

Supporting Information

Two new luminescence cadmium coordination polymers constructed by 4,4'-di(4H-1,2,4-triazol-4-yl)-1,1'-biphenyl and polycarboxylic acids: Syntheses, Structures, Fe³⁺ identifying and photo-degradable properties

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Table S1 Selected bond distances (Å) and angles (°) for **CP 1**

1			
Cd(1)-O(3)#2	2.2357(19)	O(13)-Cd(1)-O(5)#3	103.98(8)
Cd(1)-O(1)	2.258(2)	N(2)-Cd(1)-O(5)#3	78.39(7)
Cd(1)-O(13)	2.360(3)	O(6)#3-Cd(1)-O(5)#3	51.89(6)
Cd(1)-N(2)	2.373(2)	N(5)-Cd(2)-N(8)	164.89(9)
Cd(1)-O(6)#3	2.440(2)	N(5)-Cd(2)-O(14)	82.86(9)
Cd(1)-O(5)#3	2.526(2)	N(8)-Cd(2)-O(14)	83.48(9)
Cd(2)-N(5)	2.278(2)	N(5)-Cd(2)-O(8)	99.24(9)
Cd(2)-N(8)	2.294(3)	N(8)-Cd(2)-O(8)	88.84(9)
Cd(2)-O(14)	2.319(2)	O(14)-Cd(2)-O(8)	147.33(8)
Cd(2)-O(8)	2.335(2)	N(5)-Cd(2)-O(11)#4	105.04(9)
Cd(2)-O(11)#4	2.354(2)	N(8)-Cd(2)-O(11)#4	88.76(9)
Cd(2)-O(12)#4	2.574(2)	O(14)-Cd(2)-O(11)#4	130.27(8)
Cd(2)-O(7)	2.595(2)	O(8)-Cd(2)-O(11)#4	81.01(7)
Cd(3)-O(16)	2.245(2)	N(5)-Cd(2)-O(12)#4	86.38(10)
Cd(3)-N(3)#5	2.302(2)	N(8)-Cd(2)-O(12)#4	97.71(10)
Cd(3)-O(15)	2.318(2)	O(14)-Cd(2)-O(12)#4	80.50(8)
Cd(3)-O(10)	2.326(2)	O(8)-Cd(2)-O(12)#4	132.09(7)
Cd(3)-O(5)#6	2.382(2)	O(11)#4-Cd(2)-O(12)#4	51.96(7)
Cd(3)-O(9)	2.455(2)	N(5)-Cd(2)-O(7)	85.13(8)
N(3)-Cd(3)#5	2.302(2)	N(8)-Cd(2)-O(7)	89.79(9)
O(3)-Cd(1)#2	2.2357(19)	O(14)-Cd(2)-O(7)	95.55(8)
O(5)-Cd(3)#7	2.382(2)	O(8)-Cd(2)-O(7)	52.58(7)
O(5)-Cd(1)#3	2.526(2)	O(11)#4-Cd(2)-O(7)	133.59(7)
O(6)-Cd(1)#3	2.440(2)	O(12)#4-Cd(2)-O(7)	171.03(8)
O(11)-Cd(2)#8	2.354(2)	O(16)-Cd(3)-N(3)#5	154.98(8)

O(12)-Cd(2)#8	2.574(2)	O(16)-Cd(3)-O(15)	92.56(8)
O(3)#2-Cd(1)-O(1)	100.40(8)	N(3)#5-Cd(3)-O(15)	84.14(9)
O(3)#2-Cd(1)-O(13)	91.03(9)	O(16)-Cd(3)-O(10)	123.07(8)
O(1)-Cd(1)-O(13)	164.94(7)	N(3)#5-Cd(3)-O(10)	79.83(9)
O(3)#2-Cd(1)-N(2)	150.23(8)	O(15)-Cd(3)-O(10)	116.84(7)
O(1)-Cd(1)-N(2)	83.37(8)	N(3)#5-Cd(3)-O(5)#6	74.36(8)
O(13)-Cd(1)-N(2)	81.86(8)	O(15)-Cd(3)-O(5)#6	141.75(7)
O(3)#2-Cd(1)-O(6)#3	82.20(7)	O(10)-Cd(3)-O(5)#6	90.38(8)
O(1)-Cd(1)-O(6)#3	99.65(8)	O(16)-Cd(3)-O(9)	89.20(8)
O(13)-Cd(1)-O(6)#3	91.54(9)	N(3)#5-Cd(3)-O(9)	114.32(8)
N(2)-Cd(1)-O(6)#3	126.62(8)	O(15)-Cd(3)-O(9)	79.17(8)
O(3)#2-Cd(1)-O(5)#3	131.29(7)	O(10)-Cd(3)-O(9)	54.59(8)
O(1)-Cd(1)-O(5)#3	75.77(8)	O(5)#6-Cd(3)-O(9)	138.50(8)

Symmetric codes: #1 -x+1,-y+3,-z+2; #2 -x+1,-y+1,-z+1; #3 -x,-y+1,-z+1; #4 x-1,y,z; #5 -x,-y+2,-z+1; #6 x,y+1,z; #7 x,y-1,z; #8 x+1,y,z

Table S2 Selected bond distances (Å) and angles (°) for **CP 2**

2			
Cd(1)-O(6)#3	2.233(3)	N(2)-Cd(1)-O(7)#3	84.30(12)
Cd(1)-N(2)	2.262(3)	O(4)#4-Cd(1)-O(7)#3	163.09(10)
Cd(1)-O(4)#4	2.287(3)	O(1)-Cd(1)-O(7)#3	77.53(9)
Cd(1)-O(1)	2.360(3)	O(6)#3-Cd(1)-O(2)	85.50(10)
Cd(1)-O(7)#3	2.369(3)	N(2)-Cd(1)-O(2)	167.82(12)
Cd(1)-O(2)	2.448(3)	O(4)#4-Cd(1)-O(2)	78.71(11)
Cd(2)-O(5)#5	2.282(3)	O(1)-Cd(1)-O(2)	54.41(9)
Cd(2)-O(7)#3	2.289(3)	O(7)#3-Cd(1)-O(2)	99.71(11)
Cd(2)-N(4)	2.315(3)	O(5)#5-Cd(2)-O(7)#3	92.45(10)
Cd(2)-O(3)	2.335(3)	O(5)#5-Cd(2)-N(4)	93.37(12)
Cd(2)-O(9)	2.346(3)	O(7)#3-Cd(2)-N(4)	152.74(11)
Cd(2)-O(1)	2.429(3)	O(5)#5-Cd(2)-O(3)	102.56(10)

O(4)-Cd(1)#6	2.287(3)	O(7)#3-Cd(2)-O(3)	110.83(11)
O(5)-Cd(2)#7	2.282(3)	N(4)-Cd(2)-O(3)	93.81(12)
O(6)-Cd(1)#8	2.233(3)	O(5)#5-Cd(2)-O(9)	98.79(11)
O(7)-Cd(2)#8	2.289(3)	O(7)#3-Cd(2)-O(9)	75.58(10)
O(7)-Cd(1)#8	2.369(3)	N(4)-Cd(2)-O(9)	77.23(11)
O(6)#3-Cd(1)-N(2)	106.58(12)	O(3)-Cd(2)-O(9)	157.30(11)
O(6)#3-Cd(1)-O(4)#4	116.77(11)	O(5)#5-Cd(2)-O(1)	169.74(10)
N(2)-Cd(1)-O(4)#4	94.08(13)	O(7)#3-Cd(2)-O(1)	77.68(9)
O(6)#3-Cd(1)-O(1)	128.56(11)	N(4)-Cd(2)-O(1)	96.69(11)
N(2)-Cd(1)-O(1)	116.12(11)	O(3)-Cd(2)-O(1)	78.76(10)
O(4)#4-Cd(1)-O(1)	88.20(10)	O(9)-Cd(2)-O(1)	81.60(10)
O(6)#3-Cd(1)-O(7)#3	79.65(10)		

Symmetric codes: #1 -x+3,-y,-z+3; #2 -x+1,-y,-z; #3 x+1,-y+1/2,z+1/2 ; #4 x,-y+1/2,z+1/2 ; #5 x+1,y,z ; #6 x,-y+1/2,z-1/2 ; #7 x-1,y,z ; #8 x-1,-y+1/2,z-1/2

Synthesis of {4-[4-(1H-1, 2, 4-triazol-1-yl) phenyl] phenyl}-1H-1, 2, 4-tri-azole (L). The past obtained after mixing 4,4'-diaminodiphenyl-y mass methane (0.925 g, 4.66 mmol), 1 equiv) and 1 (2 g, 9.33mmol, 2 equiv) in toluene(25 mL) was stirred vigorously and refluxed for 8 h. The pale yellow solid obtained was filtered, and washed with cold EtOH (1 × 3 mL). The solid was dissolved in hot EtOH (10 mL), treated with a pinch of charcoal and filtered. White crystals obtained was separated and dried under vacuum; yield: 2.10g (75%); mp 262 °C.IR (KBr): 3095 (m), 2775 (m), 1635 (m), 1562 (m), 1523 (s), 1243(s), 1095 (s), 998 (m), 867 (m), 817 (m), 792 (s), 636 cm⁻¹(s). ¹H NMR (300 MHz, DMSO-d₆, 298 K): d = 9.1 (s, 4 H), 7.65 (d, J= 8.5 Hz, 4 H), 7.45 (d, J= 8.5 Hz, 4 H), 4.0 (s, 2 H). ¹³C NMR (75 MHz, DMSO-d₆, 298 K): d = 141.6, 133, 132, 130.2,121.8, 34.8. MS: m/z = 303.04 (M⁺ H⁺).Anal. Calcd for C₁₇H₁₄N₆ (302.34): C, 67.54; H, 4.67; N, 27.80.Found: C, 67.79, H, 5.03, N, 27.36.

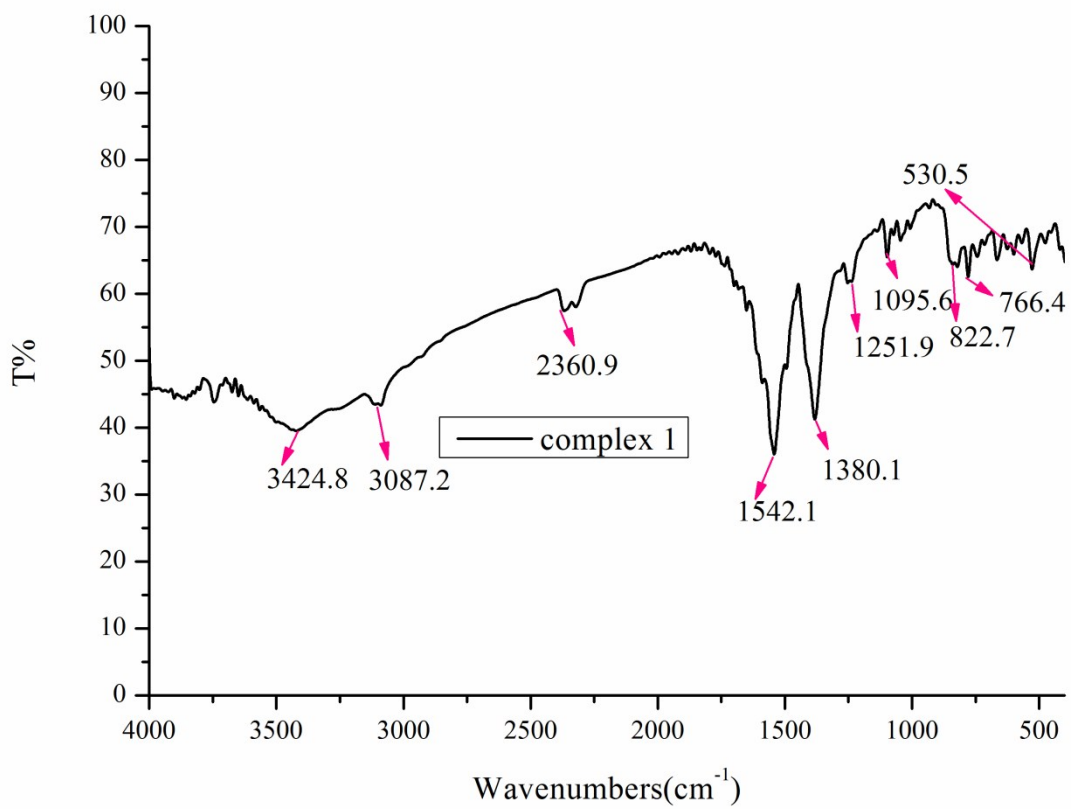


Figure S1 The IR spectra of CP 1

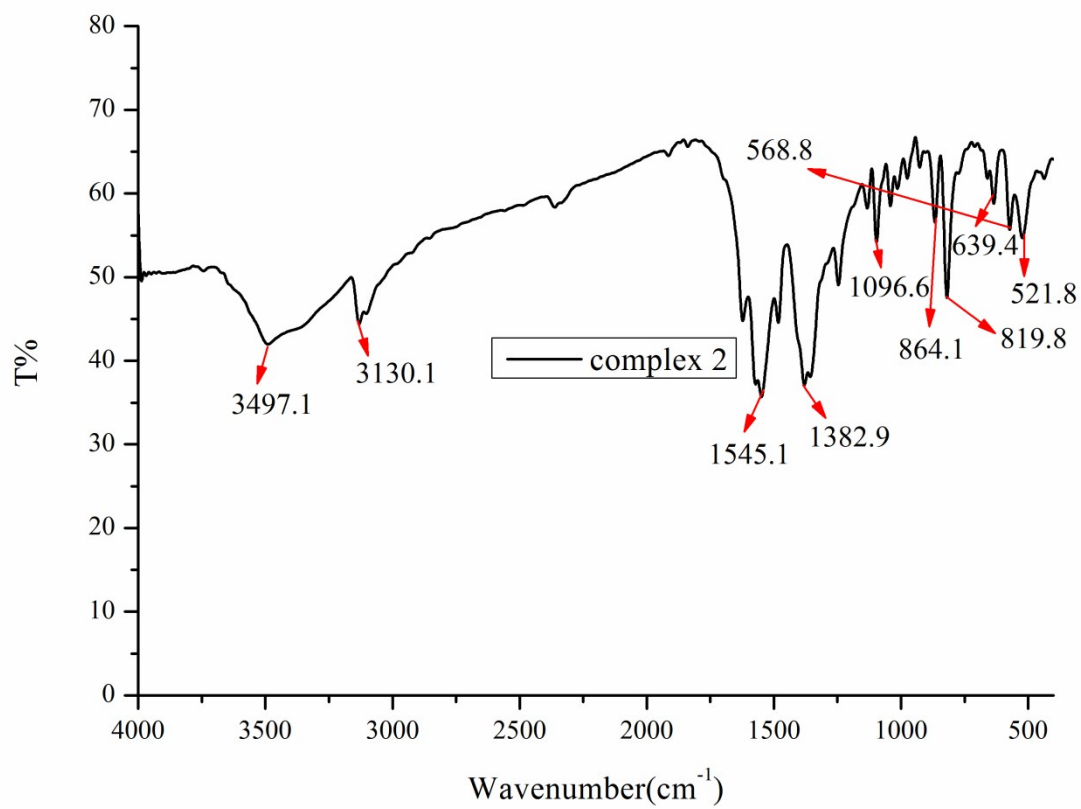


Figure S2 The IR spectra of CP 2

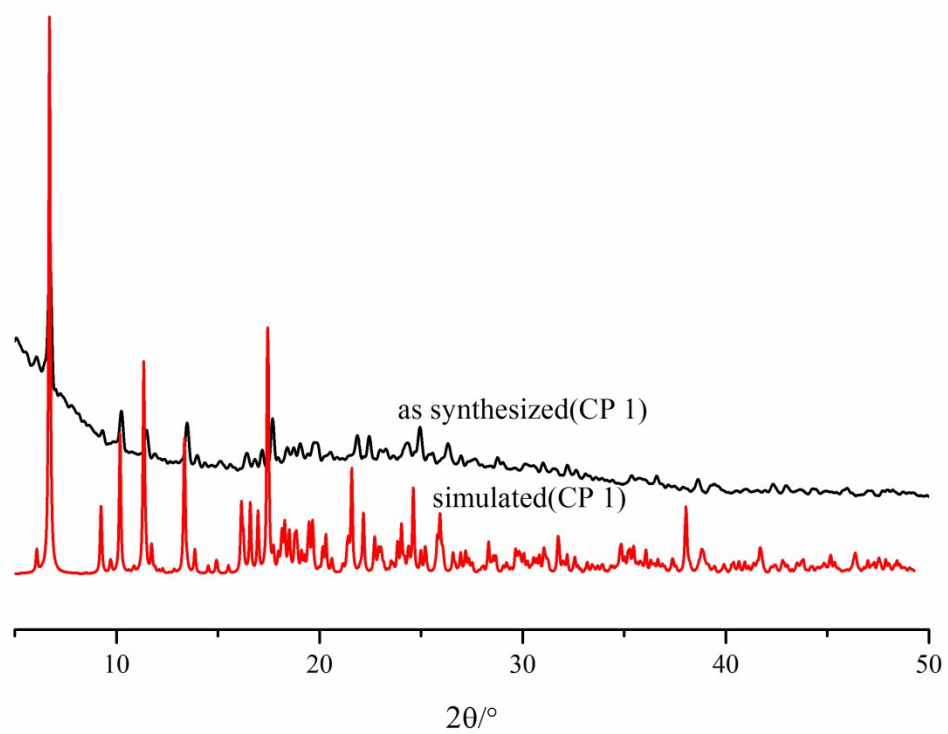


Figure S3 PXRD patterns of CP 1

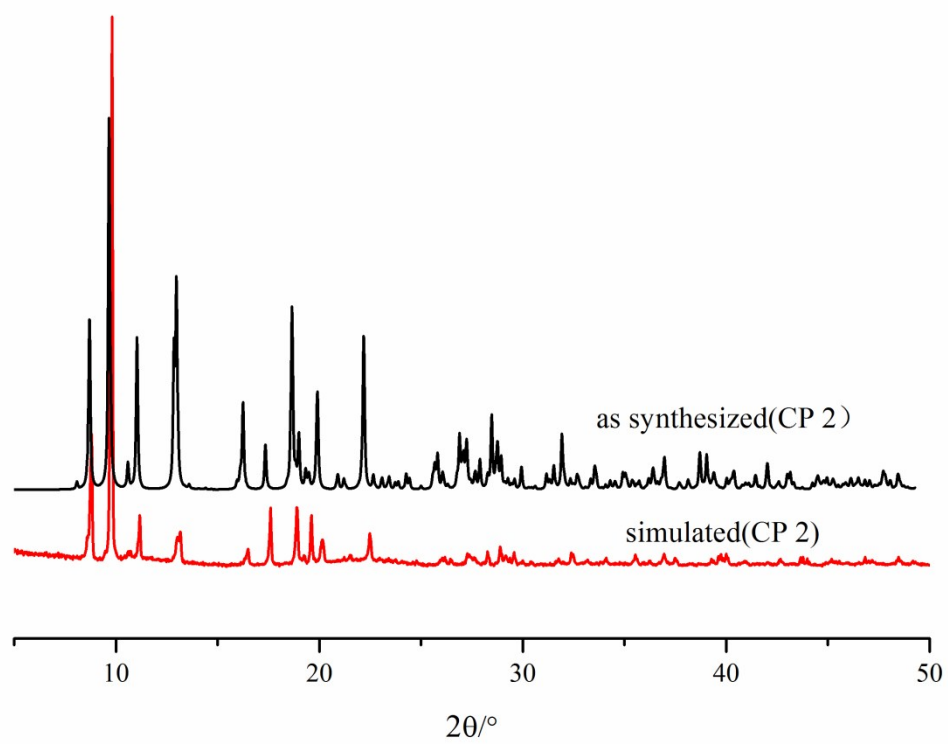


Figure S4 PXRD patterns of CP 2

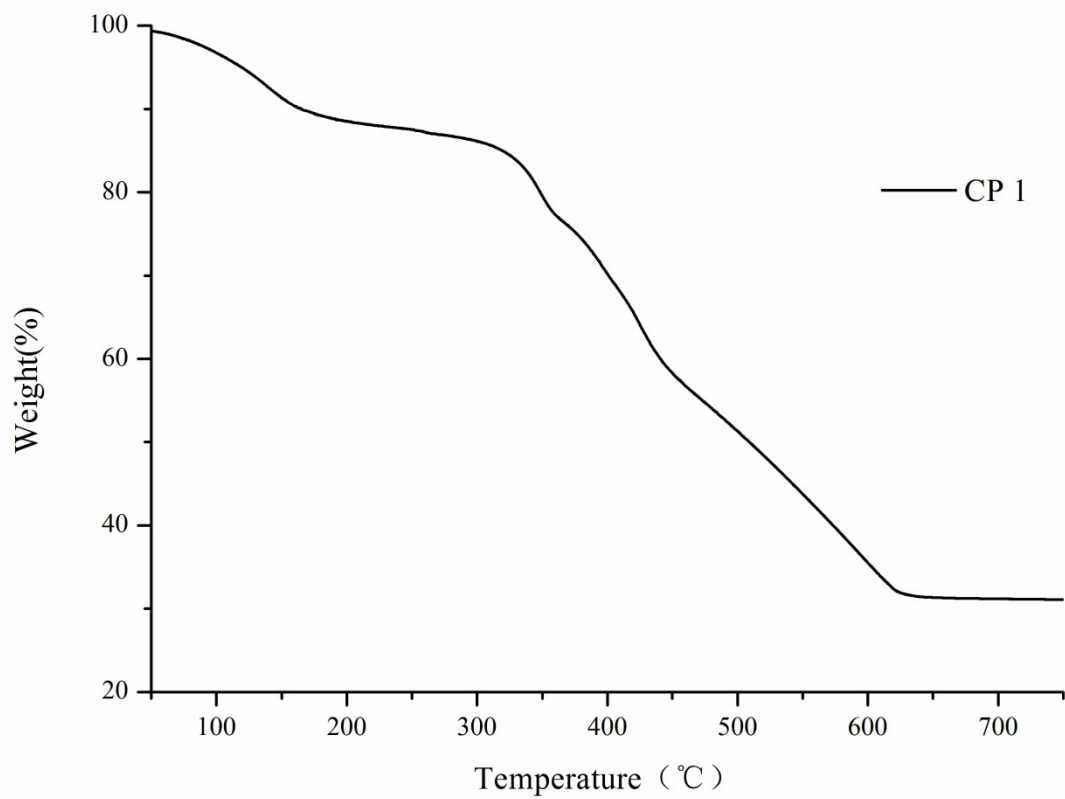


Figure S5 The TGA diagram of CP 1

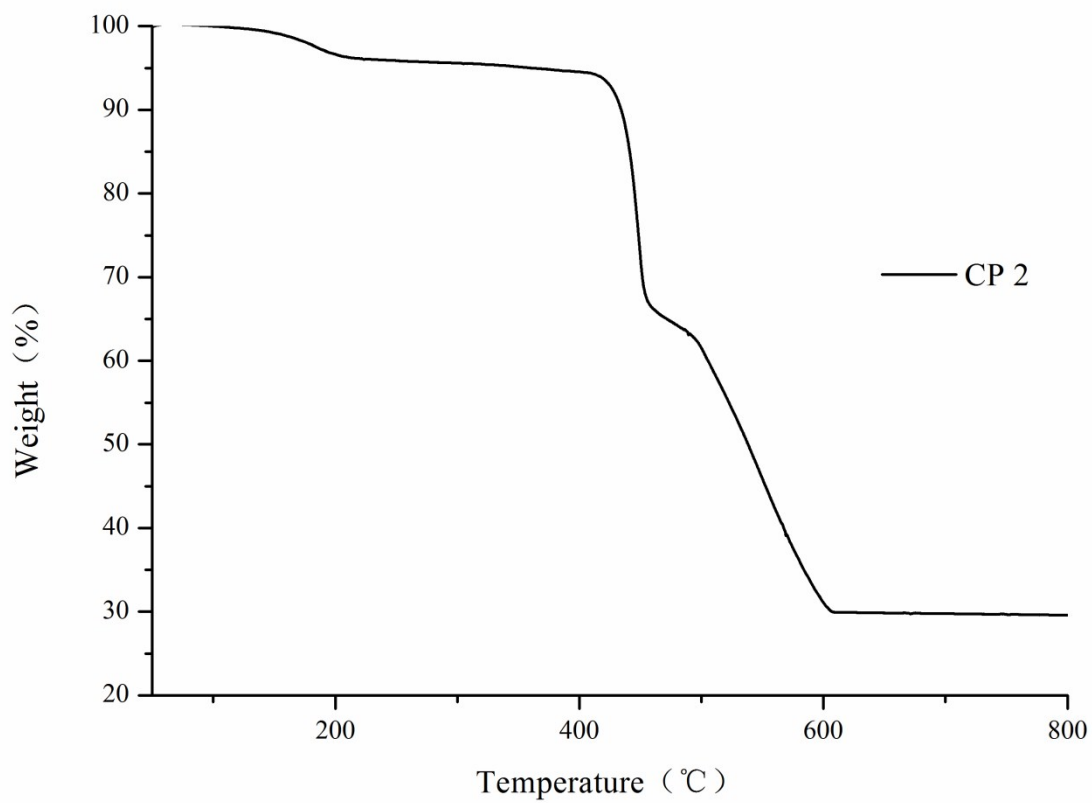


Figure S6 The TGA diagram of CP 2

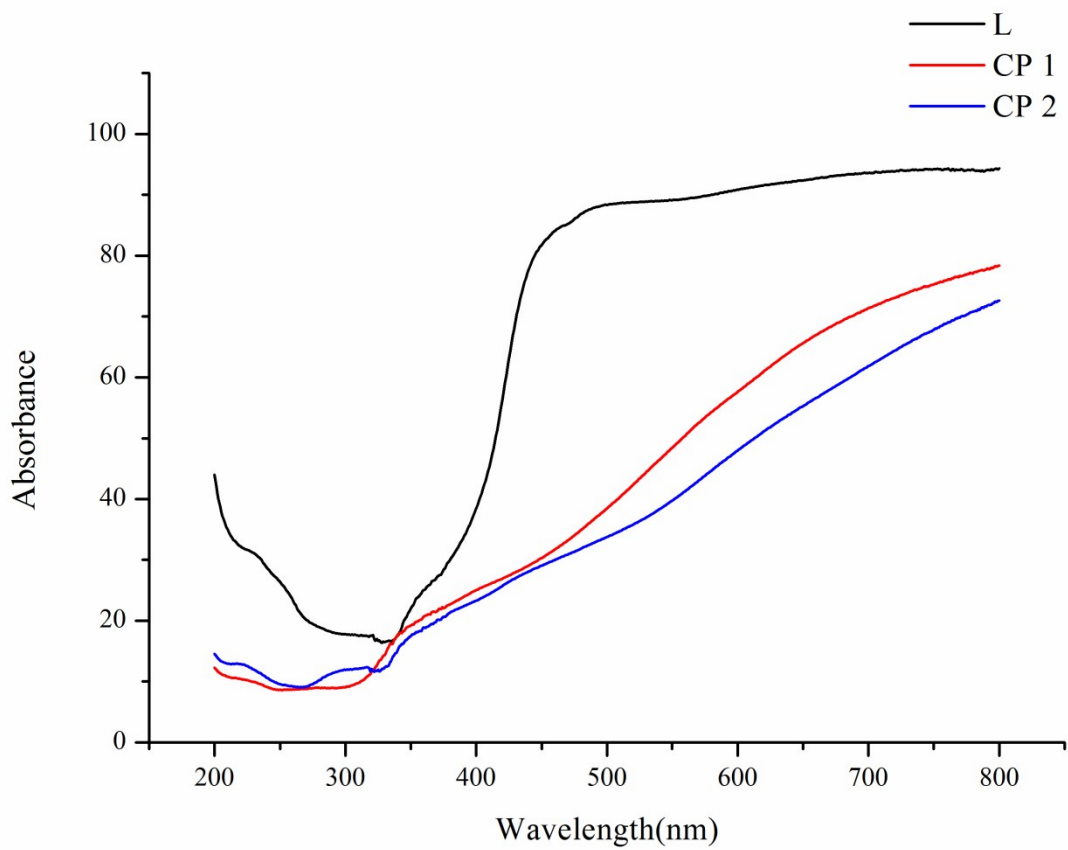


Figure S7 Solid UV of L, CP 1 and CP 2