Supplemental Material

The Lanthanide Complexes of 2,2'-Bipyridyl-6,6'-dicarboxylic Dimethylanilides: the Influence of Secondary Coordination Sphere on the Stability, Structure, Luminescence and f-Elements Extraction

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Stability constants

Table 1. Log β_1 values for the binding of trivalent lanthanides ions with all ligands (***1-5***) in "dry" (30 ppm of water) acetonitrile

Ln^{3+} / L	La	Ce	Pr	Nd	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
BPDA	6.2 ±0.2	5.6 ±0.1	5.9 ±0.1	5.9 ±0.1	5.7 ±0.1	5.6 ±0.1	5.7 ±0.1	5.7 ±0.1	5.7 ±0.1	5.7 ±0.2	5.4 ±0.1	5.9 ±0.2	5.6 ±0.2	5.5 ±0.2
2.5-diMe	6.11 ±0.03	6.42 ±0.04	6.59 ±0.03	6.82 ±0.04	6.71 ±0.08	6.40 ±0.05	6.30 ±0.04	6.76 ±0.05	6.9 ±0.2	7.1 ±0.1	6.7 ±0.2	6.33 ±0.05	6.5 ±0.2	6.85 ±0.08
2.4-diMe	6.45 ±0.02	6.41 ±0.05	7.11 ±0.09	7.36 ±0.03	6.96 ±0.05	6.7 ±0.2	6.59 ±0.05	6.63 ±0.05	6.98 ±0.04	7.10 ±0.05	7.29 ±0.07	6.91 ±0.05	7.05 ±0.08	7.49 ±0.04
3.5-diMe	6.00 ±0.02	6.51 ±0.01	7.19 ±0.03	7.6 ±0.2	6.89 ±0.05	6.86 ±0.02	6.69 ±0.02	7.44 ±0.08	7.4 ±0.2	7.2 ±0.2	7.3 ±0.2	7.23 ±0.04	6.86 ±0.09	7.65 ±0.09
3.4-diMe	5.60 ±0.02	6.91 ±0.01	7.6 ±0.1	8.3 ±0.1	7.6 ±0.1	6.87 ±0.07	6.76 ±0.03	8.0 ±0.1	8.9 ±0.1	8.40 ±0.08	7.35 ±0.03	7.28 ±0.07	6.9 ±0.2	6.7 ±0.2

Table 2. Log β_1 values for the binding of trivalent lanthanides ions with all ligands (***2-3***) in "wet" (400 ppm of water) acetonitrile

Ln^{3+} / L	La	Ce	Pr	Nd	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
2.5-diMe	4.6 ±0.3	5.0 ±0.1	4.7 ±0.1	4.83 ±0.03	4.5 ±0.2		4.87 ±0.06		4.69 ±0.07	4.81 ±0.06	4.5 ±0.2		5.08 ±0.02	
2.4-diMe	4.83 ±0.03		4.85 ±0.06	4.5 ±0.3	4.4 ±0.1	5.02 ±0.02	4.63 ±0.06	4.59 ±0.08						

X-Ray Data

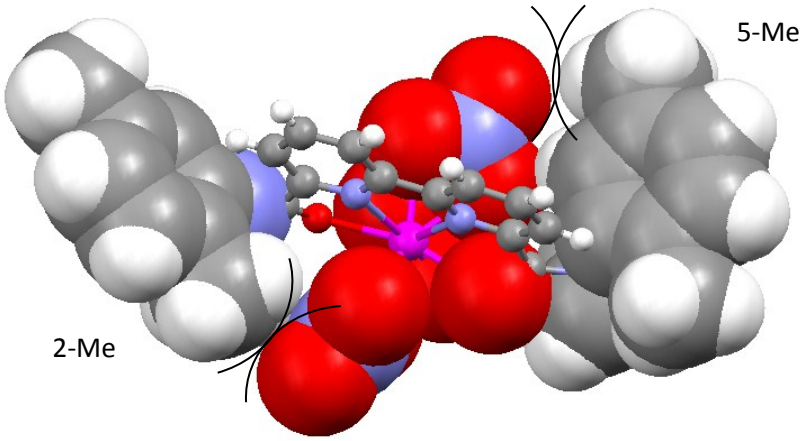


Figure 1. Spacefill representation of 2,5-diMeGd$(NO_3)_3$ complex with pointed sterical hindrance of methyl-groups with nitrate-counterions

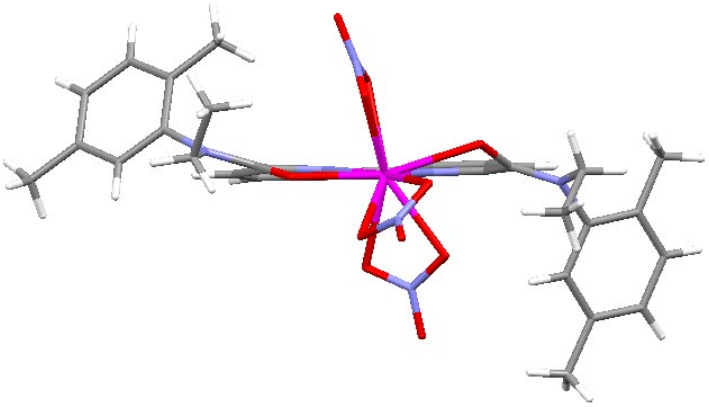


Figure 2. The deviation of oxygen atom of one of carboxamidic groups from bipyridyl plane for 2,5-diMeGd$(NO_3)_3$ complex.

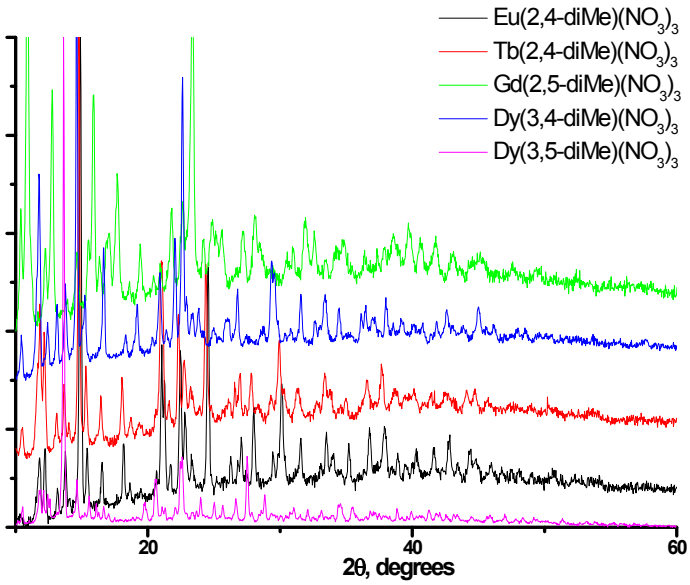


Figure 3. The XRD spectra of diMe complexes.

Table 1 Comparison of the interatomic distances (Å) and angles (°) in the coordination sphere of the metal ions for complexes with BPDAs ligands

	HNd[1]	**H**Pr[1]	**H**Gd[1]	**H**Tb[1]	**3,4diMe** Dy	**3,5diMe Dy**	**2,4diMe Eu**	**2,4diMe Tb**
Ln-O(1)	2.481	2.490	2.414	2.402	2.397(2)	2.323(2)	2.422(5)	2.404(6)
Ln-O(1')	2.409	2.414	2.346	2.325	2.333(3)	2.390(2)	2.389(5)	2.359(6)
Ln-O(1N)	2.570	2.582	2.513	2.495	2.505(2)	2.463(2)	2.494(5)	2.480(6)
Ln-O(2N)	2.575	2.589	2.519	2.529	2.479(3)	2.466(2)	2.525(6)	2.540(6)
Ln-O(4N)	2.525	2.542	2.492	2.474	2.431(3)	2.526(2)	2.491(5)	2.457(6)
ln-O(5N)	2.525	2.544	2.498	2.475	2.480(3)	2.415(2)	2.504(6)	2.492(7)
Ln-O(7N)	2.535	2.552	2.474	2.457	2.384(4)	2.489(2)	2.44(1)	2.42(2)
Ln-O(8N)	2.535	2.551	2.478	2.477	2.804(7)	2.468(2)	2.56(1)	2.53(1)
Ln-N(2)	2.605	2.623	2.530	2.514	2.475(3)	2.581(2)	2.555(5)	2.518(6)
Ln-N(2')	2.683	2.694	2.625	2.611	2.496(2)	2.481(2)	2.572(6)	2.507(6)
O1 C7	1.255	1.261	1.251	1.254	1.252(4)	1.250(4)	1.266(8)	1.25(1)
O1' C7'	1.246	1.250	1.245	1.246	1.275(4)	1.258(4)	1.24(1)	1.25(1)
N2C1-C1'N2'	5.01	4.57	12.79	11.07	-4.2(4)	15.5(4)	4.9(8)	7(1)
O(1)C(7)-C(3)N(2)	25.42	25.26	28.47	28.86	21.6(4)	-16.5(4)	-23.1(8)	22(1)
O(1')C(7')-C(3')N(2')	7.54	7.85	7.7	7.21	20.9(4)	-31.7(4)	-18.7(9)	-19(1)
delta(C=O)	0.072	0.076	0.068	0.077	0.064	0.067	0.033	0.045
delta(py)	0.078	0.071	0.095	0.097	0.021	0.100	0.017	0.011

Table 2. Crystal data and structure refinement for 2,5diMeGd**.**

Identification code	a	
Empirical formula	C36 H40 Gd N9 O11	
Formula weight	932.02	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.4044(3) Å	α= 71.4040(10)°.
	b = 13.4377(5) Å	β= 86.0310(10)°.
	c = 16.6972(6) Å	γ = 77.4430(10)°.
Volume	1952.08(12) $Å^3$	
Z	2	
Density (calculated)	1.586 Mg/m^3	
Absorption coefficient	1.770 mm^{-1}	
F(000)	942	
Crystal size	0.211 x 0.143 x 0.096 mm^3	
Theta range for data collection	1.634 to 30.000°.	
Index ranges	-13<=h<=13, -18<=k<=18, -23<=l<=23	
Reflections collected	25328	
Independent reflections	11368 [R(int) = 0.0190]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.858 and 0.692	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11368 / 0 / 522	
Goodness-of-fit on F^2	1.015	
Final R indices [I>2sigma(I)]	R1 = 0.0204, wR2 = 0.0480	
R indices (all data)	R1 = 0.0234, wR2 = 0.0492	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.678 and -0.409 e. $Å^{-3}$	

Table 3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 2,5diMeGd. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Gd(01)	2851(1)	4288(1)	2905(1)	12(1)
O(1)	4180(1)	5375(1)	1896(1)	18(1)
O(2)	825(1)	3503(1)	3684(1)	15(1)
N(1)	4833(2)	6931(1)	1179(1)	16(1)
N(2)	3772(1)	5760(1)	3326(1)	13(1)
N(3)	2348(1)	4399(1)	4416(1)	12(1)

N(4)	620(1)	2154(1)	4891(1)	15(1)
C(1)	4502(2)	6229(1)	1897(1)	15(1)
C(2)	5015(2)	6596(1)	406(1)	23(1)
C(3)	3609(2)	6784(2)	-53(1)	40(1)
C(4)	4981(2)	8002(1)	1106(1)	16(1)
C(5)	6380(2)	8224(1)	965(1)	18(1)
C(6)	6610(2)	9224(1)	933(1)	19(1)
C(6A)	8124(2)	9460(2)	792(1)	25(1)
C(7)	5408(2)	9983(1)	1041(1)	21(1)
C(8)	4017(2)	9761(1)	1165(1)	22(1)
C(9)	3762(2)	8761(1)	1194(1)	18(1)
C(9A)	2250(2)	8539(2)	1314(1)	25(1)
C(10)	4500(2)	6417(1)	2746(1)	14(1)
C(11)	5200(2)	7119(1)	2948(1)	17(1)
C(12)	5083(2)	7169(1)	3770(1)	17(1)
C(13)	4286(2)	6528(1)	4359(1)	16(1)
C(14)	3652(2)	5823(1)	4114(1)	13(1)
C(15)	993(2)	3090(1)	4465(1)	14(1)
C(16)	-49(2)	1623(1)	4403(1)	19(1)
C(17)	1070(2)	1012(2)	3942(1)	26(1)
C(18)	1252(2)	1464(1)	5699(1)	15(1)
C(19)	2752(2)	1067(1)	5736(1)	17(1)
C(20)	3414(2)	352(1)	6482(1)	19(1)
C(20A)	5040(2)	-62(2)	6523(1)	27(1)
C(21)	2522(2)	23(1)	7175(1)	22(1)
C(22)	1023(2)	415(1)	7133(1)	22(1)
C(23)	354(2)	1155(1)	6396(1)	18(1)
C(23A)	-1260(2)	1612(1)	6383(1)	24(1)
C(24)	1549(2)	3726(1)	4925(1)	13(1)
C(25)	1143(2)	3737(1)	5741(1)	16(1)
C(26)	1580(2)	4481(1)	6037(1)	16(1)
C(27)	2403(2)	5175(1)	5521(1)	16(1)
C(28)	2776(2)	5108(1)	4711(1)	13(1)
N(1N)	3483(2)	2762(1)	1948(1)	22(1)
N(2N)	657(2)	6018(1)	1897(1)	23(1)
N(3N)	5126(2)	2637(1)	3970(1)	17(1)
O(1N)	4441(1)	3239(1)	2069(1)	25(1)
O(2N)	2248(1)	2969(1)	2283(1)	24(1)
O(3N)	3741(2)	2141(1)	1529(1)	34(1)
O(4N)	1203(1)	5198(1)	1669(1)	25(1)
O(5N)	1015(1)	5967(1)	2638(1)	21(1)
O(6N)	-133(2)	6805(1)	1442(1)	38(1)
O(7N)	5319(1)	3592(1)	3608(1)	19(1)
O(8N)	3874(1)	2472(1)	3881(1)	18(1)
O(9N)	6083(1)	1931(1)	4386(1)	29(1)
N(1S)	-173(3)	8468(2)	-978(1)	51(1)
N(2S)	7717(2)	5090(2)	2151(2)	54(1)
C(1S)	-351(2)	7606(2)	-720(1)	37(1)
C(2S)	-554(3)	6499(2)	-397(2)	42(1)
C(3S)	7896(2)	4203(2)	2214(1)	40(1)
C(4S)	8122(3)	3063(2)	2300(2)	48(1)

Table 4. Bond lengths [Å] and angles [°] for 2,5diMeGd.

Gd(01)-O(1)	2.3383(11)	N(1)-C(2)	1.485(2)
Gd(01)-O(5N)	2.4592(12)	N(2)-C(14)	1.3403(19)
Gd(01)-O(2)	2.4680(11)	N(2)-C(10)	1.3456(19)
Gd(01)-O(4N)	2.4827(12)	N(3)-C(28)	1.3432(19)
Gd(01)-O(8N)	2.4885(11)	N(3)-C(24)	1.3493(19)
Gd(01)-O(1N)	2.4932(12)	N(4)-C(15)	1.3410(19)
Gd(01)-O(2N)	2.4968(12)	N(4)-C(18)	1.4509(19)
Gd(01)-O(7N)	2.5239(12)	N(4)-C(16)	1.485(2)
Gd(01)-N(3)	2.5810(12)	C(1)-C(10)	1.518(2)
Gd(01)-N(2)	2.6229(12)	C(2)-C(3)	1.507(3)
Gd(01)-N(2N)	2.8977(14)	C(2)-H(2A)	0.9900
Gd(01)-N(1N)	2.9226(14)	C(2)-H(2B)	0.9900
O(1)-C(1)	1.2492(18)	C(3)-H(3A)	0.9800
O(2)-C(15)	1.2499(18)	C(3)-H(3B)	0.9800
N(1)-C(1)	1.3331(19)	C(3)-H(3C)	0.9800
N(1)-C(4)	1.442(2)	C(4)-C(9)	1.393(2)

C(4)-C(5)	1.399(2)	C(2S)-H(2SB)	0.9800
C(5)-C(6)	1.391(2)	C(2S)-H(2SC)	0.9800
C(5)-H(5A)	0.9500	C(3S)-C(4S)	1.461(4)
C(6)-C(7)	1.392(2)	C(4S)-H(4SA)	0.9800
C(6)-C(6A)	1.512(2)	C(4S)-H(4SB)	0.9800
C(6A)-H(6AA)	0.9800	C(4S)-H(4SC)	0.9800
C(6A)-H(6AB)	0.9800		
C(6A)-H(6AC)	0.9800	O(1)-Gd(01)-O(5N)	83.03(4)
C(7)-C(8)	1.391(2)	O(1)-Gd(01)-O(2)	162.29(4)
C(7)-H(7A)	0.9500	O(5N)-Gd(01)-O(2)	82.58(4)
C(8)-C(9)	1.401(2)	O(1)-Gd(01)-O(4N)	74.50(4)
C(8)-H(8A)	0.9500	O(5N)-Gd(01)-O(4N)	51.82(4)
C(9)-C(9A)	1.503(2)	O(2)-Gd(01)-O(4N)	88.47(4)
C(9A)-H(9AA)	0.9800	O(1)-Gd(01)-O(8N)	125.36(4)
C(9A)-H(9AB)	0.9800	O(5N)-Gd(01)-O(8N)	148.36(4)
C(9A)-H(9AC)	0.9800	O(2)-Gd(01)-O(8N)	71.38(4)
C(10)-C(11)	1.393(2)	O(4N)-Gd(01)-O(8N)	141.44(4)
C(11)-C(12)	1.391(2)	O(1)-Gd(01)-O(1N)	69.26(4)
C(11)-H(11A)	0.9500	O(5N)-Gd(01)-O(1N)	138.07(4)
C(12)-C(13)	1.382(2)	O(2)-Gd(01)-O(1N)	116.38(4)
C(12)-H(12A)	0.9500	O(4N)-Gd(01)-O(1N)	89.72(4)
C(13)-C(14)	1.395(2)	O(8N)-Gd(01)-O(1N)	71.77(4)
C(13)-H(13A)	0.9500	O(1)-Gd(01)-O(2N)	107.61(4)
C(14)-C(28)	1.488(2)	O(5N)-Gd(01)-O(2N)	114.28(4)
C(15)-C(24)	1.505(2)	O(2)-Gd(01)-O(2N)	69.44(4)
C(16)-C(17)	1.513(2)	O(4N)-Gd(01)-O(2N)	68.69(4)
C(16)-H(16A)	0.9900	O(8N)-Gd(01)-O(2N)	73.45(4)
C(16)-H(16B)	0.9900	O(1N)-Gd(01)-O(2N)	51.23(4)
C(17)-H(17A)	0.9800	O(1)-Gd(01)-O(7N)	81.04(4)
C(17)-H(17B)	0.9800	O(5N)-Gd(01)-O(7N)	134.97(4)
C(17)-H(17C)	0.9800	O(2)-Gd(01)-O(7N)	116.54(4)
C(18)-C(19)	1.394(2)	O(4N)-Gd(01)-O(7N)	153.62(4)
C(18)-C(23)	1.395(2)	O(8N)-Gd(01)-O(7N)	51.15(4)
C(19)-C(20)	1.395(2)	O(1N)-Gd(01)-O(7N)	72.24(4)
C(19)-H(19A)	0.9500	O(2N)-Gd(01)-O(7N)	110.66(4)
C(20)-C(21)	1.393(2)	O(1)-Gd(01)-N(3)	123.91(4)
C(20)-C(20A)	1.508(2)	O(5N)-Gd(01)-N(3)	78.64(4)
C(20A)-H(20A)	0.9800	O(2)-Gd(01)-N(3)	62.80(4)
C(20A)-H(20B)	0.9800	O(4N)-Gd(01)-N(3)	126.19(4)
C(20A)-H(20C)	0.9800	O(8N)-Gd(01)-N(3)	73.68(4)
C(21)-C(22)	1.391(3)	O(1N)-Gd(01)-N(3)	143.02(4)
C(21)-H(21A)	0.9500	O(2N)-Gd(01)-N(3)	128.30(4)
C(22)-C(23)	1.398(2)	O(7N)-Gd(01)-N(3)	76.09(4)
C(22)-H(22A)	0.9500	O(1)-Gd(01)-N(2)	62.57(4)
C(23)-C(23A)	1.508(2)	O(5N)-Gd(01)-N(2)	67.63(4)
C(23A)-H(23A)	0.9800	O(2)-Gd(01)-N(2)	120.34(4)
C(23A)-H(23B)	0.9800	O(4N)-Gd(01)-N(2)	108.21(4)
C(23A)-H(23C)	0.9800	O(8N)-Gd(01)-N(2)	110.34(4)
C(24)-C(25)	1.392(2)	O(1N)-Gd(01)-N(2)	120.37(4)
C(25)-C(26)	1.390(2)	O(2N)-Gd(01)-N(2)	170.06(4)
C(25)-H(25A)	0.9500	O(7N)-Gd(01)-N(2)	67.62(4)
C(26)-C(27)	1.386(2)	N(3)-Gd(01)-N(2)	61.40(4)
C(26)-H(26A)	0.9500	O(1)-Gd(01)-N(2N)	75.52(4)
C(27)-C(28)	1.400(2)	O(5N)-Gd(01)-N(2N)	26.07(4)
C(27)-H(27A)	0.9500	O(2)-Gd(01)-N(2N)	87.05(4)
N(1N)-O(3N)	1.2255(18)	O(4N)-Gd(01)-N(2N)	25.89(4)
N(1N)-O(2N)	1.2685(19)	O(8N)-Gd(01)-N(2N)	157.18(4)
N(1N)-O(1N)	1.2742(19)	O(1N)-Gd(01)-N(2N)	113.47(4)
N(2N)-O(6N)	1.2128(19)	O(2N)-Gd(01)-N(2N)	92.38(4)
N(2N)-O(4N)	1.271(2)	O(7N)-Gd(01)-N(2N)	151.23(4)
N(2N)-O(5N)	1.2816(19)	N(3)-Gd(01)-N(2N)	103.48(4)
N(3N)-O(9N)	1.2194(18)	N(2)-Gd(01)-N(2N)	86.68(4)
N(3N)-O(8N)	1.2716(17)	O(1)-Gd(01)-N(1N)	88.16(4)
N(3N)-O(7N)	1.2789(17)	O(5N)-Gd(01)-N(1N)	129.46(4)
N(1S)-C(1S)	1.146(3)	O(2)-Gd(01)-N(1N)	93.06(4)
N(2S)-C(3S)	1.139(3)	O(4N)-Gd(01)-N(1N)	77.84(4)
C(1S)-C(2S)	1.461(3)	O(8N)-Gd(01)-N(1N)	71.04(4)
C(2S)-H(2SA)	0.9800	O(1N)-Gd(01)-N(1N)	25.68(4)

O(2N)-Gd(01)-N(1N)	25.55(4)
O(7N)-Gd(01)-N(1N)	91.82(4)
N(3)-Gd(01)-N(1N)	142.22(4)
N(2)-Gd(01)-N(1N)	145.73(4)
N(2N)-Gd(01)-N(1N)	103.73(4)
C(1)-O(1)-Gd(01)	128.27(10)
C(15)-O(2)-Gd(01)	115.90(9)
C(1)-N(1)-C(4)	123.93(13)
C(1)-N(1)-C(2)	117.75(13)
C(4)-N(1)-C(2)	118.30(12)
C(14)-N(2)-C(10)	118.96(13)
C(14)-N(2)-Gd(01)	122.38(9)
C(10)-N(2)-Gd(01)	118.41(9)
C(28)-N(3)-C(24)	118.56(13)
C(28)-N(3)-Gd(01)	124.25(10)
C(24)-N(3)-Gd(01)	117.13(9)
C(15)-N(4)-C(18)	123.40(13)
C(15)-N(4)-C(16)	117.41(13)
C(18)-N(4)-C(16)	115.74(12)
O(1)-C(1)-N(1)	120.73(14)
O(1)-C(1)-C(10)	116.85(13)
N(1)-C(1)-C(10)	122.42(13)
N(1)-C(2)-C(3)	113.80(16)
N(1)-C(2)-H(2A)	108.8
C(3)-C(2)-H(2A)	108.8
N(1)-C(2)-H(2B)	108.8
C(3)-C(2)-H(2B)	108.8
H(2A)-C(2)-H(2B)	107.7
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(9)-C(4)-C(5)	122.62(15)
C(9)-C(4)-N(1)	119.91(14)
C(5)-C(4)-N(1)	117.46(14)
C(6)-C(5)-C(4)	120.35(15)
C(6)-C(5)-H(5A)	119.8
C(4)-C(5)-H(5A)	119.8
C(5)-C(6)-C(7)	117.71(15)
C(5)-C(6)-C(6A)	120.36(16)
C(7)-C(6)-C(6A)	121.93(15)
C(6)-C(6A)-H(6AA)	109.5
C(6)-C(6A)-H(6AB)	109.5
H(6AA)-C(6A)-H(6AB)	109.5
C(6)-C(6A)-H(6AC)	109.5
H(6AA)-C(6A)-H(6AC)	109.5
H(6AB)-C(6A)-H(6AC)	109.5
C(8)-C(7)-C(6)	121.53(16)
C(8)-C(7)-H(7A)	119.2
C(6)-C(7)-H(7A)	119.2
C(7)-C(8)-C(9)	121.56(16)
C(7)-C(8)-H(8A)	119.2
C(9)-C(8)-H(8A)	119.2
C(4)-C(9)-C(8)	116.20(15)
C(4)-C(9)-C(9A)	122.85(15)
C(8)-C(9)-C(9A)	120.95(15)
C(9)-C(9A)-H(9AA)	109.5
C(9)-C(9A)-H(9AB)	109.5
H(9AA)-C(9A)-H(9AB)	109.5
C(9)-C(9A)-H(9AC)	109.5
H(9AA)-C(9A)-H(9AC)	109.5
H(9AB)-C(9A)-H(9AC)	109.5
N(2)-C(10)-C(11)	122.20(14)
N(2)-C(10)-C(1)	110.85(13)
C(11)-C(10)-C(1)	126.87(14)
C(12)-C(11)-C(10)	118.33(14)
C(12)-C(11)-H(11A)	120.8
C(10)-C(11)-H(11A)	120.8
C(13)-C(12)-C(11)	119.61(14)
C(13)-C(12)-H(12A)	120.2
C(11)-C(12)-H(12A)	120.2
C(12)-C(13)-C(14)	118.63(14)
C(12)-C(13)-H(13A)	120.7
C(14)-C(13)-H(13A)	120.7
N(2)-C(14)-C(13)	122.18(14)
N(2)-C(14)-C(28)	115.96(13)
C(13)-C(14)-C(28)	121.86(13)
O(2)-C(15)-N(4)	122.42(14)
O(2)-C(15)-C(24)	116.91(13)
N(4)-C(15)-C(24)	120.55(13)
N(4)-C(16)-C(17)	112.59(13)
N(4)-C(16)-H(16A)	109.1
C(17)-C(16)-H(16A)	109.1
N(4)-C(16)-H(16B)	109.1
C(17)-C(16)-H(16B)	109.1
H(16A)-C(16)-H(16B)	107.8
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(19)-C(18)-C(23)	121.77(14)
C(19)-C(18)-N(4)	117.98(14)
C(23)-C(18)-N(4)	120.09(14)
C(18)-C(19)-C(20)	120.72(15)
C(18)-C(19)-H(19A)	119.6
C(20)-C(19)-H(19A)	119.6
C(21)-C(20)-C(19)	117.84(15)
C(21)-C(20)-C(20A)	121.55(15)
C(19)-C(20)-C(20A)	120.61(16)
C(20)-C(20A)-H(20A)	109.5
C(20)-C(20A)-H(20B)	109.5
H(20A)-C(20A)-H(20B)	109.5
C(20)-C(20A)-H(20C)	109.5
H(20A)-C(20A)-H(20C)	109.5
H(20B)-C(20A)-H(20C)	109.5
C(22)-C(21)-C(20)	121.20(15)
C(22)-C(21)-H(21A)	119.4
C(20)-C(21)-H(21A)	119.4
C(21)-C(22)-C(23)	121.38(16)
C(21)-C(22)-H(22A)	119.3
C(23)-C(22)-H(22A)	119.3
C(18)-C(23)-C(22)	117.05(15)
C(18)-C(23)-C(23A)	122.69(15)
C(22)-C(23)-C(23A)	120.23(15)
C(23)-C(23A)-H(23A)	109.5
C(23)-C(23A)-H(23B)	109.5
H(23A)-C(23A)-H(23B)	109.5
C(23)-C(23A)-H(23C)	109.5
H(23A)-C(23A)-H(23C)	109.5
H(23B)-C(23A)-H(23C)	109.5
N(3)-C(24)-C(25)	122.91(14)
N(3)-C(24)-C(15)	111.79(13)
C(25)-C(24)-C(15)	124.79(13)
C(26)-C(25)-C(24)	118.10(14)
C(26)-C(25)-H(25A)	121.0
C(24)-C(25)-H(25A)	121.0
C(27)-C(26)-C(25)	119.61(14)
C(27)-C(26)-H(26A)	120.2
C(25)-C(26)-H(26A)	120.2
C(26)-C(27)-C(28)	118.82(14)
C(26)-C(27)-H(27A)	120.6
C(28)-C(27)-H(27A)	120.6

N(3)-C(28)-C(27)	122.00(14)	N(1N)-O(1N)-Gd(01)	96.34(9)
N(3)-C(28)-C(14)	115.51(13)	N(1N)-O(2N)-Gd(01)	96.33(9)
C(27)-C(28)-C(14)	122.48(13)	N(2N)-O(4N)-Gd(01)	95.60(9)
O(3N)-N(1N)-O(2N)	122.05(15)	N(2N)-O(5N)-Gd(01)	96.43(9)
O(3N)-N(1N)-O(1N)	121.87(16)	N(3N)-O(7N)-Gd(01)	95.34(9)
O(2N)-N(1N)-O(1N)	116.08(13)	N(3N)-O(8N)-Gd(01)	97.24(9)
O(3N)-N(1N)-Gd(01)	178.53(12)	N(1S)-C(1S)-C(2S)	179.0(3)
O(2N)-N(1N)-Gd(01)	58.12(8)	C(1S)-C(2S)-H(2SA)	109.5
O(1N)-N(1N)-Gd(01)	57.98(8)	C(1S)-C(2S)-H(2SB)	109.5
O(6N)-N(2N)-O(4N)	122.55(16)	H(2SA)-C(2S)-H(2SB)	109.5
O(6N)-N(2N)-O(5N)	121.92(16)	C(1S)-C(2S)-H(2SC)	109.5
O(4N)-N(2N)-O(5N)	115.52(13)	H(2SA)-C(2S)-H(2SC)	109.5
O(6N)-N(2N)-Gd(01)	172.52(12)	H(2SB)-C(2S)-H(2SC)	109.5
O(4N)-N(2N)-Gd(01)	58.51(8)	N(2S)-C(3S)-C(4S)	179.6(3)
O(5N)-N(2N)-Gd(01)	57.50(8)	C(3S)-C(4S)-H(4SA)	109.5
O(9N)-N(3N)-O(8N)	122.07(14)	C(3S)-C(4S)-H(4SB)	109.5
O(9N)-N(3N)-O(7N)	121.83(14)	H(4SA)-C(4S)-H(4SB)	109.5
O(8N)-N(3N)-O(7N)	116.09(13)	C(3S)-C(4S)-H(4SC)	109.5
O(9N)-N(3N)-Gd(01)	177.26(11)	H(4SA)-C(4S)-H(4SC)	109.5
O(8N)-N(3N)-Gd(01)	57.29(7)	H(4SB)-C(4S)-H(4SC)	109.5
O(7N)-N(3N)-Gd(01)	58.93(7)		

Table 5. Anisotropic displacement parameters ($Å^2$x 10^3) for 2,5diMeGd. 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}
Gd(01)	14(1)	11(1)	10(1)	-4(1)	1(1)	-4(1)
O(1)	25(1)	17(1)	14(1)	-6(1)	3(1)	-11(1)
O(2)	16(1)	15(1)	14(1)	-3(1)	-1(1)	-4(1)
N(1)	21(1)	17(1)	12(1)	-4(1)	2(1)	-8(1)
N(2)	15(1)	11(1)	12(1)	-4(1)	0(1)	-3(1)
N(3)	12(1)	11(1)	13(1)	-3(1)	0(1)	-2(1)
N(4)	16(1)	14(1)	15(1)	-4(1)	-1(1)	-5(1)
C(1)	16(1)	15(1)	14(1)	-3(1)	1(1)	-5(1)
C(2)	36(1)	24(1)	14(1)	-7(1)	7(1)	-14(1)
C(3)	44(1)	59(1)	24(1)	-17(1)	-2(1)	-21(1)
C(4)	21(1)	15(1)	12(1)	-2(1)	0(1)	-6(1)
C(5)	20(1)	19(1)	14(1)	-3(1)	2(1)	-6(1)
C(6)	25(1)	21(1)	13(1)	-3(1)	0(1)	-10(1)
C(6A)	25(1)	26(1)	26(1)	-8(1)	1(1)	-12(1)
C(7)	30(1)	17(1)	17(1)	-3(1)	-2(1)	-7(1)
C(8)	26(1)	21(1)	18(1)	-7(1)	-2(1)	1(1)
C(9)	20(1)	20(1)	13(1)	-2(1)	-1(1)	-4(1)
C(9A)	20(1)	29(1)	24(1)	-7(1)	2(1)	-6(1)
C(10)	15(1)	13(1)	14(1)	-3(1)	0(1)	-3(1)
C(11)	19(1)	14(1)	16(1)	-2(1)	-1(1)	-6(1)
C(12)	19(1)	14(1)	19(1)	-5(1)	-4(1)	-5(1)
C(13)	17(1)	15(1)	15(1)	-6(1)	-2(1)	-3(1)
C(14)	13(1)	11(1)	14(1)	-4(1)	-1(1)	-2(1)
C(15)	11(1)	14(1)	17(1)	-5(1)	2(1)	-2(1)
C(16)	21(1)	20(1)	19(1)	-4(1)	-3(1)	-11(1)
C(17)	35(1)	22(1)	29(1)	-13(1)	3(1)	-13(1)
C(18)	18(1)	11(1)	15(1)	-3(1)	-2(1)	-4(1)
C(19)	18(1)	14(1)	19(1)	-6(1)	1(1)	-4(1)
C(20)	21(1)	14(1)	22(1)	-7(1)	-6(1)	-1(1)
C(20A)	22(1)	22(1)	34(1)	-9(1)	-8(1)	2(1)
C(21)	29(1)	18(1)	18(1)	-2(1)	-7(1)	-3(1)
C(22)	30(1)	21(1)	16(1)	-4(1)	2(1)	-8(1)
C(23)	20(1)	15(1)	19(1)	-6(1)	2(1)	-5(1)
C(23A)	20(1)	24(1)	26(1)	-7(1)	4(1)	-4(1)
C(24)	12(1)	12(1)	14(1)	-4(1)	0(1)	-2(1)
C(25)	16(1)	15(1)	15(1)	-4(1)	2(1)	-2(1)
C(26)	18(1)	18(1)	13(1)	-6(1)	2(1)	-1(1)
C(27)	17(1)	16(1)	15(1)	-7(1)	0(1)	-3(1)
C(28)	13(1)	11(1)	14(1)	-4(1)	-2(1)	-1(1)
N(1N)	37(1)	16(1)	13(1)	-6(1)	3(1)	-7(1)
N(2N)	19(1)	21(1)	25(1)	-1(1)	-4(1)	-6(1)
N(3N)	19(1)	18(1)	16(1)	-8(1)	-1(1)	-1(1)
O(1N)	32(1)	24(1)	24(1)	-12(1)	9(1)	-11(1)
O(2N)	27(1)	26(1)	24(1)	-14(1)	1(1)	-8(1)

O(3N)	57(1)	25(1)	27(1)	-18(1)	9(1)	-11(1)
O(4N)	27(1)	27(1)	22(1)	-9(1)	-5(1)	-3(1)
O(5N)	20(1)	21(1)	20(1)	-6(1)	-1(1)	-2(1)
O(6N)	38(1)	26(1)	41(1)	1(1)	-20(1)	1(1)
O(7N)	21(1)	17(1)	19(1)	-6(1)	0(1)	-6(1)
O(8N)	18(1)	17(1)	20(1)	-6(1)	1(1)	-5(1)
O(9N)	26(1)	22(1)	34(1)	-7(1)	-11(1)	4(1)
N(1S)	60(1)	44(1)	52(1)	-20(1)	9(1)	-11(1)
N(2S)	36(1)	71(2)	61(2)	-29(1)	-3(1)	-9(1)
C(1S)	38(1)	41(1)	35(1)	-17(1)	2(1)	-4(1)
C(2S)	53(1)	40(1)	36(1)	-12(1)	-6(1)	-12(1)
C(3S)	23(1)	66(2)	33(1)	-23(1)	-2(1)	-1(1)
C(4S)	45(1)	62(2)	34(1)	-23(1)	-7(1)	8(1)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for 2,5diMeGd.

	x	y	z	U(eq)
H(2A)	5469	5822	565	28
H(2B)	5689	6994	17	28
H(3A)	3809	6552	-557	59
H(3B)	3157	7550	-222	59
H(3C)	2945	6373	321	59
H(5A)	7176	7689	891	22
H(6AA)	8483	9409	239	38
H(6AB)	8778	8938	1235	38
H(6AC)	8093	10186	812	38
H(7A)	5541	10668	1030	26
H(8A)	3220	10301	1232	27
H(9AA)	1549	9197	1311	37
H(9AB)	2195	7981	1856	37
H(9AC)	2020	8294	854	37
H(11A)	5745	7553	2534	20
H(12A)	5548	7641	3925	20
H(13A)	4173	6566	4919	19
H(16A)	-742	2174	3987	23
H(16B)	-605	1121	4794	23
H(17A)	577	675	3633	40
H(17B)	1751	457	4351	40
H(17C)	1608	1508	3543	40
H(19A)	3331	1286	5247	20
H(20A)	5490	331	6006	40
H(20B)	5254	-828	6578	40
H(20C)	5433	41	7013	40
H(21A)	2944	-479	7685	27
H(22A)	442	175	7616	27
H(23A)	-1649	1750	5820	35
H(23B)	-1432	2285	6520	35
H(23C)	-1747	1098	6801	35
H(25A)	585	3250	6085	19
H(26A)	1315	4513	6589	20
H(27A)	2709	5688	5714	19
H(2SA)	255	6056	-20	63
H(2SB)	-582	6222	-871	63
H(2SC)	-1473	6479	-83	63
H(4SA)	7603	2702	2801	72
H(4SB)	9166	2743	2361	72
H(4SC)	7750	2980	1797	72

Table 7. Torsion angles [°] for 2,5diMeGd.

Gd(01)-O(1)-C(1)-N(1)	-157.93(11)	C(9)-C(4)-C(5)-C(6)	2.0(2)
Gd(01)-O(1)-C(1)-C(10)	22.3(2)	N(1)-C(4)-C(5)-C(6)	-176.55(14)
C(4)-N(1)-C(1)-O(1)	169.43(15)	C(4)-C(5)-C(6)-C(7)	-0.3(2)
C(2)-N(1)-C(1)-O(1)	-8.7(2)	C(4)-C(5)-C(6)-C(6A)	179.23(15)
C(4)-N(1)-C(1)-C(10)	-10.8(2)	C(5)-C(6)-C(7)-C(8)	-0.9(2)
C(2)-N(1)-C(1)-C(10)	171.10(14)	C(6A)-C(6)-C(7)-C(8)	179.56(16)
C(1)-N(1)-C(2)-C(3)	85.8(2)	C(6)-C(7)-C(8)-C(9)	0.5(3)
C(4)-N(1)-C(2)-C(3)	-92.42(19)	C(5)-C(4)-C(9)-C(8)	-2.3(2)
C(1)-N(1)-C(4)-C(9)	-67.9(2)	N(1)-C(4)-C(9)-C(8)	176.20(14)
C(2)-N(1)-C(4)-C(9)	110.13(17)	C(5)-C(4)-C(9)-C(9A)	177.78(15)
C(1)-N(1)-C(4)-C(5)	110.61(18)	N(1)-C(4)-C(9)-C(9A)	-3.7(2)
C(2)-N(1)-C(4)-C(5)	-71.32(19)	C(7)-C(8)-C(9)-C(4)	1.0(2)

C(7)-C(8)-C(9)-C(9A)	-179.03(16)	C(19)-C(18)-C(23)-C(23A)	177.08(15)
C(14)-N(2)-C(10)-C(11)	3.5(2)	N(4)-C(18)-C(23)-C(23A)	-7.6(2)
Gd(01)-N(2)-C(10)-C(11)	-170.92(11)	C(21)-C(22)-C(23)-C(18)	1.3(2)
C(14)-N(2)-C(10)-C(1)	-179.49(13)	C(21)-C(22)-C(23)-C(23A)	-176.63(16)
Gd(01)-N(2)-C(10)-C(1)	6.06(16)	C(28)-N(3)-C(24)-C(25)	0.3(2)
O(1)-C(1)-C(10)-N(2)	-16.68(19)	Gd(01)-N(3)-C(24)-C(25)	-177.00(11)
N(1)-C(1)-C(10)-N(2)	163.56(14)	C(28)-N(3)-C(24)-C(15)	172.42(12)
O(1)-C(1)-C(10)-C(11)	160.12(15)	Gd(01)-N(3)-C(24)-C(15)	-4.85(15)
N(1)-C(1)-C(10)-C(11)	-19.6(2)	O(2)-C(15)-C(24)-N(3)	-26.54(19)
N(2)-C(10)-C(11)-C(12)	-2.8(2)	N(4)-C(15)-C(24)-N(3)	157.31(13)
C(1)-C(10)-C(11)-C(12)	-179.26(15)	O(2)-C(15)-C(24)-C(25)	145.43(15)
C(10)-C(11)-C(12)-C(13)	0.1(2)	N(4)-C(15)-C(24)-C(25)	-30.7(2)
C(11)-C(12)-C(13)-C(14)	1.7(2)	N(3)-C(24)-C(25)-C(26)	0.4(2)
C(10)-N(2)-C(14)-C(13)	-1.6(2)	C(15)-C(24)-C(25)-C(26)	-170.76(14)
Gd(01)-N(2)-C(14)-C(13)	172.64(11)	C(24)-C(25)-C(26)-C(27)	-0.5(2)
C(10)-N(2)-C(14)-C(28)	177.36(13)	C(25)-C(26)-C(27)-C(28)	0.0(2)
Gd(01)-N(2)-C(14)-C(28)	-8.41(17)	C(24)-N(3)-C(28)-C(27)	-0.8(2)
C(12)-C(13)-C(14)-N(2)	-1.0(2)	Gd(01)-N(3)-C(28)-C(27)	176.26(11)
C(12)-C(13)-C(14)-C(28)	-179.91(14)	C(24)-N(3)-C(28)-C(14)	-179.94(13)
Gd(01)-O(2)-C(15)-N(4)	-137.77(12)	Gd(01)-N(3)-C(28)-C(14)	-2.89(17)
Gd(01)-O(2)-C(15)-C(24)	46.16(15)	C(26)-C(27)-C(28)-N(3)	0.7(2)
C(18)-N(4)-C(15)-O(2)	156.58(14)	C(26)-C(27)-C(28)-C(14)	179.77(14)
C(16)-N(4)-C(15)-O(2)	-1.5(2)	N(2)-C(14)-C(28)-N(3)	7.19(19)
C(18)-N(4)-C(15)-C(24)	-27.5(2)	C(13)-C(14)-C(28)-N(3)	-173.86(13)
C(16)-N(4)-C(15)-C(24)	174.39(13)	N(2)-C(14)-C(28)-C(27)	-171.95(14)
C(15)-N(4)-C(16)-C(17)	80.43(18)	C(13)-C(14)-C(28)-C(27)	7.0(2)
C(18)-N(4)-C(16)-C(17)	-79.37(17)	O(3N)-N(1N)-O(1N)-Gd(01)	178.28(14)
C(15)-N(4)-C(18)-C(19)	-60.1(2)	O(2N)-N(1N)-O(1N)-Gd(01)	-1.55(14)
C(16)-N(4)-C(18)-C(19)	98.32(16)	O(3N)-N(1N)-O(2N)-Gd(01)	-178.28(14)
C(15)-N(4)-C(18)-C(23)	124.37(16)	O(1N)-N(1N)-O(2N)-Gd(01)	1.55(14)
C(16)-N(4)-C(18)-C(23)	-77.18(18)	O(6N)-N(2N)-O(4N)-Gd(01)	171.26(15)
C(23)-C(18)-C(19)-C(20)	-0.9(2)	O(5N)-N(2N)-O(4N)-Gd(01)	-7.75(14)
N(4)-C(18)-C(19)-C(20)	-176.35(14)	O(6N)-N(2N)-O(5N)-Gd(01)	-171.18(15)
C(18)-C(19)-C(20)-C(21)	2.2(2)	O(4N)-N(2N)-O(5N)-Gd(01)	7.84(14)
C(18)-C(19)-C(20)-C(20A)	-179.03(15)	O(9N)-N(3N)-O(7N)-Gd(01)	176.91(13)
C(19)-C(20)-C(21)-C(22)	-1.7(2)	O(8N)-N(3N)-O(7N)-Gd(01)	-4.10(13)
C(20A)-C(20)-C(21)-C(22)	179.53(16)	O(9N)-N(3N)-O(8N)-Gd(01)	-176.84(13)
C(20)-C(21)-C(22)-C(23)	-0.1(3)	O(7N)-N(3N)-O(8N)-Gd(01)	4.17(13)
C(19)-C(18)-C(23)-C(22)	-0.8(2)		
N(4)-C(18)-C(23)-C(22)	174.47(14)		

Table 8. Crystal data and structure refinement for 3,5diMeDy.

Identification code	3,5diMeDy	
Empirical formula	C32 H34 Dy N7 O11	
Formula weight	855.16	
Temperature	120(2) K	
Wavelength	0.71073 E	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 26.0636(18) Å	α= 90°.
	b = 8.1361(6) Å	β= 93.831(2)°.
	c = 16.2987(11) Å	γ = 90°.
Volume	3448.5(4) Å^3	
Z	4	
Density (calculated)	1.647 Mg/m^3	
Absorption coefficient	2.237 mm^{-1}	
F(000)	1716	
Crystal size	0.330 x 0.220 x 0.050 mm^3	
Theta range for data collection	0.783 to 31.557°.	
Index ranges	-38<=h<=38, -11<=k<=11, -23<=l<=23	
Reflections collected	47587	
Independent reflections	11477 [R(int) = 0.0768]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11477 / 0 / 466	
Goodness-of-fit on F^2	0.999	
Final R indices for 8808 refl. with [I>2sigma(I)]	R1 = 0.0400, wR2 = 0.0718	

R indices (all data)	R1 = 0.0637, wR2 = 0.0804
Extinction coefficient	n/a
Largest diff. peak and hole	1.154 and -1.182 e. Å^{-3}

Table 9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for 3,5diMeDy. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Dy(1)	2494(1)	4754(1)	5723(1)	10(1)
O(1)	3067(1)	2621(3)	6035(1)	17(1)
O(1N)	1554(1)	4927(2)	5779(1)	16(1)
N(1N)	1538(1)	4233(3)	6485(2)	18(1)
N(1)	3635(1)	1035(3)	6745(2)	15(1)
C(1)	3292(1)	2263(4)	6713(2)	14(1)
O(2)	2238(1)	7228(2)	5020(1)	12(1)
N(2N)	2046(1)	2667(3)	4467(1)	9(1)
O(2N)	1958(1)	3593(3)	6771(1)	16(1)
N(2)	1484(1)	8629(3)	4999(2)	14(1)
C(2)	3718(1)	188(4)	5955(2)	20(1)
O(3N)	1148(1)	4226(4)	6861(2)	33(1)
N(3N)	3445(1)	6025(4)	5165(2)	24(1)
C(3)	4088(1)	1133(5)	5461(2)	27(1)
O(4N)	2153(1)	2042(3)	5164(1)	24(1)
C(4)	3990(1)	620(4)	7424(2)	14(1)
O(5N)	2159(1)	4112(3)	4343(1)	25(1)
C(5)	4349(1)	1748(4)	7739(2)	16(1)
O(6N)	1821(1)	1817(3)	3904(2)	29(1)
C(6)	4710(1)	1285(4)	8364(2)	18(1)
C(6A)	4395(1)	-3279(4)	8560(2)	30(1)
O(7N)	3156(1)	5094(3)	4704(1)	22(1)
C(7)	4717(1)	-352(4)	8626(2)	21(1)
C(7A)	5087(1)	2518(5)	8746(2)	29(1)
O(8N)	3307(1)	6313(3)	5874(1)	20(1)
C(8)	4365(1)	-1505(4)	8299(2)	19(1)
O(9N)	3834(1)	6638(5)	4921(2)	62(1)
C(9)	3995(1)	-993(4)	7703(2)	18(1)
C(10)	3155(1)	3255(4)	7447(2)	12(1)
C(11)	3228(1)	2821(4)	8270(2)	14(1)
C(12)	3063(1)	3912(4)	8856(2)	16(1)
C(13)	2844(1)	5389(4)	8610(2)	14(1)
C(14)	2760(1)	5716(4)	7771(2)	12(1)
N(15)	2912(1)	4653(3)	7203(2)	12(1)
C(16)	1912(1)	8042(4)	5386(2)	11(1)
C(17)	1400(1)	8347(4)	4098(2)	18(1)
C(18)	1130(1)	6723(4)	3907(2)	26(1)
C(19)	1057(1)	9302(4)	5412(2)	14(1)
C(20)	900(1)	10907(4)	5228(2)	16(1)
C(21)	484(1)	11564(4)	5599(2)	19(1)
C(21A)	307(1)	13290(4)	5415(2)	24(1)
C(22)	231(1)	10581(4)	6148(2)	20(1)
C(22A)	85(1)	7922(5)	6898(2)	32(1)
C(23)	381(1)	8971(4)	6325(2)	21(1)
C(24)	800(1)	8327(4)	5947(2)	17(1)
C(25)	2037(1)	8340(4)	6289(2)	11(1)
C(26)	1938(1)	9761(4)	6708(2)	15(1)
C(27)	2133(1)	9897(4)	7524(2)	17(1)
C(28)	2402(1)	8598(4)	7894(2)	17(1)
C(29)	2483(1)	7189(4)	7437(2)	12(1)
N(30)	2310(1)	7085(3)	6640(1)	10(1)

Table 10. Bond lengths [Å] and angles [°] for 3,5diMeDy.

Dy(1)-O(1)	2.323(2)	Dy(1)-N(2N)	2.849(2)
Dy(1)-O(2)	2.390(2)	Dy(1)-N(1N)	2.888(3)
Dy(1)-O(5N)	2.416(2)	O(1)-C(1)	1.250(3)
Dy(1)-O(1N)	2.463(2)	O(1N)-N(1N)	1.284(3)
Dy(1)-O(2N)	2.466(2)	N(1N)-O(3N)	1.223(3)
Dy(1)-O(8N)	2.467(2)	N(1N)-O(2N)	1.272(3)
Dy(1)-N(30)	2.481(2)	N(1)-C(1)	1.340(4)
Dy(1)-O(7N)	2.489(2)	N(1)-C(4)	1.435(4)
Dy(1)-O(4N)	2.526(2)	N(1)-C(2)	1.490(4)
Dy(1)-N(15)	2.581(2)	C(1)-C(10)	1.506(4)

O(2)-C(16)	1.258(3)	C(25)-C(26)	1.376(4)
N(2N)-O(5N)	1.232(3)	C(26)-C(27)	1.396(4)
N(2N)-O(4N)	1.259(3)	C(26)-H(26A)	0.9500
N(2N)-O(6N)	1.262(3)	C(27)-C(28)	1.384(4)
N(2)-C(16)	1.332(4)	C(27)-H(27A)	0.9500
N(2)-C(19)	1.447(4)	C(28)-C(29)	1.390(4)
N(2)-C(17)	1.487(4)	C(28)-H(28A)	0.9500
C(2)-C(3)	1.508(5)	C(29)-N(30)	1.349(4)
C(2)-H(2A)	0.9900	O(1)-Dy(1)-O(2)	152.81(7)
C(2)-H(2B)	0.9900	O(1)-Dy(1)-O(5N)	103.28(8)
N(3N)-O(9N)	1.220(4)	O(2)-Dy(1)-O(5N)	70.33(7)
N(3N)-O(8N)	1.255(3)	O(1)-Dy(1)-O(1N)	131.39(7)
N(3N)-O(7N)	1.277(3)	O(2)-Dy(1)-O(1N)	73.87(7)
C(3)-H(3A)	0.9800	O(5N)-Dy(1)-O(1N)	75.40(8)
C(3)-H(3B)	0.9800	O(1)-Dy(1)-O(2N)	87.01(7)
C(3)-H(3C)	0.9800	O(2)-Dy(1)-O(2N)	120.08(7)
C(4)-C(5)	1.384(4)	O(5N)-Dy(1)-O(2N)	112.08(8)
C(4)-C(9)	1.389(4)	O(1N)-Dy(1)-O(2N)	52.04(7)
C(5)-C(6)	1.392(4)	O(1)-Dy(1)-O(8N)	80.05(8)
C(5)-H(5A)	0.9500	O(2)-Dy(1)-O(8N)	79.96(7)
C(6)-C(7)	1.398(5)	O(5N)-Dy(1)-O(8N)	117.31(8)
C(6)-C(7A)	1.508(5)	O(1N)-Dy(1)-O(8N)	144.77(7)
C(6A)-C(8)	1.505(5)	O(2N)-Dy(1)-O(8N)	130.55(7)
C(6A)-H(6AA)	0.9800	O(1)-Dy(1)-N(30)	125.90(8)
C(6A)-H(6AB)	0.9800	O(2)-Dy(1)-N(30)	65.50(7)
C(6A)-H(6AC)	0.9800	O(5N)-Dy(1)-N(30)	130.81(8)
C(7)-C(8)	1.392(5)	O(1N)-Dy(1)-N(30)	72.60(7)
C(7)-H(7A)	0.9500	O(2N)-Dy(1)-N(30)	74.59(7)
C(7A)-H(7AA)	0.9800	O(8N)-Dy(1)-N(30)	75.29(8)
C(7A)-H(7AB)	0.9800	O(1)-Dy(1)-O(7N)	76.41(8)
C(7A)-H(7AC)	0.9800	O(2)-Dy(1)-O(7N)	76.76(7)
C(8)-C(9)	1.387(4)	O(5N)-Dy(1)-O(7N)	68.07(8)
C(9)-H(9A)	0.9500	O(1N)-Dy(1)-O(7N)	138.99(7)
C(10)-N(15)	1.349(4)	O(2N)-Dy(1)-O(7N)	162.73(7)
C(10)-C(11)	1.387(4)	O(8N)-Dy(1)-O(7N)	51.71(7)
C(11)-C(12)	1.392(4)	N(30)-Dy(1)-O(7N)	119.16(8)
C(11)-H(11A)	0.9500	O(1)-Dy(1)-O(4N)	68.41(8)
C(12)-C(13)	1.379(4)	O(2)-Dy(1)-O(4N)	118.85(7)
C(12)-H(12A)	0.9500	O(5N)-Dy(1)-O(4N)	51.58(8)
C(13)-C(14)	1.397(4)	O(1N)-Dy(1)-O(4N)	74.71(7)
C(13)-H(13A)	0.9500	O(2N)-Dy(1)-O(4N)	73.35(7)
C(14)-N(15)	1.345(4)	O(8N)-Dy(1)-O(4N)	139.83(8)
C(14)-C(29)	1.484(4)	N(30)-Dy(1)-O(4N)	143.85(8)
C(16)-C(25)	1.505(4)	O(7N)-Dy(1)-O(4N)	95.71(8)
C(17)-C(18)	1.519(5)	O(1)-Dy(1)-N(15)	63.06(7)
C(17)-H(17A)	0.9900	O(2)-Dy(1)-N(15)	124.18(7)
C(17)-H(17B)	0.9900	O(5N)-Dy(1)-N(15)	165.35(8)
C(18)-H(18A)	0.9800	O(1N)-Dy(1)-N(15)	109.01(7)
C(18)-H(18B)	0.9800	O(2N)-Dy(1)-N(15)	64.11(7)
C(18)-H(18C)	0.9800	O(8N)-Dy(1)-N(15)	67.50(8)
C(19)-C(24)	1.383(4)	N(30)-Dy(1)-N(15)	63.11(8)
C(19)-C(20)	1.395(4)	O(7N)-Dy(1)-N(15)	111.05(8)
C(20)-C(21)	1.385(4)	O(4N)-Dy(1)-N(15)	115.20(8)
C(20)-H(20A)	0.9500	O(1)-Dy(1)-N(2N)	86.49(7)
C(21)-C(22)	1.398(5)	O(2)-Dy(1)-N(2N)	93.98(7)
C(21)-C(21A)	1.502(5)	O(5N)-Dy(1)-N(2N)	25.39(7)
C(21A)-H(21A)	0.9800	O(1N)-Dy(1)-N(2N)	72.52(7)
C(21A)-H(21B)	0.9800	O(2N)-Dy(1)-N(2N)	92.62(7)
C(21A)-H(21C)	0.9800	O(8N)-Dy(1)-N(2N)	133.31(7)
C(22)-C(23)	1.392(5)	N(30)-Dy(1)-N(2N)	143.30(7)
C(22)-H(22A)	0.9500	O(7N)-Dy(1)-N(2N)	81.72(7)
C(22A)-C(23)	1.515(5)	O(4N)-Dy(1)-N(2N)	26.22(7)
C(22A)-H(22B)	0.9800	N(15)-Dy(1)-N(2N)	141.24(7)
C(22A)-H(22C)	0.9800	O(1)-Dy(1)-N(1N)	110.88(8)
C(22A)-H(22D)	0.9800	O(2)-Dy(1)-N(1N)	96.18(7)
C(23)-C(24)	1.392(4)	O(5N)-Dy(1)-N(1N)	95.73(8)
C(24)-H(24A)	0.9500	O(1N)-Dy(1)-N(1N)	26.26(7)
C(25)-N(30)	1.350(4)	O(2N)-Dy(1)-N(1N)	25.98(7)

O(8N)-Dy(1)-N(1N)	142.38(7)	C(8)-C(7)-H(7A)	119.0
N(30)-Dy(1)-N(1N)	69.29(8)	C(6)-C(7)-H(7A)	119.0
O(7N)-Dy(1)-N(1N)	163.66(8)	C(6)-C(7A)-H(7AA)	109.5
O(4N)-Dy(1)-N(1N)	74.58(8)	C(6)-C(7A)-H(7AB)	109.5
N(15)-Dy(1)-N(1N)	85.16(8)	H(7AA)-C(7A)-H(7AB)	109.5
N(2N)-Dy(1)-N(1N)	84.12(7)	C(6)-C(7A)-H(7AC)	109.5
C(1)-O(1)-Dy(1)	128.6(2)	H(7AA)-C(7A)-H(7AC)	109.5
N(1N)-O(1N)-Dy(1)	95.65(17)	H(7AB)-C(7A)-H(7AC)	109.5
O(3N)-N(1N)-O(2N)	122.6(3)	N(3N)-O(8N)-Dy(1)	96.32(18)
O(3N)-N(1N)-O(1N)	121.9(3)	C(9)-C(8)-C(7)	118.3(3)
O(2N)-N(1N)-O(1N)	115.5(2)	C(9)-C(8)-C(6A)	120.5(3)
O(3N)-N(1N)-Dy(1)	170.8(2)	C(7)-C(8)-C(6A)	121.2(3)
O(2N)-N(1N)-Dy(1)	58.14(14)	C(8)-C(9)-C(4)	120.3(3)
O(1N)-N(1N)-Dy(1)	58.08(14)	C(8)-C(9)-H(9A)	119.9
C(1)-N(1)-C(4)	126.9(3)	C(4)-C(9)-H(9A)	119.9
C(1)-N(1)-C(2)	116.5(3)	N(15)-C(10)-C(11)	122.1(3)
C(4)-N(1)-C(2)	115.7(2)	N(15)-C(10)-C(1)	110.4(2)
O(1)-C(1)-N(1)	118.7(3)	C(11)-C(10)-C(1)	127.4(3)
O(1)-C(1)-C(10)	117.2(3)	C(10)-C(11)-C(12)	118.2(3)
N(1)-C(1)-C(10)	124.1(3)	C(10)-C(11)-H(11A)	120.9
C(16)-O(2)-Dy(1)	113.08(18)	C(12)-C(11)-H(11A)	120.9
O(5N)-N(2N)-O(4N)	119.6(2)	C(13)-C(12)-C(11)	119.9(3)
O(5N)-N(2N)-O(6N)	120.5(2)	C(13)-C(12)-H(12A)	120.1
O(4N)-N(2N)-O(6N)	119.9(2)	C(11)-C(12)-H(12A)	120.1
O(5N)-N(2N)-Dy(1)	57.22(14)	C(12)-C(13)-C(14)	119.0(3)
O(4N)-N(2N)-Dy(1)	62.42(15)	C(12)-C(13)-H(13A)	120.5
O(6N)-N(2N)-Dy(1)	175.8(2)	C(14)-C(13)-H(13A)	120.5
N(1N)-O(2N)-Dy(1)	95.88(17)	N(15)-C(14)-C(13)	121.2(3)
C(16)-N(2)-C(19)	124.1(2)	N(15)-C(14)-C(29)	115.2(3)
C(16)-N(2)-C(17)	118.5(2)	C(13)-C(14)-C(29)	123.6(3)
C(19)-N(2)-C(17)	116.7(2)	C(14)-N(15)-C(10)	119.5(3)
N(1)-C(2)-C(3)	111.1(3)	C(14)-N(15)-Dy(1)	119.83(19)
N(1)-C(2)-H(2A)	109.4	C(10)-N(15)-Dy(1)	117.58(19)
C(3)-C(2)-H(2A)	109.4	O(2)-C(16)-N(2)	122.2(3)
N(1)-C(2)-H(2B)	109.4	O(2)-C(16)-C(25)	116.1(3)
C(3)-C(2)-H(2B)	109.4	N(2)-C(16)-C(25)	121.7(3)
H(2A)-C(2)-H(2B)	108.0	N(2)-C(17)-C(18)	111.9(3)
O(9N)-N(3N)-O(8N)	121.3(3)	N(2)-C(17)-H(17A)	109.2
O(9N)-N(3N)-O(7N)	121.4(3)	C(18)-C(17)-H(17A)	109.2
O(8N)-N(3N)-O(7N)	117.2(3)	N(2)-C(17)-H(17B)	109.2
O(9N)-N(3N)-Dy(1)	176.7(3)	C(18)-C(17)-H(17B)	109.2
O(8N)-N(3N)-Dy(1)	58.10(15)	H(17A)-C(17)-H(17B)	107.9
O(7N)-N(3N)-Dy(1)	59.17(15)	C(17)-C(18)-H(18A)	109.5
C(2)-C(3)-H(3A)	109.5	C(17)-C(18)-H(18B)	109.5
C(2)-C(3)-H(3B)	109.5	H(18A)-C(18)-H(18B)	109.5
H(3A)-C(3)-H(3B)	109.5	C(17)-C(18)-H(18C)	109.5
C(2)-C(3)-H(3C)	109.5	H(18A)-C(18)-H(18C)	109.5
H(3A)-C(3)-H(3C)	109.5	H(18B)-C(18)-H(18C)	109.5
H(3B)-C(3)-H(3C)	109.5	C(24)-C(19)-C(20)	121.7(3)
N(2N)-O(4N)-Dy(1)	91.36(16)	C(24)-C(19)-N(2)	119.7(3)
C(5)-C(4)-C(9)	120.9(3)	C(20)-C(19)-N(2)	118.6(3)
C(5)-C(4)-N(1)	121.0(3)	C(21)-C(20)-C(19)	119.7(3)
C(9)-C(4)-N(1)	117.8(3)	C(21)-C(20)-H(20A)	120.2
N(2N)-O(5N)-Dy(1)	97.39(17)	C(19)-C(20)-H(20A)	120.2
C(4)-C(5)-C(6)	119.9(3)	C(20)-C(21)-C(22)	118.4(3)
C(4)-C(5)-H(5A)	120.0	C(20)-C(21)-C(21A)	120.9(3)
C(6)-C(5)-H(5A)	120.0	C(22)-C(21)-C(21A)	120.7(3)
C(5)-C(6)-C(7)	118.4(3)	C(21)-C(21A)-H(21A)	109.5
C(5)-C(6)-C(7A)	120.7(3)	C(21)-C(21A)-H(21B)	109.5
C(7)-C(6)-C(7A)	120.9(3)	H(21A)-C(21A)-H(21B)	109.5
C(8)-C(6A)-H(6AA)	109.5	C(21)-C(21A)-H(21C)	109.5
C(8)-C(6A)-H(6AB)	109.5	H(21A)-C(21A)-H(21C)	109.5
H(6AA)-C(6A)-H(6AB)	109.5	H(21B)-C(21A)-H(21C)	109.5
C(8)-C(6A)-H(6AC)	109.5	C(23)-C(22)-C(21)	122.1(3)
H(6AA)-C(6A)-H(6AC)	109.5	C(23)-C(22)-H(22A)	118.9
H(6AB)-C(6A)-H(6AC)	109.5	C(21)-C(22)-H(22A)	118.9
N(3N)-O(7N)-Dy(1)	94.68(17)	C(23)-C(22A)-H(22B)	109.5
C(8)-C(7)-C(6)	122.1(3)	C(23)-C(22A)-H(22C)	109.5

H(22B)-C(22A)-H(22C)	109.5	C(25)-C(26)-H(26A)	120.9
C(23)-C(22A)-H(22D)	109.5	C(27)-C(26)-H(26A)	120.9
H(22B)-C(22A)-H(22D)	109.5	C(28)-C(27)-C(26)	119.7(3)
H(22C)-C(22A)-H(22D)	109.5	C(28)-C(27)-H(27A)	120.2
C(24)-C(23)-C(22)	118.8(3)	C(26)-C(27)-H(27A)	120.2
C(24)-C(23)-C(22A)	120.6(3)	C(29)-C(28)-C(27)	119.2(3)
C(22)-C(23)-C(22A)	120.6(3)	C(29)-C(28)-H(28A)	120.4
C(19)-C(24)-C(23)	119.3(3)	C(27)-C(28)-H(28A)	120.4
C(19)-C(24)-H(24A)	120.3	N(30)-C(29)-C(28)	120.9(3)
C(23)-C(24)-H(24A)	120.3	N(30)-C(29)-C(14)	115.2(3)
N(30)-C(25)-C(26)	122.4(3)	C(28)-C(29)-C(14)	123.9(3)
N(30)-C(25)-C(16)	111.5(2)	C(25)-N(30)-C(29)	119.6(3)
C(26)-C(25)-C(16)	125.8(3)	C(25)-N(30)-Dy(1)	116.15(19)
C(25)-C(26)-C(27)	118.1(3)	C(29)-N(30)-Dy(1)	124.21(19)

Table 11. Anisotropic displacement parameters (E^2x 10^3) for 3,5diMeDy. 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}
Dy(1)	13(1)	9(1)	7(1)	0(1)	0(1)	1(1)
O(1)	23(1)	16(1)	11(1)	0(1)	-4(1)	8(1)
O(1N)	17(1)	15(1)	15(1)	5(1)	-2(1)	-1(1)
N(1N)	20(1)	17(1)	17(1)	-1(1)	1(1)	-4(1)
N(1)	17(1)	13(1)	13(1)	-2(1)	-1(1)	6(1)
C(1)	16(2)	13(2)	14(2)	0(1)	2(1)	3(1)
O(2)	15(1)	12(1)	8(1)	1(1)	2(1)	1(1)
N(2N)	12(1)	9(1)	6(1)	2(1)	2(1)	2(1)
O(2N)	17(1)	15(1)	14(1)	3(1)	1(1)	2(1)
N(2)	18(1)	15(1)	10(1)	1(1)	2(1)	4(1)
C(2)	26(2)	15(2)	18(2)	-6(1)	-4(1)	9(1)
O(3N)	22(1)	51(2)	28(2)	6(1)	11(1)	0(1)
N(3N)	21(2)	32(2)	18(2)	-7(1)	6(1)	-7(1)
C(3)	26(2)	35(2)	20(2)	-7(2)	2(2)	6(2)
O(4N)	35(2)	19(1)	18(1)	3(1)	-3(1)	-1(1)
C(4)	14(2)	13(2)	15(2)	1(1)	0(1)	4(1)
O(5N)	38(2)	20(1)	17(1)	2(1)	-1(1)	-8(1)
C(5)	17(2)	15(2)	17(2)	2(1)	2(1)	-1(1)
O(6N)	39(2)	29(2)	20(1)	-8(1)	-4(1)	-12(1)
C(6)	15(2)	23(2)	16(2)	2(1)	1(1)	2(1)
C(6A)	30(2)	26(2)	33(2)	12(2)	1(2)	6(2)
O(7N)	22(1)	27(1)	17(1)	-7(1)	3(1)	-5(1)
C(7)	18(2)	31(2)	14(2)	6(1)	-2(1)	6(2)
C(7A)	21(2)	37(2)	28(2)	0(2)	-5(2)	-5(2)
O(8N)	20(1)	27(1)	13(1)	-4(1)	4(1)	-6(1)
C(8)	18(2)	23(2)	16(2)	6(1)	7(1)	7(1)
O(9N)	45(2)	105(3)	39(2)	-30(2)	26(2)	-46(2)
C(9)	18(2)	15(2)	20(2)	4(1)	1(1)	2(1)
C(10)	11(1)	13(2)	11(1)	1(1)	0(1)	0(1)
C(11)	12(1)	15(2)	16(2)	4(1)	0(1)	3(1)
C(12)	16(2)	23(2)	10(1)	3(1)	1(1)	1(1)
C(13)	15(1)	18(2)	8(1)	-1(1)	-1(1)	1(1)
C(14)	12(1)	13(1)	10(1)	-1(1)	2(1)	-1(1)
N(15)	14(1)	12(1)	10(1)	2(1)	1(1)	2(1)
C(16)	16(2)	9(1)	10(1)	1(1)	3(1)	-2(1)
C(17)	20(2)	24(2)	10(2)	1(1)	-2(1)	5(1)
C(18)	24(2)	29(2)	25(2)	-6(2)	-5(2)	2(2)
C(19)	13(1)	16(2)	12(1)	-2(1)	-1(1)	2(1)
C(20)	15(2)	16(2)	17(2)	2(1)	-1(1)	0(1)
C(21)	18(2)	18(2)	20(2)	-3(1)	-4(1)	3(1)
C(21A)	21(2)	17(2)	34(2)	-2(2)	2(2)	5(1)
C(22)	17(2)	24(2)	18(2)	-6(1)	1(1)	5(1)
C(22A)	30(2)	38(2)	30(2)	6(2)	12(2)	-2(2)
C(23)	21(2)	27(2)	14(2)	-1(1)	0(1)	0(1)
C(24)	19(2)	18(2)	14(2)	0(1)	0(1)	3(1)
C(25)	12(1)	13(2)	9(1)	1(1)	-1(1)	-1(1)
C(26)	21(2)	11(1)	12(1)	1(1)	1(1)	3(1)
C(27)	28(2)	10(2)	14(2)	-4(1)	2(1)	0(1)
C(28)	20(2)	19(2)	11(2)	-4(1)	0(1)	2(1)
C(29)	14(1)	14(2)	9(1)	1(1)	1(1)	1(1)
N(30)	12(1)	10(1)	9(1)	1(1)	2(1)	-1(1)

Table 12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (E^2x 10^3) for 3,5diMeDy.

	x	y	z	U(eq)
H(2A)	3385	74	5630	24
H(2B)	3856	-929	6070	24
H(3A)	4147	529	4955	40
H(3B)	4415	1269	5786	40
H(3C)	3943	2216	5320	40
H(5A)	4348	2837	7529	19
H(6AA)	4048	-3746	8544	44
H(6AB)	4554	-3352	9122	44
H(6AC)	4604	-3893	8186	44
H(7A)	4969	-687	9040	26
H(7AA)	5163	3347	8335	44
H(7AB)	5405	1954	8937	44
H(7AC)	4937	3053	9212	44
H(9A)	3743	-1748	7485	21
H(11A)	3386	1807	8429	17
H(12A)	3102	3639	9423	19
H(13A)	2751	6173	9006	17
H(17A)	1736	8354	3848	22
H(17B)	1190	9255	3850	22
H(18A)	1052	6630	3313	39
H(18B)	810	6678	4189	39
H(18C)	1355	5815	4097	39
H(20A)	1078	11546	4851	19
H(21A)	587	13915	5190	36
H(21B)	208	13815	5923	36
H(21C)	10	13267	5013	36
H(22A)	-53	11026	6410	24
H(22B)	32	8540	7401	48
H(22C)	280	6919	7037	48
H(22D)	-249	7628	6626	48
H(24A)	909	7229	6055	21
H(26A)	1743	10626	6449	18
H(27A)	2081	10877	7825	21
H(28A)	2530	8668	8452	20

Table 13. Crystal data and structure refinement for 2,4diMeEu.

Identification code	2,4diMeEu	
Empirical formula	C32 H34 Eu N7 O11	
Formula weight	844.62	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 47.880(4) Å	α= 90°.
	b = 8.6436(7) Å	β= 101.877(2)°.
	c = 17.1229(13) Å	γ = 90°.
Volume	6934.7(9) $Å^3$	
Z	8	
Density (calculated)	1.618 Mg/m^3	
Absorption coefficient	1.879 mm^{-1}	
F(000)	3408	
Crystal size	0.136 x 0.034 x 0.021 mm^3	
Theta range for data collection	1.738 to 26.998°.	
Index ranges	-60<=h<=60, -11<=k<=11, -21<=l<=21	
Reflections collected	29263	
Independent reflections	7561 [R(int) = 0.0737]	
Completeness to theta = 25.242°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7561 / 83 / 499	
Goodness-of-fit on F^2	1.062	
Final R indices [I>2sigma(I)]	R1 = 0.0543, wR2 = 0.1220	
R indices (all data)	R1 = 0.0952, wR2 = 0.1414	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.456 and -1.378 e.$Å^{-3}$	

Table 14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 2,4diMeEu. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Eu(1)	1256(1)	7088(1)	1909(1)	37(1)
O(1)	1067(1)	5034(6)	2613(3)	52(1)
O(2)	1450(1)	9310(6)	1385(3)	62(1)
N(1)	690(1)	3410(7)	2539(4)	55(2)
N(2)	1807(1)	10390(6)	926(3)	44(1)
N(15)	1110(1)	4598(6)	1127(3)	33(1)
N(30)	1442(1)	6705(5)	617(3)	35(1)
C(1)	902(1)	4015(8)	2240(4)	48(2)
C(2)	667(2)	3887(12)	3369(5)	78(3)
C(3)	495(2)	5315(13)	3362(6)	101(4)
C(4)	468(2)	2407(9)	2105(5)	56(2)
C(5)	264(2)	2946(11)	1470(5)	65(2)
C(5A)	254(2)	4486(14)	1131(7)	70(3)
C(9A)	659(6)	480(40)	3204(19)	70(3)
C(6)	54(2)	1940(15)	1089(5)	85(3)
C(7)	51(2)	415(14)	1335(5)	75(3)
C(7A)	-178(2)	-701(14)	892(6)	105(4)
C(8)	252(2)	-80(11)	1972(5)	70(2)
C(9)	460(2)	886(9)	2364(5)	58(2)
C(10)	962(1)	3503(8)	1444(4)	39(2)
C(11)	899(1)	2050(7)	1092(4)	42(2)
C(12)	984(1)	1745(7)	397(4)	44(2)
C(13)	1134(1)	2853(7)	64(4)	42(2)
C(14)	1193(1)	4259(7)	448(4)	36(1)
C(16)	1618(2)	9238(8)	921(4)	47(2)
C(17)	1801(2)	11716(7)	1482(5)	52(2)
C(18)	2002(2)	11447(10)	2280(5)	72(2)
C(19)	2026(2)	10386(12)	434(5)	36(2)
C(20)	2268(2)	9538(11)	626(5)	40(2)
C(20A)	2334(2)	8482(13)	1342(7)	67(3)
C(21)	2462(2)	9639(11)	132(6)	50(2)
C(22A)	2629(3)	10661(15)	-1097(8)	84(4)
C(22)	2419(2)	10562(12)	-547(6)	52(2)
C(23)	2166(2)	11413(12)	-715(6)	54(3)
C(24)	1974(2)	11358(11)	-230(6)	44(2)
C(19')	2063(4)	10350(30)	653(12)	36(2)
C(20')	2274(4)	9280(20)	952(10)	40(2)
C(21')	2505(4)	9090(20)	587(12)	50(2)
C(22')	2525(4)	9970(20)	-78(12)	52(2)
C(23')	2314(4)	11050(20)	-377(11)	54(3)
C(24')	2083(4)	11240(20)	-11(12)	44(2)
C(24A)	1847(5)	12370(30)	-356(17)	67(3)
C(22B)	2789(5)	9840(40)	-441(19)	84(4)
C(25)	1589(1)	7871(7)	363(4)	41(2)
C(26)	1671(2)	7817(9)	-360(4)	58(2)
C(27)	1596(2)	6545(9)	-850(4)	65(2)
C(28)	1438(2)	5376(8)	-602(4)	55(2)
C(29)	1369(1)	5479(7)	155(4)	38(1)
O(4N)	1636(1)	5109(6)	2325(3)	62(1)
O(5N)	1788(1)	7411(7)	2370(4)	81(2)
O(6N)	2083(1)	5531(7)	2809(4)	82(2)
O(7N)	899(1)	7963(6)	720(3)	63(1)
O(8N)	722(1)	7123(7)	1683(4)	74(2)
O(9N)	445(2)	7719(10)	557(5)	127(3)
N(1N)	1151(3)	9179(16)	3164(8)	46(2)
O(1N)	1251(3)	7726(15)	3297(7)	59(2)
O(2N)	1089(2)	9582(13)	2483(7)	44(2)
O(3N)	1109(3)	10010(12)	3707(6)	57(2)
O(3N')	1277(4)	9938(18)	3893(9)	57(2)
O(2N')	1220(3)	9617(19)	2557(10)	44(2)
N(1N')	1279(4)	9150(20)	3283(11)	46(2)
O(1N')	1381(4)	7900(20)	3332(11)	59(2)
N(2N)	1838(1)	5965(7)	2539(4)	56(2)
N(3N)	681(2)	7646(8)	973(5)	64(2)

Table 15. Bond lengths [Å] and angles [°] for 2,4diMeEu.

Eu(1)-O(2)	2.389(5)	C(18)-H(18B)	0.9800
Eu(1)-O(1)	2.422(4)	C(18)-H(18C)	0.9800
Eu(1)-O(1N)	2.444(13)	C(19)-C(20)	1.355(12)
Eu(1)-O(2N')	2.473(17)	C(19)-C(24)	1.394(12)
Eu(1)-O(1N')	2.488(19)	C(20)-C(21)	1.381(13)
Eu(1)-O(7N)	2.491(5)	C(20)-C(20A)	1.509(13)
Eu(1)-O(4N)	2.494(5)	C(20A)-H(20A)	0.9800
Eu(1)-O(8N)	2.504(5)	C(20A)-H(20B)	0.9800
Eu(1)-O(5N)	2.525(6)	C(20A)-H(20C)	0.9800
Eu(1)-N(15)	2.555(5)	C(21)-C(22)	1.390(14)
Eu(1)-O(2N)	2.564(11)	C(21)-H(21A)	0.9500
Eu(1)-N(30)	2.573(5)	C(22A)-C(22)	1.516(14)
O(1)-C(1)	1.265(8)	C(22A)-H(22A)	0.9800
O(2)-C(16)	1.242(8)	C(22A)-H(22B)	0.9800
N(1)-C(1)	1.334(8)	C(22A)-H(22C)	0.9800
N(1)-C(4)	1.451(10)	C(22)-C(23)	1.392(14)
N(1)-C(2)	1.505(10)	C(23)-C(24)	1.360(13)
N(2)-C(16)	1.345(8)	C(23)-H(23A)	0.9500
N(2)-C(19')	1.396(15)	C(24)-H(24A)	0.9500
N(2)-C(19)	1.474(10)	C(19')-C(20')	1.3900
N(2)-C(17)	1.494(8)	C(19')-C(24')	1.3900
N(15)-C(14)	1.338(8)	C(20')-C(21')	1.3900
N(15)-C(10)	1.360(7)	C(20')-H(20D)	0.9500
N(30)-C(29)	1.326(7)	C(21')-C(22')	1.3900
N(30)-C(25)	1.350(8)	C(21')-H(21B)	0.9500
C(1)-C(10)	1.516(9)	C(22')-C(23')	1.3900
C(2)-C(3)	1.483(13)	C(22')-C(22B)	1.522(8)
C(2)-H(2A)	0.9900	C(23')-C(24')	1.3900
C(2)-H(2B)	0.9900	C(23')-H(23B)	0.9500
C(3)-H(3A)	0.9800	C(24')-C(24A)	1.518(8)
C(3)-H(3B)	0.9800	C(24A)-H(24B)	0.9800
C(3)-H(3C)	0.9800	C(24A)-H(24C)	0.9800
C(4)-C(5)	1.386(11)	C(24A)-H(24D)	0.9800
C(4)-C(9)	1.391(10)	C(22B)-H(22D)	0.9800
C(5)-C(6)	1.384(13)	C(22B)-H(22E)	0.9800
C(5)-C(5A)	1.449(13)	C(22B)-H(22F)	0.9800
C(5)-H(5A)	0.9500	C(25)-C(26)	1.375(9)
C(5A)-H(5AA)	0.9800	C(26)-C(27)	1.385(10)
C(5A)-H(5AB)	0.9800	C(26)-H(26A)	0.9500
C(5A)-H(5AC)	0.9800	C(27)-C(28)	1.379(9)
C(9A)-C(9)	1.59(3)	C(27)-H(27A)	0.9500
C(9A)-H(9AA)	0.9800	C(28)-C(29)	1.405(9)
C(9A)-H(9AB)	0.9800	C(28)-H(28A)	0.9500
C(9A)-H(9AC)	0.9800	O(4N)-N(2N)	1.214(7)
C(6)-C(7)	1.385(14)	O(5N)-N(2N)	1.295(8)
C(6)-H(6A)	0.9500	O(6N)-N(2N)	1.224(7)
C(7)-C(8)	1.365(12)	O(7N)-N(3N)	1.241(9)
C(7)-C(7A)	1.540(12)	O(8N)-N(3N)	1.273(9)
C(7A)-H(7AA)	0.9800	O(9N)-N(3N)	1.206(9)
C(7A)-H(7AB)	0.9800	N(1N)-O(2N)	1.194(16)
C(7A)-H(7AC)	0.9800	N(1N)-O(3N)	1.226(16)
C(8)-C(9)	1.365(11)	N(1N)-O(1N)	1.346(18)
C(8)-H(8A)	0.9500	O(3N')-N(1N')	1.25(2)
C(9)-H(9A)	0.9500	O(2N')-N(1N')	1.28(2)
C(10)-C(11)	1.398(9)	N(1N')-O(1N')	1.18(3)
C(11)-C(12)	1.359(9)		
C(11)-H(11A)	0.9500	O(2)-Eu(1)-O(1)	172.05(16)
C(12)-C(13)	1.389(8)	O(2)-Eu(1)-O(1N)	105.4(3)
C(12)-H(12A)	0.9500	O(1)-Eu(1)-O(1N)	66.6(3)
C(13)-C(14)	1.383(8)	O(2)-Eu(1)-O(2N')	61.7(4)
C(13)-H(13A)	0.9500	O(1)-Eu(1)-O(2N')	111.0(4)
C(14)-C(29)	1.499(8)	O(2)-Eu(1)-O(1N')	96.1(5)
C(16)-C(25)	1.508(8)	O(1)-Eu(1)-O(1N')	76.1(4)
C(17)-C(18)	1.518(11)	O(2N')-Eu(1)-O(1N')	48.3(6)
C(17)-H(17A)	0.9900	O(2)-Eu(1)-O(7N)	72.75(19)
C(17)-H(17B)	0.9900	O(1)-Eu(1)-O(7N)	111.45(18)
C(18)-H(18A)	0.9800	O(1N)-Eu(1)-O(7N)	125.7(3)

O(2N')-Eu(1)-O(7N)	90.0(4)	O(1)-C(1)-C(10)	116.2(6)
O(1N')-Eu(1)-O(7N)	134.5(5)	N(1)-C(1)-C(10)	122.0(7)
O(2)-Eu(1)-O(4N)	109.90(19)	O(1)-C(1)-Eu(1)	39.4(3)
O(1)-Eu(1)-O(4N)	71.37(18)	N(1)-C(1)-Eu(1)	148.2(5)
O(1N)-Eu(1)-O(4N)	91.7(3)	C(10)-C(1)-Eu(1)	83.1(4)
O(2N')-Eu(1)-O(4N)	126.3(4)	C(3)-C(2)-N(1)	111.7(7)
O(1N')-Eu(1)-O(4N)	84.3(4)	C(3)-C(2)-H(2A)	109.3
O(7N)-Eu(1)-O(4N)	141.25(18)	N(1)-C(2)-H(2A)	109.3
O(2)-Eu(1)-O(8N)	113.3(2)	C(3)-C(2)-H(2B)	109.3
O(1)-Eu(1)-O(8N)	67.23(19)	N(1)-C(2)-H(2B)	109.3
O(1N)-Eu(1)-O(8N)	86.2(3)	H(2A)-C(2)-H(2B)	107.9
O(2N')-Eu(1)-O(8N)	84.1(4)	C(2)-C(3)-H(3A)	109.5
O(1N')-Eu(1)-O(8N)	100.4(4)	C(2)-C(3)-H(3B)	109.5
O(7N)-Eu(1)-O(8N)	50.5(2)	H(3A)-C(3)-H(3B)	109.5
O(4N)-Eu(1)-O(8N)	135.63(19)	C(2)-C(3)-H(3C)	109.5
O(2)-Eu(1)-O(5N)	65.3(2)	H(3A)-C(3)-H(3C)	109.5
O(1)-Eu(1)-O(5N)	112.45(19)	H(3B)-C(3)-H(3C)	109.5
O(1N)-Eu(1)-O(5N)	83.2(3)	C(5)-C(4)-C(9)	120.4(8)
O(2N')-Eu(1)-O(5N)	85.4(4)	C(5)-C(4)-N(1)	121.7(7)
O(1N')-Eu(1)-O(5N)	68.8(4)	C(9)-C(4)-N(1)	117.8(7)
O(7N)-Eu(1)-O(5N)	134.5(2)	C(6)-C(5)-C(4)	119.0(9)
O(4N)-Eu(1)-O(5N)	49.84(18)	C(6)-C(5)-C(5A)	115.4(9)
O(8N)-Eu(1)-O(5N)	168.4(2)	C(4)-C(5)-C(5A)	125.6(9)
O(2)-Eu(1)-N(15)	124.47(16)	C(6)-C(5)-H(5A)	120.5
O(1)-Eu(1)-N(15)	63.47(16)	C(4)-C(5)-H(5A)	120.5
O(1N)-Eu(1)-N(15)	130.0(3)	C(5)-C(5A)-H(5AA)	109.5
O(2N')-Eu(1)-N(15)	160.5(4)	C(5)-C(5A)-H(5AB)	109.5
O(1N')-Eu(1)-N(15)	137.5(5)	H(5AA)-C(5A)-H(5AB)	109.5
O(7N)-Eu(1)-N(15)	76.10(16)	C(5)-C(5A)-H(5AC)	109.5
O(4N)-Eu(1)-N(15)	71.18(16)	H(5AA)-C(5A)-H(5AC)	109.5
O(8N)-Eu(1)-N(15)	76.61(18)	H(5AB)-C(5A)-H(5AC)	109.5
O(5N)-Eu(1)-N(15)	114.02(18)	C(9)-C(9A)-H(9AA)	109.5
O(2)-Eu(1)-O(2N)	69.1(3)	C(9)-C(9A)-H(9AB)	109.5
O(1)-Eu(1)-O(2N)	104.4(3)	H(9AA)-C(9A)-H(9AB)	109.5
O(1N)-Eu(1)-O(2N)	51.1(4)	C(9)-C(9A)-H(9AC)	109.5
O(7N)-Eu(1)-O(2N)	81.0(3)	H(9AA)-C(9A)-H(9AC)	109.5
O(4N)-Eu(1)-O(2N)	137.2(3)	H(9AB)-C(9A)-H(9AC)	109.5
O(8N)-Eu(1)-O(2N)	70.2(3)	C(7)-C(6)-C(5)	120.4(9)
O(5N)-Eu(1)-O(2N)	99.3(3)	C(7)-C(6)-H(6A)	119.8
N(15)-Eu(1)-O(2N)	146.7(3)	C(5)-C(6)-H(6A)	119.8
O(2)-Eu(1)-N(30)	63.17(16)	C(8)-C(7)-C(6)	119.4(9)
O(1)-Eu(1)-N(30)	124.38(15)	C(8)-C(7)-C(7A)	120.7(10)
O(1N)-Eu(1)-N(30)	160.0(3)	C(6)-C(7)-C(7A)	119.8(9)
O(2N')-Eu(1)-N(30)	124.6(4)	C(7)-C(7A)-H(7AA)	109.5
O(1N')-Eu(1)-N(30)	145.3(4)	C(7)-C(7A)-H(7AB)	109.5
O(7N)-Eu(1)-N(30)	68.73(18)	H(7AA)-C(7A)-H(7AB)	109.5
O(4N)-Eu(1)-N(30)	78.18(17)	C(7)-C(7A)-H(7AC)	109.5
O(8N)-Eu(1)-N(30)	113.08(19)	H(7AA)-C(7A)-H(7AC)	109.5
O(5N)-Eu(1)-N(30)	77.0(2)	H(7AB)-C(7A)-H(7AC)	109.5
N(15)-Eu(1)-N(30)	63.07(15)	C(9)-C(8)-C(7)	121.6(9)
O(2N)-Eu(1)-N(30)	128.9(3)	C(9)-C(8)-H(8A)	119.2
C(1)-O(1)-Eu(1)	121.2(4)	C(7)-C(8)-H(8A)	119.2
C(16)-O(2)-Eu(1)	123.6(4)	C(8)-C(9)-C(4)	119.1(8)
C(1)-N(1)-C(4)	124.9(6)	C(8)-C(9)-C(9A)	123.4(13)
C(1)-N(1)-C(2)	117.6(7)	C(4)-C(9)-C(9A)	116.4(13)
C(4)-N(1)-C(2)	117.4(6)	C(8)-C(9)-H(9A)	120.4
C(16)-N(2)-C(19')	128.0(12)	C(4)-C(9)-H(9A)	120.4
C(16)-N(2)-C(19)	123.5(6)	N(15)-C(10)-C(11)	122.4(6)
C(16)-N(2)-C(17)	118.0(6)	N(15)-C(10)-C(1)	111.4(6)
C(19')-N(2)-C(17)	111.4(12)	C(11)-C(10)-C(1)	125.9(6)
C(19)-N(2)-C(17)	118.5(6)	C(12)-C(11)-C(10)	118.4(6)
C(14)-N(15)-C(10)	117.8(5)	C(12)-C(11)-H(11A)	120.8
C(14)-N(15)-Eu(1)	122.8(4)	C(10)-C(11)-H(11A)	120.8
C(10)-N(15)-Eu(1)	119.1(4)	C(11)-C(12)-C(13)	119.9(6)
C(29)-N(30)-C(25)	119.7(5)	C(11)-C(12)-H(12A)	120.1
C(29)-N(30)-Eu(1)	121.3(4)	C(13)-C(12)-H(12A)	120.1
C(25)-N(30)-Eu(1)	118.5(4)	C(14)-C(13)-C(12)	118.9(6)
O(1)-C(1)-N(1)	121.7(7)	C(14)-C(13)-H(13A)	120.5

C(12)-C(13)-H(13A)	120.5	C(22')-C(23')-H(23B)	120.0
N(15)-C(14)-C(13)	122.5(5)	C(24')-C(23')-H(23B)	120.0
N(15)-C(14)-C(29)	115.2(5)	C(23')-C(24')-C(19')	120.0
C(13)-C(14)-C(29)	122.2(5)	C(23')-C(24')-C(24A)	119.9(6)
O(2)-C(16)-N(2)	118.9(6)	C(19')-C(24')-C(24A)	120.0(6)
O(2)-C(16)-C(25)	117.1(6)	C(24')-C(24A)-H(24B)	109.5
N(2)-C(16)-C(25)	124.0(6)	C(24')-C(24A)-H(24C)	109.5
O(2)-C(16)-Eu(1)	37.8(3)	H(24B)-C(24A)-H(24C)	109.5
N(2)-C(16)-Eu(1)	148.5(5)	C(24')-C(24A)-H(24D)	109.5
C(25)-C(16)-Eu(1)	83.8(4)	H(24B)-C(24A)-H(24D)	109.5
N(2)-C(17)-C(18)	111.3(6)	H(24C)-C(24A)-H(24D)	109.5
N(2)-C(17)-H(17A)	109.4	C(22')-C(22B)-H(22D)	109.5
C(18)-C(17)-H(17A)	109.4	C(22')-C(22B)-H(22E)	109.5
N(2)-C(17)-H(17B)	109.4	H(22D)-C(22B)-H(22E)	109.5
C(18)-C(17)-H(17B)	109.4	C(22')-C(22B)-H(22F)	109.5
H(17A)-C(17)-H(17B)	108.0	H(22D)-C(22B)-H(22F)	109.5
C(17)-C(18)-H(18A)	109.5	H(22E)-C(22B)-H(22F)	109.5
C(17)-C(18)-H(18B)	109.5	N(30)-C(25)-C(26)	121.9(6)
H(18A)-C(18)-H(18B)	109.5	N(30)-C(25)-C(16)	111.6(5)
C(17)-C(18)-H(18C)	109.5	C(26)-C(25)-C(16)	126.2(6)
H(18A)-C(18)-H(18C)	109.5	C(25)-C(26)-C(27)	119.1(6)
H(18B)-C(18)-H(18C)	109.5	C(25)-C(26)-H(26A)	120.5
C(20)-C(19)-C(24)	121.5(8)	C(27)-C(26)-H(26A)	120.5
C(20)-C(19)-N(2)	122.5(8)	C(28)-C(27)-C(26)	119.1(7)
C(24)-C(19)-N(2)	116.0(8)	C(28)-C(27)-H(27A)	120.5
C(19)-C(20)-C(21)	117.9(8)	C(26)-C(27)-H(27A)	120.5
C(19)-C(20)-C(20A)	123.3(9)	C(27)-C(28)-C(29)	119.0(6)
C(21)-C(20)-C(20A)	118.9(9)	C(27)-C(28)-H(28A)	120.5
C(20)-C(20A)-H(20A)	109.5	C(29)-C(28)-H(28A)	120.5
C(20)-C(20A)-H(20B)	109.5	N(30)-C(29)-C(28)	121.2(6)
H(20A)-C(20A)-H(20B)	109.5	N(30)-C(29)-C(14)	117.4(5)
C(20)-C(20A)-H(20C)	109.5	C(28)-C(29)-C(14)	121.3(5)
H(20A)-C(20A)-H(20C)	109.5	N(2N)-O(4N)-Eu(1)	99.1(4)
H(20B)-C(20A)-H(20C)	109.5	N(2N)-O(5N)-Eu(1)	95.3(4)
C(20)-C(21)-C(22)	123.0(9)	N(3N)-O(7N)-Eu(1)	97.6(5)
C(20)-C(21)-H(21A)	118.5	N(3N)-O(8N)-Eu(1)	96.1(5)
C(22)-C(21)-H(21A)	118.5	O(2N)-N(1N)-O(3N)	121.5(13)
C(22)-C(22A)-H(22A)	109.5	O(2N)-N(1N)-O(1N)	116.5(13)
C(22)-C(22A)-H(22B)	109.5	O(3N)-N(1N)-O(1N)	121.9(13)
H(22A)-C(22A)-H(22B)	109.5	O(2N)-N(1N)-Eu(1)	60.6(8)
C(22)-C(22A)-H(22C)	109.5	O(3N)-N(1N)-Eu(1)	177.8(10)
H(22A)-C(22A)-H(22C)	109.5	O(1N)-N(1N)-Eu(1)	56.0(7)
H(22B)-C(22A)-H(22C)	109.5	N(1N)-O(1N)-Eu(1)	96.9(8)
C(21)-C(22)-C(23)	116.8(9)	N(1N)-O(2N)-Eu(1)	95.4(9)
C(21)-C(22)-C(22A)	123.2(10)	N(1N')-O(2N')-Eu(1)	97.9(13)
C(23)-C(22)-C(22A)	120.0(10)	O(1N')-N(1N')-O(3N')	121(2)
C(24)-C(23)-C(22)	121.5(10)	O(1N')-N(1N')-O(2N')	111.1(19)
C(24)-C(23)-H(23A)	119.3	O(3N')-N(1N')-O(2N')	127(2)
C(22)-C(23)-H(23A)	119.3	O(1N')-N(1N')-Eu(1)	56.5(12)
C(23)-C(24)-C(19)	119.4(9)	O(3N')-N(1N')-Eu(1)	174.8(15)
C(23)-C(24)-H(24A)	120.3	O(2N')-N(1N')-Eu(1)	56.5(11)
C(19)-C(24)-H(24A)	120.3	N(1N')-O(1N')-Eu(1)	100.3(14)
C(20')-C(19')-C(24')	120.0	O(4N)-N(2N)-O(6N)	124.6(6)
C(20')-C(19')-N(2)	120.8(11)	O(4N)-N(2N)-O(5N)	114.9(6)
C(24')-C(19')-N(2)	118.4(11)	O(6N)-N(2N)-O(5N)	119.9(7)
C(21')-C(20')-C(19')	120.0	O(4N)-N(2N)-Eu(1)	56.8(3)
C(21')-C(20')-H(20D)	120.0	O(6N)-N(2N)-Eu(1)	178.5(5)
C(19')-C(20')-H(20D)	120.0	O(5N)-N(2N)-Eu(1)	58.7(4)
C(20')-C(21')-C(22')	120.0	O(9N)-N(3N)-O(7N)	122.3(9)
C(20')-C(21')-H(21B)	120.0	O(9N)-N(3N)-O(8N)	121.7(8)
C(22')-C(21')-H(21B)	120.0	O(7N)-N(3N)-O(8N)	115.8(7)
C(21')-C(22')-C(23')	120.0	O(9N)-N(3N)-Eu(1)	173.1(6)
C(21')-C(22')-C(22B)	119.7(6)	O(7N)-N(3N)-Eu(1)	57.5(4)
C(23')-C(22')-C(22B)	120.1(6)	O(8N)-N(3N)-Eu(1)	58.3(4)
C(22')-C(23')-C(24')	120.0		

Table 16. Anisotropic displacement parameters ($Å^2$x 10^3) for 2,4diMeEu. 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)	39(1)	37(1)	36(1)	-3(1)	10(1)	-2(1)
O(1)	54(3)	61(3)	48(3)	3(2)	27(2)	-12(3)
O(2)	74(4)	46(3)	74(4)	-15(3)	30(3)	-21(3)
N(1)	46(4)	61(4)	67(4)	17(3)	29(3)	0(3)
N(2)	49(3)	27(3)	55(3)	-4(3)	12(3)	-9(2)
N(15)	29(3)	33(3)	37(3)	4(2)	6(2)	-3(2)
N(30)	39(3)	32(3)	34(3)	1(2)	8(2)	-9(2)
C(1)	39(4)	51(4)	59(4)	19(4)	21(3)	7(3)
C(2)	66(6)	118(8)	58(5)	10(5)	34(4)	-20(6)
C(3)	97(8)	129(9)	93(7)	-16(7)	61(6)	6(7)
C(4)	36(4)	75(6)	63(5)	16(4)	24(4)	0(4)
C(5)	51(5)	85(6)	72(5)	24(5)	37(4)	16(5)
C(5A)	59(7)	70(7)	85(8)	12(6)	25(6)	8(6)
C(9A)	59(7)	70(7)	85(8)	12(6)	25(6)	8(6)
C(6)	36(5)	167(11)	58(5)	17(7)	21(4)	9(6)
C(7)	59(5)	127(9)	46(5)	1(5)	28(4)	-24(6)
C(7A)	85(6)	147(8)	86(6)	-13(6)	27(5)	-35(6)
C(8)	72(6)	87(6)	61(5)	15(5)	37(5)	-18(5)
C(9)	41(4)	66(5)	73(5)	25(4)	24(4)	-9(4)
C(10)	29(3)	41(3)	47(4)	16(3)	11(3)	6(3)
C(11)	32(3)	32(3)	64(4)	17(3)	17(3)	3(3)
C(12)	43(4)	29(4)	59(4)	1(3)	11(3)	-6(3)
C(13)	52(4)	36(3)	41(3)	0(3)	13(3)	-8(3)
C(14)	33(3)	35(3)	41(3)	1(3)	9(3)	-4(3)
C(16)	52(4)	43(4)	48(4)	-4(3)	12(3)	-14(3)
C(17)	51(4)	33(4)	72(5)	-12(3)	15(4)	-7(3)
C(18)	91(7)	54(5)	65(5)	-20(4)	0(5)	-1(5)
C(19)	39(3)	32(3)	35(4)	-11(3)	3(3)	-13(3)
C(20)	47(4)	36(3)	34(4)	-2(3)	1(3)	-7(3)
C(20A)	75(6)	53(5)	69(6)	5(5)	3(5)	0(5)
C(21)	50(4)	41(4)	59(4)	-12(4)	11(4)	-5(3)
C(22A)	86(7)	78(7)	100(7)	-17(6)	44(6)	-36(6)
C(22)	49(4)	51(4)	59(4)	-9(4)	17(4)	-16(3)
C(23)	60(5)	42(4)	60(4)	4(4)	13(4)	-11(4)
C(24)	43(4)	36(3)	50(4)	-3(3)	1(3)	-4(3)
C(19')	39(3)	32(3)	35(4)	-11(3)	3(3)	-13(3)
C(20')	47(4)	36(3)	34(4)	-2(3)	1(3)	-7(3)
C(21')	50(4)	41(4)	59(4)	-12(4)	11(4)	-5(3)
C(22')	49(4)	51(4)	59(4)	-9(4)	17(4)	-16(3)
C(23')	60(5)	42(4)	60(4)	4(4)	13(4)	-11(4)
C(24')	43(4)	36(3)	50(4)	-3(3)	1(3)	-4(3)
C(24A)	75(6)	53(5)	69(6)	5(5)	3(5)	0(5)
C(22B)	86(7)	78(7)	100(7)	-17(6)	44(6)	-36(6)
C(25)	45(4)	39(3)	40(3)	-4(3)	9(3)	-18(3)
C(26)	79(6)	54(4)	44(4)	-6(4)	18(4)	-37(4)
C(27)	97(6)	61(5)	40(4)	-10(4)	23(4)	-48(5)
C(28)	87(6)	47(4)	37(4)	-11(3)	26(4)	-35(4)
C(29)	43(4)	35(3)	35(3)	-1(3)	7(3)	-13(3)
O(4N)	58(3)	45(3)	74(4)	-3(3)	-9(3)	7(3)
O(5N)	65(4)	66(4)	103(5)	-6(4)	-5(4)	5(3)
O(6N)	48(3)	68(4)	119(5)	-1(4)	-6(3)	15(3)
O(7N)	73(4)	45(3)	64(3)	16(3)	-2(3)	7(3)
O(8N)	51(3)	88(4)	82(4)	13(4)	14(3)	17(3)
O(9N)	63(5)	153(7)	138(7)	27(6)	-39(5)	10(5)
N(1N)	52(5)	46(3)	40(4)	-3(3)	14(4)	-4(4)
O(1N)	80(6)	51(4)	45(3)	5(3)	9(4)	6(4)
O(2N)	50(5)	41(3)	41(3)	3(2)	7(4)	1(4)
O(3N)	80(7)	41(3)	50(5)	-11(3)	17(5)	0(6)
O(3N')	80(7)	41(3)	50(5)	-11(3)	17(5)	0(6)
O(2N')	50(5)	41(3)	41(3)	3(2)	7(4)	1(4)
N(1N')	52(5)	46(3)	40(4)	-3(3)	14(4)	-4(4)
O(1N')	80(6)	51(4)	45(3)	5(3)	9(4)	6(4)
N(2N)	49(4)	41(4)	75(4)	-3(3)	5(3)	10(3)
N(3N)	57(5)	53(4)	78(5)	10(4)	0(4)	9(3)

Table 17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 2,4diMeEu.

	x	y	z	U(eq)
H(2A)	578	3039	3621	93
H(2B)	861	4064	3693	93

H(3A)	474	5552	3907	151
H(3B)	306	5160	3020	151
H(3C)	591	6177	3156	151
H(5A)	267	3990	1298	79
H(5AA)	57	4746	880	105
H(5AB)	373	4519	729	105
H(5AC)	326	5235	1554	105
H(9AA)	668	-642	3274	105
H(9AB)	579	951	3631	105
H(9AC)	851	893	3223	105
H(6A)	-88	2298	656	102
H(7AA)	-256	-1309	1282	157
H(7AB)	-93	-1398	555	157
H(7AC)	-332	-106	559	157
H(8A)	247	-1121	2146	84
H(9A)	597	523	2808	70
H(11A)	800	1293	1333	50
H(12A)	940	776	139	53
H(13A)	1195	2650	-420	51
H(17A)	1604	11854	1568	62
H(17B)	1857	12676	1238	62
H(18A)	2012	12386	2606	108
H(18B)	2192	11195	2192	108
H(18C)	1931	10587	2557	108
H(20A)	2155	8119	1471	101
H(20B)	2444	9048	1798	101
H(20C)	2445	7593	1220	101
H(21A)	2633	9050	262	60
H(22A)	2648	11741	-1252	127
H(22B)	2560	10036	-1575	127
H(22C)	2815	10271	-819	127
H(23A)	2128	12045	-1178	65
H(24A)	1807	11976	-343	53
H(20D)	2260	8676	1406	48
H(21B)	2649	8353	791	60
H(23B)	2328	11649	-831	65
H(24B)	1902	13411	-155	101
H(24C)	1670	12062	-195	101
H(24D)	1818	12363	-939	101
H(22D)	2955	9586	-21	127
H(22E)	2822	10821	-691	127
H(22F)	2760	9015	-844	127
H(26A)	1778	8640	-521	70
H(27A)	1652	6478	-1350	77
H(28A)	1377	4514	-938	66

Table 18. Torsion angles [°] for 2,4diMeEu.

Eu(1)-O(1)-C(1)-N(1)	-145.1(5)	C(6)-C(7)-C(8)-C(9)	-1.3(12)
Eu(1)-O(1)-C(1)-C(10)	35.9(7)	C(7A)-C(7)-C(8)-C(9)	179.0(8)
C(4)-N(1)-C(1)-O(1)	170.9(7)	C(7)-C(8)-C(9)-C(4)	-0.4(12)
C(2)-N(1)-C(1)-O(1)	-4.7(10)	C(7)-C(8)-C(9)-C(9A)	167.2(15)
C(4)-N(1)-C(1)-C(10)	-10.3(11)	C(5)-C(4)-C(9)-C(8)	1.7(11)
C(2)-N(1)-C(1)-C(10)	174.1(6)	N(1)-C(4)-C(9)-C(8)	179.4(7)
C(4)-N(1)-C(1)-Eu(1)	127.4(9)	C(5)-C(4)-C(9)-C(9A)	-166.9(13)
C(2)-N(1)-C(1)-Eu(1)	-48.2(12)	N(1)-C(4)-C(9)-C(9A)	10.8(15)
C(1)-N(1)-C(2)-C(3)	87.5(9)	C(14)-N(15)-C(10)-C(11)	0.9(9)
C(4)-N(1)-C(2)-C(3)	-88.4(9)	Eu(1)-N(15)-C(10)-C(11)	-173.4(4)
C(1)-N(1)-C(4)-C(5)	-67.9(10)	C(14)-N(15)-C(10)-C(1)	175.8(5)
C(2)-N(1)-C(4)-C(5)	107.7(8)	Eu(1)-N(15)-C(10)-C(1)	1.5(6)
C(1)-N(1)-C(4)-C(9)	114.4(8)	O(1)-C(1)-C(10)-N(15)	-23.1(8)
C(2)-N(1)-C(4)-C(9)	-70.0(9)	N(1)-C(1)-C(10)-N(15)	158.0(6)
C(9)-C(4)-C(5)-C(6)	-1.2(11)	Eu(1)-C(1)-C(10)-N(15)	-1.0(4)
N(1)-C(4)-C(5)-C(6)	-178.8(7)	O(1)-C(1)-C(10)-C(11)	151.6(6)
C(9)-C(4)-C(5)-C(5A)	-178.1(8)	N(1)-C(1)-C(10)-C(11)	-27.4(10)
N(1)-C(4)-C(5)-C(5A)	4.3(12)	Eu(1)-C(1)-C(10)-C(11)	173.6(6)
C(4)-C(5)-C(6)-C(7)	-0.6(12)	N(15)-C(10)-C(11)-C(12)	-1.8(9)
C(5A)-C(5)-C(6)-C(7)	176.7(8)	C(1)-C(10)-C(11)-C(12)	-175.9(6)
C(5)-C(6)-C(7)-C(8)	1.8(12)	C(10)-C(11)-C(12)-C(13)	1.5(10)
C(5)-C(6)-C(7)-C(7A)	-178.5(8)	C(11)-C(12)-C(13)-C(14)	-0.4(10)

C(10)-N(15)-C(14)-C(13)	0.3(9)	C(22B)-C(22')-C(23')-C(24')	-176(3)
Eu(1)-N(15)-C(14)-C(13)	174.3(5)	C(22')-C(23')-C(24')-C(19')	0.0
C(10)-N(15)-C(14)-C(29)	-176.8(5)	C(22')-C(23')-C(24')-C(24A)	-178(2)
Eu(1)-N(15)-C(14)-C(29)	-2.7(7)	C(20')-C(19')-C(24')-C(23')	0.0
C(12)-C(13)-C(14)-N(15)	-0.5(10)	N(2)-C(19')-C(24')-C(23')	-170(2)
C(12)-C(13)-C(14)-C(29)	176.3(6)	C(20')-C(19')-C(24')-C(24A)	178(2)
Eu(1)-O(2)-C(16)-N(2)	-151.3(5)	N(2)-C(19')-C(24')-C(24A)	8(2)
Eu(1)-O(2)-C(16)-C(25)	30.8(9)	C(29)-N(30)-C(25)-C(26)	-1.3(10)
C(19')-N(2)-C(16)-O(2)	159.0(12)	Eu(1)-N(30)-C(25)-C(26)	-173.5(6)
C(19)-N(2)-C(16)-O(2)	176.7(7)	C(29)-N(30)-C(25)-C(16)	172.6(6)
C(17)-N(2)-C(16)-O(2)	-1.1(10)	Eu(1)-N(30)-C(25)-C(16)	0.4(7)
C(19')-N(2)-C(16)-C(25)	-23.2(15)	O(2)-C(16)-C(25)-N(30)	-18.7(9)
C(19)-N(2)-C(16)-C(25)	-5.6(11)	N(2)-C(16)-C(25)-N(30)	163.5(6)
C(17)-N(2)-C(16)-C(25)	176.6(6)	Eu(1)-C(16)-C(25)-N(30)	-0.3(5)
C(19')-N(2)-C(16)-Eu(1)	124.8(13)	O(2)-C(16)-C(25)-C(26)	154.9(8)
C(19)-N(2)-C(16)-Eu(1)	142.4(8)	N(2)-C(16)-C(25)-C(26)	-22.9(12)
C(17)-N(2)-C(16)-Eu(1)	-35.3(12)	Eu(1)-C(16)-C(25)-C(26)	173.3(8)
C(16)-N(2)-C(17)-C(18)	91.5(8)	N(30)-C(25)-C(26)-C(27)	1.4(12)
C(19')-N(2)-C(17)-C(18)	-71.7(11)	C(16)-C(25)-C(26)-C(27)	-171.6(8)
C(19)-N(2)-C(17)-C(18)	-86.3(8)	C(25)-C(26)-C(27)-C(28)	0.6(13)
C(16)-N(2)-C(19)-C(20)	-77.4(10)	C(26)-C(27)-C(28)-C(29)	-2.7(13)
C(17)-N(2)-C(19)-C(20)	100.3(9)	C(25)-N(30)-C(29)-C(28)	-0.8(10)
C(16)-N(2)-C(19)-C(24)	105.0(9)	Eu(1)-N(30)-C(29)-C(28)	171.1(5)
C(17)-N(2)-C(19)-C(24)	-77.3(9)	C(25)-N(30)-C(29)-C(14)	-176.9(6)
C(24)-C(19)-C(20)-C(21)	-1.4(13)	Eu(1)-N(30)-C(29)-C(14)	-5.0(8)
N(2)-C(19)-C(20)-C(21)	-178.8(8)	C(27)-C(28)-C(29)-N(30)	2.9(12)
C(24)-C(19)-C(20)-C(20A)	179.5(9)	C(27)-C(28)-C(29)-C(14)	178.8(7)
N(2)-C(19)-C(20)-C(20A)	2.1(13)	N(15)-C(14)-C(29)-N(30)	5.0(9)
C(19)-C(20)-C(21)-C(22)	-0.1(13)	C(13)-C(14)-C(29)-N(30)	-172.1(6)
C(20A)-C(20)-C(21)-C(22)	179.0(9)	N(15)-C(14)-C(29)-C(28)	-171.1(7)
C(20)-C(21)-C(22)-C(23)	0.3(14)	C(13)-C(14)-C(29)-C(28)	11.8(10)
C(20)-C(21)-C(22)-C(22A)	-179.2(10)	O(2N)-N(1N)-O(1N)-Eu(1)	4.1(12)
C(21)-C(22)-C(23)-C(24)	0.9(14)	O(3N)-N(1N)-O(1N)-Eu(1)	179.4(10)
C(22A)-C(22)-C(23)-C(24)	-179.5(9)	O(3N)-N(1N)-O(2N)-Eu(1)	-179.2(11)
C(22)-C(23)-C(24)-C(19)	-2.4(14)	O(1N)-N(1N)-O(2N)-Eu(1)	-3.9(11)
C(20)-C(19)-C(24)-C(23)	2.6(13)	Eu(1)-O(2N')-N(1N')-O(1N')	15.3(17)
N(2)-C(19)-C(24)-C(23)	-179.8(8)	Eu(1)-O(2N')-N(1N')-O(3N')	-175.5(17)
C(16)-N(2)-C(19')-C(20')	-56.7(19)	O(3N')-N(1N')-O(1N')-Eu(1)	174.7(15)
C(17)-N(2)-C(19')-C(20')	104.5(14)	O(2N')-N(1N')-O(1N')-Eu(1)	-15.3(17)
C(16)-N(2)-C(19')-C(24')	112.9(13)	Eu(1)-O(4N)-N(2N)-O(6N)	179.5(7)
C(17)-N(2)-C(19')-C(24')	-85.9(14)	Eu(1)-O(4N)-N(2N)-O(5N)	-9.1(7)
C(24')-C(19')-C(20')-C(21')	0.0	Eu(1)-O(5N)-N(2N)-O(4N)	9.0(7)
N(2)-C(19')-C(20')-C(21')	169(2)	Eu(1)-O(5N)-N(2N)-O(6N)	-179.3(6)
C(19')-C(20')-C(21')-C(22')	0.0	Eu(1)-O(7N)-N(3N)-O(9N)	-171.8(7)
C(20')-C(21')-C(22')-C(23')	0.0	Eu(1)-O(7N)-N(3N)-O(8N)	3.0(7)
C(20')-C(21')-C(22')-C(22B)	176(3)	Eu(1)-O(8N)-N(3N)-O(9N)	171.9(8)
C(21')-C(22')-C(23')-C(24')	0.0	Eu(1)-O(8N)-N(3N)-O(7N)	-3.0(7)

Table 19. Crystal data and structure refinement for 2,4diMeTb.

Identification code	2,4diMeTb	
Empirical formula	C32 H34 N7 O11 Tb	
Formula weight	851.58	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 48.332(9) Å	α= 90°.
	b = 8.6695(16) Å	β= 101.483(5)°.
	c = 16.778(3) Å	γ = 90°.
Volume	6889(2) Å^3	
Z	8	
Density (calculated)	1.642 Mg/m^3	
Absorption coefficient	2.123 mm^{-1}	
F(000)	3424	
Crystal size	0.136 x 0.034 x 0.021 mm^3	
Theta range for data collection	1.720 to 27.000°.	
Index ranges	-61<=h<=61, -11<=k<=11, -21<=l<=21	
Reflections collected	29690	

Independent reflections	7515 [R(int) = 0.1187]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.962 and 0.750
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7515 / 70 / 499
Goodness-of-fit on F^2	1.007
Final R indices [I>2sigma(I)]	R1 = 0.0599, wR2 = 0.1318
R indices (all data)	R1 = 0.1053, wR2 = 0.1558
Extinction coefficient	n/a
Largest diff. peak and hole	2.102 and -2.391 e. $Å^{-3}$

Table 20. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 2,4diMeTb. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Tb(1)	1256(1)	7157(1)	1888(1)	34(1)
O(1)	1058(1)	5209(7)	2627(3)	47(1)
O(2)	1445(1)	9369(6)	1377(3)	45(1)
N(1)	693(2)	3563(9)	2577(4)	51(2)
N(2)	1811(1)	10409(7)	929(4)	40(2)
N(15)	1111(1)	4683(7)	1133(4)	34(1)
N(30)	1448(1)	6761(7)	620(3)	33(1)
C(1)	903(2)	4175(10)	2258(5)	43(2)
C(2)	667(2)	4073(13)	3407(6)	66(3)
C(3)	487(3)	5471(15)	3393(7)	92(4)
C(4)	478(2)	2550(10)	2151(5)	48(2)
C(5)	275(2)	3042(11)	1501(6)	53(2)
C(5A)	256(3)	4575(16)	1142(9)	62(3)
C(9A)	673(7)	610(40)	3270(20)	62(3)
C(6)	74(2)	2027(15)	1116(6)	68(3)
C(7)	70(2)	487(14)	1361(6)	63(3)
C(7A)	-146(2)	-664(16)	925(7)	96(4)
C(8)	279(2)	25(12)	2028(6)	62(3)
C(9)	473(2)	1031(11)	2433(5)	52(2)
C(10)	964(2)	3614(9)	1455(4)	35(2)
C(11)	904(2)	2178(9)	1114(5)	40(2)
C(12)	997(2)	1826(9)	415(5)	44(2)
C(13)	1148(2)	2904(9)	68(5)	42(2)
C(14)	1206(2)	4320(9)	448(4)	36(2)
C(16)	1620(2)	9293(9)	919(5)	39(2)
C(17)	1799(2)	11730(9)	1476(5)	47(2)
C(18)	1998(2)	11484(12)	2304(6)	67(3)
C(19)	2023(2)	10416(14)	434(6)	37(2)
C(20)	2267(2)	9569(12)	645(6)	40(2)
C(20A)	2330(3)	8539(14)	1382(7)	55(3)
C(21)	2465(2)	9655(13)	149(7)	46(3)
C(22A)	2632(3)	10621(18)	-1112(9)	77(4)
C(22)	2421(3)	10563(14)	-555(7)	50(3)
C(23)	2176(2)	11406(14)	-732(7)	51(3)
C(24)	1982(2)	11362(13)	-243(7)	42(3)
C(19')	2070(5)	10390(30)	644(16)	37(2)
C(20')	2270(5)	9290(30)	963(14)	40(2)
C(21')	2504(5)	9050(30)	610(14)	46(3)
C(22')	2537(5)	9910(30)	-63(15)	50(3)
C(23')	2337(5)	11020(30)	-382(14)	51(3)
C(24')	2104(5)	11260(30)	-28(15)	42(3)
C(24A)	1884(6)	12450(40)	-380(20)	55(3)
C(22B)	2816(6)	9840(50)	-360(20)	77(4)
C(25)	1596(2)	7906(9)	360(4)	37(2)
C(26)	1683(2)	7837(10)	-381(5)	54(2)
C(27)	1609(2)	6564(11)	-867(5)	61(3)
C(28)	1458(2)	5407(9)	-605(5)	51(2)
C(29)	1379(2)	5514(9)	143(4)	36(2)
O(4N)	1617(1)	5146(7)	2352(3)	47(1)
O(5N)	1787(1)	7424(7)	2354(4)	54(2)
O(6N)	2065(1)	5502(7)	2791(4)	63(2)
O(7N)	915(1)	8004(7)	679(4)	59(2)
O(8N)	730(1)	7204(8)	1642(5)	71(2)
O(9N)	463(2)	7835(10)	479(6)	105(3)

N(1N)	1178(3)	9217(18)	3205(9)	40(3)
O(1N)	1316(3)	7810(30)	3316(13)	53(3)
O(2N)	1071(3)	9520(15)	2490(8)	44(2)
O(3N)	1139(3)	10014(14)	3760(7)	53(3)
O(3N')	1302(5)	9920(20)	3911(11)	53(3)
O(2N')	1197(4)	9650(20)	2568(12)	44(2)
N(1N')	1292(5)	9090(30)	3287(14)	40(3)
O(1N')	1396(5)	7980(40)	3340(20)	53(3)
N(2N)	1827(2)	5982(7)	2509(4)	41(2)
N(3N)	699(2)	7711(9)	917(6)	61(2)

Table 21. Bond lengths [Å] and angles [°] for 2,4diMeTb.

Tb(1)-O(2)	2.360(5)	C(12)-C(13)	1.383(11)
Tb(1)-O(1)	2.404(5)	C(12)-H(12A)	0.9500
Tb(1)-O(1N)	2.42(2)	C(13)-C(14)	1.386(10)
Tb(1)-O(7N)	2.458(6)	C(13)-H(13A)	0.9500
Tb(1)-O(2N')	2.49(2)	C(14)-C(29)	1.484(10)
Tb(1)-O(4N)	2.480(5)	C(16)-C(25)	1.515(11)
Tb(1)-O(1N')	2.49(3)	C(17)-C(18)	1.539(12)
Tb(1)-O(8N)	2.492(7)	C(17)-H(17A)	0.9900
Tb(1)-N(30)	2.507(6)	C(17)-H(17B)	0.9900
Tb(1)-N(15)	2.518(6)	C(18)-H(18A)	0.9800
Tb(1)-O(2N)	2.526(13)	C(18)-H(18B)	0.9800
Tb(1)-O(5N)	2.540(6)	C(18)-H(18C)	0.9800
O(1)-C(1)	1.250(10)	C(19)-C(20)	1.373(14)
O(2)-C(16)	1.252(9)	C(19)-C(24)	1.383(15)
N(1)-C(1)	1.347(10)	C(20)-C(21)	1.391(15)
N(1)-C(4)	1.438(11)	C(20)-C(20A)	1.506(15)
N(1)-C(2)	1.491(12)	C(20A)-H(20A)	0.9800
N(2)-C(16)	1.334(10)	C(20A)-H(20B)	0.9800
N(2)-C(19')	1.428(19)	C(20A)-H(20C)	0.9800
N(2)-C(19)	1.443(12)	C(21)-C(22)	1.400(16)
N(2)-C(17)	1.476(10)	C(21)-H(21A)	0.9500
N(15)-C(10)	1.344(9)	C(22A)-C(22)	1.515(17)
N(15)-C(14)	1.356(9)	C(22A)-H(22A)	0.9800
N(30)-C(29)	1.347(9)	C(22A)-H(22B)	0.9800
N(30)-C(25)	1.347(9)	C(22A)-H(22C)	0.9800
C(1)-C(10)	1.515(11)	C(22)-C(23)	1.372(17)
C(2)-C(3)	1.488(15)	C(23)-C(24)	1.364(15)
C(2)-H(2A)	0.9900	C(23)-H(23A)	0.9500
C(2)-H(2B)	0.9900	C(24)-H(24A)	0.9500
C(3)-H(3A)	0.9800	C(19')-C(20')	1.3900
C(3)-H(3B)	0.9800	C(19')-C(24')	1.3900
C(3)-H(3C)	0.9800	C(20')-C(21')	1.3900
C(4)-C(5)	1.381(13)	C(20')-H(20D)	0.9500
C(4)-C(9)	1.402(12)	C(21')-C(22')	1.3900
C(5)-C(6)	1.371(14)	C(21')-H(21B)	0.9500
C(5)-C(5A)	1.454(15)	C(22')-C(23')	1.3900
C(5)-H(5A)	0.9500	C(22')-C(22B)	1.527(9)
C(5A)-H(5AA)	0.9800	C(23')-C(24')	1.3900
C(5A)-H(5AB)	0.9800	C(23')-H(23B)	0.9500
C(5A)-H(5AC)	0.9800	C(24')-C(24A)	1.517(8)
C(9A)-C(9)	1.57(3)	C(24A)-H(24B)	0.9800
C(9A)-H(9AA)	0.9800	C(24A)-H(24C)	0.9800
C(9A)-H(9AB)	0.9800	C(24A)-H(24D)	0.9800
C(9A)-H(9AC)	0.9800	C(22B)-H(22D)	0.9800
C(6)-C(7)	1.398(15)	C(22B)-H(22E)	0.9800
C(6)-H(6A)	0.9500	C(22B)-H(22F)	0.9800
C(7)-C(8)	1.408(14)	C(25)-C(26)	1.389(11)
C(7)-C(7A)	1.523(14)	C(26)-C(27)	1.377(12)
C(7A)-H(7AA)	0.9800	C(26)-H(26A)	0.9500
C(7A)-H(7AB)	0.9800	C(27)-C(28)	1.364(11)
C(7A)-H(7AC)	0.9800	C(27)-H(27A)	0.9500
C(8)-C(9)	1.360(13)	C(28)-C(29)	1.386(10)
C(8)-H(8A)	0.9500	C(28)-H(28A)	0.9500
C(9)-H(9A)	0.9500	O(4N)-N(2N)	1.231(8)
C(10)-C(11)	1.377(11)	O(5N)-N(2N)	1.284(8)
C(11)-C(12)	1.370(11)	O(6N)-N(2N)	1.227(8)
C(11)-H(11A)	0.9500	O(7N)-N(3N)	1.217(10)

O(8N)-N(3N)	1.273(10)
O(9N)-N(3N)	1.232(10)
N(1N)-O(3N)	1.204(18)
N(1N)-O(2N)	1.237(19)
N(1N)-O(1N)	1.38(3)
O(3N')-N(1N')	1.26(3)
O(2N')-N(1N')	1.30(3)
N(1N')-O(1N')	1.08(4)

O(2)-Tb(1)-O(1)	169.09(18)
O(2)-Tb(1)-O(1N)	100.9(5)
O(1)-Tb(1)-O(1N)	68.7(5)
O(2)-Tb(1)-O(7N)	72.7(2)
O(1)-Tb(1)-O(7N)	111.4(2)
O(1N)-Tb(1)-O(7N)	132.4(5)
O(2)-Tb(1)-O(2N')	63.2(5)
O(1)-Tb(1)-O(2N')	106.3(5)
O(7N)-Tb(1)-O(2N')	89.9(5)
O(2)-Tb(1)-O(4N)	112.7(2)
O(1)-Tb(1)-O(4N)	70.9(2)
O(1N)-Tb(1)-O(4N)	85.2(5)
O(7N)-Tb(1)-O(4N)	141.6(2)
O(2N')-Tb(1)-O(4N)	127.2(5)
O(2)-Tb(1)-O(1N')	94.2(7)
O(1)-Tb(1)-O(1N')	75.9(7)
O(7N)-Tb(1)-O(1N')	136.6(7)
O(2N')-Tb(1)-O(1N')	48.6(9)
O(4N)-Tb(1)-O(1N')	81.8(7)
O(2)-Tb(1)-O(8N)	112.5(2)
O(1)-Tb(1)-O(8N)	66.4(2)
O(1N)-Tb(1)-O(8N)	94.4(4)
O(7N)-Tb(1)-O(8N)	50.5(2)
O(2N')-Tb(1)-O(8N)	81.6(5)
O(4N)-Tb(1)-O(8N)	134.0(2)
O(1N')-Tb(1)-O(8N)	103.1(6)
O(2)-Tb(1)-N(30)	64.33(18)
O(1)-Tb(1)-N(30)	126.45(19)
O(1N)-Tb(1)-N(30)	151.6(4)
O(7N)-Tb(1)-N(30)	69.0(2)
O(2N')-Tb(1)-N(30)	127.1(5)
O(4N)-Tb(1)-N(30)	79.32(19)
O(1N')-Tb(1)-N(30)	142.4(6)
O(8N)-Tb(1)-N(30)	113.5(2)
O(2)-Tb(1)-N(15)	126.78(19)
O(1)-Tb(1)-N(15)	64.01(19)
O(1N)-Tb(1)-N(15)	131.6(5)
O(7N)-Tb(1)-N(15)	76.4(2)
O(2N')-Tb(1)-N(15)	157.6(5)
O(4N)-Tb(1)-N(15)	70.59(19)
O(1N')-Tb(1)-N(15)	136.7(8)
O(8N)-Tb(1)-N(15)	76.0(2)
N(30)-Tb(1)-N(15)	64.51(19)
O(2)-Tb(1)-O(2N)	71.4(3)
O(1)-Tb(1)-O(2N)	98.9(3)
O(1N)-Tb(1)-O(2N)	52.8(6)
O(7N)-Tb(1)-O(2N)	81.7(3)
O(4N)-Tb(1)-O(2N)	136.7(3)
O(8N)-Tb(1)-O(2N)	67.8(4)
N(30)-Tb(1)-O(2N)	132.1(3)
N(15)-Tb(1)-O(2N)	143.8(3)
O(2)-Tb(1)-O(5N)	66.18(19)
O(1)-Tb(1)-O(5N)	112.78(19)
O(1N)-Tb(1)-O(5N)	76.1(4)
O(7N)-Tb(1)-O(5N)	134.2(2)
O(2N')-Tb(1)-O(5N)	88.9(5)
O(4N)-Tb(1)-O(5N)	50.40(18)
O(1N')-Tb(1)-O(5N)	67.2(6)
O(8N)-Tb(1)-O(5N)	169.7(2)
N(30)-Tb(1)-O(5N)	75.6(2)
N(15)-Tb(1)-O(5N)	113.29(19)
O(2N)-Tb(1)-O(5N)	102.7(3)
C(1)-O(1)-Tb(1)	120.6(5)
C(16)-O(2)-Tb(1)	122.6(5)
C(1)-N(1)-C(4)	124.8(7)
C(1)-N(1)-C(2)	117.7(8)
C(4)-N(1)-C(2)	117.3(7)
C(16)-N(2)-C(19')	129.7(14)
C(16)-N(2)-C(19)	124.4(7)
C(16)-N(2)-C(17)	117.3(7)
C(19')-N(2)-C(17)	111.2(15)
C(19)-N(2)-C(17)	118.3(7)
C(10)-N(15)-C(14)	118.4(6)
C(10)-N(15)-Tb(1)	120.1(5)
C(14)-N(15)-Tb(1)	121.1(5)
C(29)-N(30)-C(25)	118.9(6)
C(29)-N(30)-Tb(1)	121.6(5)
C(25)-N(30)-Tb(1)	119.0(5)
O(1)-C(1)-N(1)	120.6(8)
O(1)-C(1)-C(10)	117.9(7)
N(1)-C(1)-C(10)	121.5(8)
C(3)-C(2)-N(1)	112.6(8)
C(3)-C(2)-H(2A)	109.1
N(1)-C(2)-H(2A)	109.1
C(3)-C(2)-H(2B)	109.1
N(1)-C(2)-H(2B)	109.1
H(2A)-C(2)-H(2B)	107.8
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(5)-C(4)-C(9)	119.9(9)
C(5)-C(4)-N(1)	122.3(8)
C(9)-C(4)-N(1)	117.7(8)
C(6)-C(5)-C(4)	119.9(9)
C(6)-C(5)-C(5A)	114.3(10)
C(4)-C(5)-C(5A)	125.8(10)
C(6)-C(5)-H(5A)	120.0
C(4)-C(5)-H(5A)	120.0
C(5)-C(5A)-H(5AA)	109.5
C(5)-C(5A)-H(5AB)	109.5
H(5AA)-C(5A)-H(5AB)	109.5
C(5)-C(5A)-H(5AC)	109.5
H(5AA)-C(5A)-H(5AC)	109.5
H(5AB)-C(5A)-H(5AC)	109.5
C(9)-C(9A)-H(9AA)	109.5
C(9)-C(9A)-H(9AB)	109.5
H(9AA)-C(9A)-H(9AB)	109.5
C(9)-C(9A)-H(9AC)	109.5
H(9AA)-C(9A)-H(9AC)	109.5
H(9AB)-C(9A)-H(9AC)	109.5
C(5)-C(6)-C(7)	121.6(10)
C(5)-C(6)-H(6A)	119.2
C(7)-C(6)-H(6A)	119.2
C(6)-C(7)-C(8)	117.1(9)
C(6)-C(7)-C(7A)	122.2(11)
C(8)-C(7)-C(7A)	120.6(11)
C(7)-C(7A)-H(7AA)	109.5
C(7)-C(7A)-H(7AB)	109.5
H(7AA)-C(7A)-H(7AB)	109.5
C(7)-C(7A)-H(7AC)	109.5
H(7AA)-C(7A)-H(7AC)	109.5
H(7AB)-C(7A)-H(7AC)	109.5
C(9)-C(8)-C(7)	121.9(10)
C(9)-C(8)-H(8A)	119.1

C(7)-C(8)-H(8A)	119.1	C(24')-C(19')-N(2)	121.1(13)
C(8)-C(9)-C(4)	119.4(9)	C(19')-C(20')-C(21')	120.0
C(8)-C(9)-C(9A)	122.4(15)	C(19')-C(20')-H(20D)	120.0
C(4)-C(9)-C(9A)	117.9(14)	C(21')-C(20')-H(20D)	120.0
C(8)-C(9)-H(9A)	120.3	C(22')-C(21')-C(20')	120.0
C(4)-C(9)-H(9A)	120.3	C(22')-C(21')-H(21B)	120.0
N(15)-C(10)-C(11)	122.7(7)	C(20')-C(21')-H(21B)	120.0
N(15)-C(10)-C(1)	110.4(7)	C(21')-C(22')-C(23')	120.0
C(11)-C(10)-C(1)	126.7(7)	C(21')-C(22')-C(22B)	119.6(6)
C(12)-C(11)-C(10)	118.7(7)	C(23')-C(22')-C(22B)	119.6(6)
C(12)-C(11)-H(11A)	120.7	C(24')-C(23')-C(22')	120.0
C(10)-C(11)-H(11A)	120.7	C(24')-C(23')-H(23B)	120.0
C(11)-C(12)-C(13)	119.9(8)	C(22')-C(23')-H(23B)	120.0
C(11)-C(12)-H(12A)	120.0	C(23')-C(24')-C(19')	120.0
C(13)-C(12)-H(12A)	120.0	C(23')-C(24')-C(24A)	119.9(6)
C(14)-C(13)-C(12)	118.8(8)	C(19')-C(24')-C(24A)	120.1(6)
C(14)-C(13)-H(13A)	120.6	C(24')-C(24A)-H(24B)	109.5
C(12)-C(13)-H(13A)	120.6	C(24')-C(24A)-H(24C)	109.5
N(15)-C(14)-C(13)	121.5(7)	H(24B)-C(24A)-H(24C)	109.5
N(15)-C(14)-C(29)	116.1(6)	C(24')-C(24A)-H(24D)	109.5
C(13)-C(14)-C(29)	122.4(7)	H(24B)-C(24A)-H(24D)	109.5
O(2)-C(16)-N(2)	120.2(7)	H(24C)-C(24A)-H(24D)	109.5
O(2)-C(16)-C(25)	116.3(7)	C(22')-C(22B)-H(22D)	109.5
N(2)-C(16)-C(25)	123.5(7)	C(22')-C(22B)-H(22E)	109.5
N(2)-C(17)-C(18)	111.1(7)	H(22D)-C(22B)-H(22E)	109.5
N(2)-C(17)-H(17A)	109.4	C(22')-C(22B)-H(22F)	109.5
C(18)-C(17)-H(17A)	109.4	H(22D)-C(22B)-H(22F)	109.5
N(2)-C(17)-H(17B)	109.4	H(22E)-C(22B)-H(22F)	109.5
C(18)-C(17)-H(17B)	109.4	N(30)-C(25)-C(26)	122.2(7)
H(17A)-C(17)-H(17B)	108.0	N(30)-C(25)-C(16)	111.4(6)
C(17)-C(18)-H(18A)	109.5	C(26)-C(25)-C(16)	126.0(7)
C(17)-C(18)-H(18B)	109.5	C(27)-C(26)-C(25)	118.5(8)
H(18A)-C(18)-H(18B)	109.5	C(27)-C(26)-H(26A)	120.8
C(17)-C(18)-H(18C)	109.5	C(25)-C(26)-H(26A)	120.8
H(18A)-C(18)-H(18C)	109.5	C(28)-C(27)-C(26)	119.4(8)
H(18B)-C(18)-H(18C)	109.5	C(28)-C(27)-H(27A)	120.3
C(20)-C(19)-C(24)	120.4(10)	C(26)-C(27)-H(27A)	120.3
C(20)-C(19)-N(2)	121.4(9)	C(27)-C(28)-C(29)	120.3(7)
C(24)-C(19)-N(2)	118.1(10)	C(27)-C(28)-H(28A)	119.9
C(19)-C(20)-C(21)	118.3(10)	C(29)-C(28)-H(28A)	119.9
C(19)-C(20)-C(20A)	123.5(10)	N(30)-C(29)-C(28)	120.8(7)
C(21)-C(20)-C(20A)	118.2(10)	N(30)-C(29)-C(14)	116.4(6)
C(20)-C(20A)-H(20A)	109.5	C(28)-C(29)-C(14)	122.8(7)
C(20)-C(20A)-H(20B)	109.5	N(2N)-O(4N)-Tb(1)	98.7(4)
H(20A)-C(20A)-H(20B)	109.5	N(2N)-O(5N)-Tb(1)	94.4(4)
C(20)-C(20A)-H(20C)	109.5	N(3N)-O(7N)-Tb(1)	98.3(5)
H(20A)-C(20A)-H(20C)	109.5	N(3N)-O(8N)-Tb(1)	95.0(5)
H(20B)-C(20A)-H(20C)	109.5	O(3N)-N(1N)-O(2N)	121.9(14)
C(20)-C(21)-C(22)	121.8(11)	O(3N)-N(1N)-O(1N)	123.1(16)
C(20)-C(21)-H(21A)	119.1	O(2N)-N(1N)-O(1N)	114.5(15)
C(22)-C(21)-H(21A)	119.1	O(3N)-N(1N)-Tb(1)	177.0(12)
C(22)-C(22A)-H(22A)	109.5	O(2N)-N(1N)-Tb(1)	59.3(8)
C(22)-C(22A)-H(22B)	109.5	O(1N)-N(1N)-Tb(1)	55.4(10)
H(22A)-C(22A)-H(22B)	109.5	N(1N)-O(1N)-Tb(1)	96.6(12)
C(22)-C(22A)-H(22C)	109.5	N(1N)-O(2N)-Tb(1)	95.9(9)
H(22A)-C(22A)-H(22C)	109.5	N(1N')-O(2N')-Tb(1)	92.9(15)
H(22B)-C(22A)-H(22C)	109.5	O(1N')-N(1N')-O(3N')	120(3)
C(23)-C(22)-C(21)	117.5(11)	O(1N')-N(1N')-O(2N')	118(3)
C(23)-C(22)-C(22A)	120.5(12)	O(3N')-N(1N')-O(2N')	121(2)
C(21)-C(22)-C(22A)	122.0(12)	O(1N')-N(1N')-Tb(1)	59(2)
C(24)-C(23)-C(22)	121.5(11)	O(3N')-N(1N')-Tb(1)	178.0(18)
C(24)-C(23)-H(23A)	119.2	O(2N')-N(1N')-Tb(1)	60.2(13)
C(22)-C(23)-H(23A)	119.2	N(1N')-O(1N')-Tb(1)	99(2)
C(23)-C(24)-C(19)	120.3(11)	O(6N)-N(2N)-O(4N)	123.5(7)
C(23)-C(24)-H(24A)	119.9	O(6N)-N(2N)-O(5N)	120.0(7)
C(19)-C(24)-H(24A)	119.9	O(4N)-N(2N)-O(5N)	116.4(7)
C(20')-C(19')-C(24')	120.0	O(6N)-N(2N)-Tb(1)	178.2(5)
C(20')-C(19')-N(2)	117.9(13)	O(4N)-N(2N)-Tb(1)	56.8(4)

O(5N)-N(2N)-Tb(1)	59.8(4)	O(7N)-N(3N)-Tb(1)	57.1(4)
O(7N)-N(3N)-O(9N)	122.5(10)	O(9N)-N(3N)-Tb(1)	175.0(7)
O(7N)-N(3N)-O(8N)	116.0(7)	O(8N)-N(3N)-Tb(1)	59.0(4)
O(9N)-N(3N)-O(8N)	121.4(9)		

Table 22. Anisotropic displacement parameters ($Å^2$x 10^3) for 2,4diMeTb. 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)	42(1)	28(1)	31(1)	-1(1)	4(1)	-1(1)
O(1)	55(4)	44(3)	44(3)	0(3)	16(3)	-12(3)
O(2)	58(4)	23(3)	54(3)	-3(2)	16(3)	-7(3)
N(1)	49(4)	54(5)	57(4)	6(4)	24(4)	-1(4)
N(2)	48(4)	28(3)	40(4)	-3(3)	4(3)	-7(3)
N(15)	38(4)	26(3)	38(3)	3(3)	5(3)	0(3)
N(30)	41(4)	25(3)	30(3)	2(2)	0(3)	-1(3)
C(1)	42(5)	40(5)	50(5)	12(4)	14(4)	9(4)
C(2)	58(6)	87(8)	58(6)	14(5)	24(5)	-7(6)
C(3)	99(9)	106(10)	80(8)	-14(7)	40(7)	16(8)
C(4)	45(5)	51(6)	54(5)	10(4)	20(4)	-6(4)
C(5)	53(6)	56(6)	55(5)	13(4)	26(4)	4(5)
C(5A)	58(8)	55(8)	70(8)	2(7)	7(6)	-5(6)
C(9A)	58(8)	55(8)	70(8)	2(7)	7(6)	-5(6)
C(6)	49(6)	107(10)	47(5)	6(6)	12(4)	11(6)
C(7)	60(6)	86(8)	50(6)	-8(5)	31(5)	-26(6)
C(7A)	88(9)	139(12)	63(7)	-15(7)	21(6)	-47(8)
C(8)	76(7)	61(6)	59(6)	9(5)	33(5)	-14(5)
C(9)	45(5)	56(6)	54(5)	13(4)	9(4)	-7(4)
C(10)	41(4)	27(4)	35(4)	10(3)	2(3)	6(3)
C(11)	38(4)	28(4)	56(5)	8(4)	11(4)	-4(4)
C(12)	44(5)	33(5)	53(5)	-1(4)	6(4)	-2(4)
C(13)	51(5)	32(4)	42(4)	0(4)	9(4)	-7(4)
C(14)	39(4)	32(4)	36(4)	-3(3)	0(3)	0(3)
C(16)	50(5)	26(4)	38(4)	6(3)	4(4)	0(4)
C(17)	56(5)	23(4)	58(5)	-8(4)	7(4)	-5(4)
C(18)	79(7)	48(5)	66(6)	-23(5)	-8(5)	-2(5)
C(19)	44(6)	29(4)	35(6)	-13(5)	1(5)	-14(4)
C(20)	45(4)	32(4)	38(5)	0(4)	-1(4)	-4(3)
C(20A)	63(6)	45(6)	54(6)	-2(5)	2(5)	7(5)
C(21)	48(4)	40(4)	50(5)	-7(4)	9(4)	-1(4)
C(22A)	77(7)	77(8)	83(7)	-8(6)	28(6)	-21(6)
C(22)	50(5)	48(5)	54(5)	-2(4)	10(4)	-10(4)
C(23)	55(5)	45(4)	52(4)	1(4)	9(4)	-10(4)
C(24)	43(5)	35(4)	47(4)	3(3)	3(4)	-3(4)
C(19')	44(6)	29(4)	35(6)	-13(5)	1(5)	-14(4)
C(20')	45(4)	32(4)	38(5)	0(4)	-1(4)	-4(3)
C(21')	48(4)	40(4)	50(5)	-7(4)	9(4)	-1(4)
C(22')	50(5)	48(5)	54(5)	-2(4)	10(4)	-10(4)
C(23')	55(5)	45(4)	52(4)	1(4)	9(4)	-10(4)
C(24')	43(5)	35(4)	47(4)	3(3)	3(4)	-3(4)
C(24A)	63(6)	45(6)	54(6)	-2(5)	2(5)	7(5)
C(22B)	77(7)	77(8)	83(7)	-8(6)	28(6)	-21(6)
C(25)	43(4)	34(4)	34(4)	3(3)	2(3)	-7(4)
C(26)	80(6)	46(5)	38(4)	-3(4)	16(4)	-30(5)
C(27)	103(8)	46(5)	38(4)	-8(4)	27(5)	-35(5)
C(28)	83(7)	35(5)	36(4)	-14(4)	16(4)	-27(5)
C(29)	48(5)	31(4)	27(4)	4(3)	1(3)	-8(4)
O(4N)	47(4)	38(3)	51(3)	3(3)	-4(3)	4(3)
O(5N)	55(4)	38(4)	62(4)	4(3)	-7(3)	-2(3)
O(6N)	48(4)	51(4)	83(5)	-3(3)	-4(3)	10(3)
O(7N)	57(4)	56(4)	56(4)	12(3)	-4(3)	8(3)
O(8N)	55(4)	76(5)	82(5)	18(4)	15(4)	16(4)
O(9N)	61(5)	108(7)	128(8)	25(6)	-27(5)	10(5)
N(1N)	45(6)	36(4)	38(4)	-4(3)	11(5)	0(5)
O(1N)	60(6)	53(4)	46(3)	0(3)	9(5)	3(5)
O(2N)	51(5)	36(3)	46(3)	1(3)	9(4)	6(4)
O(3N)	73(8)	43(4)	41(5)	-11(4)	10(6)	2(6)
O(3N')	73(8)	43(4)	41(5)	-11(4)	10(6)	2(6)
O(2N')	51(5)	36(3)	46(3)	1(3)	9(4)	6(4)
N(1N')	45(6)	36(4)	38(4)	-4(3)	11(5)	0(5)

O(1N')	60(6)	53(4)	46(3)	0(3)	9(5)	3(5)
N(2N)	51(4)	28(4)	41(4)	-4(3)	4(3)	7(3)
N(3N)	44(5)	50(5)	80(6)	16(4)	-7(4)	8(4)

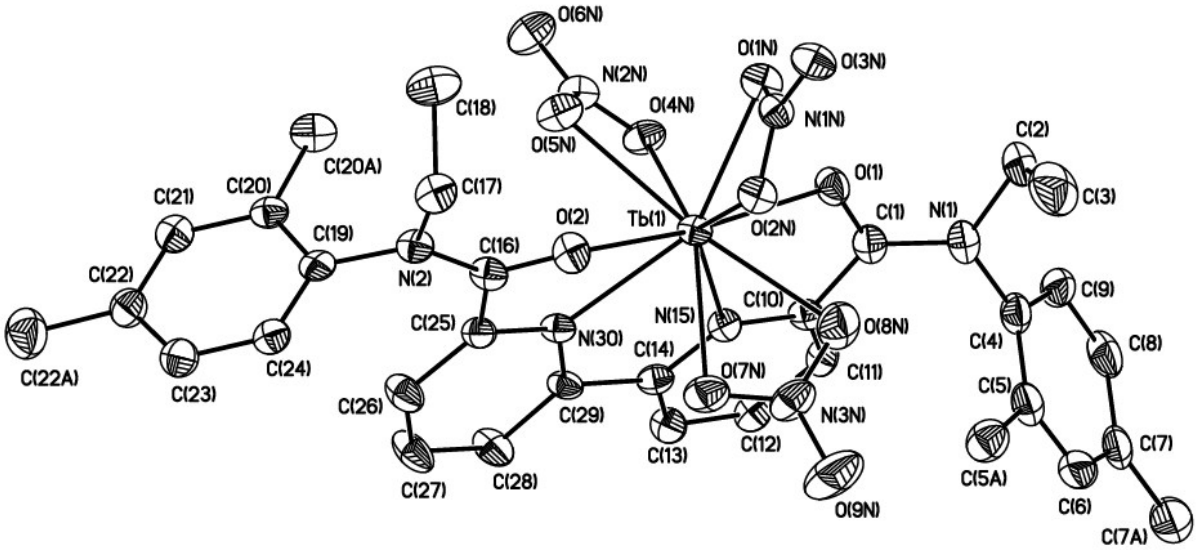
Table 23. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 2,4diMeTb.

	x	y	z	U(eq)
H(2A)	585	3224	3679	79
H(2B)	857	4295	3730	79
H(3A)	462	5701	3945	138
H(3B)	303	5285	3041	138
H(3C)	579	6348	3183	138
H(5A)	274	4081	1321	63
H(5AA)	71	4705	784	92
H(5AB)	404	4699	825	92
H(5AC)	280	5352	1574	92
H(9AA)	739	-452	3245	92
H(9AB)	569	716	3708	92
H(9AC)	835	1314	3362	92
H(6A)	-65	2379	672	81
H(7AA)	-257	-1069	1308	143
H(7AB)	-48	-1515	713	143
H(7AC)	-272	-148	474	143
H(8A)	284	-1020	2201	75
H(9A)	604	708	2904	62
H(11A)	801	1446	1359	48
H(12A)	957	843	169	52
H(13A)	1210	2679	-421	50
H(17A)	1603	11861	1558	56
H(17B)	1854	12683	1221	56
H(18A)	1992	12393	2647	101
H(18B)	2191	11327	2222	101
H(18C)	1937	10574	2570	101
H(20A)	2153	8172	1513	83
H(20B)	2437	9120	1844	83
H(20C)	2443	7654	1268	83
H(21A)	2636	9082	292	55
H(22A)	2655	11690	-1277	116
H(22B)	2564	9988	-1594	116
H(22C)	2815	10222	-823	116
H(23A)	2141	12034	-1205	61
H(24A)	1817	11985	-369	51
H(20D)	2248	8696	1422	47
H(21B)	2640	8291	827	55
H(23B)	2360	11607	-841	61
H(24B)	1978	13410	-484	83
H(24C)	1760	12648	2	83
H(24D)	1772	12065	-896	83
H(22D)	2908	8848	-207	116
H(22E)	2940	10677	-101	116
H(22F)	2780	9966	-948	116
H(26A)	1790	8650	-548	65
H(27A)	1663	6491	-1380	73
H(28A)	1406	4525	-938	61

Table 24. Torsion angles [°] for 2,4diMeTb.

Tb(1)-O(1)-C(1)-N(1)	-148.5(6)	N(1)-C(4)-C(5)-C(5A)	2.8(15)
Tb(1)-O(1)-C(1)-C(10)	32.9(9)	C(4)-C(5)-C(6)-C(7)	-0.4(14)
C(4)-N(1)-C(1)-O(1)	170.0(8)	C(5A)-C(5)-C(6)-C(7)	177.1(9)
C(2)-N(1)-C(1)-O(1)	-4.7(12)	C(5)-C(6)-C(7)-C(8)	0.9(14)
C(4)-N(1)-C(1)-C(10)	-11.4(12)	C(5)-C(6)-C(7)-C(7A)	-178.4(9)
C(2)-N(1)-C(1)-C(10)	174.0(7)	C(6)-C(7)-C(8)-C(9)	1.4(14)
C(1)-N(1)-C(2)-C(3)	88.4(11)	C(7A)-C(7)-C(8)-C(9)	-179.3(9)
C(4)-N(1)-C(2)-C(3)	-86.6(11)	C(7)-C(8)-C(9)-C(4)	-4.1(14)
C(1)-N(1)-C(4)-C(5)	-67.5(12)	C(7)-C(8)-C(9)-C(9A)	169.2(17)
C(2)-N(1)-C(4)-C(5)	107.2(10)	C(5)-C(4)-C(9)-C(8)	4.5(13)
C(1)-N(1)-C(4)-C(9)	114.8(9)	N(1)-C(4)-C(9)-C(8)	-177.7(8)
C(2)-N(1)-C(4)-C(9)	-70.6(11)	C(5)-C(4)-C(9)-C(9A)	-169.1(16)
C(9)-C(4)-C(5)-C(6)	-2.3(13)	N(1)-C(4)-C(9)-C(9A)	8.7(18)
N(1)-C(4)-C(5)-C(6)	-180.0(8)	C(14)-N(15)-C(10)-C(11)	-0.7(11)
C(9)-C(4)-C(5)-C(5A)	-179.5(10)	Tb(1)-N(15)-C(10)-C(11)	-173.1(5)

C(14)-N(15)-C(10)-C(1)	174.2(6)
Tb(1)-N(15)-C(10)-C(1)	1.8(8)
O(1)-C(1)-C(10)-N(15)	-21.8(10)
N(1)-C(1)-C(10)-N(15)	159.6(7)
O(1)-C(1)-C(10)-C(11)	152.9(8)
N(1)-C(1)-C(10)-C(11)	-25.8(12)
N(15)-C(10)-C(11)-C(12)	-0.4(11)
C(1)-C(10)-C(11)-C(12)	-174.4(7)
C(10)-C(11)-C(12)-C(13)	0.2(12)
C(11)-C(12)-C(13)-C(14)	1.0(12)
C(10)-N(15)-C(14)-C(13)	1.9(11)
Tb(1)-N(15)-C(14)-C(13)	174.3(6)
C(10)-N(15)-C(14)-C(29)	-177.0(6)
Tb(1)-N(15)-C(14)-C(29)	-4.7(9)
C(12)-C(13)-C(14)-N(15)	-2.1(12)
C(12)-C(13)-C(14)-C(29)	176.8(7)
Tb(1)-O(2)-C(16)-N(2)	-150.1(5)
Tb(1)-O(2)-C(16)-C(25)	31.1(9)
C(19')-N(2)-C(16)-O(2)	161.2(14)
C(19)-N(2)-C(16)-O(2)	179.1(8)
C(17)-N(2)-C(16)-O(2)	-1.8(11)
C(19')-N(2)-C(16)-C(25)	-20.1(17)
C(19)-N(2)-C(16)-C(25)	-2.3(12)
C(17)-N(2)-C(16)-C(25)	176.8(7)
C(16)-N(2)-C(17)-C(18)	93.6(9)
C(19')-N(2)-C(17)-C(18)	-72.5(13)
C(19)-N(2)-C(17)-C(18)	-87.3(10)
C(16)-N(2)-C(19)-C(20)	-79.8(12)
C(17)-N(2)-C(19)-C(20)	101.1(11)
C(16)-N(2)-C(19)-C(24)	103.2(11)
C(17)-N(2)-C(19)-C(24)	-75.8(11)
C(24)-C(19)-C(20)-C(21)	-1.8(15)
N(2)-C(19)-C(20)-C(21)	-178.7(10)
C(24)-C(19)-C(20)-C(20A)	178.7(10)
N(2)-C(19)-C(20)-C(20A)	1.9(15)
C(19)-C(20)-C(21)-C(22)	-0.6(16)
C(20A)-C(20)-C(21)-C(22)	178.9(10)
C(20)-C(21)-C(22)-C(23)	1.6(17)
C(20)-C(21)-C(22)-C(22A)	-178.0(12)
C(21)-C(22)-C(23)-C(24)	-0.2(17)
C(22A)-C(22)-C(23)-C(24)	179.4(11)
C(22)-C(23)-C(24)-C(19)	-2.2(17)
C(20)-C(19)-C(24)-C(23)	3.2(16)
N(2)-C(19)-C(24)-C(23)	-179.8(10)
C(16)-N(2)-C(19')-C(20')	-57(2)
C(17)-N(2)-C(19')-C(20')	106.7(16)
C(16)-N(2)-C(19')-C(24')	111.6(17)
C(17)-N(2)-C(19')-C(24')	-84.6(19)
C(24')-C(19')-C(20')-C(21')	0.0
N(2)-C(19')-C(20')-C(21')	169(3)
C(19')-C(20')-C(21')-C(22')	0.0
C(20')-C(21')-C(22')-C(23')	0.0
C(20')-C(21')-C(22')-C(22B)	169(3)
C(21')-C(22')-C(23')-C(24')	0.0
C(22B)-C(22')-C(23')-C(24')	-169(3)
C(22')-C(23')-C(24')-C(19')	0.0
C(22')-C(23')-C(24')-C(24A)	-179(3)
C(20')-C(19')-C(24')-C(23')	0.0
N(2)-C(19')-C(24')-C(23')	-169(3)
C(20')-C(19')-C(24')-C(24A)	179(3)
N(2)-C(19')-C(24')-C(24A)	11(3)
C(29)-N(30)-C(25)-C(26)	-0.6(12)
Tb(1)-N(30)-C(25)-C(26)	-172.9(7)
C(29)-N(30)-C(25)-C(16)	172.5(6)
Tb(1)-N(30)-C(25)-C(16)	0.1(8)
O(2)-C(16)-C(25)-N(30)	-18.9(10)
N(2)-C(16)-C(25)-N(30)	162.4(7)
O(2)-C(16)-C(25)-C(26)	153.8(8)
N(2)-C(16)-C(25)-C(26)	-24.9(13)
N(30)-C(25)-C(26)-C(27)	1.1(14)
C(16)-C(25)-C(26)-C(27)	-170.9(9)
C(25)-C(26)-C(27)-C(28)	-0.8(16)
C(26)-C(27)-C(28)-C(29)	0.0(16)
C(25)-N(30)-C(29)-C(28)	-0.3(12)
Tb(1)-N(30)-C(29)-C(28)	171.9(6)
C(25)-N(30)-C(29)-C(14)	-177.7(7)
Tb(1)-N(30)-C(29)-C(14)	-5.6(9)
C(27)-C(28)-C(29)-N(30)	0.6(14)
C(27)-C(28)-C(29)-C(14)	177.8(9)
N(15)-C(14)-C(29)-N(30)	6.6(10)
C(13)-C(14)-C(29)-N(30)	-172.4(7)
N(15)-C(14)-C(29)-C(28)	-170.8(8)
C(13)-C(14)-C(29)-C(28)	10.3(12)
O(3N)-N(1N)-O(1N)-Tb(1)	176.8(13)
O(2N)-N(1N)-O(1N)-Tb(1)	4.3(15)
O(3N)-N(1N)-O(2N)-Tb(1)	-176.7(13)
O(1N)-N(1N)-O(2N)-Tb(1)	-4.2(14)
Tb(1)-O(2N')-N(1N')-O(1N')	12(3)
Tb(1)-O(2N')-N(1N')-O(3N')	-177.9(19)
O(3N')-N(1N')-O(1N')-Tb(1)	177.7(19)
O(2N')-N(1N')-O(1N')-Tb(1)	-12(3)
Tb(1)-O(4N)-N(2N)-O(6N)	177.8(6)
Tb(1)-O(4N)-N(2N)-O(5N)	-2.9(7)
Tb(1)-O(5N)-N(2N)-O(6N)	-177.9(6)
Tb(1)-O(5N)-N(2N)-O(4N)	2.8(7)
Tb(1)-O(7N)-N(3N)-O(9N)	-174.1(8)
Tb(1)-O(7N)-N(3N)-O(8N)	3.1(9)
Tb(1)-O(8N)-N(3N)-O(7N)	-3.0(9)
Tb(1)-O(8N)-N(3N)-O(9N)	174.2(8)



A general view of the 2,4diMeTb complex in crystal. The non-hydrogen atoms are only given for clarity by probability ellipsoids of atomic displacements (p=0.5).

Table 25. Crystal data and structure refinement for 3,4diMeDy.

Identification code	3,4diMeDy	
Empirical formula	C32 H34 Dy N7 O11	
Formula weight	855.16	
Temperature	120(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 48.3072(8) Å	α= 90°.
	b = 8.49250(10) Å	β= 98.8150(10)°.
	c = 16.9413(3) Å	γ = 90°.
Volume	6868.05(19) Å^3	
Z	8	
Density (calculated)	1.654 Mg/m^3	
Absorption coefficient	12.248 mm^{-1}	
F(000)	3432	
Crystal size	0.34 x 0.28 x 0.07 mm^3	
Theta range for data collection	1.85 to 72.34°.	
Index ranges	-55<=h<=50, -10<=k<=10, -20<=l<=20	
Reflections collected	79105	
Independent reflections	6624 [R(int) = 0.0633]	
Completeness to theta = 68.00°	98.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.864 and 0.471	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6624 / 96 / 570	
Goodness-of-fit on F^2	1.030	
Final R indices for 6194 refl. with [I>2sigma(I)]	R1 = 0.0325, wR2 = 0.0810	
R indices (all data)	R1 = 0.0351, wR2 = 0.0829	
Largest diff. peak and hole	0.849 and -0.885 e.Å-3	

Table 26. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for 3,4diMeDy. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Dy(1)	1246(1)	1835(1)	6980(1)	28(1)
O(1)	1100(1)	-284(3)	6077(1)	38(1)
O(2)	1426(1)	4162(3)	7588(2)	34(1)
O(2')	1557(3)	3771(16)	7533(7)	32(3)
N(1)	1127(1)	-639(3)	7622(1)	24(1)
N(2)	1435(1)	1590(3)	8431(2)	25(1)

N(3)	739(1)	-1975(3)	5766(2)	36(1)
N(4)	1778(1)	5344(3)	8408(2)	36(1)
C(1)	982(1)	-1739(3)	7160(2)	28(1)
C(2)	917(1)	-3188(3)	7462(2)	32(1)
C(3)	1005(1)	-3493(4)	8262(2)	34(1)
C(4)	1152(1)	-2367(4)	8743(2)	32(1)
C(5)	1212(1)	-928(3)	8395(2)	25(1)
C(6)	1576(1)	2813(3)	8810(2)	28(1)
C(7)	1656(1)	2826(4)	9631(2)	33(1)
C(8)	1595(1)	1528(4)	10067(2)	35(1)
C(9)	1457(1)	258(4)	9678(2)	30(1)
C(10)	1376(1)	336(3)	8859(2)	25(1)
C(11)	935(1)	-1281(4)	6290(2)	32(1)
C(12)	736(1)	-1657(5)	4903(2)	51(1)
C(13)	575(1)	-187(6)	4624(3)	67(1)
C(14)	487(1)	-2668(4)	5986(2)	38(1)
C(15)	427(1)	-4244(4)	5843(2)	45(1)
C(16)	176(1)	-4888(5)	6030(2)	49(1)
C(17)	-11(1)	-3899(6)	6336(2)	54(1)
C(18)	53(1)	-2344(6)	6471(3)	55(1)
C(19)	302(1)	-1704(5)	6301(2)	46(1)
C(20)	112(1)	-6578(5)	5901(3)	66(1)
C(21)	-289(1)	-4533(8)	6526(3)	84(2)
C(22)	1601(1)	4151(4)	8232(2)	38(1)
C(23)	1777(1)	6612(4)	7801(2)	46(1)
C(24)	1963(1)	6237(5)	7194(3)	64(1)
C(25)	2023(4)	5300(20)	9052(13)	33(4)
C(26)	2027(2)	6180(11)	9705(5)	41(2)
C(27)	2245(3)	6159(14)	10328(7)	48(3)
C(28)	2464(3)	5199(17)	10241(6)	48(3)
C(29)	2471(2)	4300(12)	9518(5)	50(2)
C(30)	2240(2)	4343(10)	8918(5)	37(2)
C(31)	2275(3)	6960(14)	11046(7)	87(4)
C(32)	2730(2)	5012(14)	10862(6)	81(3)
C(25')	1962(4)	5540(30)	9107(17)	31(4)
C(26')	2231(2)	4886(12)	9221(8)	47(3)
C(27')	2436(3)	5031(17)	9910(11)	55(4)
C(28')	2345(3)	5904(19)	10494(11)	54(4)
C(29')	2077(2)	6659(10)	10433(5)	42(2)
C(30')	1896(2)	6477(9)	9728(5)	26(2)
C(31')	2705(3)	4252(17)	9907(11)	106(5)
C(32')	2538(3)	6176(16)	11322(8)	91(4)
N(1N)	688(1)	2109(3)	7410(2)	39(1)
O(1N)	724(1)	1540(3)	6736(2)	40(1)
O(2N)	899(1)	2709(3)	7825(1)	39(1)
N(2N)	1185(1)	4059(3)	5683(2)	46(1)
O(3N)	461(1)	2015(4)	7639(2)	59(1)
O(4N)	1380(1)	2968(3)	5775(2)	40(1)
O(5N)	1026(1)	4077(4)	6180(2)	41(1)
O(4N')	1151(3)	2483(16)	5548(8)	44(3)
O(5N')	1143(3)	4380(16)	6352(9)	34(3)
O(6N)	1169(1)	5021(4)	5144(2)	82(1)
N(3N)	1832(1)	764(4)	7071(4)	45(1)
O(7N)	1634(1)	137(6)	6902(2)	60(1)
O(8N)	1830(1)	2176(6)	7288(4)	113(3)
O(9N)	2076(1)	146(6)	7055(4)	78(1)
N(3N')	1831(4)	830(30)	6740(14)	44(6)
O(7N')	1685(3)	1710(14)	6236(8)	41(3)
O(8N')	1721(4)	267(19)	7291(10)	44(4)
O(9N')	2067(4)	520(30)	6594(13)	70(6)

Table 27. Bond lengths [Å] and angles [°] for 3,4diMeDy.

Dy(1)-O(2')	2.324(13)	Dy(1)-O(7N)	2.384(3)
Dy(1)-O(2)	2.333(3)	Dy(1)-O(1)	2.398(2)

Dy(1)-O(5N')	2.426(14)	C(23)-H(23B)	0.9900
Dy(1)-O(4N)	2.431(3)	C(24)-H(24A)	0.9800
Dy(1)-O(4N')	2.460(13)	C(24)-H(24B)	0.9800
Dy(1)-N(1)	2.476(2)	C(24)-H(24C)	0.9800
Dy(1)-O(2N)	2.479(2)	C(25)-C(26)	1.33(2)
Dy(1)-O(5N)	2.480(3)	C(25)-C(30)	1.371(19)
Dy(1)-N(2)	2.496(3)	C(26)-C(27)	1.370(16)
Dy(1)-O(1N)	2.505(2)	C(26)-H(26A)	0.9500
O(1)-C(11)	1.252(4)	C(27)-C(28)	1.36(2)
O(2)-C(22)	1.275(4)	C(27)-C(31)	1.381(17)
O(2')-C(22)	1.215(13)	C(28)-C(29)	1.448(13)
N(1)-C(5)	1.334(4)	C(28)-C(32)	1.538(14)
N(1)-C(1)	1.345(4)	C(29)-C(30)	1.389(10)
N(2)-C(10)	1.344(4)	C(29)-H(29A)	0.9500
N(2)-C(6)	1.349(4)	C(30)-H(30A)	0.9500
N(3)-C(11)	1.332(4)	C(31)-H(31A)	0.9800
N(3)-C(14)	1.451(4)	C(31)-H(31B)	0.9800
N(3)-C(12)	1.485(5)	C(31)-H(31C)	0.9800
N(4)-C(22)	1.329(4)	C(32)-H(32A)	0.9800
N(4)-C(25')	1.38(3)	C(32)-H(32B)	0.9800
N(4)-C(25)	1.484(19)	C(32)-H(32C)	0.9800
N(4)-C(23)	1.488(4)	C(25')-C(30')	1.39(3)
C(1)-C(2)	1.386(4)	C(25')-C(26')	1.40(2)
C(1)-C(11)	1.507(5)	C(26')-C(27')	1.42(2)
C(2)-C(3)	1.382(5)	C(26')-H(26B)	0.9500
C(2)-H(2A)	0.9500	C(27')-C(28')	1.36(3)
C(3)-C(4)	1.381(5)	C(27')-C(31')	1.46(2)
C(3)-H(3A)	0.9500	C(28')-C(29')	1.434(17)
C(4)-C(5)	1.404(4)	C(28')-C(32')	1.577(17)
C(4)-H(4A)	0.9500	C(29')-C(30')	1.375(12)
C(5)-C(10)	1.485(4)	C(29')-H(29B)	0.9500
C(6)-C(7)	1.386(4)	C(30')-H(30B)	0.9500
C(6)-C(22)	1.518(4)	C(31')-H(31D)	0.9800
C(7)-C(8)	1.383(4)	C(31')-H(31E)	0.9800
C(7)-H(7A)	0.9500	C(31')-H(31F)	0.9800
C(8)-C(9)	1.381(4)	C(32')-H(32D)	0.9800
C(8)-H(8A)	0.9500	C(32')-H(32E)	0.9800
C(9)-C(10)	1.386(4)	C(32')-H(32F)	0.9800
C(9)-H(9A)	0.9500	N(1N)-O(3N)	1.222(4)
C(12)-C(13)	1.508(7)	N(1N)-O(2N)	1.255(4)
C(12)-H(12A)	0.9900	N(1N)-O(1N)	1.277(4)
C(12)-H(12B)	0.9900	N(2N)-O(5N')	1.213(15)
C(13)-H(13A)	0.9800	N(2N)-O(6N)	1.218(4)
C(13)-H(13B)	0.9800	N(2N)-O(5N)	1.224(5)
C(13)-H(13C)	0.9800	N(2N)-O(4N)	1.312(4)
C(14)-C(19)	1.378(5)	N(2N)-O(4N')	1.363(14)
C(14)-C(15)	1.383(5)	N(3N)-O(7N)	1.095(6)
C(15)-C(16)	1.412(5)	N(3N)-O(8N)	1.255(6)
C(15)-H(15A)	0.9500	N(3N)-O(9N)	1.293(6)
C(16)-C(17)	1.391(7)	N(3N')-O(9N')	1.23(3)
C(16)-C(20)	1.477(6)	N(3N')-O(8N')	1.24(3)
C(17)-C(18)	1.368(7)	N(3N')-O(7N')	1.26(2)
C(17)-C(21)	1.524(6)		
C(18)-C(19)	1.392(6)	O(2')-Dy(1)-O(2)	18.1(3)
C(18)-H(18A)	0.9500	O(2')-Dy(1)-O(7N)	89.2(4)
C(19)-H(19A)	0.9500	O(2)-Dy(1)-O(7N)	107.15(16)
C(20)-H(20A)	0.9800	O(2')-Dy(1)-O(1)	153.8(4)
C(20)-H(20B)	0.9800	O(2)-Dy(1)-O(1)	166.13(9)
C(20)-H(20C)	0.9800	O(7N)-Dy(1)-O(1)	70.59(13)
C(21)-H(21A)	0.9800	O(2')-Dy(1)-O(5N')	67.9(5)
C(21)-H(21B)	0.9800	O(2)-Dy(1)-O(5N')	58.5(4)
C(21)-H(21C)	0.9800	O(7N)-Dy(1)-O(5N')	128.7(4)
C(23)-C(24)	1.499(6)	O(1)-Dy(1)-O(5N')	111.6(4)
C(23)-H(23A)	0.9900	O(2')-Dy(1)-O(4N)	79.7(3)

O(2)-Dy(1)-O(4N)	84.70(10)	C(11)-N(3)-C(14)	123.2(3)
O(7N)-Dy(1)-O(4N)	83.18(13)	C(11)-N(3)-C(12)	118.4(3)
O(1)-Dy(1)-O(4N)	81.45(9)	C(14)-N(3)-C(12)	116.3(3)
O(5N')-Dy(1)-O(4N)	48.9(3)	C(22)-N(4)-C(25')	126.3(11)
O(2')-Dy(1)-O(4N')	104.5(5)	C(22)-N(4)-C(25)	123.8(8)
O(2)-Dy(1)-O(4N')	104.3(3)	C(22)-N(4)-C(23)	117.6(3)
O(7N)-Dy(1)-O(4N')	96.3(3)	C(25')-N(4)-C(23)	116.1(10)
O(1)-Dy(1)-O(4N')	63.0(3)	C(25)-N(4)-C(23)	116.4(8)
O(5N')-Dy(1)-O(4N')	51.3(5)	N(1)-C(1)-C(2)	121.8(3)
O(4N)-Dy(1)-O(4N')	28.0(3)	N(1)-C(1)-C(11)	112.1(3)
O(2')-Dy(1)-N(1)	127.1(3)	C(2)-C(1)-C(11)	125.6(3)
O(2)-Dy(1)-N(1)	128.37(9)	C(3)-C(2)-C(1)	118.5(3)
O(7N)-Dy(1)-N(1)	75.48(14)	C(3)-C(2)-H(2A)	120.8
O(1)-Dy(1)-N(1)	64.99(8)	C(1)-C(2)-H(2A)	120.8
O(5N')-Dy(1)-N(1)	154.5(4)	C(4)-C(3)-C(2)	120.1(3)
O(4N)-Dy(1)-N(1)	144.57(9)	C(4)-C(3)-H(3A)	120.0
O(4N')-Dy(1)-N(1)	127.0(3)	C(2)-C(3)-H(3A)	120.0
O(2')-Dy(1)-O(2N)	90.4(4)	C(3)-C(4)-C(5)	118.4(3)
O(2)-Dy(1)-O(2N)	74.32(11)	C(3)-C(4)-H(4A)	120.8
O(7N)-Dy(1)-O(2N)	145.05(12)	C(5)-C(4)-H(4A)	120.8
O(1)-Dy(1)-O(2N)	115.72(8)	N(1)-C(5)-C(4)	121.3(3)
O(5N')-Dy(1)-O(2N)	82.8(4)	N(1)-C(5)-C(10)	116.4(2)
O(4N)-Dy(1)-O(2N)	131.01(9)	C(4)-C(5)-C(10)	122.3(3)
O(4N')-Dy(1)-O(2N)	117.5(3)	N(2)-C(6)-C(7)	121.9(3)
N(1)-Dy(1)-O(2N)	77.05(8)	N(2)-C(6)-C(22)	110.7(3)
O(2')-Dy(1)-O(5N)	82.7(4)	C(7)-C(6)-C(22)	127.1(3)
O(2)-Dy(1)-O(5N)	71.95(12)	C(8)-C(7)-C(6)	118.6(3)
O(7N)-Dy(1)-O(5N)	135.18(14)	C(8)-C(7)-H(7A)	120.7
O(1)-Dy(1)-O(5N)	99.69(12)	C(6)-C(7)-H(7A)	120.7
O(5N')-Dy(1)-O(5N)	15.1(3)	C(9)-C(8)-C(7)	119.7(3)
O(4N)-Dy(1)-O(5N)	52.00(11)	C(9)-C(8)-H(8A)	120.2
O(4N')-Dy(1)-O(5N)	44.8(3)	C(7)-C(8)-H(8A)	120.2
N(1)-Dy(1)-O(5N)	141.48(12)	C(8)-C(9)-C(10)	118.8(3)
O(2N)-Dy(1)-O(5N)	79.29(10)	C(8)-C(9)-H(9A)	120.6
O(2')-Dy(1)-N(2)	63.0(3)	C(10)-C(9)-H(9A)	120.6
O(2)-Dy(1)-N(2)	65.22(8)	N(2)-C(10)-C(9)	121.8(3)
O(7N)-Dy(1)-N(2)	80.35(12)	N(2)-C(10)-C(5)	115.4(3)
O(1)-Dy(1)-N(2)	126.37(8)	C(9)-C(10)-C(5)	122.8(3)
O(5N')-Dy(1)-N(2)	121.7(3)	O(1)-C(11)-N(3)	121.7(3)
O(4N)-Dy(1)-N(2)	139.14(10)	O(1)-C(11)-C(1)	116.8(3)
O(4N')-Dy(1)-N(2)	166.9(3)	N(3)-C(11)-C(1)	121.4(3)
N(1)-Dy(1)-N(2)	64.58(8)	N(3)-C(12)-C(13)	112.8(3)
O(2N)-Dy(1)-N(2)	68.50(8)	N(3)-C(12)-H(12A)	109.0
O(5N)-Dy(1)-N(2)	131.56(10)	C(13)-C(12)-H(12A)	109.0
O(2')-Dy(1)-O(1N)	135.2(4)	N(3)-C(12)-H(12B)	109.0
O(2)-Dy(1)-O(1N)	117.02(11)	C(13)-C(12)-H(12B)	109.0
O(7N)-Dy(1)-O(1N)	135.24(14)	H(12A)-C(12)-H(12B)	107.8
O(1)-Dy(1)-O(1N)	68.20(8)	C(12)-C(13)-H(13A)	109.5
O(5N')-Dy(1)-O(1N)	83.2(4)	C(12)-C(13)-H(13B)	109.5
O(4N)-Dy(1)-O(1N)	106.88(10)	H(13A)-C(13)-H(13B)	109.5
O(4N')-Dy(1)-O(1N)	80.2(3)	C(12)-C(13)-H(13C)	109.5
N(1)-Dy(1)-O(1N)	71.97(8)	H(13A)-C(13)-H(13C)	109.5
O(2N)-Dy(1)-O(1N)	51.15(8)	H(13B)-C(13)-H(13C)	109.5
O(5N)-Dy(1)-O(1N)	69.51(12)	C(19)-C(14)-C(15)	120.8(3)
N(2)-Dy(1)-O(1N)	111.16(8)	C(19)-C(14)-N(3)	118.5(3)
C(11)-O(1)-Dy(1)	117.50(19)	C(15)-C(14)-N(3)	120.6(3)
C(22)-O(2)-Dy(1)	121.7(2)	C(14)-C(15)-C(16)	120.0(4)
C(22)-O(2')-Dy(1)	126.0(9)	C(14)-C(15)-H(15A)	120.0
C(5)-N(1)-C(1)	119.9(3)	C(16)-C(15)-H(15A)	120.0
C(5)-N(1)-Dy(1)	122.03(18)	C(17)-C(16)-C(15)	118.8(4)
C(1)-N(1)-Dy(1)	118.0(2)	C(17)-C(16)-C(20)	120.6(4)
C(10)-N(2)-C(6)	119.1(3)	C(15)-C(16)-C(20)	120.6(4)
C(10)-N(2)-Dy(1)	121.42(18)	C(18)-C(17)-C(16)	120.1(4)
C(6)-N(2)-Dy(1)	119.09(19)	C(18)-C(17)-C(21)	119.3(5)

C(16)-C(17)-C(21)	120.6(5)	C(28')-C(27')-C(26')	112.6(12)
C(17)-C(18)-C(19)	121.5(4)	C(28')-C(27')-C(31')	129.5(17)
C(17)-C(18)-H(18A)	119.2	C(26')-C(27')-C(31')	117.9(16)
C(19)-C(18)-H(18A)	119.2	C(27')-C(28')-C(29')	125.4(13)
C(14)-C(19)-C(18)	118.8(4)	C(27')-C(28')-C(32')	120.9(15)
C(14)-C(19)-H(19A)	120.6	C(29')-C(28')-C(32')	113.7(16)
C(18)-C(19)-H(19A)	120.6	C(30')-C(29')-C(28')	117.3(11)
C(16)-C(20)-H(20A)	109.5	C(30')-C(29')-H(29B)	121.4
C(16)-C(20)-H(20B)	109.5	C(28')-C(29')-H(29B)	121.4
H(20A)-C(20)-H(20B)	109.5	C(29')-C(30')-C(25')	122.0(13)
C(16)-C(20)-H(20C)	109.5	C(29')-C(30')-H(30B)	119.0
H(20A)-C(20)-H(20C)	109.5	C(25')-C(30')-H(30B)	119.0
H(20B)-C(20)-H(20C)	109.5	C(27')-C(31')-H(31D)	109.5
C(17)-C(21)-H(21A)	109.5	C(27')-C(31')-H(31E)	109.5
C(17)-C(21)-H(21B)	109.5	H(31D)-C(31')-H(31E)	109.5
H(21A)-C(21)-H(21B)	109.5	C(27')-C(31')-H(31F)	109.5
C(17)-C(21)-H(21C)	109.5	H(31D)-C(31')-H(31F)	109.5
H(21A)-C(21)-H(21C)	109.5	H(31E)-C(31')-H(31F)	109.5
H(21B)-C(21)-H(21C)	109.5	C(28')-C(32')-H(32D)	109.5
O(2')-C(22)-N(4)	115.6(7)	C(28')-C(32')-H(32E)	109.5
O(2)-C(22)-N(4)	120.4(3)	H(32D)-C(32')-H(32E)	109.5
O(2')-C(22)-C(6)	114.3(7)	C(28')-C(32')-H(32F)	109.5
O(2)-C(22)-C(6)	116.6(3)	H(32D)-C(32')-H(32F)	109.5
N(4)-C(22)-C(6)	122.6(3)	H(32E)-C(32')-H(32F)	109.5
N(4)-C(23)-C(24)	112.5(3)	O(3N)-N(1N)-O(2N)	122.7(3)
N(4)-C(23)-H(23A)	109.1	O(3N)-N(1N)-O(1N)	120.9(3)
C(24)-C(23)-H(23A)	109.1	O(2N)-N(1N)-O(1N)	116.4(3)
N(4)-C(23)-H(23B)	109.1	O(3N)-N(1N)-Dy(1)	170.7(2)
C(24)-C(23)-H(23B)	109.1	O(2N)-N(1N)-Dy(1)	57.82(16)
H(23A)-C(23)-H(23B)	107.8	O(1N)-N(1N)-Dy(1)	59.09(16)
C(23)-C(24)-H(24A)	109.5	N(1N)-O(1N)-Dy(1)	94.97(18)
C(23)-C(24)-H(24B)	109.5	N(1N)-O(2N)-Dy(1)	96.80(18)
H(24A)-C(24)-H(24B)	109.5	O(5N')-N(2N)-O(6N)	123.3(7)
C(23)-C(24)-H(24C)	109.5	O(6N)-N(2N)-O(5N)	122.2(4)
H(24A)-C(24)-H(24C)	109.5	O(5N')-N(2N)-O(4N)	105.5(7)
H(24B)-C(24)-H(24C)	109.5	O(6N)-N(2N)-O(4N)	121.6(3)
C(26)-C(25)-C(30)	123.7(14)	O(5N)-N(2N)-O(4N)	116.2(3)
C(26)-C(25)-N(4)	120.2(13)	O(5N')-N(2N)-O(4N')	110.1(9)
C(30)-C(25)-N(4)	116.1(14)	O(6N)-N(2N)-O(4N')	122.8(6)
C(25)-C(26)-C(27)	123.0(12)	O(5N)-N(2N)-O(4N')	93.2(6)
C(25)-C(26)-H(26A)	118.5	O(4N)-N(2N)-O(4N')	52.5(6)
C(27)-C(26)-H(26A)	118.5	O(5N')-N(2N)-Dy(1)	56.4(7)
C(28)-C(27)-C(26)	116.1(10)	O(6N)-N(2N)-Dy(1)	177.5(3)
C(28)-C(27)-C(31)	114.3(13)	O(5N)-N(2N)-Dy(1)	58.98(19)
C(26)-C(27)-C(31)	129.5(14)	O(4N)-N(2N)-Dy(1)	57.18(16)
C(27)-C(28)-C(29)	121.8(10)	O(4N')-N(2N)-Dy(1)	58.6(6)
C(27)-C(28)-C(32)	124.6(11)	N(2N)-O(4N)-Dy(1)	95.9(2)
C(29)-C(28)-C(32)	113.5(12)	N(2N)-O(5N)-Dy(1)	96.0(2)
C(30)-C(29)-C(28)	119.0(10)	N(2N)-O(4N')-Dy(1)	93.2(7)
C(30)-C(29)-H(29A)	120.5	N(2N)-O(5N')-Dy(1)	99.0(8)
C(28)-C(29)-H(29A)	120.5	O(7N)-N(3N)-O(8N)	119.7(6)
C(25)-C(30)-C(29)	116.3(11)	O(7N)-N(3N)-O(9N)	124.0(5)
C(25)-C(30)-H(30A)	121.8	O(8N)-N(3N)-O(9N)	116.3(6)
C(29)-C(30)-H(30A)	121.8	N(3N)-O(7N)-Dy(1)	110.8(4)
N(4)-C(25')-C(30')	121.6(14)	N(3N)-O(8N)-Dy(1)	84.3(4)
N(4)-C(25')-C(26')	122.3(19)	O(9N')-N(3N')-O(8N')	126(2)
C(30')-C(25')-C(26')	116(2)	O(9N')-N(3N')-O(7N')	115(2)
C(25')-C(26')-C(27')	126.6(16)	O(8N')-N(3N')-O(7N')	118(2)
C(25')-C(26')-H(26B)	116.7	N(3N')-O(7N')-Dy(1)	96.2(13)
C(27')-C(26')-H(26B)	116.7	N(3N')-O(8N')-Dy(1)	96.7(13)

Table 28. Anisotropic displacement parameters (Å2x 103) for 3,4diMeDy. The anisotropic displacement factor exponent takes the form: -2□2[h2 a*2U11 + ... + 2 h k a* b* U12]

U11	U22	U33	U23	U13	U12

Dy(1)	37(1)	23(1)	24(1)	-2(1)	5(1)	-7(1)
O(1)	44(1)	43(1)	30(1)	-14(1)	13(1)	-23(1)
O(2)	37(2)	25(1)	36(2)	5(1)	-8(1)	-10(1)
N(1)	24(1)	22(1)	30(1)	-6(1)	10(1)	-3(1)
N(2)	28(1)	21(1)	28(1)	-3(1)	8(1)	-5(1)
N(3)	31(1)	42(2)	37(2)	-13(1)	7(1)	-14(1)
N(4)	51(2)	25(1)	31(1)	1(1)	0(1)	-15(1)
C(1)	23(1)	26(2)	35(2)	-9(1)	9(1)	-4(1)
C(2)	28(2)	24(2)	44(2)	-10(1)	12(1)	-7(1)
C(3)	36(2)	22(1)	47(2)	-2(1)	13(1)	-7(1)
C(4)	40(2)	24(2)	34(2)	-1(1)	11(1)	-5(1)
C(5)	25(1)	21(1)	31(2)	-3(1)	9(1)	-2(1)
C(6)	34(2)	23(1)	28(2)	-3(1)	6(1)	-7(1)
C(7)	42(2)	29(2)	29(2)	-5(1)	4(1)	-13(1)
C(8)	41(2)	38(2)	27(2)	0(1)	6(1)	-12(1)
C(9)	33(2)	28(2)	31(2)	2(1)	8(1)	-7(1)
C(10)	27(1)	21(1)	28(2)	-2(1)	8(1)	-3(1)
C(11)	31(2)	30(2)	36(2)	-13(1)	12(1)	-9(1)
C(12)	48(2)	70(3)	37(2)	-22(2)	11(2)	-31(2)
C(13)	76(3)	85(3)	39(2)	6(2)	3(2)	-23(3)
C(14)	28(2)	43(2)	40(2)	-1(2)	0(1)	-13(1)
C(15)	35(2)	44(2)	50(2)	-4(2)	-9(2)	-10(2)
C(16)	46(2)	53(2)	40(2)	11(2)	-15(2)	-22(2)
C(17)	36(2)	80(3)	42(2)	10(2)	-4(2)	-17(2)
C(18)	33(2)	81(3)	50(2)	4(2)	7(2)	-2(2)
C(19)	37(2)	55(2)	45(2)	4(2)	6(2)	-3(2)
C(20)	61(3)	59(3)	69(3)	10(2)	-19(2)	-17(2)
C(21)	49(3)	135(5)	70(3)	3(3)	13(2)	-40(3)
C(22)	52(2)	28(2)	31(2)	-1(1)	3(1)	-15(1)
C(23)	67(3)	28(2)	40(2)	7(1)	-2(2)	-19(2)
C(24)	97(4)	47(2)	51(3)	10(2)	22(2)	-16(2)
C(25)	24(7)	34(7)	38(5)	9(5)	-4(5)	-13(5)
C(26)	42(5)	38(4)	44(4)	-3(3)	5(4)	-21(4)
C(27)	52(7)	43(5)	52(5)	4(4)	14(5)	-25(5)
C(28)	56(5)	54(6)	34(5)	-3(4)	9(4)	-34(4)
C(29)	35(4)	59(5)	53(4)	1(4)	-4(3)	-16(3)
C(30)	40(4)	37(4)	32(4)	1(3)	3(3)	-17(3)
C(31)	92(7)	89(7)	81(6)	-1(5)	18(5)	-32(5)
C(32)	68(5)	90(6)	75(6)	16(5)	-25(4)	-35(5)
C(25')	25(8)	23(5)	48(6)	11(4)	10(5)	-4(5)
C(26')	59(6)	24(4)	66(6)	4(4)	34(5)	-2(4)
C(27')	58(6)	33(5)	78(9)	20(6)	27(7)	-5(5)
C(28')	33(6)	41(6)	81(8)	32(5)	-15(5)	-17(5)
C(29')	46(5)	38(4)	40(4)	-2(3)	-3(4)	-14(4)
C(30')	21(4)	23(3)	32(4)	-5(3)	1(3)	-1(3)
C(31')	55(6)	89(7)	170(10)	72(7)	8(6)	-2(5)
C(32')	80(7)	90(7)	86(7)	44(6)	-45(5)	-50(6)
N(1N)	43(2)	34(2)	39(2)	-3(1)	5(1)	9(1)
O(1N)	41(1)	38(1)	38(1)	-9(1)	0(1)	2(1)
O(2N)	48(1)	30(1)	38(1)	-10(1)	7(1)	-1(1)
N(2N)	84(2)	27(1)	26(2)	-2(1)	11(1)	4(1)
O(3N)	40(2)	74(2)	65(2)	-12(2)	17(1)	4(1)
O(4N)	61(2)	31(2)	34(2)	1(1)	22(1)	3(1)
O(5N)	45(2)	42(2)	37(2)	8(1)	8(2)	10(2)
O(6N)	173(4)	36(2)	43(2)	14(1)	33(2)	19(2)
N(3N)	87(4)	19(2)	37(3)	7(2)	32(3)	11(2)
O(7N)	47(2)	95(3)	37(2)	-11(2)	7(2)	23(2)
O(8N)	167(6)	56(3)	144(5)	-35(3)	115(5)	-49(3)
O(9N)	38(2)	75(3)	119(4)	13(3)	7(2)	5(2)

Table 29. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 3,4diMeDy.

	x	y	z	U(eq)
H(2A)	815	-3953	7127	38

H(3A)	964	-4479	8483	41
H(4A)	1212	-2560	9295	39
H(7A)	1751	3709	9890	40
H(8A)	1649	1509	10630	42
H(9A)	1418	-652	9968	36
H(12A)	651	-2567	4590	61
H(12B)	931	-1548	4798	61
H(13A)	577	-39	4051	101
H(13B)	662	725	4918	101
H(13C)	381	-290	4721	101
H(15A)	555	-4894	5619	54
H(18A)	-76	-1684	6686	66
H(19A)	344	-623	6400	55
H(20A)	-59	-6695	5513	100
H(20B)	85	-7065	6408	100
H(20C)	268	-7095	5697	100
H(21A)	-380	-3724	6808	127
H(21B)	-254	-5470	6865	127
H(21C)	-410	-4812	6029	127
H(23A)	1841	7607	8075	55
H(23B)	1583	6772	7525	55
H(24A)	1970	7145	6841	95
H(24B)	1888	5324	6878	95
H(24C)	2152	5998	7467	95
H(26A)	1873	6855	9739	49
H(29A)	2631	3691	9454	60
H(30A)	2233	3744	8442	44
H(31A)	2099	7498	11098	131
H(31B)	2425	7737	11062	131
H(31C)	2321	6212	11487	131
H(32A)	2813	6050	10994	122
H(32B)	2865	4345	10642	122
H(32C)	2681	4522	11346	122
H(26B)	2282	4284	8792	56
H(29B)	2027	7260	10861	51
H(30B)	1721	7007	9663	31
H(31D)	2705	3709	9396	159
H(31E)	2736	3485	10344	159
H(31F)	2855	5038	9980	159
H(32D)	2615	5165	11531	137
H(32E)	2427	6643	11699	137
H(32F)	2691	6887	11249	137

Table 30. Torsion angles [°] for 3,4diMeDy.

O(2')-Dy(1)-O(1)-C(11)	152.4(8)	N(2)-Dy(1)-O(2)-C(22)	21.7(3)
O(2)-Dy(1)-O(1)-C(11)	-166.1(4)	O(1N)-Dy(1)-O(2)-C(22)	123.9(3)
O(7N)-Dy(1)-O(1)-C(11)	111.0(3)	O(2)-Dy(1)-O(2')-C(22)	67.7(12)
O(5N')-Dy(1)-O(1)-C(11)	-124.0(4)	O(7N)-Dy(1)-O(2')-C(22)	-104.4(12)
O(4N)-Dy(1)-O(1)-C(11)	-163.3(3)	O(1)-Dy(1)-O(2')-C(22)	-143.0(7)
O(4N')-Dy(1)-O(1)-C(11)	-141.0(4)	O(5N')-Dy(1)-O(2')-C(22)	122.7(13)
N(1)-Dy(1)-O(1)-C(11)	28.4(2)	O(4N)-Dy(1)-O(2')-C(22)	172.4(12)
O(2N)-Dy(1)-O(1)-C(11)	-31.6(3)	O(4N')-Dy(1)-O(2')-C(22)	159.4(11)
O(5N)-Dy(1)-O(1)-C(11)	-114.4(3)	N(1)-Dy(1)-O(2')-C(22)	-33.3(14)
N(2)-Dy(1)-O(1)-C(11)	49.7(3)	O(2N)-Dy(1)-O(2')-C(22)	40.7(12)
O(1N)-Dy(1)-O(1)-C(11)	-51.2(2)	O(5N)-Dy(1)-O(2')-C(22)	119.9(12)
O(2')-Dy(1)-O(2)-C(22)	-57.0(10)	N(2)-Dy(1)-O(2')-C(22)	-24.8(10)
O(7N)-Dy(1)-O(2)-C(22)	-48.7(4)	O(1N)-Dy(1)-O(2')-C(22)	68.8(13)
O(1)-Dy(1)-O(2)-C(22)	-127.1(4)	O(2')-Dy(1)-N(1)-C(5)	8.8(5)
O(5N')-Dy(1)-O(2)-C(22)	-174.0(5)	O(2)-Dy(1)-N(1)-C(5)	-14.1(3)
O(4N)-Dy(1)-O(2)-C(22)	-129.9(3)	O(7N)-Dy(1)-N(1)-C(5)	86.5(2)
O(4N')-Dy(1)-O(2)-C(22)	-150.0(5)	O(1)-Dy(1)-N(1)-C(5)	161.5(2)
N(1)-Dy(1)-O(2)-C(22)	36.1(4)	O(5N')-Dy(1)-N(1)-C(5)	-110.4(8)
O(2N)-Dy(1)-O(2)-C(22)	94.9(3)	O(4N)-Dy(1)-N(1)-C(5)	141.3(2)
O(5N)-Dy(1)-O(2)-C(22)	178.5(4)	O(4N')-Dy(1)-N(1)-C(5)	173.4(4)

O(2N)-Dy(1)-N(1)-C(5)	-71.7(2)
O(5N)-Dy(1)-N(1)-C(5)	-125.2(2)
N(2)-Dy(1)-N(1)-C(5)	0.4(2)
O(1N)-Dy(1)-N(1)-C(5)	-124.7(2)
O(2')-Dy(1)-N(1)-C(1)	-168.3(5)
O(2)-Dy(1)-N(1)-C(1)	168.8(2)
O(7N)-Dy(1)-N(1)-C(1)	-90.6(2)
O(1)-Dy(1)-N(1)-C(1)	-15.6(2)
O(5N')-Dy(1)-N(1)-C(1)	72.5(8)
O(4N)-Dy(1)-N(1)-C(1)	-35.8(3)
O(4N')-Dy(1)-N(1)-C(1)	-3.7(5)
O(2N)-Dy(1)-N(1)-C(1)	111.2(2)
O(5N)-Dy(1)-N(1)-C(1)	57.7(3)
N(2)-Dy(1)-N(1)-C(1)	-176.7(2)
O(1N)-Dy(1)-N(1)-C(1)	58.2(2)
O(2')-Dy(1)-N(2)-C(10)	-175.3(5)
O(2)-Dy(1)-N(2)-C(10)	164.6(3)
O(7N)-Dy(1)-N(2)-C(10)	-81.3(2)
O(1)-Dy(1)-N(2)-C(10)	-24.2(3)
O(5N')-Dy(1)-N(2)-C(10)	148.9(5)
O(4N)-Dy(1)-N(2)-C(10)	-148.9(2)
O(4N')-Dy(1)-N(2)-C(10)	-157.4(14)
N(1)-Dy(1)-N(2)-C(10)	-2.9(2)
O(2N)-Dy(1)-N(2)-C(10)	82.6(2)
O(5N)-Dy(1)-N(2)-C(10)	134.5(2)
O(1N)-Dy(1)-N(2)-C(10)	53.7(2)
O(2')-Dy(1)-N(2)-C(6)	11.5(5)
O(2)-Dy(1)-N(2)-C(6)	-8.5(2)
O(7N)-Dy(1)-N(2)-C(6)	105.6(3)
O(1)-Dy(1)-N(2)-C(6)	162.6(2)
O(5N')-Dy(1)-N(2)-C(6)	-24.3(5)
O(4N)-Dy(1)-N(2)-C(6)	37.9(3)
O(4N')-Dy(1)-N(2)-C(6)	29.5(14)
N(1)-Dy(1)-N(2)-C(6)	-176.0(2)
O(2N)-Dy(1)-N(2)-C(6)	-90.6(2)
O(5N)-Dy(1)-N(2)-C(6)	-38.6(3)
O(1N)-Dy(1)-N(2)-C(6)	-119.5(2)
C(5)-N(1)-C(1)-C(2)	-0.3(4)
Dy(1)-N(1)-C(1)-C(2)	176.8(2)
C(5)-N(1)-C(1)-C(11)	-172.9(2)
Dy(1)-N(1)-C(1)-C(11)	4.3(3)
N(1)-C(1)-C(2)-C(3)	0.3(5)
C(11)-C(1)-C(2)-C(3)	171.8(3)
C(1)-C(2)-C(3)-C(4)	0.2(5)
C(2)-C(3)-C(4)-C(5)	-0.6(5)
C(1)-N(1)-C(5)-C(4)	-0.2(4)
Dy(1)-N(1)-C(5)-C(4)	-177.2(2)
C(1)-N(1)-C(5)-C(10)	178.8(3)
Dy(1)-N(1)-C(5)-C(10)	1.8(3)
C(3)-C(4)-C(5)-N(1)	0.6(5)
C(3)-C(4)-C(5)-C(10)	-178.3(3)
C(10)-N(2)-C(6)-C(7)	-1.2(5)
Dy(1)-N(2)-C(6)-C(7)	172.1(2)
C(10)-N(2)-C(6)-C(22)	-175.6(3)
Dy(1)-N(2)-C(6)-C(22)	-2.3(3)
N(2)-C(6)-C(7)-C(8)	1.5(5)
C(22)-C(6)-C(7)-C(8)	174.9(3)
C(6)-C(7)-C(8)-C(9)	-0.1(5)
C(7)-C(8)-C(9)-C(10)	-1.6(5)
C(6)-N(2)-C(10)-C(9)	-0.6(4)
Dy(1)-N(2)-C(10)-C(9)	-173.7(2)
C(6)-N(2)-C(10)-C(5)	177.9(3)
Dy(1)-N(2)-C(10)-C(5)	4.8(3)
C(8)-C(9)-C(10)-N(2)	2.0(5)
C(8)-C(9)-C(10)-C(5)	-176.4(3)
N(1)-C(5)-C(10)-N(2)	-4.2(4)
C(4)-C(5)-C(10)-N(2)	174.7(3)
N(1)-C(5)-C(10)-C(9)	174.3(3)
C(4)-C(5)-C(10)-C(9)	-6.8(4)
Dy(1)-O(1)-C(11)-N(3)	145.8(3)
Dy(1)-O(1)-C(11)-C(1)	-38.0(4)
C(14)-N(3)-C(11)-O(1)	-157.0(3)
C(12)-N(3)-C(11)-O(1)	5.8(5)
C(14)-N(3)-C(11)-C(1)	27.1(5)
C(12)-N(3)-C(11)-C(1)	-170.2(3)
N(1)-C(1)-C(11)-O(1)	21.6(4)
C(2)-C(1)-C(11)-O(1)	-150.6(3)
N(1)-C(1)-C(11)-N(3)	-162.2(3)
C(2)-C(1)-C(11)-N(3)	25.5(5)
C(11)-N(3)-C(12)-C(13)	-85.7(4)
C(14)-N(3)-C(12)-C(13)	78.3(4)
C(11)-N(3)-C(14)-C(19)	62.0(5)
C(12)-N(3)-C(14)-C(19)	-101.1(4)
C(11)-N(3)-C(14)-C(15)	-121.3(4)
C(12)-N(3)-C(14)-C(15)	75.6(4)
C(19)-C(14)-C(15)-C(16)	-0.8(5)
N(3)-C(14)-C(15)-C(16)	-177.5(3)
C(14)-C(15)-C(16)-C(17)	1.9(5)
C(14)-C(15)-C(16)-C(20)	-178.4(3)
C(15)-C(16)-C(17)-C(18)	-1.8(6)
C(20)-C(16)-C(17)-C(18)	178.4(4)
C(15)-C(16)-C(17)-C(21)	178.4(4)
C(20)-C(16)-C(17)-C(21)	-1.4(6)
C(16)-C(17)-C(18)-C(19)	0.7(6)
C(21)-C(17)-C(18)-C(19)	-179.5(4)
C(15)-C(14)-C(19)-C(18)	-0.3(6)
N(3)-C(14)-C(19)-C(18)	176.5(3)
C(17)-C(18)-C(19)-C(14)	0.3(6)
Dy(1)-O(2')-C(22)-O(2)	-69.7(11)
Dy(1)-O(2')-C(22)-N(4)	-176.8(7)
Dy(1)-O(2')-C(22)-C(6)	32.5(13)
Dy(1)-O(2)-C(22)-O(2')	62.7(11)
Dy(1)-O(2)-C(22)-N(4)	154.3(3)
Dy(1)-O(2)-C(22)-C(6)	-31.9(5)
C(25')-N(4)-C(22)-O(2')	-146.8(14)
C(25)-N(4)-C(22)-O(2')	-129.0(12)
C(23)-N(4)-C(22)-O(2')	33.9(9)
C(25')-N(4)-C(22)-O(2)	174.7(11)
C(25)-N(4)-C(22)-O(2)	-167.5(10)
C(23)-N(4)-C(22)-O(2)	-4.6(6)
C(25')-N(4)-C(22)-C(6)	1.2(12)
C(25)-N(4)-C(22)-C(6)	19.0(10)
C(23)-N(4)-C(22)-C(6)	-178.1(3)
N(2)-C(6)-C(22)-O(2')	-17.0(9)
C(7)-C(6)-C(22)-O(2')	169.0(8)
N(2)-C(6)-C(22)-O(2)	20.9(5)
C(7)-C(6)-C(22)-O(2)	-153.1(4)
N(2)-C(6)-C(22)-N(4)	-165.4(3)
C(7)-C(6)-C(22)-N(4)	20.6(6)
C(22)-N(4)-C(23)-C(24)	-85.7(4)
C(25')-N(4)-C(23)-C(24)	94.9(10)
C(25)-N(4)-C(23)-C(24)	78.5(9)
C(22)-N(4)-C(25)-C(26)	-111.4(15)
C(25')-N(4)-C(25)-C(26)	-7(6)
C(23)-N(4)-C(25)-C(26)	85.5(17)
C(22)-N(4)-C(25)-C(30)	70.4(17)
C(25')-N(4)-C(25)-C(30)	175(8)
C(23)-N(4)-C(25)-C(30)	-92.7(15)

C(30)-C(25)-C(26)-C(27) -4(2)
N(4)-C(25)-C(26)-C(27) 178.4(11)
C(25)-C(26)-C(27)-C(28) 1.5(17)
C(25)-C(26)-C(27)-C(31) -177.7(14)
C(26)-C(27)-C(28)-C(29) 2.2(15)
C(31)-C(27)-C(28)-C(29) -178.5(10)
C(26)-C(27)-C(28)-C(32) 179.4(10)
C(31)-C(27)-C(28)-C(32) -1.3(16)
C(27)-C(28)-C(29)-C(30) -4.1(15)
C(32)-C(28)-C(29)-C(30) 178.5(8)
C(26)-C(25)-C(30)-C(29) 1(2)
N(4)-C(25)-C(30)-C(29) 179.6(10)
C(28)-C(29)-C(30)-C(25) 2.1(15)
C(22)-N(4)-C(25')-C(30') -96.8(19)
C(25)-N(4)-C(25')-C(30') 178(9)
C(23)-N(4)-C(25')-C(30') 83(2)
C(22)-N(4)-C(25')-C(26') 87(2)
C(25)-N(4)-C(25')-C(26') 1(5)
C(23)-N(4)-C(25')-C(26') -93.8(19)
N(4)-C(25')-C(26')-C(27') 179.3(13)
C(30')-C(25')-C(26')-C(27') 3(3)
C(25')-C(26')-C(27')-C(28') 0(2)
C(25')-C(26')-C(27')-C(31') 179.9(16)
C(26')-C(27')-C(28')-C(29') -2.1(19)
C(31')-C(27')-C(28')-C(29') 178.4(12)
C(26')-C(27')-C(28')-C(32') 178.4(11)
C(31')-C(27')-C(28')-C(32') -1(2)
C(27')-C(28')-C(29')-C(30') 0.5(19)
C(32')-C(28')-C(29')-C(30') -179.9(8)
C(28')-C(29')-C(30')-C(25') 3.0(18)
N(4)-C(25')-C(30')-C(29') 179.0(13)
C(26')-C(25')-C(30')-C(29') -4(3)
O(2')-Dy(1)-N(1N)-O(2N) -22.4(4)
O(2)-Dy(1)-N(1N)-O(2N) -27.8(2)
O(7N)-Dy(1)-N(1N)-O(2N) 107.1(3)
O(1)-Dy(1)-N(1N)-O(2N) 163.37(19)
O(5N')-Dy(1)-N(1N)-O(2N) -85.1(4)
O(4N)-Dy(1)-N(1N)-O(2N) -115.92(19)
O(4N')-Dy(1)-N(1N)-O(2N) -133.8(4)
N(1)-Dy(1)-N(1N)-O(2N) 100.57(19)
O(5N)-Dy(1)-N(1N)-O(2N) -97.0(2)
N(2)-Dy(1)-N(1N)-O(2N) 37.02(19)
O(1N)-Dy(1)-N(1N)-O(2N) -171.2(3)
O(2')-Dy(1)-N(1N)-O(1N) 148.8(4)
O(2)-Dy(1)-N(1N)-O(1N) 143.38(19)
O(7N)-Dy(1)-N(1N)-O(1N) -81.7(3)
O(1)-Dy(1)-N(1N)-O(1N) -25.45(19)
O(5N')-Dy(1)-N(1N)-O(1N) 86.1(4)
O(4N)-Dy(1)-N(1N)-O(1N) 55.3(2)
O(4N')-Dy(1)-N(1N)-O(1N) 37.4(4)
N(1)-Dy(1)-N(1N)-O(1N) -88.25(19)
O(2N)-Dy(1)-N(1N)-O(1N) 171.2(3)
O(5N)-Dy(1)-N(1N)-O(1N) 74.2(2)
N(2)-Dy(1)-N(1N)-O(1N) -151.80(19)
O(3N)-N(1N)-O(1N)-Dy(1) -169.2(3)
O(2N)-N(1N)-O(1N)-Dy(1) 8.3(3)
O(2')-Dy(1)-O(1N)-N(1N) -42.1(5)
O(2)-Dy(1)-O(1N)-N(1N) -41.7(2)
O(7N)-Dy(1)-O(1N)-N(1N) 128.2(2)
O(1)-Dy(1)-O(1N)-N(1N) 152.4(2)
O(5N')-Dy(1)-O(1N)-N(1N) -91.0(4)
O(4N)-Dy(1)-O(1N)-N(1N) -134.34(19)
O(4N')-Dy(1)-O(1N)-N(1N) -142.8(4)
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O(2N)-Dy(1)-O(1N)-N(1N) -4.84(17)
O(5N)-Dy(1)-O(1N)-N(1N) -97.5(2)
N(2)-Dy(1)-O(1N)-N(1N) 30.4(2)
O(3N)-N(1N)-O(2N)-Dy(1) 169.1(3)
O(1N)-N(1N)-O(2N)-Dy(1) -8.4(3)
O(2')-Dy(1)-O(2N)-N(1N) 159.7(4)
O(2)-Dy(1)-O(2N)-N(1N) 151.2(2)
O(7N)-Dy(1)-O(2N)-N(1N) -111.1(3)
O(1)-Dy(1)-O(2N)-N(1N) -18.5(2)
O(5N')-Dy(1)-O(2N)-N(1N) 92.0(4)
O(4N)-Dy(1)-O(2N)-N(1N) 83.0(2)
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N(2)-Dy(1)-O(2N)-N(1N) -139.7(2)
O(1N)-Dy(1)-O(2N)-N(1N) 4.94(17)
O(2')-Dy(1)-N(2N)-O(5N') -57.5(9)
O(2)-Dy(1)-N(2N)-O(5N') -39.4(9)
O(7N)-Dy(1)-N(2N)-O(5N') -143.0(9)
O(1)-Dy(1)-N(2N)-O(5N') 147.3(9)
O(4N)-Dy(1)-N(2N)-O(5N') -144.2(9)
O(4N')-Dy(1)-N(2N)-O(5N') 152.9(11)
N(1)-Dy(1)-N(2N)-O(5N') 119.6(9)
O(2N)-Dy(1)-N(2N)-O(5N') 30.4(9)
O(5N)-Dy(1)-N(2N)-O(5N') 36.5(8)
N(2)-Dy(1)-N(2N)-O(5N') -42.8(9)
O(1N)-Dy(1)-N(2N)-O(5N') 79.2(9)
O(2')-Dy(1)-N(2N)-O(5N) -94.0(4)
O(2)-Dy(1)-N(2N)-O(5N) -75.8(3)
O(7N)-Dy(1)-N(2N)-O(5N) -179.5(3)
O(1)-Dy(1)-N(2N)-O(5N) 110.8(3)
O(5N')-Dy(1)-N(2N)-O(5N) -36.5(8)
O(4N)-Dy(1)-N(2N)-O(5N) 179.3(4)
O(4N')-Dy(1)-N(2N)-O(5N) 116.4(7)
N(1)-Dy(1)-N(2N)-O(5N) 83.1(3)
O(2N)-Dy(1)-N(2N)-O(5N) -6.1(3)
N(2)-Dy(1)-N(2N)-O(5N) -79.2(3)
O(1N)-Dy(1)-N(2N)-O(5N) 42.7(3)
O(2')-Dy(1)-N(2N)-O(4N) 86.7(4)
O(2)-Dy(1)-N(2N)-O(4N) 104.9(2)
O(7N)-Dy(1)-N(2N)-O(4N) 1.2(3)
O(1)-Dy(1)-N(2N)-O(4N) -68.5(2)
O(5N')-Dy(1)-N(2N)-O(4N) 144.2(9)
O(4N')-Dy(1)-N(2N)-O(4N) -62.9(7)
N(1)-Dy(1)-N(2N)-O(4N) -96.2(3)
O(2N)-Dy(1)-N(2N)-O(4N) 174.6(2)
O(5N)-Dy(1)-N(2N)-O(4N) -179.3(4)
N(2)-Dy(1)-N(2N)-O(4N) 101.5(2)
O(1N)-Dy(1)-N(2N)-O(4N) -136.6(2)
O(2')-Dy(1)-N(2N)-O(4N') 149.6(8)
O(2)-Dy(1)-N(2N)-O(4N') 167.8(7)
O(7N)-Dy(1)-N(2N)-O(4N') 64.1(7)
O(1)-Dy(1)-N(2N)-O(4N') -5.6(7)
O(5N')-Dy(1)-N(2N)-O(4N') -152.9(11)
O(4N)-Dy(1)-N(2N)-O(4N') 62.9(7)
N(1)-Dy(1)-N(2N)-O(4N') -33.3(7)
O(2N)-Dy(1)-N(2N)-O(4N') -122.5(7)
O(5N)-Dy(1)-N(2N)-O(4N') -116.4(7)
N(2)-Dy(1)-N(2N)-O(4N') 164.4(7)
O(1N)-Dy(1)-N(2N)-O(4N') -73.7(7)
O(5N')-N(2N)-O(4N)-Dy(1) 30.3(8)
O(6N)-N(2N)-O(4N)-Dy(1) 177.5(3)
O(5N)-N(2N)-O(4N)-Dy(1) -0.7(4)
O(4N')-N(2N)-O(4N)-Dy(1) -73.4(7)

O(2')-Dy(1)-O(4N)-N(2N) -88.4(4)
O(2)-Dy(1)-O(4N)-N(2N) -70.8(2)
O(7N)-Dy(1)-O(4N)-N(2N) -178.8(2)
O(1)-Dy(1)-O(4N)-N(2N) 109.9(2)
O(5N')-Dy(1)-O(4N)-N(2N) -18.8(5)
O(4N')-Dy(1)-O(4N)-N(2N) 63.8(7)
N(1)-Dy(1)-O(4N)-N(2N) 128.3(2)
O(2N)-Dy(1)-O(4N)-N(2N) -6.9(3)
O(5N)-Dy(1)-O(4N)-N(2N) 0.4(2)
N(2)-Dy(1)-O(4N)-N(2N) -112.2(2)
O(1N)-Dy(1)-O(4N)-N(2N) 45.8(2)
O(5N')-N(2N)-O(5N)-Dy(1) -75.3(14)
O(6N)-N(2N)-O(5N)-Dy(1) -177.5(3)
O(4N)-N(2N)-O(5N)-Dy(1) 0.7(4)
O(4N')-N(2N)-O(5N)-Dy(1) 50.0(6)
O(2')-Dy(1)-O(5N)-N(2N) 82.2(4)
O(2)-Dy(1)-O(5N)-N(2N) 97.1(3)
O(7N)-Dy(1)-O(5N)-N(2N) 0.7(4)
O(1)-Dy(1)-O(5N)-N(2N) -71.4(3)
O(5N')-Dy(1)-O(5N)-N(2N) 71.8(14)
O(4N)-Dy(1)-O(5N)-N(2N) -0.4(2)
O(4N')-Dy(1)-O(5N)-N(2N) -36.9(5)
N(1)-Dy(1)-O(5N)-N(2N) -133.2(2)
O(2N)-Dy(1)-O(5N)-N(2N) 174.0(3)
N(2)-Dy(1)-O(5N)-N(2N) 125.8(2)
O(1N)-Dy(1)-O(5N)-N(2N) -133.7(3)
O(5N')-N(2N)-O(4N')-Dy(1) -23.9(10)
O(6N)-N(2N)-O(4N')-Dy(1) 177.6(4)
O(5N)-N(2N)-O(4N')-Dy(1) -50.3(4)
O(4N)-N(2N)-O(4N')-Dy(1) 70.6(5)
O(2')-Dy(1)-O(4N')-N(2N) -31.0(8)
O(2)-Dy(1)-O(4N')-N(2N) -12.3(7)
O(7N)-Dy(1)-O(4N')-N(2N) -121.8(6)
O(1)-Dy(1)-O(4N')-N(2N) 173.7(8)
O(5N')-Dy(1)-O(4N')-N(2N) 14.1(6)
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O(6N)-N(2N)-O(5N')-Dy(1) -177.1(4)
O(5N)-N(2N)-O(5N')-Dy(1) 84.7(13)
O(4N)-N(2N)-O(5N')-Dy(1) -30.6(7)
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O(2')-Dy(1)-O(5N')-N(2N) 116.2(9)
O(2)-Dy(1)-O(5N')-N(2N) 133.6(10)
O(7N)-Dy(1)-O(5N')-N(2N) 46.4(11)
O(1)-Dy(1)-O(5N')-N(2N) -35.5(9)
O(4N)-Dy(1)-O(5N')-N(2N) 20.6(6)
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N(1)-Dy(1)-O(5N')-N(2N) -112.5(9)
O(2N)-Dy(1)-O(5N')-N(2N) -150.4(9)
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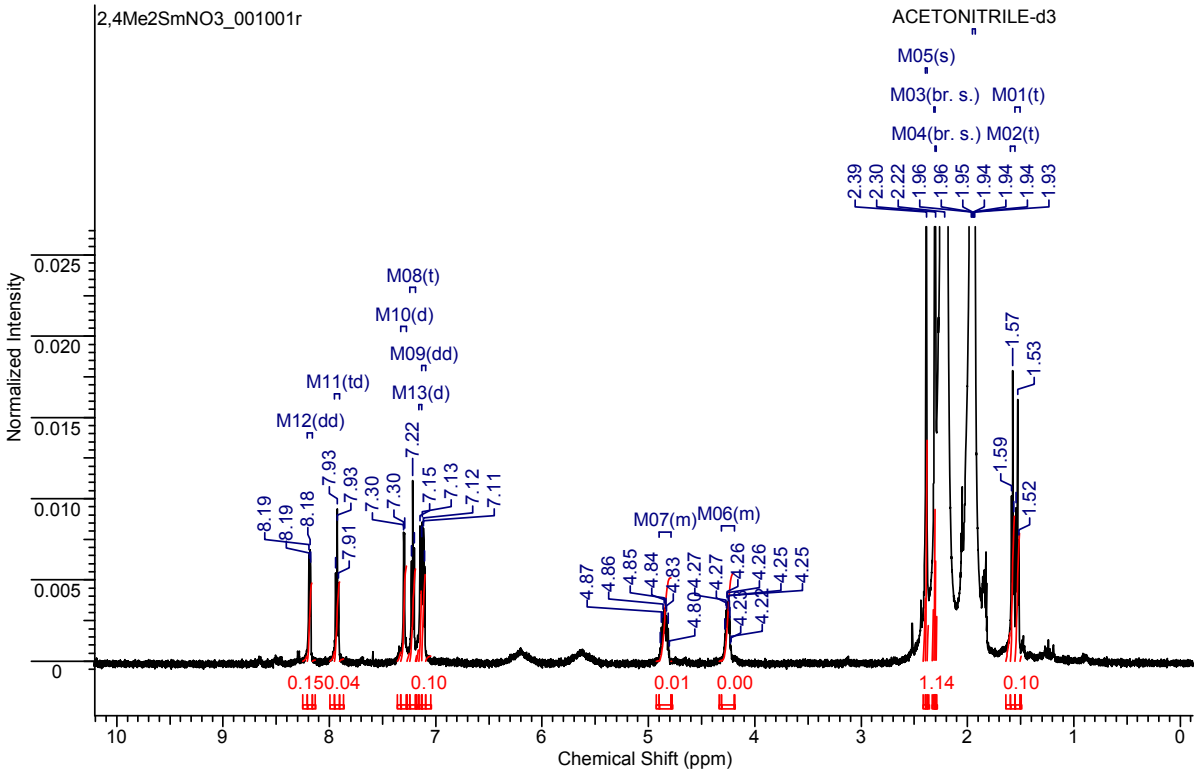
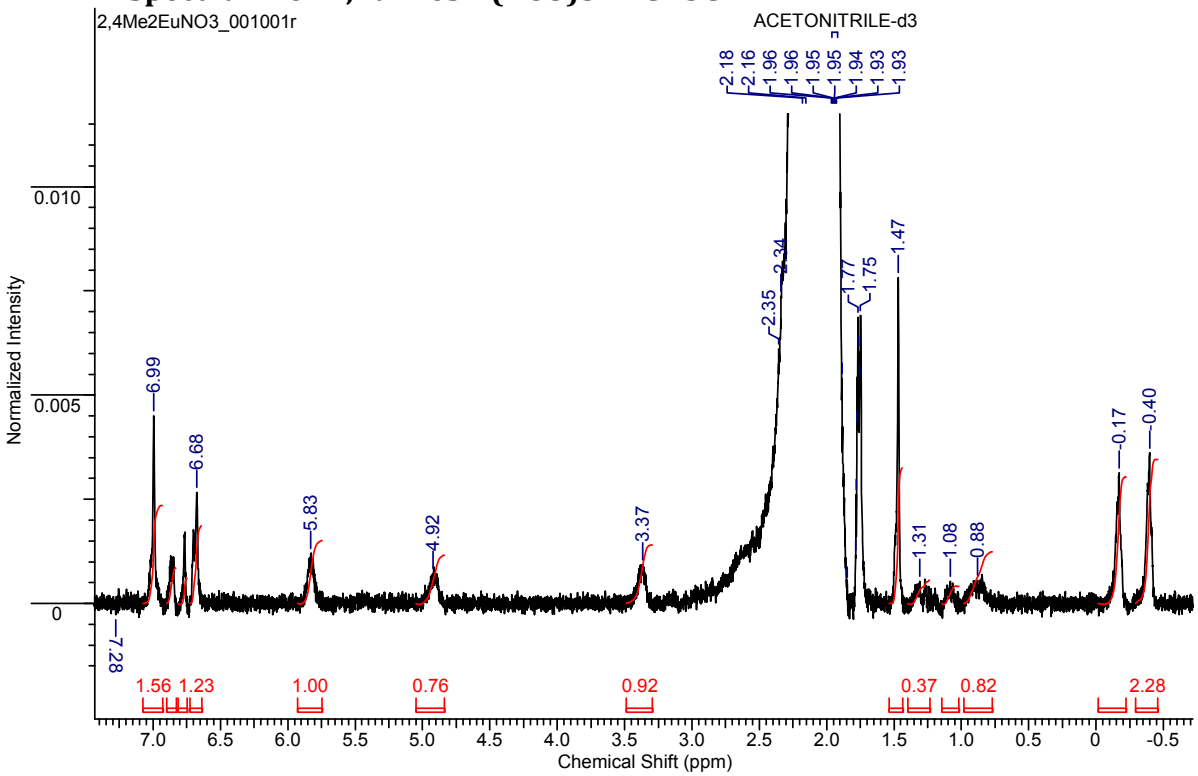
N(2)-Dy(1)-O(5N')-N(2N) 150.4(6)
O(1N)-Dy(1)-O(5N')-N(2N) -98.8(8)
O(8N)-N(3N)-O(7N)-Dy(1) 1.8(8)
O(9N)-N(3N)-O(7N)-Dy(1) -177.4(5)
O(2')-Dy(1)-O(7N)-N(3N) -6.2(6)
O(2)-Dy(1)-O(7N)-N(3N) -8.8(5)
O(1)-Dy(1)-O(7N)-N(3N) 156.8(5)
O(5N')-Dy(1)-O(7N)-N(3N) 54.2(7)
O(4N)-Dy(1)-O(7N)-N(3N) 73.5(5)
O(4N')-Dy(1)-O(7N)-N(3N) 98.3(6)
N(1)-Dy(1)-O(7N)-N(3N) -135.0(5)
O(2N)-Dy(1)-O(7N)-N(3N) -95.8(5)
O(5N)-Dy(1)-O(7N)-N(3N) 72.6(6)
N(2)-Dy(1)-O(7N)-N(3N) -69.0(5)
O(1N)-Dy(1)-O(7N)-N(3N) -179.4(4)
O(7N)-N(3N)-O(8N)-Dy(1) -1.4(7)
O(9N)-N(3N)-O(8N)-Dy(1) 177.9(5)
O(2')-Dy(1)-O(8N)-N(3N) 173.3(6)
O(2)-Dy(1)-O(8N)-N(3N) 172.4(4)
O(7N)-Dy(1)-O(8N)-N(3N) 0.8(4)
O(1)-Dy(1)-O(8N)-N(3N) -22.0(4)
O(5N')-Dy(1)-O(8N)-N(3N) -139.0(5)
O(4N)-Dy(1)-O(8N)-N(3N) -95.3(4)
O(4N')-Dy(1)-O(8N)-N(3N) -87.2(5)
N(1)-Dy(1)-O(8N)-N(3N) 47.7(4)
O(2N)-Dy(1)-O(8N)-N(3N) 134.6(3)
O(5N)-Dy(1)-O(8N)-N(3N) -132.8(4)
N(2)-Dy(1)-O(8N)-N(3N) 99.6(4)
O(9N')-N(3N')-O(7N')-Dy(1) -178.6(18)
O(8N')-N(3N')-O(7N')-Dy(1) 7(2)
O(2')-Dy(1)-O(7N')-N(3N') 85.0(12)
O(2)-Dy(1)-O(7N')-N(3N') 94.2(11)
O(7N)-Dy(1)-O(7N')-N(3N') -24.2(11)
O(1)-Dy(1)-O(7N')-N(3N') -94.9(11)
O(5N')-Dy(1)-O(7N')-N(3N') 152.7(12)
O(4N)-Dy(1)-O(7N')-N(3N') 178.1(13)
O(4N')-Dy(1)-O(7N')-N(3N') -159.3(13)
N(1)-Dy(1)-O(7N')-N(3N') -38.4(12)
O(2N)-Dy(1)-O(7N')-N(3N') 97.8(14)
O(5N)-Dy(1)-O(7N')-N(3N') 166.0(11)
N(2)-Dy(1)-O(7N')-N(3N') 30.5(12)
O(1N)-Dy(1)-O(7N')-N(3N') -131.6(11)
O(9N')-N(3N')-O(8N')-Dy(1) 179(2)
O(7N')-N(3N')-O(8N')-Dy(1) -7(2)
O(2')-Dy(1)-O(8N')-N(3N') -73.7(13)
O(2)-Dy(1)-O(8N')-N(3N') -79.6(13)
O(7N)-Dy(1)-O(8N')-N(3N') 61.6(18)
O(1)-Dy(1)-O(8N')-N(3N') 86.5(13)
O(5N')-Dy(1)-O(8N')-N(3N') -27.7(16)
O(4N)-Dy(1)-O(8N')-N(3N') 5.3(13)
O(4N')-Dy(1)-O(8N')-N(3N') 27.5(14)
N(1)-Dy(1)-O(8N')-N(3N') 152.0(14)
O(2N)-Dy(1)-O(8N')-N(3N') -152.8(12)
O(5N)-Dy(1)-O(8N')-N(3N') -12.6(17)
N(2)-Dy(1)-O(8N')-N(3N') -139.4(14)
O(1N)-Dy(1)-O(8N')-N(3N') 127.7(12)

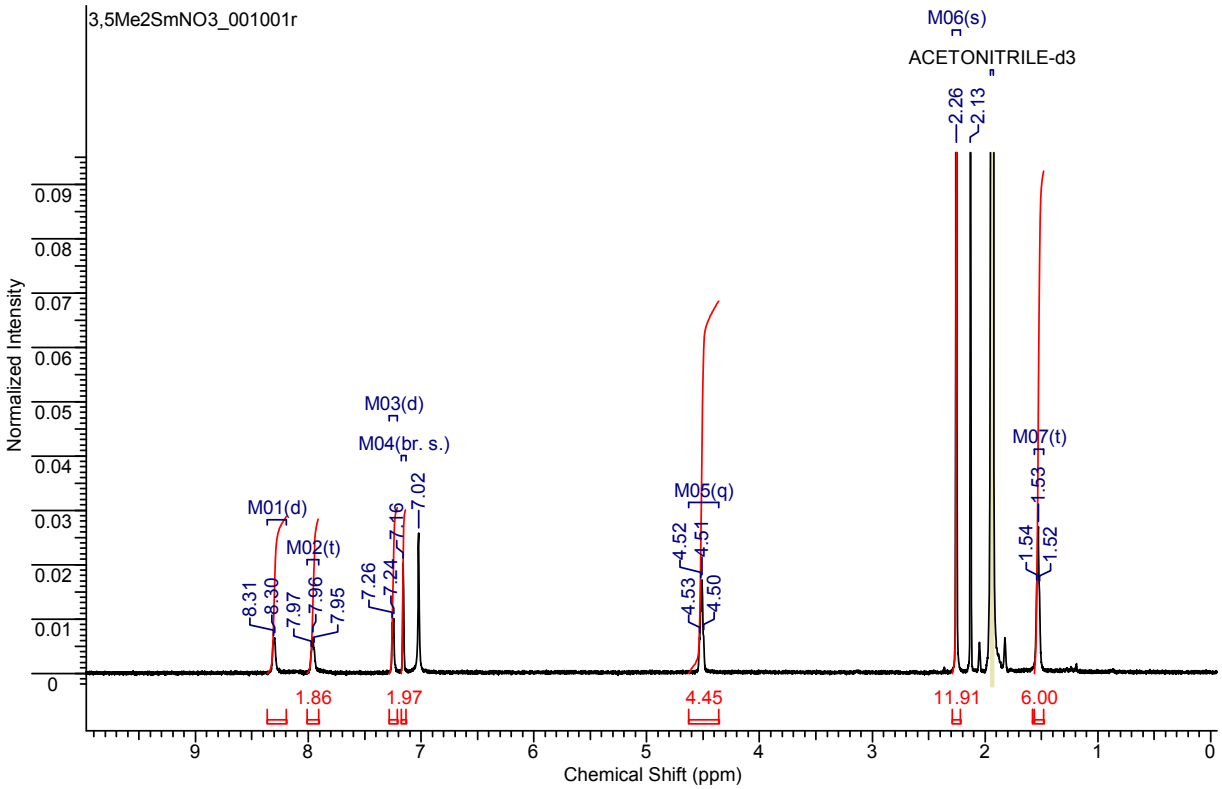
NMR Spectra



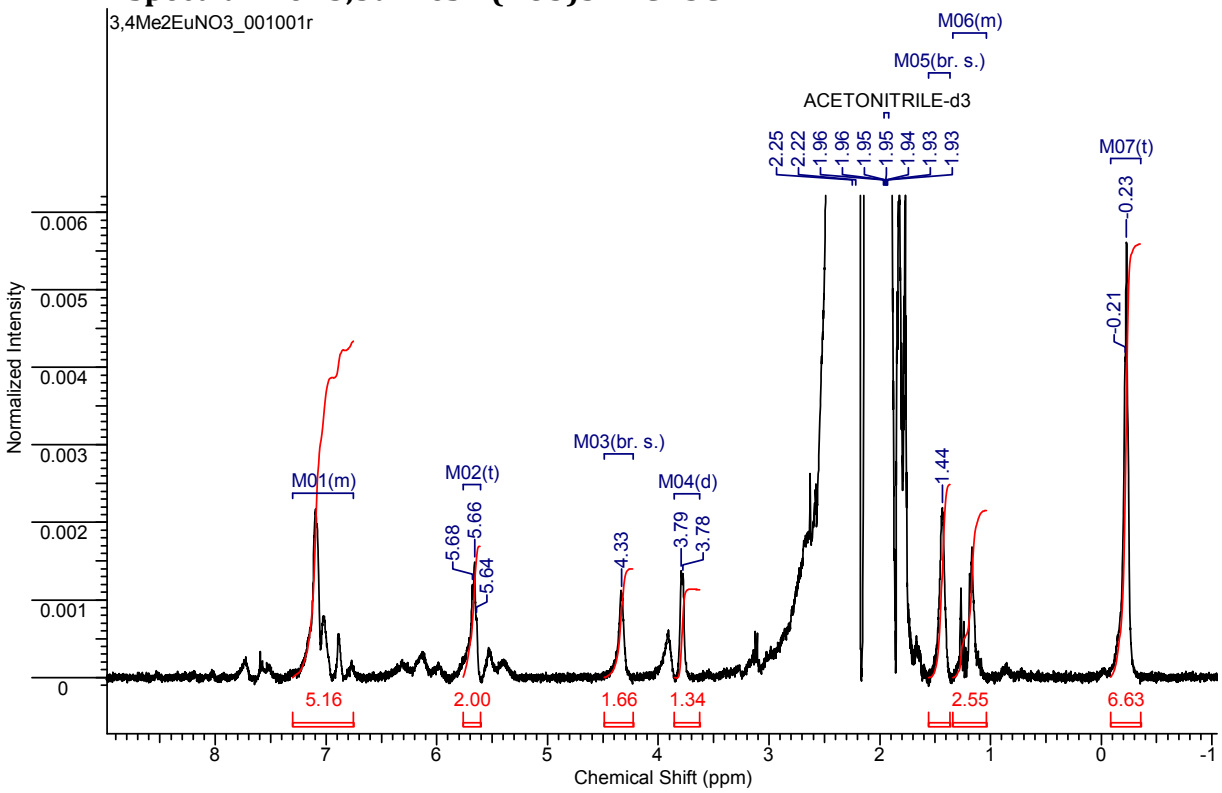
1H NMR Spectrum for 2,4diMeSm(NO3)3 in CD3CN.



1H NMR Spectrum for 2,4diMeEu(NO3)3 in CD3CN.



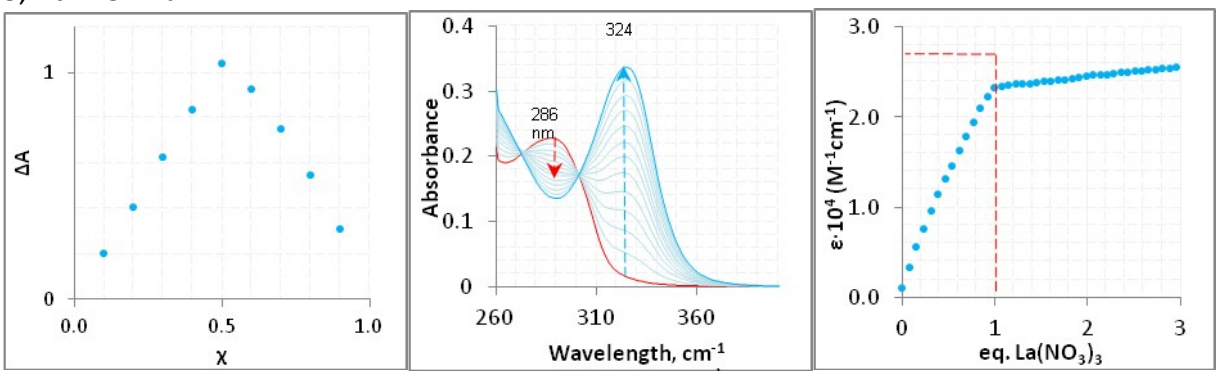
1H NMR Spectrum for 3,5diMeSm(NO3)3 in CD3CN.



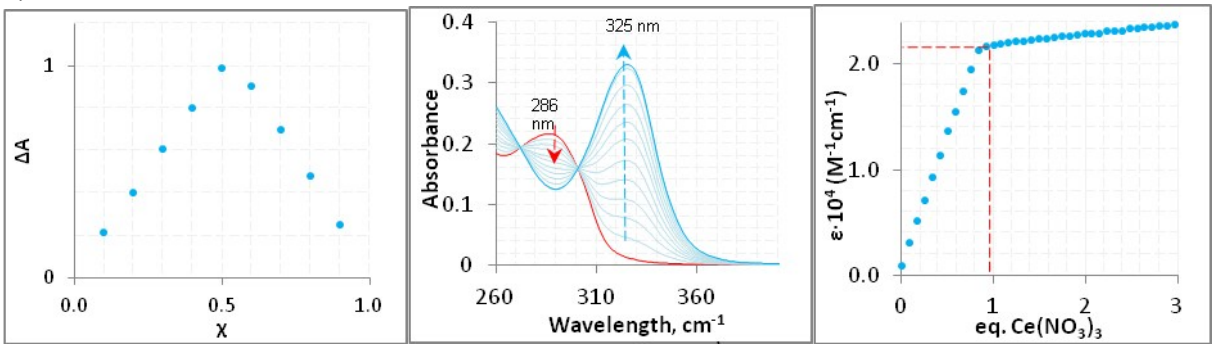
1H NMR Spectrum for 3,4diMeEu(NO3)3 in CD3CN.

UV-VIS Titration Data

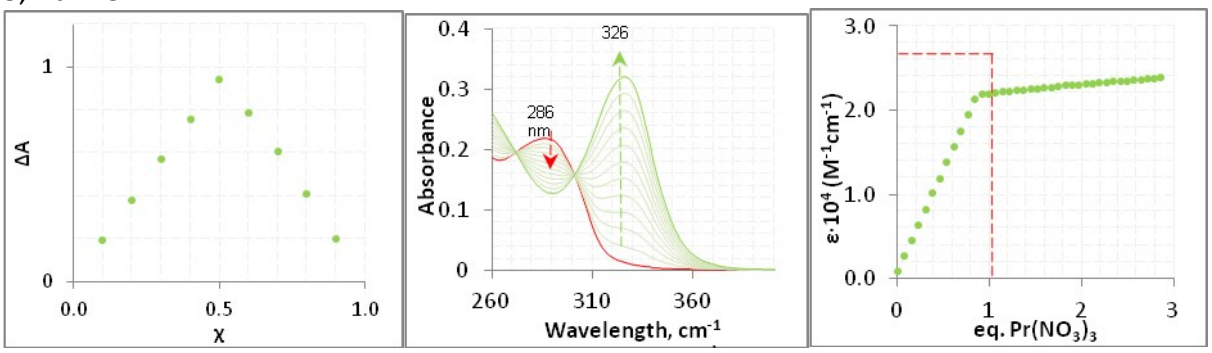
3,4-diMe + La^{3+}



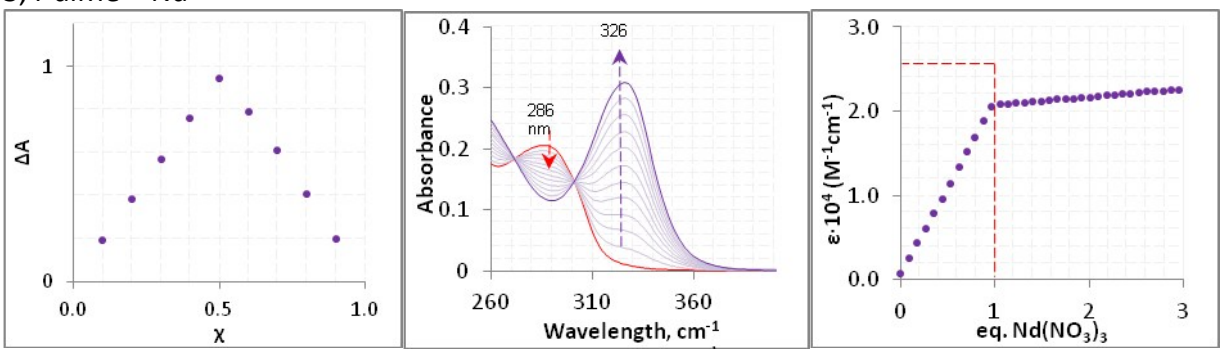
3,4-diMe + Ce^{3+}



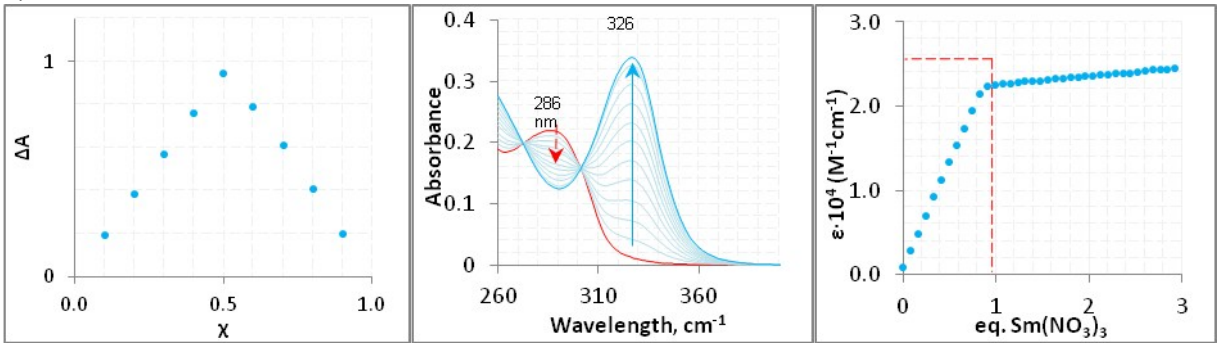
3,4-diMe + Pr^{3+}



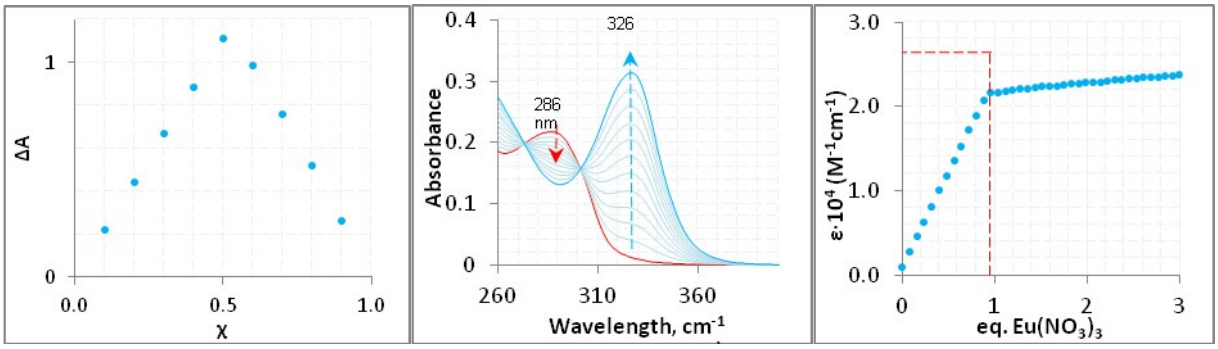
3,4-diMe + Nd^{3+}



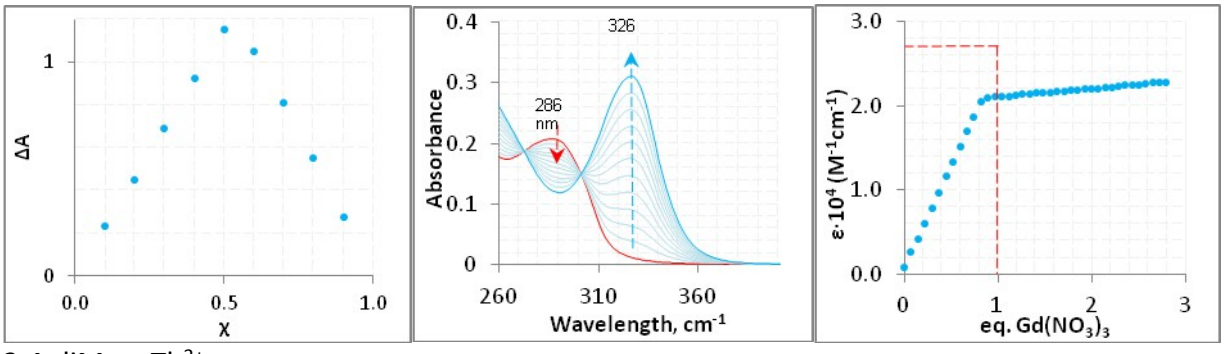
3,4-diMe + Sm^{3+}



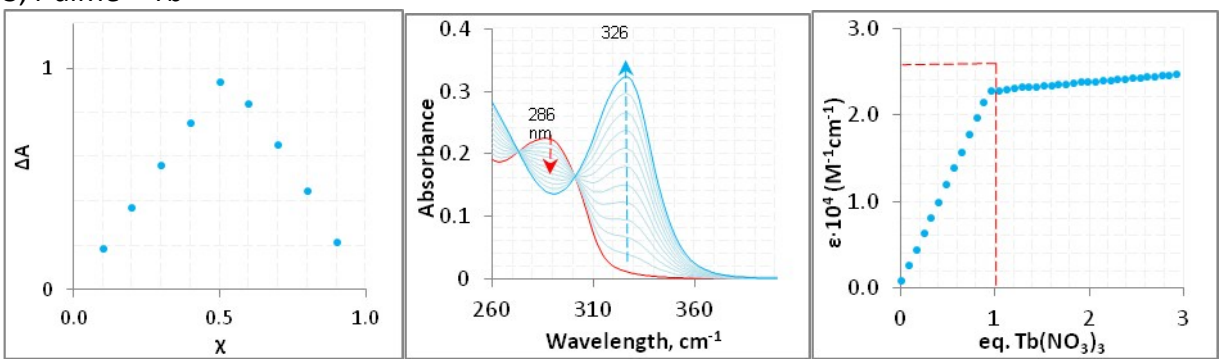
3,4-diMe + Eu^{3+}



3,4-diMe + Gd^{3+}



3,4-diMe + Tb^{3+}



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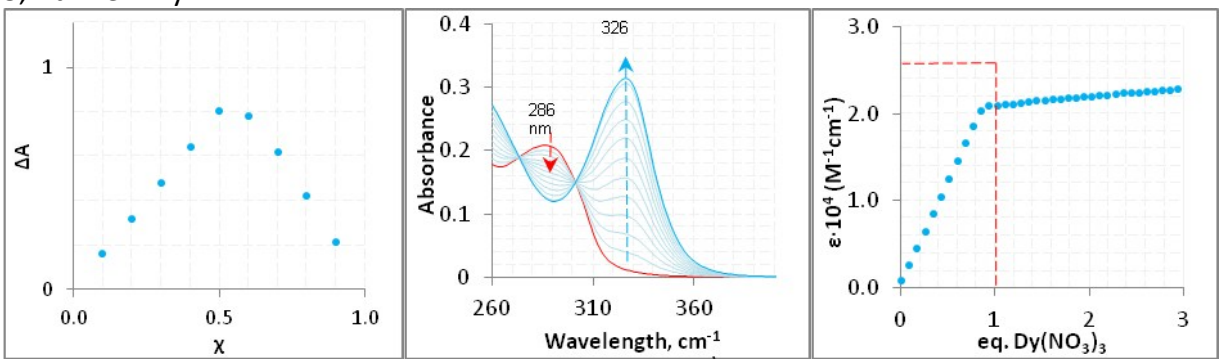
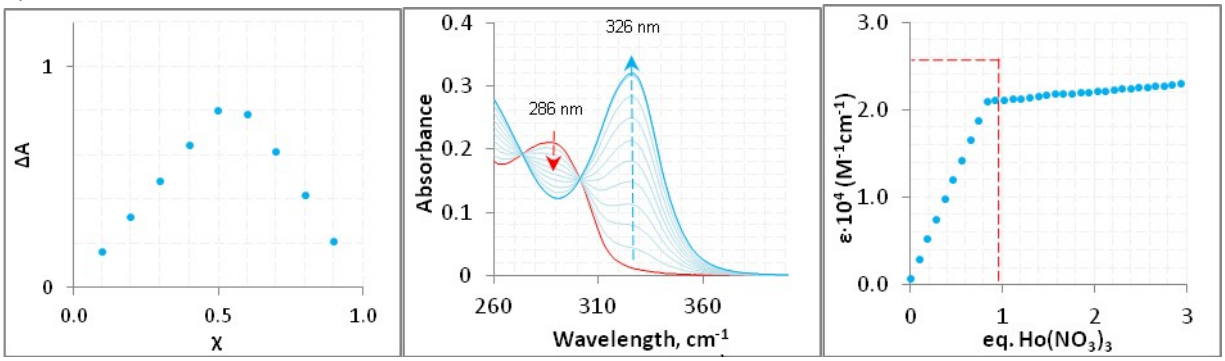


3,4-diMe + Ho^{3+}



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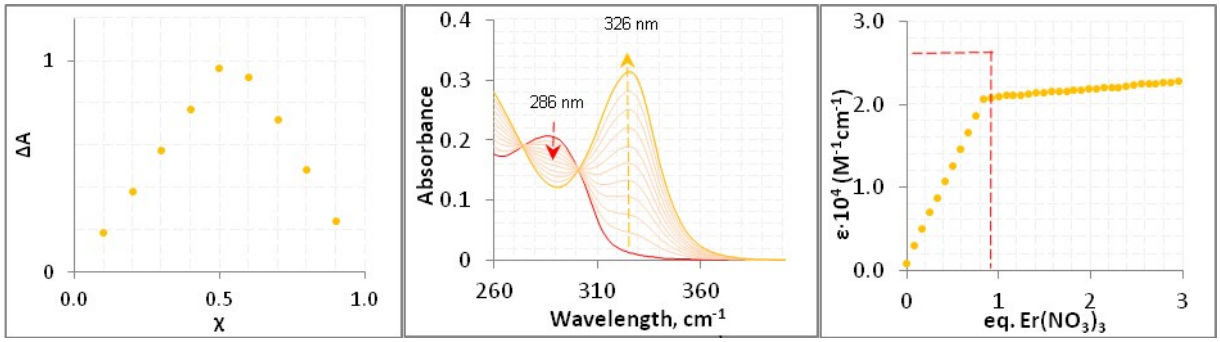
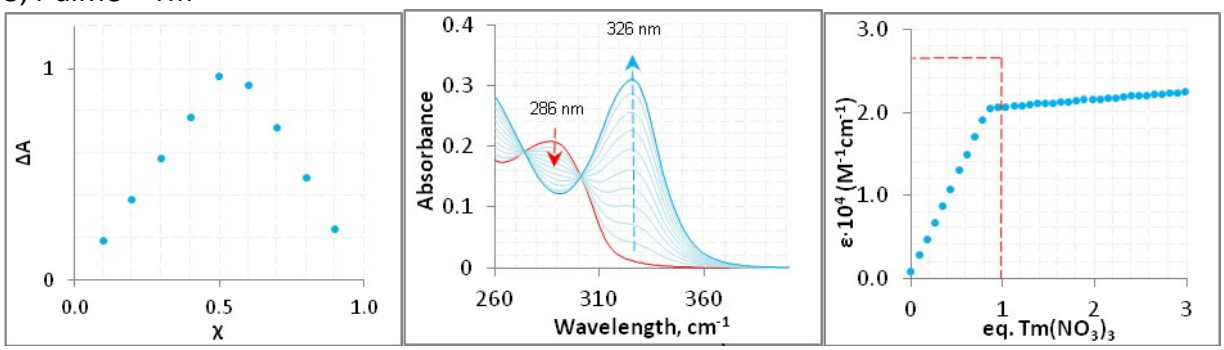
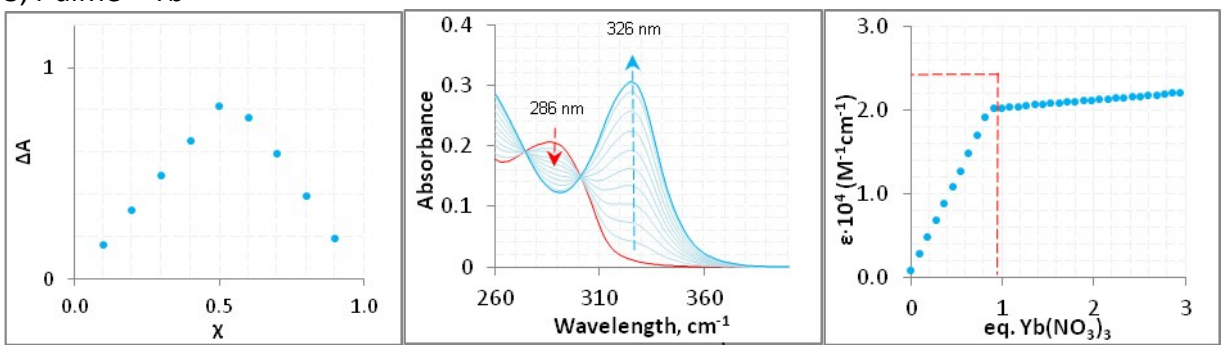


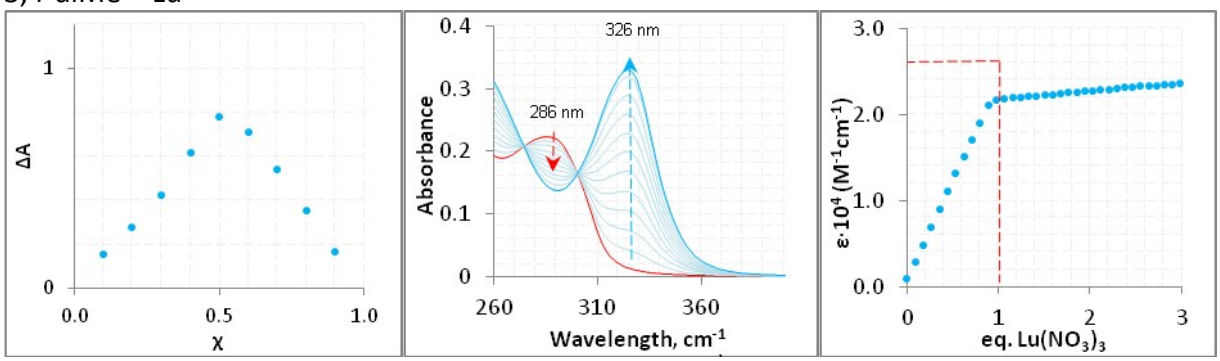
3,4-diMe + Tm^{3+}



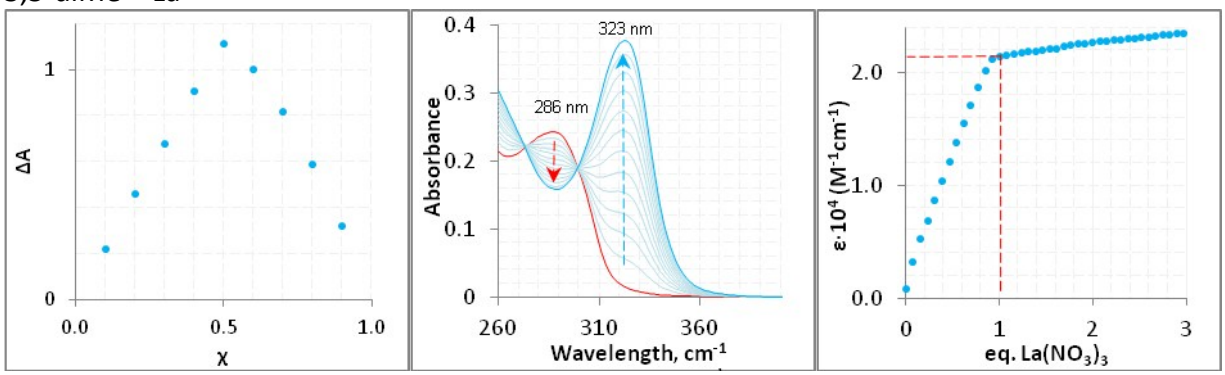
3,4-diMe + Yb^{3+}



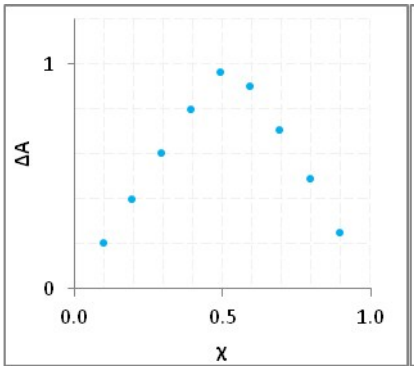
3,4-diMe + Lu^{3+}

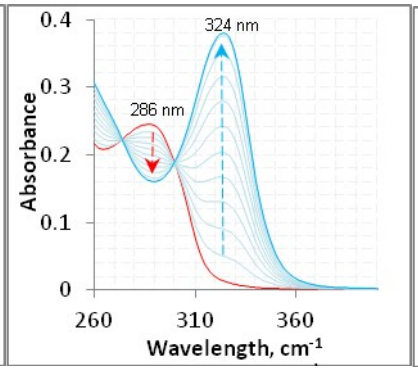


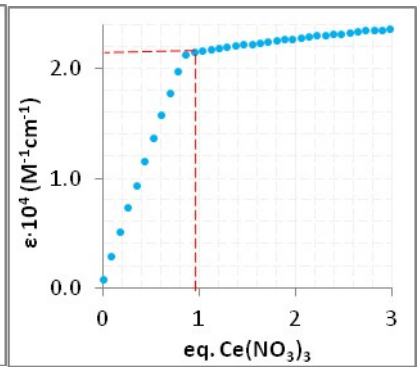
3,5-diMe + La^{3+}



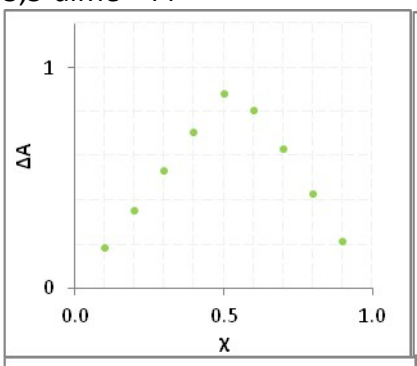
3,5-diMe + Ce^{3+}

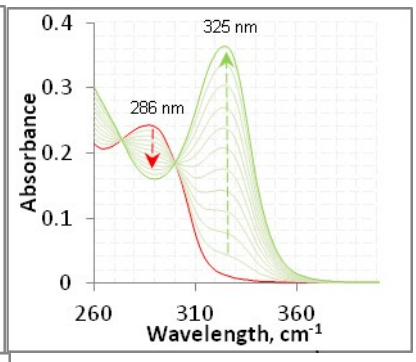


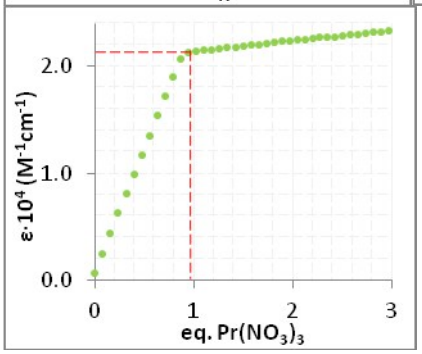




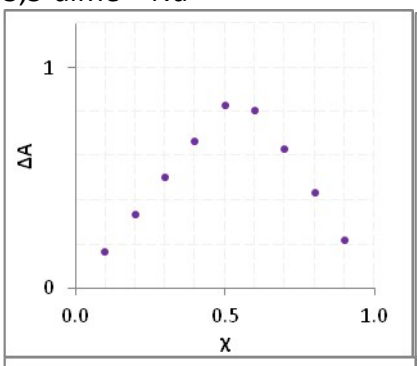
3,5-diMe + Pr^{3+}

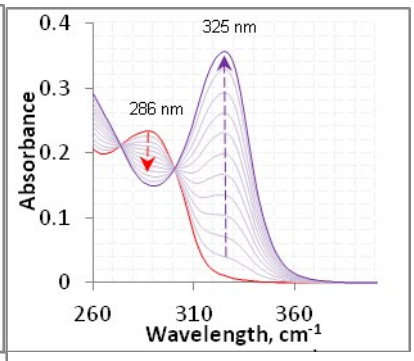


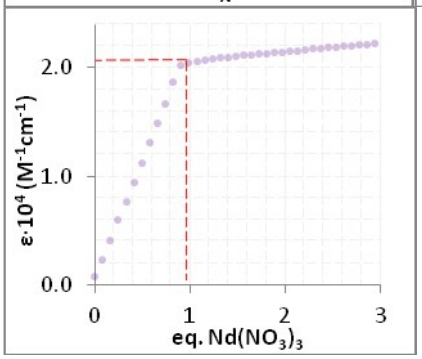




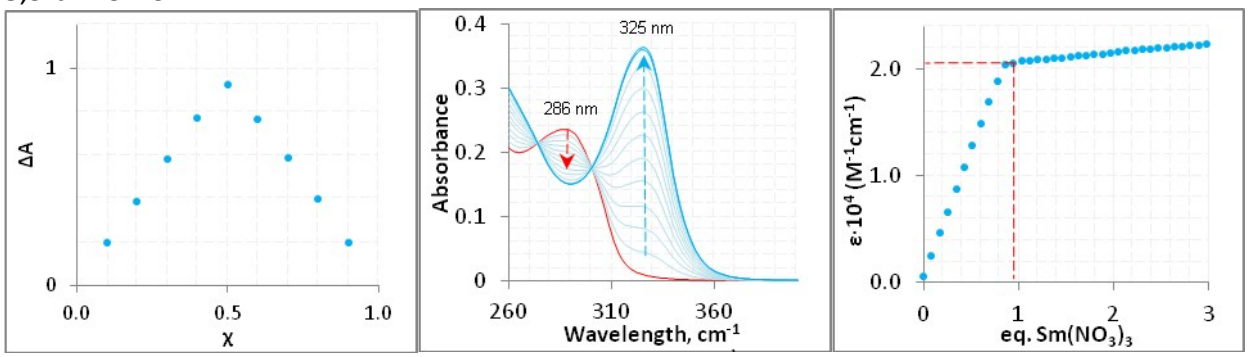
3,5-diMe + Nd^{3+}



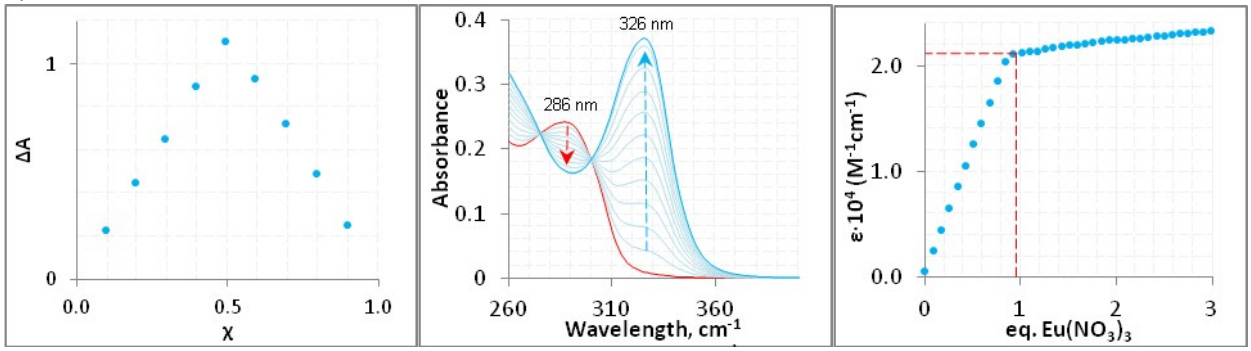




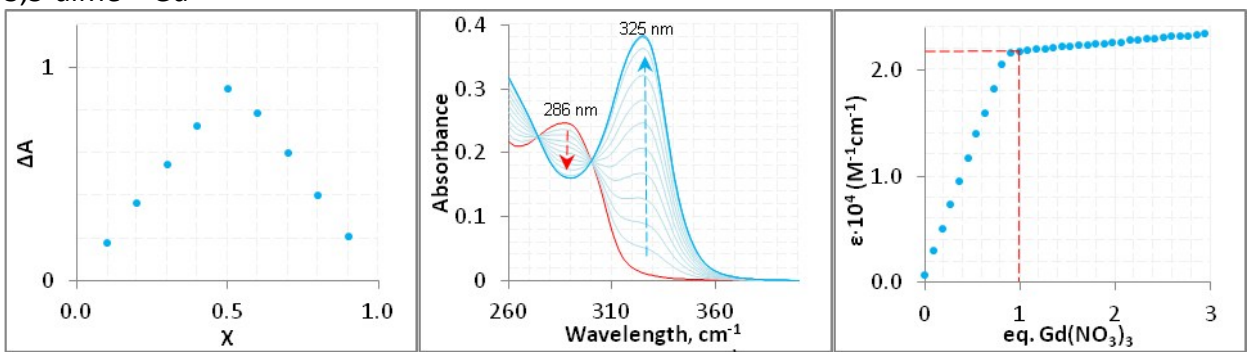
3,5-diMe + Sm^{3+}



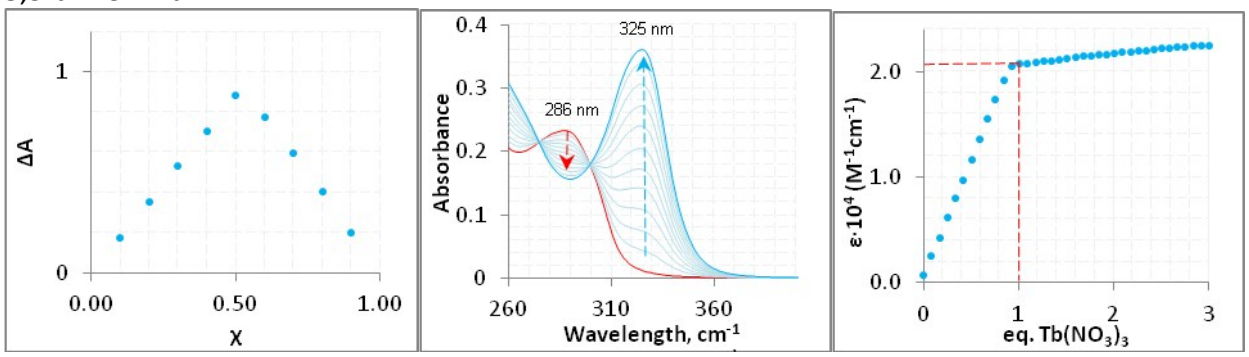
3,5-diMe + Eu^{3+}



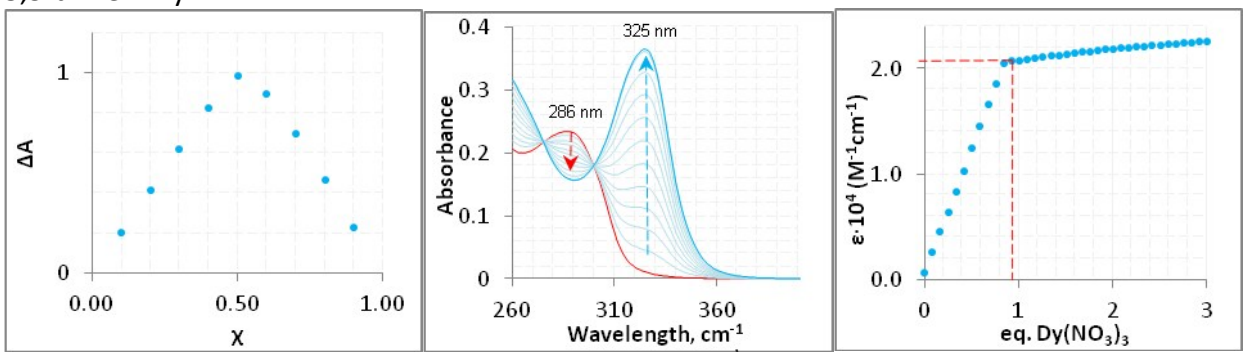
3,5-diMe + Gd^{3+}



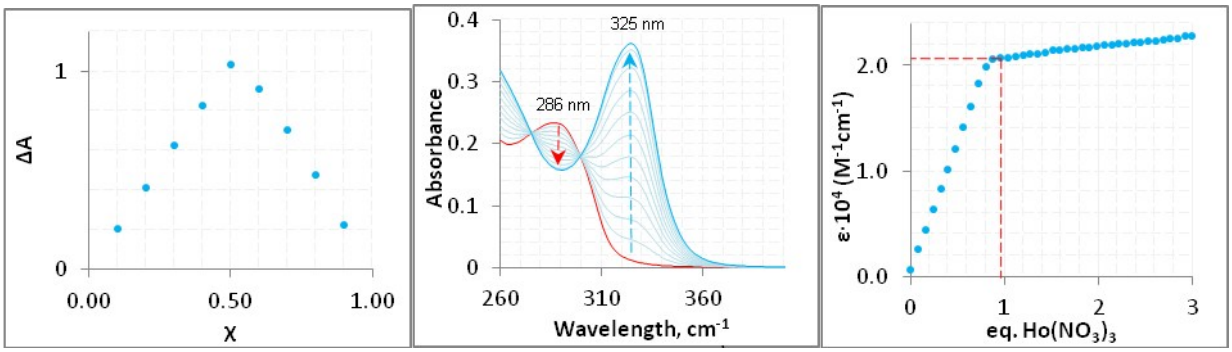
3,5-diMe + Tb^{3+}



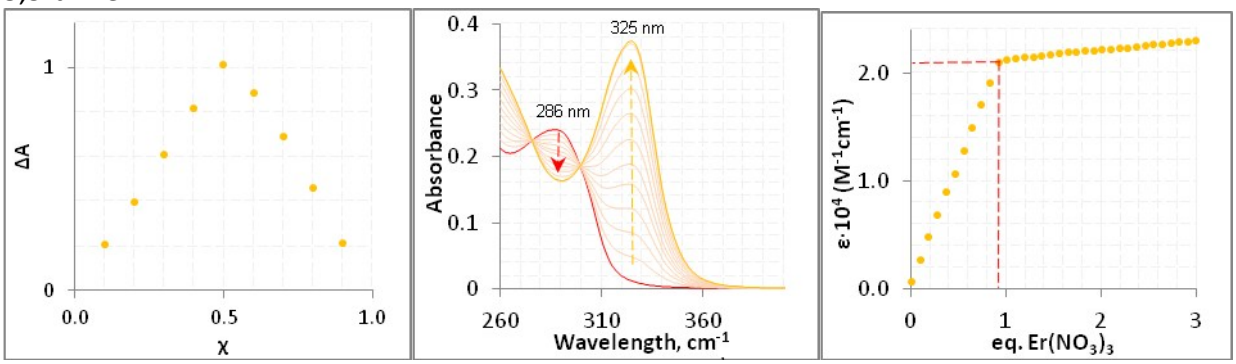
3,5-diMe + Dy^{3+}



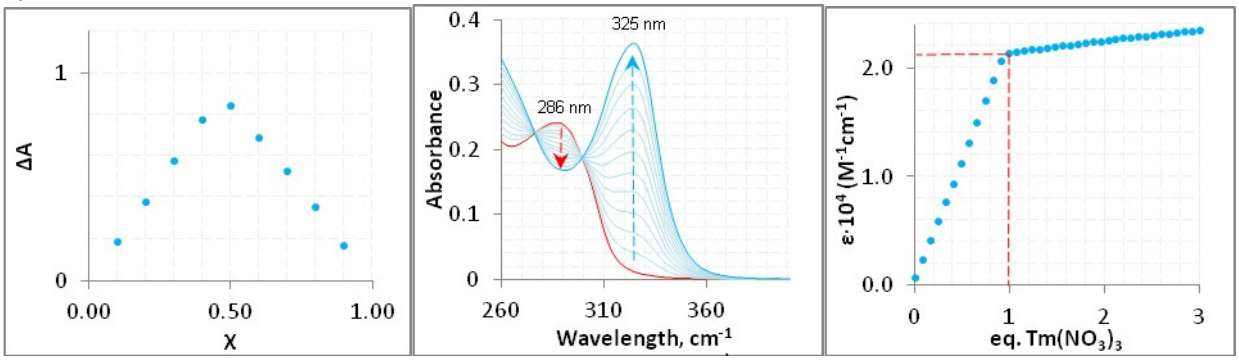
3,5-diMe + Ho^{3+}



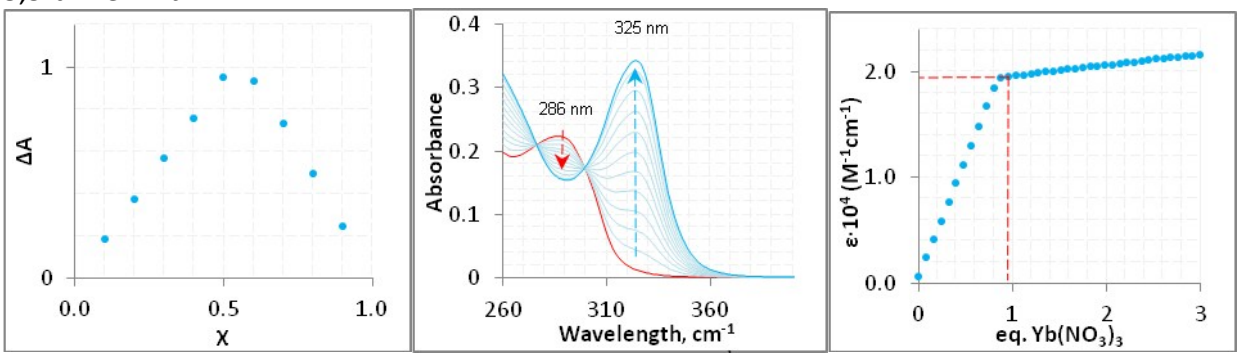
3,5-diMe + Er^{3+}



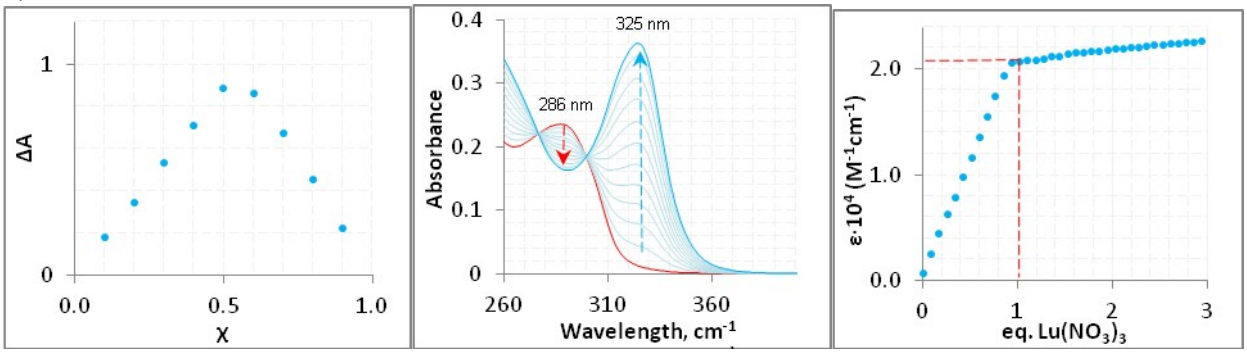
3,5-diMe + Tm^{3+}



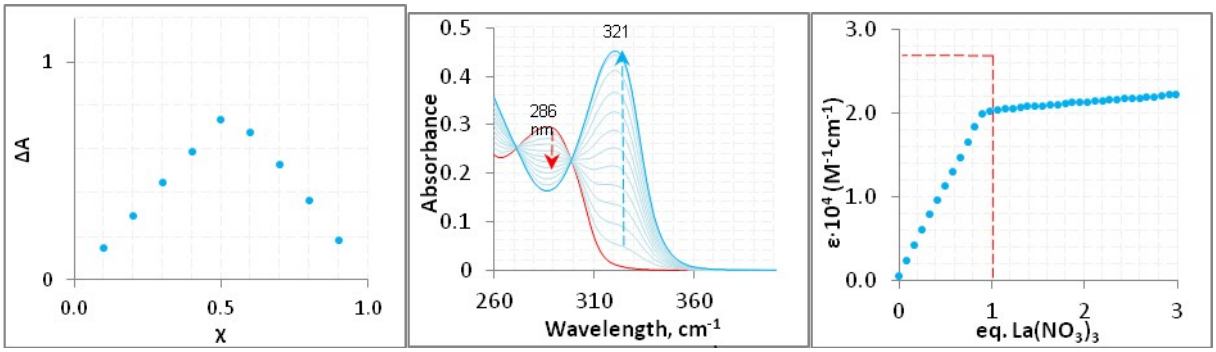
3,5-diMe + Yb^{3+}



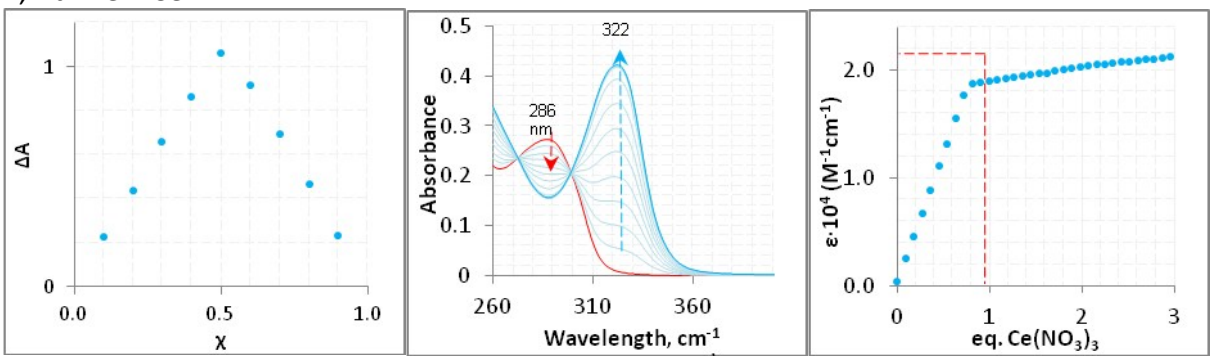
3,5-diMe + Lu^{3+}



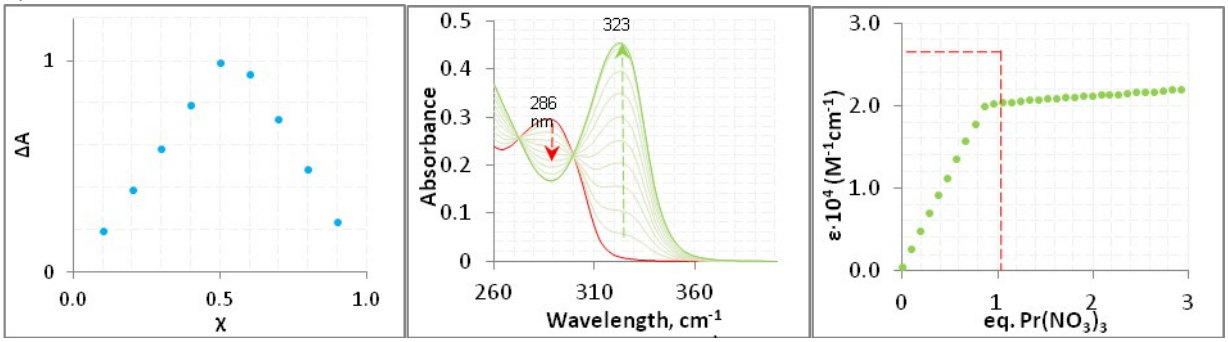
2,4-diMe + La^{3+}



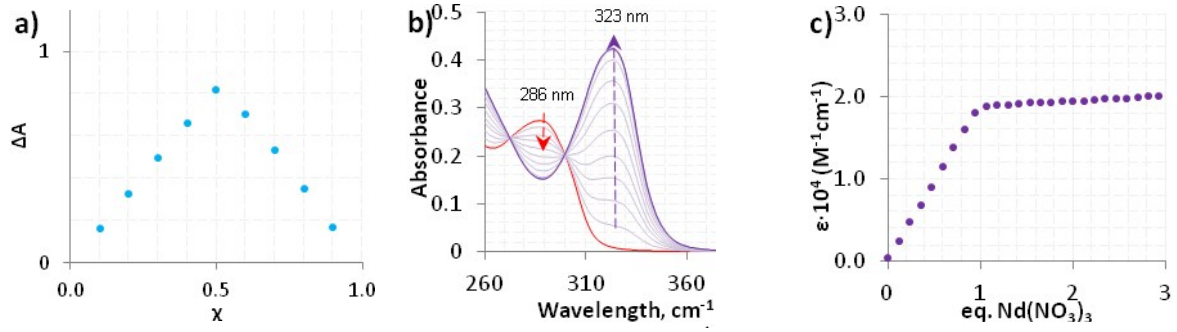
2,4-diMe + Ce^{3+}



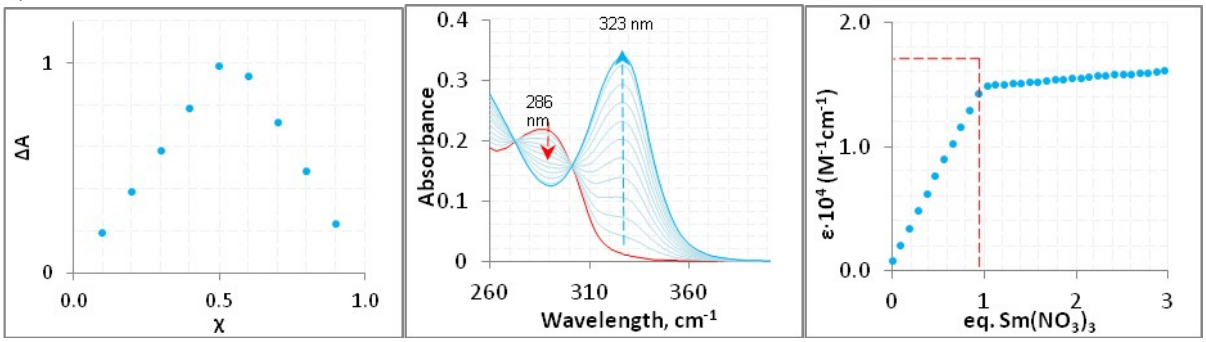
2,4-diMe + Pr^{3+}



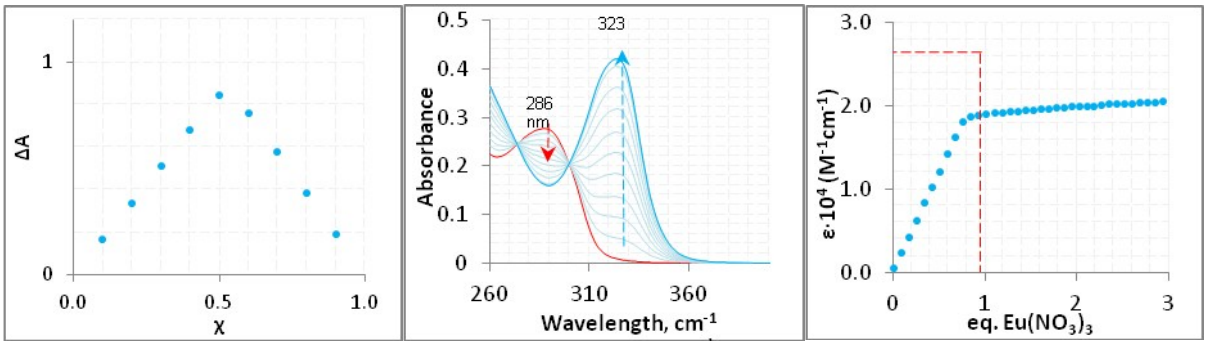
2,4-diMe + Nd^{3+}



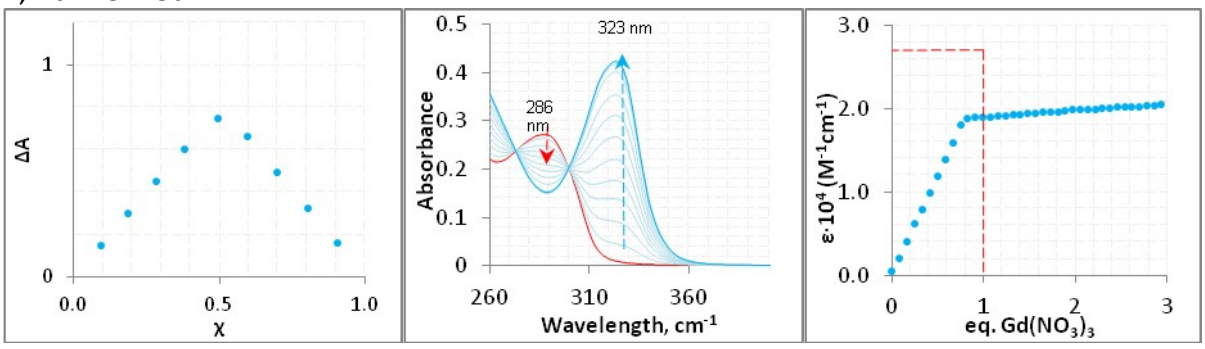
2,4-diMe + Sm^{3+}



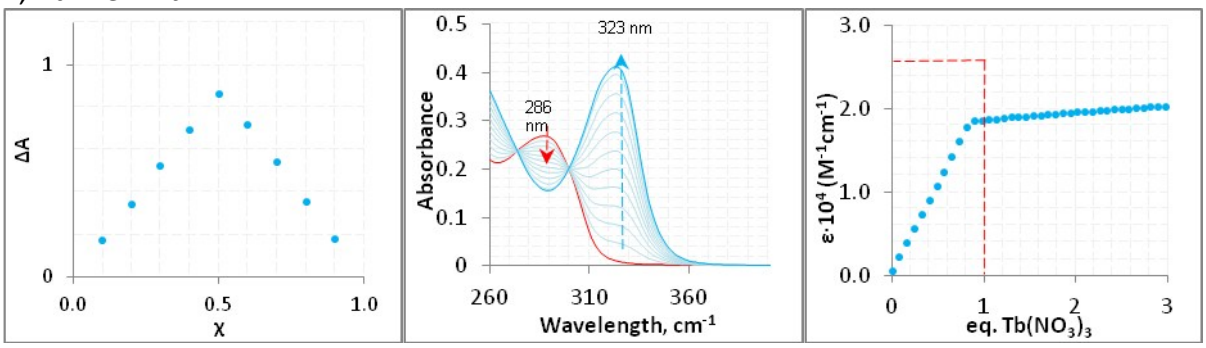
2,4-diMe + Eu^{3+}



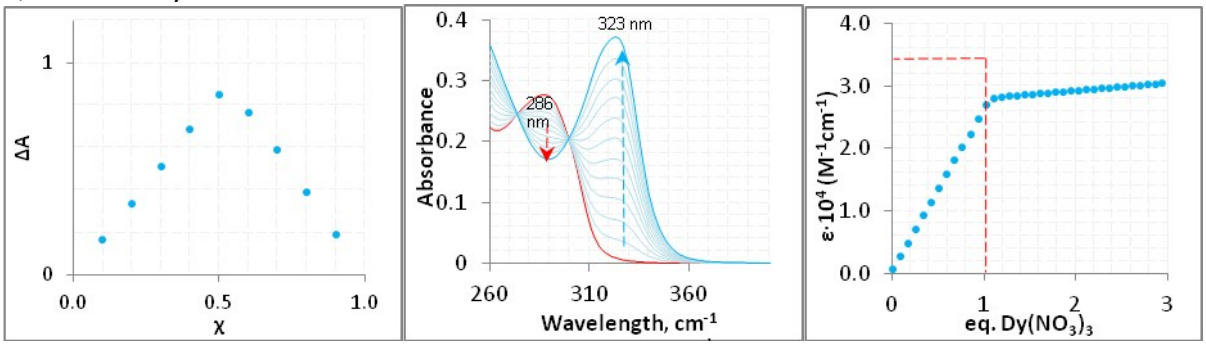
2,4-diMe + Gd^{3+}



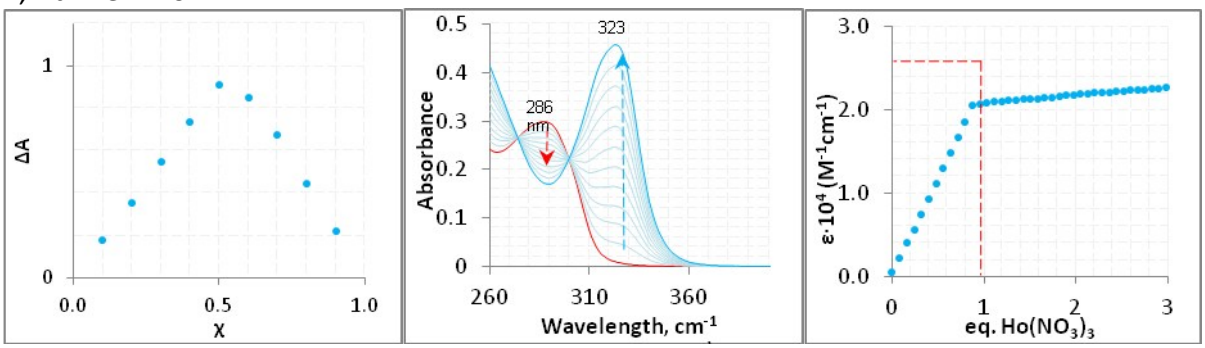
2,4-diMe + Tb^{3+}



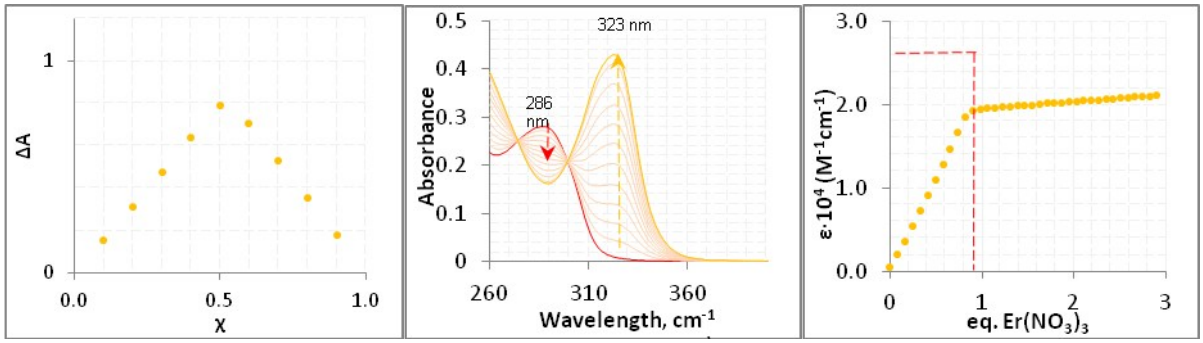
2,4-diMe + Dy^{3+}



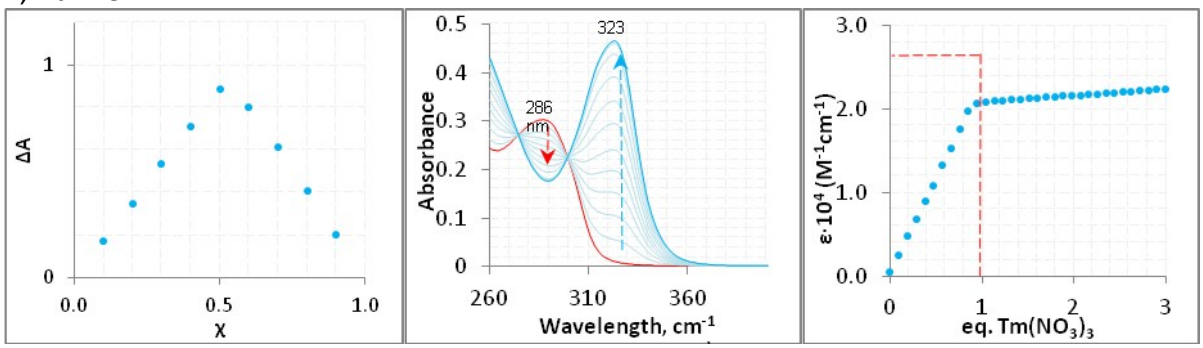
2,4-diMe + Ho^{3+}



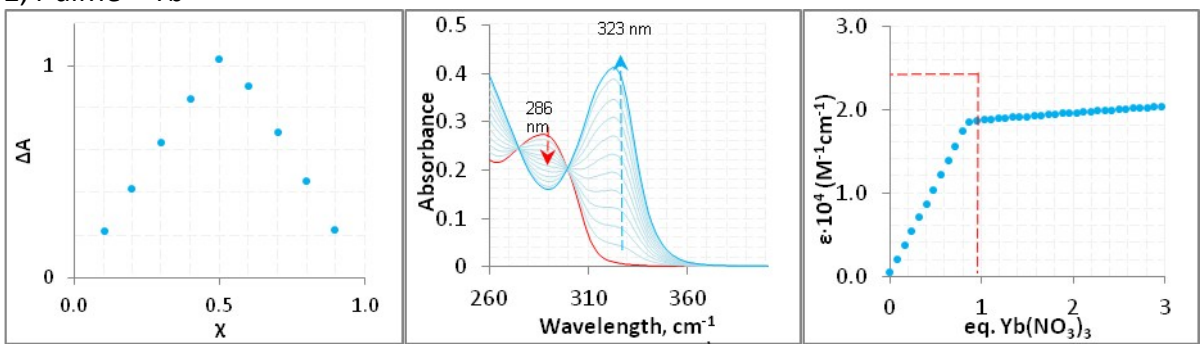
2,4-diMe + Er^{3+}



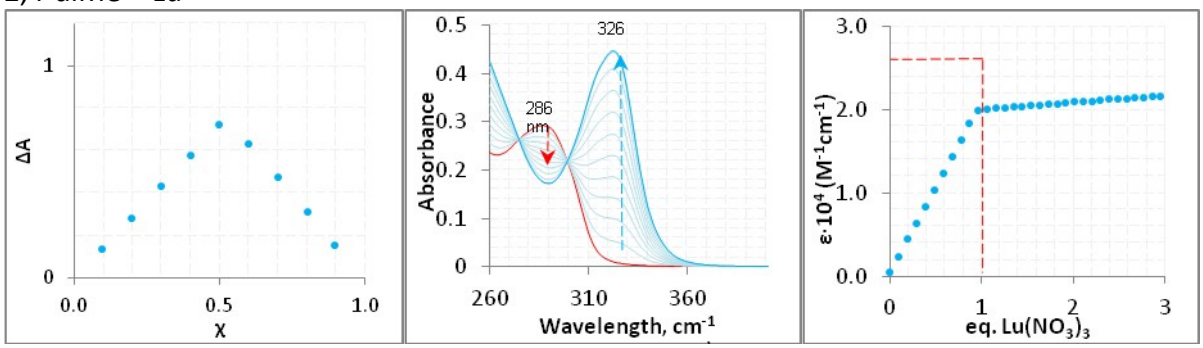
2,4-diMe + Tm^{3+}



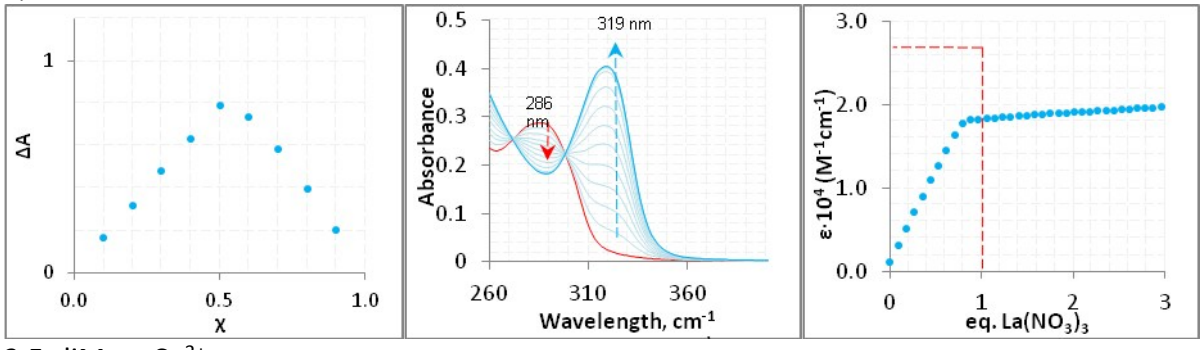
2,4-diMe + Yb^{3+}



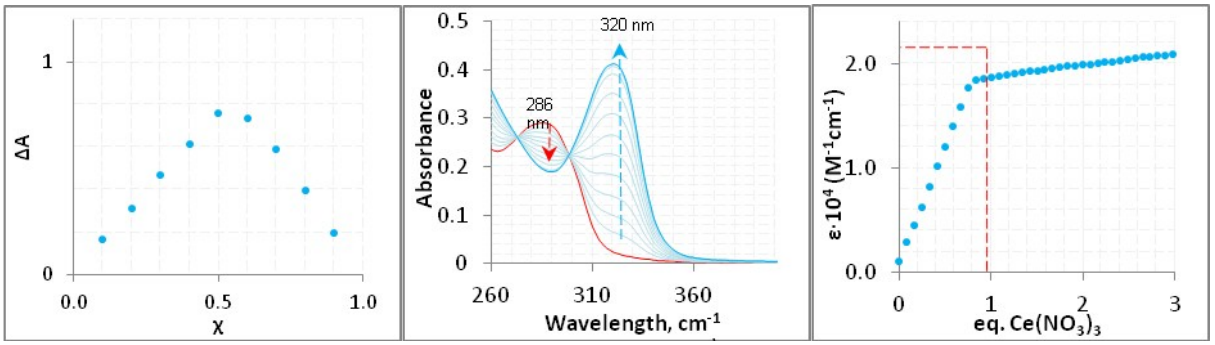
2,4-diMe + Lu^{3+}



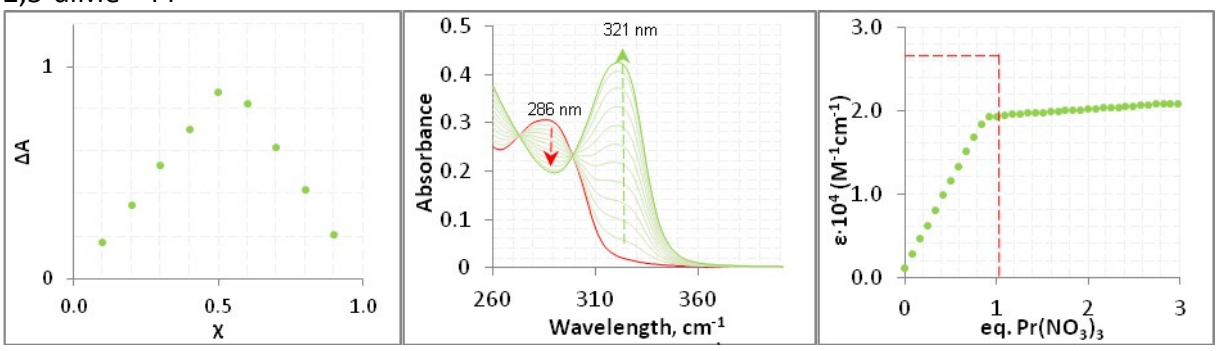
2,5-diMe + La^{3+}



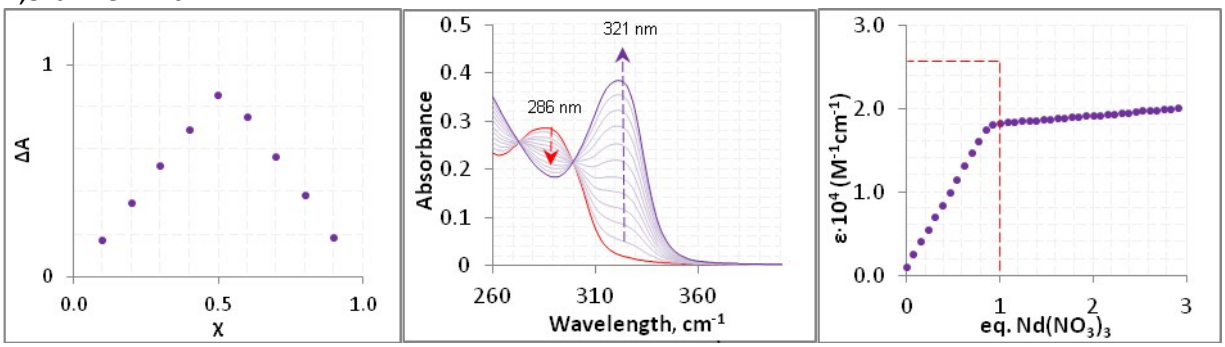
2,5-diMe + Ce^{3+}



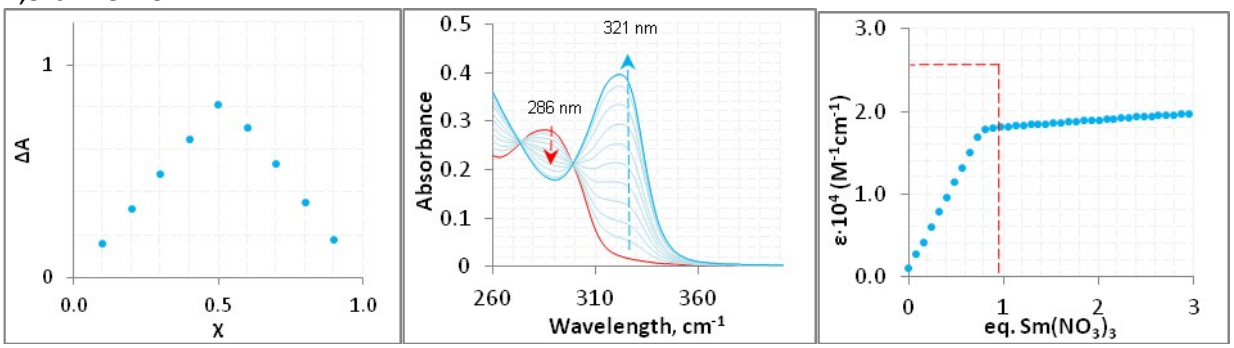
2,5-diMe + Pr^{3+}



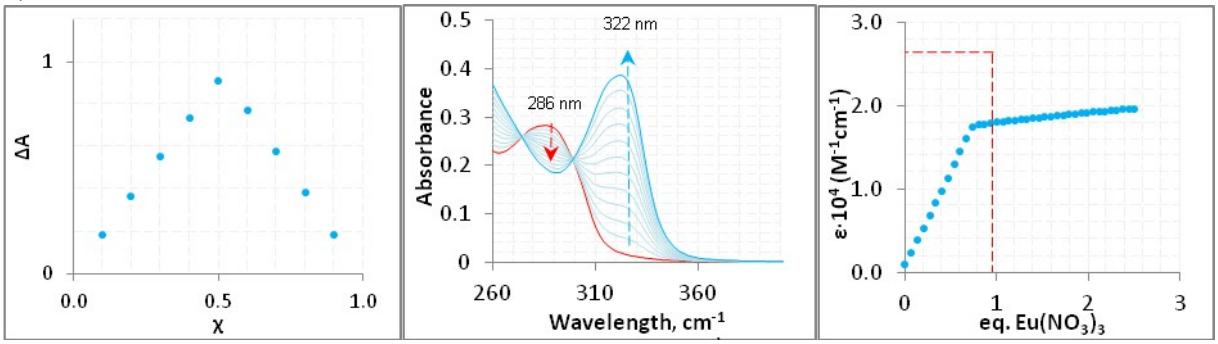
2,5-diMe + Nd^{3+}



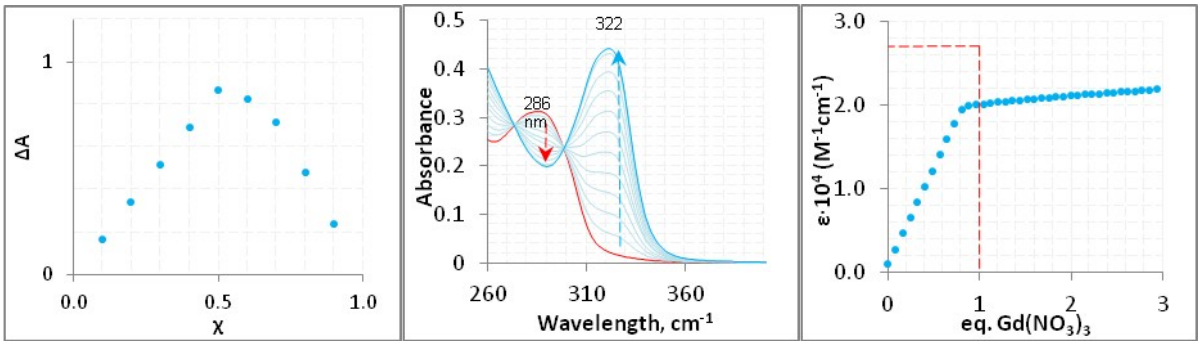
2,5-diMe + Sm^{3+}



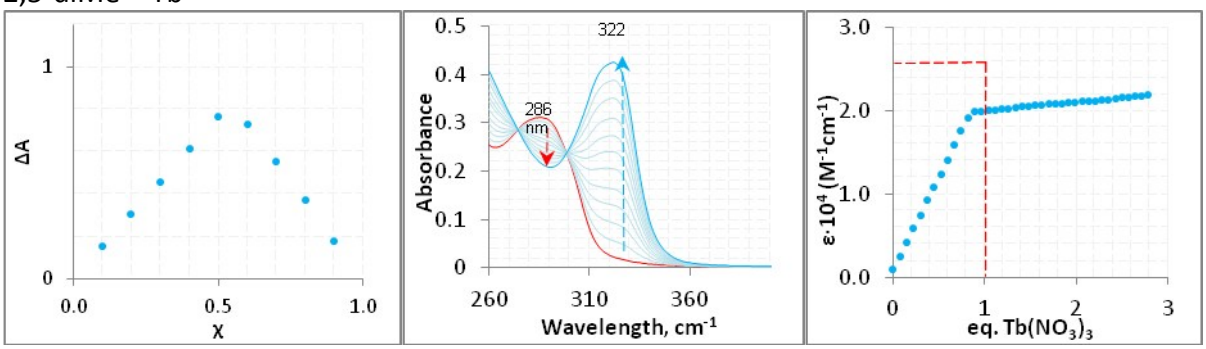
2,5-diMe + Eu^{3+}



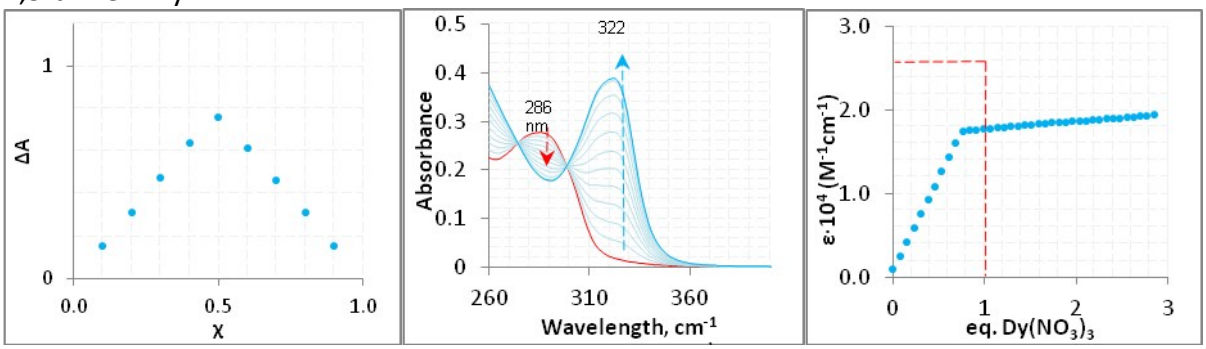
2,5-diMe + Gd^{3+}



2,5-diMe + Tb^{3+}



2,5-diMe + Dy^{3+}



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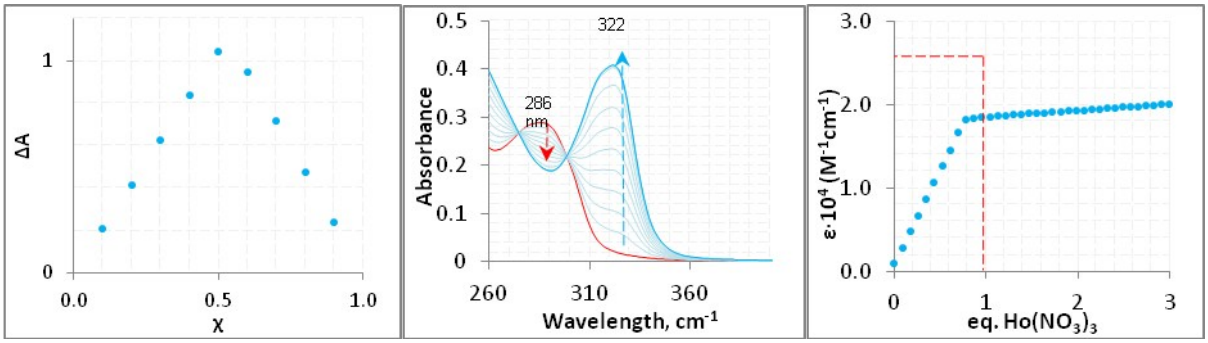
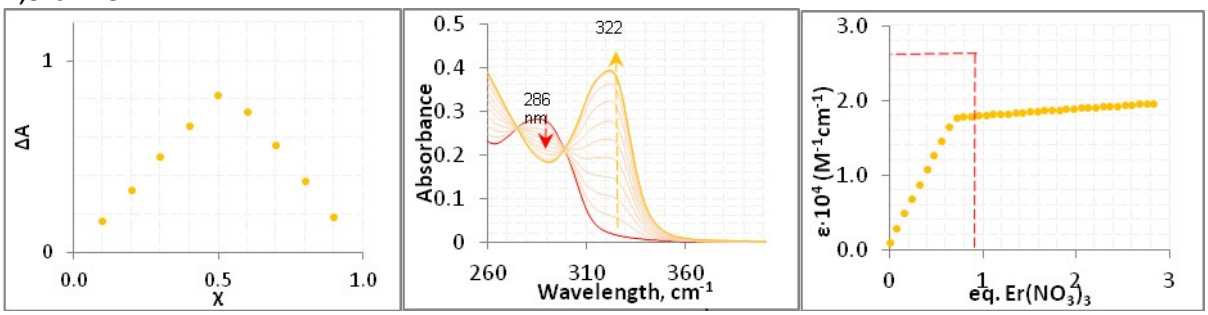
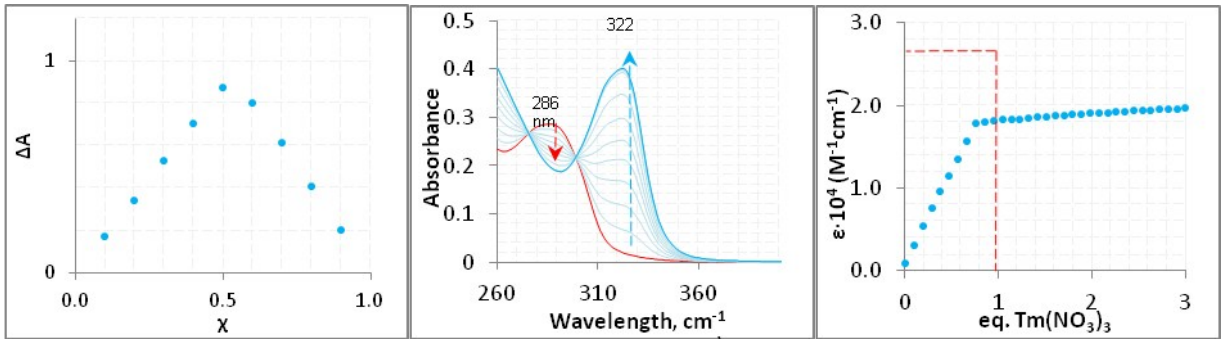


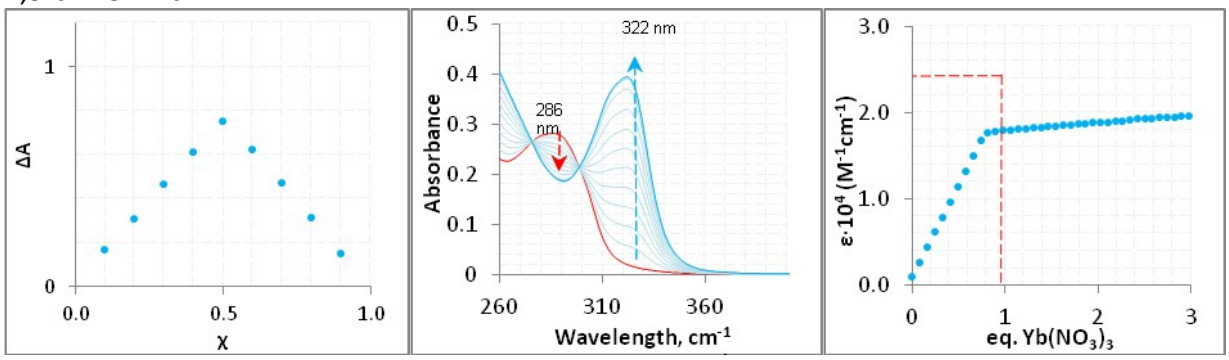
2,5-diMe + Er^{3+}



2,5-diMe + Tm^{3+}



2,5-diMe + Yb^{3+}



2,5-diMe + Lu^{3+}