

Supplementary Information

Synthesis, Structures, and Luminescent Properties of f-element bearing 2,4,6-tri- α -pyridyl-1,3,5-triazine Coordination Polymers

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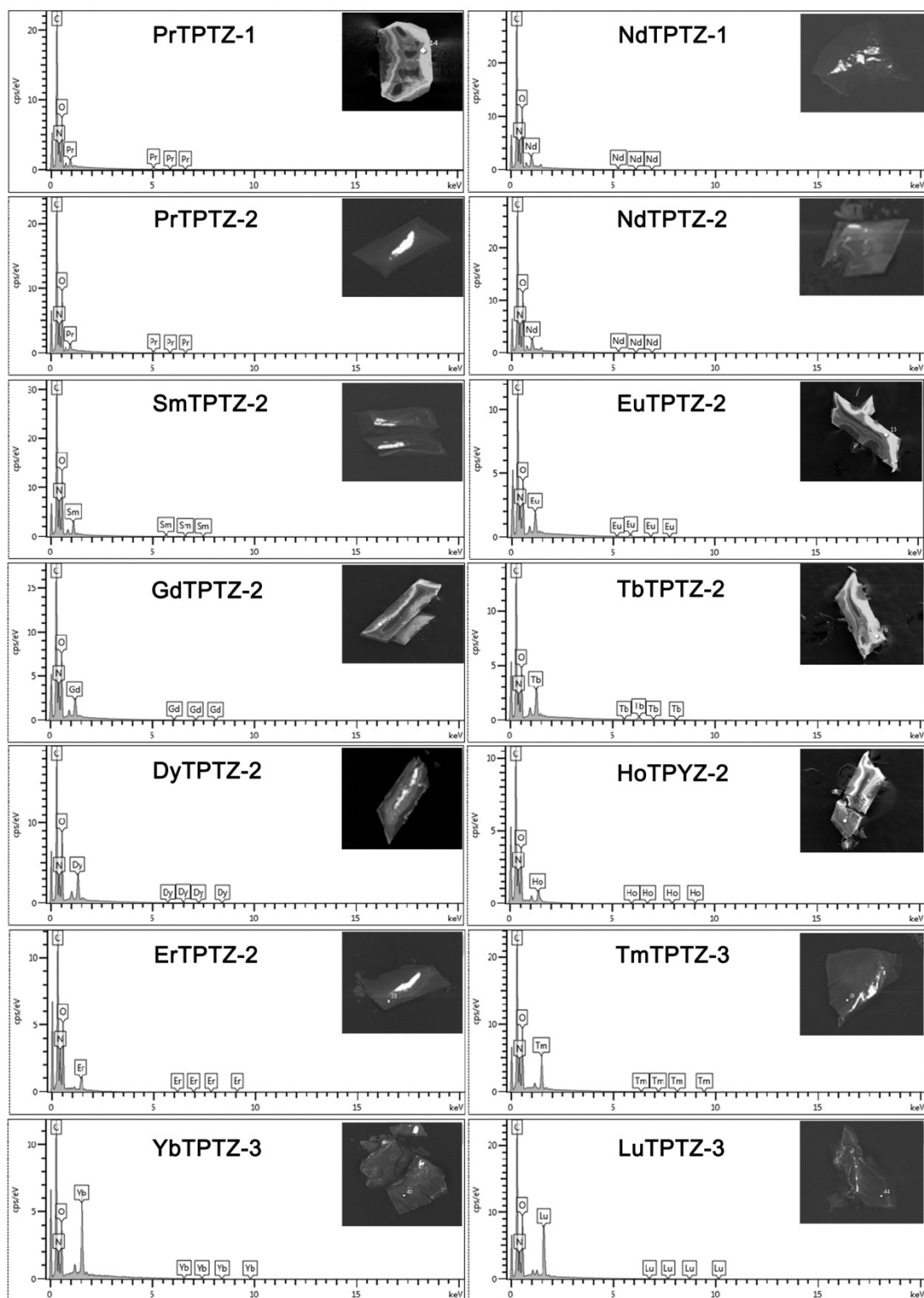


Fig S1. SEM images and EDS spectra of LnTPTZ.

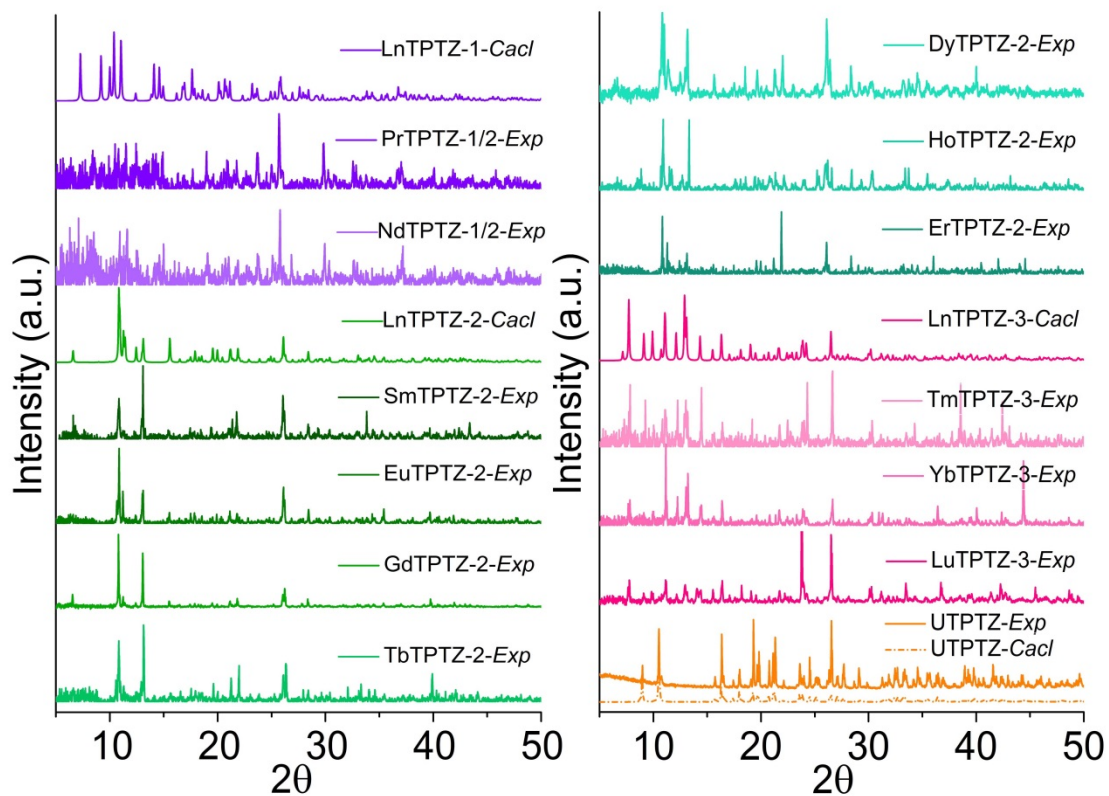


Fig S2. The Powder X-ray diffraction (PXRD) patterns of **LnTPTZ** and **UTPTZ**.

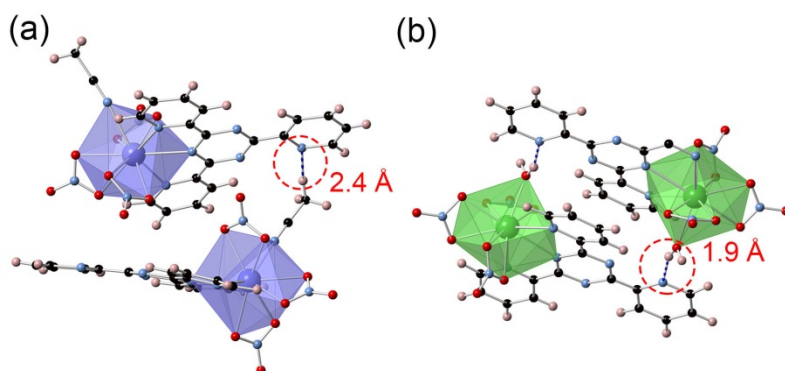


Fig S3. Intermolecular hydrogen bonds in (a) **LnTPTZ-1** and (b) **LnTPTZ-2**

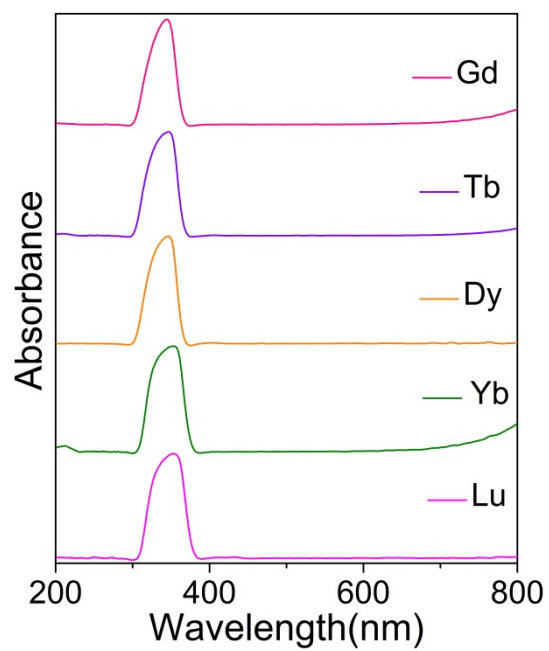


Fig S4. UV-Vis spectra of GdTPTZ-2, TbTPTZ-2, DyTPTZ-2, YbTPTZ-3, and LuTPTZ-3.

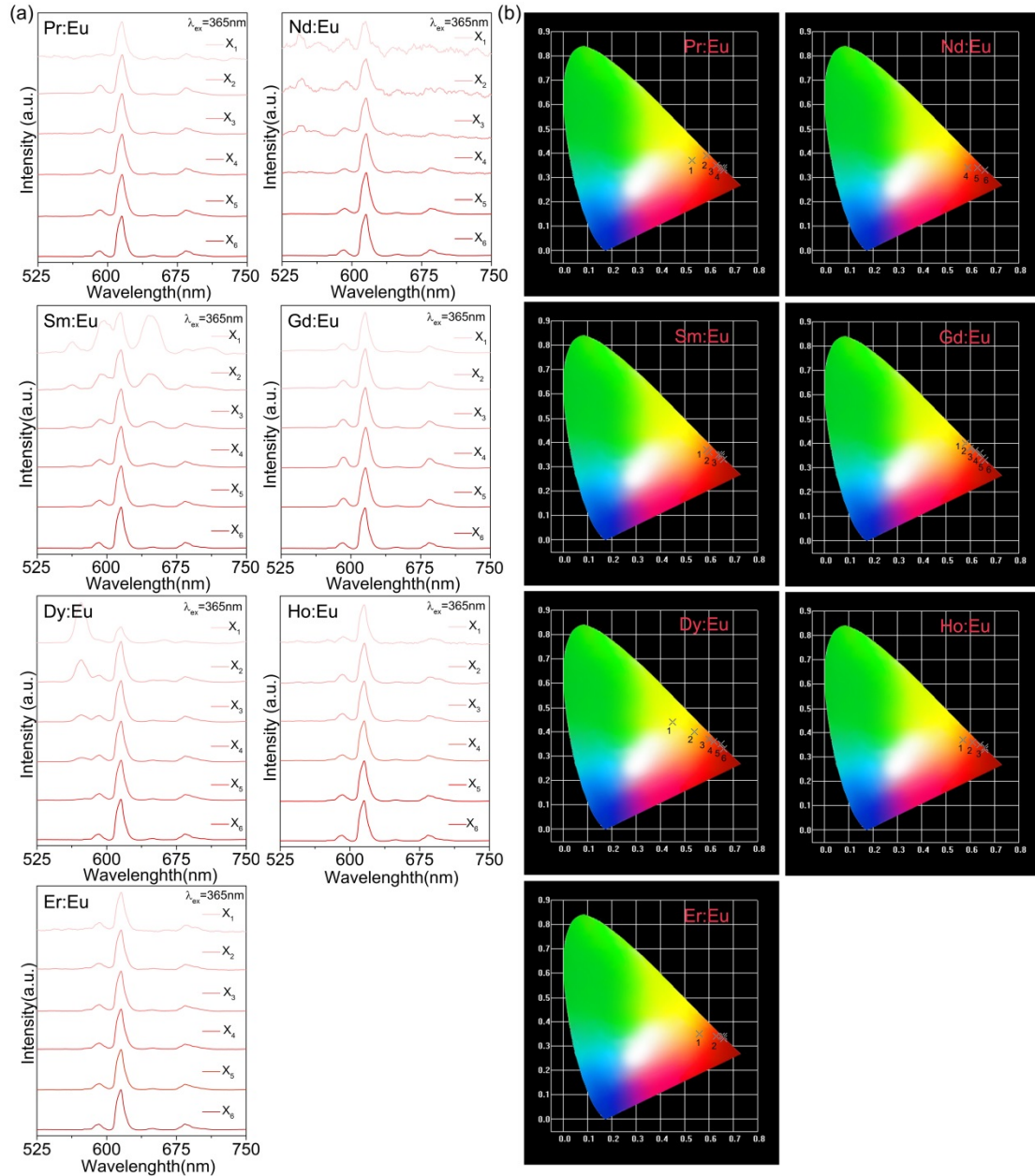


Fig S5. (a) Emission spectra and (b) CIE chromaticity diagrams for $\text{Eu}_x\text{Ln}_{1-x}\text{TPTZ-2}$ ($x = 0.01, 0.06, 0.1, 0.2, \text{ and } 0.4$).

Table S4. Crystallographic data for **LnTPTZ** and **UTPTZ**.

Compound	PrTPTZ-1	NdTPTZ-1	PrTPTZ-2	NdTPTZ-2	SmTPTZ-2	EuTPTZ-2	GdTPTZ-2
Formula Mass	680.33	683.66	698.34	701.67	707.79	709.40	714.68
Color	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow
Habit	Block	Block	Block	Block	Block	Block	Block
Space Group	<i>P2(1)/n</i>	<i>P2(1)/n</i>	<i>P-1</i>	<i>P-1</i>	<i>P-1</i>	<i>P-1</i>	<i>P-1</i>
<i>a</i> (Å)	14.6447(10)	14.6200(7)	9.5833(12)	9.5728(2)	9.5666(6)	9.5675(5)	9.5677(2)
<i>b</i> (Å)	10.5774(8)	10.5736(5)	10.6466(13)	10.6394(3)	10.6253(6)	10.6223(6)	10.6207(2)
<i>c</i> (Å)	16.4505(12)	16.4263(7)	13.7055(15)	13.7014(3)	13.6627(7)	13.6502(7)	13.6374(3)
α (°)	90	90	89.780(4)	89.9080(10)	89.966(2)	90.020(2)	90.0320(10)
β (°)	103.302(2)	103.2810(10)	84.840(4)	84.9420(10)	84.946(2)	84.971(2)	84.9710(10)
γ (°)	90	90	69.902(4)	69.8010(10)	69.600(2)	69.520(2)	69.4360(10)
<i>V</i> (Å ³)	2479.9(3)	2471.4(2)	1307.3(3)	1303.93(5)	1295.95(13)	1293.85(12)	1291.75(5)
<i>Z</i>	4	4	2	2	2	2	2
<i>T</i> (K)	302(2)	302(2)	296(2) K	302(2)	302(2)	302(2)	302(2)
λ (Å)	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
Maximum 2θ (°)	27.613	27.506	27.514	27.501	27.538	27.567	27.537
ρ_{calcd} (g cm ⁻³)	1.822	1.837	1.774	1.787	1.814	1.821	1.837
μ (Mo K α) (mm ⁻¹)	2.037	2.173	1.937	2.065	2.340	2.498	2.642
GoF on F ²	1.078	1.094	1.042	1.045	1.041	1.036	1.042
R ₁ , ^a wR ₂ [I > 2 σ (I)] ^b	0.0551,0.1580	0.0410, 0.0915	0.0382,0.0962	0.0356,0.0842	0.0333,0.0821	0.0323, 0.0816	0.0317,0.0804
R ₁ , ^a wR ₂ (all data) ^b	0.0875,0.1988	0.0501, 0.0974	0.0410,0.0990	0.0400, 0.0876	0.0375,0.0856	0.0339, 0.0830	0.0337,0.0820
($\Delta\rho$) _{max} , ($\Delta\rho$) _{min} /e (Å ⁻³)	1.530, -1.424	1.606, -1.392	1.803, -1.672	1.768, -1.579	1.866, -1.744	1.852, -1.778	1.850, -1.748

Compound	TbTPTZ-2	DyTPTZ-2	HoTPTZ-2	ErTPTZ-2	TmTPTZ-3	YbTPTZ-3	LuTPTZ-3	UTPTZ
Formula Mass	716.35	719.93	722.36	721.67	767.42	771.53	773.46	706.39
Color	Yellow	Yellow	Orange	Orange	Yellow	Yellow	Yellow	Yellow
Habit	Block	Block	Block	Block	Block	Block	Block	Block
Space Group	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1	<i>P</i> 2(1)/ <i>c</i>
<i>a</i> (Å)	9.5688(5)	9.5733(3)	9.5767(2)	9.5825(2)	9.926(2)	9.9111(11)	9.9120(13)	9.345(3)
<i>b</i> (Å)	10.6168(5)	10.6196(3)	10.6201(2)	10.6229(3)	11.740(3)	11.7258(12)	11.7216(16)	19.718(5)
<i>c</i> (Å)	13.6158(7)	13.5996(4)	13.5852(3)	13.5597(3)	12.473(3)	12.4564(13)	12.4564(17)	11.382(3)
α (°)	90.041(2)	90.0780(10)	90.1030(10)	90.0710(10)	95.343(8)	95.469(4)	95.570(5)	90
β (°)	84.944(2)	84.9110(10)	84.9030(10)	84.8310(10)	94.291(8)	94.225(4)	94.166(5)	96.384(9)
γ (°)	69.288(2)	69.1590(10)	69.0670(10)	68.9060(10)	100.894(8)	100.880(4)	100.890(4)	90
<i>V</i> (Å ³)	1288.04(11)	1286.24(7)	1284.56(5)	1281.72(5)	1414.7(5)	1408.9(3)	1408.3(3)	2084.4(9)
<i>Z</i>	2	2	2	2	2	2	2	4
<i>T</i> (K)	280(2)	303(2)	303(2)	288(2)	292(2)	302 (2)	292(2)	283(2)
λ (Å)	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
Maximum 2θ (°)	27.535	27.564	27.506	27.580	27.575	39.307	27.511	27.562
ρ_{calcd} (g cm ⁻³)	1.847	1.859	1.868	1.878	1.802	1.819	1.824	2.251
μ (Mo <i>K</i> α) (mm ⁻¹)	2.820	2.979	3.155	3.349	3.210	3.394	3.580	7.855
GoF on <i>F</i> ²	1.049	1.038	1.039	1.065	1.027	1.046	1.054	1.048
<i>R</i> ₁ , ^{<i>a</i>} <i>wR</i> ₂ [<i>I</i> > 2 σ (<i>I</i>)] ^{<i>b</i>}	0.0323, 0.0828	0.0304, 0.0784	0.0302, 0.0772	0.0323, 0.0798	0.0325, 0.0845	0.0440, 0.0988	0.0316, 0.0826	0.0195, 0.0433
<i>R</i> ₁ , ^{<i>a</i>} <i>wR</i> ₂ (all data) ^{<i>b</i>}	0.0343, 0.0845	0.0323, 0.0800	0.0318, 0.0786	0.0362, 0.0867	0.0342, 0.0861	0.0767, 0.1253	0.0328, 0.0837	0.0282, 0.0476
($\Delta\rho$) _{max} , ($\Delta\rho$) _{min} /e (Å ⁻³)	1.935, -1.755	1.953, -1.723	1.850, -1.770	1.897, -1.809	1.582, -1.501	2.019, -1.932	1.629, -1.512	0.428, -0.723