Electronic Supplementary Information (ESI)

Visible and NIR emitting Yb(III) and Er(III) complexes sensitized by β-diketonates and phenanthroline derivatives

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Abreviations

Hbta = benzoyltrifluoroacetone

Htta = 2-thenoyltrifluoroacetone

me-phen = 5-methyl-1,10-phenanthroline

pyz-phen = pyrazino[2,3-f][1,10]phenanthroline

[Er$(bta)_3$(me-phen)] **(1),** [Yb$(bta)_3$(me-phen)] **(2)**, [Gd(bta)3(me-phen)] (**3**), [Yb$(bta)_3$(pyz-phen)] **(4)**, and [Er$(tta)_3$(pyz-phen)] **(5)**

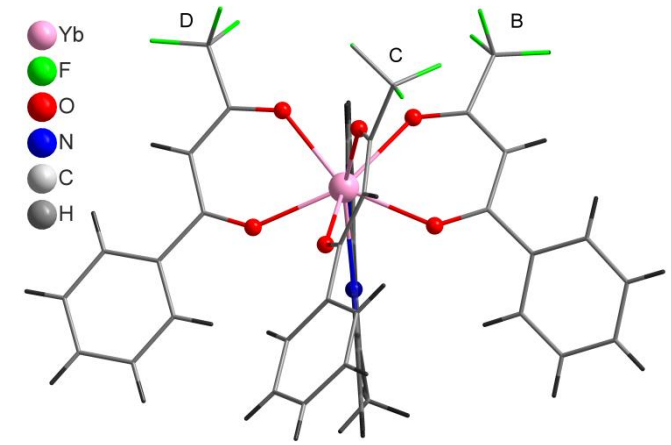

Fig. S1 Molecular structure of **2** with the bta$^-$ ligands labelled as B, C and D.

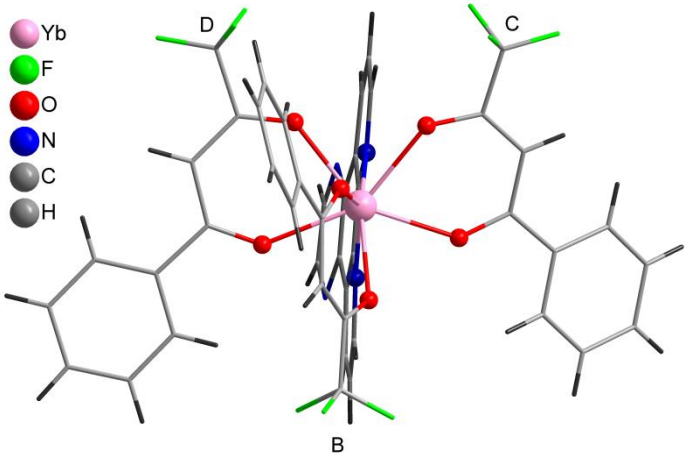

Fig. S2 Molecular structure of **4** with the bta$^-$ ligands labelled as B, C and D.

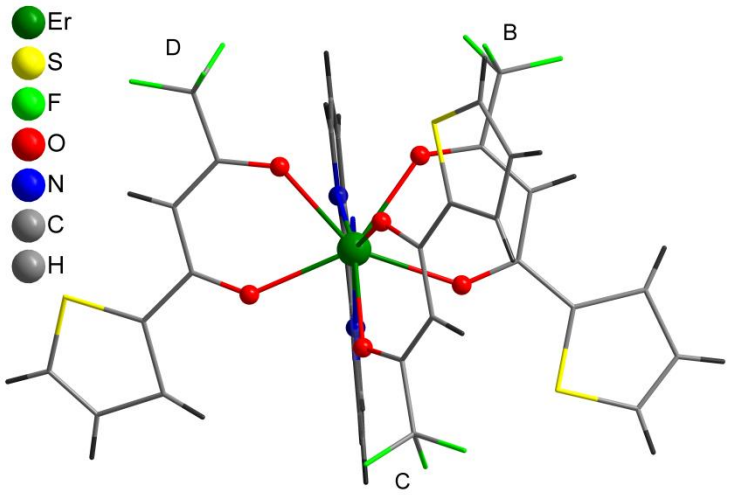

Fig. S3 Molecular structure of **5** with the tta$^-$ ligands labelled as B, C and D.

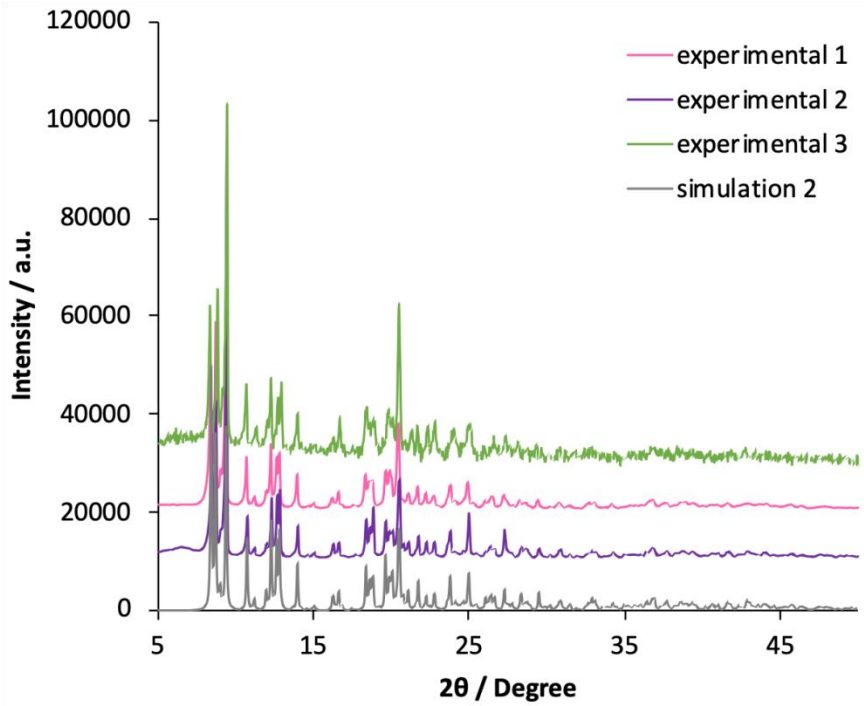

Fig. S4 Powder diffraction patterns of **1** - **3**, together with the simulation of **2** from the single crystal X-ray structure.

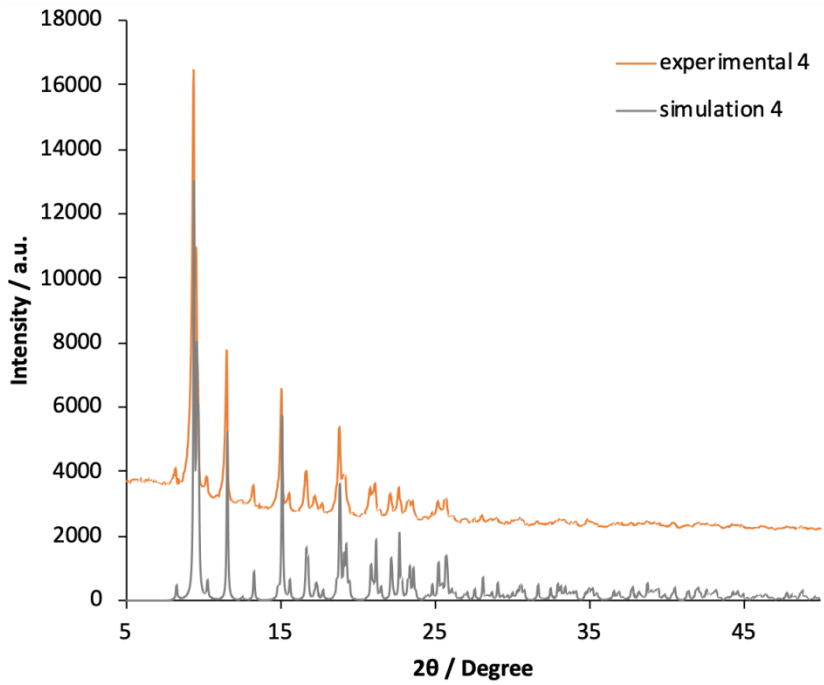

Fig. S5 Powder diffraction pattern of **4** compared with the simulation from single crystal

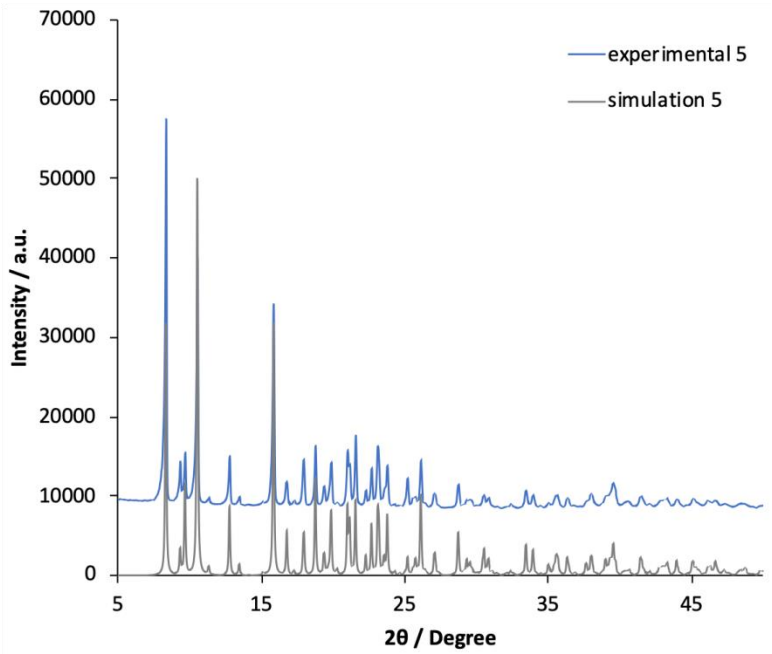

Fig. S6 Powder diffraction pattern of **5** compared with the simulation from single crystal.

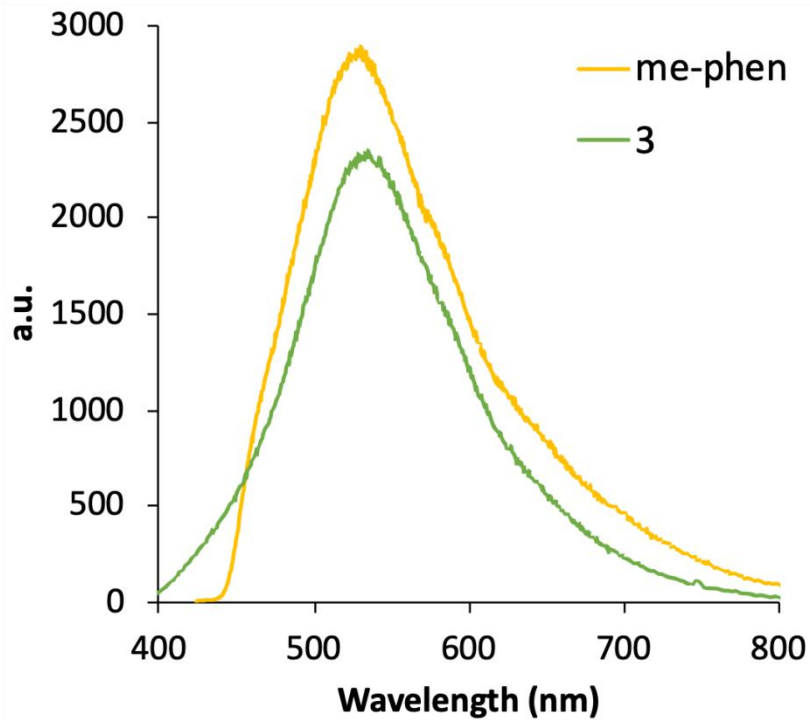

Fig. S7 Photoluminescence spectra of me-phen ligand and [Gd(me-phen)$(bta)_3$] (**3**) complex excited at 375 nm.

Table S1. Distances [Å] and angles [°] for the shortest π-π interactions in [Yb(bta)$_3$(me-phen)](2).

π-π interaction Cg(I)···Cg(J)	d[Cg(I)···Cg(J)]	α	β	γ	d[Cg1···P_2]	d[Cg2···P_1]
Cg1···Cg2^{i}	3.931(5)	26.1	8.4	31.8	3.339	3.889

Cg: ring centroid; α: dihedral angle between planes I and J, β: Angle between Cg(I)-Cg(J) vector and normal to plane; γ: Angle between Cg(I) and Cg(J) vector and normal to plane J Cg···P: perpendicular distance of Cg on ring plane P; d

Cg1: C4A-C5A-C6A-C7A-C11A-C12A; Cg2: C5B-C6B-C7B-C8B-C9B-C10B

Symmetry transformations: i=x,1/2-y,1/2+z

Table S2. Distances [Å] and angles [°] for the shortest π-π interactions in [Yb(bta)$_3$(pyz-phen)](**4**).

π-π interaction Cg(I)···Cg(J)	d[Cg(I)···Cg(J)]	α	β	γ	d[Cg1···P_2]	d[Cg2···P_1]
Cg1···Cg2^{i}	3.711(11)	12	14	11.2	3.669	3.659
Cg1···Cg3^{ii}	3.724(10)	3.4	23.3	26.6	3.330	3.422
Cg4···Cg3^{ii}	3.685(6)	3.8	21	24.6	3.351	3.441

Cg: ring centroid; α: dihedral angle between planes I and J, β: Angle between Cg(I)-Cg(J) vector and normal to plane; γ: Angle between Cg(I) and Cg(J) vector and normal to plane J Cg···P: perpendicular distance of Cg on ring plane P; d

Cg1: N3A-C5A-C6A-N4A-C14A-C13A; Cg2: C5B-C6B-C7B-C8B-C9B- C10B; Cg3: C5C-C6C-C7C-C8C-C9C-C10C; Cg4: C4A-C5A-C6A-C7A-C11A- C12A

Symmetry transformations: i=-1/2+x,3/2-y,z ii= 1-x,1-y,1/2+z

Table S3. Distances [Å] and angles [°] for the shortest π-π interactions in [Er(tta)$_3$(pyz-phen)](**5**).

π-π interaction Cg(I)···Cg(J)	d[Cg(I)···Cg(J)]	α	β	γ	d[Cg1···P_2]	d[Cg2···P_1]
Cg1···Cg2^{i}	3.795(7)	3.7	24.8	22.3	3.509	3.445
Cg1···Cg3^{i}	3.726(8)	5.2	17.1	21.8	3.459	3.561

Cg: ring centroid; α: dihedral angle between planes I and J, β: Angle between Cg(I)-Cg(J) vector and normal to plane; γ: Angle between Cg(I) and Cg(J) vector and normal to plane J Cg···P: perpendicular distance of Cg on ring plane P; d

Cg1: S2D–C5D–C6D–C7D–C8D; Cg2: N3A–C5A–C6A–N4A–C14A–C13A; Cg3: C4A–C5A–C6A–C7A–C11A–C12A.

Symmetry transformations: i= 1/2-x,-1/2+y, z.

Table S4. Selected geometric parameters (Å,˚) for compounds **2**, **4** and **5**

Compound **2**		Compound **4**		Compound **5**	
Yb1—O2D	2.263 (4)	Yb01—O2D	2.263 (4)	Er1—O2C	2.270 (3)
Yb1—O2C	2.271 (4)	Yb01—O2B	2.264 (5)	Er1—O1D	2.290 (3)
Yb1—O1C	2.282 (4)	Yb01—O2C	2.274 (5)	Er1—O2B	2.306 (3)
Yb1—O2B	2.283 (4)	Yb01—O1B	2.277 (5)	Er1—O1B	2.311 (3)
Yb1—O1D	2.286 (4)	Yb01—O1C	2.278 (4)	Er1—O2D	2.311 (3)
Yb1—O1B	2.319 (4)	Yb01—O1D	2.288 (5)	Er1—O1C	2.320 (3)
Yb1—N1A	2.491 (5)	Yb01—N2A	2.499 (7)	Er1—N2A	2.518 (4)
Yb1—N2A	2.524 (5)	Yb01—N1A	2.512 (7)	Er1—N1A	2.543 (4)
O1C—Yb1—O1B	74.41 (18)	O1B—Yb01—O1C	120.8 (2)	O1B—Er1—O1C	133.18 (12)
O2C—Yb1—O1B	137.45 (17)	O2C—Yb01—O1B	77.03 (19)	O2C—Er1—O1B	73.74 (14)
O1D—Yb1—O1B	80.08 (15)	O1B—Yb01—O1D	137.00 (19)	O1D—Er1—O1B	78.25 (12)
O2D—Yb1—O1B	147.37 (16)	O2D—Yb01—O1B	77.07 (19)	O1B—Er1—O2D	147.06 (11)
O1B—Yb1—N2A	116.29 (17)	O1B—Yb01—N1A	144.4 (2)	O1B—Er1—N1A	70.77 (14)
O1B—Yb1—N1A	73.10 (17)	O1B—Yb01—N2A	80.5 (2)	O1B—Er1—N2A	117.00 (13)
O2B—Yb1—O1B	73.30 (15)	O2B—Yb01—O1B	72.9 (2)	O2B—Er1—O1B	72.97 (11)
O2C—Yb1—O1C	73.35 (17)	O2C—Yb01—O1C	72.66 (16)	O2C—Er1—O1C	72.67 (13)
O2D—Yb1—O1D	73.61 (15)	O2D—Yb01—O1D	73.10 (17)	O1D—Er1—O2D	73.33 (12)
N1A—Yb1—N2A	64.46 (19)	N2A—Yb01—N1A	65.0 (3)	N2A—Er1—N1A	64.09 (12)