Supporting Materials

Syntheses, structures and photocatalytic properties of three coordination polymers based on 1,2-bis(1,2,4-triazol-4-yl)ethane and benzenetricarboxylate

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Table S1 Seleted bond lengths and angles for **1**, **2** and **3** (Å and °).

		1	
Cu(1)-O(1)	1.970(5)	Cu(1)-O(5)#2	1.954(5)
Cu(1)-O(7)	2.402(5)	Cu(1)-O(7)#1	1.943(5)
Cu(1)-N(1)	1.951(6)	Cu(2)-O(2)	2.088(5)
Cu(2)-O(4)#3	2.222(5)	Cu(2)-O(7)	1.922(5)
Cu(2)-O(8)	1.944(5)	Cu(2)-N(2)#1	2.098(6)
O(5)#2-Cu(1)-O(1)	94.9(2)	O(1)-Cu(1)-O(7)	103.40(19)
O(7)#1-Cu(1)-O(1)	171.2(2)	N(1)-Cu(1)-O(1)	88.0(2)
O(5)#2-Cu(1)-O(7)	78.69(19)	O(7)#1-Cu(1)-O(5)#2	89.3(2)
N(1)-Cu(1)-O(5)#2	173.8(2)	N(1)-Cu(1)-O(7)	106.0(2)
O(7)#1-Cu(1)-O(7)	84.94(19)	O(7)#1-Cu(1)-N(1)	87.1(2)
O(2)-Cu(2)-O(4)#3	91.5(2)	O(7)-Cu(2)-O(2)	92.2(2)
O(8)-Cu(2)-O(2)	84.4(2)	O(2)-Cu(2)-N(2)#1	168.6(2)
O(7)-Cu(2)-O(4)#3	99.9(2)	O(8)-Cu(2)-O(4)#3	86.7(2)
N(2)#1-Cu(2)-O(4)#3	99.9(2)	O(7)-Cu(2)-O(8)	172.7(2)
O(7)-Cu(2)-N(2)#1	86.6(2)	O(8)-Cu(2)-N(2)#1	95.4(2)
Cu(2)-O(7)-Cu(1)	94.53(19)	Cu(2)-O(7)-Cu(1)#1	124.6(3)
Cu(1)#1-O(7)-Cu(1)	95.06(19)		
		2	
Zn(1)-O(1)	2.102(6)	Zn(1)-O(4)#2	2.227(5)
Zn(1)-O(7)	2.076(6)	Zn(1)-O(7)#1	2.085(6)
Zn(1)-O(8)	2.087(6)	Zn(1)-N(1)	2.146(7)
Zn(2)-O(2)#1	2.052(6)	Zn(2)-O(3)#3	2.062(6)

Zn(2)-O(7)	2.022(5)	Zn(2)-O(9)	2.165(6)
Zn(2)-N(2)	2.071(7)		
O(1)-Zn(1)-O(4)#2	87.9(2)	O(7)-Zn(1)-O(1)	174.9(2)
O(7)#1-Zn(1)-O(1)	92.8(2)	O(8)-Zn(1)-O(1)	83.1(2)
O(1)-Zn(1)-N(1)	92.1(2)	O(7)-Zn(1)-O(4)#2	92.9(2)
O(7)#1-Zn(1)-O(4)#2	83.9(2)	O(8)-Zn(1)-O(4)#2	87.1(2)
N(1)-Zn(1)-O(4)#2	173.1(2)	O(7)-Zn(1)-O(7)#1	82.3(2)
O(7)-Zn(1)-O(8)	102.0(2)	O(7)-Zn(1)-N(1)	87.8(2)
O(7)#1-Zn(1)-O(8)	170.3(2)	O(7)#1-Zn(1)-N(1)	102.9(2)
O(8)-Zn(1)-N(1)	86.1(2)	O(2)#1-Zn(2)-O(3)#3	87.2(2)
O(7)-Zn(2)-O(2)#1	94.1(2)	O(2)#1-Zn(2)-O(9)	85.3(2)
O(2)#1-Zn(2)-N(2)	164.9(3)	O(7)-Zn(2)-O(3)#3	99.7(2)
O(3)#3-Zn(2)-O(9)	87.7(2)	O(3)#3-Zn(2)-N(2)	105.4(2)
O(7)-Zn(2)-O(9)	172.5(2)	O(7)-Zn(2)-N(2)	92.0(2)
N(2)-Zn(2)-O(9)	86.8(3)		

3

Cd(1)-O(1)	2.487(4)	Cd(1)-O(2)	2.286(4)
Cd(1)-O(3)#2	2.277(4)	Cd(1)-O(4)#2	2.567(4)
Cd(1)-O(12)#1	2.269(4)	Cd(1)-N(1)	2.256(4)
Cd(2)-O(5)#2	2.351(4)	Cd(2)-O(13)	2.285(4)
Cd(2)-O(14)	2.251(4)	Cd(2)-O(15)	2.274(4)
Cd(2)-N(2)	2.354(4)	Cd(2)-N(4)	2.317(5)
Cd(3)-O(6)#2	2.229(4)	Cd(3)-O(7)	2.382(4)
Cd(3)-O(8)	2.419(4)	Cd(3)-O(10)#1	2.238(4)
Cd(3)-O(13)	2.524(4)	Cd(3)-N(5)	2.358(4)
O(2)-Cd(1)-O(1)	54.22(14)	O(3)#2-Cd(1)-O(1)	139.33(14)
O(1)-Cd(1)-O(4)#2	126.68(13)	O(12)#1-Cd(1)-O(1)	88.03(14)
N(1)-Cd(1)-O(1)	82.70(16)	O(3)#2-Cd(1)-O(2)	89.30(14)
O(2)-Cd(1)-O(4)#2	83.07(14)	O(12)#1-Cd(1)-O(2)	115.35(15)
N(1)-Cd(1)-O(2)	118.17(17)	O(3)#2-Cd(1)-O(4)#2	53.48(12)
O(12)#1-Cd(1)-O(3)#2	93.51(14)	N(1)-Cd(1)-O(3)#2	135.66(14)
O(12)#1-Cd(1)-O(4)#2	143.37(13)	N(1)-Cd(1)-O(4)#2	93.55(14)
N(1)-Cd(1)-O(12)#1	103.30(16)	O(13)-Cd(2)-O(5)#2	80.43(15)
O(14)-Cd(2)-O(5)#2	84.35(15)	O(15)-Cd(2)-O(5)#2	161.66(16)
O(5)#2-Cd(2)-N(2)	113.92(15)	N(4)-Cd(2)-O(5)#2	84.49(15)
O(14)-Cd(2)-O(13)	158.67(15)	O(15)-Cd(2)-O(13)	107.90(16)
O(13)-Cd(2)-N(2)	87.53(15)	O(13)-Cd(2)-N(4)	80.95(15)
O(14)-Cd(2)-O(15)	91.07(16)	O(14)-Cd(2)-N(2)	85.06(16)
O(14)-Cd(2)-N(4)	112.46(16)	O(15)-Cd(2)-N(2)	83.24(17)
O(15)-Cd(2)-N(4)	80.87(17)	N(4)-Cd(2)-N(2)	156.42(18)
O(6)#2-Cd(3)-O(7)	84.15(14)	O(6)#2-Cd(3)-O(8)	136.77(14)
O(6)#2-Cd(3)-	117.78(15)	O(6)#2-Cd(3)-O(13)	110.87(14)

O(10)#1			
O(6)#2-Cd(3)-N(5)	91.25(16)	O(7)-Cd(3)-O(8)	54.37(13)
O(10)#1-Cd(3)-O(7)	122.21(15)	O(7)-Cd(3)-O(13)	154.08(14)
N(5)-Cd(3)-O(7)	81.23(16)	O(10)#1-Cd(3)-O(8)	81.27(14)
O(8)-Cd(3)-O(13)	112.11(14)	N(5)-Cd(3)-O(8)	93.51(15)
O(10)#1-Cd(3)-O(13)	70.51(14)	O(10)#1-Cd(3)-N(5)	142.61(16)
N(5)-Cd(3)-O(13)	77.57(14)		

Symmetry transformations used to generate equivalent atoms: #1 -x+1, -y+1, -z; #2 -x+2, y-1/2, -z+1/2; #3 -x+1, y-1/2, -z+1/2 for **1**; #1 -x+1, -y+4, -z; #2 -x+1, -y+3, -z; #3 x+1, y+1, z for **2**; #1 -x+1, -y+2, -z ; #2 -x+1, -y+1, -z+1 for **3**.

Table S2 Hydrogen bonds for **1**, **2** and **3** (Å and °).

D-H···A	d(D-H)	d(H···A)	D(D···A)	<(DHA)
		1		
O(7)-H(1W)···O(6)^{i}	0.89(2)	1.87(3)	2.748(7)	167(7)
O(8)-H(2W)···O(9)^{i}	0.877(19)	1.752(19)	2.621(9)	171(5)
O(8)-H(3W)···O(3)^{ii}	0.89(2)	1.72(2)	2.606(7)	171(7)
O(9)-H(4W)···O(6)^{i}	0.91(2)	1.94(4)	2.640(9)	132(4)
O(9)-H(5W)···O(7)	0.91(2)	2.42(6)	3.067(9)	128(6)
		2		
O(7)-H(1W)···O(5)^{i}	0.90(2)	2.13(6)	2.875(8)	138(7)
O(8)-H(2W)···O(5)^{ii}	0.91(2)	1.73(3)	2.609(8)	163(6)
O(8)-H(3W)···O(3)^{i}	0.90(2)	1.80(4)	2.627(8)	151(7)
O(9)-H(4W)···O(8)^{iii}	0.91(2)	2.35(7)	2.968(9)	125(6)
O(9)-H(5W)···O(10)^{iv}	1.019(15)	2.520(16)	3.538(9)	177(6)
O(10)-H(6W)···O(8)^{v}	0.90(2)	2.41(7)	3.098(10)	133(7)
O(10)-H(7W)···O(6)	0.90(2)	1.88(4)	2.751(10)	161(10)
O(11)-H(8W)···O(10)	0.90(2)	2.08(6)	2.918(12)	154(12)
O(11)-H(9W)···O(10)^{vi}	0.90(2)	2.06(5)	2.895(13)	153(10)
		3		
O(13)-H(1W)···O(11)^{i}	0.891(19)	1.92(3)	2.726(5)	149(5)
O(13)-H(2W)···O(17)	0.890(19)	1.78(3)	2.617(7)	156(6)
O(14)-H(3W)···O(16)^{ii}	0.899(19)	1.84(2)	2.706(7)	161(5)
O(14)-H(4W)···O(4)^{iii}	0.886(19)	1.98(4)	2.732(6)	142(6)
O(15)-H(5W)...O(3)^{iv}	0.967(17)	2.069(19)	2.733(6)	124.2(16)
O(15)-H(6W)...O(9)^{v}	0.86(2)	2.05(4)	2.627(6)	123(4)
O(16)-H(7W)...O(4)	0.89(2)	1.98(2)	2.868(6)	173(7)
O(16)-H(8W)...O(3)^{iii}	0.89(2)	2.05(2)	2.921(6)	165(6)
O(17)-H(9W)...O(8)^{v}	0.89(2)	2.40(2)	2.866(7)	1113(2)
O(17)-H(10W)...O(18)	0.90(2)	1.93(3)	2.785(9)	158(6)
O(18)-H(11W)...O(10)^{i}	0.90(2)	2.03(3)	2.896(7)	162(5)
O(18)-H(12W)...O(9)	0.89(2)	2.13(3)	3.011(7)	168(7)

Symmetry transformations used to generate equivalent atoms: i -x+1, y-1/2,- z+1/2; ii -x+2, y-1/2, -z+1/2 for **1**; i -x+1, -y+3, -z; ii x+1, y+1, z; iii x, y+1, z; iv x+1, y+2, z; v x-1, y-1, z; vi -x-1, -y+1, -z-1 for **2**; i -x+1, -y+2, -z; ii x+1, y, z; iii -x+1, -y+1, -z+1; iv -x+2, -y+1, -z+1; v -x+2, -y+2, -z for **3**.

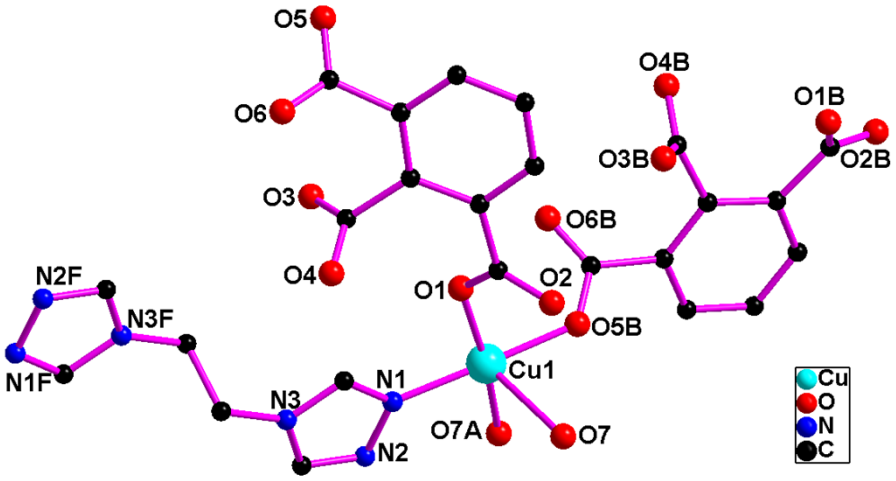

Fig. S1 The coordination environment of Cu1(II) atom in **1**.

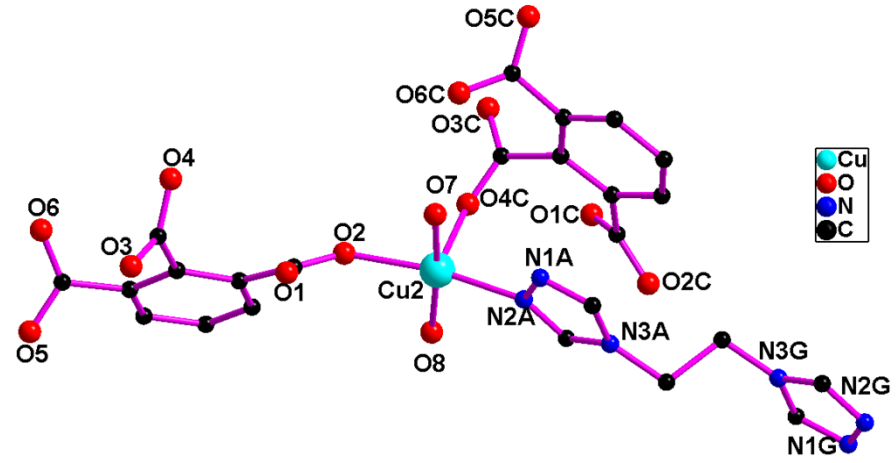

Fig. S2 The coordination environment of Cu2(II) atom in **1**.

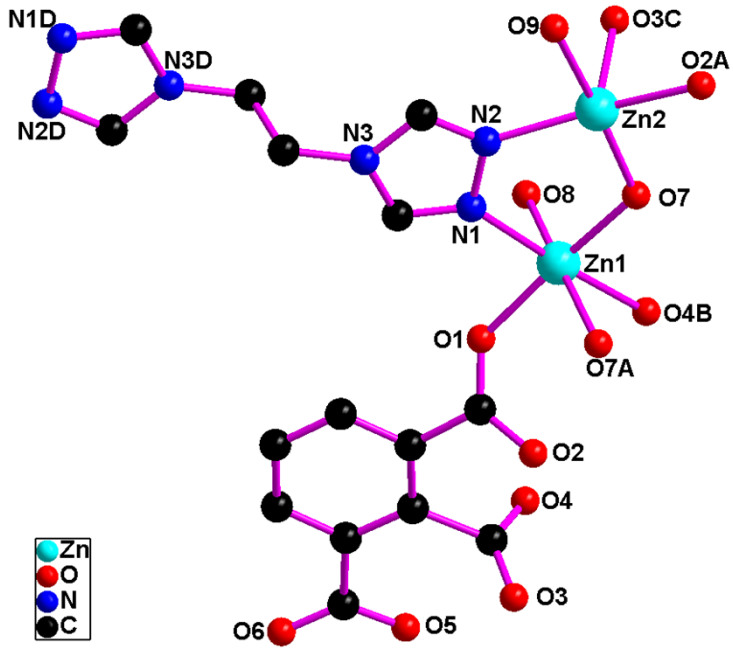

Fig. S3 The coordination environment of Zn(II) atoms in **2**.

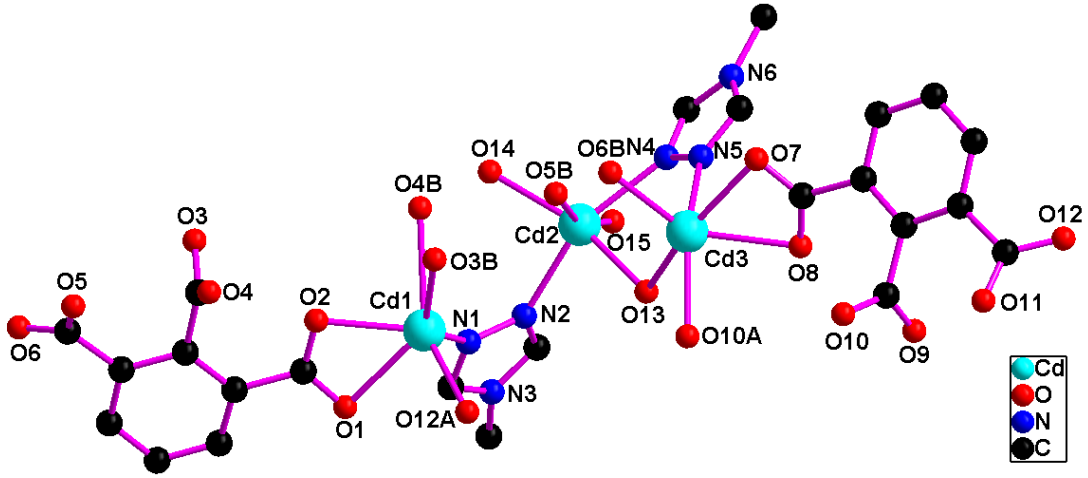

Fig. S4 The coordination environment of Cd(II) atoms in **3**.

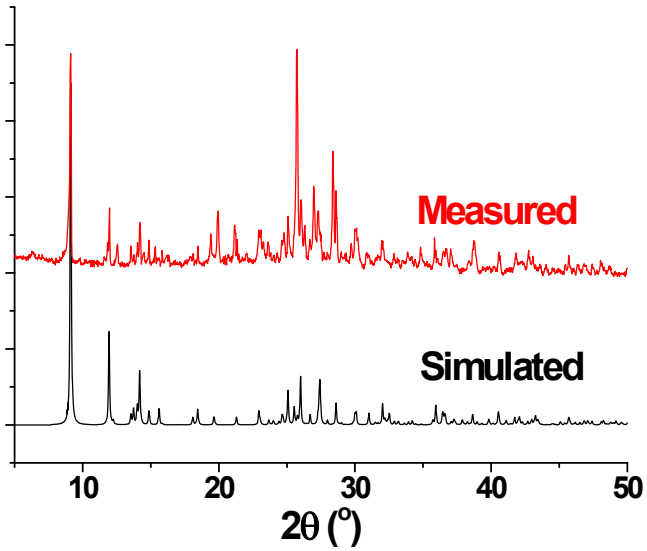

Fig. S5 PXRD patterns of the measured and simulated diagram from single crystal data of **1**.

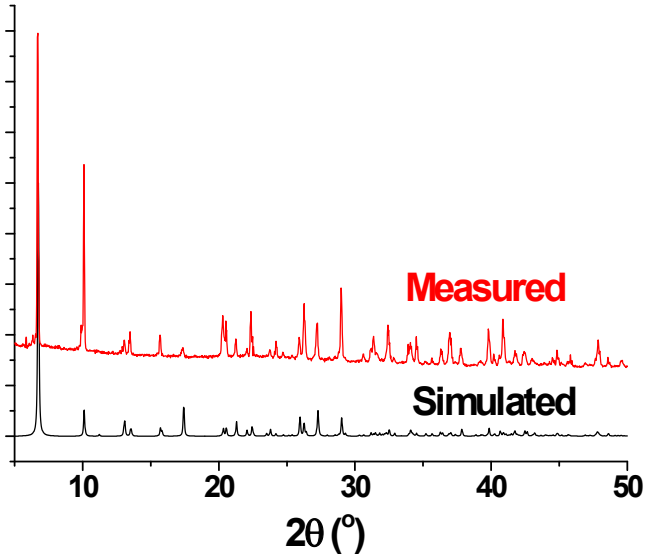

Fig. S6 PXRD patterns of the measured and simulated diagram from single crystal data of **2**.

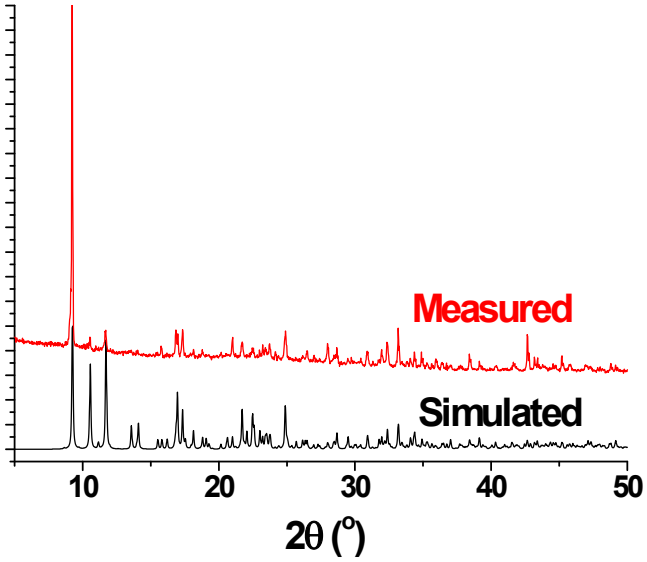

Fig. S7 PXRD patterns of the measured and simulated diagram from single crystal data of **3**.

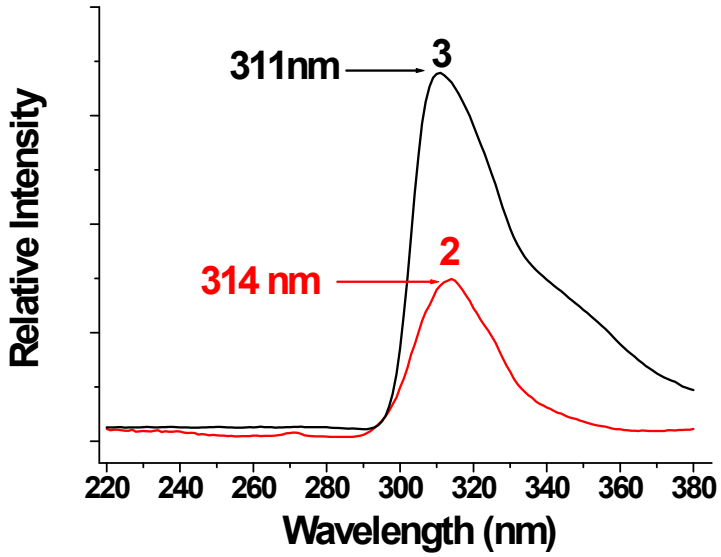

Fig. S8 The excitation spectra of **2** and **3** in the solid state at room temperature.