Electronic supporting information available

Single-component Eu^{3+}-Tb^{3+}-Gd^{3+}-grafted polymer with ultra-high color rendering index white-light emission

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Supporting information

X-ray Crystallography. Single crystals of complex monomer $[Gd(TTA)_3(4\text{-VB-PBI})]$ (**4**) of suitable dimensions were mounted onto thin glass fibers. All the intensity data were collected on a Bruker SMART CCD diffractometer ((Mo-Kα radiation and $\lambda = 0.71073$ Å) in Φ and ω scan modes. Structures were solved by direct methods followed by difference Fourier syntheses, and then refined by full-matrix least-squares techniques against F^2 using SHELXTL.[1] All other non-hydrogen atoms were refined with anisotropic thermal parameters. Absorption corrections were applied using SADABS.[2] All hydrogen atoms were placed in calculated positions and refined isotropically using a riding model. Crystallographic data and selected atomic distances and bond angles are presented in Tables 1-2S, respectively. CCDC reference number 1494131 for **4**.

Synthesis of PMMA in activation with AIBN. To a solution of MMA (9.5 mmol, 1 mL) in dry THF (30 mL), AIBN initiator (1.5 mol% of MMA) was added, and the resultant

mixture was heated to 60 °C with continuous stirring for 48 h under a reduced N_2 atmosphere. The reaction mixture remained clear throughout the polymerization process. After cooling to RT, each viscous mixture was diluted with dry THF (20 mL) and precipitated with absolute diethyl ether (50 mL) three times. The resulting solid product was collected by filtration and dried at 45 °C under vacuum to constant weight. For PMMA: Yield: 92%. FT-IR (KBr, cm^{-1}): 3002 (w), 2951 (m), 2841 (w), 1732 (s), 1639 (m), 1602 (m), 1484 (w), 1454 (w), 1432 (w), 1398 (m), 1384 (m), 1335 (w), 1267 (w), 1237 (w), 1138 (vs), 992 (m), 914 (w), 841 (m), 809 (w), 751 (m), 617 (w), 545 (w), 513 (w), 484 (w). ^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) 3.57 (s, 3H, -COOMe), 1.85 (b, 2H, -CH_2), 0.95-0.75 (m, 3H, -CH_3).

References

1 G. M. Sheldrick, *SHELXL-97: Program for crystal structure refinement*, Göttingen, Germany, 1997.

2 G. M. Sheldrick, *SADABS*, University of Göttingen, 1996.

Table 1S. Crystal data and structure refinement for complex monomer **4**

Compound	**4**
Empirical formula	$C_{45}H_{29}F_9GdN_3O_6S_3$
Formula weight	1132.14
Crystal size/mm	0.31 × 0.27 × 0.25
T/K	293(2)
λ/Å	0.71073
Crystal system	triclinic
Space group	*P-1*
a/Å	9.6659(19)
b/Å	10.381(2)
c/Å	23.145(5)
α/°	82.71(3)
β/°	81.94(3)
γ/°	83.31(3)
V/Å^3	2269.3(8)
Z	2
ρ/g·cm^{-3}	1.657
μ/mm^{-1}	1.688
F(000)	1122
Data/restraints/parameters	7978/7/604
Quality-of-fit indicator	1.056
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0564$
	$wR_2 = 0.1389$
R indices (all data)	$R_1 = 0.0811$
	$wR_2 = 0.1476$

Table 2S. Selected bond lengths (Å) and bond angles (°) in complex monomer **4**

4			
Gd(1)-O(1)	2.355(5)	Gd(1)-O(2)	2.367(4)
Gd(1)-O(3)	2.334(4)	Gd(1)-O(4)	2.337(4)
Gd(1)-O(5)	2.352(4)	Gd(1)-O(6)	2.367(4)
Gd(1)-N(1)	2.602(6)	Gd(1)-N(2)	2.525(5)
C(44)-C(45)	1.2996(12)		
O(1)-Gd(1)-O(2)	72.01(15)	O(3)-Gd(1)-O(4)	72.45(16)
O(5)-Gd(1)-O(6)	72.25(15)	N(1)-Gd(1)-N(2)	63.19(18)

Table 3S. GPC data of the samples of PMMA, **Poly(MMA-*co*-1)**, **Poly(MMA-*co*-2)**, **Poly(MMA-*co*-3)**, **Poly(MMA-*co*-4)** and **Poly(MMA-*co*-2-*co*-3-*co*-4)**

Sample	Monomer	MMA / Monomer	M_n[a]/g·mol	PDI[b]
PMMA	MMA	**-**	42187	1.16
Poly(MMA-*co*-1)	MMA and **1**	200:1	20721	1.25
Poly(MMA-*co*-2)	MMA and **2**	100:1	12914	1.38
Poly(MMA-*co*-2)	MMA and **2**	200:1	19795	1.26
Poly(MMA-*co*-2)	MMA and **2**	400:1	34216	1.19
Poly(MMA-*co*-2)	MMA and **2**	600:1	38814	1.18
Poly(MMA-*co*-3)	MMA and **3**	100:1	12868	1.37
Poly(MMA-*co*-3)	MMA and **3**	200:1	19678	1.25
Poly(MMA-*co*-3)	MMA and **3**	400:1	34383	1.20
Poly(MMA-*co*-3)	MMA and **3**	600:1	39015	1.17
Poly(MMA-*co*-4)	MMA and **4**	200:1	19712	1.23
Poly(MMA-*co*-2-*co*-3-*co*-4)	MMA, **2**, **3** and **4**	200:1[**2**/**3**/**4** = 1:7:4]	19664	1.24
Poly(MMA-*co*-2-*co*-3-*co*-4)	MMA, **2**, **3** and **4**	200:1[**2**/**3**/**4** = 1:7:8]	19688	1.22
Poly(MMA-*co*-2-*co*-3-*co*-4)	MMA, **2**, **3** and **4**	200:1[**2**/**3**/**4** = 1:7:12]	19725	1.21

[a]M_n is number average molecular weight.

[b]PDI = M_w/M_n, where M_w is weight average molecular weight.

Figure 1S. ^{1}H NMR spectra of 4-VP-PBI, complex monomer **1** and **Poly(MMA-*co*-1)** (200:1) in DMSO-δ_6 at room temperature.

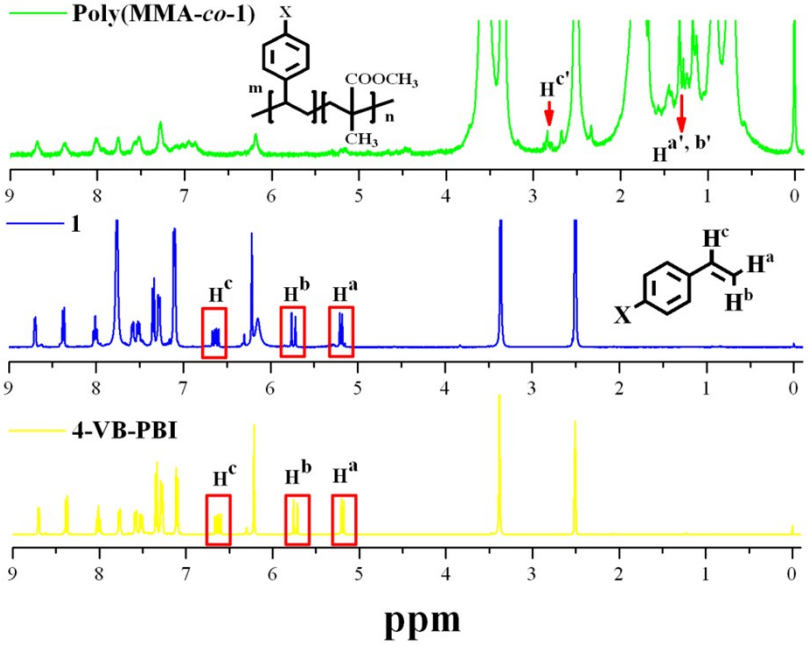

Figure 2S. UV-visible absorption spectra of ligands HTTA and 4-VP-BPI and complex monomers **2**-**4** in MeCN at 2 × 10^{-5} M at room temperature.

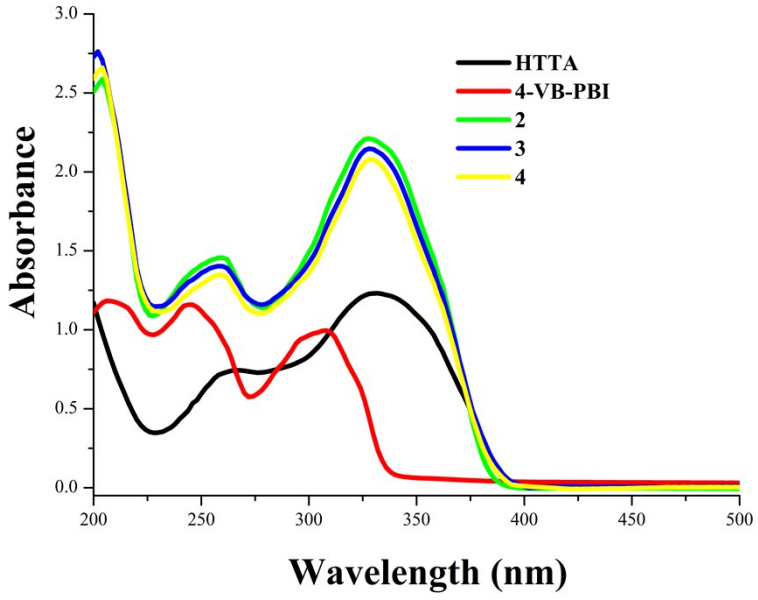

Figure 3S. Schematic energy level diagram and energy transfer process of Eu^{3+} or Tb^{3+} ion for complex monomers **2-4** in solution.

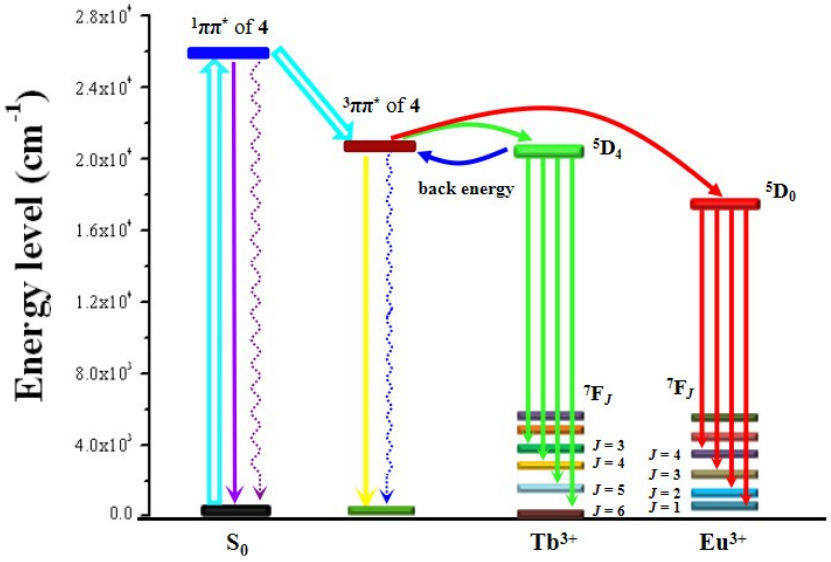

Figure 4S. Emission and excitation spectra of PMMA and **Poly(MMA-*co*-4)** (200:1) in solid state at room temperature.