APPENDIX F

Crystallographic Data for TBA·Tb(DO2A)(F-DPA)

CALIFORNIA INSTITUTE OF TECHNOLOGY

BECKMAN INSTITUTE

X-RAY CRYSTALLOGRAPHY LABORATORY

Date 11 January 2010

Crystal Structure Analysis of:

MLC23

(shown below)

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Account Number: AP1.HSARPA3-1-HSARPA.PONCE

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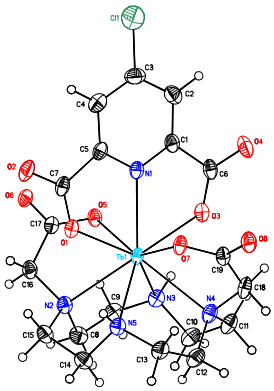

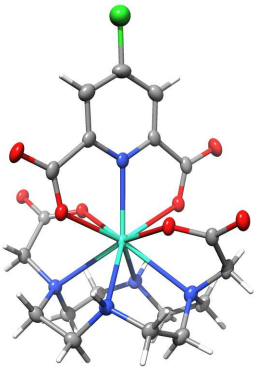

MLC23

Note: The crystallographic data have been deposited in the Cambridge Database (CCDC) and has been placed on hold pending further instructions from me. The deposition number is 761002. Ideally the CCDC would like the publication to contain a footnote of the type: "Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 761002."

Table 1. Crystal data and structure refinement for MLC23 (CCDC 761002).

Empirical formula	$[C_{19}H_{24}Cl_{0.63}F_{0.37}N_5O_8Tb]^-[C_{16}H_{36}N]^+ \bullet C_3H_6O \bullet 2(H_2O)$
Formula weight	975.45
Crystallization Solvent	Acetone/water
Crystal Habit	Trapezoidal
Crystal size	0.15 x 0.15 x 0.15 mm^3
Crystal color	Colorless

Data Collection

Type of diffractometer	Bruker KAPPA APEX II
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 9873 reflections used in lattice determination	2.33 to 38.01°
Unit cell dimensions	a = 13.2324(6) Å b = 12.9812(6) Å β= 90.528(2)° c = 26.2126(11) Å
Volume	4502.4(3) $Å^3$
Z	4
Crystal system	Monoclinic
Space group	P $2_1/c$
Density (calculated)	1.439 Mg/m^3
F(000)	2028
θ range for data collection	1.54 to 39.88°
Completeness to θ = 39.88°	96.2 %
Index ranges	$-22 \le h \le 23$, $-23 \le k \le 21$, $-44 \le l \le 46$
Data collection scan type	ω scans; 16 settings
Reflections collected	172388
Independent reflections	26652 [R_{int}= 0.0331]
Absorption coefficient	1.671 mm^{-1}
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7478 and 0.6753

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 2008)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 2008)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	26652 / 0 / 525
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	2.025
Final R indices [$I>2\sigma(I)$, 18685 reflections]	R1 = 0.0285, *w*R2 = 0.0499
R indices (all data)	R1 = 0.0534, *w*R2 = 0.0518
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.005
Average shift/error	0.000
Largest diff. peak and hole	2.226 and -1.457 e.Å^{-3}

Special Refinement Details

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

The DPA ligand is disordered at the halogen site, composed of 63% Cl and 37% F. The fluorine was refined isotropically and the two were restrained to a total occupancy of unity

Hydrogen atoms on water were located in the map then assigned to ride the corresponding oxygen. All other hydrogen atoms were restrained as riding at calculated positions.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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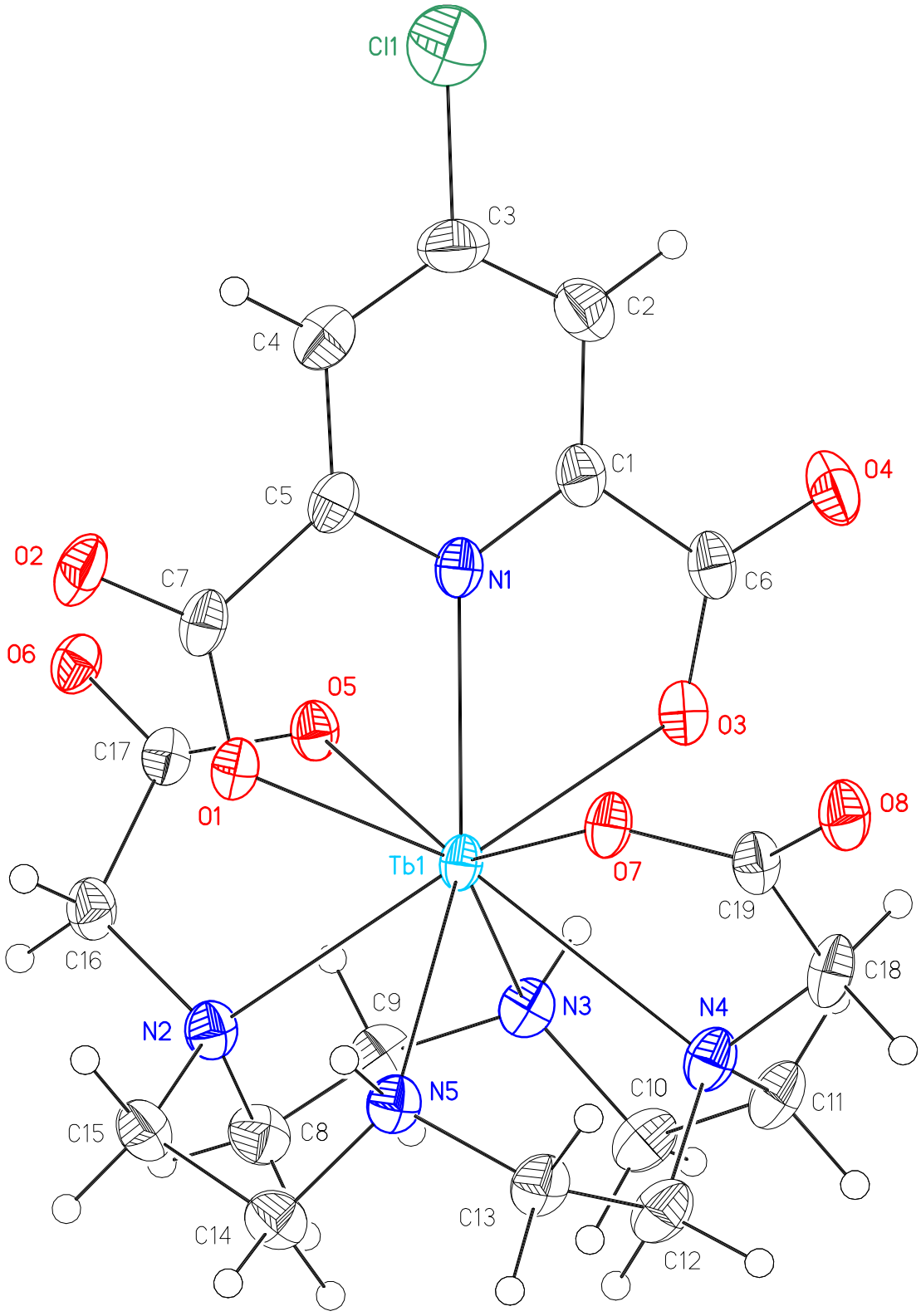
Cl1
C3
C2
C4
C1
O4
C5
O2
C7
N1
C6
O6
O5
O3
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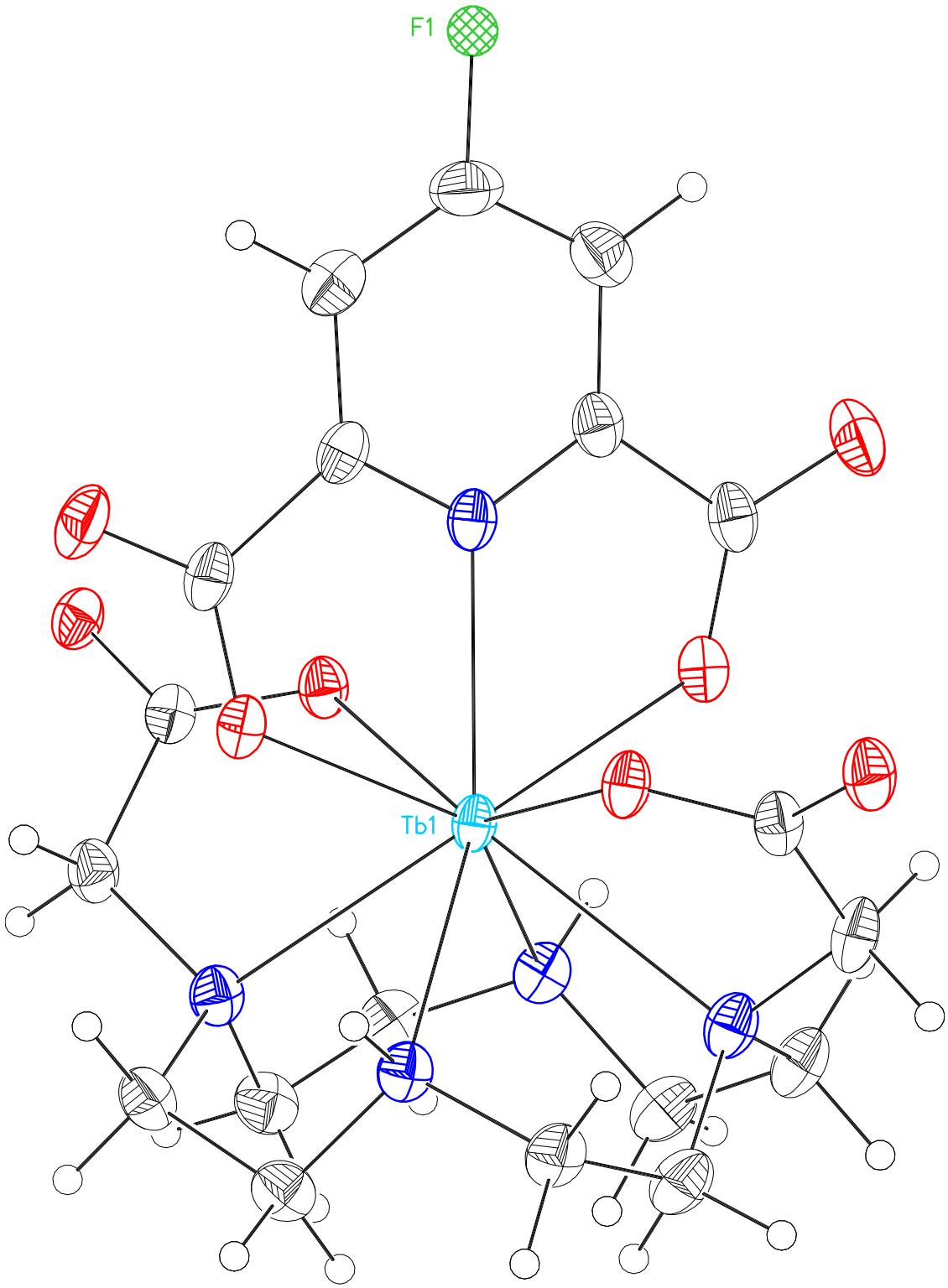
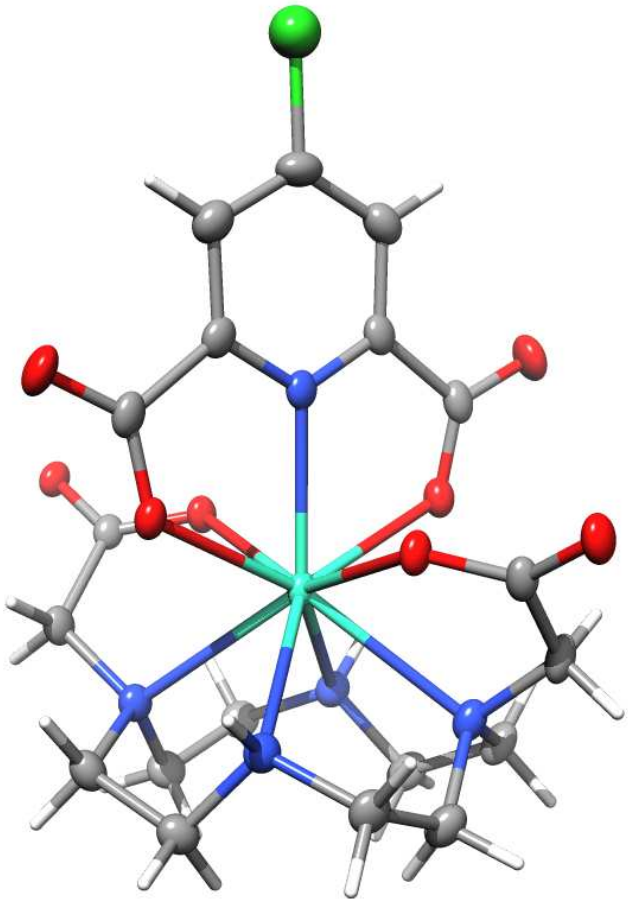
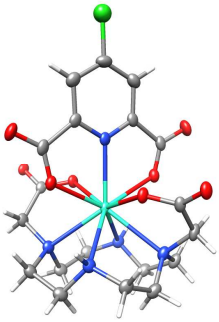
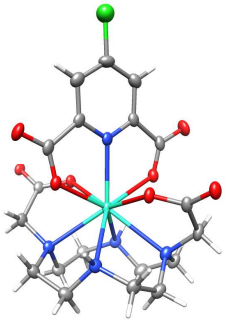
O1
O8
Tb1
O7
C19
C16
C18
C9
N3
N4
N2
N5
C10
C11
C15
C8
C14
C13
C12

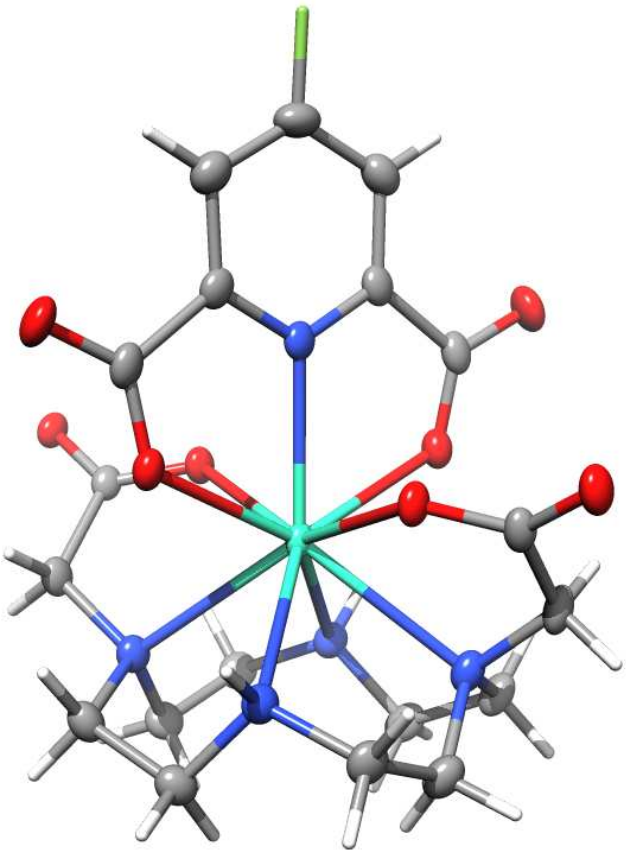
F6

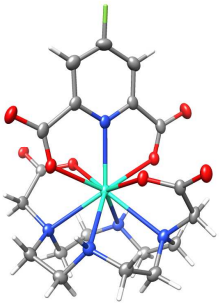


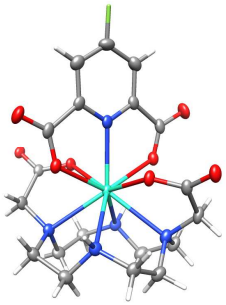












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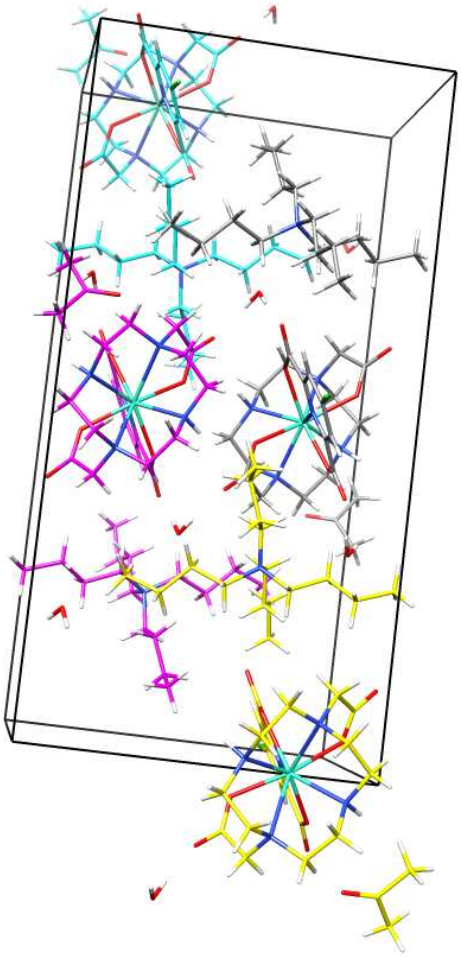

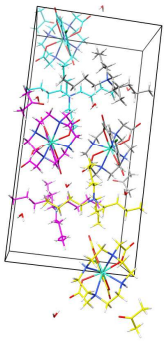

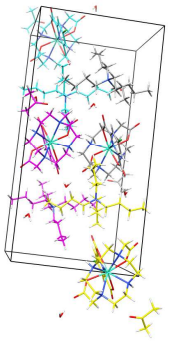

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for MLC23 (CCDC 761002). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
Tb(1)	2472(1)	5024(1)	4974(1)	16(1)	1
Cl(1)	2658(1)	-260(1)	4804(1)	54(1)	0.630(6)
F(1)	2514(4)	26(5)	4774(2)	50(2)	0.370(6)
O(1)	1696(1)	4120(1)	5658(1)	21(1)	1
O(2)	1372(1)	2667(1)	6091(1)	31(1)	1
O(3)	3290(1)	4354(1)	4236(1)	22(1)	1
O(4)	3678(1)	3059(1)	3708(1)	33(1)	1
O(5)	3911(1)	4403(1)	5406(1)	20(1)	1
O(6)	4661(1)	4001(1)	6142(1)	21(1)	1
O(7)	1048(1)	4548(1)	4494(1)	21(1)	1
O(8)	251(1)	4439(1)	3745(1)	26(1)	1
N(1)	2495(1)	3110(1)	4902(1)	19(1)	1
N(2)	2939(1)	6079(1)	5808(1)	21(1)	1
N(3)	3895(1)	6320(1)	4811(1)	22(1)	1
N(4)	2011(1)	6340(1)	4240(1)	22(1)	1
N(5)	1062(1)	6248(1)	5245(1)	21(1)	1
C(1)	2898(1)	2665(1)	4494(1)	22(1)	1
C(2)	2938(1)	1600(1)	4441(1)	28(1)	1
C(3)	2555(1)	1026(1)	4835(1)	32(1)	1
C(4)	2144(1)	1462(1)	5263(1)	28(1)	1
C(5)	2123(1)	2534(1)	5279(1)	21(1)	1
C(6)	3322(1)	3415(1)	4108(1)	23(1)	1
C(7)	1693(1)	3151(1)	5719(1)	23(1)	1
C(8)	3635(1)	6939(1)	5687(1)	25(1)	1
C(9)	4406(1)	6661(1)	5286(1)	24(1)	1
C(10)	3629(1)	7187(1)	4474(1)	27(1)	1
C(11)	2949(1)	6816(1)	4043(1)	26(1)	1
C(12)	1319(1)	7148(1)	4429(1)	27(1)	1
C(13)	554(1)	6744(1)	4804(1)	24(1)	1
C(14)	1323(1)	6993(1)	5649(1)	25(1)	1
C(15)	2004(1)	6487(1)	6043(1)	24(1)	1
C(16)	3432(1)	5334(1)	6155(1)	23(1)	1
C(17)	4057(1)	4520(1)	5881(1)	18(1)	1
C(18)	1513(1)	5724(1)	3834(1)	25(1)	1
C(19)	874(1)	4837(1)	4038(1)	21(1)	1
N(6)	3611(1)	2719(1)	2232(1)	19(1)	1
C(20)	3314(1)	1590(1)	2225(1)	21(1)	1
C(21)	3168(1)	1107(1)	2747(1)	30(1)	1
C(22)	2891(1)	-15(1)	2696(1)	31(1)	1
C(23)	2702(1)	-521(1)	3209(1)	38(1)	1
C(24)	4582(1)	2875(1)	2535(1)	22(1)	1
C(25)	5502(1)	2309(1)	2337(1)	26(1)	1
C(26)	6319(1)	2248(1)	2749(1)	27(1)	1
C(27)	7271(1)	1721(1)	2570(1)	36(1)	1
C(28)	3744(1)	3042(1)	1681(1)	21(1)	1

C(29)	3955(1)	4177(1)	1593(1)	26(1)	1
C(30)	4358(1)	4338(1)	1057(1)	29(1)	1
C(31)	4402(1)	5473(1)	908(1)	48(1)	1
C(32)	2798(1)	3365(1)	2488(1)	22(1)	1
C(33)	1746(1)	3240(1)	2265(1)	26(1)	1
C(34)	1004(1)	3960(1)	2523(1)	36(1)	1
C(35)	-72(1)	3767(1)	2336(1)	47(1)	1
O(41)	5766(1)	5083(1)	6854(1)	28(1)	1
O(42)	9136(1)	5853(1)	3129(1)	37(1)	1
O(51)	1422(1)	9456(1)	6247(1)	57(1)	1
C(51)	17(1)	8655(2)	6648(1)	61(1)	1
C(52)	525(1)	9313(1)	6258(1)	52(1)	1
C(53)	-148(2)	9784(3)	5859(1)	121(1)	1

Table 3. Selected bond lengths [Å] and angles [°] for MLC23 (CCDC 761002).

Tb(1)-O(7)	2.3392(8)	O(7)-Tb(1)-O(5)	144.47(3)
Tb(1)-O(5)	2.3492(7)	O(7)-Tb(1)-O(1)	85.65(3)
Tb(1)-O(1)	2.3835(7)	O(5)-Tb(1)-O(1)	79.68(3)
Tb(1)-O(3)	2.3889(8)	O(7)-Tb(1)-O(3)	80.64(3)
Tb(1)-N(1)	2.4924(9)	O(5)-Tb(1)-O(3)	83.90(3)
Tb(1)-N(5)	2.5562(9)	O(1)-Tb(1)-O(3)	129.13(3)
Tb(1)-N(3)	2.5634(9)	O(7)-Tb(1)-N(1)	72.93(3)
Tb(1)-N(4)	2.6409(9)	O(5)-Tb(1)-N(1)	71.54(3)
Tb(1)-N(2)	2.6476(9)	O(1)-Tb(1)-N(1)	64.62(3)
		O(3)-Tb(1)-N(1)	64.52(3)
		O(7)-Tb(1)-N(5)	74.14(3)
		O(5)-Tb(1)-N(5)	132.09(3)
		O(1)-Tb(1)-N(5)	77.12(3)
		O(3)-Tb(1)-N(5)	142.03(3)
		N(1)-Tb(1)-N(5)	130.57(3)
		O(7)-Tb(1)-N(3)	132.31(3)
		O(5)-Tb(1)-N(3)	73.28(3)
		O(1)-Tb(1)-N(3)	140.40(3)
		O(3)-Tb(1)-N(3)	76.41(3)
		N(1)-Tb(1)-N(3)	129.19(3)
		N(5)-Tb(1)-N(3)	100.23(3)
		O(7)-Tb(1)-N(4)	66.38(3)
		O(5)-Tb(1)-N(4)	138.96(3)
		O(1)-Tb(1)-N(4)	140.26(3)
		O(3)-Tb(1)-N(4)	75.45(3)
		N(1)-Tb(1)-N(4)	126.36(3)
		N(5)-Tb(1)-N(4)	68.64(3)
		N(3)-Tb(1)-N(4)	67.62(3)
		O(7)-Tb(1)-N(2)	139.59(3)
		O(5)-Tb(1)-N(2)	66.28(3)
		O(1)-Tb(1)-N(2)	74.50(3)
		O(3)-Tb(1)-N(2)	138.80(3)
		N(1)-Tb(1)-N(2)	125.11(3)
		N(5)-Tb(1)-N(2)	67.36(3)
		N(3)-Tb(1)-N(2)	68.39(3)
		N(4)-Tb(1)-N(2)	108.52(3)

Table 4. Bond lengths [Å] and angles [°] for MLC23 (CCDC 761002).

Tb(1)-O(7)	2.3392(8)	C(24)-C(25)	1.5179(16)
Tb(1)-O(5)	2.3492(7)	C(25)-C(26)	1.5223(17)
Tb(1)-O(1)	2.3835(7)	C(26)-C(27)	1.5126(18)
Tb(1)-O(3)	2.3889(8)	C(28)-C(29)	1.5171(16)
Tb(1)-N(1)	2.4924(9)	C(29)-C(30)	1.5225(17)
Tb(1)-N(5)	2.5562(9)	C(30)-C(31)	1.525(2)
Tb(1)-N(3)	2.5634(9)	C(32)-C(33)	1.5135(16)
Tb(1)-N(4)	2.6409(9)	C(33)-C(34)	1.5191(17)
Tb(1)-N(2)	2.6476(9)	C(34)-C(35)	1.5219(19)
Cl(1)-C(3)	1.676(2)	O(51)-C(52)	1.202(2)
F(1)-C(3)	1.309(6)	C(51)-C(52)	1.496(3)
O(1)-C(7)	1.2683(14)	C(52)-C(53)	1.500(3)
O(2)-C(7)	1.2385(13)		
O(3)-C(6)	1.2662(14)	O(7)-Tb(1)-O(5)	144.47(3)
O(4)-C(6)	1.2430(13)	O(7)-Tb(1)-O(1)	85.65(3)
O(5)-C(17)	1.2681(12)	O(5)-Tb(1)-O(1)	79.68(3)
O(6)-C(17)	1.2455(12)	O(7)-Tb(1)-O(3)	80.64(3)
O(7)-C(19)	1.2731(12)	O(5)-Tb(1)-O(3)	83.90(3)
O(8)-C(19)	1.2358(13)	O(1)-Tb(1)-O(3)	129.13(3)
N(1)-C(1)	1.3312(14)	O(7)-Tb(1)-N(1)	72.93(3)
N(1)-C(5)	1.3362(14)	O(5)-Tb(1)-N(1)	71.54(3)
N(2)-C(16)	1.4759(14)	O(1)-Tb(1)-N(1)	64.62(3)
N(2)-C(8)	1.4822(15)	O(3)-Tb(1)-N(1)	64.52(3)
N(2)-C(15)	1.4854(15)	O(7)-Tb(1)-N(5)	74.14(3)
N(3)-C(10)	1.4722(14)	O(5)-Tb(1)-N(5)	132.09(3)
N(3)-C(9)	1.4788(14)	O(1)-Tb(1)-N(5)	77.12(3)
N(4)-C(18)	1.4812(15)	O(3)-Tb(1)-N(5)	142.03(3)
N(4)-C(12)	1.4812(15)	N(1)-Tb(1)-N(5)	130.57(3)
N(4)-C(11)	1.4834(15)	O(7)-Tb(1)-N(3)	132.31(3)
N(5)-C(14)	1.4726(15)	O(5)-Tb(1)-N(3)	73.28(3)
N(5)-C(13)	1.4786(14)	O(1)-Tb(1)-N(3)	140.40(3)
C(1)-C(2)	1.3913(16)	O(3)-Tb(1)-N(3)	76.41(3)
C(1)-C(6)	1.5163(16)	N(1)-Tb(1)-N(3)	129.19(3)
C(2)-C(3)	1.3741(18)	N(5)-Tb(1)-N(3)	100.23(3)
C(3)-C(4)	1.3740(18)	O(7)-Tb(1)-N(4)	66.38(3)
C(4)-C(5)	1.3924(16)	O(5)-Tb(1)-N(4)	138.96(3)
C(5)-C(7)	1.5190(17)	O(1)-Tb(1)-N(4)	140.26(3)
C(8)-C(9)	1.5157(17)	O(3)-Tb(1)-N(4)	75.45(3)
C(10)-C(11)	1.5158(17)	N(1)-Tb(1)-N(4)	126.36(3)
C(12)-C(13)	1.5114(17)	N(5)-Tb(1)-N(4)	68.64(3)
C(14)-C(15)	1.5136(16)	N(3)-Tb(1)-N(4)	67.62(3)
C(16)-C(17)	1.5237(16)	O(7)-Tb(1)-N(2)	139.59(3)
C(18)-C(19)	1.5267(16)	O(5)-Tb(1)-N(2)	66.28(3)
N(6)-C(28)	1.5163(14)	O(1)-Tb(1)-N(2)	74.50(3)
N(6)-C(24)	1.5172(14)	O(3)-Tb(1)-N(2)	138.80(3)
N(6)-C(20)	1.5176(14)	N(1)-Tb(1)-N(2)	125.11(3)
N(6)-C(32)	1.5254(14)	N(5)-Tb(1)-N(2)	67.36(3)
C(20)-C(21)	1.5195(16)	N(3)-Tb(1)-N(2)	68.39(3)
C(21)-C(22)	1.5076(17)	N(4)-Tb(1)-N(2)	108.52(3)
C(22)-C(23)	1.5185(18)	C(7)-O(1)-Tb(1)	125.80(7)

C(6)-O(3)-Tb(1)	125.65(7)	N(2)-C(16)-C(17)	113.78(9)
C(17)-O(5)-Tb(1)	123.19(7)	O(6)-C(17)-O(5)	124.44(10)
C(19)-O(7)-Tb(1)	124.39(7)	O(6)-C(17)-C(16)	117.70(9)
C(1)-N(1)-C(5)	120.22(10)	O(5)-C(17)-C(16)	117.85(9)
C(1)-N(1)-Tb(1)	119.92(7)	N(4)-C(18)-C(19)	113.58(9)
C(5)-N(1)-Tb(1)	119.84(7)	O(8)-C(19)-O(7)	125.07(11)
C(16)-N(2)-C(8)	110.70(9)	O(8)-C(19)-C(18)	117.80(9)
C(16)-N(2)-C(15)	110.13(9)	O(7)-C(19)-C(18)	117.10(9)
C(8)-N(2)-C(15)	110.00(9)	C(28)-N(6)-C(24)	110.89(8)
C(16)-N(2)-Tb(1)	105.52(6)	C(28)-N(6)-C(20)	106.70(8)
C(8)-N(2)-Tb(1)	110.72(6)	C(24)-N(6)-C(20)	110.73(8)
C(15)-N(2)-Tb(1)	109.68(6)	C(28)-N(6)-C(32)	110.84(8)
C(10)-N(3)-C(9)	112.41(9)	C(24)-N(6)-C(32)	107.08(8)
C(10)-N(3)-Tb(1)	115.48(7)	C(20)-N(6)-C(32)	110.64(8)
C(9)-N(3)-Tb(1)	112.80(7)	N(6)-C(20)-C(21)	114.96(9)
C(18)-N(4)-C(12)	110.56(9)	C(22)-C(21)-C(20)	110.55(10)
C(18)-N(4)-C(11)	110.10(9)	C(21)-C(22)-C(23)	112.37(11)
C(12)-N(4)-C(11)	110.11(9)	N(6)-C(24)-C(25)	115.73(9)
C(18)-N(4)-Tb(1)	105.79(6)	C(24)-C(25)-C(26)	110.42(9)
C(12)-N(4)-Tb(1)	110.67(6)	C(27)-C(26)-C(25)	113.09(10)
C(11)-N(4)-Tb(1)	109.52(7)	N(6)-C(28)-C(29)	115.86(9)
C(14)-N(5)-C(13)	112.21(9)	C(28)-C(29)-C(30)	109.86(9)
C(14)-N(5)-Tb(1)	116.13(7)	C(29)-C(30)-C(31)	112.58(11)
C(13)-N(5)-Tb(1)	112.44(7)	C(33)-C(32)-N(6)	114.90(9)
N(1)-C(1)-C(2)	121.91(11)	C(32)-C(33)-C(34)	110.95(9)
N(1)-C(1)-C(6)	114.30(10)	C(33)-C(34)-C(35)	111.23(11)
C(2)-C(1)-C(6)	123.78(10)	O(51)-C(52)-C(51)	123.83(17)
C(3)-C(2)-C(1)	116.63(11)	O(51)-C(52)-C(53)	119.93(18)
F(1)-C(3)-C(4)	119.4(3)	C(51)-C(52)-C(53)	116.22(17)
F(1)-C(3)-C(2)	117.5(2)		
C(4)-C(3)-C(2)	122.86(11)		
F(1)-C(3)-Cl(1)	8.1(2)		
C(4)-C(3)-Cl(1)	118.84(11)		
C(2)-C(3)-Cl(1)	118.20(11)		
C(3)-C(4)-C(5)	116.35(11)		
N(1)-C(5)-C(4)	122.02(11)		
N(1)-C(5)-C(7)	114.13(10)		
C(4)-C(5)-C(7)	123.85(10)		
O(4)-C(6)-O(3)	126.63(11)		
O(4)-C(6)-C(1)	118.09(11)		
O(3)-C(6)-C(1)	115.27(9)		
O(2)-C(7)-O(1)	127.06(11)		
O(2)-C(7)-C(5)	117.71(10)		
O(1)-C(7)-C(5)	115.23(9)		
N(2)-C(8)-C(9)	113.13(9)		
N(3)-C(9)-C(8)	110.43(9)		
N(3)-C(10)-C(11)	109.95(9)		
N(4)-C(11)-C(10)	111.51(9)		
N(4)-C(12)-C(13)	113.09(9)		
N(5)-C(13)-C(12)	110.87(9)		
N(5)-C(14)-C(15)	109.87(9)		
N(2)-C(15)-C(14)	111.42(9)		

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for MLC23 (CCDC 761002). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Tb(1)	134(1)	221(1)	136(1)	19(1)	-16(1)	-6(1)
Cl(1)	719(7)	453(7)	442(5)	9(4)	-18(4)	-15(5)
O(1)	200(4)	274(4)	165(3)	36(3)	1(3)	3(3)
O(2)	362(5)	360(5)	219(4)	127(3)	37(4)	14(4)
O(3)	207(4)	287(4)	170(3)	2(3)	2(3)	-23(3)
O(4)	401(5)	401(5)	189(4)	-69(3)	50(4)	-25(4)
O(5)	173(4)	266(4)	164(3)	-3(3)	-30(3)	5(3)
O(6)	199(4)	241(4)	188(3)	33(3)	-46(3)	-20(3)
O(7)	172(4)	301(4)	164(3)	33(3)	-32(3)	-15(3)
O(8)	234(4)	371(5)	186(4)	-9(3)	-52(3)	8(4)
N(1)	159(4)	254(4)	164(4)	10(3)	-44(3)	-9(4)
N(2)	179(4)	252(5)	197(4)	-4(3)	-25(3)	1(4)
N(3)	171(4)	246(5)	229(4)	25(4)	-5(3)	-9(4)
N(4)	176(4)	288(5)	209(4)	57(4)	-8(3)	1(4)
N(5)	174(4)	247(5)	212(4)	12(3)	-9(3)	6(4)
C(1)	181(5)	293(6)	176(5)	-17(4)	-44(4)	-3(4)
C(2)	282(6)	312(6)	256(6)	-61(5)	-25(5)	27(5)
C(3)	367(7)	202(6)	374(7)	-9(5)	-60(6)	15(5)
C(4)	280(6)	288(6)	286(6)	61(5)	-31(5)	-3(5)
C(5)	175(5)	265(6)	197(5)	48(4)	-46(4)	2(4)
C(6)	193(5)	339(6)	164(5)	-23(4)	-25(4)	-18(5)
C(7)	183(5)	322(6)	179(5)	56(4)	-31(4)	7(4)
C(8)	226(6)	258(6)	275(6)	-33(4)	-38(5)	-34(5)
C(9)	175(5)	263(6)	288(6)	4(4)	-36(4)	-41(4)
C(10)	208(6)	271(6)	322(6)	80(5)	-2(5)	-24(5)
C(11)	214(6)	320(6)	250(6)	109(5)	14(4)	-12(5)
C(12)	225(6)	299(6)	294(6)	81(5)	-9(5)	38(5)
C(13)	171(5)	301(6)	262(5)	32(4)	-24(4)	48(4)
C(14)	209(6)	272(6)	277(6)	-37(5)	-14(5)	26(5)
C(15)	211(5)	294(6)	218(5)	-49(4)	-1(4)	21(4)
C(16)	215(5)	293(6)	176(5)	-11(4)	-42(4)	14(4)
C(17)	148(5)	226(5)	175(5)	13(4)	-18(4)	-42(4)
C(18)	208(5)	380(7)	174(5)	80(4)	-32(4)	-9(5)
C(19)	151(4)	314(6)	164(4)	0(4)	-7(3)	42(4)
N(6)	181(4)	211(4)	175(4)	-56(3)	-2(3)	-8(3)
C(20)	209(5)	206(5)	215(5)	-51(4)	1(4)	-24(4)
C(21)	382(7)	267(6)	246(6)	-26(5)	44(5)	-44(5)
C(22)	352(6)	260(6)	322(6)	30(5)	-66(5)	-37(6)
C(23)	418(8)	316(7)	410(8)	91(6)	-44(6)	-23(6)
C(24)	189(5)	260(6)	195(5)	-47(4)	-18(4)	-20(4)
C(25)	201(6)	333(6)	244(6)	-66(5)	-26(4)	18(5)
C(26)	262(6)	280(6)	273(6)	-3(5)	-59(5)	14(5)
C(27)	248(7)	422(8)	420(8)	-25(6)	-78(6)	63(6)
C(28)	220(5)	231(5)	172(5)	-40(4)	3(4)	7(4)
C(29)	295(6)	231(6)	257(6)	-29(4)	25(5)	10(5)

C(30)	321(7)	280(6)	279(6)	16(5)	25(5)	0(5)
C(31)	585(11)	350(8)	514(9)	137(7)	132(8)	3(7)
C(32)	197(5)	248(5)	202(5)	-75(4)	17(4)	6(4)
C(33)	208(5)	329(6)	245(5)	-102(5)	-7(4)	9(5)
C(34)	224(6)	468(8)	396(7)	-181(6)	5(5)	50(6)
C(35)	214(7)	608(10)	576(10)	-195(8)	-3(6)	70(7)
O(41)	377(5)	274(4)	197(3)	-19(3)	-69(3)	-69(4)
O(42)	423(6)	442(5)	254(4)	-3(4)	-102(4)	145(4)
O(51)	382(7)	675(8)	643(8)	-57(6)	-31(6)	-51(6)
C(51)	461(10)	646(12)	725(12)	-19(10)	42(9)	22(9)
C(52)	399(9)	676(11)	480(9)	-122(8)	-12(8)	71(8)
C(53)	558(14)	2270(30)	808(17)	690(20)	19(13)	157(19)

Table 6. Hydrogen bonds for MLC23 (CCDC 761002) [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(3)-H(3)...O(5)#1	0.93	2.31	3.1089(12)	144.0
N(3)-H(3)...O(6)#1	0.93	2.41	3.1876(12)	141.2
N(5)-H(5)...O(7)#2	0.93	2.22	3.0600(12)	149.4
N(5)-H(5)...O(8)#2	0.93	2.55	3.3037(12)	137.9
O(41)-H(41A)...O(6)	0.83	1.92	2.7457(11)	172.4
O(41)-H(41B)...O(4)#1	0.87	2.05	2.9239(12)	176.6
O(42)-H(42A)...O(8)#3	0.81	2.04	2.8477(12)	171.1
O(42)-H(42B)...O(2)#1	0.85	2.04	2.8888(13)	175.5

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