Construction of d^{10} metal coordination polymers based on *in situ* formed 3,5-di(1H-1,2,4-triazol-1-yl)benzoic acid from different precursors: influence of *in situ* hydrolysis reactions on assembly process

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Supporting information

Table S**1** Selected bond lengths [Å] and angles[°] for the compounds **1**-**7**.[a]

Compound **1**			
Zn(1)-O(1)	1.9415(15)	Zn(1)-N(6)#1	1.9975(17)
Zn(1)-O(3)	1.9445(16)	Zn(1)-N(3)#2	2.0372(17)
O(1)-Zn(1)-O(3)	106.47(7)	O(1)-Zn(1)-N(3)#2	96.18(7)
O(1)-Zn(1)-N(6)#1	120.24(8)	O(3)-Zn(1)-N(3)#2	112.13(7)
O(3)-Zn(1)-N(6)#1	115.48(7)	N(6)#1-Zn(1)-N(3)#2	104.67(7)
Compound **2**			
Cd(1)-O(2)	2.282(3)	Cd(1)-N(6)#3	2.395(3)
Cd(1)-O(2)#1	2.282(3)	Cd(1)-N(1)#4	2.444(3)
Cd(1)-N(6)#2	2.395(3)	Cd(1)-N(1)#5	2.444(3)
O(2)-Cd(1)-O(2)#1	180	N(6)#2-Cd(1)-N(1)#4	88.54(11)
O(2)-Cd(1)-N(6)#2	89.16(14)	N(6)#3-Cd(1)-N(1)#4	91.46(11)
O(2)#1-Cd(1)-N(6)#2	90.84(14)	O(2)-Cd(1)-N(1)#5	103.22(12)
O(2)-Cd(1)-N(6)#3	90.84(14)	O(2)#1-Cd(1)-N(1)#5	76.78(12)
O(2)#1-Cd(1)-N(6)#3	89.16(14)	N(6)#2-Cd(1)-N(1)#5	91.46(11)
N(6)#2-Cd(1)-N(6)#3	180	N(6)#3-Cd(1)-N(1)#5	88.54(11)
O(2)-Cd(1)-N(1)#4	76.78(12)	N(1)#4-Cd(1)-N(1)#5	180
O(2)#1-Cd(1)-N(1)#4	103.22(12)		
Compound **3**			
Cd(1)-O(3)#1	2.282(4)	Cd(1)-O(4)#3	2.320(4)
Cd(1)-O(2)#2	2.288(4)	Cd(1)-N(12)	2.323(4)
Cd(1)-N(6)#3	2.315(4)	Cd(1)-O(1)	2.327(4)
O(3)#1-Cd(1)-O(2)#2	179.81(19)	N(6)#3-Cd(1)-N(12)	179.89(19)
O(3)#1-Cd(1)-N(6)#3	82.45(15)	O(4)#3-Cd(1)-N(12)	84.82(16)
O(2)#2-Cd(1)-N(6)#3	97.50(15)	O(3)#1-Cd(1)-O(1)	99.22(15)
O(3)#1-Cd(1)-O(4)#3	80.95(15)	O(2)#2-Cd(1)-O(1)	80.59(15)
O(2)#2-Cd(1)-O(4)#3	99.24(15)	N(6)#3-Cd(1)-O(1)	85.18(15)
N(6)#3-Cd(1)-O(4)#3	95.12(16)	O(4)#3-Cd(1)-O(1)	179.67(16)
O(3)#1-Cd(1)-N(12)	97.45(16)	N(12)-Cd(1)-O(1)	94.88(16)
O(2)#2-Cd(1)-N(12)	82.60(16)		
Compound **4**			
Cd(1)-N(9)	2.3246(19)	Cd(1)-N(6)#3	2.364(2)
Cd(1)-N(3)	2.328(2)	Cd(1)-O(4)#1	2.4600(18)
Cd(1)-O(3)#1	2.3473(18)	Cd(1)-O(2)#2	2.582(2)
Cd(1)-O(1)#2	2.3526(18)	N(9)-Cd(1)-O(4)#1	90.32(7)
N(9)-Cd(1)-N(3)	176.91(7)	N(3)-Cd(1)-O(4)#1	92.44(8)
N(9)-Cd(1)-O(3)#1	97.17(7)	O(3)#1-Cd(1)-O(4)#1	54.26(6)

N(3)-Cd(1)-O(3)#1	85.58(8)	O(1)#2-Cd(1)-O(4)#1	159.19(7)
N(9)-Cd(1)-O(1)#2	81.64(7)	N(6)#3-Cd(1)-O(4)#1	80.57(7)
N(3)-Cd(1)-O(1)#2	95.29(8)	N(9)-Cd(1)-O(2)#2	94.27(7)
O(3)#1-Cd(1)-O(1)#2	145.60(7)	N(3)-Cd(1)-O(2)#2	84.13(8)
N(9)-Cd(1)-N(6)#3	89.35(8)	O(3)#1-Cd(1)-O(2)#2	93.68(6)
N(3)-Cd(1)-N(6)#3	89.72(8)	O(1)#2-Cd(1)-O(2)#2	52.43(7)
O(3)#1-Cd(1)-N(6)#3	134.22(7)	N(6)#3-Cd(1)-O(2)#2	131.10(7)
O(1)#2-Cd(1)-N(6)#3	80.17(7)	O(4)#1-Cd(1)-O(2)#2	147.95(6)

Compound **5**

Zn(1)-O(2)#1	1.9630(14)	Zn(1)-N(6)	2.0324(15)
Zn(1)-N(3)#2	2.0309(15)	Zn(1)-Cl(1)	2.1948(6)
O(2)#1-Zn(1)-N(3)#2	104.37(7)	O(2)#1-Zn(1)-Cl(1)	127.03(5)
O(2)#1-Zn(1)-N(6)	94.06(6)	N(3)#2-Zn(1)-Cl(1)	106.37(5)
N(3)#2-Zn(1)-N(6)	108.02(7)	N(6)-Zn(1)-Cl(1)	115.42(5)

Compound **6**

Zn(1)-O(2)#1	1.924(2)	Zn(1)-O(3)	2.003(3)
Zn(1)-N(6)#2	1.988(3)	Zn(1)-N(1)	2.032(3)
O(2)#1-Zn(1)-N(6)#2	122.07(12)	O(2)#1-Zn(1)-N(1)	95.00(11)
O(2)#1-Zn(1)-O(3)	104.20(12)	N(6)#2-Zn(1)-N(1)	112.19(12)
N(6)#2-Zn(1)-O(3)	111.32(11)	O(3)-Zn(1)-N(1)	110.77(12)

Compound **7**

Cd(1)-N(1)	2.251(16)	Cd(1)-O(3)	2.34(2)
Cd(1)-N(6)#1	2.283(16)	Cd(1)-O(1W)	2.35(2)
Cd(1)-O(2)#2	2.322(14)	Cd(1)-O(1)#2	2.458(15)
N(1)-Cd(1)-N(6)#1	119.0(6)	O(2)#2-Cd(1)-O(1W)	87.8(8)
N(1)-Cd(1)-O(2)#2	140.7(6)	O(3)-Cd(1)-O(1W)	175.7(8)
N(6)#1-Cd(1)-O(2)#2	99.0(6)	N(1)-Cd(1)-O(1)#2	86.7(5)
N(1)-Cd(1)-O(3)	99.1(7)	N(6)#1-Cd(1)-O(1)#2	153.5(5)
N(6)#1-Cd(1)-O(3)	90.9(7)	O(2)#2-Cd(1)-O(1)#2	54.6(5)
O(2)#2-Cd(1)-O(3)	89.2(7)	O(3)-Cd(1)-O(1)#2	91.4(6)
N(1)-Cd(1)-O(1W)	85.2(8)	O(1W)-Cd(1)-O(1)#2	89.4(8)
N(6)#1-Cd(1)-O(1W)	86.5(8)		

[a]Symmetry transformations used to generate equivalentatoms : #1 x + 1, y, z, #2 x, y - 1, z, #3 x - 1, y, z, #4 x, y + 1, z for compound **1**; #1 -x + 1, -y + 1, -z, #2 -x + 2, y - 1/2, -z + 1/2, #3 x- 1, -y + 3/2, z - 1/2, #4 x, y, z – 1, #5 -x + 1, -y + 1, -z + 1, #6 -x + 2, y + 1/2, -z + 1/2, #7 x, y, z + 1 for compound **2**; #1 x, y, z + 1, #2 x - 1, y, z, #3 x - 1, y, z + 1, #4 x + 1, y, z – 1, #5 x, y, z – 1, #6 x + 1, y, z for compound **3**; #1 -x + 3/2, y - 1/2, - z+ 1/2, #2 -x + 1, y + 1, -z + 1/2, #3 x, -y - 1, z - 1/2, #4 -x + 3/2, y + 1/2, -z + 1/2, #5 -x + 1, y - 1, -z + 1/2, #6 x, -y -1, z + 1/2 for compound 4; #1 -x + 1, -y + 1, -z + 1, #2 -x + 2, y + 1/2, -z + 3/2, #3 -x + 2, y - 1/2, -z + 3/2 for compound **5** ; #1 x - 1, y, z, #2 x - 1/2, -y + 3/2, z + 1/2, #3 x + 1/2, -y + 3/2, z - 1/2, #4 x + 1, y, z for compound **6** ; #1 x + 1, y, z + 1, #2 -x - 1, y + 1/2, -z + 1/2, #3 -x - 1, y - 1/2, -z + 1/2, #4 x - 1, y, z - 1 for compound **7** ;

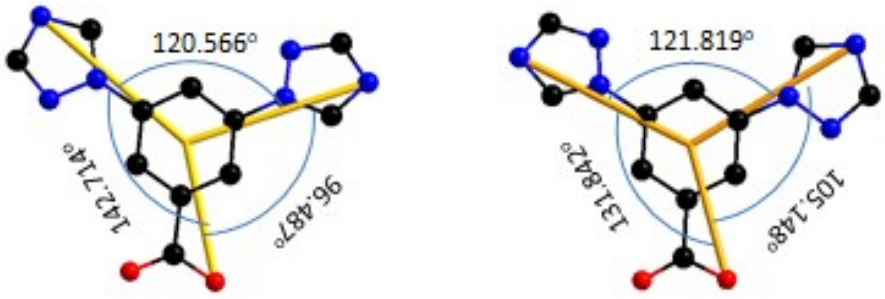

Figure S1. The angles between the center of benzene ring and the three terminal coordination atoms in compounds **5** and **6**.

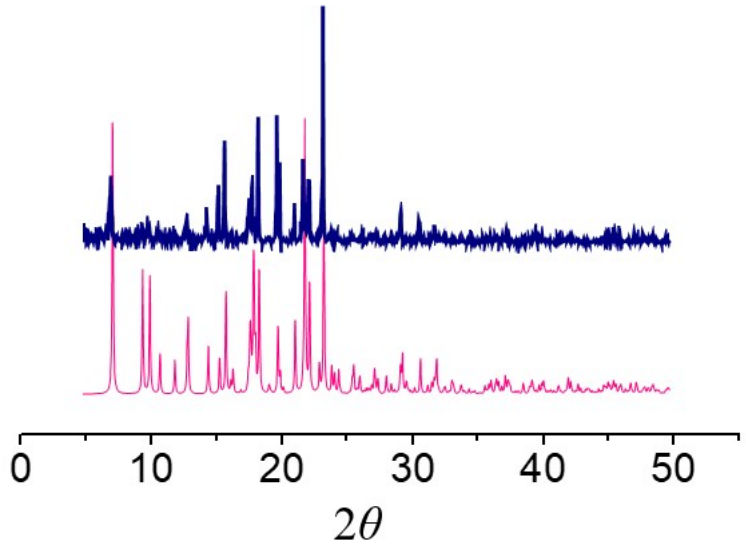

Figure S2. The simulated X-ray powder diffraction patterns (lower) and the measured one (upper) of compound **1**.

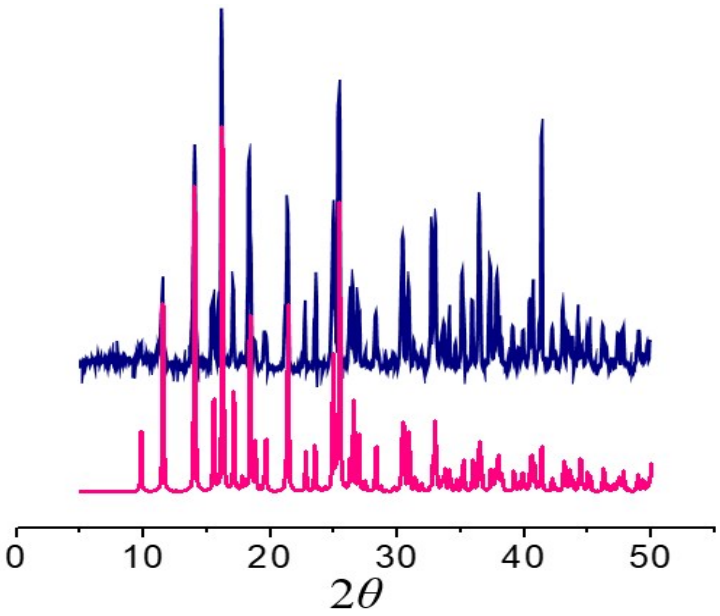

Figure S3. The simulated X-ray powder diffraction patterns (lower) and the measured one (upper) of compound **2**.

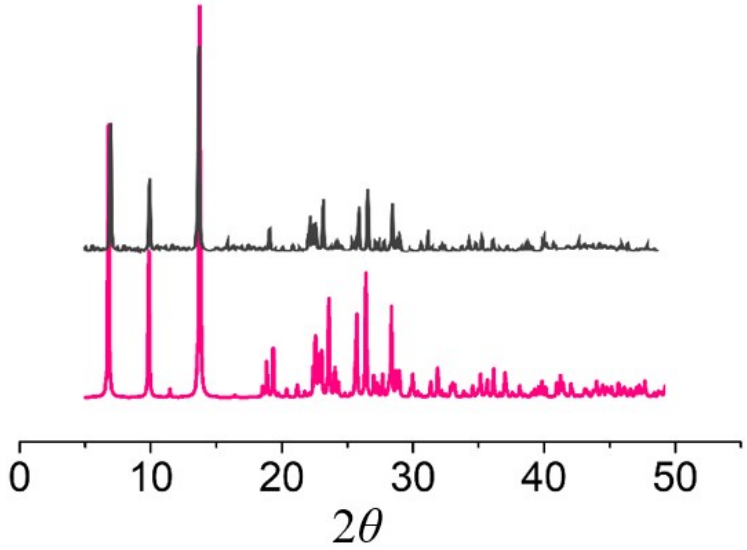

Figure S4. The simulated X-ray powder diffraction patterns (lower) and the measured one (upper) of compound **3**.

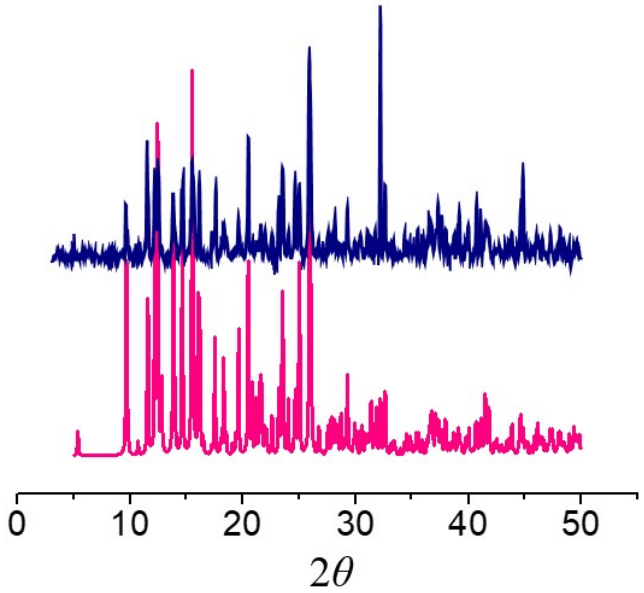

Figure S5. The simulated X-ray powder diffraction patterns (lower) and the measured one (upper) of compound **4**.

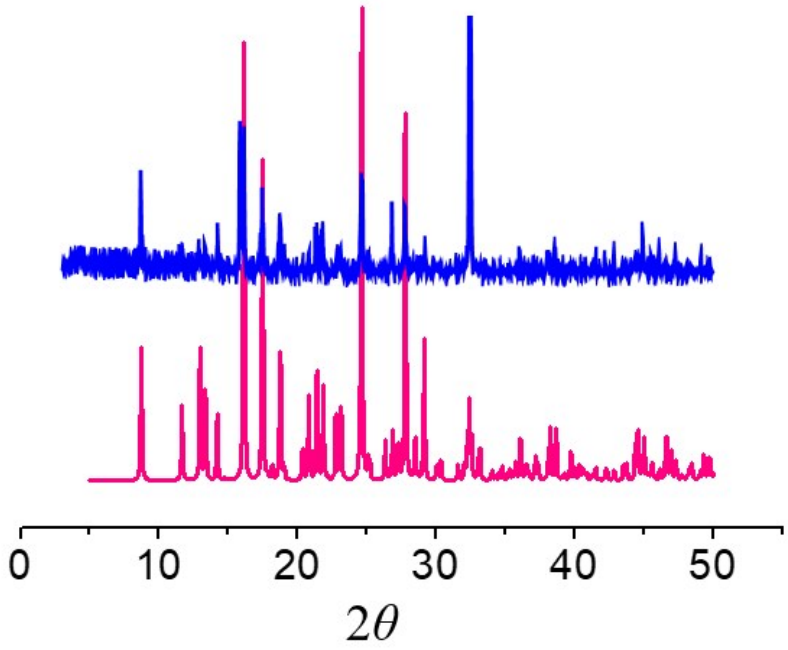

Figure S6. The simulated X-ray powder diffraction patterns (lower) and the measured one (upper) of compound **5**.

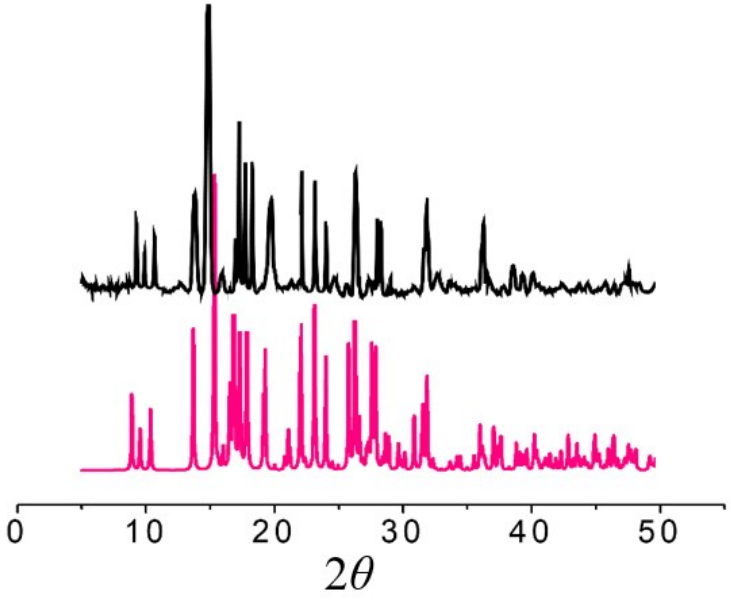

Figure S7. The simulated X-ray powder diffraction patterns (lower) and the measured one (upper) of compound **6**.

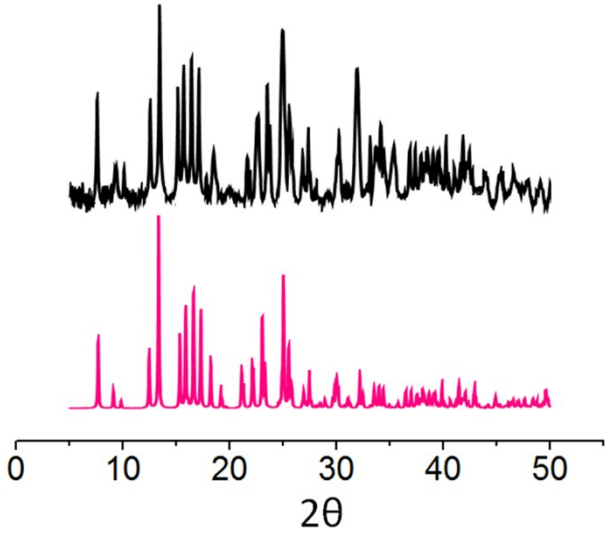

Figure S8. The simulated X-ray powder diffraction patterns (lower) and the measured one (upper) of compound **7**.

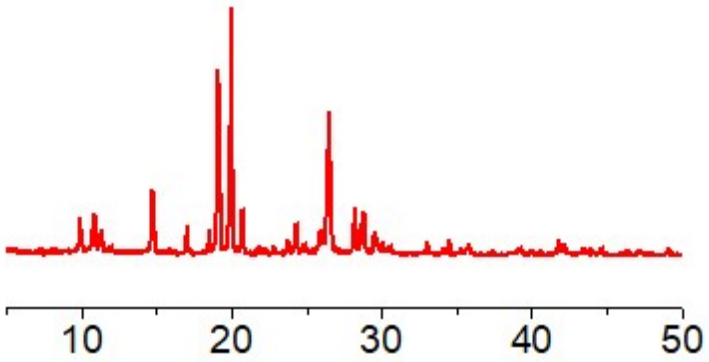

Figure S9. The measured PXRD of product obtained by reaction of $Zn(NO_3)_2 \cdot 6H_2O$ with HDTBA.

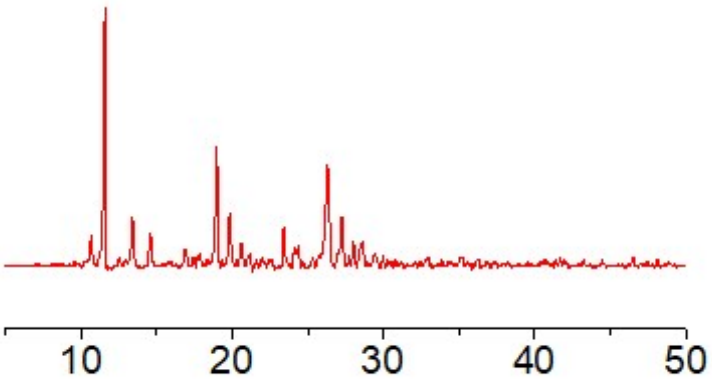

Figure S10. The measured PXRD of product obtained by reaction of $ZnCl_2 \cdot 2H_2O$ with HDTBA.

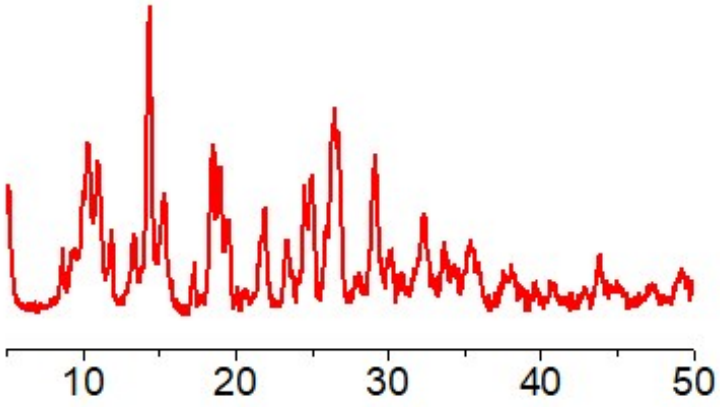

Figure S11. The measured PXRD of product obtained by reaction of $Cd(NO_3)_2 \cdot 4H_2O$ with HDTBA.

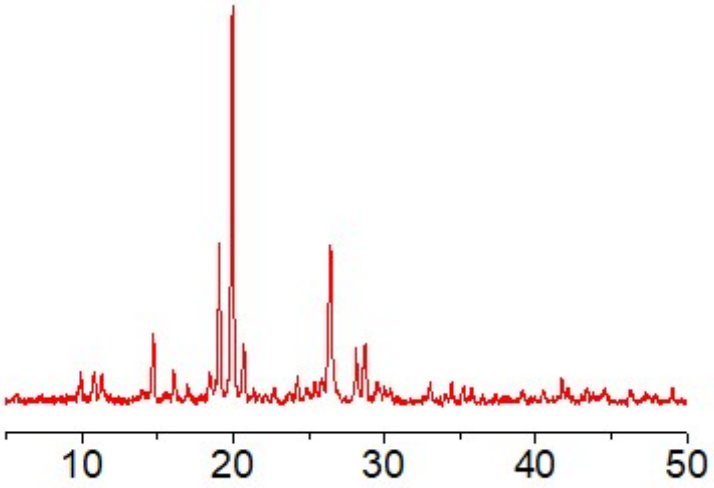

Figure S12. The measured PXRD of product obtained by reaction of $Cd(NO_3)_2 \cdot 4H_2O$ with HDTBA at the present of $NH_3 \cdot H_2O$.

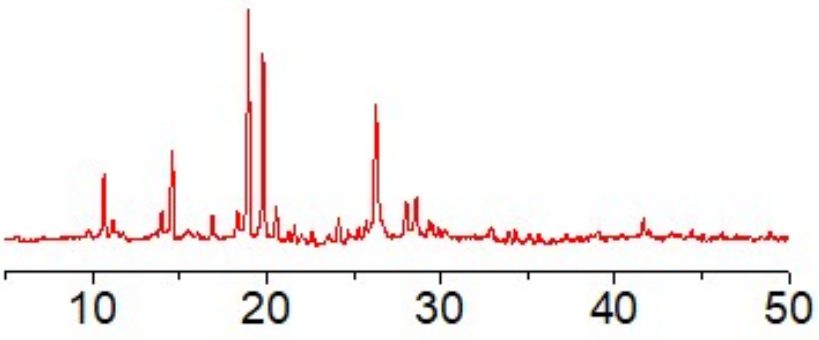

Figure S13. The measured PXRD of product obtained by reaction of $Cd(ClO_4)_2 \cdot 6H_2O$ with HDTBA.

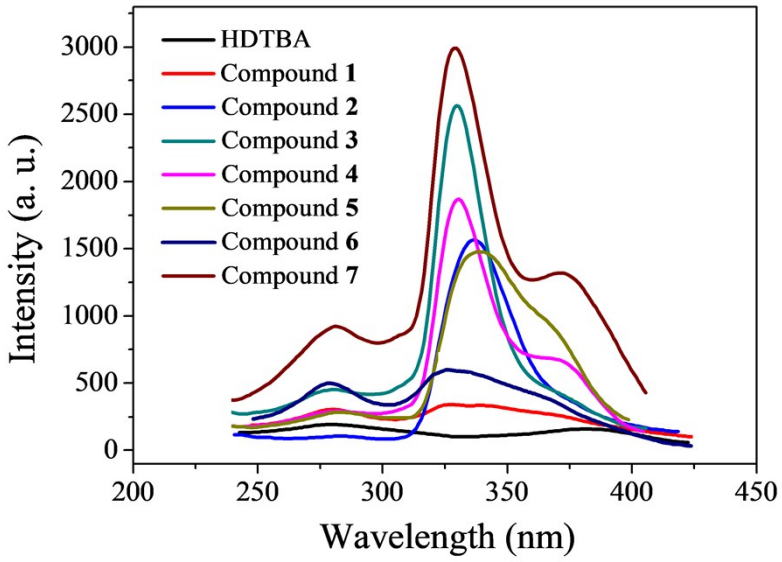

Figure S14. The solid-state excitation spectra for compounds **1-7** at room temperature.