APPENDIX E

Crystallographic Data for TBA·Eu(DO2A)(DPA) Temperature Dependence

Temperature	Designation	CCDC	Page
100 K	MLC18	761599	E2
200 K	MLC17	762705	E17
300 K	MLC19	763335	E31

CALIFORNIA INSTITUTE OF TECHNOLOGY

BECKMAN INSTITUTE

X-RAY CRYSTALLOGRAPHY LABORATORY

Date 15 January 2010

Crystal Structure Analysis of:

MLC18

(shown below)

For Investigator: Morgan Cable ext. (818) 354-4345

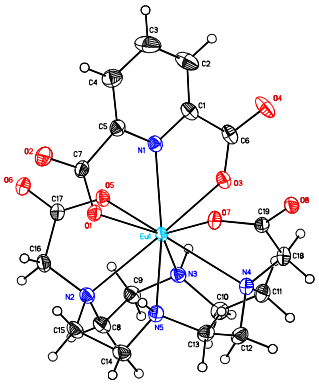
Advisor: Adrian Ponce ext. (818) 354-8196

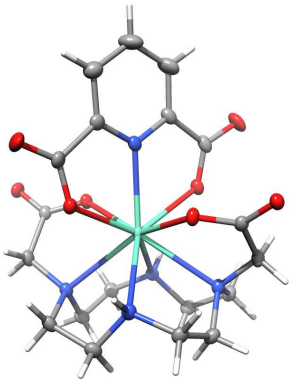
Account Number: AP1.HSARPA3-1-HSARPA.PONCE

By Michael W. Day 116 Beckman ext. 2734

e-mail: mikeday@caltech.edu

Contents



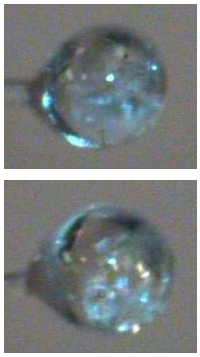


MLC18

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 761599. 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 761599."

Table 1. Crystal data and structure refinement for MLC18 (CCDC 761599).

Empirical formula	$[C_{19}H_{25}N_5O_8Eu]^-$ $[C_{16}H_{36}N]^+ \bullet C_3H_6O \bullet 3.68(H_2O)$
Formula weight	970.23
Crystallization Solvent	Acetone
Crystal Habit	Fragment
Crystal size	0.22 x 0.19 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 9759 reflections used in lattice determination	2.22 to 39.59°
Unit cell dimensions	a = 13.0309(5) Å b = 13.4740(5) Å β= 90.600(2)° c = 26.1088(9) Å
Volume	4583.9(3) $Å^3$
Z	4
Crystal system	Monoclinic
Space group	P $2_1/c$
Density (calculated)	1.406 Mg/m^3
F(000)	2035
θ range for data collection	1.56 to 40.90°
Completeness to θ = 40.90°	97.8 %
Index ranges	$-23 \le h \le 23$, $-24 \le k \le 23$, $-47 \le l \le 46$
Data collection scan type	ω scans; 19 settings
Reflections collected	219049
Independent reflections	29345 [R_{int}= 0.0420]
Absorption coefficient	1.432 mm^{-1}
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7480 and 0.6761

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	29345 / 0 / 544
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	2.444
Final R indices [$I>2\sigma(I)$, 19989 reflections]	R1 = 0.0341, *w*R2 = 0.0624
R indices (all data)	R1 = 0.0648, *w*R2 = 0.0638
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.003
Average shift/error	0.000
Largest diff. peak and hole	3.339 and -2.101 e.Å^{-3}

Special Refinement Details

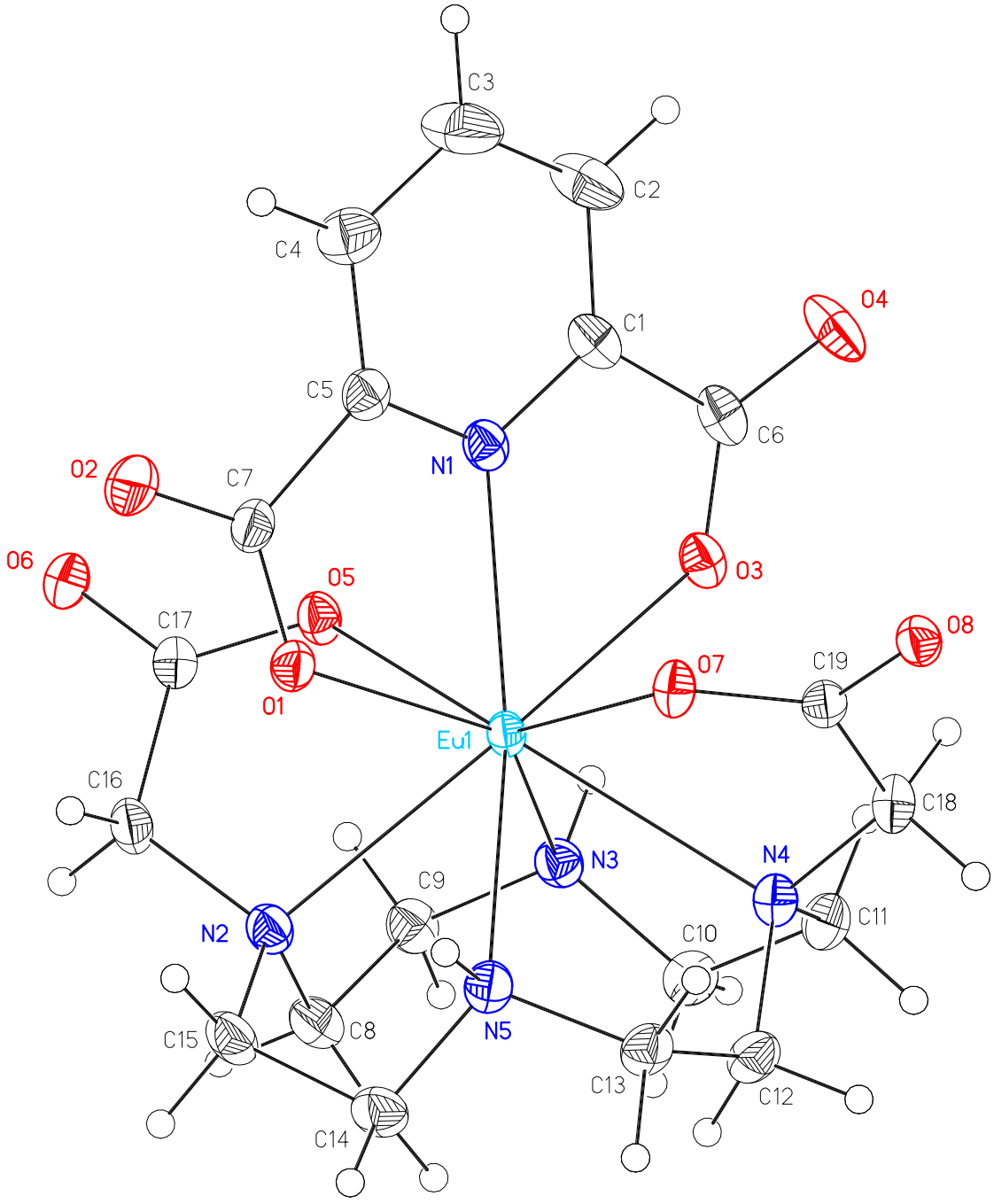
Crystals were mounted on a glass fiber using, coated with epoxy then placed on the diffractometer under a nitrogen stream at 100K.

The asymmetric unit contains acetone at one site that is disordered between two orientations. The major orientation (69%), O51-C53 is accompanied by a water molecule, O44, that is hydrogen bonded to two other waters, O42 and O43. The minor orientation does not contain a discernable water. Hydrogen atoms on water were located in the electron density difference map and were constrained to ride the appropriate oxygen. All other hydrogens were placed at geometric positions and refined as riding atoms. No other restraints were placed on the model.

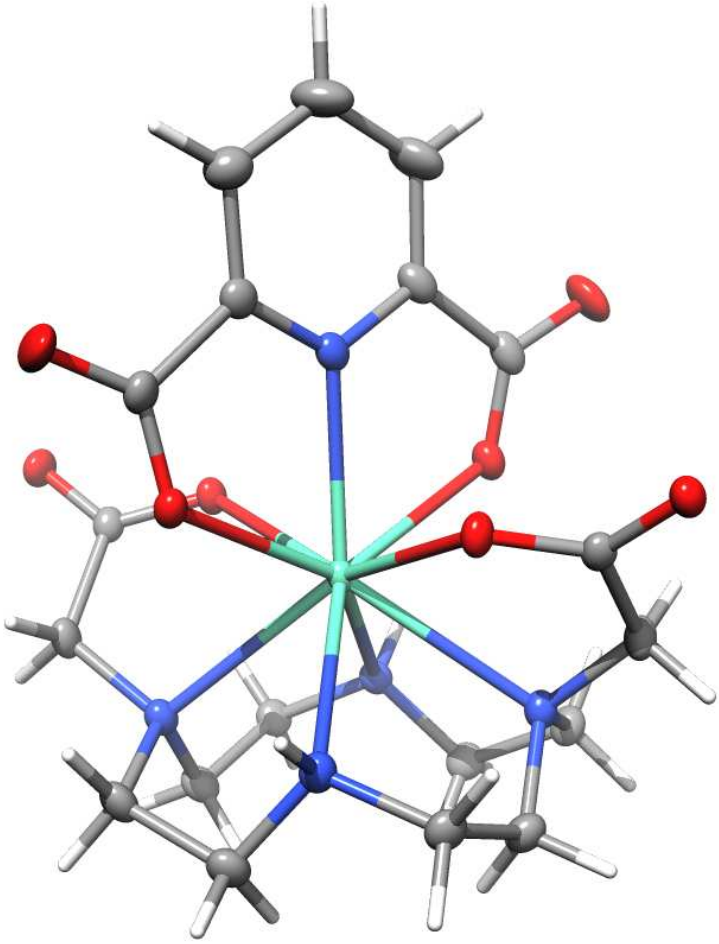
Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not 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.

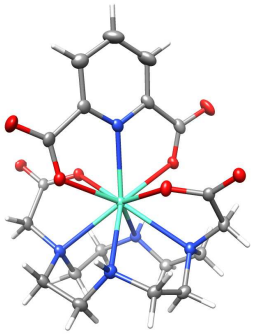
All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when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

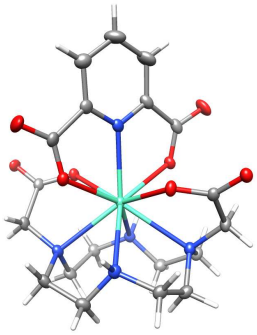
E5


C3
C2
C4
C1
O4
C5
N1
C6
O2
C7
O6
O5
O3
C17
O8
O1
O7
C19
Eu1
C16
C18
N3
N4
C9
N2
C10
C11
C15
C8
N5
C13
C12
C14

E6







E7

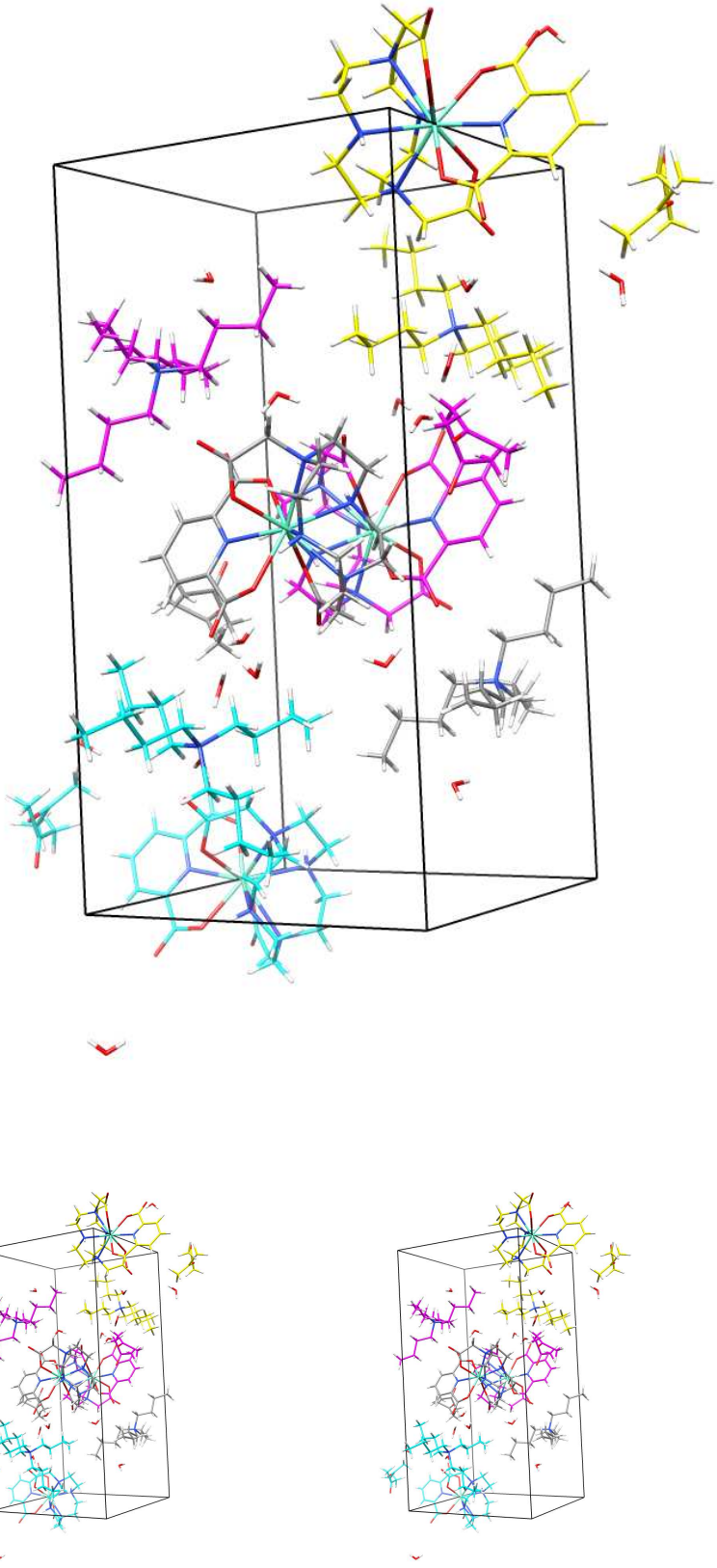


Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for MLC18 (CCDC 761599). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
Eu(1)	7492(1)	4903(1)	4994(1)	14(1)	1
O(1)	8306(1)	5479(1)	5775(1)	18(1)	1
O(2)	8565(1)	6661(1)	6360(1)	42(1)	1
O(3)	6699(1)	5871(1)	4322(1)	19(1)	1
O(4)	6432(1)	7320(1)	3919(1)	31(1)	1
O(5)	6045(1)	5286(1)	5504(1)	18(1)	1
O(6)	5344(1)	5321(1)	6275(1)	23(1)	1
O(7)	8971(1)	5551(1)	4584(1)	18(1)	1
O(8)	9676(1)	6058(1)	3858(1)	18(1)	1
N(1)	7502(1)	6747(1)	5124(1)	17(1)	1
N(2)	7026(1)	3510(1)	5684(1)	18(1)	1
N(3)	6038(1)	3765(1)	4670(1)	18(1)	1
N(4)	7955(1)	3995(1)	4122(1)	17(1)	1
N(5)	8935(1)	3605(1)	5124(1)	18(1)	1
C(1)	7130(1)	7348(1)	4758(1)	20(1)	1
C(2)	7127(2)	8365(1)	4817(1)	32(1)	1
C(3)	7510(2)	8769(1)	5267(1)	37(1)	1
C(4)	7885(1)	8142(1)	5646(1)	26(1)	1
C(5)	7877(1)	7133(1)	5556(1)	18(1)	1
C(6)	6718(1)	6808(1)	4291(1)	21(1)	1
C(7)	8283(1)	6363(1)	5932(1)	20(1)	1
C(8)	6320(1)	2765(1)	5452(1)	22(1)	1
C(9)	5532(1)	3222(1)	5091(1)	20(1)	1
C(10)	6301(1)	3113(1)	4240(1)	21(1)	1
C(11)	6990(1)	3653(1)	3870(1)	20(1)	1
C(12)	8644(1)	3141(1)	4220(1)	21(1)	1
C(13)	9436(1)	3345(1)	4638(1)	20(1)	1
C(14)	8665(1)	2726(1)	5429(1)	23(1)	1
C(15)	7981(1)	3018(1)	5867(1)	22(1)	1
C(16)	6530(1)	4032(1)	6113(1)	20(1)	1
C(17)	5911(1)	4945(1)	5952(1)	16(1)	1
C(18)	8463(1)	4744(1)	3802(1)	20(1)	1
C(19)	9098(1)	5510(1)	4103(1)	16(1)	1
N(6)	1363(1)	2123(1)	7182(1)	20(1)	1
C(20)	1674(1)	3209(1)	7193(1)	21(1)	1
C(21)	1850(1)	3646(1)	7721(1)	28(1)	1
C(22)	2079(1)	4747(1)	7682(1)	29(1)	1
C(23)	2313(2)	5212(1)	8203(1)	39(1)	1
C(24)	2194(1)	1484(1)	7439(1)	25(1)	1
C(25)	3264(1)	1634(1)	7243(1)	30(1)	1
C(26)	3996(2)	873(2)	7480(1)	53(1)	1
C(27)	5107(2)	1117(2)	7360(1)	56(1)	1
C(28)	1228(1)	1845(1)	6622(1)	22(1)	1
C(29)	911(2)	773(1)	6522(1)	36(1)	1
C(30)	706(2)	582(1)	5967(1)	43(1)	1

C(31)	462(2)	-459(2)	5822(1)	63(1)	1
C(32)	380(1)	1958(1)	7474(1)	23(1)	1
C(33)	-555(1)	2516(1)	7273(1)	26(1)	1
C(34)	-1414(1)	2506(1)	7660(1)	27(1)	1
C(35)	-2376(1)	3033(1)	7471(1)	35(1)	1
O(41)	761(1)	5077(1)	3094(1)	28(1)	1
O(42)	4212(1)	3975(1)	6888(1)	37(1)	1
O(43)	3882(2)	2263(1)	8520(1)	92(1)	1
O(44)	5098(2)	8671(2)	7083(1)	69(1)	0.689(2)
O(51)	3588(2)	9313(1)	5364(1)	56(1)	0.689(2)
C(51)	3427(3)	9395(3)	6244(2)	57(1)	0.689(2)
C(52)	4006(3)	9500(2)	5753(1)	45(1)	0.689(2)
C(53)	5099(5)	9768(5)	5796(2)	111(2)	0.689(2)
O(61)	3597(11)	9491(10)	6027(5)	120(5)	0.311(2)
C(61)	4945(7)	8811(6)	6490(3)	71(2)	0.311(2)
C(62)	4450(9)	9449(7)	6180(4)	75(3)	0.311(2)
C(63)	5015(10)	10326(7)	5883(4)	66(3)	0.311(2)

Table 3. Selected bond lengths [Å] and angles [°] for MLC18 (CCDC 761599).

Eu(1)-O(5)	2.3747(10)	O(5)-Eu(1)-N(4)	140.15(3)
Eu(1)-O(7)	2.3813(10)	O(7)-Eu(1)-N(4)	65.88(3)
Eu(1)-O(3)	2.4104(8)	O(3)-Eu(1)-N(4)	74.06(3)
Eu(1)-O(1)	2.4156(8)	O(1)-Eu(1)-N(4)	140.21(4)
Eu(1)-N(1)	2.5067(11)	N(1)-Eu(1)-N(4)	124.77(3)
Eu(1)-N(3)	2.5728(11)	N(3)-Eu(1)-N(4)	67.50(4)
Eu(1)-N(5)	2.5882(11)	N(5)-Eu(1)-N(4)	68.26(3)
Eu(1)-N(4)	2.6595(11)	O(5)-Eu(1)-N(2)	65.70(3)
Eu(1)-N(2)	2.6759(11)	O(7)-Eu(1)-N(2)	138.66(3)
Eu(1)-C(19)	3.2513(14)	O(3)-Eu(1)-N(2)	140.46(4)
Eu(1)-C(17)	3.2569(14)	O(1)-Eu(1)-N(2)	76.02(3)
		N(1)-Eu(1)-N(2)	127.27(3)
O(5)-Eu(1)-O(7)	145.43(4)	N(3)-Eu(1)-N(2)	68.39(3)
O(5)-Eu(1)-O(3)	87.33(3)	N(5)-Eu(1)-N(2)	66.89(4)
O(7)-Eu(1)-O(3)	79.43(3)	N(4)-Eu(1)-N(2)	107.96(3)
O(5)-Eu(1)-O(1)	78.58(3)	O(5)-Eu(1)-C(19)	150.10(3)
O(7)-Eu(1)-O(1)	84.92(3)	O(3)-Eu(1)-C(19)	67.47(3)
O(3)-Eu(1)-O(1)	128.40(3)	O(1)-Eu(1)-C(19)	104.05(3)
O(5)-Eu(1)-N(1)	73.29(4)	N(1)-Eu(1)-C(19)	81.05(4)
O(7)-Eu(1)-N(1)	72.19(4)	N(3)-Eu(1)-C(19)	113.07(3)
O(3)-Eu(1)-N(1)	64.11(3)	N(5)-Eu(1)-C(19)	77.96(3)
O(1)-Eu(1)-N(1)	64.30(3)	N(4)-Eu(1)-C(19)	49.42(3)
O(5)-Eu(1)-N(3)	74.19(4)	N(2)-Eu(1)-C(19)	144.18(3)
O(7)-Eu(1)-N(3)	131.85(3)	O(7)-Eu(1)-C(17)	149.39(3)
O(3)-Eu(1)-N(3)	76.99(3)	O(3)-Eu(1)-C(17)	106.25(3)
O(1)-Eu(1)-N(3)	141.63(4)	O(1)-Eu(1)-C(17)	67.80(3)
N(1)-Eu(1)-N(3)	129.60(4)	N(1)-Eu(1)-C(17)	83.21(3)
O(5)-Eu(1)-N(5)	130.81(3)	N(3)-Eu(1)-C(17)	78.09(3)
O(7)-Eu(1)-N(5)	73.51(4)	N(5)-Eu(1)-C(17)	112.09(3)
O(3)-Eu(1)-N(5)	140.01(4)	N(4)-Eu(1)-C(17)	144.72(3)
O(1)-Eu(1)-N(5)	78.18(3)	N(2)-Eu(1)-C(17)	49.13(3)
N(1)-Eu(1)-N(5)	130.51(4)	C(19)-Eu(1)-C(17)	164.23(3)
N(3)-Eu(1)-N(5)	99.87(4)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Bond lengths [Å] and angles [°] for MLC18 (CCDC 761599).

Eu(1)-O(5)	2.3747(10)	C(24)-C(25)	1.504(2)
Eu(1)-O(7)	2.3813(10)	C(25)-C(26)	1.525(2)
Eu(1)-O(3)	2.4104(8)	C(26)-C(27)	1.521(3)
Eu(1)-O(1)	2.4156(8)	C(28)-C(29)	1.525(2)
Eu(1)-N(1)	2.5067(11)	C(29)-C(30)	1.494(2)
Eu(1)-N(3)	2.5728(11)	C(30)-C(31)	1.487(3)
Eu(1)-N(5)	2.5882(11)	C(32)-C(33)	1.520(2)
Eu(1)-N(4)	2.6595(11)	C(33)-C(34)	1.517(2)
Eu(1)-N(2)	2.6759(11)	C(34)-C(35)	1.520(2)
Eu(1)-C(19)	3.2513(14)	O(51)-C(52)	1.174(3)
Eu(1)-C(17)	3.2569(14)	C(51)-C(52)	1.502(7)
O(1)-C(7)	1.2597(16)	C(52)-C(53)	1.473(7)
O(2)-C(7)	1.2386(15)	O(61)-C(62)	1.179(15)
O(3)-C(6)	1.2647(16)	C(61)-C(62)	1.341(11)
O(4)-C(6)	1.2447(15)	C(62)-C(63)	1.597(16)
O(5)-C(17)	1.2716(15)		
O(6)-C(17)	1.2353(17)	O(5)-Eu(1)-O(7)	145.43(4)
O(7)-C(19)	1.2696(15)	O(5)-Eu(1)-O(3)	87.33(3)
O(8)-C(19)	1.2375(17)	O(7)-Eu(1)-O(3)	79.43(3)
N(1)-C(5)	1.3316(16)	O(5)-Eu(1)-O(1)	78.58(3)
N(1)-C(1)	1.3389(16)	O(7)-Eu(1)-O(1)	84.92(3)
N(2)-C(16)	1.4762(18)	O(3)-Eu(1)-O(1)	128.40(3)
N(2)-C(15)	1.4849(18)	O(5)-Eu(1)-N(1)	73.29(4)
N(2)-C(8)	1.4862(18)	O(7)-Eu(1)-N(1)	72.19(4)
N(3)-C(10)	1.4701(18)	O(3)-Eu(1)-N(1)	64.11(3)
N(3)-C(9)	1.4805(19)	O(1)-Eu(1)-N(1)	64.30(3)
N(4)-C(18)	1.4740(18)	O(5)-Eu(1)-N(3)	74.19(4)
N(4)-C(12)	1.4794(18)	O(7)-Eu(1)-N(3)	131.85(3)
N(4)-C(11)	1.4867(17)	O(3)-Eu(1)-N(3)	76.99(3)
N(5)-C(14)	1.4712(18)	O(1)-Eu(1)-N(3)	141.63(4)
N(5)-C(13)	1.4752(19)	N(1)-Eu(1)-N(3)	129.60(4)
C(1)-C(2)	1.378(2)	O(5)-Eu(1)-N(5)	130.81(3)
C(1)-C(6)	1.5149(19)	O(7)-Eu(1)-N(5)	73.51(4)
C(2)-C(3)	1.382(2)	O(3)-Eu(1)-N(5)	140.01(4)
C(3)-C(4)	1.387(2)	O(1)-Eu(1)-N(5)	78.18(3)
C(4)-C(5)	1.381(2)	N(1)-Eu(1)-N(5)	130.51(4)
C(5)-C(7)	1.5204(19)	N(3)-Eu(1)-N(5)	99.87(4)
C(8)-C(9)	1.5165(19)	O(5)-Eu(1)-N(4)	140.15(3)
C(10)-C(11)	1.512(2)	O(7)-Eu(1)-N(4)	65.88(3)
C(12)-C(13)	1.5204(18)	O(3)-Eu(1)-N(4)	74.06(3)
C(14)-C(15)	1.510(2)	O(1)-Eu(1)-N(4)	140.21(4)
C(16)-C(17)	1.5274(18)	N(1)-Eu(1)-N(4)	124.77(3)
C(18)-C(19)	1.5346(19)	N(3)-Eu(1)-N(4)	67.50(4)
N(6)-C(32)	1.515(2)	N(5)-Eu(1)-N(4)	68.26(3)
N(6)-C(20)	1.5180(18)	O(5)-Eu(1)-N(2)	65.70(3)
N(6)-C(28)	1.5191(17)	O(7)-Eu(1)-N(2)	138.66(3)
N(6)-C(24)	1.5324(18)	O(3)-Eu(1)-N(2)	140.46(4)
C(20)-C(21)	1.515(2)	O(1)-Eu(1)-N(2)	76.02(3)
C(21)-C(22)	1.517(2)	N(1)-Eu(1)-N(2)	127.27(3)
C(22)-C(23)	1.525(2)	N(3)-Eu(1)-N(2)	68.39(3)

N(5)-Eu(1)-N(2)	66.89(4)	N(1)-C(5)-C(4)	122.14(12)
N(4)-Eu(1)-N(2)	107.96(3)	N(1)-C(5)-C(7)	113.81(11)
O(5)-Eu(1)-C(19)	150.10(3)	C(4)-C(5)-C(7)	124.05(12)
O(7)-Eu(1)-C(19)	19.13(3)	O(4)-C(6)-O(3)	126.74(13)
O(3)-Eu(1)-C(19)	67.47(3)	O(4)-C(6)-C(1)	117.54(12)
O(1)-Eu(1)-C(19)	104.05(3)	O(3)-C(6)-C(1)	115.72(11)
N(1)-Eu(1)-C(19)	81.05(4)	O(2)-C(7)-O(1)	126.38(12)
N(3)-Eu(1)-C(19)	113.07(3)	O(2)-C(7)-C(5)	117.34(12)
N(5)-Eu(1)-C(19)	77.96(3)	O(1)-C(7)-C(5)	116.27(11)
N(4)-Eu(1)-C(19)	49.42(3)	N(2)-C(8)-C(9)	113.08(11)
N(2)-Eu(1)-C(19)	144.18(3)	N(3)-C(9)-C(8)	110.90(12)
O(5)-Eu(1)-C(17)	18.95(3)	N(3)-C(10)-C(11)	110.18(11)
O(7)-Eu(1)-C(17)	149.39(3)	N(4)-C(11)-C(10)	111.80(10)
O(3)-Eu(1)-C(17)	106.25(3)	N(4)-C(12)-C(13)	112.87(11)
O(1)-Eu(1)-C(17)	67.80(3)	N(5)-C(13)-C(12)	110.92(12)
N(1)-Eu(1)-C(17)	83.21(3)	N(5)-C(14)-C(15)	110.31(11)
N(3)-Eu(1)-C(17)	78.09(3)	N(2)-C(15)-C(14)	111.81(10)
N(5)-Eu(1)-C(17)	112.09(3)	N(2)-C(16)-C(17)	114.22(10)
N(4)-Eu(1)-C(17)	144.72(3)	O(6)-C(17)-O(5)	124.68(12)
N(2)-Eu(1)-C(17)	49.13(3)	O(6)-C(17)-C(16)	117.48(11)
C(19)-Eu(1)-C(17)	164.23(3)	O(5)-C(17)-C(16)	117.78(12)
C(7)-O(1)-Eu(1)	124.58(8)	O(6)-C(17)-Eu(1)	156.72(9)
C(6)-O(3)-Eu(1)	125.38(8)	O(5)-C(17)-Eu(1)	37.35(7)
C(17)-O(5)-Eu(1)	123.70(9)	C(16)-C(17)-Eu(1)	81.98(8)
C(19)-O(7)-Eu(1)	122.95(9)	N(4)-C(18)-C(19)	114.36(10)
C(5)-N(1)-C(1)	119.64(12)	O(8)-C(19)-O(7)	124.83(12)
C(5)-N(1)-Eu(1)	120.17(8)	O(8)-C(19)-C(18)	117.69(11)
C(1)-N(1)-Eu(1)	120.18(9)	O(7)-C(19)-C(18)	117.46(12)
C(16)-N(2)-C(15)	109.96(10)	O(8)-C(19)-Eu(1)	156.91(9)
C(16)-N(2)-C(8)	110.94(12)	O(7)-C(19)-Eu(1)	37.92(7)
C(15)-N(2)-C(8)	110.07(11)	C(18)-C(19)-Eu(1)	81.39(8)
C(16)-N(2)-Eu(1)	106.26(8)	C(32)-N(6)-C(20)	111.11(12)
C(15)-N(2)-Eu(1)	109.53(9)	C(32)-N(6)-C(28)	111.06(11)
C(8)-N(2)-Eu(1)	110.01(7)	C(20)-N(6)-C(28)	106.47(10)
C(10)-N(3)-C(9)	112.36(11)	C(32)-N(6)-C(24)	107.12(10)
C(10)-N(3)-Eu(1)	115.53(9)	C(20)-N(6)-C(24)	110.25(11)
C(9)-N(3)-Eu(1)	112.53(8)	C(28)-N(6)-C(24)	110.88(12)
C(18)-N(4)-C(12)	110.77(12)	C(21)-C(20)-N(6)	115.37(11)
C(18)-N(4)-C(11)	110.10(10)	C(20)-C(21)-C(22)	110.29(12)
C(12)-N(4)-C(11)	110.11(10)	C(21)-C(22)-C(23)	112.28(13)
C(18)-N(4)-Eu(1)	106.19(7)	C(25)-C(24)-N(6)	115.44(11)
C(12)-N(4)-Eu(1)	110.73(7)	C(24)-C(25)-C(26)	110.51(13)
C(11)-N(4)-Eu(1)	108.86(8)	C(27)-C(26)-C(25)	111.36(15)
C(14)-N(5)-C(13)	112.65(11)	N(6)-C(28)-C(29)	115.23(11)
C(14)-N(5)-Eu(1)	115.90(9)	C(30)-C(29)-C(28)	111.91(13)
C(13)-N(5)-Eu(1)	112.07(7)	C(31)-C(30)-C(29)	116.42(16)
N(1)-C(1)-C(2)	121.55(12)	N(6)-C(32)-C(33)	115.56(11)
N(1)-C(1)-C(6)	113.93(12)	C(34)-C(33)-C(32)	111.05(11)
C(2)-C(1)-C(6)	124.52(12)	C(33)-C(34)-C(35)	113.03(12)
C(1)-C(2)-C(3)	119.04(13)	O(51)-C(52)-C(51)	119.1(4)
C(2)-C(3)-C(4)	119.21(14)	O(51)-C(52)-C(53)	123.9(4)
C(5)-C(4)-C(3)	118.41(13)	C(51)-C(52)-C(53)	116.9(3)

O(61)-C(62)-C(61)	133.0(12)
O(61)-C(62)-C(63)	103.8(10)
C(61)-C(62)-C(63)	123.0(10)

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for MLC18 (CCDC 761599). 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}
Eu(1)	130(1)	164(1)	114(1)	17(1)	11(1)	19(1)
O(1)	211(6)	207(5)	138(4)	-4(3)	-5(4)	36(4)
O(2)	816(11)	293(6)	152(5)	-67(4)	-98(6)	111(6)
O(3)	195(6)	228(5)	160(4)	42(3)	-11(4)	10(4)
O(4)	367(8)	291(6)	265(5)	151(4)	-89(5)	-43(5)
O(5)	161(5)	216(5)	149(4)	27(3)	25(3)	18(4)
O(6)	273(6)	239(5)	172(4)	-9(4)	71(4)	26(4)
O(7)	166(5)	248(5)	134(4)	-1(3)	19(3)	-3(4)
O(8)	197(6)	195(5)	162(4)	26(3)	32(4)	19(4)
N(1)	144(6)	195(5)	164(5)	28(3)	24(4)	7(4)
N(2)	181(6)	197(5)	168(5)	30(4)	10(4)	31(4)
N(3)	162(6)	184(5)	178(5)	19(4)	5(4)	18(4)
N(4)	158(6)	204(5)	146(5)	3(4)	6(4)	-2(4)
N(5)	162(6)	217(6)	168(5)	-2(4)	-2(4)	31(4)
C(1)	169(7)	218(7)	225(6)	67(5)	-2(5)	-5(5)
C(2)	359(11)	226(8)	389(9)	93(6)	-95(8)	6(7)
C(3)	440(12)	182(7)	478(10)	1(7)	-99(9)	0(7)
C(4)	266(9)	236(7)	294(7)	-34(5)	-17(6)	-7(6)
C(5)	158(7)	211(6)	183(6)	5(5)	34(5)	13(5)
C(6)	169(7)	262(7)	196(6)	75(5)	-2(5)	-19(5)
C(7)	223(8)	234(7)	147(5)	-12(5)	30(5)	37(5)
C(8)	240(8)	194(7)	236(6)	51(5)	11(6)	-5(5)
C(9)	172(7)	220(7)	217(6)	22(5)	24(5)	-12(5)
C(10)	183(8)	219(7)	224(6)	-21(5)	-2(5)	-21(5)
C(11)	191(8)	243(7)	170(6)	-27(5)	-11(5)	-10(5)
C(12)	192(8)	224(7)	207(6)	-39(5)	8(5)	42(5)
C(13)	163(7)	231(7)	211(6)	-16(5)	19(5)	49(5)
C(14)	221(8)	221(7)	250(7)	42(5)	7(6)	78(6)
C(15)	216(8)	235(7)	208(6)	76(5)	-2(5)	61(6)
C(16)	211(8)	254(7)	147(5)	44(5)	31(5)	43(5)
C(17)	140(6)	194(6)	146(5)	-1(4)	1(4)	-27(5)
C(18)	196(7)	253(7)	138(5)	-2(4)	18(5)	-23(5)
C(19)	145(7)	190(6)	155(5)	8(4)	9(4)	42(5)
N(6)	166(6)	242(6)	202(5)	101(4)	-22(4)	-20(5)
C(20)	199(8)	237(7)	200(6)	87(5)	-31(5)	-35(5)
C(21)	315(10)	316(8)	211(7)	66(6)	-41(6)	-58(7)
C(22)	309(10)	324(8)	242(7)	36(6)	-17(6)	-65(7)
C(23)	420(12)	418(10)	319(8)	-25(7)	-33(8)	-96(9)
C(24)	178(8)	298(8)	280(7)	168(6)	-37(6)	-5(6)
C(25)	187(8)	365(9)	331(8)	187(6)	-31(6)	-3(7)
C(26)	236(11)	624(13)	724(14)	446(11)	-39(10)	54(9)
C(27)	207(11)	664(14)	807(16)	367(12)	-17(10)	65(10)
C(28)	198(8)	252(7)	206(6)	65(5)	-20(5)	4(5)
C(29)	400(12)	300(9)	371(9)	41(6)	7(8)	-133(8)
C(30)	632(15)	268(9)	389(10)	-26(7)	-157(10)	63(9)

C(31)	686(19)	479(13)	734(16)	-205(11)	-45(14)	-157(12)
C(32)	180(8)	291(7)	225(6)	107(5)	-12(5)	-38(6)
C(33)	199(8)	355(8)	225(7)	109(6)	4(6)	18(6)
C(34)	258(9)	297(8)	252(7)	63(5)	48(6)	-2(6)
C(35)	269(10)	395(10)	394(9)	61(7)	86(7)	36(7)
O(41)	403(8)	249(5)	179(4)	-4(4)	64(4)	95(5)
O(42)	461(9)	430(7)	229(5)	46(5)	59(5)	-184(6)
O(43)	902(17)	1005(15)	850(13)	180(11)	175(12)	-21(13)
O(44)	850(20)	802(17)	423(12)	-117(11)	-116(12)	469(14)
O(51)	950(20)	216(9)	523(12)	40(8)	-274(13)	9(10)
C(51)	420(20)	750(30)	540(20)	-178(19)	-84(19)	166(18)
C(52)	740(30)	178(12)	422(16)	60(10)	-114(17)	127(13)
C(53)	920(50)	1500(60)	920(40)	550(40)	-370(30)	-390(50)

Table 6. Hydrogen bonds for MLC18 (CCDC 761599) [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(3)-H(3)...O(5)#1	0.93	2.18	3.0310(15)	151.2
N(3)-H(3)...O(6)#1	0.93	2.50	3.2799(14)	141.9
N(5)-H(5)...O(7)#2	0.93	2.20	3.0464(16)	150.6
N(5)-H(5)...O(8)#2	0.93	2.44	3.2325(13)	143.6
O(41)-H(41A)...O(8)#3	0.75	2.05	2.7908(15)	170.8
O(41)-H(41B)...O(2)#1	0.74	2.13	2.8745(14)	179.0
O(42)-H(42A)...O(6)	0.77	2.10	2.8418(16)	163.0
O(42)-H(42B)...O(4)#1	0.80	2.06	2.8542(15)	171.9
O(43)-H(43A)...O(6)#4	0.59	2.45	2.853(2)	128.9
O(43)-H(43B)...O(2)#4	0.94	2.40	3.309(3)	163.3
O(44)-H(44A)...O(42)#5	0.82	2.03	2.854(2)	177.2
O(44)-H(44B)...O(43)#5	0.81	2.01	2.808(3)	166.9

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

CALIFORNIA INSTITUTE OF TECHNOLOGY

BECKMAN INSTITUTE

X-RAY CRYSTALLOGRAPHY LABORATORY

Date 21 January 2010

Crystal Structure Analysis of:

MLC17

(shown below)

For Investigator: Morgan Cable ext. (818) 354-4345

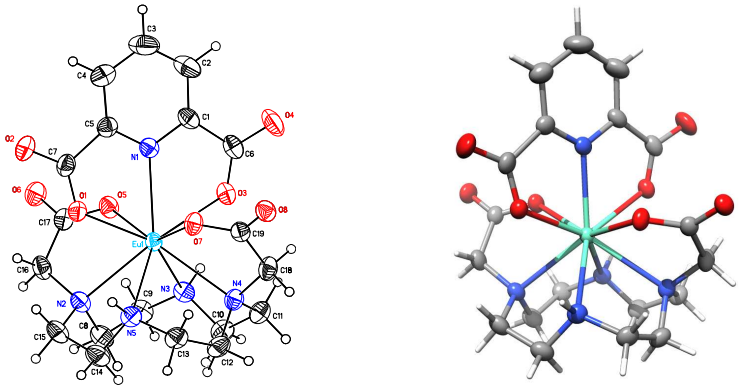
Advisor: Adrian Ponce ext. (818) 354-8196

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

By Michael W. Day 116 Beckman ext. 2734

e-mail: mikeday@caltech.edu

Contents

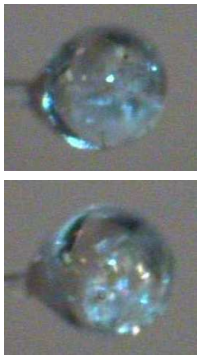


MLC17

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 762705. 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 762705."

Table 1. Crystal data and structure refinement for MLC18 (CCDC 762705).

Empirical formula	$[C_{19}H_{25}N_5O_8Eu]^-$ $[C_{16}H_{36}N]^+ \bullet C_3H_6O \bullet 3.68(H_2O)$
Formula weight	970.23
Crystallization Solvent	Acetone
Crystal Habit	Fragment
Crystal size	0.22 x 0.19 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	200(2) K
θ range for 9964 reflections used in lattice determination	2.21 to 33.31°
Unit cell dimensions	a = 13.1516(5) Å b = 13.5276(5) Å β= 90.701(2)° c = 26.1946(9) Å
Volume	4659.9(3) $Å^3$
Z	4
Crystal system	Monoclinic
Space group	P $2_1/c$
Density (calculated)	1.383 Mg/m^3
F(000)	2035
θ range for data collection	1.55 to 39.51°
Completeness to θ = 39.51°	99.7 %
Index ranges	$-23 \le h \le 23$, $-24 \le k \le 23$, $-46 \le l \le 46$
Data collection scan type	ω scans; 17 settings
Reflections collected	197040
Independent reflections	27945 [R_{int}= 0.0446]
Absorption coefficient	1.409 mm^{-1}
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7478 and 0.6642

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	27945 / 0 / 546
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.916
Final R indices [$I>2\sigma(I)$, 16515 reflections]	R1 = 0.0337, *w*R2 = 0.0550
R indices (all data)	R1 = 0.0775, *w*R2 = 0.0576
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.007
Average shift/error	0.000
Largest diff. peak and hole	1.688 and -2.002 e.Å^{-3}

Special Refinement Details

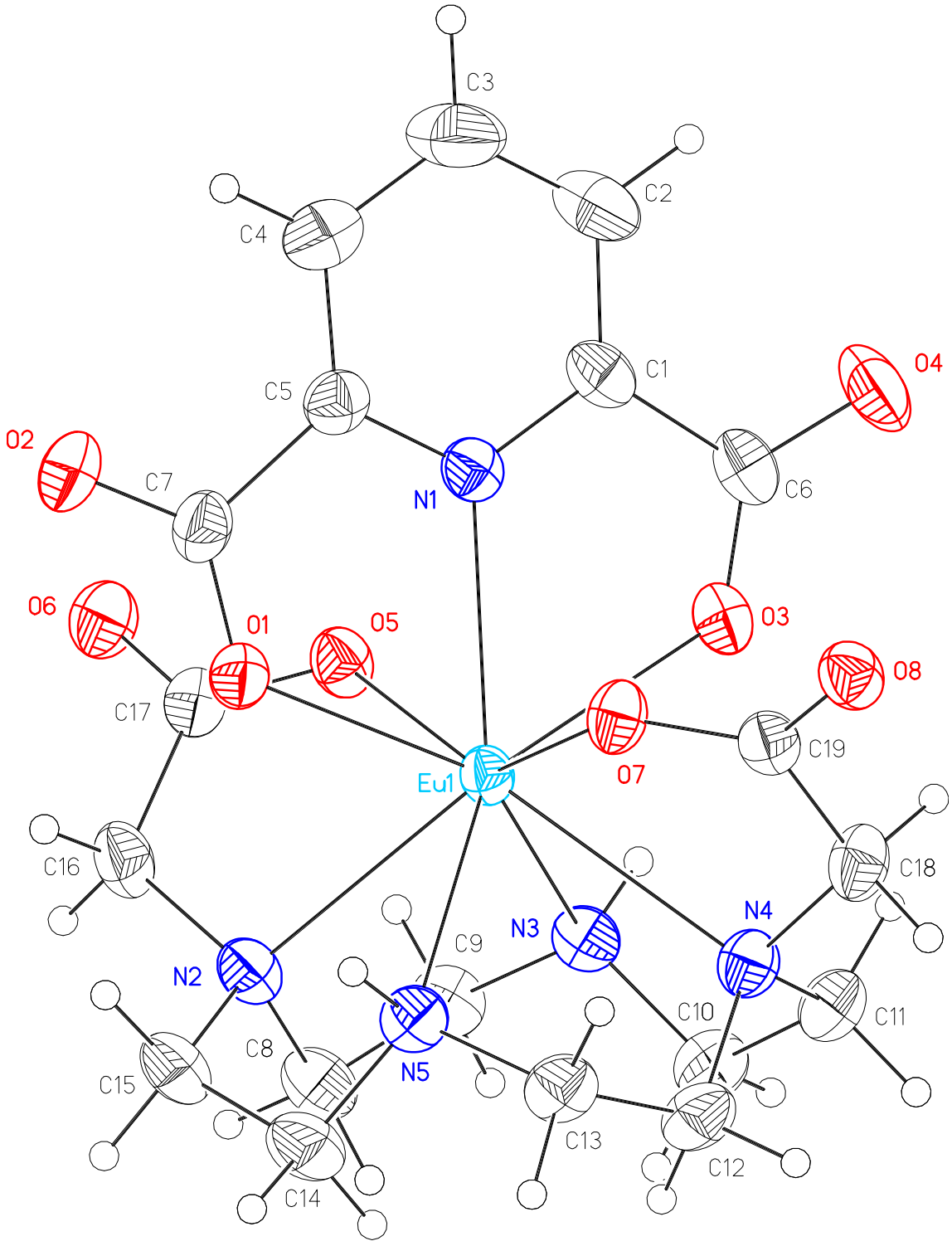
Crystals were mounted on a glass fiber using Paratone oil then coated in epoxy and placed on the diffractometer under a nitrogen stream at 200K.

This is the same exact crystal as MLC18. ∴ The asymmetric unit contains acetone at one site that is disordered between two orientations. **This acetone site was refined as a rigid body starting with the coordinates from MLC18.** The major orientation (69%), O51-C53 is accompanied by a water molecule, O44, that is hydrogen bonded to two other waters, O42 and O43. The minor orientation does not contain a discernable water. Hydrogen atoms on water were located in the electron density difference map and were constrained to ride the appropriate oxygen. All other hydrogens were placed at geometric positions and refined as riding atoms. No other restraints were placed on the model.

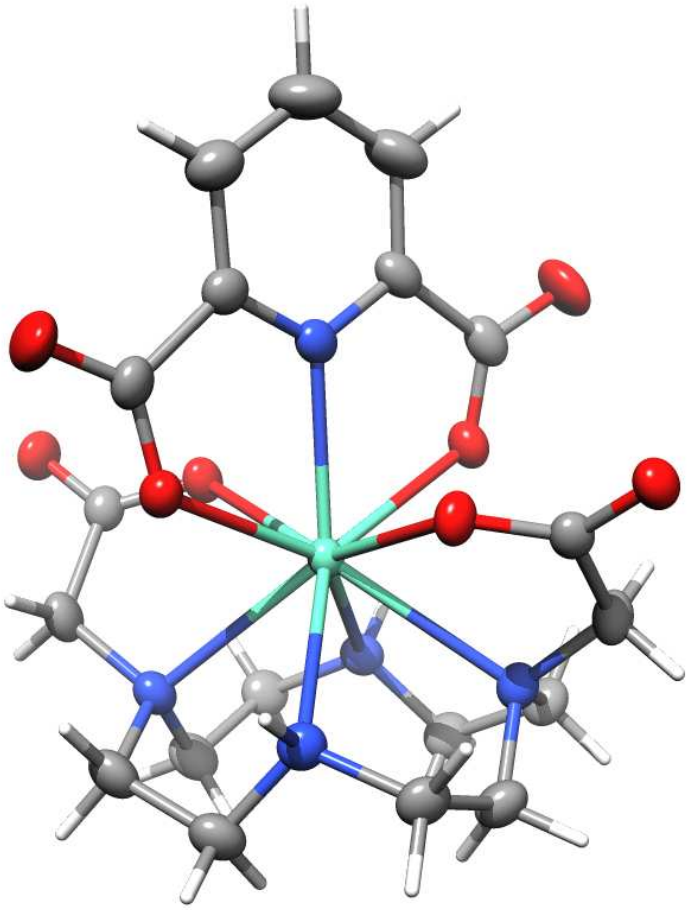
Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not 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.

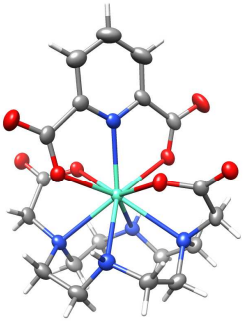
All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when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

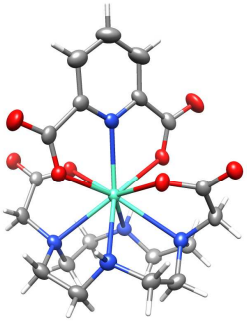
E20

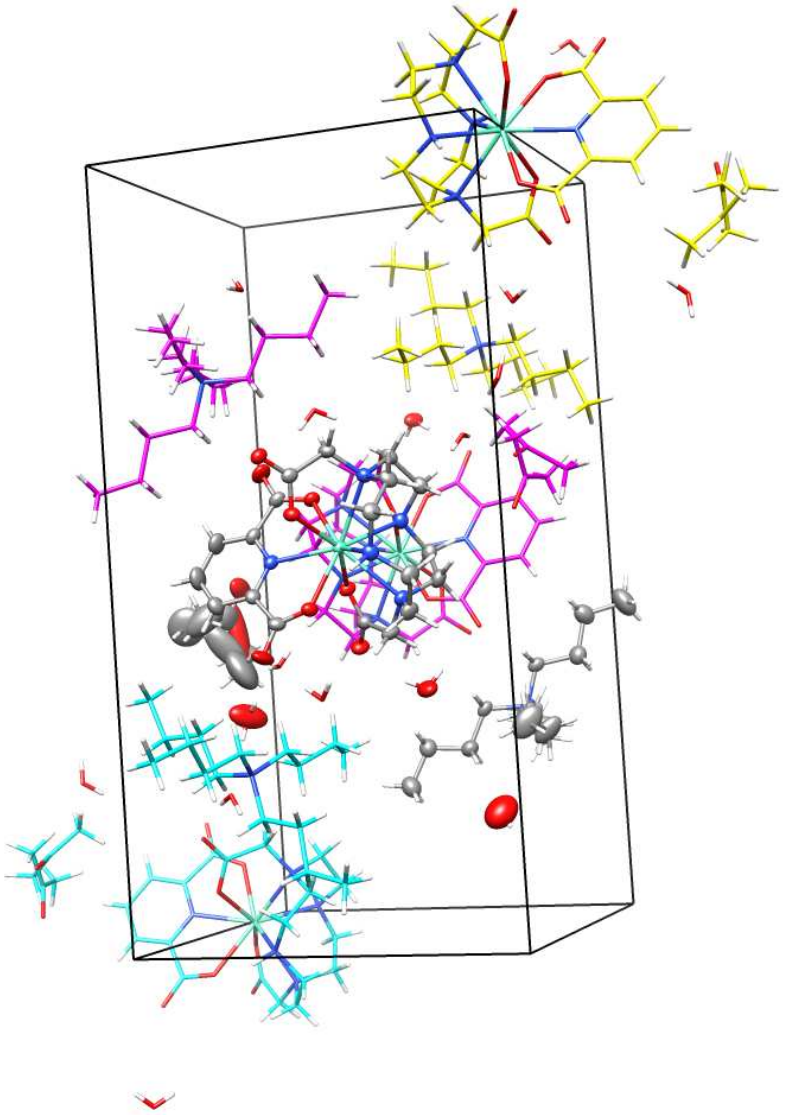

C3
C2
C4
C1
C5
O4
O2
C7
N1
C6
O6
O1
O5
O3
O8
C17
O7
C19
Eu1
C16
C18
N3
N4
N2
C9
C10
C11
C8
N5
C15
C13
C12
C14

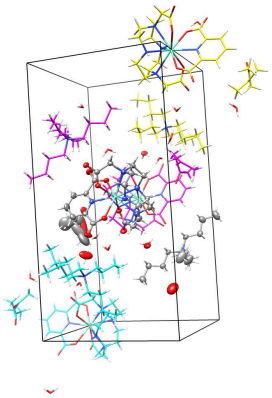
E21











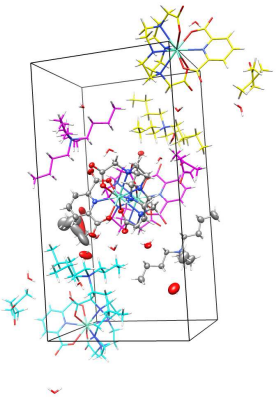


Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for MLC18 (CCDC 762705). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
Eu(1)	7497(1)	4924(1)	5002(1)	22(1)	1
O(1)	8318(1)	5503(1)	5774(1)	30(1)	1
O(2)	8635(1)	6689(1)	6344(1)	57(1)	1
O(3)	6704(1)	5883(1)	4331(1)	31(1)	1
O(4)	6440(1)	7318(1)	3928(1)	49(1)	1
O(5)	6066(1)	5318(1)	5508(1)	30(1)	1
O(6)	5343(1)	5340(1)	6267(1)	38(1)	1
O(7)	8962(1)	5558(1)	4586(1)	29(1)	1
O(8)	9664(1)	6037(1)	3861(1)	31(1)	1
N(1)	7518(1)	6761(1)	5125(1)	26(1)	1
N(2)	7028(1)	3546(1)	5693(1)	30(1)	1
N(3)	6050(1)	3786(1)	4684(1)	29(1)	1
N(4)	7952(1)	3999(1)	4138(1)	28(1)	1
N(5)	8919(1)	3621(1)	5135(1)	29(1)	1
C(1)	7140(1)	7353(1)	4760(1)	31(1)	1
C(2)	7142(2)	8365(1)	4818(1)	47(1)	1
C(3)	7536(2)	8768(1)	5261(1)	54(1)	1
C(4)	7922(1)	8152(1)	5639(1)	41(1)	1
C(5)	7908(1)	7148(1)	5554(1)	29(1)	1
C(6)	6725(1)	6814(1)	4299(1)	32(1)	1
C(7)	8320(1)	6385(1)	5927(1)	32(1)	1
C(8)	6325(1)	2807(1)	5463(1)	37(1)	1
C(9)	5549(1)	3258(1)	5104(1)	34(1)	1
C(10)	6316(1)	3130(1)	4260(1)	34(1)	1
C(11)	6993(1)	3656(1)	3888(1)	33(1)	1
C(12)	8635(1)	3148(1)	4239(1)	35(1)	1
C(13)	9416(1)	3355(1)	4654(1)	33(1)	1
C(14)	8644(1)	2754(1)	5442(1)	37(1)	1
C(15)	7972(1)	3056(1)	5876(1)	36(1)	1
C(16)	6543(1)	4078(1)	6117(1)	34(1)	1
C(17)	5920(1)	4975(1)	5953(1)	28(1)	1
C(18)	8457(1)	4740(1)	3813(1)	32(1)	1
C(19)	9088(1)	5502(1)	4108(1)	26(1)	1
N(6)	1373(1)	2174(1)	7200(1)	32(1)	1
C(20)	1689(1)	3253(1)	7206(1)	35(1)	1
C(21)	1859(2)	3693(1)	7731(1)	47(1)	1
C(22)	2105(2)	4778(1)	7694(1)	51(1)	1
C(23)	2323(2)	5245(2)	8210(1)	67(1)	1
C(24)	2198(1)	1537(1)	7459(1)	38(1)	1
C(25)	3251(1)	1663(1)	7258(1)	46(1)	1
C(26)	3977(2)	916(2)	7495(1)	75(1)	1
C(27)	5075(2)	1135(2)	7364(1)	94(1)	1
C(28)	1239(1)	1888(1)	6643(1)	35(1)	1
C(29)	929(2)	818(1)	6546(1)	51(1)	1
C(30)	719(2)	622(1)	5996(1)	64(1)	1

C(31)	479(2)	-427(2)	5861(1)	98(1)	1
C(32)	401(1)	2017(1)	7491(1)	36(1)	1
C(33)	-522(1)	2572(1)	7294(1)	44(1)	1
C(34)	-1373(1)	2546(1)	7670(1)	47(1)	1
C(35)	-2331(2)	3068(2)	7492(1)	66(1)	1
O(41)	733(1)	5045(1)	3100(1)	48(1)	1
O(42)	4224(1)	3983(1)	6873(1)	64(1)	1
O(43)	3931(2)	2311(2)	8542(1)	141(1)	1
O(44)	5079(3)	8661(2)	7101(1)	125(1)	0.687(3)
O(51)	3577(2)	9293(1)	5363(1)	97(1)	0.687(3)
C(51)	3473(3)	9448(3)	6226(1)	112(2)	0.687(3)
C(52)	4047(2)	9495(1)	5753(1)	70(1)	0.687(3)
C(53)	5149(2)	9716(4)	5768(2)	172(4)	0.687(3)
O(61)	3595(2)	9410(2)	6019(1)	289(12)	0.313(3)
C(61)	4986(4)	8804(3)	6471(1)	184(7)	0.313(3)
C(62)	4456(2)	9461(2)	6145(1)	199(11)	0.313(3)
C(63)	5036(3)	10280(4)	5847(2)	173(9)	0.313(3)

Table 3. Selected bond lengths [Å] and angles [°] for MLC18 (CCDC 762705).

Eu(1)-O(5)	2.3757(11)	O(5)-Eu(1)-O(7)	145.56(3)
Eu(1)-O(7)	2.3837(10)	O(5)-Eu(1)-O(3)	86.96(3)
Eu(1)-O(3)	2.4098(8)	O(7)-Eu(1)-O(3)	79.58(3)
Eu(1)-O(1)	2.4126(8)	O(5)-Eu(1)-O(1)	78.97(3)
Eu(1)-N(1)	2.5051(10)	O(7)-Eu(1)-O(1)	84.90(3)
Eu(1)-N(3)	2.5785(11)	O(3)-Eu(1)-O(1)	128.47(3)
Eu(1)-N(5)	2.5907(11)	O(5)-Eu(1)-N(1)	73.33(4)
Eu(1)-N(4)	2.6606(11)	O(7)-Eu(1)-N(1)	72.26(4)
Eu(1)-N(2)	2.6758(11)	O(3)-Eu(1)-N(1)	64.19(3)
		O(1)-Eu(1)-N(1)	64.27(3)
		O(5)-Eu(1)-N(3)	74.15(4)
		O(7)-Eu(1)-N(3)	131.66(3)
		O(3)-Eu(1)-N(3)	76.99(3)
		O(1)-Eu(1)-N(3)	141.75(4)
		N(1)-Eu(1)-N(3)	129.84(4)
		O(5)-Eu(1)-N(5)	130.74(3)
		O(7)-Eu(1)-N(5)	73.75(4)
		O(3)-Eu(1)-N(5)	140.34(4)
		O(1)-Eu(1)-N(5)	78.05(3)
		N(1)-Eu(1)-N(5)	130.62(4)
		N(3)-Eu(1)-N(5)	99.53(4)
		O(5)-Eu(1)-N(4)	140.17(3)
		O(7)-Eu(1)-N(4)	65.73(3)
		O(3)-Eu(1)-N(4)	74.54(3)
		O(1)-Eu(1)-N(4)	139.74(4)
		N(1)-Eu(1)-N(4)	125.05(3)
		N(3)-Eu(1)-N(4)	67.51(4)
		N(5)-Eu(1)-N(4)	67.97(3)
		O(5)-Eu(1)-N(2)	65.64(3)
		O(7)-Eu(1)-N(2)	138.93(3)
		O(3)-Eu(1)-N(2)	140.00(4)
		O(1)-Eu(1)-N(2)	76.30(3)
		N(1)-Eu(1)-N(2)	127.27(4)
		N(3)-Eu(1)-N(2)	68.07(3)
		N(5)-Eu(1)-N(2)	66.85(4)
		N(4)-Eu(1)-N(2)	107.68(4)

Table 4. Bond lengths [Å] and angles [°] for MLC18 (CCDC 762705).

Eu(1)-O(5)	2.3757(11)	C(26)-C(27)	1.517(3)
Eu(1)-O(7)	2.3837(10)	C(28)-C(29)	1.525(2)
Eu(1)-O(3)	2.4098(8)	C(29)-C(30)	1.489(2)
Eu(1)-O(1)	2.4126(8)	C(30)-C(31)	1.496(3)
Eu(1)-N(1)	2.5051(10)	C(32)-C(33)	1.512(2)
Eu(1)-N(3)	2.5785(11)	C(33)-C(34)	1.500(3)
Eu(1)-N(5)	2.5907(11)	C(34)-C(35)	1.513(3)
Eu(1)-N(4)	2.6606(11)	O(51)-C(52)	1.2187
Eu(1)-N(2)	2.6758(11)	C(51)-C(52)	1.4609
O(1)-C(7)	1.2582(16)	C(52)-C(53)	1.4807
O(2)-C(7)	1.2348(15)	O(61)-C(62)	1.1779
O(3)-C(6)	1.2636(16)	C(61)-C(62)	1.4098
O(4)-C(6)	1.2407(15)	C(62)-C(63)	1.5596
O(5)-C(17)	1.2715(16)		
O(6)-C(17)	1.2309(18)	O(5)-Eu(1)-O(7)	145.56(3)
O(7)-C(19)	1.2668(16)	O(5)-Eu(1)-O(3)	86.96(3)
O(8)-C(19)	1.2358(17)	O(7)-Eu(1)-O(3)	79.58(3)
N(1)-C(5)	1.3351(16)	O(5)-Eu(1)-O(1)	78.97(3)
N(1)-C(1)	1.3381(16)	O(7)-Eu(1)-O(1)	84.90(3)
N(2)-C(16)	1.4759(19)	O(3)-Eu(1)-O(1)	128.47(3)
N(2)-C(8)	1.4840(18)	O(5)-Eu(1)-N(1)	73.33(4)
N(2)-C(15)	1.4837(18)	O(7)-Eu(1)-N(1)	72.26(4)
N(3)-C(10)	1.4676(19)	O(3)-Eu(1)-N(1)	64.19(3)
N(3)-C(9)	1.473(2)	O(1)-Eu(1)-N(1)	64.27(3)
N(4)-C(18)	1.4762(19)	O(5)-Eu(1)-N(3)	74.15(4)
N(4)-C(12)	1.4820(18)	O(7)-Eu(1)-N(3)	131.66(3)
N(4)-C(11)	1.4880(17)	O(3)-Eu(1)-N(3)	76.99(3)
N(5)-C(14)	1.4700(19)	O(1)-Eu(1)-N(3)	141.75(4)
N(5)-C(13)	1.471(2)	N(1)-Eu(1)-N(3)	129.84(4)
C(1)-C(2)	1.376(2)	O(5)-Eu(1)-N(5)	130.74(3)
C(1)-C(6)	1.509(2)	O(7)-Eu(1)-N(5)	73.75(4)
C(2)-C(3)	1.378(2)	O(3)-Eu(1)-N(5)	140.34(4)
C(3)-C(4)	1.384(2)	O(1)-Eu(1)-N(5)	78.05(3)
C(4)-C(5)	1.3764(19)	N(1)-Eu(1)-N(5)	130.62(4)
C(5)-C(7)	1.5171(19)	N(3)-Eu(1)-N(5)	99.53(4)
C(8)-C(9)	1.5087(19)	O(5)-Eu(1)-N(4)	140.17(3)
C(10)-C(11)	1.506(2)	O(7)-Eu(1)-N(4)	65.73(3)
C(12)-C(13)	1.5126(19)	O(3)-Eu(1)-N(4)	74.54(3)
C(14)-C(15)	1.506(2)	O(1)-Eu(1)-N(4)	139.74(4)
C(16)-C(17)	1.5231(19)	N(1)-Eu(1)-N(4)	125.05(3)
C(18)-C(19)	1.5271(19)	N(3)-Eu(1)-N(4)	67.51(4)
N(6)-C(28)	1.5164(18)	N(5)-Eu(1)-N(4)	67.97(3)
N(6)-C(20)	1.5185(17)	O(5)-Eu(1)-N(2)	65.64(3)
N(6)-C(32)	1.512(2)	O(7)-Eu(1)-N(2)	138.93(3)
N(6)-C(24)	1.5363(18)	O(3)-Eu(1)-N(2)	140.00(4)
C(20)-C(21)	1.514(2)	O(1)-Eu(1)-N(2)	76.30(3)
C(21)-C(22)	1.507(2)	N(1)-Eu(1)-N(2)	127.27(4)
C(22)-C(23)	1.516(3)	N(3)-Eu(1)-N(2)	68.07(3)
C(24)-C(25)	1.498(2)	N(5)-Eu(1)-N(2)	66.85(4)
C(25)-C(26)	1.518(2)	N(4)-Eu(1)-N(2)	107.68(4)

C(7)-O(1)-Eu(1)	124.94(8)	N(4)-C(18)-C(19)	114.39(11)
C(6)-O(3)-Eu(1)	125.18(8)	O(8)-C(19)-O(7)	124.80(13)
C(17)-O(5)-Eu(1)	124.03(9)	O(8)-C(19)-C(18)	117.64(12)
C(19)-O(7)-Eu(1)	123.11(9)	O(7)-C(19)-C(18)	117.54(13)
C(5)-N(1)-C(1)	120.01(11)	C(28)-N(6)-C(20)	106.45(10)
C(5)-N(1)-Eu(1)	120.09(8)	C(28)-N(6)-C(32)	111.17(11)
C(1)-N(1)-Eu(1)	119.90(8)	C(20)-N(6)-C(32)	111.27(12)
C(16)-N(2)-C(8)	111.13(13)	C(28)-N(6)-C(24)	110.81(12)
C(16)-N(2)-C(15)	109.96(10)	C(20)-N(6)-C(24)	110.02(11)
C(8)-N(2)-C(15)	110.17(11)	C(32)-N(6)-C(24)	107.16(10)
C(16)-N(2)-Eu(1)	106.02(8)	C(21)-C(20)-N(6)	115.13(11)
C(8)-N(2)-Eu(1)	110.09(8)	C(20)-C(21)-C(22)	110.72(13)
C(15)-N(2)-Eu(1)	109.38(9)	C(21)-C(22)-C(23)	112.73(15)
C(10)-N(3)-C(9)	112.60(11)	C(25)-C(24)-N(6)	115.61(12)
C(10)-N(3)-Eu(1)	115.08(9)	C(24)-C(25)-C(26)	111.09(14)
C(9)-N(3)-Eu(1)	112.59(8)	C(25)-C(26)-C(27)	111.85(17)
C(18)-N(4)-C(12)	110.76(13)	N(6)-C(28)-C(29)	115.41(12)
C(18)-N(4)-C(11)	110.10(10)	C(30)-C(29)-C(28)	112.05(14)
C(12)-N(4)-C(11)	110.16(10)	C(31)-C(30)-C(29)	115.69(18)
C(18)-N(4)-Eu(1)	106.11(8)	N(6)-C(32)-C(33)	116.01(12)
C(12)-N(4)-Eu(1)	110.86(8)	C(34)-C(33)-C(32)	111.51(13)
C(11)-N(4)-Eu(1)	108.76(9)	C(33)-C(34)-C(35)	114.37(14)
C(14)-N(5)-C(13)	112.86(11)	O(51)-C(52)-C(51)	116.1
C(14)-N(5)-Eu(1)	115.76(9)	O(51)-C(52)-C(53)	123.7
C(13)-N(5)-Eu(1)	112.23(8)	C(51)-C(52)-C(53)	120.1
N(1)-C(1)-C(2)	121.13(13)	O(61)-C(62)-C(61)	126.8
N(1)-C(1)-C(6)	114.23(11)	O(61)-C(62)-C(63)	112.0
C(2)-C(1)-C(6)	124.64(12)	C(61)-C(62)-C(63)	120.7
C(1)-C(2)-C(3)	119.07(14)		
C(2)-C(3)-C(4)	119.63(14)		
C(5)-C(4)-C(3)	118.29(14)		
N(1)-C(5)-C(4)	121.86(12)		
N(1)-C(5)-C(7)	113.87(11)		
C(4)-C(5)-C(7)	124.27(12)		
O(4)-C(6)-O(3)	126.46(13)		
O(4)-C(6)-C(1)	117.70(12)		
O(3)-C(6)-C(1)	115.83(11)		
O(2)-C(7)-O(1)	126.53(13)		
O(2)-C(7)-C(5)	117.24(12)		
O(1)-C(7)-C(5)	116.22(11)		
N(2)-C(8)-C(9)	113.17(11)		
N(3)-C(9)-C(8)	110.89(13)		
N(3)-C(10)-C(11)	110.58(11)		
N(4)-C(11)-C(10)	111.67(11)		
N(4)-C(12)-C(13)	112.87(11)		
N(5)-C(13)-C(12)	110.88(13)		
N(5)-C(14)-C(15)	110.35(12)		
N(2)-C(15)-C(14)	111.86(11)		
N(2)-C(16)-C(17)	114.26(11)		
O(6)-C(17)-O(5)	124.67(13)		
O(6)-C(17)-C(16)	117.67(12)		
O(5)-C(17)-C(16)	117.59(13)		

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for MLC18 (CCDC 762705). 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}
Eu(1)	220(1)	247(1)	202(1)	18(1)	16(1)	14(1)
O(1)	343(6)	308(5)	241(5)	-8(4)	-20(4)	38(4)
O(2)	970(12)	465(6)	264(5)	-98(5)	-133(6)	76(6)
O(3)	322(6)	341(5)	258(5)	56(4)	-26(4)	-3(4)
O(4)	621(9)	461(6)	397(6)	204(5)	-125(6)	-32(6)
O(5)	270(6)	347(5)	273(5)	49(4)	52(4)	37(4)
O(6)	413(7)	425(6)	310(5)	-5(4)	119(5)	37(5)
O(7)	266(6)	378(5)	239(5)	-15(4)	41(4)	-28(4)
O(8)	311(6)	315(5)	294(5)	45(4)	54(4)	5(4)
N(1)	242(6)	279(5)	266(6)	26(4)	52(5)	11(4)
N(2)	298(7)	297(6)	295(6)	59(4)	10(5)	31(5)
N(3)	245(7)	295(6)	325(6)	21(4)	-7(5)	10(5)
N(4)	259(7)	317(6)	258(5)	-18(4)	11(5)	-19(5)
N(5)	240(7)	317(6)	317(6)	-12(5)	-15(5)	28(5)
C(1)	274(8)	300(7)	343(7)	88(5)	30(6)	0(6)
C(2)	526(12)	319(8)	567(11)	123(7)	-49(9)	23(8)
C(3)	635(14)	274(8)	701(12)	-19(8)	-50(10)	3(8)
C(4)	448(11)	351(8)	439(9)	-79(6)	14(8)	-11(7)
C(5)	269(8)	299(7)	293(7)	-17(5)	53(6)	9(6)
C(6)	270(9)	380(8)	314(7)	102(6)	3(6)	-14(6)
C(7)	330(9)	378(8)	238(7)	-27(5)	40(6)	27(6)
C(8)	370(10)	332(7)	415(8)	93(6)	26(7)	-46(6)
C(9)	265(9)	349(7)	391(8)	23(6)	31(7)	-59(6)
C(10)	295(9)	346(7)	380(8)	-46(6)	-3(7)	-51(6)
C(11)	322(9)	366(7)	308(7)	-71(6)	-23(6)	-28(6)
C(12)	318(9)	354(7)	367(8)	-86(6)	18(7)	59(6)
C(13)	254(8)	352(7)	373(8)	-34(6)	32(6)	71(6)
C(14)	343(10)	335(7)	446(9)	76(6)	6(7)	93(6)
C(15)	358(10)	352(7)	372(8)	115(6)	-34(7)	66(6)
C(16)	343(9)	405(8)	262(7)	89(5)	56(6)	39(6)
C(17)	254(8)	327(7)	261(6)	-4(5)	9(5)	-42(6)
C(18)	324(9)	403(7)	245(6)	-17(5)	48(6)	-59(6)
C(19)	229(8)	296(7)	268(7)	22(5)	21(6)	48(5)
N(6)	306(7)	347(6)	314(6)	129(5)	-20(5)	-16(5)
C(20)	361(10)	346(7)	348(8)	129(6)	-24(7)	-36(6)
C(21)	566(13)	458(9)	379(9)	67(7)	-47(8)	-78(8)
C(22)	575(14)	467(9)	488(10)	15(7)	9(9)	-97(9)
C(23)	777(18)	605(11)	615(13)	-82(9)	-16(12)	-135(11)
C(24)	321(10)	421(8)	406(8)	196(6)	-38(7)	13(7)
C(25)	338(11)	555(10)	480(9)	221(8)	-13(8)	31(8)
C(26)	418(14)	920(15)	900(16)	495(12)	-22(12)	142(11)
C(27)	391(15)	1120(19)	1320(20)	518(17)	-2(15)	171(13)
C(28)	355(10)	394(8)	303(7)	89(6)	-7(7)	8(6)
C(29)	550(13)	469(9)	511(11)	41(7)	17(9)	-91(8)
C(30)	821(18)	528(11)	565(12)	-65(8)	-137(12)	43(10)

C(31)	1050(20)	800(16)	1070(20)	-354(15)	-104(18)	-162(16)
C(32)	324(9)	412(8)	341(8)	128(6)	13(7)	-39(7)
C(33)	356(10)	551(10)	413(9)	182(7)	31(8)	55(8)
C(34)	433(11)	515(10)	458(10)	98(7)	95(8)	31(8)
C(35)	462(14)	772(14)	759(14)	123(10)	166(11)	113(11)
O(41)	715(10)	407(6)	318(5)	5(4)	118(6)	149(5)
O(42)	807(11)	743(8)	372(7)	39(6)	117(7)	-313(8)
O(43)	1400(20)	1457(18)	1388(19)	312(14)	318(16)	85(16)
O(44)	1580(30)	1330(20)	850(20)	-283(16)	-280(20)	820(20)
O(51)	1740(30)	380(11)	776(17)	36(10)	-398(18)	42(13)
C(51)	900(50)	1790(60)	650(30)	-290(30)	-120(30)	450(40)
C(52)	940(40)	371(17)	790(20)	129(15)	-110(20)	176(18)
C(53)	960(60)	2630(90)	1580(60)	990(60)	80(50)	-210(50)
O(61)	990(100)	610(60)	7100(400)	-780(120)	-580(160)	-10(50)
C(61)	1850(170)	1490(110)	2180(180)	-900(110)	-110(130)	-230(100)
C(62)	1080(140)	2030(170)	2800(200)	-1370(170)	-1080(160)	660(120)
C(63)	950(130)	2190(180)	2030(180)	320(130)	-600(120)	-30(100)

Table 6. Hydrogen bonds for MLC18 (CCDC 762705) [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(3)-H(3)...O(5)#1	0.93	2.23	3.0715(15)	149.9
N(3)-H(3)...O(6)#1	0.93	2.51	3.2945(15)	142.0
N(5)-H(5)...O(7)#2	0.93	2.24	3.0801(15)	149.4
N(5)-H(5)...O(8)#2	0.93	2.44	3.2385(14)	144.6
O(41)-H(41A)...O(8)#3	0.76	2.05	2.7967(15)	171.2
O(41)-H(41B)...O(2)#1	0.74	2.14	2.8780(14)	178.4
O(42)-H(42A)...O(6)	0.77	2.10	2.8472(17)	163.6
O(42)-H(42B)...O(4)#1	0.80	2.07	2.8658(16)	172.1
O(43)-H(43A)...O(6)#4	0.59	2.47	2.873(2)	127.9
O(43)-H(43B)...O(2)#4	0.95	2.57	3.495(3)	164.4
O(44)-H(44A)...O(42)#5	0.83	2.04	2.864(3)	178.0
O(44)-H(44B)...O(43)#5	0.81	2.02	2.815(4)	165.6

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

E31

CALIFORNIA INSTITUTE OF TECHNOLOGY

BECKMAN INSTITUTE

X-RAY CRYSTALLOGRAPHY LABORATORY

Date 26 January 2010

Crystal Structure Analysis of:

MLC19

(shown below)

For Investigator: Morgan Cable ext. (818) 354-4345

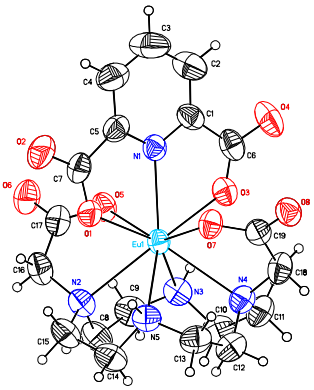
Advisor: Adrian Ponce ext. (818) 354-8196

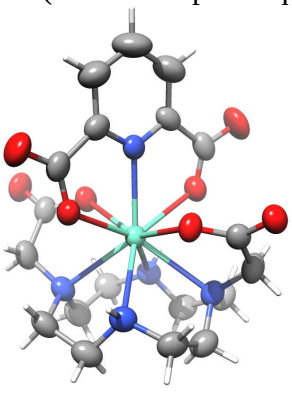
Account Number: AP1.HSARPA3-1-HSARPA.PONCE

By Michael W. Day 116 Beckman ext. 2734

e-mail: mikeday@caltech.edu

Contents





MLC19

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 763335. 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 763335."

Table 1. Crystal data and structure refinement for MLC19 (CCDC 763335).

Empirical formula	$[C_{19}H_{25}N_5O_8Eu]^-$ $[C_{16}H_{36}N]^+ \bullet C_3H_6O \bullet 2.50(H_2O)$
Formula weight	949.07
Crystallization Solvent	Acetone
Crystal Habit	Fragment
Crystal size	0.22 x 0.19 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	300(2) K
θ range for 9548 reflections used in lattice determination	2.18 to 27.72°
Unit cell dimensions	a = 13.3306(9) Å b = 13.4557(9) Å β= 90.450(3)° c = 26.3443(17) Å
Volume	4725.3(5) $Å^3$
Z	4
Crystal system	Monoclinic
Space group	P $2_1/c$
Density (calculated)	1.334 Mg/m^3
F(000)	1988
θ range for data collection	1.53 to 39.59°
Completeness to θ = 39.59°	98.5 %
Index ranges	$-23 \le h \le 23$, $-24 \le k \le 23$, $-46 \le l \le 47$
Data collection scan type	ω scans; 19 settings
Reflections collected	220185
Independent reflections	28102 [R_{int}= 0.0620]
Absorption coefficient	1.386 mm^{-1}
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7477 and 0.6515

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	28102 / 0 / 482
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.682
Final R indices [$I>2\sigma(I)$, 11411 reflections]	R1 = 0.0469, *w*R2 = 0.0623
R indices (all data)	R1 = 0.1399, *w*R2 = 0.0679
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.014
Average shift/error	0.000
Largest diff. peak and hole	2.053 and -1.042 e.Å^{-3}

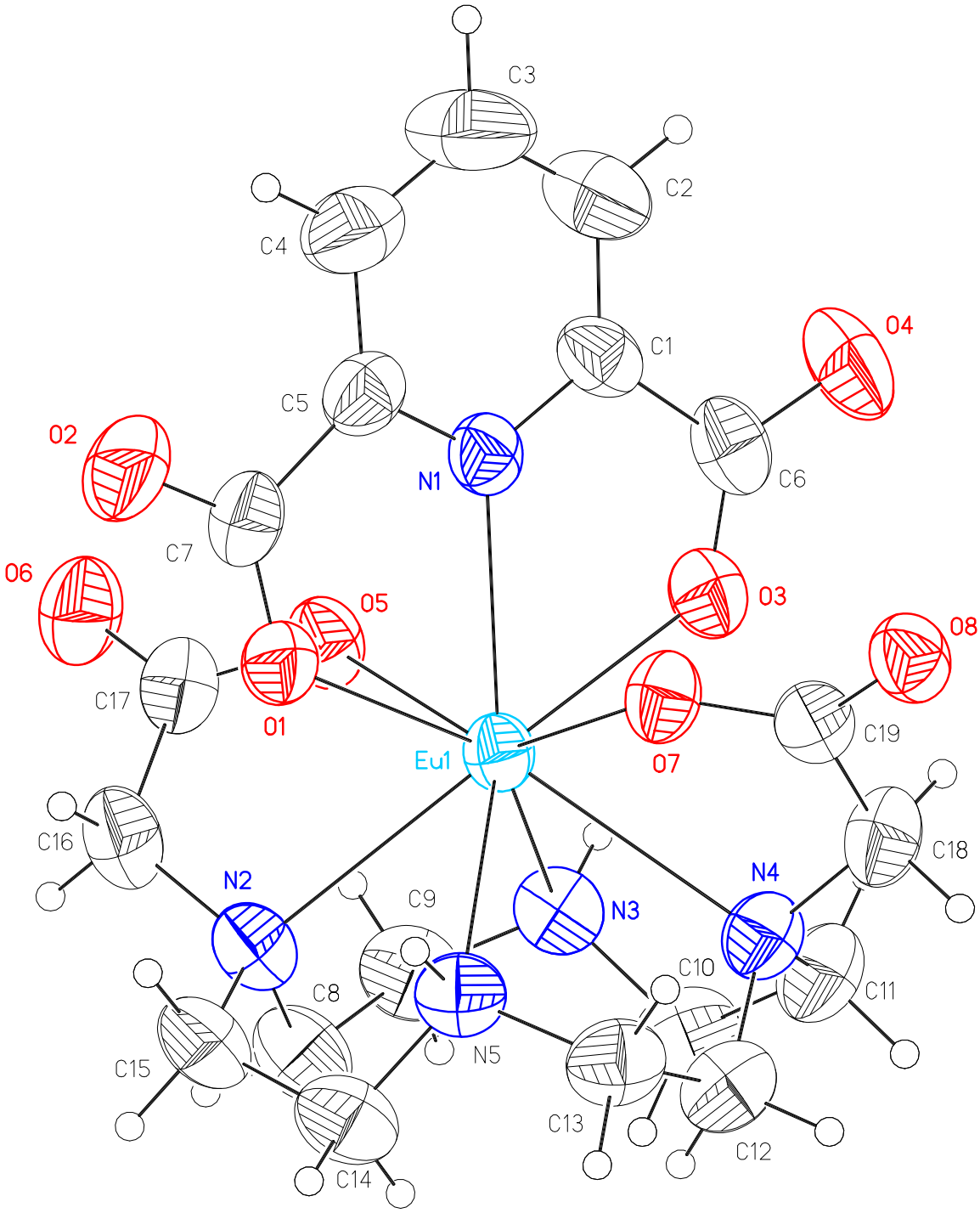
Special Refinement Details

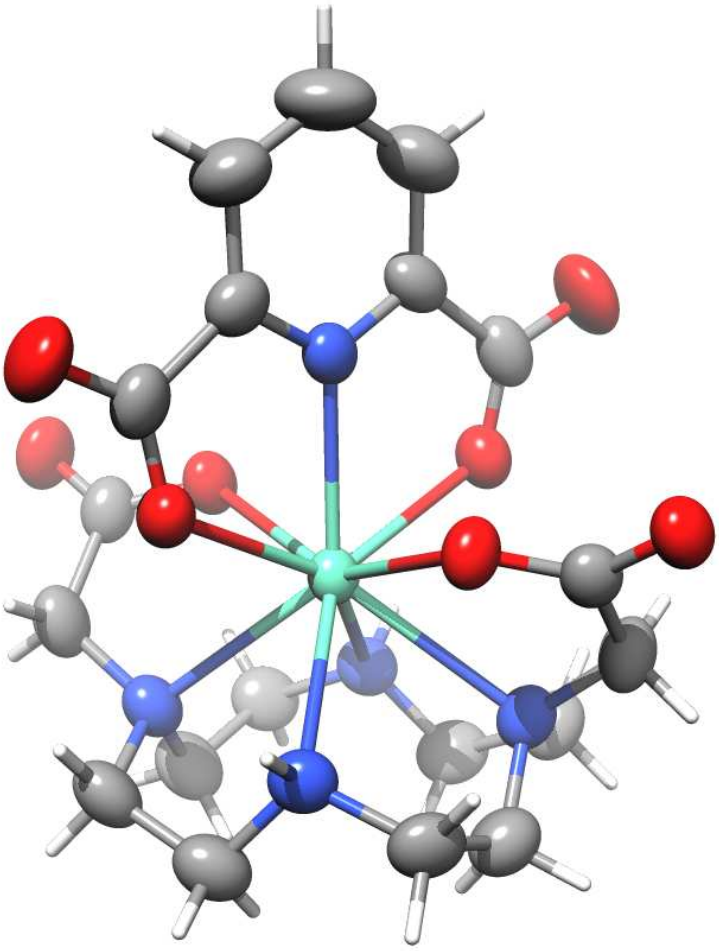
Crystals were mounted on a glass fiber using Paratone oil then coated in epoxy and placed on the diffractometer under a nitrogen stream at 300K.

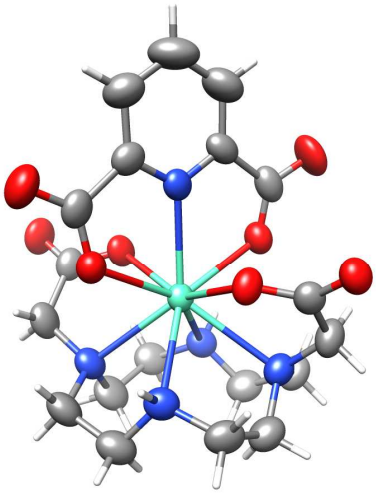
This is the same exact crystal as MLC18. ∴ The asymmetric unit contains acetone at one site that is disordered between two orientations. **This acetone site was refined as a rigid body starting with the coordinates from MLC18.** The relative occupancies refine to different ratios than the lower temperature studies, with the major orientation (50.3%), O51-C53 accompanied by a water molecule, O44, that is hydrogen bonded to two other waters, O42 and O43. The minor orientation does not contain a discernable water. Hydrogen atoms on water were located in the electron density difference map and were constrained to ride the appropriate oxygen. All other hydrogens were placed at geometric positions and refined as riding atoms. No other restraints were placed on the model. **Note, one water molecule (O43) was removed from the model as the position appeared to become so diffuse as to disappear from maps.**

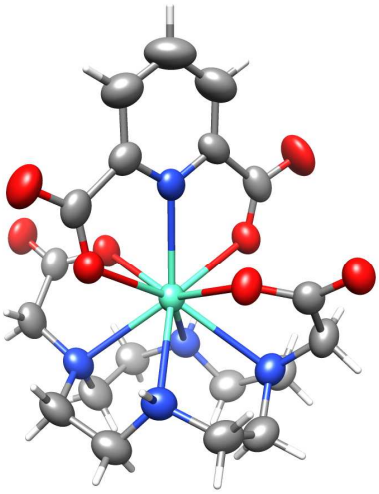
Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not 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.

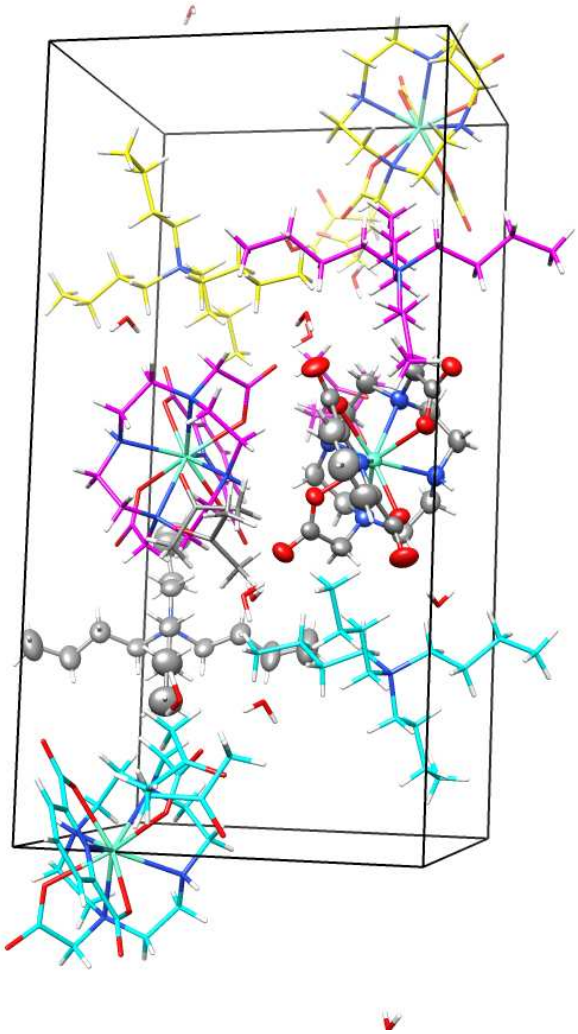

C3
C2
C4
C1
O4
C5
O2
N1
C6
C7
O6
O3
O5
O8
C17
O1
Eu1
O7
C19
C16
C18
N2
N4
C9
N3
C10
C11
C8
N5
C15
C13
C12
C14



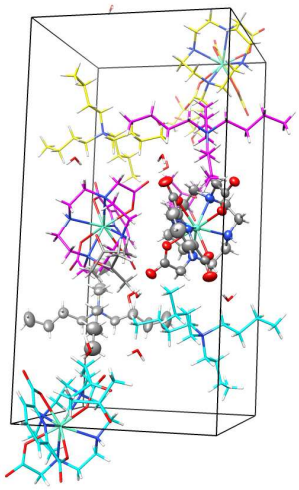




E36



E37



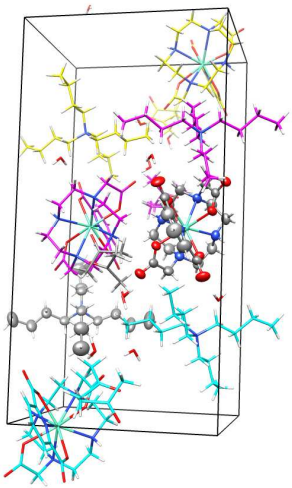


Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for MLC19 (CCDC 763335). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
Eu(1)	7500(1)	4978(1)	5016(1)	40(1)	1
O(1)	8333(1)	5567(1)	5772(1)	51(1)	1
O(2)	8717(1)	6773(1)	6321(1)	79(1)	1
O(3)	6717(1)	5932(1)	4353(1)	51(1)	1
O(4)	6437(1)	7371(1)	3950(1)	81(1)	1
O(5)	6085(1)	5391(1)	5512(1)	51(1)	1
O(6)	5298(1)	5386(1)	6246(1)	66(1)	1
O(7)	8945(1)	5588(1)	4590(1)	49(1)	1
O(8)	9641(1)	6022(1)	3861(1)	53(1)	1
N(1)	7533(1)	6829(1)	5130(1)	44(1)	1
N(2)	7034(1)	3615(1)	5714(1)	53(1)	1
N(3)	6068(1)	3814(1)	4713(1)	51(1)	1
N(4)	7941(1)	4002(1)	4166(1)	49(1)	1
N(5)	8905(1)	3658(1)	5156(1)	51(1)	1
C(1)	7147(2)	7422(2)	4773(1)	50(1)	1
C(2)	7150(2)	8424(2)	4820(1)	78(1)	1
C(3)	7565(2)	8841(2)	5255(1)	95(1)	1
C(4)	7953(2)	8230(2)	5624(1)	75(1)	1
C(5)	7940(2)	7217(2)	5549(1)	51(1)	1
C(6)	6725(2)	6860(2)	4316(1)	54(1)	1
C(7)	8363(2)	6455(2)	5913(1)	53(1)	1
C(8)	6342(2)	2869(2)	5501(1)	68(1)	1
C(9)	5573(2)	3301(2)	5138(1)	61(1)	1
C(10)	6322(2)	3139(2)	4296(1)	64(1)	1
C(11)	6984(2)	3657(2)	3925(1)	61(1)	1
C(12)	8605(2)	3146(2)	4275(1)	63(1)	1
C(13)	9385(2)	3365(2)	4677(1)	59(1)	1
C(14)	8630(2)	2801(2)	5470(1)	65(1)	1
C(15)	7968(2)	3131(2)	5900(1)	63(1)	1
C(16)	6555(2)	4172(2)	6128(1)	62(1)	1
C(17)	5915(2)	5046(2)	5952(1)	50(1)	1
C(18)	8438(2)	4732(2)	3837(1)	58(1)	1
C(19)	9070(2)	5507(2)	4115(1)	46(1)	1
N(6)	1442(1)	2262(1)	7233(1)	56(1)	1
C(20)	1744(2)	3344(2)	7231(1)	63(1)	1
C(21)	1885(2)	3805(2)	7747(1)	80(1)	1
C(22)	2153(3)	4867(2)	7711(1)	100(1)	1
C(23)	2304(3)	5365(2)	8219(1)	119(1)	1
C(24)	2239(2)	1629(2)	7495(1)	62(1)	1
C(25)	3277(2)	1717(2)	7292(1)	79(1)	1
C(26)	3998(2)	1094(3)	7583(1)	129(1)	1
C(27)	5074(3)	1278(4)	7440(2)	170(2)	1
C(28)	1329(2)	1943(2)	6678(1)	62(1)	1
C(29)	1039(2)	878(2)	6587(1)	81(1)	1
C(30)	785(3)	670(3)	6048(1)	110(1)	1

C(31)	623(4)	-374(3)	5912(2)	159(2)	1
C(32)	477(2)	2107(2)	7518(1)	62(1)	1
C(33)	-437(2)	2661(2)	7319(1)	73(1)	1
C(34)	-1280(2)	2627(2)	7687(1)	88(1)	1
C(35)	-2221(3)	3137(3)	7525(1)	129(1)	1
O(41)	698(1)	4987(1)	3117(1)	77(1)	1
O(42)	4175(2)	4013(2)	6845(1)	106(1)	1
O(44)	5030(30)	8240(30)	6864(18)	1210(40)	0.503(5)
O(51)	3635(4)	9301(4)	5422(2)	192(3)	0.503(5)
C(51)	3518(4)	9433(4)	6286(2)	201(6)	0.503(5)
C(52)	4099(3)	9494(2)	5815(2)	123(3)	0.503(5)
C(53)	5201(3)	9717(6)	5836(2)	317(10)	0.503(5)
O(61)	3644(3)	9401(3)	6078(2)	344(8)	0.497(5)
C(61)	5029(6)	8785(5)	6531(2)	210(5)	0.497(5)
C(62)	4503(4)	9450(3)	6208(2)	142(3)	0.497(5)
C(63)	5085(4)	10278(5)	5918(3)	212(6)	0.497(5)

Table 3. Selected bond lengths [Å] and angles [°] for MLC19 (CCDC 763335).

Eu(1)-O(5)	2.3674(15)	O(7)-Eu(1)-N(4)	65.77(5)
Eu(1)-O(7)	2.3836(14)	O(3)-Eu(1)-N(4)	75.46(5)
Eu(1)-O(3)	2.4004(12)	O(1)-Eu(1)-N(4)	138.90(5)
Eu(1)-O(1)	2.4059(11)	N(1)-Eu(1)-N(4)	125.83(5)
Eu(1)-N(1)	2.5085(16)	N(3)-Eu(1)-N(4)	67.03(5)
Eu(1)-N(3)	2.5904(16)	N(5)-Eu(1)-N(4)	67.65(5)
Eu(1)-N(5)	2.6055(16)	O(5)-Eu(1)-N(2)	65.94(5)
Eu(1)-N(4)	2.6661(15)	O(7)-Eu(1)-N(2)	138.84(5)
Eu(1)-N(2)	2.6724(16)	O(3)-Eu(1)-N(2)	139.95(5)
Eu(1)-C(19)	3.256(2)	O(1)-Eu(1)-N(2)	76.44(5)
Eu(1)-C(17)	3.259(2)	N(1)-Eu(1)-N(2)	127.12(5)
		N(3)-Eu(1)-N(2)	67.84(5)
O(5)-Eu(1)-O(7)	146.00(5)	N(5)-Eu(1)-N(2)	66.75(6)
O(5)-Eu(1)-O(3)	86.12(5)	N(4)-Eu(1)-N(2)	107.05(6)
O(7)-Eu(1)-O(3)	79.73(5)	O(5)-Eu(1)-C(19)	150.44(5)
O(5)-Eu(1)-O(1)	80.31(5)	O(7)-Eu(1)-C(19)	19.03(4)
O(7)-Eu(1)-O(1)	84.61(4)	O(3)-Eu(1)-C(19)	68.32(5)
O(3)-Eu(1)-O(1)	128.45(5)	O(1)-Eu(1)-C(19)	103.63(5)
O(5)-Eu(1)-N(1)	73.42(5)	N(1)-Eu(1)-C(19)	81.90(5)
O(7)-Eu(1)-N(1)	72.59(5)	N(3)-Eu(1)-C(19)	112.55(5)
O(3)-Eu(1)-N(1)	64.11(4)	N(5)-Eu(1)-C(19)	77.67(5)
O(1)-Eu(1)-N(1)	64.35(4)	N(4)-Eu(1)-C(19)	49.30(5)
O(5)-Eu(1)-N(3)	73.97(5)	N(2)-Eu(1)-C(19)	143.62(5)
O(7)-Eu(1)-N(3)	131.25(5)	O(5)-Eu(1)-C(17)	18.76(5)
O(3)-Eu(1)-N(3)	77.47(5)	O(7)-Eu(1)-C(17)	151.34(5)
O(1)-Eu(1)-N(3)	142.07(5)	O(3)-Eu(1)-C(17)	104.77(5)
N(1)-Eu(1)-N(3)	130.47(5)	O(1)-Eu(1)-C(17)	70.33(5)
O(5)-Eu(1)-N(5)	131.07(5)	N(1)-Eu(1)-C(17)	83.86(6)
O(7)-Eu(1)-N(5)	73.64(5)	N(3)-Eu(1)-C(17)	76.70(5)
O(3)-Eu(1)-N(5)	140.82(5)	N(5)-Eu(1)-C(17)	112.44(5)
O(1)-Eu(1)-N(5)	77.34(5)	N(4)-Eu(1)-C(17)	142.89(5)
N(1)-Eu(1)-N(5)	130.41(5)	N(2)-Eu(1)-C(17)	49.03(6)
N(3)-Eu(1)-N(5)	99.12(6)	C(19)-Eu(1)-C(17)	165.75(6)
O(5)-Eu(1)-N(4)	139.51(5)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Bond lengths [Å] and angles [°] for MLC19 (CCDC 763335).

Eu(1)-O(5)	2.3674(15)	C(24)-C(25)	1.492(3)
Eu(1)-O(7)	2.3836(14)	C(25)-C(26)	1.484(3)
Eu(1)-O(3)	2.4004(12)	C(26)-C(27)	1.506(5)
Eu(1)-O(1)	2.4059(11)	C(28)-C(29)	1.503(3)
Eu(1)-N(1)	2.5085(16)	C(29)-C(30)	1.483(3)
Eu(1)-N(3)	2.5904(16)	C(30)-C(31)	1.465(4)
Eu(1)-N(5)	2.6055(16)	C(32)-C(33)	1.519(3)
Eu(1)-N(4)	2.6661(15)	C(33)-C(34)	1.492(4)
Eu(1)-N(2)	2.6724(16)	C(34)-C(35)	1.489(4)
Eu(1)-C(19)	3.256(2)	O(51)-C(52)	1.2294
Eu(1)-C(17)	3.259(2)	C(51)-C(52)	1.4697
O(1)-C(7)	1.253(2)	C(52)-C(53)	1.4999
O(2)-C(7)	1.247(2)	O(61)-C(62)	1.1945
O(3)-C(6)	1.254(2)	C(61)-C(62)	1.4162
O(4)-C(6)	1.242(2)	C(62)-C(63)	1.5608
O(5)-C(17)	1.271(2)		
O(6)-C(17)	1.224(2)	O(5)-Eu(1)-O(7)	146.00(5)
O(7)-C(19)	1.269(2)	O(5)-Eu(1)-O(3)	86.12(5)
O(8)-C(19)	1.232(2)	O(7)-Eu(1)-O(3)	79.73(5)
N(1)-C(5)	1.333(2)	O(5)-Eu(1)-O(1)	80.31(5)
N(1)-C(1)	1.334(2)	O(7)-Eu(1)-O(1)	84.61(4)
N(2)-C(8)	1.472(3)	O(3)-Eu(1)-O(1)	128.45(5)
N(2)-C(16)	1.474(3)	O(5)-Eu(1)-N(1)	73.42(5)
N(2)-C(15)	1.484(3)	O(7)-Eu(1)-N(1)	72.59(5)
N(3)-C(10)	1.468(3)	O(3)-Eu(1)-N(1)	64.11(4)
N(3)-C(9)	1.476(3)	O(1)-Eu(1)-N(1)	64.35(4)
N(4)-C(18)	1.470(3)	O(5)-Eu(1)-N(3)	73.97(5)
N(4)-C(12)	1.479(3)	O(7)-Eu(1)-N(3)	131.25(5)
N(4)-C(11)	1.495(2)	O(3)-Eu(1)-N(3)	77.47(5)
N(5)-C(14)	1.467(3)	O(1)-Eu(1)-N(3)	142.07(5)
N(5)-C(13)	1.474(3)	N(1)-Eu(1)-N(3)	130.47(5)
C(1)-C(2)	1.354(3)	O(5)-Eu(1)-N(5)	131.07(5)
C(1)-C(6)	1.524(3)	O(7)-Eu(1)-N(5)	73.64(5)
C(2)-C(3)	1.387(3)	O(3)-Eu(1)-N(5)	140.82(5)
C(3)-C(4)	1.373(3)	O(1)-Eu(1)-N(5)	77.34(5)
C(4)-C(5)	1.378(3)	N(1)-Eu(1)-N(5)	130.41(5)
C(5)-C(7)	1.510(3)	N(3)-Eu(1)-N(5)	99.12(6)
C(8)-C(9)	1.512(3)	O(5)-Eu(1)-N(4)	139.51(5)
C(10)-C(11)	1.494(3)	O(7)-Eu(1)-N(4)	65.77(5)
C(12)-C(13)	1.507(3)	O(3)-Eu(1)-N(4)	75.46(5)
C(14)-C(15)	1.508(3)	O(1)-Eu(1)-N(4)	138.90(5)
C(16)-C(17)	1.522(3)	N(1)-Eu(1)-N(4)	125.83(5)
C(18)-C(19)	1.525(3)	N(3)-Eu(1)-N(4)	67.03(5)
N(6)-C(32)	1.510(3)	N(5)-Eu(1)-N(4)	67.65(5)
N(6)-C(20)	1.511(3)	O(5)-Eu(1)-N(2)	65.94(5)
N(6)-C(24)	1.524(3)	O(7)-Eu(1)-N(2)	138.84(5)
N(6)-C(28)	1.529(2)	O(3)-Eu(1)-N(2)	139.95(5)
C(20)-C(21)	1.506(3)	O(1)-Eu(1)-N(2)	76.44(5)
C(21)-C(22)	1.477(3)	N(1)-Eu(1)-N(2)	127.12(5)
C(22)-C(23)	1.509(4)	N(3)-Eu(1)-N(2)	67.84(5)

N(5)-Eu(1)-N(2)	66.75(6)	N(1)-C(5)-C(4)	120.79(19)
N(4)-Eu(1)-N(2)	107.05(6)	N(1)-C(5)-C(7)	114.04(18)
O(5)-Eu(1)-C(19)	150.44(5)	C(4)-C(5)-C(7)	125.17(18)
O(7)-Eu(1)-C(19)	19.03(4)	O(4)-C(6)-O(3)	127.5(2)
O(3)-Eu(1)-C(19)	68.32(5)	O(4)-C(6)-C(1)	116.7(2)
O(1)-Eu(1)-C(19)	103.63(5)	O(3)-C(6)-C(1)	115.87(16)
N(1)-Eu(1)-C(19)	81.90(5)	O(2)-C(7)-O(1)	126.47(19)
N(3)-Eu(1)-C(19)	112.55(5)	O(2)-C(7)-C(5)	116.9(2)
N(5)-Eu(1)-C(19)	77.67(5)	O(1)-C(7)-C(5)	116.67(16)
N(4)-Eu(1)-C(19)	49.30(5)	N(2)-C(8)-C(9)	113.52(18)
N(2)-Eu(1)-C(19)	143.62(5)	N(3)-C(9)-C(8)	110.76(19)
O(5)-Eu(1)-C(17)	18.76(5)	N(3)-C(10)-C(11)	109.99(18)
O(7)-Eu(1)-C(17)	151.34(5)	N(4)-C(11)-C(10)	111.92(16)
O(3)-Eu(1)-C(17)	104.77(5)	N(4)-C(12)-C(13)	113.12(17)
O(1)-Eu(1)-C(17)	70.33(5)	N(5)-C(13)-C(12)	110.62(18)
N(1)-Eu(1)-C(17)	83.86(6)	N(5)-C(14)-C(15)	109.97(19)
N(3)-Eu(1)-C(17)	76.70(5)	N(2)-C(15)-C(14)	112.03(16)
N(5)-Eu(1)-C(17)	112.44(5)	N(2)-C(16)-C(17)	114.37(15)
N(4)-Eu(1)-C(17)	142.89(5)	O(6)-C(17)-O(5)	124.6(2)
N(2)-Eu(1)-C(17)	49.03(6)	O(6)-C(17)-C(16)	118.24(17)
C(19)-Eu(1)-C(17)	165.75(6)	O(5)-C(17)-C(16)	117.17(19)
C(7)-O(1)-Eu(1)	124.96(11)	O(6)-C(17)-Eu(1)	158.82(17)
C(6)-O(3)-Eu(1)	125.81(12)	O(5)-C(17)-Eu(1)	36.80(10)
C(17)-O(5)-Eu(1)	124.44(13)	C(16)-C(17)-Eu(1)	81.03(12)
C(19)-O(7)-Eu(1)	123.21(12)	N(4)-C(18)-C(19)	115.07(15)
C(5)-N(1)-C(1)	120.16(18)	O(8)-C(19)-O(7)	125.14(19)
C(5)-N(1)-Eu(1)	119.63(12)	O(8)-C(19)-C(18)	117.70(17)
C(1)-N(1)-Eu(1)	120.21(12)	O(7)-C(19)-C(18)	117.13(19)
C(8)-N(2)-C(16)	110.77(19)	O(8)-C(19)-Eu(1)	157.45(15)
C(8)-N(2)-C(15)	110.44(17)	O(7)-C(19)-Eu(1)	37.76(10)
C(16)-N(2)-C(15)	110.23(15)	C(18)-C(19)-Eu(1)	81.03(12)
C(8)-N(2)-Eu(1)	110.75(11)	C(32)-N(6)-C(20)	111.29(18)
C(16)-N(2)-Eu(1)	105.29(12)	C(32)-N(6)-C(24)	106.86(15)
C(15)-N(2)-Eu(1)	109.25(13)	C(20)-N(6)-C(24)	110.81(16)
C(10)-N(3)-C(9)	112.69(17)	C(32)-N(6)-C(28)	111.00(16)
C(10)-N(3)-Eu(1)	115.57(14)	C(20)-N(6)-C(28)	106.97(14)
C(9)-N(3)-Eu(1)	112.42(11)	C(24)-N(6)-C(28)	109.94(17)
C(18)-N(4)-C(12)	111.21(18)	C(21)-C(20)-N(6)	115.17(16)
C(18)-N(4)-C(11)	110.09(15)	C(22)-C(21)-C(20)	111.6(2)
C(12)-N(4)-C(11)	110.38(16)	C(21)-C(22)-C(23)	113.8(2)
C(18)-N(4)-Eu(1)	105.64(11)	C(25)-C(24)-N(6)	115.90(17)
C(12)-N(4)-Eu(1)	110.89(11)	C(26)-C(25)-C(24)	111.6(2)
C(11)-N(4)-Eu(1)	108.49(12)	C(25)-C(26)-C(27)	113.1(3)
C(14)-N(5)-C(13)	112.64(17)	C(29)-C(28)-N(6)	116.35(17)
C(14)-N(5)-Eu(1)	115.69(14)	C(30)-C(29)-C(28)	113.0(2)
C(13)-N(5)-Eu(1)	112.20(11)	C(31)-C(30)-C(29)	116.5(3)
N(1)-C(1)-C(2)	121.95(19)	N(6)-C(32)-C(33)	116.40(17)
N(1)-C(1)-C(6)	113.48(18)	C(34)-C(33)-C(32)	111.48(19)
C(2)-C(1)-C(6)	124.57(19)	C(35)-C(34)-C(33)	115.9(2)
C(1)-C(2)-C(3)	118.7(2)	O(51)-C(52)-C(51)	115.8
C(4)-C(3)-C(2)	119.3(2)	O(51)-C(52)-C(53)	124.0
C(3)-C(4)-C(5)	119.1(2)	C(51)-C(52)-C(53)	120.1

O(61)-C(62)-C(61)	127.3
O(61)-C(62)-C(63)	112.2
C(61)-C(62)-C(63)	119.9

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for MLC19 (CCDC 763335). 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}
Eu(1)	375(1)	444(1)	371(1)	25(1)	26(1)	-2(1)
O(1)	593(10)	519(9)	406(6)	-13(6)	-48(6)	60(7)
O(2)	1034(15)	840(12)	486(8)	-184(7)	-161(9)	48(10)
O(3)	526(10)	569(9)	445(7)	63(6)	-44(6)	-20(7)
O(4)	964(15)	871(12)	599(9)	311(8)	-150(9)	18(10)
O(5)	455(9)	611(9)	465(7)	88(6)	78(6)	19(7)
O(6)	603(11)	867(12)	526(8)	-21(7)	157(7)	30(8)
O(7)	437(9)	611(9)	415(6)	-37(6)	44(6)	-62(7)
O(8)	527(10)	573(9)	502(7)	78(6)	99(6)	7(7)
N(1)	424(10)	491(10)	414(8)	30(6)	82(7)	13(8)
N(2)	502(12)	539(11)	537(9)	110(8)	21(8)	8(9)
N(3)	421(11)	541(11)	584(9)	31(8)	-23(8)	-25(8)
N(4)	446(11)	553(11)	480(8)	-57(7)	32(7)	-36(9)
N(5)	423(11)	523(11)	589(9)	2(8)	-27(8)	42(8)
C(1)	466(13)	468(12)	574(11)	123(9)	91(9)	20(10)
C(2)	890(20)	563(16)	878(16)	146(13)	-42(15)	48(15)
C(3)	1150(30)	465(16)	1230(20)	-46(16)	-90(20)	17(16)
C(4)	910(20)	571(15)	755(15)	-153(12)	-41(14)	23(14)
C(5)	506(14)	525(13)	502(11)	-74(9)	91(9)	-8(10)
C(6)	434(14)	693(16)	499(11)	163(10)	26(9)	-10(12)
C(7)	487(14)	688(16)	414(10)	-54(10)	54(9)	38(11)
C(8)	663(18)	624(15)	744(14)	175(11)	47(12)	-125(13)
C(9)	442(14)	622(15)	768(14)	43(11)	22(11)	-132(11)
C(10)	530(16)	605(15)	784(15)	-125(12)	-62(12)	-100(12)
C(11)	584(16)	704(16)	530(11)	-155(10)	-16(11)	-87(12)
C(12)	600(16)	632(15)	658(13)	-123(11)	48(11)	16(12)
C(13)	458(14)	593(14)	732(13)	-38(11)	70(11)	108(11)
C(14)	567(17)	581(15)	793(15)	123(12)	-23(12)	68(12)
C(15)	624(17)	602(15)	651(13)	202(11)	-34(12)	68(12)
C(16)	601(16)	761(16)	499(11)	153(10)	72(10)	20(13)
C(17)	411(11)	658(13)	442(8)	-27(12)	16(7)	-93(13)
C(18)	564(15)	727(17)	441(9)	-60(9)	85(9)	-71(11)
C(19)	385(12)	511(12)	483(10)	34(9)	45(9)	70(10)
N(6)	567(13)	601(12)	498(9)	189(8)	4(8)	-18(9)
C(20)	637(16)	640(15)	603(12)	214(10)	-4(11)	-40(12)
C(21)	980(20)	685(18)	736(15)	79(12)	-45(14)	-144(16)
C(22)	1160(30)	830(20)	999(19)	-49(16)	12(18)	-172(19)
C(23)	1430(40)	980(20)	1160(20)	-152(18)	-90(20)	-170(20)
C(24)	604(16)	711(16)	560(11)	241(11)	-22(11)	44(12)
C(25)	654(19)	980(20)	744(15)	281(14)	-8(13)	101(15)
C(26)	720(30)	1780(40)	1360(30)	710(30)	40(20)	410(20)
C(27)	790(30)	2290(50)	2010(40)	740(40)	20(30)	360(30)
C(28)	673(17)	699(16)	489(11)	140(10)	6(10)	35(13)
C(29)	940(20)	766(19)	724(15)	54(13)	30(14)	-32(16)
C(30)	1240(30)	1140(30)	920(20)	-177(18)	-90(20)	20(20)

C(31)	2150(50)	1170(30)	1460(30)	-490(30)	-230(30)	-190(30)
C(32)	657(17)	680(15)	520(11)	169(10)	29(11)	-44(13)
C(33)	641(18)	832(18)	714(14)	259(13)	81(13)	60(14)
C(34)	700(20)	1060(20)	897(18)	302(16)	175(15)	106(17)
C(35)	850(30)	1580(40)	1440(30)	240(20)	370(20)	270(20)

Table 6. Hydrogen bonds for MLC19 (CCDC 763335) [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(3)-H(3)...O(5)#1	0.91	2.30	3.115(2)	148.2
N(3)-H(3)...O(6)#1	0.91	2.53	3.284(2)	140.7
N(5)-H(5)...O(7)#2	0.91	2.30	3.108(2)	148.0
N(5)-H(5)...O(8)#2	0.91	2.47	3.2522(18)	144.3
O(41)-H(41A)...O(8)#3	0.76	2.04	2.795(2)	173.1
O(41)-H(41B)...O(2)#1	0.74	2.16	2.897(2)	176.5
O(42)-H(42A)...O(6)	0.77	2.11	2.859(3)	164.3
O(42)-H(42B)...O(4)#1	0.81	2.12	2.913(2)	168.7
O(44)-H(44A)...O(42)#4	0.83	2.88	3.70(4)	171.4

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