Phase selectivity and tunable photophysical natures of rare earth metal–organic frameworks of Eu_xY_{1-x} -PTC (H₃PTC = 2, 4, 6-pyridine tricarboxylic acid; x = 0-1)

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compound	$Eu_{0.82}Y_{0.18}$ -PTC	Eu _{0.745} Y _{0.255} -PTC	Eu _{0.66} Y _{0.34} -PTC
empirical formula	$C_{16}H_{16}Eu_{1.64}N_2O_{18}Y_{0.36}$	$C_{16}H_{16}Eu_{1.49}N_2O_{18}Y_{0.51}$	$C_{16}H_{16}Eu_{1.32}N_2O_{18}Y_{0.68}$
CCDC deposit no.	1968497	1968494	1968493
$F_w(g \text{ mol}^{-1})$	805.61	796.09	785.43
crystal system	monoclinic	monoclinic	monoclinic
space group	$P2_1/n$	$P2_1/n$	$P2_1/n$
crystal color	colorless	colorless	colorless
crystal size	0.3×0.2×0.1	0.3×0.2×0.1	0.3×0.2×0.1
temperature (K)	303(2)	306(2)	303(2)
Wavelength (Å)	0.71073	0.71073	0.71073
<i>a</i> (Å)	18.4125(10)	18.3931(12)	18.3854(4)
<i>b</i> (Å)	6.9080(3)	6.9087(5)	6.9070(2)
<i>c</i> (Å)	18.5353(10)	18.5133(12)	18.5103(5)
α (deg)	90	90	90
β (deg)	112.0386(18)	112.056(2)	112.0906(8)
γ (deg)	90	90	90
$V(Å^3)$	2185.31(19)	2180.4(3)	2178.03(10)
Ζ	4	4	4
D_c (g cm ⁻³)	2.449	2.425	2.395
<i>F</i> (000)	1549.0	1535.0	1518.8
$\theta_{\min,\max}(^{\mathrm{o}})$	3.18-27.49	3.18-27.49	3.18-27.48
GOF	1.178	1.104	1.158
$R_1,^{\mathbf{a}} \mathbf{w} R_2^{b} \left[I > 2\sigma(I) \right]$	0.0157, 0.0336	0.0160, 0.0361	0.0150, 0.0316
${}^{a} R_{1} = \sum F_{o} - F_{c} / \sum F_{o} . {}^{b} w R_{2} = \{\sum [w(F_{o}^{2} - F_{c}^{2})^{2}] / \sum [w(F_{o}^{2})^{2}] \}^{1/2}$			

Table S1: Crystallographic data and structure refinement details of Eu_xY_{1-x} -PTC

compound	Eu _{0.55} Y _{0.45} -PTC	Eu _{0.49} Y _{0.51} -PTC	Eu _{0.395} Y _{0.605} -PTC	
empirical formula	$C_{16}H_{16}Eu_{1.10}N_2O_{18}Y_{0.90}$	$C_{16}H_{16}Eu_{0.98}N_2O_{18}Y_{1.02}$	$C_{16}H_{16}Eu_{0.79}N_2O_{18}Y_{1.21}$	
CCDC deposit no.	1968487	1968473	1968463	
$F_w(g \text{ mol}^{-1})$	771.30	763.93	751.66	
crystal system	monoclinic	monoclinic	monoclinic	
space group	$P2_1/n$	$P2_{1}/n$	$P2_1/n$	
crystal color	colorless	colorless	colorless	
crystal size	0.3×0.2×0.1	$0.3\times0.2\times0.1$	$0.3\times0.2\times0.1$	
temperature (K)	301(2)	273(2)	301(2)	
Wavelength (Å)	0.71073	0.71073	0.71073	
<i>a</i> (Å)	18.356(3)	18.3578(7)	18.3663(7)	
<i>b</i> (Å)	6.8895(13)	6.9013(3)	6.8962(3)	
<i>c</i> (Å)	18.502(3)	18.4646(8)	18.4474(7)	
α (deg)	90	90	90	
β (deg)	112.176(7)	112.1571(11)	112.1762(14)	
γ (deg)	90	90	90	
$V(Å^3)$	2166.8(7)	2166.58(16)	2163.67(15)	
Ζ	4	4	4	
$D_c ({ m g}{ m cm}^{-3})$	2.364	2.342	2.307	
<i>F</i> (000)	1497.5	1486.0	1467.4	
$\theta_{\min,\max}(^{o})$	3.18-27.55	1.98-27.56	3.18-27.51	
GOF	1.130	1.047	1.151	
$R_1,^{\mathbf{a}} \mathbf{w} R_2^{b} \left[I > 2\sigma(I) \right]$	0.0216, 0.0410	0.0208, 0.0431	0.0149,0.0326	
${}^{a}R_{1} = \sum F_{o} - F_{c} / \sum F_{o} . {}^{b}wR_{2} = \{\sum [w(F_{o}^{2} - F_{c}^{2})^{2}] / \sum [w(F_{o}^{2})^{2}] \}^{1/2}$				

compound	Eu _{0.285} Y _{0.715} -PTC	Eu _{0.195} Y _{0.805} -PTC	Eu _{0.09} Y _{0.91} -PTC
empirical formula	$C_{16}H_{16}Eu_{0.57}N_2O_{18}Y_{1.43}$	$C_{16}H_{16}Eu_{0.39}N_2O_{18}Y_{1.61}$	$C_{16}H_{16}Eu_{0.18}N_2O_{18}Y_{1.82}$
CCDC deposit no.	1968449	1968480	1968448
$F_w(g \text{ mol}^{-1})$	737.88	726.72	713.35
crystal system	monoclinic	monoclinic	monoclinic
space group	$P2_1/n$	$P2_{1}/n$	$P2_{1}/n$
crystal color	colorless	colorless	colorless
crystal size	0.3×0.2×0.1	$0.3\times0.2\times0.1$	$0.3\times0.2\times0.1$
temperature (K)	301(2)	273(2)	301(2)
Wavelength (Å)	0.71073	0.71073	0.71073
<i>a</i> (Å)	18.329(4)	18.3456(16)	18.3352(9)
<i>b</i> (Å)	6.8971(18)	6.8867(6)	6.8838(4)
<i>c</i> (Å)	18.442(4)	18.3909(16)	18.3844(9)
α (deg)	90	90	90
β (deg)	112.200(9)	112.165(3)	112.22
γ (deg)	90	90	90
$V(Å^3)$	2158.6(8)	2151.8(3)	2148.16(19)
Ζ	4	4	4
$D_c (\text{g cm}^{-3})$	2.270	2.243	2.206
<i>F</i> (000)	1446.4	1429.0	1409.0
$\theta_{\min,\max}(^{o})$	3.18-27.49	1.99-27.55	3.19-27.50
GOF	1.088	1.083	1.074
$R_{1}^{a} W R_{2}^{b} [I > 2\sigma(I)]$	0.0230, 0.0423	0.0231, 0.0494	0.0197,0.0433
$a R_1 = \sum F_0 - F_c /\Sigma$	$\sum F_0 \cdot {}^{b} w R_2 = \{ \sum [w(F_0^2 - F_0^2)] \}$	$(F_{o}^{2})^{2}]/\sum[w(F_{o}^{2})^{2}]\}^{1/2}$	

	Y-I	PTC	
Bond length / Å			
Y1-N2	2.496(4)	Y1-O3	2.376(4)
Y1-05	2.405(4)	Y1-07	2.346(4)
Y1-O10	2.274(4)	Y1-011	2.349(4)
Y1-O12	2.292(4)	Y1-013	2.277(4)
Y2-N1	2.453(5)	Y2-O1	2.373(4)
Y2-O2	2.316(4)	Y2-O3	2.453(4)
Y2-O4	2.466(4)	Y2-O6	2.286(4)
Y2-O8	2.298(4)	Y2-O9	2.319(4)
Bond angles / °			
O3-Y1-N2	64.02(13)	O3-Y1-O5	127.90(12)
O5-Y1-N2	64.12(13)	O7-Y1-N2	126.93(15)
O7-Y1-O3	73.77(14)	O7-Y1-O5	147.82(14)
07-Y1-011	133.74(16)	O10-Y1-N2	73.86(15)
O10-Y1-O3	90.84(14)	O10-Y1-O5	79.69(14)
O10-Y1-O7	76.22(15)	O10-Y1-O11	143.87(16)
O10-Y1-O12	144.97(17)	O10-Y1-O13	79.89(17)
O11-Y1-N2	71.18(15)	O11-Y1-O3	82.01(13)
O11-Y1-O5	77.21(14)	O12-Y1-N2	139.09(16)
O12-Y1-O3	95.41(15)	O12-Y1-O5	121.08(16)
O12-Y1-O7	72.61(17)	O12-Y1-O11	71.15(17)
O13-Y1-N2	131.34(15)	O13-Y1-O3	156.98(15)
O13-Y1-O5	71.42(14)	O13-Y1-O7	83.53(15)
O13-Y1-O11	117.60(16)	O13-Y1-O12	81.10(17)
O3-Y2-N1	118.66(14)	N1-Y2-O4	71.63(14)
01-Y2-N1	64.70(14)	O1-Y2-O3	119.59(13)
O1-Y2-O4	79.06(14)	O2-Y2-N1	65.85(15)
O2-Y2-O1	130.36(14)	O2-Y2-O3	81.19(14)
O2-Y2-O4	81.87(15)	O2-Y2-O9	88.11(16)
O3-Y2-O4	52.89(12)	O6-Y2-N1	140.64(16)
O6-Y2-O1	142.77(15)	O6-Y2-O2	82.78(15)
O6-Y2-O3	76.50(13)	O6-Y2-O4	128.70(13)
O6-Y2-O8	76.38(15)	O6-Y2-O9	79.01(15)
O8-Y2-N1	138.71(15)	O8-Y2-O1	74.02(14)
O8-Y2-O2	155.01(15)	O8-Y2-O3	80.67(15)
O8-Y2-O4	100.48(16)	O8-Y2-O9	101.48(16)
O9-Y2-N1	76.90(16)	O9-Y2-O1	85.03(15)
O9-Y2-O3	154.29(15)	O9-Y2-O4	148.39(15)
Eu-PTC			
Bond length / Å			
Eu1-O1	2.4102(17)	Eu1-O2#2	2.5179(16)
			S-6

Table S2: Selected bond length (Å) and bond angle (°) for Y-PTC and Eu-PTC

Eu1-O3	2.3945(17)	Eu1-O9#1	2.4988(17)
Eu1-O10#1	2.5802(18)	Eu1-O13	2.4403(19)
Eu1-O14	2.446(2)	Eu1-O15	2.418(2)
Eu1-N1	2.5473(19)	Eu2-O5	2.3713(17)
Eu2-O6#3	2.4014(17)	Eu2-O7	2.3472(17)
Eu2-O8#4	2.4125(17)	Eu2-O12#4	2.4040(17)
Eu2-O16	2.3818(19)	Eu2-O17	2.4416(19)
Eu2-N2#4	2.515(2)		
Bond angles / °			
O1-Eu1-O2#2	72.68(6)	O1-Eu1-O9#1	101.49(6)
O1-Eu1-O10#1	139.11(6)	O1-Eu1-O13	86.58(7)
01-Eu1-O14	139.58(7)	O1-Eu1-O15	73.68(7)
01-Eu1-N1	63.03(6)	O2#2-Eu1-O10#1	114.84(6)
02#2-Eu1-N1	123.67(6)	O3-Eu1-O1	126.13(6)
O3-Eu1-O2#2	147.01(6)	O3-Eu1-O9#1	121.90(6)
O3-Eu1-O10#1	70.65(6)	O3-Eu1-O13	80.80(6)
O3-Eu1-O14	85.50(7)	O3-Eu1-O15	85.15(7)
03-Eu1-N1	63.28(6)	O9#1-Eu1-O2#2	71.26(6)
O9#1-Eu1-O10#1	51.25(6)	O9#1-Eu1-N1	147.76(6)
D13-Eu1-O2#2	73.08(6)	O13-Eu1-O9#1	138.92(7)
O13-Eu1-O10#1	134.30(6)	O13-Eu1-O14	73.28(7)
D13-Eu1-N1	71.35(6)	O14-Eu1-O2#2	68.10(7)
014-Eu1-O9#1	75.01(7)	O14-Eu1-O10#1	69.67(7)
014-Eu1-N1	135.66(7)	O15-Eu1-O2#2	127.81(7)
)15-Eu1-O9#1	77.82(7)	O15-Eu1-O10#1	71.08(7)
015-Eu1-O13	142.01(7)	O15-Eu1-O14	140.57(8)
D15-Eu1-N1	70.79(7)	N1-Eu1-O10#1	121.34(6)
O5-Eu2-O6#3	73.54(6)	O5-Eu2-O8#4	137.70(6)
05-Eu2-O12#4	82.93(6)	O5-Eu2-O16	79.62(7)
05-Eu2-O17	70.73(7)	O5-Eu2-N2#4	136.36(6)
D6#3-Eu2-O8#4	80.00(6)	O6#3-Eu2-O12#4	86.41(6)
D6#3-Eu2-O17	143.39(7)	O6#3-Eu2-N2#4	77.02(6)
O7-Eu2-O5	137.55(6)	O7-Eu2-O6#3	148.31(6)
O7-Eu2-O8#4	76.64(7)	O7-Eu2-O12#4	91.35(6)
07-Eu2-O16	94.02(7)	O7-Eu2-O17	66.82(7)
D7-Eu2-N2#4	73.74(6)	O8#4-Eu2-O17	133.60(7)
D8#4-Eu2-N2#4	64.54(6)	O12#4-Eu2-O8#4	128.08(6)
D12#4-Eu2-O17	81.61(7)	O12#4-Eu2-N2#4	63.60(6)
D16-Eu2-O6#3	99.15(7)	O16-Eu2-O8#4	72.64(7)
D16-Eu2-O12#4	159.28(7)	O16-Eu2-O17	82.16(8)
D16-Eu2-N2#4	137.06(7)	O17-Eu2-N2#4	125.97(7)
Symmetry codes: #1 x,1/2+y,1/2-z	= 1/2-x, 1/2+y, 3/2-z;	#2 = 1/2-x, -1/2+y, 3/2-z; #3	B = 1-x, 2-y, 1-z; #4 = 1/2-

(herein, the Eu and T site occupation factors are determined by the fer)			
compound	Eu _{0.835} Y _{0.165} -PTC	Eu _{0.745} Y _{0.255} -PTC	Eu _{0.645} Y _{0.355} -PTC
empirical formula	$C_{16}H_{16}Eu_{1.67}N_2O_{18}Y_{0.33}$	$C_{16}H_{16}Eu_{1.49}N_2O_{18}Y_{0.51}$	$C_{16}H_{16}Eu_{1.29}N_2O_{18}Y_{0.71}$
$F_w(g \text{ mol}^{-1})$	807.42	796.07	783.46
crystal system	monoclinic	monoclinic	monoclinic
space group	$P2_1/n$	$P2_1/n$	$P2_1/n$
crystal color	colorless	colorless	colorless
crystal size	0.3×0.2×0.1	0.3×0.2×0.1	0.3×0.2×0.1
temperature (K)	303(2)	306(2)	303(2)
Wavelength (Å)	0.71073	0.71073	0.71073
<i>a</i> (Å)	18.4125(10)	18.3931(12)	18.3854(4)
<i>b</i> (Å)	6.9080(3)	6.9087(5)	6.9070(2)
<i>c</i> (Å)	18.5353(10)	18.5133(12)	18.5103(5)
α (deg)	90	90	90
β (deg)	112.0386(18)	112.056(2)	112.0906(8)
γ (deg)	90	90	90
$V(\text{\AA}^3)$	2185.31(19)	2180.4(3)	2178.03(10)
Ζ	4	4	4
$D_c (\mathrm{g \ cm^{-3}})$	2.454	2.425	2.389
<i>F</i> (000)	1552.0	1535.0	1516.0
$\theta_{\min,\max}(^{\mathrm{o}})$	3.18-27.49	3.18-27.49	3.18-27.48
GOF	1.080	1.053	1.088
R_1 , ^a w $R_2^b [I > 2\sigma(I)]$	0.0171, 0.0404	0.0202, 0.0495	0.0229, 0.0614
^{<i>a</i>} $R_1 = \sum F_o - F_c / \sum F_o $. ^{<i>b</i>} $wR_2 = \{\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2] \}^{1/2}$			

Table S3: Crystallographic data and structure refinement details of Eu_xY_{1-x} -PTC (herein, the Eu and Y site occupation factors are determined by the ICP)

Continue	Table	S 3

$C_{18}Y_{0.88}$ $C_{16}H_{16}Eu_{0.85}N_2O_{18}Y_{1.1}$ 755.72	$C_{16}H_{16}Eu_{0.68}N_{2}O_{18}Y_{1.32}$
755.72	.5 10 10 .000 2 - 18 - 1.52
	745.00
monoclinic	monoclinic
$P2_1/n$	$P2_1/n$
colorless	colorless
0.3 imes 0.2 imes 0.1	$0.3\times0.2\times0.1$
273(2)	301(2)
0.71073	0.71073
18.3578(7)	18.3663(7)
6.9013(3)	6.8962(3)
18.4646(8)	18.4474(7)
90	90
112.1571(11)	112.1762(14)
90	90
2166.58(16)	2163.67(15)
4	4
2.317	2.287
1474.0	1457.0
3.18-27.51	3.18-27.49
1.135	1.107
	0.0283, 0.0778
	1.135 0.0331, 0.0897

compound	$Eu_{0.30}Y_{0.70}$ -PTC	Eu _{0.21} Y _{0.79} -PTC	Eu _{0.08} Y _{0.92} -PTC
empirical formula	$C_{16}H_{16}Eu_{0.60}N_2O_{18}Y_{1.40}$	$C_{16}H_{16}Eu_{0.42}N_2O_{18}Y_{1.58}$	$C_{16}H_{16}Eu_{0.16}N_2O_{18}Y_{1.84}$
$F_w(g \text{ mol}^{-1})$	739.96	728.61	712.22
crystal system	monoclinic	monoclinic	monoclinic
space group	$P2_{1}/n$	$P2_1/n$	$P2_{1}/n$
crystal color	colorless	colorless	colorless
crystal size	0.3×0.2×0.1	$0.3\times0.2\times0.1$	$0.3\times0.2\times0.1$
temperature (K)	301(2)	273(2)	301(2)
Wavelength (Å)	0.71073	0.71073	0.71073
<i>a</i> (Å)	18.329(4)	18.3456(16)	18.3352(9)
b (Å)	6.8971(18)	6.8867(6)	6.8838(4)
<i>c</i> (Å)	18.442(4)	18.3909(16)	18.3844(9)
α (deg)	90	90	90
β (deg)	112.200(9)	112.165(3)	112.22
γ (deg)	90	90	90
$V(Å^3)$	2158.6(8)	2151.8(3)	2148.16(19)
Ζ	4	4	4
$D_c (\text{g cm}^{-3})$	2.277	2.249	2.202
<i>F</i> (000)	1450.0	1432.0	1407.0
$\theta_{\min,\max}(^{o})$	3.18-27.49	1.99-27.55	3.19-27.50
GOF	1.052	1.073	1.087
$R_1,^{\mathrm{a}} \le R_2^{\mathrm{b}} \left[I > 2\sigma(I) \right]$	0.0338, 0.0848	0.0313, 0.0827	0.0246,0.0611
${}^{a}R_{1} = \sum F_{0} - F_{c} /\sum$	$[F_0] \cdot {}^{b}wR_2 = \{\sum [w(F_0^2 - F_c)]$	$^{2})^{2}]/\sum[w(F_{o}^{2})^{2}]\}^{1/2}$	

compound	Eu _{0.06} Y _{0.94} -PTC	Eu _{0.013} Y _{0.987} -PTC		
empirical formula	$C_{16}H_{16}Eu_{0.12}N_2O_{18}Y_{1.88}$	$C_{16}H_{16}Eu_{0.026}N_2O_{18}Y_{1.974}$		
F_w (g mol ⁻¹)	709.69	704.02		
crystal system	monoclinic	monoclinic		
space group	$P2_{1}/n$	$P2_{1}/n$		
crystal color	colorless	colorless		
crystal size	$0.3\times 0.2\times 0.1$	$0.3\times0.2\times0.1$		
temperature (K)	273(2)	296(2)		
Wavelength (Å)	0.71073	0.71073		
<i>a</i> (Å)	18.3079(4)	18.3115(5)		
<i>b</i> (Å)	6.8784(2)	6.8759(1)		
<i>c</i> (Å)	18.3684(4)	18.3669(4)		
α (deg)	90	90		
β (deg)	112.1963(8)	112.2217(9)		
γ (deg)	90	90		
$V(Å^3)$	2166.58(16)	2140.82(8)		
Z	4	4		
$D_c (\text{g cm}^{-3})$	2.201	2.184		
<i>F</i> (000)	1404.0	1395.0		
$\theta_{\min,\max}(^{\mathrm{o}})$	3.19-27.50	3.19-27.49		
GOF	1.051	1.078		
$R_1,^{a} \le R_2^{b} [I > 2\sigma(I)]$	0.0251, 0.0563	0.0284, 0.0581		
${}^{a}R_{1} = \sum F_{o} - F_{c} / \sum F_{o} . {}^{b}wR_{2} = \{\sum [w(F_{o}^{2} - F_{c}^{2})^{2}] / \sum [w(F_{o}^{2})^{2}] \}^{1/2}$				



Figure S1: The connection of Eu1 (purple) and Eu2 (green) in Eu-PTC.



Figure S2: Molar ratio of Eu:Y = x: (1-x) in Eu_xY_{1-x}-PTC.(Samples 1-11 represent x = 0.82-0.013)



Figure S3: IR spectra of (a) Y-PTC (b) Eu-PTC (c) Y-PTC and Eu-PTC (d) Eu_xY_{1-x} -PTC (x = 0.013-1).



Figure S4: TG and DTA curves of (a)Y-PTC (b)Eu-PTC (c, d) Eu_xY_{1-x} -PTC (x = 0.013-0.82).



Figure S5: The powder X-ray diffraction patterns for (a) Y-PTC (b) Eu-PTC. (a)



Figure S6: Solid-state UV-vis diffuse reflectance spectra of $Eu_x Y_{1-x}$ -PTC (x = 0.013-0.82).



Figure S7: The fine structure of solid-state emission spectra for Y-PTC at 10K excited under UV light at 326 nm.



Figure S8: Eu_xY_{1-x}-PTC (x = 0.013-1) under optimal excitation light with $\lambda = 301$ nm at room temperature.



Figure S9: Images of crystals under UV light (300–380 nm) for Eu_xY_{1-x} -PTC (x = 0.395-1).



Figure S10: Photographs of Eu_xY_{1-x} -PTC under UV light (upper row, $\lambda_{ex} = 254$ nm and lower row, $\lambda_{ex} = 365$ nm) showing different colors owing to the emission spectra being dependent on excited wavelength.







Figure S11: Emission decay of H_3 PTC and all MOFs obtained at room temperature, where the red lines and the black squares represent the fitting curves and the experimental data, respectively.



Figure S12: Excitation and emission spectra of (a) Y-PTC (b) Eu-PTC at ambient condition, excitation spectrum of $Eu_{0.06}Y_{0.94}$ -PTC (c) examined at 443 nm (d) examined at 618 nm.