Nitro-Functionalization and Luminescence Quantum Yield of Eu(III) and Tb(III) Benzoic Acid Complexes

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Supplementary Information

Table 1.   Bond lengths [Å] and angles [°] for **1**.

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C(1)-O(1)	1.261(8)	C(9)-C(14)	1.377(10)
C(1)-O(14)#1	1.261(8)	C(9)-C(10)	1.387(9)
C(1)-C(2)	1.511(9)	C(10)-C(11)	1.396(10)
C(2)-C(7)	1.383(10)	C(10)-H(10)	0.9500
C(2)-C(3)	1.386(10)	C(11)-C(12)	1.368(11)
C(3)-C(4)	1.385(10)	C(11)-H(11)	0.9500
C(3)-N(1)	1.474(10)	C(12)-C(13)	1.402(11)
C(4)-C(5)	1.366(12)	C(12)-H(12)	0.9500
C(4)-H(4)	0.9500	C(13)-C(14)	1.375(10)
C(5)-C(6)	1.395(11)	C(13)-H(13)	0.9500
C(5)-H(5)	0.9500	C(14)-N(2)	1.478(9)
C(6)-C(7)	1.398(10)	C(15)-O(11)#1	1.248(8)
C(6)-H(6)	0.9500	C(15)-O(8)	1.268(8)
C(7)-H(7)	0.9500	C(15)-C(16)	1.500(10)
C(8)-O(5)	1.249(8)	C(15)-Eu(1)	3.200(7)
C(8)-O(4)	1.279(8)	C(16)-C(17)	1.383(10)
C(8)-C(9)	1.512(9)	C(16)-C(21)	1.401(10)
C(8)-Eu(1)	2.834(7)	C(17)-C(18)	1.372(11)

C(17)-N(3)	1.479(10)	C(33)-C(34)	1.400(9)
C(18)-C(19)	1.377(11)	C(33)-H(33)	0.9500
C(18)-H(18)	0.9500	C(34)-C(35)	1.385(10)
C(19)-C(20)	1.389(11)	C(34)-H(34)	0.9500
C(19)-H(19)	0.9500	C(35)-C(36)	1.378(10)
C(20)-C(21)	1.395(11)	C(35)-H(35)	0.9500
C(20)-H(20)	0.9500	C(36)-C(37)	1.390(9)
C(21)-H(21)	0.9500	C(36)-H(36)	0.9500
C(22)-O(12)	1.416(9)	C(37)-N(5)	1.479(9)
C(22)-H(22A)	0.9800	C(38)-O(23)	1.255(8)
C(22)-H(22B)	0.9800	C(38)-O(22)	1.271(8)
C(22)-H(22C)	0.9800	C(38)-C(39)	1.499(10)
C(23)-O(13)	1.444(8)	C(38)-Eu(2)	2.930(7)
C(23)-H(23A)	0.9800	C(39)-C(44)	1.391(10)
C(23)-H(23B)	0.9800	C(39)-C(40)	1.391(10)
C(23)-H(23C)	0.9800	C(40)-C(41)	1.390(11)
C(24)-O(16)	1.261(8)	C(40)-H(40)	0.9500
C(24)-O(15)	1.266(8)	C(41)-C(42)	1.362(12)
C(24)-C(25)	1.490(9)	C(41)-H(41)	0.9500
C(24)-Eu(2)	2.800(7)	C(42)-C(43)	1.391(12)
C(25)-C(26)	1.392(9)	C(42)-H(42)	0.9500
C(25)-C(30)	1.392(10)	C(43)-C(44)	1.367(11)
C(26)-C(27)	1.387(10)	C(43)-H(43)	0.9500
C(26)-H(26)	0.9500	C(44)-N(6)	1.501(10)
C(27)-C(28)	1.379(11)	C(45)-O(27)	1.425(8)
C(27)-H(27)	0.9500	C(45)-H(45A)	0.9800
C(28)-C(29)	1.372(10)	C(45)-H(45B)	0.9800
C(28)-H(28)	0.9500	C(45)-H(45C)	0.9800
C(29)-C(30)	1.365(10)	C(46)-O(28)	1.426(8)
C(29)-H(29)	0.9500	C(46)-H(46A)	0.9800
C(30)-N(4)	1.473(9)	C(46)-H(46B)	0.9800
C(31)-O(19)	1.241(7)	C(46)-H(46C)	0.9800
C(31)-O(26)#2	1.258(8)	Eu(1)-O(11)	2.282(5)
C(31)-C(32)	1.521(9)	Eu(1)-O(14)	2.354(5)
C(32)-C(33)	1.386(10)	Eu(1)-O(1)	2.382(5)
C(32)-C(37)	1.387(10)	Eu(1)-O(4)	2.433(5)

Eu(1)-O(8)	2.435(5)	C(3)-C(2)-C(1)	123.9(6)
Eu(1)-O(12)	2.443(6)	C(2)-C(3)-C(4)	122.6(7)
Eu(1)-O(13)	2.461(4)	C(2)-C(3)-N(1)	119.7(7)
Eu(1)-O(5)	2.524(5)	C(4)-C(3)-N(1)	117.5(7)
Eu(1)-Eu(1)#1	4.3507(13)	C(5)-C(4)-C(3)	118.9(7)
Eu(2)-O(19)	2.377(4)	C(5)-C(4)-H(4)	120.5
Eu(2)-O(22)#2	2.388(4)	C(3)-C(4)-H(4)	120.5
Eu(2)-O(15)	2.408(5)	C(4)-C(5)-C(6)	120.6(7)
Eu(2)-O(26)	2.410(5)	C(4)-C(5)-H(5)	119.7
Eu(2)-O(28)	2.410(5)	C(6)-C(5)-H(5)	119.7
Eu(2)-O(27)	2.453(5)	C(5)-C(6)-C(7)	119.3(7)
Eu(2)-O(16)	2.494(5)	C(5)-C(6)-H(6)	120.3
Eu(2)-O(23)	2.542(5)	C(7)-C(6)-H(6)	120.3
Eu(2)-O(22)	2.573(5)	C(2)-C(7)-C(6)	121.0(7)
Eu(2)-Eu(2)#2	3.9428(11)	C(2)-C(7)-H(7)	119.5
N(1)-O(2)	1.220(8)	C(6)-C(7)-H(7)	119.5
N(1)-O(3)	1.222(8)	O(5)-C(8)-O(4)	121.6(6)
N(2)-O(7)	1.213(8)	O(5)-C(8)-C(9)	119.8(6)
N(2)-O(6)	1.235(8)	O(4)-C(8)-C(9)	118.4(6)
N(3)-O(10)	1.220(8)	O(5)-C(8)-Eu(1)	62.9(3)
N(3)-O(9)	1.230(8)	O(4)-C(8)-Eu(1)	58.9(3)
N(4)-O(18)	1.223(8)	C(9)-C(8)-Eu(1)	170.8(5)
N(4)-O(17)	1.231(8)	C(14)-C(9)-C(10)	117.4(6)
N(5)-O(20)	1.220(8)	C(14)-C(9)-C(8)	125.7(6)
N(5)-O(21)	1.230(8)	C(10)-C(9)-C(8)	116.6(6)
N(6)-O(25)	1.201(8)	C(9)-C(10)-C(11)	120.9(7)
N(6)-O(24)	1.214(9)	C(9)-C(10)-H(10)	119.6
O(11)-C(15)#1	1.248(8)	C(11)-C(10)-H(10)	119.6
O(14)-C(1)#1	1.261(8)	C(12)-C(11)-C(10)	120.1(7)
O(22)-Eu(2)#2	2.388(4)	C(12)-C(11)-H(11)	119.9
O(26)-C(31)#2	1.258(8)	C(10)-C(11)-H(11)	119.9
O(1)-C(1)-O(14)#1	127.2(6)	C(11)-C(12)-C(13)	120.1(7)
O(1)-C(1)-C(2)	116.1(6)	C(11)-C(12)-H(12)	120.0
O(14)#1-C(1)-C(2)	116.7(6)	C(13)-C(12)-H(12)	120.0
C(7)-C(2)-C(3)	117.6(7)	C(14)-C(13)-C(12)	118.2(7)
C(7)-C(2)-C(1)	118.3(6)	C(14)-C(13)-H(13)	120.9

C(12)-C(13)-H(13)	120.9	H(23A)-C(23)-H(23B)	109.5
C(13)-C(14)-C(9)	123.3(7)	O(13)-C(23)-H(23C)	109.5
C(13)-C(14)-N(2)	116.8(6)	H(23A)-C(23)-H(23C)	109.5
C(9)-C(14)-N(2)	119.8(6)	H(23B)-C(23)-H(23C)	109.5
O(11)#1-C(15)-O(8)	123.4(7)	O(16)-C(24)-O(15)	122.0(6)
O(11)#1-C(15)-C(16)	117.6(6)	O(16)-C(24)-C(25)	120.0(6)
O(8)-C(15)-C(16)	118.9(6)	O(15)-C(24)-C(25)	117.9(6)
O(11)#1-C(15)-Eu(1)	80.6(4)	O(16)-C(24)-Eu(2)	63.0(4)
O(8)-C(15)-Eu(1)	43.2(3)	O(15)-C(24)-Eu(2)	59.0(3)
C(16)-C(15)-Eu(1)	159.6(5)	C(25)-C(24)-Eu(2)	174.5(5)
C(17)-C(16)-C(21)	117.2(7)	C(26)-C(25)-C(30)	116.1(6)
C(17)-C(16)-C(15)	126.7(7)	C(26)-C(25)-C(24)	119.3(6)
C(21)-C(16)-C(15)	116.0(6)	C(30)-C(25)-C(24)	124.3(6)
C(18)-C(17)-C(16)	122.9(7)	C(27)-C(26)-C(25)	121.5(7)
C(18)-C(17)-N(3)	117.9(7)	C(27)-C(26)-H(26)	119.3
C(16)-C(17)-N(3)	119.2(7)	C(25)-C(26)-H(26)	119.3
C(17)-C(18)-C(19)	119.2(7)	C(28)-C(27)-C(26)	119.3(7)
C(17)-C(18)-H(18)	120.4	C(28)-C(27)-H(27)	120.3
C(19)-C(18)-H(18)	120.4	C(26)-C(27)-H(27)	120.3
C(18)-C(19)-C(20)	120.5(7)	C(29)-C(28)-C(27)	120.9(7)
C(18)-C(19)-H(19)	119.7	C(29)-C(28)-H(28)	119.6
C(20)-C(19)-H(19)	119.7	C(27)-C(28)-H(28)	119.6
C(19)-C(20)-C(21)	119.2(7)	C(30)-C(29)-C(28)	118.5(7)
C(19)-C(20)-H(20)	120.4	C(30)-C(29)-H(29)	120.7
C(21)-C(20)-H(20)	120.4	C(28)-C(29)-H(29)	120.7
C(20)-C(21)-C(16)	121.0(7)	C(29)-C(30)-C(25)	123.5(7)
C(20)-C(21)-H(21)	119.5	C(29)-C(30)-N(4)	116.7(6)
C(16)-C(21)-H(21)	119.5	C(25)-C(30)-N(4)	119.7(6)
O(12)-C(22)-H(22A)	109.5	O(19)-C(31)-O(26)#2	127.7(6)
O(12)-C(22)-H(22B)	109.5	O(19)-C(31)-C(32)	116.4(6)
H(22A)-C(22)-H(22B)	109.5	O(26)#2-C(31)-C(32)	115.8(6)
O(12)-C(22)-H(22C)	109.5	C(33)-C(32)-C(37)	116.0(6)
H(22A)-C(22)-H(22C)	109.5	C(33)-C(32)-C(31)	119.6(6)
H(22B)-C(22)-H(22C)	109.5	C(37)-C(32)-C(31)	124.2(6)
O(13)-C(23)-H(23A)	109.5	C(32)-C(33)-C(34)	120.8(7)
O(13)-C(23)-H(23B)	109.5	C(32)-C(33)-H(33)	119.6

C(34)-C(33)-H(33)	119.6	C(39)-C(44)-N(6)	118.7(7)
C(35)-C(34)-C(33)	121.0(7)	O(27)-C(45)-H(45A)	109.5
C(35)-C(34)-H(34)	119.5	O(27)-C(45)-H(45B)	109.5
C(33)-C(34)-H(34)	119.5	H(45A)-C(45)-H(45B)	109.5
C(36)-C(35)-C(34)	119.8(6)	O(27)-C(45)-H(45C)	109.5
C(36)-C(35)-H(35)	120.1	H(45A)-C(45)-H(45C)	109.5
C(34)-C(35)-H(35)	120.1	H(45B)-C(45)-H(45C)	109.5
C(35)-C(36)-C(37)	117.5(7)	O(28)-C(46)-H(46A)	109.5
C(35)-C(36)-H(36)	121.3	O(28)-C(46)-H(46B)	109.5
C(37)-C(36)-H(36)	121.3	H(46A)-C(46)-H(46B)	109.5
C(32)-C(37)-C(36)	124.9(7)	O(28)-C(46)-H(46C)	109.5
C(32)-C(37)-N(5)	119.0(6)	H(46A)-C(46)-H(46C)	109.5
C(36)-C(37)-N(5)	116.1(6)	H(46B)-C(46)-H(46C)	109.5
O(23)-C(38)-O(22)	120.7(7)	O(11)-Eu(1)-O(14)	76.52(17)
O(23)-C(38)-C(39)	119.9(6)	O(11)-Eu(1)-O(1)	75.83(17)
O(22)-C(38)-C(39)	119.1(6)	O(14)-Eu(1)-O(1)	124.85(16)
O(23)-C(38)-Eu(2)	59.8(4)	O(11)-Eu(1)-O(4)	134.21(17)
O(22)-C(38)-Eu(2)	61.2(4)	O(14)-Eu(1)-O(4)	147.51(16)
C(39)-C(38)-Eu(2)	179.5(5)	O(1)-Eu(1)-O(4)	80.14(16)
C(44)-C(39)-C(40)	116.7(7)	O(11)-Eu(1)-O(8)	120.45(18)
C(44)-C(39)-C(38)	124.9(6)	O(14)-Eu(1)-O(8)	79.72(17)
C(40)-C(39)-C(38)	118.3(7)	O(1)-Eu(1)-O(8)	74.84(16)
C(41)-C(40)-C(39)	119.3(8)	O(4)-Eu(1)-O(8)	89.07(16)
C(41)-C(40)-H(40)	120.3	O(11)-Eu(1)-O(12)	83.6(2)
C(39)-C(40)-H(40)	120.3	O(14)-Eu(1)-O(12)	78.47(19)
C(42)-C(41)-C(40)	122.8(8)	O(1)-Eu(1)-O(12)	142.64(18)
C(42)-C(41)-H(41)	118.6	O(4)-Eu(1)-O(12)	93.0(2)
C(40)-C(41)-H(41)	118.6	O(8)-Eu(1)-O(12)	142.19(18)
C(41)-C(42)-C(43)	118.6(7)	O(11)-Eu(1)-O(13)	147.34(17)
C(41)-C(42)-H(42)	120.7	O(14)-Eu(1)-O(13)	78.89(16)
C(43)-C(42)-H(42)	120.7	O(1)-Eu(1)-O(13)	136.59(16)
C(44)-C(43)-C(42)	118.6(8)	O(4)-Eu(1)-O(13)	68.75(16)
C(44)-C(43)-H(43)	120.7	O(8)-Eu(1)-O(13)	75.14(16)
C(42)-C(43)-H(43)	120.7	O(12)-Eu(1)-O(13)	70.60(19)
C(43)-C(44)-C(39)	123.9(7)	O(11)-Eu(1)-O(5)	83.18(17)
C(43)-C(44)-N(6)	117.4(7)	O(14)-Eu(1)-O(5)	145.92(17)

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O(1)-Eu(1)-O(5)	74.59(16)	O(22)#2-Eu(2)-O(26)	73.02(16)
O(4)-Eu(1)-O(5)	52.84(15)	O(15)-Eu(2)-O(26)	79.99(16)
O(8)-Eu(1)-O(5)	134.36(16)	O(19)-Eu(2)-O(28)	76.08(16)
O(12)-Eu(1)-O(5)	72.23(18)	O(22)#2-Eu(2)-O(28)	141.78(16)
O(13)-Eu(1)-O(5)	106.58(16)	O(15)-Eu(2)-O(28)	85.74(17)
O(11)-Eu(1)-C(8)	108.29(19)	O(26)-Eu(2)-O(28)	142.76(16)
O(14)-Eu(1)-C(8)	160.02(18)	O(19)-Eu(2)-O(27)	138.11(16)
O(1)-Eu(1)-C(8)	74.79(17)	O(22)#2-Eu(2)-O(27)	143.61(15)
O(4)-Eu(1)-C(8)	26.74(17)	O(15)-Eu(2)-O(27)	73.54(16)
O(8)-Eu(1)-C(8)	112.14(18)	O(26)-Eu(2)-O(27)	72.06(16)
O(12)-Eu(1)-C(8)	82.8(2)	O(28)-Eu(2)-O(27)	70.93(16)
O(13)-Eu(1)-C(8)	88.49(17)	O(19)-Eu(2)-O(16)	75.74(16)
O(5)-Eu(1)-C(8)	26.15(17)	O(22)#2-Eu(2)-O(16)	74.01(16)
O(11)-Eu(1)-C(15)	99.58(19)	O(15)-Eu(2)-O(16)	53.57(15)
O(14)-Eu(1)-C(15)	73.12(17)	O(26)-Eu(2)-O(16)	121.46(16)
O(1)-Eu(1)-C(15)	65.80(17)	O(28)-Eu(2)-O(16)	73.37(16)
O(4)-Eu(1)-C(15)	105.24(17)	O(27)-Eu(2)-O(16)	117.02(16)
O(8)-Eu(1)-C(15)	20.88(16)	O(19)-Eu(2)-O(23)	79.96(16)
O(12)-Eu(1)-C(15)	149.70(19)	O(22)#2-Eu(2)-O(23)	125.18(16)
O(13)-Eu(1)-C(15)	93.45(17)	O(15)-Eu(2)-O(23)	140.48(16)
O(5)-Eu(1)-C(15)	138.02(17)	O(26)-Eu(2)-O(23)	94.04(17)
C(8)-Eu(1)-C(15)	123.56(18)	O(28)-Eu(2)-O(23)	75.67(16)
O(11)-Eu(1)-Eu(1)#1	46.59(14)	O(27)-Eu(2)-O(23)	67.53(16)
O(14)-Eu(1)-Eu(1)#1	64.54(12)	O(16)-Eu(2)-O(23)	144.30(16)
O(1)-Eu(1)-Eu(1)#1	61.69(11)	O(19)-Eu(2)-O(22)	72.10(15)
O(4)-Eu(1)-Eu(1)#1	140.92(12)	O(22)#2-Eu(2)-O(22)	74.78(17)
O(8)-Eu(1)-Eu(1)#1	73.88(11)	O(15)-Eu(2)-O(22)	151.40(15)
O(12)-Eu(1)-Eu(1)#1	122.03(17)	O(26)-Eu(2)-O(22)	72.32(15)
O(13)-Eu(1)-Eu(1)#1	135.31(12)	O(28)-Eu(2)-O(22)	120.90(16)
O(5)-Eu(1)-Eu(1)#1	118.11(11)	O(27)-Eu(2)-O(22)	103.74(16)
C(8)-Eu(1)-Eu(1)#1	133.06(13)	O(16)-Eu(2)-O(22)	139.15(15)
C(15)-Eu(1)-Eu(1)#1	53.04(12)	O(23)-Eu(2)-O(22)	50.84(15)
O(19)-Eu(2)-O(22)#2	77.05(16)	O(19)-Eu(2)-C(24)	102.49(18)
O(19)-Eu(2)-O(15)	129.21(16)	O(22)#2-Eu(2)-C(24)	81.17(18)
O(22)#2-Eu(2)-O(15)	90.65(17)	O(15)-Eu(2)-C(24)	26.80(18)
O(19)-Eu(2)-O(26)	138.18(16)	O(26)-Eu(2)-C(24)	101.04(18)

O(28)-Eu(2)-C(24)	78.68(18)	O(6)-N(2)-C(14)	116.7(6)
O(27)-Eu(2)-C(24)	95.70(18)	O(10)-N(3)-O(9)	123.6(7)
O(16)-Eu(2)-C(24)	26.77(17)	O(10)-N(3)-C(17)	118.3(6)
O(23)-Eu(2)-C(24)	152.82(17)	O(9)-N(3)-C(17)	118.0(7)
O(22)-Eu(2)-C(24)	155.95(17)	O(18)-N(4)-O(17)	125.0(6)
O(19)-Eu(2)-C(38)	76.03(17)	O(18)-N(4)-C(30)	118.3(6)
O(22)#2-Eu(2)-C(38)	100.38(18)	O(17)-N(4)-C(30)	116.6(6)
O(15)-Eu(2)-C(38)	154.46(17)	O(20)-N(5)-O(21)	123.2(6)
O(26)-Eu(2)-C(38)	81.33(18)	O(20)-N(5)-C(37)	119.1(6)
O(28)-Eu(2)-C(38)	98.95(18)	O(21)-N(5)-C(37)	117.6(6)
O(27)-Eu(2)-C(38)	84.24(18)	O(25)-N(6)-O(24)	125.7(7)
O(16)-Eu(2)-C(38)	151.76(16)	O(25)-N(6)-C(44)	117.5(7)
O(23)-Eu(2)-C(38)	25.27(17)	O(24)-N(6)-C(44)	116.8(6)
O(22)-Eu(2)-C(38)	25.66(16)	C(1)-O(1)-Eu(1)	141.8(4)
C(24)-Eu(2)-C(38)	177.49(18)	C(8)-O(4)-Eu(1)	94.4(4)
O(19)-Eu(2)-Eu(2)#2	70.35(11)	C(8)-O(5)-Eu(1)	90.9(4)
O(22)#2-Eu(2)-Eu(2)#2	39.02(11)	C(15)-O(8)-Eu(1)	115.9(4)
O(15)-Eu(2)-Eu(2)#2	125.43(12)	C(15)#1-O(11)-Eu(1)	174.0(5)
O(26)-Eu(2)-Eu(2)#2	67.97(11)	C(22)-O(12)-Eu(1)	134.8(5)
O(28)-Eu(2)-Eu(2)#2	144.18(11)	C(23)-O(13)-Eu(1)	132.5(4)
O(27)-Eu(2)-Eu(2)#2	129.98(11)	C(1)#1-O(14)-Eu(1)	139.0(4)
O(16)-Eu(2)-Eu(2)#2	109.07(11)	C(24)-O(15)-Eu(2)	94.2(4)
O(23)-Eu(2)-Eu(2)#2	86.38(11)	C(24)-O(16)-Eu(2)	90.3(4)
O(22)-Eu(2)-Eu(2)#2	35.76(10)	C(31)-O(19)-Eu(2)	135.5(4)
C(24)-Eu(2)-Eu(2)#2	120.19(14)	C(38)-O(22)-Eu(2)#2	161.3(4)
C(38)-Eu(2)-Eu(2)#2	61.38(14)	C(38)-O(22)-Eu(2)	93.1(4)
O(2)-N(1)-O(3)	123.9(7)	Eu(2)#2-O(22)-Eu(2)	105.22(17)
O(2)-N(1)-C(3)	117.6(7)	C(38)-O(23)-Eu(2)	94.9(4)
O(3)-N(1)-C(3)	118.4(6)	C(31)#2-O(26)-Eu(2)	137.9(4)
O(7)-N(2)-O(6)	125.0(6)	C(45)-O(27)-Eu(2)	130.6(4)
O(7)-N(2)-C(14)	118.3(6)	C(46)-O(28)-Eu(2)	130.4(4)

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Symmetry transformations used to generate equivalent atoms:

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

Table 2.   Bond lengths [Å] and angles [°] for **2**.

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C(1)-C(6)	1.390(4)	C(17)-H(17)	0.9500
C(1)-C(2)	1.394(4)	C(18)-C(19)	1.386(4)
C(1)-C(7)	1.504(4)	C(18)-H(18)	0.9500
C(2)-C(3)	1.388(4)	C(19)-C(20)	1.376(4)
C(2)-H(2A)	0.9500	C(19)-N(3)	1.467(4)
C(3)-C(4)	1.386(4)	C(20)-H(20)	0.9500
C(3)-N(1)	1.465(4)	C(21)-O(9)	1.264(3)
C(4)-C(5)	1.384(4)	C(21)-O(8)	1.265(4)
C(4)-H(4)	0.9500	C(22)-O(15)	1.442(4)
C(5)-C(6)	1.392(4)	C(22)-C(23)	1.503(5)
C(5)-H(5)	0.9500	C(22)-H(22A)	0.9900
C(6)-H(6)	0.9500	C(22)-H(22B)	0.9900
C(7)-O(13)#1	1.249(3)	C(23)-H(23A)	0.9800
C(7)-O(1)	1.252(4)	C(23)-H(23B)	0.9800
C(8)-C(9)	1.387(4)	C(23)-H(23C)	0.9800
C(8)-C(13)	1.398(4)	C(26)-O(17)	1.349(7)
C(8)-C(14)	1.496(4)	Eu(1)-O(13)	2.307(2)
C(9)-C(10)	1.383(4)	Eu(1)-O(1)	2.329(2)
C(9)-H(9)	0.9500	Eu(1)-O(14)	2.355(2)
C(10)-C(11)	1.384(4)	Eu(1)-O(4)	2.372(2)
C(10)-N(2)	1.475(4)	Eu(1)-O(12)	2.412(2)
C(11)-C(12)	1.381(5)	Eu(1)-O(8)	2.468(2)
C(11)-H(11A)	0.9500	Eu(1)-O(15)	2.509(2)
C(12)-C(13)	1.391(4)	Eu(1)-O(9)	2.541(2)
C(12)-H(12)	0.9500	N(1)-O(3)	1.213(4)
C(13)-H(13)	0.9500	N(1)-O(2)	1.235(3)
C(14)-O(4)	1.258(3)	N(2)-O(6)	1.218(4)
C(14)-O(14)#2	1.259(3)	N(2)-O(7)	1.228(4)
C(15)-C(20)	1.388(4)	N(3)-O(10)	1.228(4)
C(15)-C(16)	1.399(4)	N(3)-O(11)	1.233(4)
C(15)-C(21)	1.503(4)	O(13)-C(7)#1	1.249(3)
C(16)-C(17)	1.388(4)	O(14)-C(14)#2	1.259(3)
C(16)-H(16)	0.9500	O(17)-O(17)#3	1.509(9)
C(17)-C(18)	1.390(5)	C(6)-C(1)-C(2)	120.3(3)

C(6)-C(1)-C(7)	119.9(3)	C(12)-C(13)-H(13)	119.7
C(2)-C(1)-C(7)	119.8(3)	C(8)-C(13)-H(13)	119.7
C(3)-C(2)-C(1)	117.5(3)	O(4)-C(14)-O(14)#2	122.9(3)
C(3)-C(2)-H(2A)	121.2	O(4)-C(14)-C(8)	117.7(3)
C(1)-C(2)-H(2A)	121.2	O(14)#2-C(14)-C(8)	119.4(3)
C(4)-C(3)-C(2)	123.5(3)	C(20)-C(15)-C(16)	119.9(3)
C(4)-C(3)-N(1)	118.4(3)	C(20)-C(15)-C(21)	119.4(3)
C(2)-C(3)-N(1)	118.1(3)	C(16)-C(15)-C(21)	120.7(3)
C(5)-C(4)-C(3)	117.8(3)	C(17)-C(16)-C(15)	120.2(3)
C(5)-C(4)-H(4)	121.1	C(17)-C(16)-H(16)	119.9
C(3)-C(4)-H(4)	121.1	C(15)-C(16)-H(16)	119.9
C(4)-C(5)-C(6)	120.4(3)	C(16)-C(17)-C(18)	120.4(3)
C(4)-C(5)-H(5)	119.8	C(16)-C(17)-H(17)	119.8
C(6)-C(5)-H(5)	119.8	C(18)-C(17)-H(17)	119.8
C(1)-C(6)-C(5)	120.5(3)	C(19)-C(18)-C(17)	117.9(3)
C(1)-C(6)-H(6)	119.8	C(19)-C(18)-H(18)	121.1
C(5)-C(6)-H(6)	119.8	C(17)-C(18)-H(18)	121.1
O(13)#1-C(7)-O(1)	124.8(3)	C(20)-C(19)-C(18)	123.1(3)
O(13)#1-C(7)-C(1)	117.7(3)	C(20)-C(19)-N(3)	117.9(3)
O(1)-C(7)-C(1)	117.5(2)	C(18)-C(19)-N(3)	119.0(3)
C(9)-C(8)-C(13)	119.7(3)	C(19)-C(20)-C(15)	118.4(3)
C(9)-C(8)-C(14)	119.5(3)	C(19)-C(20)-H(20)	120.8
C(13)-C(8)-C(14)	120.8(3)	C(15)-C(20)-H(20)	120.8
C(10)-C(9)-C(8)	118.3(3)	O(9)-C(21)-O(8)	121.5(3)
C(10)-C(9)-H(9)	120.9	O(9)-C(21)-C(15)	119.7(3)
C(8)-C(9)-H(9)	120.9	O(8)-C(21)-C(15)	118.9(3)
C(9)-C(10)-C(11)	123.0(3)	O(15)-C(22)-C(23)	112.5(3)
C(9)-C(10)-N(2)	118.1(3)	O(15)-C(22)-H(22A)	109.1
C(11)-C(10)-N(2)	118.8(3)	C(23)-C(22)-H(22A)	109.1
C(12)-C(11)-C(10)	118.2(3)	O(15)-C(22)-H(22B)	109.1
C(12)-C(11)-H(11A)	120.9	C(23)-C(22)-H(22B)	109.1
C(10)-C(11)-H(11A)	120.9	H(22A)-C(22)-H(22B)	107.8
C(11)-C(12)-C(13)	120.2(3)	C(22)-C(23)-H(23A)	109.5
C(11)-C(12)-H(12)	119.9	C(22)-C(23)-H(23B)	109.5
C(13)-C(12)-H(12)	119.9	H(23A)-C(23)-H(23B)	109.5
C(12)-C(13)-C(8)	120.6(3)	C(22)-C(23)-H(23C)	109.5

H(23A)-C(23)-H(23C)	109.5	O(1)-Eu(1)-O(9)	77.46(8)
H(23B)-C(23)-H(23C)	109.5	O(14)-Eu(1)-O(9)	79.41(7)
O(13)-Eu(1)-O(1)	103.64(8)	O(4)-Eu(1)-O(9)	129.41(7)
O(13)-Eu(1)-O(14)	149.25(8)	O(12)-Eu(1)-O(9)	147.42(8)
O(1)-Eu(1)-O(14)	83.20(8)	O(8)-Eu(1)-O(9)	52.25(7)
O(13)-Eu(1)-O(4)	79.06(8)	O(15)-Eu(1)-O(9)	128.06(7)
O(1)-Eu(1)-O(4)	151.19(8)	O(3)-N(1)-O(2)	122.8(3)
O(14)-Eu(1)-O(4)	109.36(7)	O(3)-N(1)-C(3)	118.6(3)
O(13)-Eu(1)-O(12)	137.64(8)	O(2)-N(1)-C(3)	118.6(3)
O(1)-Eu(1)-O(12)	83.14(8)	O(6)-N(2)-O(7)	124.0(3)
O(14)-Eu(1)-O(12)	72.45(8)	O(6)-N(2)-C(10)	118.3(3)
O(4)-Eu(1)-O(12)	76.62(9)	O(7)-N(2)-C(10)	117.8(3)
O(13)-Eu(1)-O(8)	79.13(8)	O(10)-N(3)-O(11)	124.4(3)
O(1)-Eu(1)-O(8)	127.00(8)	O(10)-N(3)-C(19)	117.7(3)
O(14)-Eu(1)-O(8)	73.18(8)	O(11)-N(3)-C(19)	118.0(3)
O(4)-Eu(1)-O(8)	81.81(7)	C(7)-O(1)-Eu(1)	143.42(19)
O(12)-Eu(1)-O(8)	129.96(7)	C(14)-O(4)-Eu(1)	120.24(19)
O(13)-Eu(1)-O(15)	72.48(8)	C(21)-O(8)-Eu(1)	94.78(18)
O(1)-Eu(1)-O(15)	74.29(8)	C(21)-O(9)-Eu(1)	91.36(17)
O(14)-Eu(1)-O(15)	137.38(8)	C(7)#1-O(13)-Eu(1)	166.4(2)
O(4)-Eu(1)-O(15)	79.45(7)	C(14)#2-O(14)-Eu(1)	169.8(2)
O(12)-Eu(1)-O(15)	69.33(8)	C(22)-O(15)-Eu(1)	127.34(17)
O(8)-Eu(1)-O(15)	148.38(7)	C(26)-O(17)-O(17)#3	100.8(5)
O(13)-Eu(1)-O(9)	73.12(8)		

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Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z+1   #2 -x+1,-y+2,-z+1   #3 -x+1,-y+1,-z+1

Table 3. Bond lengths [Å] and angles [°] for **3**.

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C(1)-O(2)	1.250(5)	C(3)-H(3)	0.9500
C(1)-O(1)	1.255(5)	C(4)-C(5)	1.381(7)
C(1)-C(2)	1.501(6)	C(4)-H(4)	0.9500
C(2)-C(3)	1.385(6)	C(5)-C(6)	1.380(7)
C(2)-C(7)	1.406(6)	C(5)-N(1)	1.475(6)
C(3)-C(4)	1.395(6)	C(6)-C(7)	1.386(6)

C(6)-H(6)	0.9500	C(24)-H(24)	0.9500
C(7)-H(7)	0.9500	C(25)-C(26)	1.383(7)
C(8)-O(6)	1.257(5)	C(25)-H(25)	0.9500
C(8)-O(5)	1.261(5)	C(26)-C(27)	1.381(7)
C(8)-C(9)	1.506(6)	C(26)-N(4)	1.476(6)
C(9)-C(14)	1.386(6)	C(27)-C(28)	1.389(6)
C(9)-C(10)	1.387(6)	C(27)-H(27)	0.9500
C(10)-C(11)	1.385(7)	C(28)-H(28)	0.9500
C(10)-H(10)	0.9500	C(29)-O(17)	1.251(5)
C(11)-C(12)	1.377(7)	C(29)-O(18)	1.273(5)
C(11)-H(11)	0.9500	C(29)-C(30)	1.495(6)
C(12)-C(13)	1.380(6)	C(30)-C(35)	1.391(6)
C(12)-N(2)	1.484(6)	C(30)-C(31)	1.395(6)
C(13)-C(14)	1.381(6)	C(31)-C(32)	1.378(6)
C(13)-H(13)	0.9500	C(31)-H(31)	0.9500
C(14)-H(14)	0.9500	C(32)-C(33)	1.381(7)
C(15)-O(9)	1.262(5)	C(32)-H(32)	0.9500
C(15)-O(10)	1.266(5)	C(33)-C(34)	1.382(7)
C(15)-C(16)	1.495(6)	C(33)-N(5)	1.473(6)
C(16)-C(17)	1.397(6)	C(34)-C(35)	1.399(6)
C(16)-C(21)	1.399(6)	C(34)-H(34)	0.9500
C(17)-C(18)	1.383(6)	C(35)-H(35)	0.9500
C(17)-H(17)	0.9500	C(36)-O(21)	1.255(5)
C(18)-C(19)	1.384(6)	C(36)-O(22)	1.265(5)
C(18)-H(18)	0.9500	C(36)-C(37)	1.508(6)
C(19)-C(20)	1.381(7)	C(37)-C(42)	1.375(6)
C(19)-N(3)	1.477(6)	C(37)-C(38)	1.408(6)
C(20)-C(21)	1.386(6)	C(38)-C(39)	1.371(7)
C(20)-H(20)	0.9500	C(38)-H(38)	0.9500
C(21)-H(21)	0.9500	C(39)-C(40)	1.364(8)
C(22)-O(14)	1.253(5)	C(39)-H(39)	0.9500
C(22)-O(13)	1.260(5)	C(40)-C(41)	1.391(7)
C(22)-C(23)	1.503(6)	C(40)-N(6)	1.479(6)
C(23)-C(28)	1.392(6)	C(41)-C(42)	1.396(6)
C(23)-C(24)	1.397(6)	C(41)-H(41)	0.9500
C(24)-C(25)	1.390(7)	C(42)-H(42)	0.9500

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Eu(1)-O(14)#1	2.327(3)	C(3)-C(2)-C(1)	120.9(4)
Eu(1)-O(2)	2.353(3)	C(7)-C(2)-C(1)	119.3(4)
Eu(1)-O(5)	2.402(3)	C(2)-C(3)-C(4)	120.4(4)
Eu(1)-O(21)	2.428(3)	C(2)-C(3)-H(3)	119.8
Eu(1)-O(17)	2.452(3)	C(4)-C(3)-H(3)	119.8
Eu(1)-O(27)	2.465(3)	C(5)-C(4)-C(3)	118.1(4)
Eu(1)-O(26)	2.490(3)	C(5)-C(4)-H(4)	120.9
Eu(1)-O(25)	2.506(3)	C(3)-C(4)-H(4)	120.9
Eu(1)-O(18)	2.709(3)	C(6)-C(5)-C(4)	123.3(4)
Eu(2)-O(22)	2.317(3)	C(6)-C(5)-N(1)	117.9(5)
Eu(2)-O(13)	2.357(3)	C(4)-C(5)-N(1)	118.8(4)
Eu(2)-O(1)#2	2.362(3)	C(5)-C(6)-C(7)	117.9(4)
Eu(2)-O(18)	2.391(3)	C(5)-C(6)-H(6)	121.0
Eu(2)-O(6)	2.494(3)	C(7)-C(6)-H(6)	121.0
Eu(2)-O(28)	2.509(3)	C(6)-C(7)-C(2)	120.5(4)
Eu(2)-O(9)	2.535(3)	C(6)-C(7)-H(7)	119.7
Eu(2)-O(10)	2.548(3)	C(2)-C(7)-H(7)	119.7
Eu(2)-O(5)	2.719(3)	O(6)-C(8)-O(5)	121.4(4)
N(1)-O(3)	1.219(6)	O(6)-C(8)-C(9)	118.3(4)
N(1)-O(4)	1.220(6)	O(5)-C(8)-C(9)	120.0(4)
N(2)-O(8)	1.216(6)	C(14)-C(9)-C(10)	120.0(4)
N(2)-O(7)	1.218(5)	C(14)-C(9)-C(8)	121.2(4)
N(3)-O(11)	1.217(5)	C(10)-C(9)-C(8)	118.6(4)
N(3)-O(12)	1.233(5)	C(11)-C(10)-C(9)	120.0(4)
N(4)-O(15)	1.215(6)	C(11)-C(10)-H(10)	120.0
N(4)-O(16)	1.232(6)	C(9)-C(10)-H(10)	120.0
N(5)-O(20)	1.218(6)	C(12)-C(11)-C(10)	118.7(4)
N(5)-O(19)	1.235(6)	C(12)-C(11)-H(11)	120.6
N(6)-O(24)	1.231(7)	C(10)-C(11)-H(11)	120.6
N(6)-O(23)	1.232(7)	C(11)-C(12)-C(13)	122.4(4)
O(1)-Eu(2)#1	2.362(3)	C(11)-C(12)-N(2)	117.8(4)
O(14)-Eu(1)#2	2.327(3)	C(13)-C(12)-N(2)	119.8(4)
O(2)-C(1)-O(1)	124.7(4)	C(12)-C(13)-C(14)	118.3(4)
O(2)-C(1)-C(2)	117.7(4)	C(12)-C(13)-H(13)	120.9
O(1)-C(1)-C(2)	117.7(4)	C(14)-C(13)-H(13)	120.9
C(3)-C(2)-C(7)	119.7(4)	C(13)-C(14)-C(9)	120.6(4)

C(13)-C(14)-H(14)	119.7	C(27)-C(26)-N(4)	118.3(5)
C(9)-C(14)-H(14)	119.7	C(25)-C(26)-N(4)	118.2(4)
O(9)-C(15)-O(10)	120.8(4)	C(26)-C(27)-C(28)	117.5(4)
O(9)-C(15)-C(16)	119.1(4)	C(26)-C(27)-H(27)	121.2
O(10)-C(15)-C(16)	120.0(4)	C(28)-C(27)-H(27)	121.2
C(17)-C(16)-C(21)	120.0(4)	C(27)-C(28)-C(23)	120.8(4)
C(17)-C(16)-C(15)	119.7(4)	C(27)-C(28)-H(28)	119.6
C(21)-C(16)-C(15)	120.2(4)	C(23)-C(28)-H(28)	119.6
C(18)-C(17)-C(16)	120.4(4)	O(17)-C(29)-O(18)	121.8(4)
C(18)-C(17)-H(17)	119.8	O(17)-C(29)-C(30)	118.8(4)
C(16)-C(17)-H(17)	119.8	O(18)-C(29)-C(30)	119.4(3)
C(19)-C(18)-C(17)	117.7(4)	C(35)-C(30)-C(31)	120.3(4)
C(19)-C(18)-H(18)	121.2	C(35)-C(30)-C(29)	119.4(4)
C(17)-C(18)-H(18)	121.2	C(31)-C(30)-C(29)	120.2(4)
C(20)-C(19)-C(18)	123.8(4)	C(32)-C(31)-C(30)	120.5(4)
C(20)-C(19)-N(3)	118.3(4)	C(32)-C(31)-H(31)	119.7
C(18)-C(19)-N(3)	117.9(4)	C(30)-C(31)-H(31)	119.7
C(19)-C(20)-C(21)	117.8(4)	C(31)-C(32)-C(33)	117.8(4)
C(19)-C(20)-H(20)	121.1	C(31)-C(32)-H(32)	121.1
C(21)-C(20)-H(20)	121.1	C(33)-C(32)-H(32)	121.1
C(20)-C(21)-C(16)	120.2(4)	C(32)-C(33)-C(34)	123.7(4)
C(20)-C(21)-H(21)	119.9	C(32)-C(33)-N(5)	117.7(4)
C(16)-C(21)-H(21)	119.9	C(34)-C(33)-N(5)	118.5(4)
O(14)-C(22)-O(13)	124.2(4)	C(33)-C(34)-C(35)	117.5(4)
O(14)-C(22)-C(23)	118.7(4)	C(33)-C(34)-H(34)	121.2
O(13)-C(22)-C(23)	117.1(4)	C(35)-C(34)-H(34)	121.2
C(28)-C(23)-C(24)	120.0(4)	C(30)-C(35)-C(34)	119.9(4)
C(28)-C(23)-C(22)	120.6(4)	C(30)-C(35)-H(35)	120.1
C(24)-C(23)-C(22)	119.3(4)	C(34)-C(35)-H(35)	120.1
C(25)-C(24)-C(23)	120.0(4)	O(21)-C(36)-O(22)	125.6(4)
C(25)-C(24)-H(24)	120.0	O(21)-C(36)-C(37)	118.2(4)
C(23)-C(24)-H(24)	120.0	O(22)-C(36)-C(37)	116.2(4)
C(26)-C(25)-C(24)	118.1(4)	C(42)-C(37)-C(38)	119.9(4)
C(26)-C(25)-H(25)	120.9	C(42)-C(37)-C(36)	121.2(4)
C(24)-C(25)-H(25)	120.9	C(38)-C(37)-C(36)	118.9(4)
C(27)-C(26)-C(25)	123.5(4)	C(39)-C(38)-C(37)	119.7(5)

C(39)-C(38)-H(38)	120.1	O(2)-Eu(1)-O(25)	73.02(11)
C(37)-C(38)-H(38)	120.1	O(5)-Eu(1)-O(25)	76.56(10)
C(40)-C(39)-C(38)	119.2(5)	O(21)-Eu(1)-O(25)	71.15(10)
C(40)-C(39)-H(39)	120.4	O(17)-Eu(1)-O(25)	141.48(10)
C(38)-C(39)-H(39)	120.4	O(27)-Eu(1)-O(25)	134.40(10)
C(39)-C(40)-C(41)	123.1(5)	O(26)-Eu(1)-O(25)	127.44(10)
C(39)-C(40)-N(6)	119.5(5)	O(14)#1-Eu(1)-O(18)	130.05(10)
C(41)-C(40)-N(6)	117.3(5)	O(2)-Eu(1)-O(18)	135.58(10)
C(40)-C(41)-C(42)	117.1(5)	O(5)-Eu(1)-O(18)	68.41(10)
C(40)-C(41)-H(41)	121.4	O(21)-Eu(1)-O(18)	69.44(10)
C(42)-C(41)-H(41)	121.4	O(17)-Eu(1)-O(18)	50.30(9)
C(37)-C(42)-C(41)	120.8(4)	O(27)-Eu(1)-O(18)	66.44(10)
C(37)-C(42)-H(42)	119.6	O(26)-Eu(1)-O(18)	105.32(9)
C(41)-C(42)-H(42)	119.6	O(25)-Eu(1)-O(18)	127.09(10)
O(14)#1-Eu(1)-O(2)	92.45(11)	O(22)-Eu(2)-O(13)	80.47(11)
O(14)#1-Eu(1)-O(5)	147.29(11)	O(22)-Eu(2)-O(1)#2	135.00(11)
O(2)-Eu(1)-O(5)	82.16(11)	O(13)-Eu(2)-O(1)#2	104.49(11)
O(14)#1-Eu(1)-O(21)	77.38(10)	O(22)-Eu(2)-O(18)	75.80(11)
O(2)-Eu(1)-O(21)	144.15(10)	O(13)-Eu(2)-O(18)	79.52(10)
O(5)-Eu(1)-O(21)	88.23(10)	O(1)#2-Eu(2)-O(18)	149.13(11)
O(14)#1-Eu(1)-O(17)	85.70(11)	O(22)-Eu(2)-O(6)	87.11(11)
O(2)-Eu(1)-O(17)	140.11(11)	O(13)-Eu(2)-O(6)	155.42(10)
O(5)-Eu(1)-O(17)	118.67(10)	O(1)#2-Eu(2)-O(6)	70.00(11)
O(21)-Eu(1)-O(17)	74.11(11)	O(18)-Eu(2)-O(6)	117.96(10)
O(14)#1-Eu(1)-O(27)	139.06(11)	O(22)-Eu(2)-O(28)	71.47(10)
O(2)-Eu(1)-O(27)	72.63(10)	O(13)-Eu(2)-O(28)	76.38(11)
O(5)-Eu(1)-O(27)	69.86(10)	O(1)#2-Eu(2)-O(28)	66.69(11)
O(21)-Eu(1)-O(27)	135.37(10)	O(18)-Eu(2)-O(28)	141.91(10)
O(17)-Eu(1)-O(27)	82.94(10)	O(6)-Eu(2)-O(28)	79.59(10)
O(14)#1-Eu(1)-O(26)	72.49(11)	O(22)-Eu(2)-O(9)	136.23(10)
O(2)-Eu(1)-O(26)	72.12(11)	O(13)-Eu(2)-O(9)	122.81(10)
O(5)-Eu(1)-O(26)	134.27(10)	O(1)#2-Eu(2)-O(9)	78.97(10)
O(21)-Eu(1)-O(26)	133.67(11)	O(18)-Eu(2)-O(9)	73.59(10)
O(17)-Eu(1)-O(26)	69.36(10)	O(6)-Eu(2)-O(9)	80.50(10)
O(27)-Eu(1)-O(26)	66.68(10)	O(28)-Eu(2)-O(9)	144.50(10)
O(14)#1-Eu(1)-O(25)	71.03(11)	O(22)-Eu(2)-O(10)	148.69(10)

O(13)-Eu(2)-O(10)	75.35(10)	Eu(1)-O(5)-Eu(2)	109.08(11)
O(1)#2-Eu(2)-O(10)	71.35(11)	C(8)-O(6)-Eu(2)	95.5(3)
O(18)-Eu(2)-O(10)	80.44(10)	C(15)-O(9)-Eu(2)	94.1(2)
O(6)-Eu(2)-O(10)	122.38(10)	C(15)-O(10)-Eu(2)	93.4(3)
O(28)-Eu(2)-O(10)	120.39(9)	C(22)-O(13)-Eu(2)	133.0(3)
O(9)-Eu(2)-O(10)	51.24(9)	C(22)-O(14)-Eu(1)#2	154.3(3)
O(22)-Eu(2)-O(5)	74.55(10)	C(29)-O(17)-Eu(1)	100.3(3)
O(13)-Eu(2)-O(5)	143.09(10)	C(29)-O(18)-Eu(2)	157.7(3)
O(1)#2-Eu(2)-O(5)	112.40(10)	C(29)-O(18)-Eu(1)	87.6(2)
O(18)-Eu(2)-O(5)	68.38(10)	Eu(2)-O(18)-Eu(1)	109.77(11)
O(6)-Eu(2)-O(5)	49.58(9)	C(36)-O(21)-Eu(1)	132.6(3)
O(28)-Eu(2)-O(5)	119.14(10)	C(36)-O(22)-Eu(2)	137.4(3)
O(9)-Eu(2)-O(5)	65.47(9)		
O(10)-Eu(2)-O(5)	114.98(9)		
O(3)-N(1)-O(4)	124.8(4)		
O(3)-N(1)-C(5)	117.8(5)		
O(4)-N(1)-C(5)	117.4(4)		
O(8)-N(2)-O(7)	124.2(4)		
O(8)-N(2)-C(12)	117.8(4)		
O(7)-N(2)-C(12)	118.0(4)		
O(11)-N(3)-O(12)	123.5(4)		
O(11)-N(3)-C(19)	119.2(4)		
O(12)-N(3)-C(19)	117.3(4)		
O(15)-N(4)-O(16)	123.5(5)		
O(15)-N(4)-C(26)	118.7(5)		
O(16)-N(4)-C(26)	117.7(5)		
O(20)-N(5)-O(19)	123.6(4)		
O(20)-N(5)-C(33)	118.8(4)		
O(19)-N(5)-C(33)	117.5(4)		
O(24)-N(6)-O(23)	124.1(5)		
O(24)-N(6)-C(40)	117.5(5)		
O(23)-N(6)-C(40)	118.4(5)		
C(1)-O(1)-Eu(2)#1	142.0(3)		
C(1)-O(2)-Eu(1)	144.8(3)		
C(8)-O(5)-Eu(1)	165.7(3)		
C(8)-O(5)-Eu(2)	85.2(2)		

Table 4.   Bond lengths [Å] and angles [°] for **4**.

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C(1)-O(2)	1.264(4)	C(15)-C(16)	1.502(4)
C(1)-O(1)	1.264(4)	C(16)-C(21)	1.394(5)
C(1)-C(2)	1.501(5)	C(16)-C(17)	1.401(5)
C(2)-C(7)	1.390(5)	C(17)-C(18)	1.381(5)
C(2)-C(3)	1.394(5)	C(17)-H(17)	0.9500
C(3)-C(4)	1.387(5)	C(18)-C(19)	1.382(5)
C(3)-H(3)	0.9500	C(18)-H(18)	0.9500
C(4)-C(5)	1.388(5)	C(19)-C(20)	1.381(6)
C(4)-H(4)	0.9500	C(19)-N(3)	1.482(5)
C(5)-C(6)	1.380(5)	C(20)-C(21)	1.390(5)
C(5)-N(1)	1.470(4)	C(20)-H(20)	0.9500
C(6)-C(7)	1.386(5)	C(21)-H(21)	0.9500
C(6)-H(6)	0.9500	C(22)-O(14)	1.251(4)
C(7)-H(7)	0.9500	C(22)-O(13)	1.259(4)
C(8)-O(6)	1.256(4)	C(22)-C(23)	1.507(4)
C(8)-O(5)	1.257(4)	C(23)-C(24)	1.385(5)
C(8)-C(9)	1.505(4)	C(23)-C(28)	1.392(5)
C(9)-C(14)	1.380(5)	C(24)-C(25)	1.383(5)
C(9)-C(10)	1.385(5)	C(24)-H(24)	0.9500
C(10)-C(11)	1.389(5)	C(25)-C(26)	1.391(6)
C(10)-H(10)	0.9500	C(25)-H(25)	0.9500
C(11)-C(12)	1.381(6)	C(26)-C(27)	1.385(6)
C(11)-H(11)	0.9500	C(26)-N(4)	1.475(5)
C(12)-C(13)	1.365(6)	C(27)-C(28)	1.377(5)
C(12)-N(2)	1.479(4)	C(27)-H(27)	0.9500
C(13)-C(14)	1.391(5)	C(28)-H(28)	0.9500
C(13)-H(13)	0.9500	C(29)-O(18)	1.256(4)
C(14)-H(14)	0.9500	C(29)-O(17)	1.266(4)
C(15)-O(9)	1.251(4)	C(29)-C(30)	1.496(4)
C(15)-O(10)	1.254(4)	C(30)-C(31)	1.392(5)

C(30)-C(35)	1.395(5)	O(1)-Tb(1)	2.523(2)
C(31)-C(32)	1.390(5)	O(2)-Tb(1)	2.507(2)
C(31)-H(31)	0.9500	O(5)-Tb(1)	2.428(2)
C(32)-C(33)	1.386(6)	O(6)-Tb(2)	2.349(2)
C(32)-H(32)	0.9500	O(6)-Tb(1)	2.893(3)
C(33)-C(34)	1.381(6)	O(9)-Tb(2)	2.318(2)
C(33)-N(5)	1.471(5)	O(10)-Tb(1)#1	2.323(2)
C(34)-C(35)	1.383(5)	O(13)-Tb(1)	2.283(2)
C(34)-H(34)	0.9500	O(14)-Tb(2)	2.403(2)
C(35)-H(35)	0.9500	O(17)-Tb(1)	2.352(2)
C(36)-O(21)	1.256(4)	O(17)-Tb(2)	2.778(2)
C(36)-O(22)	1.263(4)	O(18)-Tb(2)	2.405(2)
C(36)-C(37)	1.506(4)	O(21)-Tb(2)#2	2.299(2)
C(37)-C(38)	1.389(5)	O(22)-Tb(1)	2.319(2)
C(37)-C(42)	1.390(5)	O(25)-Tb(1)	2.464(2)
C(38)-C(39)	1.381(5)	O(26)-Tb(2)	2.432(2)
C(38)-H(38)	0.9500	O(27)-Tb(2)	2.482(2)
C(39)-C(40)	1.387(5)	O(28)-Tb(2)	2.472(2)
C(39)-H(39)	0.9500	Tb(1)-O(10)#2	2.323(2)
C(40)-C(41)	1.382(6)	Tb(2)-O(21)#1	2.299(2)
C(40)-N(6)	1.477(5)	O(2)-C(1)-O(1)	121.2(3)
C(41)-C(42)	1.388(5)	O(2)-C(1)-C(2)	119.4(3)
C(41)-H(41)	0.9500	O(1)-C(1)-C(2)	119.4(3)
C(42)-H(42)	0.9500	C(7)-C(2)-C(3)	120.0(3)
N(1)-O(4)	1.226(4)	C(7)-C(2)-C(1)	119.9(3)
N(1)-O(3)	1.231(4)	C(3)-C(2)-C(1)	120.0(3)
N(2)-O(7)	1.210(5)	C(4)-C(3)-C(2)	120.4(3)
N(2)-O(8)	1.229(5)	C(4)-C(3)-H(3)	119.8
N(3)-O(11)	1.215(5)	C(2)-C(3)-H(3)	119.8
N(3)-O(12)	1.217(5)	C(3)-C(4)-C(5)	117.7(3)
N(4)-O(16)	1.224(5)	C(3)-C(4)-H(4)	121.2
N(4)-O(15)	1.234(6)	C(5)-C(4)-H(4)	121.2
N(5)-O(19)	1.224(5)	C(6)-C(5)-C(4)	123.4(3)
N(5)-O(20)	1.229(5)	C(6)-C(5)-N(1)	118.6(3)
N(6)-O(24)	1.214(5)	C(4)-C(5)-N(1)	118.0(3)
N(6)-O(23)	1.232(5)	C(5)-C(6)-C(7)	117.8(3)

C(5)-C(6)-H(6)	121.1	C(17)-C(18)-H(18)	121.1
C(7)-C(6)-H(6)	121.1	C(19)-C(18)-H(18)	121.1
C(6)-C(7)-C(2)	120.7(3)	C(20)-C(19)-C(18)	123.5(3)
C(6)-C(7)-H(7)	119.7	C(20)-C(19)-N(3)	119.0(4)
C(2)-C(7)-H(7)	119.7	C(18)-C(19)-N(3)	117.5(4)
O(6)-C(8)-O(5)	121.6(3)	C(19)-C(20)-C(21)	118.2(3)
O(6)-C(8)-C(9)	119.9(3)	C(19)-C(20)-H(20)	120.9
O(5)-C(8)-C(9)	118.2(3)	C(21)-C(20)-H(20)	120.9
C(14)-C(9)-C(10)	120.2(3)	C(20)-C(21)-C(16)	119.8(3)
C(14)-C(9)-C(8)	118.5(3)	C(20)-C(21)-H(21)	120.1
C(10)-C(9)-C(8)	121.1(3)	C(16)-C(21)-H(21)	120.1
C(9)-C(10)-C(11)	120.3(3)	O(14)-C(22)-O(13)	125.5(3)
C(9)-C(10)-H(10)	119.9	O(14)-C(22)-C(23)	118.6(3)
C(11)-C(10)-H(10)	119.9	O(13)-C(22)-C(23)	115.8(3)
C(12)-C(11)-C(10)	118.2(3)	C(24)-C(23)-C(28)	120.1(3)
C(12)-C(11)-H(11)	120.9	C(24)-C(23)-C(22)	120.9(3)
C(10)-C(11)-H(11)	120.9	C(28)-C(23)-C(22)	119.0(3)
C(13)-C(12)-C(11)	122.5(3)	C(25)-C(24)-C(23)	120.3(4)
C(13)-C(12)-N(2)	118.6(3)	C(25)-C(24)-H(24)	119.8
C(11)-C(12)-N(2)	118.9(3)	C(23)-C(24)-H(24)	119.8
C(12)-C(13)-C(14)	118.8(4)	C(24)-C(25)-C(26)	118.0(4)
C(12)-C(13)-H(13)	120.6	C(24)-C(25)-H(25)	121.0
C(14)-C(13)-H(13)	120.6	C(26)-C(25)-H(25)	121.0
C(9)-C(14)-C(13)	120.0(4)	C(27)-C(26)-C(25)	122.9(3)
C(9)-C(14)-H(14)	120.0	C(27)-C(26)-N(4)	118.6(4)
C(13)-C(14)-H(14)	120.0	C(25)-C(26)-N(4)	118.5(4)
O(9)-C(15)-O(10)	124.8(3)	C(28)-C(27)-C(26)	117.8(4)
O(9)-C(15)-C(16)	116.9(3)	C(28)-C(27)-H(27)	121.1
O(10)-C(15)-C(16)	118.3(3)	C(26)-C(27)-H(27)	121.1
C(21)-C(16)-C(17)	120.2(3)	C(27)-C(28)-C(23)	120.8(4)
C(21)-C(16)-C(15)	120.2(3)	C(27)-C(28)-H(28)	119.6
C(17)-C(16)-C(15)	119.5(3)	C(23)-C(28)-H(28)	119.6
C(18)-C(17)-C(16)	120.5(3)	O(18)-C(29)-O(17)	121.5(3)
C(18)-C(17)-H(17)	119.8	O(18)-C(29)-C(30)	118.9(3)
C(16)-C(17)-H(17)	119.8	O(17)-C(29)-C(30)	119.5(3)
C(17)-C(18)-C(19)	117.8(3)	C(31)-C(30)-C(35)	120.7(3)

C(31)-C(30)-C(29)	119.6(3)	C(41)-C(42)-H(42)	119.9
C(35)-C(30)-C(29)	119.7(3)	C(37)-C(42)-H(42)	119.9
C(32)-C(31)-C(30)	120.0(3)	O(4)-N(1)-O(3)	123.4(3)
C(32)-C(31)-H(31)	120.0	O(4)-N(1)-C(5)	118.7(3)
C(30)-C(31)-H(31)	120.0	O(3)-N(1)-C(5)	117.9(3)
C(33)-C(32)-C(31)	118.0(3)	O(7)-N(2)-O(8)	124.1(3)
C(33)-C(32)-H(32)	121.0	O(7)-N(2)-C(12)	119.0(3)
C(31)-C(32)-H(32)	121.0	O(8)-N(2)-C(12)	116.9(3)
C(34)-C(33)-C(32)	123.0(3)	O(11)-N(3)-O(12)	124.8(4)
C(34)-C(33)-N(5)	117.8(4)	O(11)-N(3)-C(19)	117.7(4)
C(32)-C(33)-N(5)	119.2(4)	O(12)-N(3)-C(19)	117.5(4)
C(33)-C(34)-C(35)	118.6(4)	O(16)-N(4)-O(15)	124.4(4)
C(33)-C(34)-H(34)	120.7	O(16)-N(4)-C(26)	117.6(4)
C(35)-C(34)-H(34)	120.7	O(15)-N(4)-C(26)	118.0(4)
C(34)-C(35)-C(30)	119.7(3)	O(19)-N(5)-O(20)	124.3(4)
C(34)-C(35)-H(35)	120.2	O(19)-N(5)-C(33)	118.9(4)
C(30)-C(35)-H(35)	120.2	O(20)-N(5)-C(33)	116.8(4)
O(21)-C(36)-O(22)	123.9(3)	O(24)-N(6)-O(23)	123.8(4)
O(21)-C(36)-C(37)	118.3(3)	O(24)-N(6)-C(40)	118.8(4)
O(22)-C(36)-C(37)	117.8(3)	O(23)-N(6)-C(40)	117.4(4)
C(38)-C(37)-C(42)	120.5(3)	C(1)-O(1)-Tb(1)	92.74(19)
C(38)-C(37)-C(36)	120.1(3)	C(1)-O(2)-Tb(1)	93.51(19)
C(42)-C(37)-C(36)	119.4(3)	C(8)-O(5)-Tb(1)	101.5(2)
C(39)-C(38)-C(37)	120.3(3)	C(8)-O(6)-Tb(2)	172.4(2)
C(39)-C(38)-H(38)	119.9	C(8)-O(6)-Tb(1)	80.07(18)
C(37)-C(38)-H(38)	119.9	Tb(2)-O(6)-Tb(1)	107.29(9)
C(38)-C(39)-C(40)	117.9(3)	C(15)-O(9)-Tb(2)	144.6(2)
C(38)-C(39)-H(39)	121.1	C(15)-O(10)-Tb(1)#1	144.4(2)
C(40)-C(39)-H(39)	121.1	C(22)-O(13)-Tb(1)	139.7(2)
C(41)-C(40)-C(39)	123.4(3)	C(22)-O(14)-Tb(2)	134.5(2)
C(41)-C(40)-N(6)	118.3(4)	C(29)-O(17)-Tb(1)	157.8(2)
C(39)-C(40)-N(6)	118.3(4)	C(29)-O(17)-Tb(2)	85.45(18)
C(40)-C(41)-C(42)	117.7(3)	Tb(1)-O(17)-Tb(2)	110.96(9)
C(40)-C(41)-H(41)	121.2	C(29)-O(18)-Tb(2)	103.4(2)
C(42)-C(41)-H(41)	121.2	C(36)-O(21)-Tb(2)#2	155.9(2)
C(41)-C(42)-C(37)	120.2(3)	C(36)-O(22)-Tb(1)	135.7(2)

O(13)-Tb(1)-O(22)	81.05(9)	O(21)#1-Tb(2)-O(9)	94.11(8)
O(13)-Tb(1)-O(10)#2	136.13(9)	O(21)#1-Tb(2)-O(6)	146.83(9)
O(22)-Tb(1)-O(10)#2	103.78(9)	O(9)-Tb(2)-O(6)	80.89(9)
O(13)-Tb(1)-O(17)	75.07(8)	O(21)#1-Tb(2)-O(14)	77.95(8)
O(22)-Tb(1)-O(17)	81.49(8)	O(9)-Tb(2)-O(14)	144.44(8)
O(10)#2-Tb(1)-O(17)	148.61(8)	O(6)-Tb(2)-O(14)	87.22(8)
O(13)-Tb(1)-O(5)	86.56(8)	O(21)#1-Tb(2)-O(18)	84.84(8)
O(22)-Tb(1)-O(5)	155.53(8)	O(9)-Tb(2)-O(18)	140.18(9)
O(10)#2-Tb(1)-O(5)	71.28(9)	O(6)-Tb(2)-O(18)	119.65(8)
O(17)-Tb(1)-O(5)	115.62(8)	O(14)-Tb(2)-O(18)	74.28(9)
O(13)-Tb(1)-O(25)	71.91(8)	O(21)#1-Tb(2)-O(26)	139.70(9)
O(22)-Tb(1)-O(25)	77.77(9)	O(9)-Tb(2)-O(26)	72.85(8)
O(10)#2-Tb(1)-O(25)	66.88(8)	O(6)-Tb(2)-O(26)	70.19(8)
O(17)-Tb(1)-O(25)	143.18(8)	O(14)-Tb(2)-O(26)	133.57(8)
O(5)-Tb(1)-O(25)	78.35(8)	O(18)-Tb(2)-O(26)	82.45(8)
O(13)-Tb(1)-O(2)	134.96(8)	O(21)#1-Tb(2)-O(28)	72.85(9)
O(22)-Tb(1)-O(2)	124.28(8)	O(9)-Tb(2)-O(28)	71.44(9)
O(10)#2-Tb(1)-O(2)	78.40(8)	O(6)-Tb(2)-O(28)	133.93(8)
O(17)-Tb(1)-O(2)	73.45(8)	O(14)-Tb(2)-O(28)	135.43(8)
O(5)-Tb(1)-O(2)	79.02(8)	O(18)-Tb(2)-O(28)	70.28(8)
O(25)-Tb(1)-O(2)	143.09(8)	O(26)-Tb(2)-O(28)	66.85(8)
O(13)-Tb(1)-O(1)	147.76(8)	O(21)#1-Tb(2)-O(27)	70.50(9)
O(22)-Tb(1)-O(1)	75.41(8)	O(9)-Tb(2)-O(27)	73.02(9)
O(10)#2-Tb(1)-O(1)	71.88(9)	O(6)-Tb(2)-O(27)	76.72(9)
O(17)-Tb(1)-O(1)	79.88(8)	O(14)-Tb(2)-O(27)	71.65(8)
O(5)-Tb(1)-O(1)	122.96(8)	O(18)-Tb(2)-O(27)	141.22(8)
O(25)-Tb(1)-O(1)	122.73(8)	O(26)-Tb(2)-O(27)	135.34(8)
O(2)-Tb(1)-O(1)	51.93(8)	O(28)-Tb(2)-O(27)	125.91(8)
O(13)-Tb(1)-O(6)	72.79(8)	O(21)#1-Tb(2)-O(17)	128.61(8)
O(22)-Tb(1)-O(6)	143.71(7)	O(9)-Tb(2)-O(17)	135.17(8)
O(10)#2-Tb(1)-O(6)	112.51(8)	O(6)-Tb(2)-O(17)	70.06(8)
O(17)-Tb(1)-O(6)	67.91(7)	O(14)-Tb(2)-O(17)	68.69(8)
O(5)-Tb(1)-O(6)	47.73(7)	O(18)-Tb(2)-O(17)	49.62(7)
O(25)-Tb(1)-O(6)	115.80(8)	O(26)-Tb(2)-O(17)	65.61(8)
O(2)-Tb(1)-O(6)	65.94(7)	O(28)-Tb(2)-O(17)	105.32(7)
O(1)-Tb(1)-O(6)	115.78(8)	O(27)-Tb(2)-O(17)	128.59(8)

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Symmetry transformations used to generate equivalent atoms:

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

Table 5. NMR titration data (chemical shifts in ppm) for 2-nitrobenzoic acid and Eu(III) in 90% methanol/10%water (v/v). Initial concentrations were [L]=0.1266 M, [Eu(III)]=0.0127 M at I=0.1 M (KCl).

Spectrum	A	B	C	D	E	F	G	H	I	J
H1	5.332	5.335	5.337	5.359	5.384	5.404	5.432	5.458	5.496	5.5317
H2	6.731	6.732	6.736	6.742	6.75	6.757	6.765	6.773	6.785	6.798
H3	6.793	6.795	6.799	6.807	6.816	6.826	6.836	6.847	6.862	6.879
H4	6.992	6.99	6.991	6.995	6.999	7.004	7.009	7.013	7.02	7.027

Table 6. NMR titration data (chemical shifts in ppm) for 3-nitrobenzoic acid and Eu(III) in 90% methanol/10%water (v/v). Initial concentrations were [L]=0.1008 M, [Eu(III)]=0.0424 M at I=0.1 M (KCl).

Spectrum	A	B	C	D	F	G	H	I	J	K
H1	5.2117	5.2427	5.2551	5.2577	5.2644	5.2697	5.2762	5.2873	5.3039	5.3331
H2	5.548	5.5703	5.5828	5.5838	5.5809	5.5801	5.5782	5.585	5.5937	5.6145
H3	6.4084	5.4182	6.4217	6.404	6.4026	6.3995	6.3966	6.3946	6.3937	6.3948
H4	7.4034	7.4091	7.4099	7.405	7.4018	7.3968	7.3919	7.3869	7.3817	7.3794

Table 7. NMR titration data (chemical shifts in ppm) for 2-nitrobenzoic acid and Eu(III) in methanol. Initial concentrations were [L]=0.1696 M, [Eu(III)]=0.030 M at I=0.1 M (Et$_4$NCl).

Spectrum	A	B	C	D	F	G	H	I
H1	6.5301	6.5258	6.5109	6.5113	6.4876	6.4786	6.4621	6.455
H2	6.8991	6.8881	6.8655	6.858	6.8327	6.8103	6.7888	6.7679

Table 8. NMR titration data (chemical shifts in ppm) for 3-nitrobenzoic acid and Eu(III) in methanol. Initial concentrations were [L]=0.1654 M, [Eu(III)]=0.030 M at I=0.1 M (Et$_4$NCl).

Spectrum	A	B	C	D	E	F	G
H1	6.0564	6.0633	6.084	6.0962	6.1122	6.124	6.1316
H2	7.1683	7.1797	7.2013	7.2215	7.2454	7.2681	7.2811

Table 9. NMR titration data (chemical shifts in ppm) for 4-nitrobenzoic acid and Eu(III) in methanol. Initial concentrations were [L]=0.2331 M, [Eu(III)]=0.030 M at I=0.1 M (Et$_4$NCl).

Spectrum	A	B	C	D	E	F	G	H	I	J
H1	6.4616	6.4588	6.4487	6.4538	6.4389	6.4358	6.4294	6.4019	6.3938	6.3821