Supplementary materials

Synthesis, structure and long-lived NIR luminescence of lanthanide ate complexes with perfluorinated 2-mercaptobenzothiazole

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Table 1S. Details of crystallographic, collection and refinement data for **1** – **3**, **6**.

Complex	**1**	**2**	**3**	**6**
Empirical formula	$C_{40}H_{30}F_{16}N_4NaNdO_6S_8$	$C_{40}H_{30}F_{16}N_4NaSmO_6S_8$	$C_{40}H_{30}F_{16}N_4NaTbO_6S_8$	$C_{40}H_{30}F_{16}N_4LiYbO_6S_8$
Formula weight	1390.39	1396.50	1405.07	1403.14
Temperature [K]	100(2)	100(2)	100(2)	100(2)
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/n$	$P2_1/n$	P2(1)/n	P2(1)/n
Unit cell dimensions				
a[Å]	14.2673(4)	14.2403(7)	15.6988(5)	13.8956(8)
b[Å]	32.3497(9)	32.3402(15)	20.5029(7)	32.1223(17)
c[Å]	23.1902(6)	23.1367(11)	16.0116(7)	23.7949(14)
α[°]	90	90	90	90
β[°]	100.0860(10)	100.2170(10)	91.6090(10)	106.296(2)
γ[°]	90	90	90	90
Volume [Å^3]	10537.9(5)	10486.3(9)	5151.6(3)	10194.4(10)
Z	8	8	4	8
Calculated density [Mg/m^3]	1.753	1.769	1.812	1.828
Absorption coefficient [mm^{-1}]	1.416	1.552	1.813	2.271
F(000)	5512	5528	2776	5528
Crystal size [mm^3]	0.24×0.17×0.11	0.44×0.33×0.18	0.12×0.08×0.04	0.20×0.15×0.04
θ [°]	1.936 - 27.000	2.188 - 27.000	2.359 - 29.000	1.902 - 25.030
Reflections collected / unique	122590 / 22994	113916 / 22884	64235 / 13621	118646 / 18191
R(int)	0.0515	0.0324	0.0491	0.0635
Final R indices [I>2sigma(I)]	R_1=0.0429, wR_2=0.0796	R_1=0.0286, wR_2=0.0569	R_1=0.0343, wR_2=0.0648	R_1=0.0684, wR_2=0.1869
R indices (all data)	R_1=0.0578, wR_2=0.0831	R_1=0.0348, wR_2=0.0584	R_1=0.0485, wR_2=0.0678	R_1=0.0834, wR_2=0.2098
S	1.076	1.089	1.066	1.042
Largest diff. peak and hole [e/Å^3]	0.962/-1.046	0.780/-0.662	1.187/-1.594	3.473/-2.986

Table 2S. Selected bond lengths (Å) and angles (°) in the complexes **1 – 3**, **6**.

Distances and Angles	**1** (Ln = Nd)	**2** (Ln = Sm)	**3** (Ln = Tb)	**4** (Ln = Yb)
Ln-S, Å	2.8634(10) - 2.8961(9)	2.8346(6) - 2.8671(6)	2.8325(7) - 2.8417(7)	2.770(3) - 2.795(3)
Ln-N, Å	2.564(3) - 2.612(3)	2.5343(18) - 2.5863(18)	2.501(2) - 2.543(2)	2.455(10) - 2.480(10)
N^L-Ln-S^L, °	57.64(6) - 58.42(7)	58.16(4) - 58.93(5)	59.16(5) - 59.32(5)	59.6(3) - 60.6(2)