4)	2.725(15)
Yb-C(5)	2.761(14)
Cl-Yb#1	2.688(3)
Li-O(1)	1.87(2)
Li-N(2)#1	1.98(2)
Li-N(1)	2.02(2)
N(1)-C(2)	1.376(18)
N(1)-C(5)	1.381(16)
N(2)-C(11)	1.370(17)
N(2)-C(8)	1.393(16)
N(2)-Li#1	1.98(2)
O(1)-C(15)	1.460(19)
O(1)-C(13)	1.437(17)
C(1)-C(2)	1.48(2)
C(2)-C(3)	1.420(19)
C(3)-C(4)	1.38(2)
C(4)-C(5)	1.36(2)
C(5)-C(6)	1.48(2)
C(7)-C(8)	1.486(19)
C(8)-C(9)	1.361(19)
C(9)-C(10)	1.43(2)
C(10)-C(11)	1.408(19)
C(11)-C(12)	1.48(2)
C(13)-C(14)	1.44(2)
C(15)-C(16)	1.48(3)
Cl#1-Yb-C(2)	118.9(4)
Cl#1-Yb-Cl	87.63(11)
C(2)-Yb-Cl	84.8(3)
Cl#1-Yb-C(3)	132.1(4)
C(2)-Yb-C(3)	30.4(4)
Cl-Yb-C(3)	111.2(4)

Cl#1-Yb-C(9)	132.9(4)
C(2)-Yb-C(9)	106.9(5)
Cl-Yb-C(9)	108.0(4)
C(3)-Yb-C(9)	84.2(4)
Cl#1-Yb-C(10)	108.5(4)
C(2)-Yb-C(10)	120.7(4)
Cl-Yb-C(10)	132.4(4)
C(3)-Yb-C(10)	91.0(4)
C(9)-Yb-C(10)	30.5(4)
Cl#1-Yb-C(11)	84.1(3)
C(2)-Yb-C(11)	150.7(4)
Cl-Yb-C(11)	116.2(3)
C(3)-Yb-C(11)	120.7(4)
C(9)-Yb-C(11)	48.9(5)
C(10)-Yb-C(11)	30.0(4)
Cl#1-Yb-C(8)	118.2(3)
C(2)-Yb-C(8)	121.0(5)
Cl-Yb-C(8)	83.8(3)
C(3)-Yb-C(8)	107.7(5)
C(9)-Yb-C(8)	28.9(4)
C(10)-Yb-C(8)	48.9(5)
C(11)-Yb-C(8)	47.9(5)
Cl#1-Yb-N(1)	89.9(2)
C(2)-Yb-N(1)	29.4(4)
Cl-Yb-N(1)	87.6(2)
C(3)-Yb-N(1)	49.7(4)
C(9)-Yb-N(1)	133.6(4)
C(10)-Yb-N(1)	135.0(3)
C(11)-Yb-N(1)	155.1(4)
C(8)-Yb-N(1)	150.1(4)
Cl#1-Yb-N(2)	89.2(2)
C(2)-Yb-N(2)	150.5(4)
Cl-Yb-N(2)	87.9(2)
C(3)-Yb-N(2)	133.1(4)
C(9)-Yb-N(2)	48.9(4)
C(10)-Yb-N(2)	49.4(4)
C(11)-Yb-N(2)	29.1(4)
C(8)-Yb-N(2)	29.6(3)
N(1)-Yb-N(2)	175.4(3)
Cl#1-Yb-C(4)	106.6(5)
C(2)-Yb-C(4)	48.5(5)
Cl-Yb-C(4)	132.5(4)
C(3)-Yb-C(4)	29.4(4)
C(9)-Yb-C(4)	94.9(5)
C(10)-Yb-C(4)	86.4(5)
C(11)-Yb-C(4)	110.3(5)

C(8)-Yb-C(4)	123.5(5)
N(1)-Yb-C(4)	48.7(4)
N(2)-Yb-C(4)	135.8(4)
Cl#1-Yb-C(5)	84.0(4)
C(2)-Yb-C(5)	47.5(5)
Cl-Yb-C(5)	115.6(3)
C(3)-Yb-C(5)	48.2(5)
C(9)-Yb-C(5)	123.6(4)
C(10)-Yb-C(5)	110.5(4)
C(11)-Yb-C(5)	126.0(4)
C(8)-Yb-C(5)	152.2(4)
N(1)-Yb-C(5)	29.1(3)
N(2)-Yb-C(5)	155.0(4)
C(4)-Yb-C(5)	28.7(5)
Yb#1-Cl-Yb	92.37(11)
O(1)-Li-N(2)#1	113.1(12)
O(1)-Li-N(1)	110.4(11)
N(2)#1-Li-N(1)	136.4(11)
C(2)-N(1)-C(5)	105.6(13)
C(2)-N(1)-Li	132.1(12)
C(5)-N(1)-Li	122.2(12)
C(2)-N(1)-Yb	73.6(7)
C(5)-N(1)-Yb	76.5(7)
Li-N(1)-Yb	113.2(7)
C(11)-N(2)-C(8)	106.8(13)
C(11)-N(2)-Li#1	123.2(12)
C(8)-N(2)-Li#1	129.9(12)
C(11)-N(2)-Yb	75.7(7)
C(8)-N(2)-Yb	75.3(6)
Li#1-N(2)-Yb	114.1(7)
C(15)-O(1)-C(13)	116.2(12)
C(15)-O(1)-Li	122.0(12)
C(13)-O(1)-Li	121.6(11)
N(1)-C(2)-C(3)	110.1(15)
N(1)-C(2)-C(1)	121.0(13)
C(3)-C(2)-C(1)	128.6(16)
N(1)-C(2)-Yb	77.1(7)
C(3)-C(2)-Yb	75.9(8)
C(1)-C(2)-Yb	118.6(9)
C(4)-C(3)-C(2)	104.9(14)
C(4)-C(3)-Yb	75.5(8)
C(2)-C(3)-Yb	73.6(7)
C(5)-C(4)-C(3)	109.1(15)
C(5)-C(4)-Yb	77.1(9)
C(3)-C(4)-Yb	75.1(8)
C(4)-C(5)-N(1)	110.2(16)

C(4)-C(5)-C(6)	129.9(15)
N(1)-C(5)-C(6)	119.8(13)
C(4)-C(5)-Yb	74.2(9)
N(1)-C(5)-Yb	74.4(7)
C(6)-C(5)-Yb	121.8(10)
C(9)-C(8)-N(2)	110.2(14)
C(9)-C(8)-C(7)	127.6(15)
N(2)-C(8)-C(7)	122.0(13)
C(9)-C(8)-Yb	75.3(8)
N(2)-C(8)-Yb	75.1(6)
C(7)-C(8)-Yb	120.3(8)
C(8)-C(9)-C(10)	107.5(13)
C(8)-C(9)-Yb	75.8(8)
C(10)-C(9)-Yb	74.4(8)
C(11)-C(10)-C(9)	105.5(13)
C(11)-C(10)-Yb	75.7(8)
C(9)-C(10)-Yb	75.1(8)
N(2)-C(11)-C(10)	109.9(15)
N(2)-C(11)-C(12)	121.1(13)
C(10)-C(11)-C(12)	128.9(15)
N(2)-C(11)-Yb	75.3(7)
C(10)-C(11)-Yb	74.3(8)
C(12)-C(11)-Yb	120.2(9)
O(1)-C(13)-C(14)	112.8(15)
O(1)-C(15)-C(16)	112.1(15)

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

Table 19. Anisotropic displacement parameters (A^2 x 10^3) for Complex **4**
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
Yb	33(1)	28(1)	59(1)	2(1)	-10(1)	-1(1)
Cl	54(2)	41(2)	61(2)	1(1)	6(2)	1(1)
Li	18(11)	58(12)	66(16)	-1(11)	-9(11)	-1(10)
N(1)	49(7)	40(6)	28(6)	5(5)	-2(5)	-3(5)
N(2)	32(6)	51(7)	46(7)	2(6)	3(6)	-6(5)
O(1)	39(5)	59(6)	88(8)	12(6)	-19(5)	-1(5)
C(1)	62(10)	76(11)	72(11)	21(9)	2(9)	-21(9)
C(2)	33(8)	36(8)	85(12)	-5(8)	-16(9)	-9(6)
C(3)	35(8)	41(9)	113(14)	21(9)	-14(9)	-24(7)
C(4)	60(11)	47(10)	128(16)	-31(12)	1(11)	-11(9)
C(5)	38(9)	30(8)	84(12)	-10(7)	-10(8)	7(6)
C(6)	68(12)	99(14)	64(12)	-38(9)	-16(10)	-1(9)
C(7)	54(10)	84(11)	62(10)	14(9)	8(8)	-13(8)
C(8)	29(8)	58(9)	43(9)	9(7)	-8(7)	5(6)
C(9)	41(9)	43(9)	119(14)	38(9)	0(10)	10(7)
C(10)	42(9)	21(7)	111(13)	-6(8)	-26(9)	-3(7)
C(11)	35(8)	40(9)	78(12)	14(7)	-9(8)	11(6)
C(12)	54(10)	73(11)	111(14)	9(9)	30(11)	24(8)
C(13)	56(11)	63(11)	109(15)	-3(10)	-15(11)	-27(8)
C(14)	81(15)	140(20)	122(18)	-16(14)	32(15)	-21(12)
C(15)	65(12)	56(11)	138(18)	13(11)	-13(12)	13(8)
C(16)	110(20)	170(30)	150(20)	36(19)	42(18)	23(16)

Table 20. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for Complex 4

	x	y	z	U(eq)
H(1A)	5930	3107	10031	113
H(1B)	6820	4197	10238	113
H(1C)	7157	3100	10881	113
H(3A)	7964	1100	10168	88
H(4A)	8762	968	8844	103
H(6A)	7515	2638	7179	130
H(6B)	8975	2628	7610	130
H(6C)	8233	3791	7590	130
H(7A)	11964	3151	13173	104
H(7B)	10519	3182	12659	104
H(7C)	11352	4248	12588	104
H(9A)	10734	1214	11732	90
H(10A)	11645	890	10445	85
H(12A)	13936	2567	10497	118
H(12B)	13170	3705	10114	118
H(12C)	12771	2510	9603	118
H(13A)	4944	3451	7921	104
H(13B)	3976	3989	7040	104
H(14A)	3202	3960	8197	174
H(14B)	3332	5253	7901	174
H(14C)	4316	4740	8786	174
H(15A)	5498	6585	7092	118
H(15B)	4140	6077	6813	118
H(16A)	4858	6095	5589	217
H(16B)	4565	4813	5816	217
H(16C)	5951	5254	6119	217

Table 21. Crystal data and structure refinement for Complex **5**

Identification code	sg327
Empirical formula	C48 H84 Cl4 Li4 N4 O6 Yb2
Formula weight	1331.22
Temperature	203(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 11.972(2) A alpha = 90 deg. b = 11.064(2) A beta = 99.980(3) deg. c = 23.357(3) A gamma = 90 deg.
Volume	3047.1(8) A^3
Z, Calculated density	2, 1.451 Mg/m^3
Absorption coefficient	3.269 mm^-1
F(000)	1341
Crystal size	0.12 x 0.10 x 0.03 mm
Theta range for data collection	1.73 to 20.81 deg.
Limiting indices	-11<=h<=11, 0<=k<=11, 0<=l<=23
Reflections collected / unique	19538 / 3180 [R(int) = 0.1481]
Completeness to theta = 20.81	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.928077 and 0.762312
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3180 / 478 / 353

Goodness-of-fit on F^2	1.056
Final R indices [I>2sigma(I)]	R1 = 0.0402, wR2 = 0.0722
R indices (all data)	R1 = 0.0789, wR2 = 0.0794
Largest diff. peak and hole	0.630 and -0.506 e.A^-3

Table 22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for Complex **5**
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Yb	1578(1)	2917(1)	1198(1)	44(1)
Cl(1)	2617(2)	1548(2)	501(1)	64(1)
Cl(2)	1264(2)	4985(2)	542(1)	52(1)
N(1)	3629(7)	2536(6)	1853(3)	49(2)
N(2)	-680(6)	3088(7)	943(3)	47(2)
Li(1)	4132(16)	1249(15)	1309(8)	62(3)
Li(2)	-780(14)	4739(15)	516(7)	55(3)
C(1)	4330(9)	4252(8)	1300(4)	62(3)
C(2)	3610(9)	3765(9)	1714(4)	50(2)
C(3)	2882(8)	4352(9)	2019(4)	54(2)
C(4)	2420(9)	3491(9)	2359(4)	57(2)
C(5)	2907(9)	2406(8)	2254(4)	53(2)
C(6)	2767(9)	1175(8)	2517(4)	78(4)
C(7)	-640(9)	1790(9)	62(4)	73(3)
C(8)	-453(8)	1964(9)	709(4)	57(2)
C(9)	-92(9)	1182(9)	1146(5)	65(2)
C(10)	-110(9)	1803(9)	1673(5)	66(2)
C(11)	-463(8)	2955(10)	1539(4)	55(2)
C(12)	-669(9)	3957(10)	1947(4)	75(3)
O(1)	3908(6)	-450(6)	1494(3)	77(2)
C(13)	2940(10)	-1163(10)	1281(6)	105(5)
C(14)	3163(13)	-2374(12)	1370(8)	203(8)
C(15)	4384(13)	-2434(10)	1674(8)	191(8)
C(16)	4698(11)	-1222(10)	1850(6)	120(5)
O(2)	5720(30)	1370(50)	1140(20)	96(5)
C(17)	5760(30)	730(30)	583(15)	128(8)
C(18)	5920(30)	1750(30)	103(14)	200(14)
C(19)	6820(30)	1480(40)	1416(13)	108(8)
C(20)	6740(18)	2050(20)	1995(9)	101(8)
O(3)	5490(40)	1380(60)	1120(30)	92(5)
C(21)	5720(40)	1410(40)	590(20)	111(8)
C(22)	6780(30)	740(40)	655(17)	126(9)
C(23)	7150(30)	390(40)	1220(16)	117(9)
C(24)	6530(40)	1390(50)	1600(20)	95(8)
O(4)	-1680(7)	5964(7)	859(3)	83(2)

C(25)	-2868(12)	5971(15)	636(6)	120(5)
C(26)	-3291(12)	4681(16)	506(8)	173(8)
C(27)	-1440(14)	7239(13)	999(6)	131(5)
C(28)	-354(14)	7252(12)	1366(6)	140(6)

Table 23. Bond lengths [A] and angles [deg] for Complex **5**

Yb-N(2)	2.673(7)
Yb-Cl(1)	2.682(3)
Yb-N(1)	2.691(7)
Yb-C(2)	2.690(9)
Yb-C(11)	2.698(10)
Yb-C(8)	2.714(9)
Yb-Cl(2)	2.744(2)
Yb-C(5)	2.752(9)
Yb-C(10)	2.758(10)
Yb-C(3)	2.755(9)
Yb-C(9)	2.759(10)
Yb-C(4)	2.796(9)
Cl(1)-Li(1)	2.403(17)
Cl(2)-Li(2)#1	2.457(16)
Cl(2)-Li(2)	2.452(17)
N(1)-C(5)	1.388(12)
N(1)-C(2)	1.397(11)
N(1)-Li(1)	2.07(2)
N(2)-C(11)	1.379(10)
N(2)-C(8)	1.405(11)
N(2)-Li(2)	2.074(17)
Li(1)-O(3)	1.77(4)
Li(1)-O(2)	2.01(4)
Li(1)-O(1)	1.958(18)
Li(2)-O(4)	1.985(19)
Li(2)-Cl(2)#1	2.457(16)
Li(2)-Li(2)#1	3.35(4)
C(1)-C(2)	1.502(13)
C(2)-C(3)	1.378(13)
C(3)-C(4)	1.413(13)
C(4)-C(5)	1.374(12)
C(5)-C(6)	1.514(12)
C(7)-C(8)	1.502(12)
C(8)-C(9)	1.350(12)
C(9)-C(10)	1.413(13)
C(10)-C(11)	1.361(13)
C(11)-C(12)	1.509(13)
O(1)-C(13)	1.419(11)
O(1)-C(16)	1.429(11)
C(13)-C(14)	1.375(14)
C(14)-C(15)	1.512(16)
C(15)-C(16)	1.434(14)

O(2)-C(17)	1.48(6)
O(2)-C(19)	1.38(5)
C(17)-C(18)	1.63(5)
C(19)-C(20)	1.51(3)
O(3)-C(21)	1.33(9)
O(3)-C(24)	1.52(8)
C(21)-C(22)	1.45(6)
C(22)-C(23)	1.38(4)
C(23)-C(24)	1.67(5)
O(4)-C(25)	1.428(14)
O(4)-C(27)	1.464(14)
C(25)-C(26)	1.527(17)
C(27)-C(28)	1.428(16)

N(2)-Yb-Cl(1)	117.54(17)
N(2)-Yb-N(1)	157.8(2)
Cl(1)-Yb-N(1)	77.50(18)
N(2)-Yb-C(2)	151.2(3)
Cl(1)-Yb-C(2)	89.5(2)
N(1)-Yb-C(2)	30.1(2)
N(2)-Yb-C(11)	29.8(2)
Cl(1)-Yb-C(11)	136.6(2)
N(1)-Yb-C(11)	128.2(3)
C(2)-Yb-C(11)	131.1(3)
N(2)-Yb-C(8)	30.2(2)
Cl(1)-Yb-C(8)	90.0(2)
N(1)-Yb-C(8)	147.2(3)
C(2)-Yb-C(8)	177.3(3)
C(11)-Yb-C(8)	48.7(3)
N(2)-Yb-Cl(2)	77.33(16)
Cl(1)-Yb-Cl(2)	99.48(8)
N(1)-Yb-Cl(2)	118.13(17)
C(2)-Yb-Cl(2)	89.1(2)
C(11)-Yb-Cl(2)	96.2(2)
C(8)-Yb-Cl(2)	93.6(2)
N(2)-Yb-C(5)	128.3(3)
Cl(1)-Yb-C(5)	99.9(2)
N(1)-Yb-C(5)	29.5(3)
C(2)-Yb-C(5)	48.1(3)
C(11)-Yb-C(5)	98.7(3)
C(8)-Yb-C(5)	129.3(3)
Cl(2)-Yb-C(5)	132.39(19)
N(2)-Yb-C(10)	48.5(3)
Cl(1)-Yb-C(10)	116.2(2)
N(1)-Yb-C(10)	111.2(3)
C(2)-Yb-C(10)	130.2(3)

C(11)-Yb-C(10)	28.9(3)
C(8)-Yb-C(10)	47.9(3)
Cl(2)-Yb-C(10)	123.9(2)
C(5)-Yb-C(10)	84.2(3)
N(2)-Yb-C(3)	122.9(3)
Cl(1)-Yb-C(3)	118.7(2)
N(1)-Yb-C(3)	49.0(2)
C(2)-Yb-C(3)	29.3(3)
C(11)-Yb-C(3)	102.6(3)
C(8)-Yb-C(3)	151.0(3)
Cl(2)-Yb-C(3)	85.1(2)
C(5)-Yb-C(3)	47.6(3)
C(10)-Yb-C(3)	110.2(3)
N(2)-Yb-C(9)	48.9(3)
Cl(1)-Yb-C(9)	89.4(3)
N(1)-Yb-C(9)	119.9(3)
C(2)-Yb-C(9)	148.8(3)
C(11)-Yb-C(9)	48.5(3)
C(8)-Yb-C(9)	28.5(3)
Cl(2)-Yb-C(9)	121.8(2)
C(5)-Yb-C(9)	101.5(3)
C(10)-Yb-C(9)	29.7(3)
C(3)-Yb-C(9)	138.7(3)
N(2)-Yb-C(4)	112.4(3)
Cl(1)-Yb-C(4)	126.1(2)
N(1)-Yb-C(4)	49.0(3)
C(2)-Yb-C(4)	48.7(3)
C(11)-Yb-C(4)	84.4(3)
C(8)-Yb-C(4)	130.0(3)
Cl(2)-Yb-C(4)	110.1(2)
C(5)-Yb-C(4)	28.7(2)
C(10)-Yb-C(4)	83.0(3)
C(3)-Yb-C(4)	29.5(3)
C(9)-Yb-C(4)	109.8(3)
Li(1)-Cl(1)-Yb	88.1(5)
Li(2)#1-Cl(2)-Li(2)	85.9(6)
Li(2)#1-Cl(2)-Yb	130.6(4)
Li(2)-Cl(2)-Yb	87.7(4)
C(5)-N(1)-C(2)	105.7(8)
C(5)-N(1)-Li(1)	128.7(8)
C(2)-N(1)-Li(1)	121.5(9)
C(5)-N(1)-Yb	77.7(5)
C(2)-N(1)-Yb	74.9(5)
Li(1)-N(1)-Yb	95.3(5)
C(11)-N(2)-C(8)	106.4(8)
C(11)-N(2)-Li(2)	124.4(8)

C(8)-N(2)-Li(2)	126.3(8)
C(11)-N(2)-Yb	76.1(5)
C(8)-N(2)-Yb	76.5(5)
Li(2)-N(2)-Yb	98.1(5)
O(3)-Li(1)-O(2)	3(4)
O(3)-Li(1)-O(1)	107(2)
O(2)-Li(1)-O(1)	106.2(17)
O(3)-Li(1)-N(1)	119(2)
O(2)-Li(1)-N(1)	117.5(17)
O(1)-Li(1)-N(1)	117.4(10)
O(3)-Li(1)-Cl(1)	114(2)
O(2)-Li(1)-Cl(1)	116.3(19)
O(1)-Li(1)-Cl(1)	101.0(8)
N(1)-Li(1)-Cl(1)	97.3(7)
O(3)-Li(1)-Yb	140(2)
O(2)-Li(1)-Yb	141.5(17)
O(1)-Li(1)-Yb	111.5(8)
N(1)-Li(1)-Yb	49.2(4)
Cl(1)-Li(1)-Yb	49.2(3)
O(4)-Li(2)-N(2)	113.4(9)
O(4)-Li(2)-Cl(2)#1	105.7(7)
N(2)-Li(2)-Cl(2)#1	125.2(8)
O(4)-Li(2)-Cl(2)	121.5(8)
N(2)-Li(2)-Cl(2)	96.5(6)
Cl(2)#1-Li(2)-Cl(2)	94.1(6)
O(4)-Li(2)-Li(2)#1	125.6(9)
N(2)-Li(2)-Li(2)#1	120.4(10)
Cl(2)#1-Li(2)-Li(2)#1	47.0(4)
Cl(2)-Li(2)-Li(2)#1	47.1(4)
O(4)-Li(2)-Yb	129.9(7)
N(2)-Li(2)-Yb	47.2(4)
Cl(2)#1-Li(2)-Yb	122.9(6)
Cl(2)-Li(2)-Yb	49.5(3)
Li(2)#1-Li(2)-Yb	85.6(6)
C(3)-C(2)-N(1)	108.9(10)
C(3)-C(2)-C(1)	130.4(9)
N(1)-C(2)-C(1)	120.7(10)
C(3)-C(2)-Yb	78.0(6)
N(1)-C(2)-Yb	75.0(5)
C(1)-C(2)-Yb	114.4(6)
C(2)-C(3)-C(4)	108.4(9)
C(2)-C(3)-Yb	72.7(6)
C(4)-C(3)-Yb	76.9(5)
C(5)-C(4)-C(3)	105.7(10)
C(5)-C(4)-Yb	73.9(6)
C(3)-C(4)-Yb	73.7(5)

C(4)-C(5)-N(1)	111.2(9)
C(4)-C(5)-C(6)	129.3(11)
N(1)-C(5)-C(6)	119.5(9)
C(4)-C(5)-Yb	77.4(6)
N(1)-C(5)-Yb	72.8(5)
C(6)-C(5)-Yb	117.4(6)
C(9)-C(8)-N(2)	109.4(9)
C(9)-C(8)-C(7)	130.6(11)
N(2)-C(8)-C(7)	120.0(9)
C(9)-C(8)-Yb	77.6(6)
N(2)-C(8)-Yb	73.3(5)
C(7)-C(8)-Yb	116.1(7)
C(8)-C(9)-C(10)	107.1(10)
C(8)-C(9)-Yb	73.9(6)
C(10)-C(9)-Yb	75.1(6)
C(11)-C(10)-C(9)	107.9(10)
C(11)-C(10)-Yb	73.1(6)
C(9)-C(10)-Yb	75.2(6)
C(10)-C(11)-N(2)	109.1(10)
C(10)-C(11)-C(12)	128.5(9)
N(2)-C(11)-C(12)	122.3(10)
C(10)-C(11)-Yb	78.0(6)
N(2)-C(11)-Yb	74.1(5)
C(12)-C(11)-Yb	116.9(7)
C(13)-O(1)-C(16)	106.8(8)
C(13)-O(1)-Li(1)	126.3(8)
C(16)-O(1)-Li(1)	126.9(8)
C(14)-C(13)-O(1)	111.3(10)
C(13)-C(14)-C(15)	105.1(11)
C(16)-C(15)-C(14)	106.1(11)
O(1)-C(16)-C(15)	106.2(9)
C(17)-O(2)-C(19)	106(3)
C(17)-O(2)-Li(1)	108(3)
C(19)-O(2)-Li(1)	141(4)
O(2)-C(17)-C(18)	107(3)
C(20)-C(19)-O(2)	105(3)
C(21)-O(3)-C(24)	115(4)
C(21)-O(3)-Li(1)	126(5)
C(24)-O(3)-Li(1)	120(4)
C(22)-C(21)-O(3)	101(5)
C(21)-C(22)-C(23)	112(4)
C(22)-C(23)-C(24)	103(3)
O(3)-C(24)-C(23)	89(4)
C(25)-O(4)-C(27)	102.7(10)
C(25)-O(4)-Li(2)	115.7(9)
C(27)-O(4)-Li(2)	130.5(10)

O(4)-C(25)-C(26)	110.0(12)
C(28)-C(27)-O(4)	105.5(12)

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

Table 24. Anisotropic displacement parameters (A^2 x 10^3) for Complex **5**
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
Yb	48(1)	40(1)	41(1)	2(1)	-4(1)	2(1)
Cl(1)	79(2)	59(2)	49(2)	-4(1)	-2(2)	18(2)
Cl(2)	51(2)	47(2)	53(2)	11(1)	-4(1)	-1(1)
N(1)	54(4)	38(4)	50(4)	2(3)	-8(3)	-1(3)
N(2)	45(3)	49(4)	45(4)	2(3)	0(3)	-9(4)
Li(1)	64(5)	44(6)	72(9)	2(6)	-1(6)	9(6)
Li(2)	46(6)	62(7)	55(9)	13(6)	2(6)	4(6)
C(1)	67(7)	46(7)	69(8)	12(5)	-2(5)	-4(5)
C(2)	50(4)	39(5)	55(6)	4(4)	-10(4)	-2(4)
C(3)	55(6)	41(5)	56(6)	-1(4)	-17(4)	5(4)
C(4)	63(6)	60(5)	43(4)	-7(4)	-5(3)	0(4)
C(5)	70(6)	40(5)	42(4)	3(4)	-11(3)	-8(4)
C(6)	105(10)	58(6)	59(7)	19(5)	-17(6)	-17(7)
C(7)	77(8)	73(9)	63(6)	-21(5)	-5(6)	-3(6)
C(8)	62(4)	47(5)	55(4)	-4(4)	-7(4)	-13(5)
C(9)	69(5)	41(4)	78(6)	5(4)	-6(5)	-14(4)
C(10)	65(5)	69(6)	60(5)	20(4)	2(4)	-14(4)
C(11)	58(4)	61(5)	45(4)	4(4)	7(4)	-12(5)
C(12)	75(8)	98(8)	56(7)	-2(6)	23(6)	14(7)
O(1)	75(6)	46(4)	95(6)	4(4)	-24(5)	7(4)
C(13)	86(9)	49(7)	157(11)	6(8)	-42(8)	-13(6)
C(14)	162(13)	60(7)	323(18)	6(11)	-140(13)	-6(8)
C(15)	172(13)	55(7)	279(17)	1(10)	-148(13)	7(8)
C(16)	115(10)	52(7)	160(12)	8(7)	-71(9)	17(7)
O(2)	68(7)	105(11)	118(11)	-25(9)	25(7)	-2(10)
C(17)	88(14)	159(19)	141(14)	-61(12)	26(11)	7(18)
C(18)	200(30)	290(30)	127(18)	-28(19)	70(20)	-20(30)
C(19)	72(9)	123(16)	128(15)	-13(15)	18(11)	-12(14)
C(20)	75(16)	150(20)	76(13)	41(13)	13(11)	9(16)
O(3)	65(7)	100(12)	112(12)	-34(11)	19(7)	-4(9)
C(21)	78(14)	140(20)	119(12)	-16(18)	28(10)	4(16)
C(22)	76(17)	190(20)	124(15)	-12(18)	38(15)	18(17)
C(23)	79(15)	150(20)	132(18)	9(17)	49(15)	24(14)
C(24)	57(10)	118(17)	116(14)	4(16)	27(12)	6(15)

O(4)	101(6)	82(5)	64(5)	9(4)	13(5)	44(5)
C(25)	94(8)	172(13)	104(11)	21(10)	42(9)	55(8)
C(26)	97(12)	234(17)	183(18)	53(16)	12(12)	-27(12)
C(27)	207(14)	91(8)	96(11)	5(9)	26(9)	24(10)
C(28)	213(17)	105(11)	101(12)	21(9)	24(10)	-33(11)

Table 25. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for Complex **5**

	x	y	z	U(eq)
H(1A)	4194	5112	1246	93
H(1B)	4138	3842	929	93
H(1C)	5124	4115	1459	93
H(3A)	2721	5184	2003	65
H(4A)	1891	3631	2605	69
H(6A)	3221	587	2351	116
H(6B)	1975	939	2433	116
H(6C)	3016	1212	2934	116
H(7A)	-920	2536	-129	110
H(7B)	-1192	1153	-47	110
H(7C)	70	1569	-57	110
H(9A)	130	375	1106	78
H(10A)	87	1479	2049	79
H(12A)	-966	4660	1722	113
H(12B)	39	4167	2196	113
H(12C)	-1213	3690	2183	113
H(13A)	2315	-928	1477	126
H(13B)	2705	-1012	864	126
H(14A)	3063	-2809	999	244
H(14B)	2658	-2727	1613	244
H(15A)	4458	-2969	2013	229
H(15B)	4870	-2742	1409	229
H(16A)	4656	-1104	2262	144
H(16B)	5473	-1049	1792	144
H(17A)	5049	282	458	154
H(17B)	6389	157	633	154
H(18A)	5859	1375	-276	300
H(18B)	6663	2119	209	300
H(18C)	5339	2365	92	300
H(19A)	7190	687	1470	129
H(19B)	7258	1995	1193	129
H(20A)	7478	2034	2244	152
H(20B)	6200	1605	2178	152
H(20C)	6488	2882	1935	152
H(21A)	5122	1015	310	133
H(21B)	5818	2241	461	133
H(22A)	7359	1239	524	152

H(22B)	6669	17	406	152
H(23A)	7981	434	1320	140
H(23B)	6912	-441	1288	140
H(24A)	6390	1073	1976	115
H(24B)	6921	2169	1653	115
H(25A)	-3019	6456	280	144
H(25B)	-3275	6338	922	144
H(26A)	-4099	4693	358	259
H(26B)	-3144	4205	860	259
H(26C)	-2896	4325	218	259
H(27A)	-1426	7708	645	158
H(27B)	-2018	7580	1202	158
H(28A)	-137	8080	1467	210
H(28B)	203	6889	1162	210
H(28C)	-388	6796	1717	210

Table 26. Crystal data and structure refinement for Complex **6**

Identification code	sg325
Empirical formula	C23.50 H36 I2 Li2 N2 O2 Yb
Formula weight	819.26
Temperature	203(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 9.0560(9) A alpha = 77.044(2) deg. b = 11.162(1) A beta = 86.608(2) deg. c = 15.354(2) A gamma = 76.605(2) deg.
Volume	1471.4(3) A^3
Z, Calculated density	2, 1.849 Mg/m^3
Absorption coefficient	5.296 mm^-1
F(000)	778
Crystal size	0.1 x 0.1 x 0.1 mm
Theta range for data collection	1.36 to 28.72 deg.
Limiting indices	-12<=h<=12, -14<=k<=14, 0<=l<=20
Reflections collected / unique	11552 / 6664 [R(int) = 0.0417]
Completeness to theta = 28.72	87.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.694463 and 0.335699
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6664 / 5 / 313
Goodness-of-fit on F^2	1.007

Final R indices [I>2sigma(I)] R1 = 0.0424, wR2 = 0.0990

R indices (all data) R1 = 0.0552, wR2 = 0.1040

Largest diff. peak and hole 1.579 and -1.565 e.A^-3

Table 27. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for Complex **6**
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Yb	319(1)	1621(1)	2202(1)	31(1)
I(1)	1563(1)	-469(1)	3873(1)	41(1)
I(2)	-1021(1)	-211(1)	1383(1)	39(1)
Li(1)	2(12)	-1606(11)	5406(8)	41(2)
Li(2)	1796(14)	-155(11)	445(8)	47(3)
N(1)	-1150(6)	2648(5)	3496(4)	34(1)
N(2)	2288(6)	1286(5)	863(3)	37(1)
O(1)	-1501(5)	-2186(5)	4882(4)	55(1)
O(2)	3066(6)	-1813(4)	705(3)	49(1)
C(1)	344(9)	4333(7)	3136(6)	59(2)
C(2)	-785(8)	3669(6)	2888(5)	43(2)
C(3)	-1651(8)	3934(7)	2121(5)	49(2)
C(4)	-2593(7)	3066(7)	2249(5)	46(2)
C(5)	-2290(7)	2299(6)	3108(4)	37(1)
C(6)	-2999(8)	1269(7)	3585(5)	47(2)
C(7)	435(9)	3026(7)	-107(4)	50(2)
C(8)	1545(7)	2540(6)	643(4)	40(1)
C(9)	1987(8)	3212(7)	1222(5)	49(2)
C(10)	3075(8)	2330(8)	1802(5)	52(2)
C(11)	3245(7)	1165(7)	1554(4)	39(1)
C(12)	4341(7)	-29(7)	1922(5)	50(2)
C(13)	-3079(9)	-2049(10)	5123(7)	72(3)
C(14)	-3882(10)	-1946(9)	4292(7)	73(3)
C(15)	-2708(12)	-2460(11)	3674(7)	83(3)
C(16)	-1277(11)	-2842(11)	4191(8)	93(4)
C(17)	2953(10)	-2862(8)	1426(6)	64(2)
C(18)	4152(16)	-3888(11)	1306(11)	131(6)
C(19)	5040(20)	-3482(13)	538(12)	200(11)
C(20)	4417(10)	-2165(9)	144(7)	79(3)
C(21)	6033(16)	4410(13)	4628(10)	59(8)
C(22)	5070(20)	4813(15)	3897(8)	85(7)
C(23)	3610(20)	5528(15)	3976(9)	140(20)
C(24)	3116(14)	5840(12)	4788(11)	65(5)
C(25)	4079(14)	5438(12)	5520(9)	68(10)
C(26)	5537(14)	4723(13)	5440(8)	55(4)

C(27)	6480(20)	4310(20)	6150(20)	83(12)

Table 28. Bond lengths [A] and angles [deg] for Complex **6**

Yb-N(1)	2.652(5)
Yb-C(8)	2.670(7)
Yb-N(2)	2.674(5)
Yb-C(2)	2.689(6)
Yb-C(5)	2.710(6)
Yb-C(9)	2.734(7)
Yb-C(11)	2.750(6)
Yb-C(3)	2.759(7)
Yb-C(4)	2.761(6)
Yb-C(10)	2.783(7)
Yb-I(2)	3.1174(5)
Yb-I(1)	3.1203(5)
I(1)-Li(1)#1	2.835(12)
I(1)-Li(1)	2.872(12)
I(2)-Li(2)#2	2.851(12)
I(2)-Li(2)	2.861(13)
Li(1)-O(1)	1.922(12)
Li(1)-N(1)#1	2.011(12)
Li(1)-I(1)#1	2.835(12)
Li(1)-Li(1)#1	3.52(2)
Li(1)-Yb#1	3.663(11)
Li(2)-O(2)	1.908(13)
Li(2)-N(2)	2.007(13)
Li(2)-I(2)#2	2.851(12)
Li(2)-Li(2)#2	3.52(2)
N(1)-C(5)	1.391(8)
N(1)-C(2)	1.393(9)
N(1)-Li(1)#1	2.011(12)
N(2)-C(11)	1.373(8)
N(2)-C(8)	1.380(8)
O(1)-C(16)	1.399(10)
O(1)-C(13)	1.437(10)
O(2)-C(17)	1.438(9)
O(2)-C(20)	1.483(9)
C(1)-C(2)	1.505(9)
C(2)-C(3)	1.390(10)
C(3)-C(4)	1.409(10)
C(4)-C(5)	1.407(10)
C(5)-C(6)	1.476(10)
C(7)-C(8)	1.495(9)
C(8)-C(9)	1.412(10)
C(9)-C(10)	1.412(10)

C(10)-C(11)	1.408(10)
C(11)-C(12)	1.482(9)
C(13)-C(14)	1.475(13)
C(14)-C(15)	1.483(15)
C(15)-C(16)	1.485(13)
C(17)-C(18)	1.422(13)
C(18)-C(19)	1.434(17)
C(19)-C(20)	1.449(14)
C(21)-C(22)	1.3900
C(21)-C(26)	1.3900
C(22)-C(23)	1.3900
C(23)-C(24)	1.3900
C(24)-C(25)	1.3900
C(25)-C(26)	1.3900
C(26)-C(27)	1.36(3)

N(1)-Yb-C(8)	133.99(19)
N(1)-Yb-N(2)	159.01(17)
C(8)-Yb-N(2)	29.93(18)
N(1)-Yb-C(2)	30.23(19)
C(8)-Yb-C(2)	103.8(2)
N(2)-Yb-C(2)	130.6(2)
N(1)-Yb-C(5)	30.04(16)
C(8)-Yb-C(5)	136.0(2)
N(2)-Yb-C(5)	161.47(17)
C(2)-Yb-C(5)	48.9(2)
N(1)-Yb-C(9)	109.4(2)
C(8)-Yb-C(9)	30.3(2)
N(2)-Yb-C(9)	50.1(2)
C(2)-Yb-C(9)	80.7(2)
C(5)-Yb-C(9)	126.4(2)
N(1)-Yb-C(11)	136.82(17)
C(8)-Yb-C(11)	48.08(19)
N(2)-Yb-C(11)	29.29(17)
C(2)-Yb-C(11)	120.4(2)
C(5)-Yb-C(11)	166.86(19)
C(9)-Yb-C(11)	48.7(2)
N(1)-Yb-C(3)	49.67(19)
C(8)-Yb-C(3)	89.7(2)
N(2)-Yb-C(3)	119.6(2)
C(2)-Yb-C(3)	29.5(2)
C(5)-Yb-C(3)	48.8(2)
C(9)-Yb-C(3)	78.7(2)
C(11)-Yb-C(3)	127.3(2)
N(1)-Yb-C(4)	49.82(18)
C(8)-Yb-C(4)	106.8(2)

N(2)-Yb-C(4)	132.42(19)
C(2)-Yb-C(4)	48.9(2)
C(5)-Yb-C(4)	29.8(2)
C(9)-Yb-C(4)	105.6(2)
C(11)-Yb-C(4)	153.3(2)
C(3)-Yb-C(4)	29.6(2)
N(1)-Yb-C(10)	111.27(19)
C(8)-Yb-C(10)	48.9(2)
N(2)-Yb-C(10)	49.4(2)
C(2)-Yb-C(10)	91.0(2)
C(5)-Yb-C(10)	139.2(2)
C(9)-Yb-C(10)	29.6(2)
C(11)-Yb-C(10)	29.5(2)
C(3)-Yb-C(10)	101.2(2)
C(4)-Yb-C(10)	130.6(2)
N(1)-Yb-I(2)	120.52(11)
C(8)-Yb-I(2)	92.42(14)
N(2)-Yb-I(2)	79.57(11)
C(2)-Yb-I(2)	136.52(15)
C(5)-Yb-I(2)	92.03(13)
C(9)-Yb-I(2)	122.68(16)
C(11)-Yb-I(2)	100.50(14)
C(3)-Yb-I(2)	113.06(16)
C(4)-Yb-I(2)	87.92(15)
C(10)-Yb-I(2)	128.17(16)
N(1)-Yb-I(1)	79.60(11)
C(8)-Yb-I(1)	133.80(14)
N(2)-Yb-I(1)	107.16(11)
C(2)-Yb-I(1)	103.36(15)
C(5)-Yb-I(1)	89.60(13)
C(9)-Yb-I(1)	123.56(15)
C(11)-Yb-I(1)	85.87(14)
C(3)-Yb-I(1)	129.22(16)
C(4)-Yb-I(1)	119.26(16)
C(10)-Yb-I(1)	94.21(16)
I(2)-Yb-I(1)	92.877(15)
Li(1)#1-I(1)-Li(1)	76.2(4)
Li(1)#1-I(1)-Yb	75.8(2)
Li(1)-I(1)-Yb	130.5(2)
Li(2)#2-I(2)-Li(2)	76.0(4)
Li(2)#2-I(2)-Yb	125.7(2)
Li(2)-I(2)-Yb	76.5(2)
O(1)-Li(1)-N(1)#1	121.6(7)
O(1)-Li(1)-I(1)#1	106.9(5)
N(1)#1-Li(1)-I(1)#1	98.6(4)
O(1)-Li(1)-I(1)	102.9(5)

N(1)#1-Li(1)-I(1)	120.8(5)
I(1)#1-Li(1)-I(1)	103.8(4)
O(1)-Li(1)-Li(1)#1	114.5(6)
N(1)#1-Li(1)-Li(1)#1	122.6(6)
I(1)#1-Li(1)-Li(1)#1	52.4(3)
I(1)-Li(1)-Li(1)#1	51.4(3)
O(1)-Li(1)-Yb#1	118.1(5)
N(1)#1-Li(1)-Yb#1	44.9(3)
I(1)#1-Li(1)-Yb#1	55.6(2)
I(1)-Li(1)-Yb#1	137.6(4)
Li(1)#1-Li(1)-Yb#1	98.5(4)
O(2)-Li(2)-N(2)	122.2(6)
O(2)-Li(2)-I(2)#2	103.6(5)
N(2)-Li(2)-I(2)#2	118.5(5)
O(2)-Li(2)-I(2)	108.5(5)
N(2)-Li(2)-I(2)	98.2(5)
I(2)#2-Li(2)-I(2)	104.0(4)
O(2)-Li(2)-Li(2)#2	116.7(7)
N(2)-Li(2)-Li(2)#2	120.2(6)
I(2)#2-Li(2)-Li(2)#2	52.1(3)
I(2)-Li(2)-Li(2)#2	51.9(3)
O(2)-Li(2)-Yb	122.7(5)
N(2)-Li(2)-Yb	44.5(3)
I(2)#2-Li(2)-Yb	132.7(4)
I(2)-Li(2)-Yb	54.9(2)
Li(2)#2-Li(2)-Yb	94.7(5)
C(5)-N(1)-C(2)	106.7(5)
C(5)-N(1)-Li(1)#1	124.1(6)
C(2)-N(1)-Li(1)#1	127.9(5)
C(5)-N(1)-Yb	77.3(3)
C(2)-N(1)-Yb	76.3(4)
Li(1)#1-N(1)-Yb	102.7(4)
C(11)-N(2)-C(8)	106.7(6)
C(11)-N(2)-Li(2)	125.0(5)
C(8)-N(2)-Li(2)	127.2(5)
C(11)-N(2)-Yb	78.4(4)
C(8)-N(2)-Yb	74.9(4)
Li(2)-N(2)-Yb	103.8(4)
C(16)-O(1)-C(13)	105.9(6)
C(16)-O(1)-Li(1)	126.9(6)
C(13)-O(1)-Li(1)	127.2(6)
C(17)-O(2)-C(20)	109.9(6)
C(17)-O(2)-Li(2)	129.1(6)
C(20)-O(2)-Li(2)	120.9(6)
C(3)-C(2)-N(1)	109.7(6)
C(3)-C(2)-C(1)	130.4(7)