

## Assembly of a series of coordination polymers built from rigid tetracarboxylate ligand and flexible bis(imidazole) linker: syntheses, structural diversities, luminescence sensing, and photocatalytic properties

Xiu-Tang Zhang,\* Hong-Tai Chen, Bin Li, Guang-Zeng Liu, Xin-Zheng Liu

**Table S1.** Selected bond lengths and bond angles for compounds 1-4.

Compound 1			
N(1)-Zn(1)	N(1)-Zn(1)	N(1)-Zn(1)	N(1)-Zn(1)
O(2)-Zn(1)	O(2)-Zn(1)	O(2)-Zn(1)	O(2)-Zn(1)
O(2)-Zn(1)-N(1)	O(2)-Zn(1)-N(1)	O(2)-Zn(1)-N(1)	O(2)-Zn(1)-N(1)
O(3)-Zn(1)-O(2)	O(3)-Zn(1)-O(2)	O(3)-Zn(1)-O(2)	O(3)-Zn(1)-O(2)
Symmetry transformations used to generate equivalent atoms: #1 -x+3/2,y+1/2,-z+1/2 #2 x-1/2,-y+1/2,z-1/2 #3 -x-1/2,y-1/2,-z+1/2 #4 x+1/2,-y+1/2,z+1/2 #5 -x+3/2,y-1/2,-z+1/2 #6 -x-1/2,y+1/2,-z+1/2.			
Compound 2			
N(1)-Ni(1)	2.107(5)	N(3)-Ni(2)	2.092(5)
N(5)-Ni(2)	2.077(4)	N(7)-Ni(1)	2.092(4)
Ni(1)-O(4)	2.042(3)	Ni(1)-O(1)	2.052(3)
Ni(1)-O(5)	2.082(3)	Ni(1)-O(9)	2.148(4)
Ni(2)-O(2)	2.046(4)	Ni(2)-O(3)	2.058(4)
Ni(2)-O(7)	2.066(4)	Ni(2)-O(9)	2.086(3)
O(4)-Ni(1)-O(1)	95.38(15)	O(4)-Ni(1)-O(5)	173.93(15)
O(1)-Ni(1)-O(5)	88.33(15)	O(4)-Ni(1)-N(7)	88.67(16)
O(1)-Ni(1)-N(7)	173.05(16)	O(5)-Ni(1)-N(7)	88.12(16)
O(4)-Ni(1)-N(1)	87.03(17)	O(1)-Ni(1)-N(1)	87.04(18)
O(5)-Ni(1)-N(1)	88.38(17)	N(7)-Ni(1)-N(1)	98.82(19)
O(4)-Ni(1)-O(9)	94.53(14)	O(1)-Ni(1)-O(9)	89.02(14)
O(5)-Ni(1)-O(9)	90.32(14)	N(7)-Ni(1)-O(9)	85.03(15)
N(1)-Ni(1)-O(9)	175.89(17)	O(2)-Ni(2)-O(3)	96.77(17)
O(2)-Ni(2)-O(7)	175.21(16)	O(3)-Ni(2)-O(7)	87.33(15)
O(2)-Ni(2)-N(5)	87.12(18)	O(3)-Ni(2)-N(5)	85.42(17)
O(7)-Ni(2)-N(5)	90.75(18)	O(2)-Ni(2)-O(9)	91.84(16)
O(3)-Ni(2)-O(9)	88.62(15)	O(7)-Ni(2)-O(9)	90.72(14)
N(5)-Ni(2)-O(9)	173.78(17)	O(2)-Ni(2)-N(3)	87.2(2)
O(3)-Ni(2)-N(3)	176.0(2)	O(7)-Ni(2)-N(3)	88.76(19)
N(5)-Ni(2)-N(3)	95.6(2)	O(9)-Ni(2)-N(3)	90.50(18)
Ni(2)-O(9)-Ni(1)	115.49(14)	Ni(2)-O(9)-H(1W)	114(6)
Ni(1)-O(9)-H(1W)	107(5)		
Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+2,z-1/2 #2 -x+3/2,y,z-1/2 #3 x+1/2,-y+1,z #4 x-1/2,-y+1,z #5 -x+1,-y+1,z-1/2 #6 -x+1,-y+2,z+1/2 #7 -x+3/2,y,z+1/2 #8 x+1/2,-y+2,z #9 -x+1,-y+1,z+1/2 #10 x-1/2,-y+2,z.			
Compound 3			
N(1)-Ni(1)	2.051(4)	N(4)-Ni(1)	2.032(3)

Ni(1)-O(9)	2.033(5)	Ni(1)-O(1)	2.055(3)
Ni(1)-O(4)	2.129(3)	Ni(1)-O(3)	2.212(3)
N(4)-Ni(1)-O(9)	98.00(19)	N(4)-Ni(1)-N(1)	91.23(15)
O(9)-Ni(1)-N(1)	93.75(18)	N(4)-Ni(1)-O(1)	94.44(15)
O(9)-Ni(1)-O(1)	87.03(17)	N(1)-Ni(1)-O(1)	174.11(15)
N(4)-Ni(1)-O(4)	161.22(16)	O(9)-Ni(1)-O(4)	100.78(15)
N(1)-Ni(1)-O(4)	87.19(13)	O(1)-Ni(1)-O(4)	86.93(13)
N(4)-Ni(1)-O(3)	100.83(15)	O(9)-Ni(1)-O(3)	159.57(15)
N(1)-Ni(1)-O(3)	93.69(14)	O(1)-Ni(1)-O(3)	83.71(12)
O(4)-Ni(1)-O(3)	60.65(11)		
Symmetry transformations used to generate equivalent atoms: #1 -x-1,y-1/2,-z #2 -x-1,y+1/2,-z #3 x-1,y,z #4 x+1,y,z.			
<b>Complex 4</b>			
Cd(1)-N(3)	2.233(3)	Cd(1)-N(1)	2.263(3)
Cd(1)-O(3)	2.360(2)	Cd(1)-O(1)	2.371(3)
Cd(1)-O(4)	2.383(2)	Cd(1)-O(2)	2.407(3)
N(3)-Cd(1)-N(1)	104.49(11)	N(3)-Cd(1)-O(3)	89.46(10)
N(1)-Cd(1)-O(3)	134.58(10)	N(3)-Cd(1)-O(1)	124.02(13)
N(1)-Cd(1)-O(1)	120.87(12)	O(3)-Cd(1)-O(1)	81.42(11)
N(3)-Cd(1)-O(4)	131.01(11)	N(1)-Cd(1)-O(4)	85.69(10)
O(3)-Cd(1)-O(4)	54.68(8)	O(1)-Cd(1)-O(4)	86.08(11)
N(3)-Cd(1)-O(2)	101.01(11)	N(1)-Cd(1)-O(2)	88.25(12)
O(3)-Cd(1)-O(2)	131.87(11)	O(1)-Cd(1)-O(2)	53.74(11)
O(4)-Cd(1)-O(2)	127.46(11)		
Symmetry transformations used to generate equivalent atoms: #1 x,-y+3/2,z-1/2 #2 x,-y+3/2,z+1/2 #3 -x-1,y+1/2,-z+1/2 #4 -x-1,-y+1,-z #5 -x-1,y-1/2,-z+1/2.			

**Table S2. The hydrogen bonding data for compounds 3 and 4.**

D-H...A	d(H...A) / [Å]	d(D...A) / [Å]	∠(D-H...A) / [°]
<b>Compound 3</b>			
C31-H31...O5	2.61	3.31	132
C33-H33A...O6	2.64	3.26	122
<b>Compound 4</b>			
C1-H1...O1	2.55	3.46	164
C12-H12...O1	2.42	3.33	165
C4-H4B...O3	2.45	3.22	137
C24-H24...O4	2.71	3.35	127
C11-H11B...O4	2.77	3.39	123

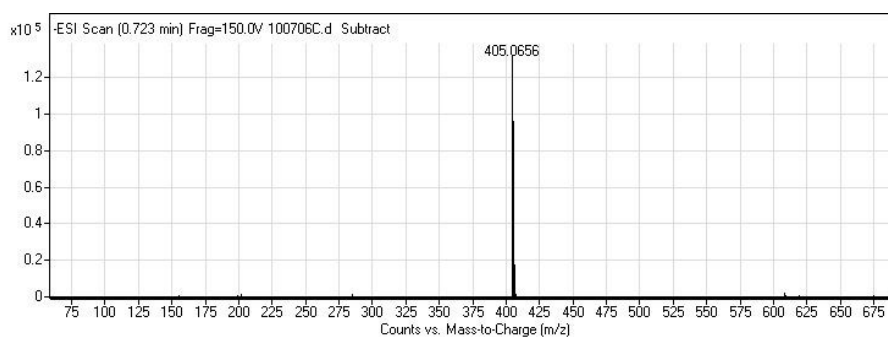


Figure S1. The mass spectrum of the as-synthesized H4tta.

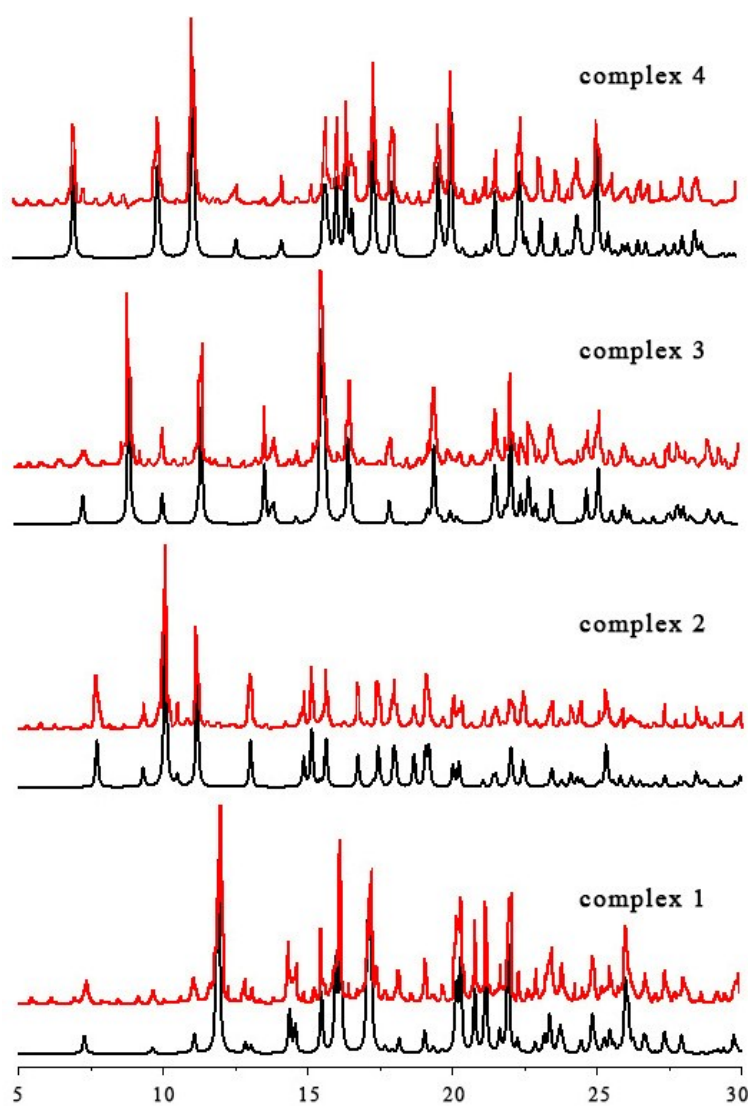


Figure S2. PXRD pattern of compounds 1–4.

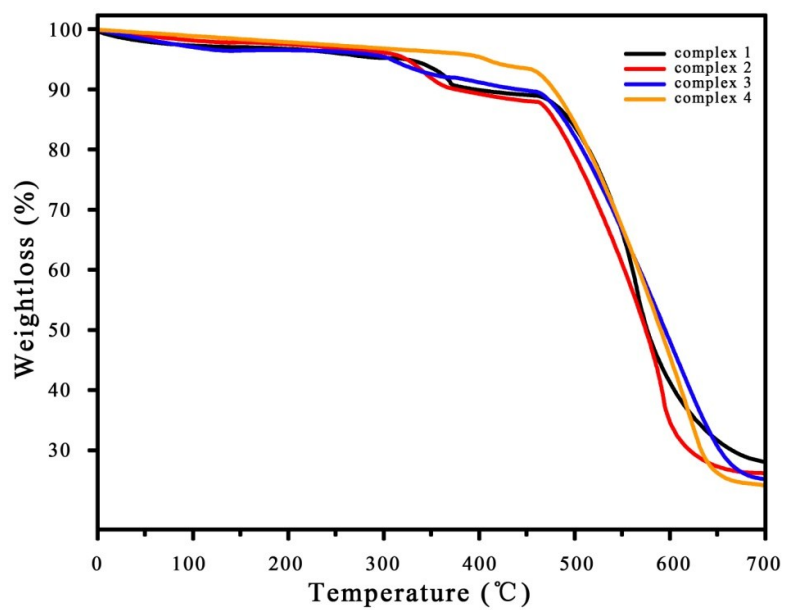


Figure S3. TGA curves for compounds 1–4.

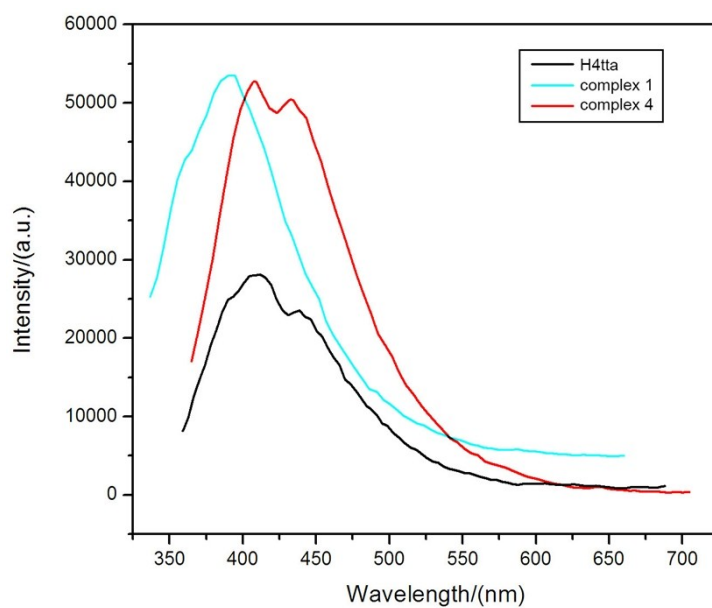
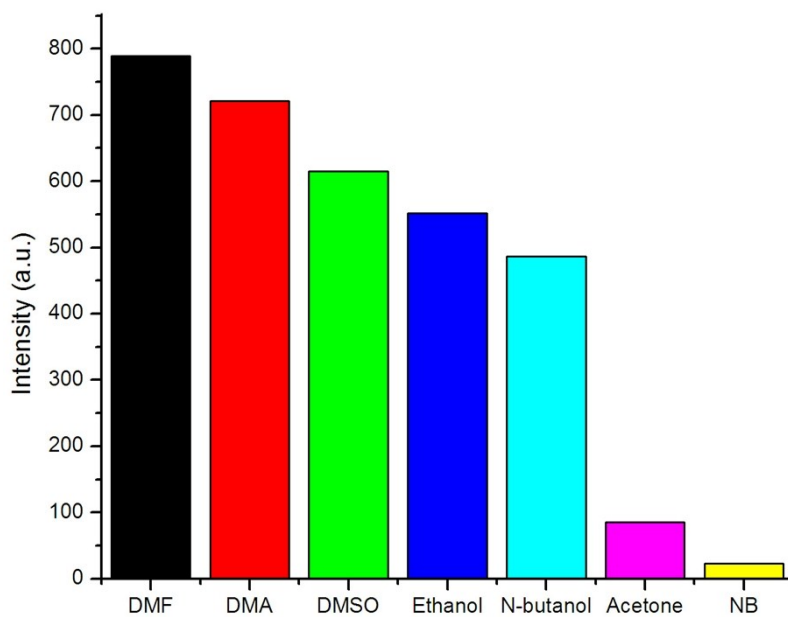
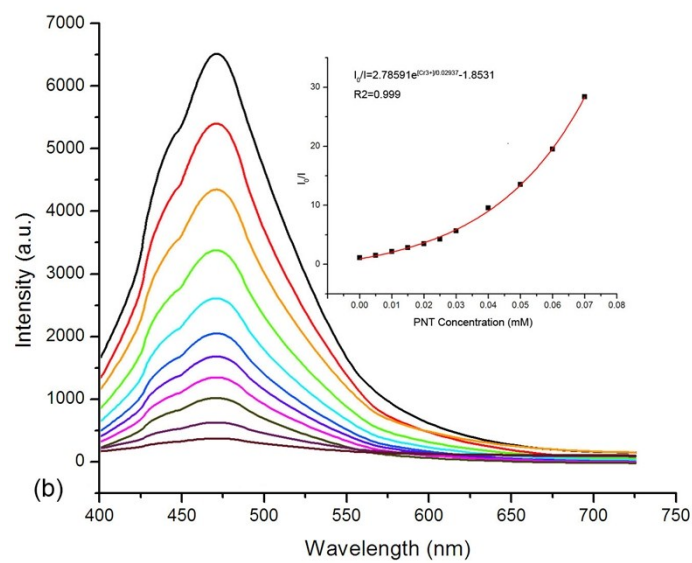
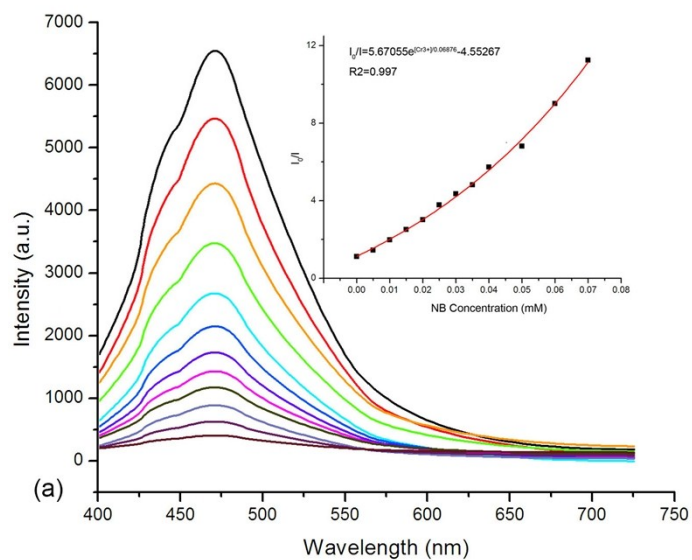


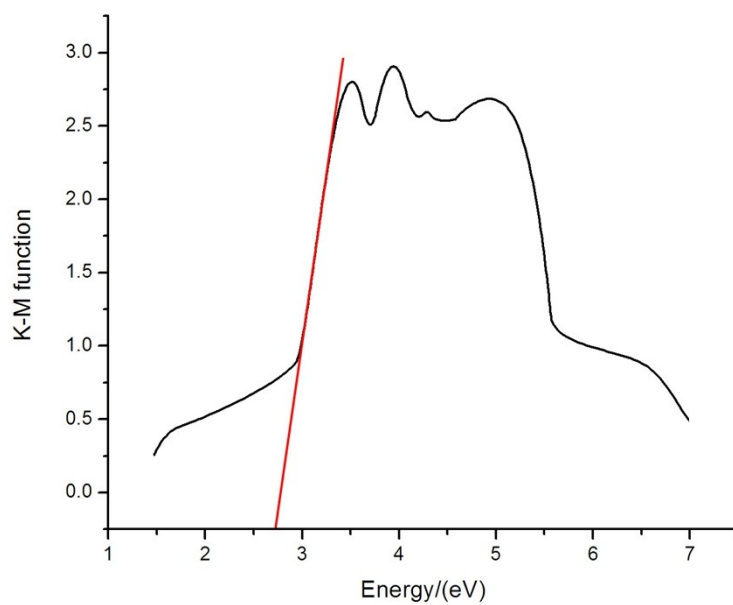
Figure S4. Emission spectra of compounds 1, 4 and H<sub>4</sub>tta ligand in the solid state at room temperature.



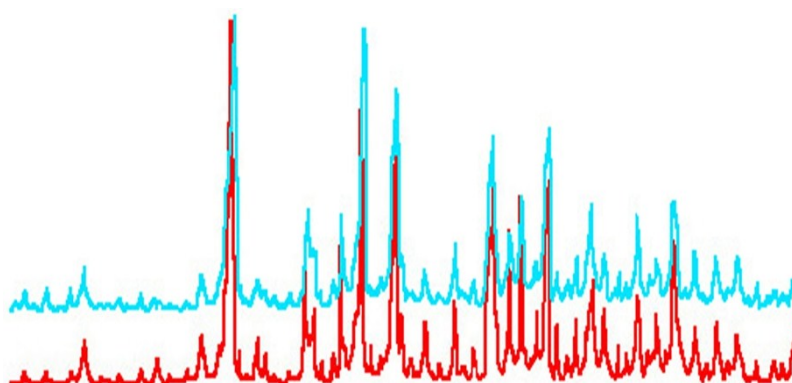
**Figure S5.** The luminescence intensities of compound **1** which were dispersed in different organic solvents.



**Figure S6.** The PL spectra of the DMF suspension of **1** upon incremental addition of NB (a), and PNT (b). Inset: The luminescent intensity ( $I_0/I$ ) versus the NACs concentration.



**Figure S7.** Diffuse reflectance spectra of Kubelka–Munk function versus energy of compound **1**.



**Figure S8.** The PXR D of compound **1** before (red) and after (blue) the photocatalysis.