

Structural and near-infrared photophysical studies on ternary lanthanide complexes containing poly(pyrazolyl)borate and 1,3-diketonate ligands

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Electronic Supporting Information: Tables S1 – S8 and figure S1.

Table S1: Coordination-sphere bond lengths and angles for $[\text{Nd}(\text{L}^2)_2(\text{dbm})_2]$

Nd(1)-O(115)	2.354(3)	Nd(2)-O(241)	2.377(3)
Nd(1)-O(141)	2.372(4)	Nd(2)-O(215)	2.380(3)
Nd(1)-O(111)	2.400(3)	Nd(2)-O(245)	2.383(3)
Nd(1)-O(145)	2.422(4)	Nd(2)-O(211)	2.390(3)
Nd(1)-N(162)	2.573(4)	Nd(2)-N(262)	2.557(4)
Nd(1)-N(171)	2.607(4)	Nd(2)-N(282)	2.584(4)
Nd(1)-N(182)	2.607(4)	Nd(2)-N(291)	2.603(5)
Nd(1)-N(191)	2.644(4)	Nd(2)-N(271)	2.636(5)

O(115)-Nd(1)-O(141)	149.66(12)	O(241)-Nd(2)-O(215)	142.26(11)
O(115)-Nd(1)-O(111)	69.23(12)	O(241)-Nd(2)-O(245)	69.22(11)
O(141)-Nd(1)-O(111)	140.63(12)	O(215)-Nd(2)-O(245)	148.42(11)
O(115)-Nd(1)-O(145)	133.54(12)	O(241)-Nd(2)-O(211)	72.75(11)
O(141)-Nd(1)-O(145)	69.72(12)	O(215)-Nd(2)-O(211)	69.67(11)
O(111)-Nd(1)-O(145)	73.50(12)	O(245)-Nd(2)-O(211)	141.91(11)
O(115)-Nd(1)-N(162)	90.36(13)	O(241)-Nd(2)-N(262)	122.68(13)
O(141)-Nd(1)-N(162)	75.27(13)	O(215)-Nd(2)-N(262)	82.32(13)
O(111)-Nd(1)-N(162)	125.41(13)	O(245)-Nd(2)-N(262)	73.11(13)
O(145)-Nd(1)-N(162)	134.55(12)	O(211)-Nd(2)-N(262)	132.67(13)
O(115)-Nd(1)-N(171)	111.01(13)	O(241)-Nd(2)-N(282)	126.25(13)
O(141)-Nd(1)-N(171)	86.71(13)	O(215)-Nd(2)-N(282)	84.15(12)
O(111)-Nd(1)-N(171)	77.06(13)	O(245)-Nd(2)-N(282)	71.26(12)
O(145)-Nd(1)-N(171)	85.92(13)	O(211)-Nd(2)-N(282)	134.07(13)
N(162)-Nd(1)-N(171)	63.70(13)	N(262)-Nd(2)-N(282)	76.61(14)
O(115)-Nd(1)-N(182)	74.15(12)	O(241)-Nd(2)-N(291)	79.02(13)
O(141)-Nd(1)-N(182)	76.20(12)	O(215)-Nd(2)-N(291)	101.00(13)
O(111)-Nd(1)-N(182)	137.89(12)	O(245)-Nd(2)-N(291)	85.41(13)
O(145)-Nd(1)-N(182)	122.47(13)	O(211)-Nd(2)-N(291)	85.33(13)
N(162)-Nd(1)-N(182)	73.85(14)	N(262)-Nd(2)-N(291)	138.49(13)
N(171)-Nd(1)-N(182)	137.05(13)	N(282)-Nd(2)-N(291)	62.82(13)
O(115)-Nd(1)-N(191)	80.85(13)	O(241)-Nd(2)-N(271)	74.64(12)
O(141)-Nd(1)-N(191)	91.22(13)	O(215)-Nd(2)-N(271)	97.27(13)
O(111)-Nd(1)-N(191)	91.23(13)	O(245)-Nd(2)-N(271)	89.13(13)
O(145)-Nd(1)-N(191)	73.14(12)	O(211)-Nd(2)-N(271)	82.98(13)
N(162)-Nd(1)-N(191)	136.35(13)	N(262)-Nd(2)-N(271)	63.10(13)
N(171)-Nd(1)-N(191)	158.30(13)	N(282)-Nd(2)-N(271)	138.97(13)
N(182)-Nd(1)-N(191)	62.59(13)	N(291)-Nd(2)-N(271)	153.33(13)

Table S2: Coordination-sphere bond lengths and angles for $[\text{Er}(\text{L}^2)_2(\text{dbm})_2]$

Er(1)-O(145)	2.264(6)	Er(2)-O(245)	2.263(6)
Er(1)-O(111)	2.278(6)	Er(2)-O(212)	2.264(6)
Er(1)-O(115)	2.286(6)	Er(2)-O(241)	2.311(6)
Er(1)-O(141)	2.301(6)	Er(2)-O(215)	2.316(6)
Er(1)-N(182)	2.462(7)	Er(2)-N(262)	2.473(7)
Er(1)-N(162)	2.469(7)	Er(2)-N(282)	2.480(8)
Er(1)-N(171)	2.508(8)	Er(2)-N(271)	2.486(8)
Er(1)-N(191)	2.525(8)	Er(2)-N(291)	2.513(8)

O(145)-Er(1)-O(111)	143.8(2)	O(245)-Er(2)-O(212)	146.5(2)
O(145)-Er(1)-O(115)	144.4(2)	O(245)-Er(2)-O(241)	72.1(2)
O(111)-Er(1)-O(115)	71.7(2)	O(212)-Er(2)-O(241)	141.2(2)
O(145)-Er(1)-O(141)	72.5(2)	O(245)-Er(2)-O(215)	137.7(2)
O(111)-Er(1)-O(141)	143.7(2)	O(212)-Er(2)-O(215)	71.5(2)
O(115)-Er(1)-O(141)	72.0(2)	O(241)-Er(2)-O(215)	71.1(2)
O(145)-Er(1)-N(182)	78.9(2)	O(245)-Er(2)-N(262)	86.6(2)
O(111)-Er(1)-N(182)	73.4(2)	O(212)-Er(2)-N(262)	74.3(2)
O(115)-Er(1)-N(182)	125.4(2)	O(241)-Er(2)-N(262)	127.4(2)
O(141)-Er(1)-N(182)	131.1(2)	O(215)-Er(2)-N(262)	132.8(2)
O(145)-Er(1)-N(162)	80.4(2)	O(245)-Er(2)-N(282)	73.4(2)
O(111)-Er(1)-N(162)	71.2(2)	O(212)-Er(2)-N(282)	75.2(2)
O(115)-Er(1)-N(162)	126.8(2)	O(241)-Er(2)-N(282)	136.6(2)
O(141)-Er(1)-N(162)	133.4(2)	O(215)-Er(2)-N(282)	124.3(2)
N(182)-Er(1)-N(162)	77.0(3)	N(262)-Er(2)-N(282)	75.1(3)
O(145)-Er(1)-N(171)	99.9(3)	O(245)-Er(2)-N(271)	109.8(2)
O(111)-Er(1)-N(171)	88.3(2)	O(212)-Er(2)-N(271)	87.6(2)
O(115)-Er(1)-N(171)	77.0(2)	O(241)-Er(2)-N(271)	76.8(2)
O(141)-Er(1)-N(171)	82.8(2)	O(215)-Er(2)-N(271)	80.9(2)
N(182)-Er(1)-N(171)	141.6(3)	N(262)-Er(2)-N(271)	66.1(3)
N(162)-Er(1)-N(171)	65.1(3)	N(282)-Er(2)-N(271)	140.6(3)
O(145)-Er(1)-N(191)	98.7(2)	O(245)-Er(2)-N(291)	83.2(2)
O(111)-Er(1)-N(191)	90.7(3)	O(212)-Er(2)-N(291)	93.9(2)
O(115)-Er(1)-N(191)	73.9(2)	O(241)-Er(2)-N(291)	85.5(2)
O(141)-Er(1)-N(191)	80.1(2)	O(215)-Er(2)-N(291)	74.0(2)
N(182)-Er(1)-N(191)	65.9(3)	N(262)-Er(2)-N(291)	140.1(3)
N(162)-Er(1)-N(191)	142.2(3)	N(282)-Er(2)-N(291)	65.1(3)
N(171)-Er(1)-N(191)	149.6(3)	N(271)-Er(2)-N(291)	152.9(3)

Table S3: Coordination-sphere bond lengths and angles for $[\text{Pr}(\text{L}^2)_2(\text{dbm})_2]$

Pr(1)-O(145)	2.390(2)	Pr(2)-O(211)	2.357(2)
Pr(1)-O(111)	2.391(2)	Pr(2)-O(245)	2.380(2)
Pr(1)-O(115)	2.397(2)	Pr(2)-O(215)	2.423(2)
Pr(1)-O(141)	2.403(2)	Pr(2)-O(241)	2.436(2)
Pr(1)-N(182)	2.589(3)	Pr(2)-N(282)	2.592(3)
Pr(1)-N(162)	2.603(3)	Pr(2)-N(262)	2.624(3)
Pr(1)-N(171)	2.627(3)	Pr(2)-N(291)	2.633(3)
Pr(1)-N(191)	2.656(3)	Pr(2)-N(271)	2.659(2)

O(145)-Pr(1)-O(111)	149.00(7)	O(211)-Pr(2)-O(245)	149.77(8)
O(145)-Pr(1)-O(115)	142.20(7)	O(211)-Pr(2)-O(215)	68.91(7)
O(111)-Pr(1)-O(115)	68.72(7)	O(245)-Pr(2)-O(215)	140.74(7)
O(145)-Pr(1)-O(141)	69.32(7)	O(211)-Pr(2)-O(241)	133.61(7)
O(111)-Pr(1)-O(141)	141.68(7)	O(245)-Pr(2)-O(241)	69.08(7)
O(115)-Pr(1)-O(141)	73.05(7)	O(215)-Pr(2)-O(241)	74.21(7)
O(145)-Pr(1)-N(182)	82.20(8)	O(211)-Pr(2)-N(282)	90.56(8)
O(111)-Pr(1)-N(182)	73.78(8)	O(245)-Pr(2)-N(282)	75.72(8)
O(115)-Pr(1)-N(182)	122.80(8)	O(215)-Pr(2)-N(282)	124.98(8)
O(141)-Pr(1)-N(182)	132.46(8)	O(241)-Pr(2)-N(282)	134.38(8)
O(145)-Pr(1)-N(162)	84.20(7)	O(211)-Pr(2)-N(262)	74.28(8)
O(111)-Pr(1)-N(162)	71.45(8)	O(245)-Pr(2)-N(262)	76.02(8)
O(115)-Pr(1)-N(162)	126.36(7)	O(215)-Pr(2)-N(262)	138.08(8)
O(141)-Pr(1)-N(162)	134.03(8)	O(241)-Pr(2)-N(262)	122.30(8)
N(182)-Pr(1)-N(162)	76.39(8)	N(282)-Pr(2)-N(262)	73.63(8)
O(145)-Pr(1)-N(171)	101.19(8)	O(211)-Pr(2)-N(291)	110.58(8)
O(111)-Pr(1)-N(171)	84.57(8)	O(245)-Pr(2)-N(291)	87.38(8)
O(115)-Pr(1)-N(171)	79.35(8)	O(215)-Pr(2)-N(291)	76.97(8)
O(141)-Pr(1)-N(171)	86.08(8)	O(241)-Pr(2)-N(291)	86.73(8)
N(182)-Pr(1)-N(171)	137.80(8)	N(282)-Pr(2)-N(291)	63.16(8)
N(162)-Pr(1)-N(171)	62.36(8)	N(262)-Pr(2)-N(291)	136.35(8)
O(145)-Pr(1)-N(191)	96.88(8)	O(211)-Pr(2)-N(271)	80.92(8)
O(111)-Pr(1)-N(191)	89.32(8)	O(245)-Pr(2)-N(271)	90.25(8)
O(115)-Pr(1)-N(191)	75.17(8)	O(215)-Pr(2)-N(271)	92.25(8)
O(141)-Pr(1)-N(191)	83.34(8)	O(241)-Pr(2)-N(271)	73.30(8)
N(182)-Pr(1)-N(191)	62.64(8)	N(282)-Pr(2)-N(271)	135.75(8)
N(162)-Pr(1)-N(191)	138.33(8)	N(262)-Pr(2)-N(271)	62.23(8)
N(171)-Pr(1)-N(191)	154.29(8)	N(291)-Pr(2)-N(271)	159.36(8)

Table S4: Coordination-sphere bond lengths and angles for [Eu(L²)₂(dbm)₂]

Eu(1)-O(115)	2.3102(15)	Eu(2)-O(215)	2.3336(15)
Eu(1)-O(145)	2.3222(15)	Eu(2)-O(245)	2.3357(15)
Eu(1)-O(111)	2.3685(14)	Eu(2)-O(241)	2.3430(15)
Eu(1)-O(141)	2.3788(14)	Eu(2)-O(211)	2.3585(15)
Eu(1)-N(172)	2.5259(19)	Eu(2)-N(272)	2.5256(18)
Eu(1)-N(182)	2.5506(19)	Eu(2)-N(282)	2.5412(18)
Eu(1)-N(161)	2.562(2)	Eu(2)-N(291)	2.5651(18)
Eu(1)-N(191)	2.584(2)	Eu(2)-N(261)	2.5912(18)

O(115)-Eu(1)-O(145)	148.28(5)	O(215)-Eu(2)-O(245)	146.61(5)
O(115)-Eu(1)-O(111)	70.46(5)	O(215)-Eu(2)-O(241)	143.02(5)
O(145)-Eu(1)-O(111)	140.88(5)	O(245)-Eu(2)-O(241)	70.31(5)
O(115)-Eu(1)-O(141)	135.79(5)	O(215)-Eu(2)-O(211)	70.85(5)
O(145)-Eu(1)-O(141)	70.29(5)	O(245)-Eu(2)-O(211)	142.54(5)
O(111)-Eu(1)-O(141)	72.49(5)	O(241)-Eu(2)-O(211)	72.27(5)
O(115)-Eu(1)-N(172)	88.68(6)	O(215)-Eu(2)-N(272)	81.08(6)
O(145)-Eu(1)-N(172)	74.90(6)	O(245)-Eu(2)-N(272)	72.98(6)
O(111)-Eu(1)-N(172)	126.32(6)	O(241)-Eu(2)-N(272)	123.79(5)
O(141)-Eu(1)-N(172)	133.42(6)	O(211)-Eu(2)-N(272)	132.39(6)
O(115)-Eu(1)-N(182)	73.40(5)	O(215)-Eu(2)-N(282)	82.60(6)
O(145)-Eu(1)-N(182)	76.11(6)	O(245)-Eu(2)-N(282)	71.41(6)
O(111)-Eu(1)-N(182)	136.92(6)	O(241)-Eu(2)-N(282)	126.54(6)
O(141)-Eu(1)-N(182)	123.63(5)	O(211)-Eu(2)-N(282)	133.57(6)
N(172)-Eu(1)-N(182)	74.58(6)	N(272)-Eu(2)-N(282)	76.76(6)
O(115)-Eu(1)-N(161)	110.46(6)	O(215)-Eu(2)-N(291)	100.52(6)
O(145)-Eu(1)-N(161)	87.06(6)	O(245)-Eu(2)-N(291)	86.73(6)
O(111)-Eu(1)-N(161)	77.12(6)	O(241)-Eu(2)-N(291)	78.07(6)
O(141)-Eu(1)-N(161)	83.42(6)	O(211)-Eu(2)-N(291)	83.99(6)
N(172)-Eu(1)-N(161)	64.60(6)	N(272)-Eu(2)-N(291)	139.81(6)
N(182)-Eu(1)-N(161)	138.68(6)	N(282)-Eu(2)-N(291)	63.83(6)
O(115)-Eu(1)-N(191)	81.92(6)	O(215)-Eu(2)-N(261)	97.39(6)
O(145)-Eu(1)-N(191)	92.23(6)	O(245)-Eu(2)-N(261)	89.96(6)
O(111)-Eu(1)-N(191)	88.78(6)	O(241)-Eu(2)-N(261)	74.77(6)
O(141)-Eu(1)-N(191)	73.97(6)	O(211)-Eu(2)-N(261)	81.93(6)
N(172)-Eu(1)-N(191)	137.93(6)	N(272)-Eu(2)-N(261)	64.10(6)
N(182)-Eu(1)-N(191)	63.42(6)	N(282)-Eu(2)-N(261)	140.24(6)
N(161)-Eu(1)-N(191)	156.17(6)	N(291)-Eu(2)-N(261)	152.13(6)

Table S5: Coordination-sphere bond lengths and angles for $[\text{Gd}(\text{L}^2)_2(\text{dbm})_2]$

Gd(1)-O(145)	2.333(2)	Gd(2)-O(215)	2.307(2)
Gd(1)-O(111)	2.336(2)	Gd(2)-O(245)	2.318(2)
Gd(1)-O(141)	2.339(2)	Gd(2)-O(211)	2.355(2)
Gd(1)-O(115)	2.346(2)	Gd(2)-O(241)	2.369(2)
Gd(1)-N(182)	2.505(3)	Gd(2)-N(262)	2.513(3)
Gd(1)-N(162)	2.529(3)	Gd(2)-N(282)	2.538(3)
Gd(1)-N(171)	2.537(3)	Gd(2)-N(271)	2.546(3)
Gd(1)-N(191)	2.566(3)	Gd(2)-N(291)	2.576(3)

O(145)-Gd(1)-O(111)	145.80(8)	O(215)-Gd(2)-O(245)	147.86(8)
O(145)-Gd(1)-O(141)	70.57(8)	O(215)-Gd(2)-O(211)	70.64(8)
O(111)-Gd(1)-O(141)	143.59(8)	O(245)-Gd(2)-O(211)	141.12(8)
O(145)-Gd(1)-O(115)	143.05(8)	O(215)-Gd(2)-O(241)	136.11(8)
O(111)-Gd(1)-O(115)	71.14(8)	O(245)-Gd(2)-O(241)	70.58(8)
O(141)-Gd(1)-O(115)	72.54(8)	O(211)-Gd(2)-O(241)	72.25(8)
O(145)-Gd(1)-N(182)	73.04(9)	O(215)-Gd(2)-N(262)	88.24(9)
O(111)-Gd(1)-N(182)	80.83(9)	O(245)-Gd(2)-N(262)	75.10(9)
O(141)-Gd(1)-N(182)	123.40(9)	O(211)-Gd(2)-N(262)	126.17(9)
O(115)-Gd(1)-N(182)	131.94(9)	O(241)-Gd(2)-N(262)	133.30(9)
O(145)-Gd(1)-N(162)	71.00(9)	O(215)-Gd(2)-N(282)	73.49(9)
O(111)-Gd(1)-N(162)	82.05(8)	O(245)-Gd(2)-N(282)	75.71(9)
O(141)-Gd(1)-N(162)	126.74(8)	O(211)-Gd(2)-N(282)	136.81(9)
O(115)-Gd(1)-N(162)	133.60(9)	O(241)-Gd(2)-N(282)	123.69(8)
N(182)-Gd(1)-N(162)	76.98(9)	N(262)-Gd(2)-N(282)	75.05(9)
O(145)-Gd(1)-N(171)	86.97(9)	O(215)-Gd(2)-N(271)	110.13(9)
O(111)-Gd(1)-N(171)	100.11(9)	O(245)-Gd(2)-N(271)	87.61(9)
O(141)-Gd(1)-N(171)	78.35(9)	O(211)-Gd(2)-N(271)	76.89(9)
O(115)-Gd(1)-N(171)	83.73(9)	O(241)-Gd(2)-N(271)	82.97(8)
N(182)-Gd(1)-N(171)	140.44(9)	N(262)-Gd(2)-N(271)	64.70(9)
N(162)-Gd(1)-N(171)	64.18(9)	N(282)-Gd(2)-N(271)	139.23(9)
O(145)-Gd(1)-N(191)	91.34(9)	O(215)-Gd(2)-N(291)	82.48(9)
O(111)-Gd(1)-N(191)	96.91(9)	O(245)-Gd(2)-N(291)	92.03(9)
O(141)-Gd(1)-N(191)	74.74(9)	O(211)-Gd(2)-N(291)	88.30(9)
O(115)-Gd(1)-N(191)	80.93(9)	O(241)-Gd(2)-N(291)	73.79(8)
N(182)-Gd(1)-N(191)	64.31(9)	N(262)-Gd(2)-N(291)	138.65(9)
N(162)-Gd(1)-N(191)	140.83(9)	N(282)-Gd(2)-N(291)	63.66(9)
N(171)-Gd(1)-N(191)	151.98(9)	N(271)-Gd(2)-N(291)	155.43(9)

Table S6: Coordination-sphere bond lengths and angles for [Yb(L²)₂(dbm)₂]

Yb(1)-O(145)	2.247(2)	Yb(2)-O(215)	2.228(2)
Yb(1)-O(115)	2.256(2)	Yb(2)-O(241)	2.232(2)
Yb(1)-O(111)	2.2743(18)	Yb(2)-O(211)	2.2841(19)
Yb(1)-O(141)	2.2879(19)	Yb(2)-O(245)	2.3051(19)
Yb(1)-N(182)	2.452(2)	Yb(2)-N(262)	2.450(2)
Yb(1)-N(162)	2.466(2)	Yb(2)-N(282)	2.475(2)
Yb(1)-N(171)	2.478(2)	Yb(2)-N(271)	2.475(2)
Yb(1)-N(191)	2.509(2)	Yb(2)-N(291)	2.496(2)

O(145)-Yb(1)-O(115)	143.33(7)	O(215)-Yb(2)-O(241)	146.07(7)
O(145)-Yb(1)-O(111)	144.44(6)	O(215)-Yb(2)-O(211)	72.39(7)
O(115)-Yb(1)-O(111)	72.20(7)	O(241)-Yb(2)-O(211)	141.34(7)
O(145)-Yb(1)-O(141)	72.92(7)	O(215)-Yb(2)-O(245)	138.20(7)
O(115)-Yb(1)-O(141)	143.75(6)	O(241)-Yb(2)-O(245)	71.71(7)
O(111)-Yb(1)-O(141)	71.56(7)	O(211)-Yb(2)-O(245)	70.99(7)
O(145)-Yb(1)-N(182)	78.96(7)	O(215)-Yb(2)-N(262)	86.19(8)
O(115)-Yb(1)-N(182)	72.86(7)	O(241)-Yb(2)-N(262)	74.35(7)
O(111)-Yb(1)-N(182)	125.01(7)	O(211)-Yb(2)-N(262)	127.04(7)
O(141)-Yb(1)-N(182)	131.39(7)	O(245)-Yb(2)-N(262)	132.63(7)
O(145)-Yb(1)-N(162)	80.19(7)	O(215)-Yb(2)-N(282)	72.91(7)
O(115)-Yb(1)-N(162)	71.16(7)	O(241)-Yb(2)-N(282)	75.45(8)
O(111)-Yb(1)-N(162)	127.10(7)	O(211)-Yb(2)-N(282)	136.24(7)
O(141)-Yb(1)-N(162)	133.29(7)	O(245)-Yb(2)-N(282)	124.53(7)
N(182)-Yb(1)-N(162)	77.22(8)	N(262)-Yb(2)-N(282)	75.71(8)
O(145)-Yb(1)-N(171)	100.13(7)	O(215)-Yb(2)-N(271)	110.12(8)
O(115)-Yb(1)-N(171)	88.64(7)	O(241)-Yb(2)-N(271)	87.47(8)
O(111)-Yb(1)-N(171)	76.72(7)	O(211)-Yb(2)-N(271)	76.46(7)
O(141)-Yb(1)-N(171)	82.17(7)	O(245)-Yb(2)-N(271)	80.01(7)
N(182)-Yb(1)-N(171)	142.31(7)	N(262)-Yb(2)-N(271)	66.35(8)
N(162)-Yb(1)-N(171)	65.66(7)	N(282)-Yb(2)-N(271)	141.40(7)
O(145)-Yb(1)-N(191)	97.97(7)	O(215)-Yb(2)-N(291)	83.55(8)
O(115)-Yb(1)-N(191)	91.34(7)	O(241)-Yb(2)-N(291)	94.15(8)
O(111)-Yb(1)-N(191)	74.25(7)	O(211)-Yb(2)-N(291)	85.16(7)
O(141)-Yb(1)-N(191)	79.93(7)	O(245)-Yb(2)-N(291)	74.00(7)
N(182)-Yb(1)-N(191)	65.54(8)	N(262)-Yb(2)-N(291)	140.85(7)
N(162)-Yb(1)-N(191)	142.24(8)	N(282)-Yb(2)-N(291)	65.16(7)
N(171)-Yb(1)-N(191)	149.47(7)	N(271)-Yb(2)-N(291)	151.95(7)

Table S7: Coordination-sphere bond lengths and angles for [Tb(L²)₂(dbm)₂]

Tb(1)-O(111)	2.305(2)	Tb(2)-O(211)	2.0876(17)
Tb(1)-O(145)	2.317(2)	Tb(2)-O(245)	2.1155(17)
Tb(1)-O(141)	2.3224(18)	Tb(2)-O(241)	2.2832(17)
Tb(1)-O(115)	2.3316(18)	Tb(2)-O(215)	2.2920(17)
Tb(1)-N(182)	2.490(2)	Tb(2)-N(272)	2.605(2)
Tb(1)-N(172)	2.558(2)	Tb(2)-N(282)	2.607(2)
Tb(1)-N(191)	2.563(2)	Tb(2)-N(261)	2.734(2)
Tb(1)-N(161)	2.617(2)	Tb(2)-N(291)	2.792(2)

O(111)-Tb(1)-O(145)	145.70(6)	O(211)-Tb(2)-O(245)	144.44(7)
O(111)-Tb(1)-O(141)	142.40(6)	O(211)-Tb(2)-O(241)	134.07(6)
O(145)-Tb(1)-O(141)	71.90(6)	O(245)-Tb(2)-O(241)	74.88(6)
O(111)-Tb(1)-O(115)	70.66(6)	O(211)-Tb(2)-O(215)	74.52(6)
O(145)-Tb(1)-O(115)	143.59(6)	O(245)-Tb(2)-O(215)	140.60(6)
O(141)-Tb(1)-O(115)	71.77(7)	O(241)-Tb(2)-O(215)	67.80(6)
O(111)-Tb(1)-N(182)	80.26(7)	O(211)-Tb(2)-N(272)	88.33(7)
O(145)-Tb(1)-N(182)	73.15(7)	O(245)-Tb(2)-N(272)	74.93(7)
O(141)-Tb(1)-N(182)	126.71(7)	O(241)-Tb(2)-N(272)	134.79(7)
O(115)-Tb(1)-N(182)	129.57(6)	O(215)-Tb(2)-N(272)	124.70(7)
O(111)-Tb(1)-N(172)	65.61(6)	O(211)-Tb(2)-N(282)	72.32(7)
O(145)-Tb(1)-N(172)	87.64(7)	O(245)-Tb(2)-N(282)	74.00(7)
O(141)-Tb(1)-N(172)	137.97(6)	O(241)-Tb(2)-N(282)	121.83(7)
O(115)-Tb(1)-N(172)	121.87(7)	O(215)-Tb(2)-N(282)	137.50(7)
N(182)-Tb(1)-N(172)	78.00(7)	N(272)-Tb(2)-N(282)	80.12(7)
O(111)-Tb(1)-N(191)	100.13(7)	O(211)-Tb(2)-N(261)	109.86(7)
O(145)-Tb(1)-N(191)	87.93(7)	O(245)-Tb(2)-N(261)	89.54(8)
O(141)-Tb(1)-N(191)	74.93(7)	O(241)-Tb(2)-N(261)	85.66(7)
O(115)-Tb(1)-N(191)	80.54(7)	O(215)-Tb(2)-N(261)	75.78(7)
N(182)-Tb(1)-N(191)	64.85(7)	N(272)-Tb(2)-N(261)	61.31(7)
N(172)-Tb(1)-N(191)	142.23(7)	N(282)-Tb(2)-N(261)	140.98(7)
O(111)-Tb(1)-N(161)	77.49(7)	O(211)-Tb(2)-N(291)	81.74(7)
O(145)-Tb(1)-N(161)	110.14(7)	O(245)-Tb(2)-N(291)	91.74(7)
O(141)-Tb(1)-N(161)	89.70(7)	O(241)-Tb(2)-N(291)	72.39(7)
O(115)-Tb(1)-N(161)	71.94(6)	O(215)-Tb(2)-N(291)	88.81(7)
N(182)-Tb(1)-N(161)	140.23(7)	N(272)-Tb(2)-N(291)	140.97(7)
N(172)-Tb(1)-N(161)	62.88(7)	N(282)-Tb(2)-N(291)	60.89(7)
N(191)-Tb(1)-N(161)	151.61(7)	N(261)-Tb(2)-N(291)	156.83(6)

Table S8: Coordination-sphere bond lengths and angles for the complex cation of $[\text{Nd}(\text{L}^1)_2][\text{Nd}(\text{dbm})_4]$

Nd(1)-N(32)	2.676(2)	Nd(1)-N(41)	2.891(2)
Nd(1)-N(52)	2.688(2)	Nd(1)-N(61)	2.922(2)
Nd(1)-N(12)	2.689(2)	Nd(1)-N(21)	2.955(2)
N(32)-Nd(1)-N(52)	112.86(6)	N(12)-Nd(1)-N(61A)	64.01(6)
N(32)-Nd(1)-N(52A)	67.14(6)	N(41)-Nd(1)-N(61A)	117.32(6)
N(32)-Nd(1)-N(12A)	67.33(6)	N(32)-Nd(1)-N(61)	64.90(6)
N(52)-Nd(1)-N(12A)	111.92(6)	N(52)-Nd(1)-N(61)	58.43(6)
N(32)-Nd(1)-N(12)	112.67(6)	N(12)-Nd(1)-N(61)	115.99(6)
N(52)-Nd(1)-N(12)	68.08(6)	N(41)-Nd(1)-N(61)	62.68(6)
N(32)-Nd(1)-N(41)	58.79(6)	N(61A)-Nd(1)-N(61)	180.0
N(52)-Nd(1)-N(41)	64.96(6)	N(32)-Nd(1)-N(21)	115.22(6)
N(12)-Nd(1)-N(41)	64.59(6)	N(32A)-Nd(1)-N(21)	64.78(6)
N(32)-Nd(1)-N(41A)	121.21(6)	N(52)-Nd(1)-N(21)	63.91(6)
N(52)-Nd(1)-N(41A)	115.04(6)	N(52A)-Nd(1)-N(21)	116.10(6)
N(12)-Nd(1)-N(41A)	115.41(6)	N(12)-Nd(1)-N(21)	121.61(6)
N(32)-Nd(1)-N(61A)	115.10(6)	N(41)-Nd(1)-N(21)	117.69(6)
N(52)-Nd(1)-N(61A)	121.57(6)	N(41A)-Nd(1)-N(21)	62.31(6)
N(52A)-Nd(1)-N(61A)	58.43(6)	N(61A)-Nd(1)-N(21)	118.62(6)
N(12A)-Nd(1)-N(61A)	115.99(6)	N(61)-Nd(1)-N(21)	61.38(6)
N(21)-Nd(1)-N(21A)	180.0	N(12)-Nd(1)-N(21A)	58.39(6)

Figure S1: Molecular structure of the complex cation of $[\text{Nd}(\text{L}^1)_2][\text{Nd}(\text{dbm})_4]$

