Electronic Supplementary Information (ESI†)

Topological structural transformation of a two-dimensional coordination polymer *via* single-crystal to single-crystal photoreaction

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Table S1 Selected Bond Lengths (Å) and Angles (º) for **1** and **1a**

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Compound **1**

Cd(1)-O(1A)	2.297(2)	Cd(1)-N(2B)	2.301(3)
Cd(1)-N(1)	2.359(3)	Cd(1)-O(1)	2.375(2)
Cd(1)-O(3)	2.417(3)	Cd(1)-O(3C)	2.467(3)
Cd(1)-O(4C)	2.533(3)		
O(1A)-Cd(1)-N(2B)	98.66(10)	O(1A)-Cd(1)-N(1)	84.25(10)
N(2B)-Cd(1)-N(1)	177.09(10)	O(1A)-Cd(1)-O(1)	76.58(9)
N(2B)-Cd(1)-O(1)	88.09(10)	N(1)-Cd(1)-O(1)	92.67(10)
O(1A)-Cd(1)-O(3)	150.12(9)	N(2B)-Cd(1)-O(3)	92.58(10)
N(1)-Cd(1)-O(3)	84.87(10)	O(1)-Cd(1)-O(3)	76.23(8)
O(1A)-Cd(1)-O(3C)	133.36(8)	N(2B)-Cd(1)-O(3C)	92.55(10)
N(1)-Cd(1)-O(3C)	85.37(10)	O(1)-Cd(1)-O(3C)	149.31(8)
O(3)-Cd(1)-O(3C)	73.10(9)	O(1A)-Cd(1)-O(4C)	81.62(8)
N(2B)-Cd(1)-O(4C)	95.49(10)	N(1)-Cd(1)-O(4C)	84.84(10)
O(1)-Cd(1)-O(4C)	158.20(8)	O(3)-Cd(1)-O(4C)	124.91(8)
O(3C)-Cd(1)-O(4C)	52.20(8)		

Compound **1a**

Cd(1)-O(1A)	2.321(4)	Cd(1)-N(1)	2.321(5)
Cd(1)-O(1)	2.364(4)	Cd(1)-N(2B)	2.365(5)

Cd(1)-O(3)	2.432(4)	Cd(1)-O(4C)	2.455(5)
Cd(1)-O(3C)	2.484(4)		
O(1A)-Cd(1)-N(1)	102.48(16)	O(1A)-Cd(1)-O(1)	75.32(15)
N(1)-Cd(1)-O(1)	88.48(16)	O(1A)-Cd(1)-N(2B)	83.45(16)
N(1)-Cd(1)-N(2B)	173.85(17)	O(1)-Cd(1)-N(2B)	91.48(16)
O(1A)-Cd(1)-O(3)	147.80(14)	N(1)-Cd(1)-O(3)	92.49(16)
O(1)-Cd(1)-O(3)	76.78(14)	N(2B)-Cd(1)-O(3)	81.51(16)
O(1A)-Cd(1)-O(4C)	82.71(14)	N(1)-Cd(1)-O(4C)	99.35(17)
O(1)-Cd(1)-O(4C)	157.82(14)	N(2B)-Cd(1)-O(4C)	82.92(17)
O(3)-Cd(1)-O(4C)	123.13(14)	O(1A)-Cd(1)-O(3C)	135.15(14)
N(1)-Cd(1)-O(3C)	91.56(16)	O(1)-Cd(1)-O(3C)	148.32(14)
N(2B)-Cd(1)-O(3C)	85.25(16)	O(3)-Cd(1)-O(3C)	71.56(16)
O(4C)-Cd(1)-O(3C)	52.84(14)		

Symmetry codes: for **1**: (A) - x + 1, - y + 1, - z + 1; (B) x, y, z - 1; (C) - x, - y + 1, - z + 1.

for **1a**: (A) - x + 2, - y + 1, - z + 1; (B) x, y, z - 1; (C) - x + 1, - y + 1, - z + 1.
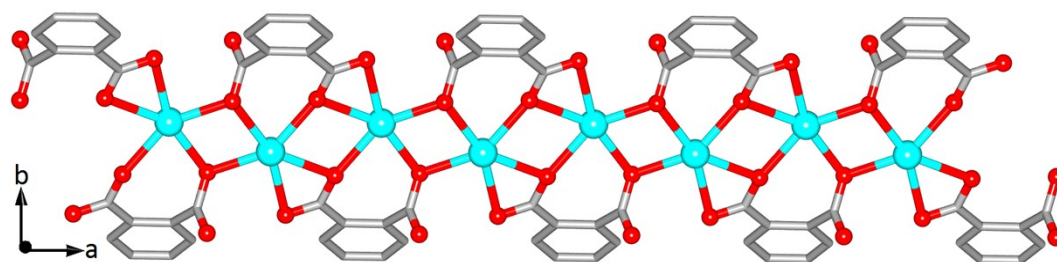
(a)
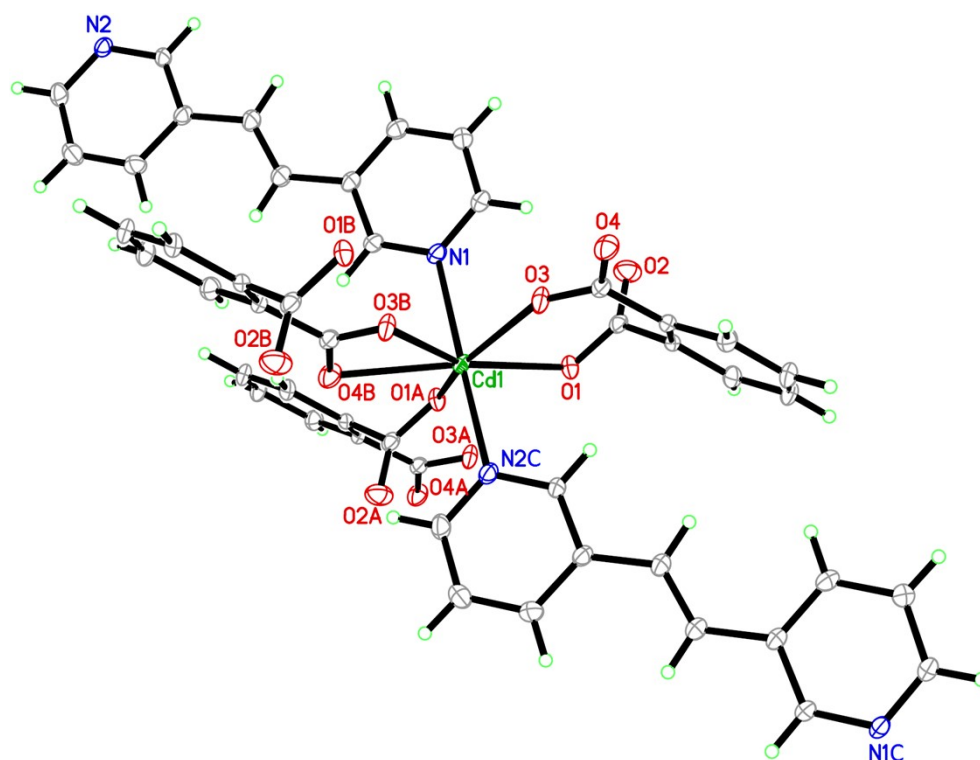
(b)

Fig. S1. (a) View of the coordination environment of Cd1 in **1** with labeling scheme. Symmetry codes: (A) - x + 1, - y + 1, - z + 1; (B) - x, - y + 1, - z + 1; (C) x, y, z - 1. (b) View of the 1D [Cd(pha)]$_n$ chain in **1** along the a axis.
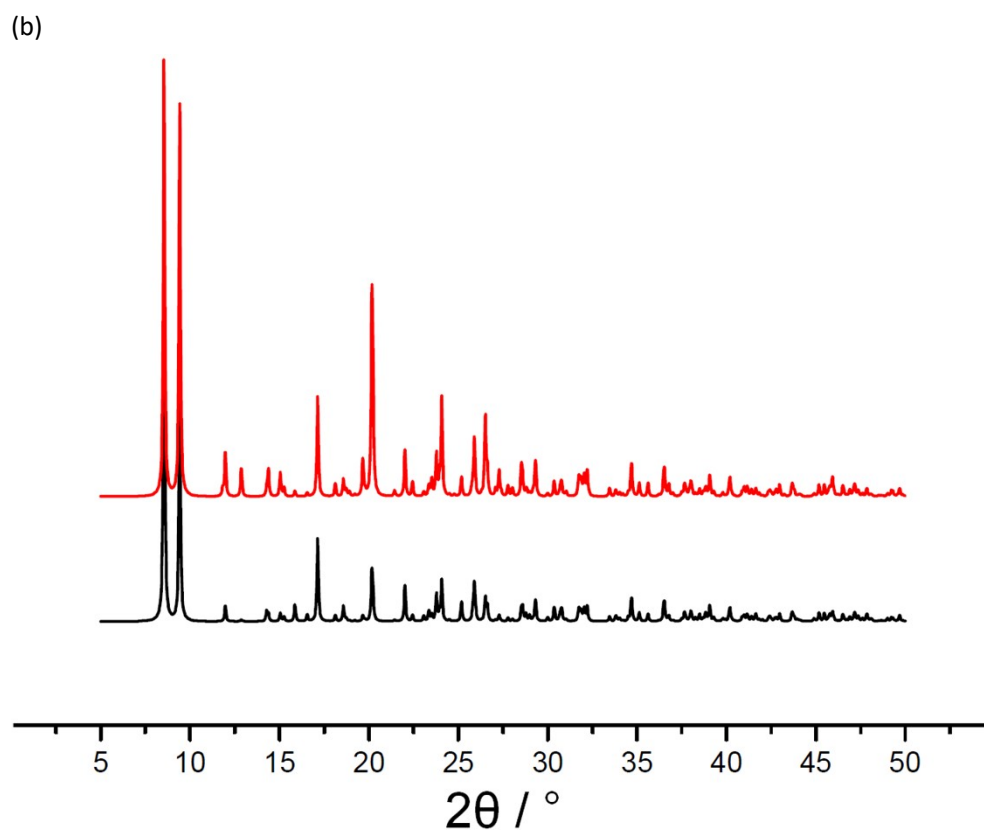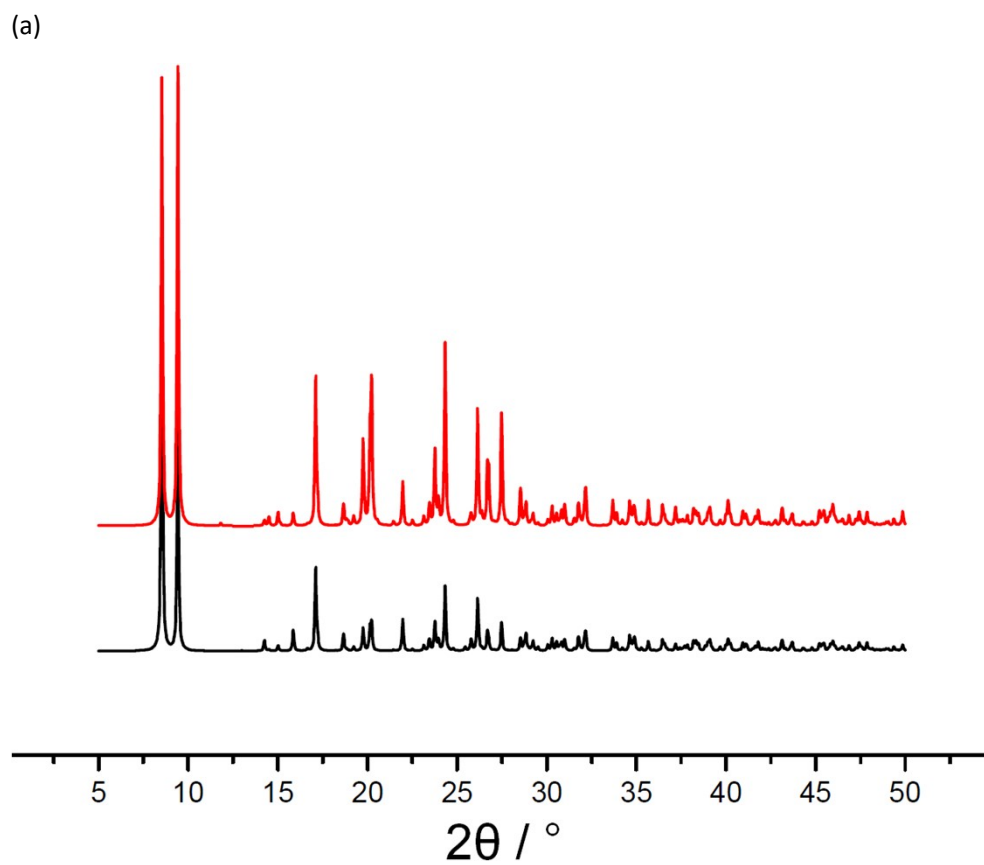
(a)

(b)

Fig. S2. PXRD patterns for **1** and **1a** (simulated pattern from single crystal: black; experimental pattern from grinding crystals: red).
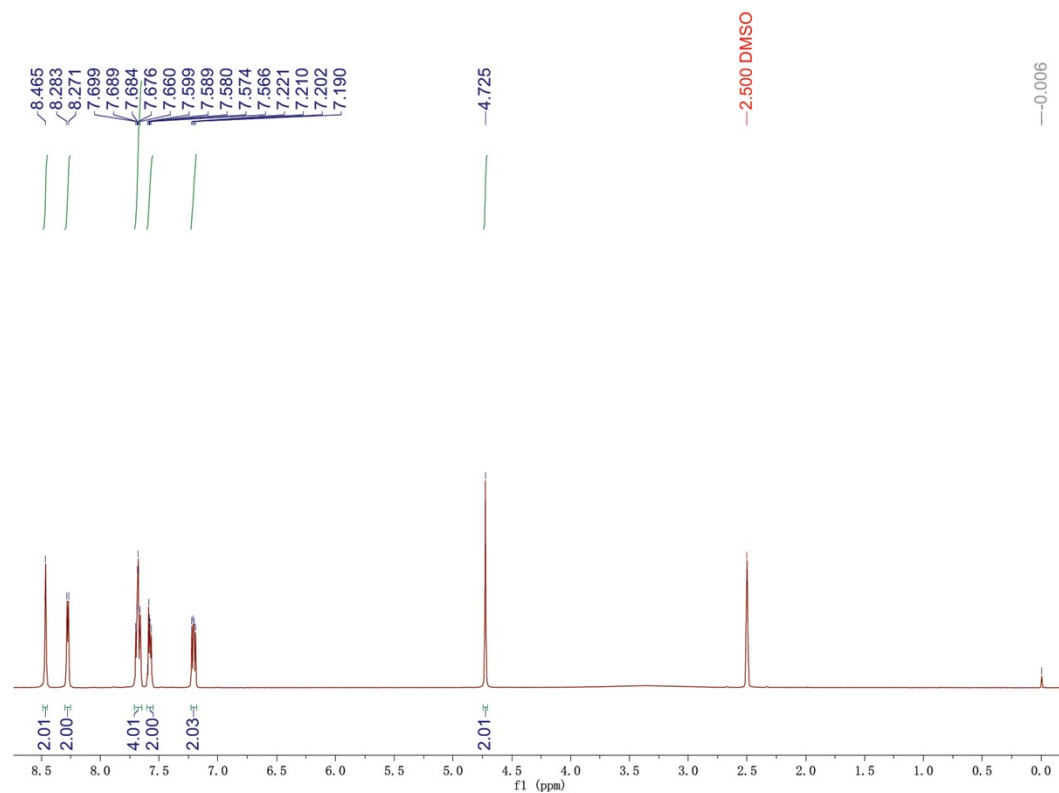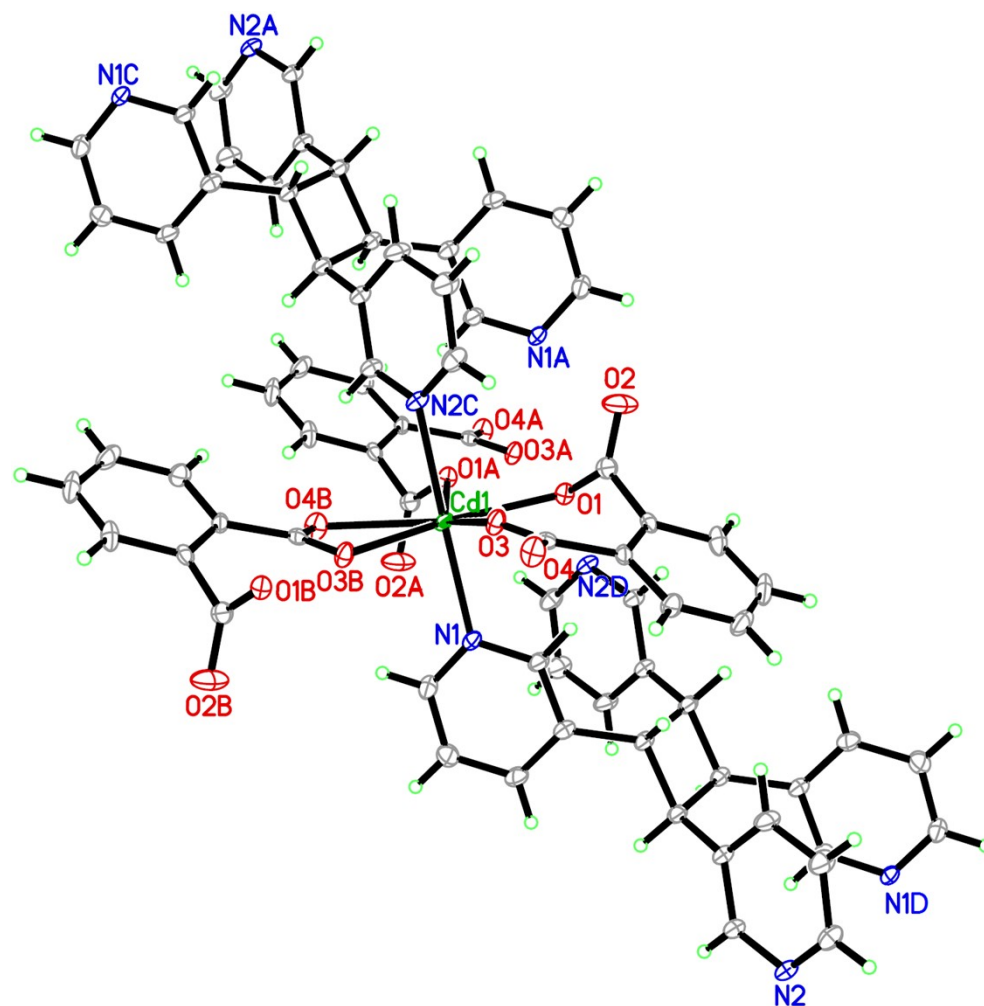
Fig. S3. The ^{1}H NMR spectra of **1a** (sunlight-irradiated sample of **1**). Due to the low solubility of 2D coordination polymer, the sample was digested by 12 mol·L^{-1} HCl aqueous solution and dried in a vacuum oven at 80 °C. The obtained solid was then dissolved in 0.6 mL d_6-DMSO for ^{1}H NMR analysis.
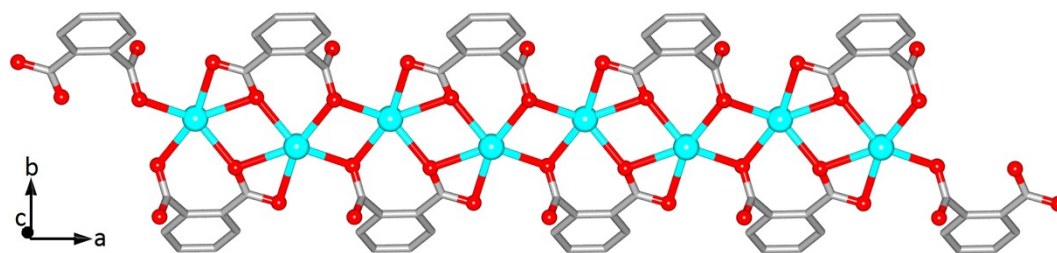
(a)

(b)

Fig. S4. (a) View of the coordination environment of Cd1 in **1a** with labeling scheme. Symmetry codes: (A) - x + 2, - y + 1, - z + 1; (B) - x + 1, - y + 1, - z + 1; (C) x, y, z - 1; (D) - x + 2, - y + 1, - z + 2. (b) View of the 1D $[Cd(pha)]_n$ chain in **1a** along the a axis.
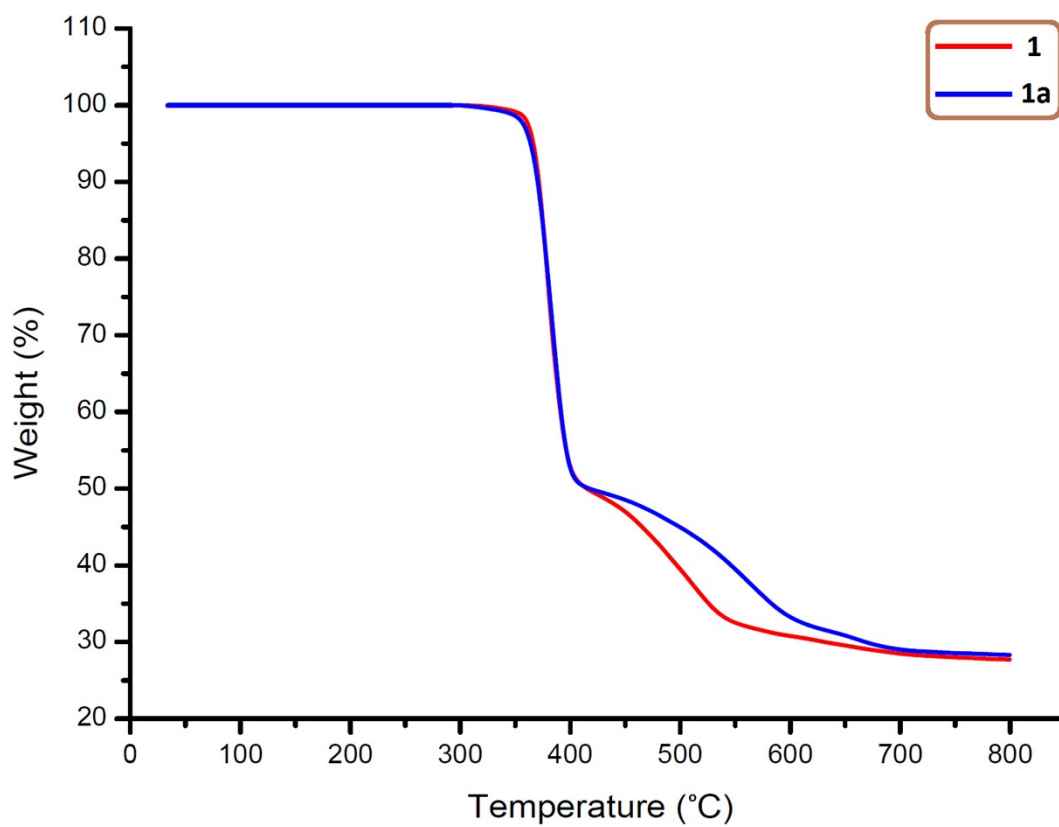
Fig. S5. The TGA curves for **1** and **1a**.