Supporting Information

New NIR-emissive tetranuclear Er(III) complexes with 4-hydroxo-2,1,3-benzothiadiazolate and dibenzoylmethanate ligands: Synthesis and characterization

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Table S1. Crystallographic data of compounds **1**·$7C_7H_8$, **1**·$3.5CH_2Cl_2$, **2**·6THF.

Compound	**1**·$7C_7H_8$	**1**·$3.5CH_2Cl_2$	**2**·6THF
Empirical formula	$C_{163}H_{136}Er_4N_8O_{18}S_4$	$C_{117.5}H_{87}Cl_7Er_4N_8O_{18}S_4$	$C_{120}H_{112}Er_4N_{12}O_{22}S_6$
Formula weight	3292.08	2944.38	2935.62
Crystal system	Triclinic	Monoclinic	Triclinic
Space group	*P*-1	$P2_1/c$	*P*-1
Unit cell dimensions *a* [Å]	14.1646(4)	15.6938(4)	14.8263(12)
b [Å]	15.2641(4)	27.3924(8)	14.8685(12)
c [Å]	16.4794(5)	26.7304(8)	16.6589(14)
α [°]	87.779(1)	90	65.675(2)
β [°]	89.776(1)	93.327(1)	68.993(2)
γ [°]	82.376(1)	90	64.225(2)
Volume [Å ^{3}]	3528.86(17)	11471.8(6)	2940.5(4)
Z	1	4	1
Density (calcd.) [g cm^{-3}]	1.549	1.705	1.658
F(000)	1650	5788	1460
Abs. coefficient [mm^{-1}]	2.483	3.202	3.006
Crystal size [mm^3]	0.18x0.12x0.10	0.25x0.25x0.04	0.18x0.08x0.02
$2\theta_{max}$ [°]	54.96	55.18	55.18
Index range	-18<=h<=18 -19<=k<=15 -21<=l<=21	-20<=h<=12 -35<=k<=35 -34<=l<=34	-9<=h<=19 -15<=k<=19 -20<=l<=21
Reflections collected	33663	85984	22102
Independent reflections	16173 [R(int) = 0.0177]	25294 [R(int) = 0.0826]	13486 [R(int) = 0.0354]
Completness to 2θ = 50.5°[%]	99.8	99.2	99.7
Reflections, $I \geq 2\sigma(I)$	13394	14004	9198
Parameters	838	1435	742
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0274, wR2 = 0.0657	R1 = 0.0705, wR2 = 0.1680	R1 = 0.0425, wR2 = 0.0906
R indices (all data)	R1 = 0.0377, wR2 = 0.0693	R1 = 0.1566, wR2 = 0.1949	R1 = 0.0809, wR2 = 0.1000
GoF	1.053	1.070	0.935
Residual electron density (min / max, *e*/Å^3)	-0.822 / 1.815	-2.733 / 4.670	-2.071 / 1.977

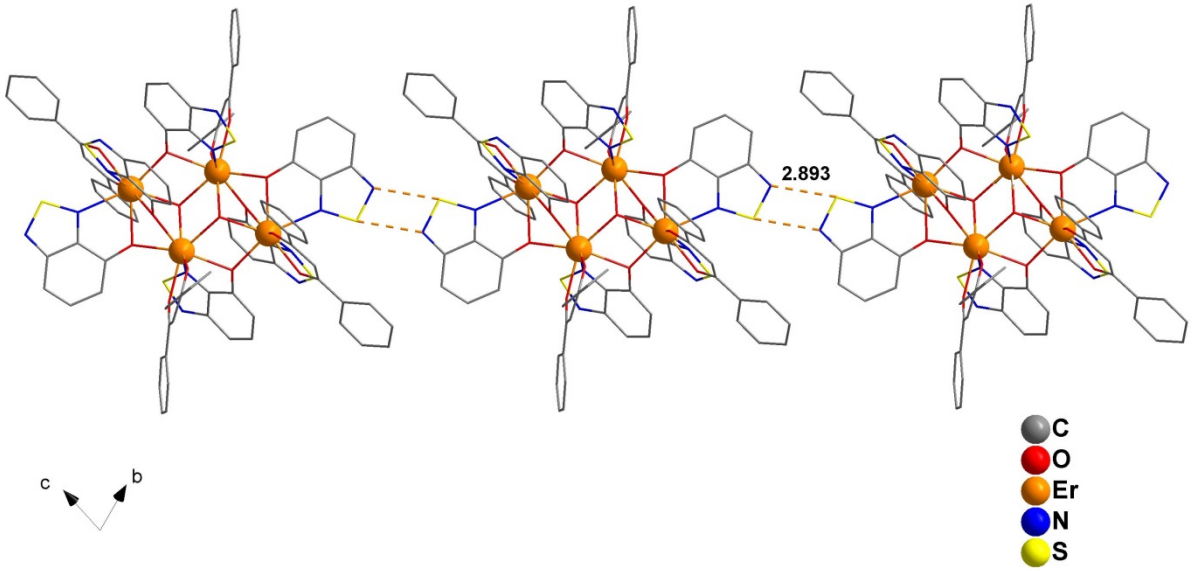
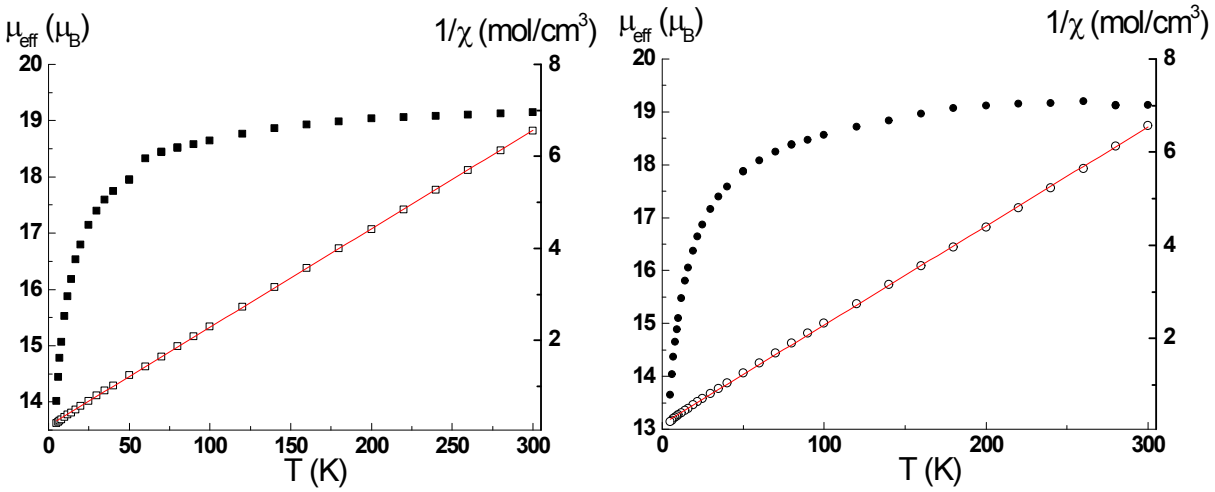


Fig. S1 Packing diagram of complex **2**·6THF viewed along *a* axis showing intermolecular S···N contacts (dashed)



a ***b***

Fig. S2 a Temperature dependences of μ_{eff} (●) and $1/\chi$ (○) for **1**. (solid lines – theoretical curves)

Fig. S2 b Temperature dependences of μ_{eff} (■) and $1/\chi$ (□) for **2**.