Electronic Supplementary Information (ESI)

A new series of Cd(II) metal-organic architectures driven by soft ether-bridged tricarboxylate spacers: synthesis, structural and topological versatility, and photocatalytic properties

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*†Electronic Supplementary Information (ESI) available: additional synthetic and analytical data, Tables S1 and S2 with structural parameters, emission wavelengths (Table S3), porosity and gas sorption data (Table S4), additional structural representations (Fig. S1), PXRD patterns (Figs. S3 and S12), diffuse reflectance spectra (Fig. S4), absorption spectra of the MB solutions in catalytic tests including kinetic data (Figs. S5–S9), catalysis in the presence of radical scavenger (Fig. S10), catalyst recycling experiments (Fig. S11); crystallographic data for **1**−**8** in CIF format: CCDC-1846591–1846598.*

Synthesis and analytical data for 2–8

Synthesis of $\{[Cd_3(\mu_5\text{-cpta})_2(phen)_3]\cdot 8H_2O\}_n$ (2). A mixture of $CdCl_2\cdot H_2O$ (60.3 mg, 0.30 mmol), H_3cpta (60.4 mg, 0.20 mmol), phen (60.0 mg, 0.3 mmol), NaOH (24.0 mg, 0.6 mmol), and H_2O (10 mL) was stirred at room temperature for 15 min, then sealed in a 25 mL Teflon-lined stainless steel vessel, and heated at 160 °C for 3 days, followed by cooling to room temperature at a rate of 10 °C·h^{-1}. Colorless block-shaped crystals of **2** were isolated manually, washed with distilled water and dried (yield 55% based on H_3cpta). Anal. Calcd for $C_{66}H_{54}Cd_3N_6O_{22}$: C, 48.92; H, 3.36; N, 5.19. Found: C, 49.17; H, 3.39; N, 5.17%. IR (KBr, cm^{-1}): 3312 m, 2920 m, 1597 s, 1568 s, 1540 s, 1510 w, 1464 w, 1376 s, 1301 w, 1230 m, 1166 w, 1143 w, 1101 w, 1044 w, 1009 w, 956 w, 858 m, 782 w, 723 m, 659 w.

Synthesis of $\{[Cd_3(\mu_5\text{-cpta})_2(2,2'\text{-bipy})_3]\cdot 6H_2O\}_n$ (3). Synthesis of **3** was similar to **2** except using 2,2′-bipy instead of phen. Colorless block-shaped crystals of **3** were isolated manually, washed with distilled water and dried (yield 65% based on H_3cpta). Anal. Calcd for $C_{60}H_{50}Cd_3N_6O_{20}$: C, 47.65; H, 3.33; N, 5.56. Found: C, 57.41; H, 3.35; N, 5.59%. IR (KBr, cm^{-1}): 3358 w, 3067 w, 1597 s, 1562 s, 1534 m, 1493 w, 1440 w, 1393 s, 1364 s, 1312 w, 1242 m, 1154 w, 1085 w, 1056 w, 1015 w, 956 w, 863 w, 828 w, 811 w, 764 m, 734 w, 647 w.

Synthesis of $\{[Cd(\mu_3\text{-cpta})(Hbpa)]\cdot 2H_2O\}$ (4). Synthesis of **4** was similar to **2** except using bpa instead of phen. Colorless block-shaped crystals of **4** were isolated manually, washed with distilled water and dried (yield 55% based on H_3cpta). Anal. Calcd for $C_{25}H_{21}CdN_3O_9$: C, 48.44; H, 3.41; N, 6.78. Found: C, 48.22; H, 3.43; N, 6.83%. IR (KBr, cm^{-1}): 3154 w, 1597 s, 1522 s, 1464 w, 1399 s, 1352 w, 1230 w, 1160 w, 1079 w, 1008 w, 950 w, 903 w, 846 w, 805 w, 782 w, 711 w, 658 w.

Synthesis of $\{[Cd_6(\mu_4\text{-cpta})_2(\mu_6\text{-cpta})_2(H_2biim)_2(H_2O)_6]\cdot 5H_2O\}_n$ (5). Synthesis of **5** was similar to **2** except using H_2biim instead of phen. Colorless block-shaped crystals of **5** were isolated manually, washed with distilled water and dried (yield 62% based on H_3cpta). Anal. Calcd for $C_{72}H_{62}Cd_6N_8O_{39}$: C, 36.99; H, 2.67; N, 4.79. Found: C, 37.21; H, 2.65; N, 4.82%. IR (KBr, cm^{-1}): 3434 w, 3131 w, 1609 m, 1546 w, 1452 w, 1399 s, 1318 w, 1230 w, 1166 w, 1137 w, 1097 w, 991 w, 950 w, 858 w, 805 w, 770

w, 746 w, 717 w, 682 w, 658 w.

Synthesis of $[Cd_3(\mu_4\text{-cpta})_2(\mu\text{-prz})(H_2O)_4]_n$ (6). A mixture of $CdCl_2 \cdot H_2O$ (60.3 mg, 0.30 mmol), H_3cpta (60.4 mg, 0.20 mmol), prz (51.6 mg, 0.60 mmol), and H_2O (10 mL) was stirred at room temperature for 15 min, then sealed in a 25 mL Teflon-lined stainless steel vessel, and heated at 160 °C for 3 days, followed by cooling to room temperature at a rate of 10 °C·h^{-1}. Colorless block-shaped crystals of **6** were isolated manually, washed with distilled water and dried (yield 63% based on H_3cpta). Anal. Calcd for $C_{34}H_{32}Cd_3N_2O_{18}$: C, 37.33; H, 2.95; N, 2.56. Found: C, 37.18; H, 2.93; N, 2.57%. IR (KBr, cm^{-1}): 3434 m, 3323 w, 3148 w, 1638 w, 1609 s, 1551 w, 1452 w, 1399 s, 1236 w, 1154 w, 1107 w, 1009 w, 950 w, 863 w, 805 w, 776 w, 705 w, 652 w.

Synthesis of $\{[Cd_3(\mu_4\text{-dbba})_2(phen)_3]\cdot H_2O\}_n$ (7). A mixture of $CdCl_2 \cdot H_2O$ (60.3 mg, 0.30 mmol), H_3dbba (63.2 mg, 0.20 mmol), phen (60.0 mg, 0.30 mmol), NaOH (24.0 mg, 0.60 mmol), and H_2O (10 mL) was stirred at room temperature for 15 min, then sealed in a 25 mL Teflon-lined stainless steel vessel, and heated at 160 °C for 3 days, followed by cooling to room temperature at a rate of 10 °C·h^{-1}. Colorless block-shaped crystals of **7** were isolated manually, washed with distilled water and dried (yield 55% based on H_3dbba). Anal. Calcd for $C_{68}H_{44}Cd_3N_6O_{15}$: C, 53.65; H, 2.91; N, 5.52. Found: C, 53.81; H, 2.92; N, 5.49%. IR (KBr, cm^{-1}): 3404 w, 3091 w, 1603 w, 1580 w, 1534 s, 1510 w, 1429 w, 1376 s, 1277 w, 1207 w, 1137 w, 1091 w, 1032 w, 1009 w, 944 w, 904 w, 858 w, 840 w, 805 w, 776 w, 717 m, 636 w.

Synthesis of $\{[Cd_3(\mu_3\text{-dbba})_2(2,2'\text{-bipy})_3(H_2O)_3]\cdot 2H_2O\}_n$ (8). Synthesis of **8** was similar to **7** except using 2,2′-bipy (46.8 mg, 0.30 mmol) instead of phen. Colorless block-shaped crystals of **8** were obtained (yield 65% based on H_3dbba). Anal. Calcd for $C_{62}H_{52}Cd_3N_6O_{19}$: C, 48.92; H, 3.44; N, 5.52. Found: C, 48.85; H, 3.41; N, 5.56%. IR (KBr, cm^{-1}): 3438 m, 3329 w, 3125 m, 1662 s, 1638 w, 1609 s, 1552 w, 1452 m, 1393 s, 1289 w, 1242 w, 1170 w, 1096 w, 1050 w, 1015 w, 904 w, 852 w, 770 m, 734 w, 664 w.

Table S1. Selected bond lengths [Å] and angles [°] for the compounds **1**–**8**[a].

1					
Cd(1)-O(1)	2.304(4)	Cd(1)-O(2)	2.591(4)	Cd(1)-O(3)#1	2.440(5)
Cd(1)-O(4)#1	2.344(5)	Cd(1)-N(1)	2.365(6)	Cd(1)-N(2)	2.380(5)
Cd(1)-N(3)	2.313(6)				
O(1)-Cd(1)-N(3)	137.41(16)	O(1)-Cd(1)-O(4)#1	88.17(17)	N(3)-Cd(1)-O(4)#1	127.47(19)
O(1)-Cd(1)-N(1)	86.96(19)	N(3)-Cd(1)-N(1)	106.9(2)	N(1)-Cd(1)-O(4)#1	98.2(2)
O(1)-Cd(1)-N(2)	85.90(19)	N(3)-Cd(1)-N(2)	70.8(2)	O(4)#1-Cd(1)-N(2)	94.16(18)
N(1)-Cd(1)-N(2)	165.48(19)	O(1)-Cd(1)-O(3)#1	141.66(17)	N(3)-Cd(1)-O(3)#1	79.90(18)
O(4)#1-Cd(1)-O(3)#1	54.69(17)	N(1)-Cd(1)-O(3)#1	89.24(19)	N(2)-Cd(1)-O(3)#1	104.15(19)
O(1)-Cd(1)-O(2)	53.00(15)	N(3)-Cd(1)-O(2)	87.26(17)	O(4)#1-Cd(1)-O(2)	140.84(17)
N(1)-Cd(1)-O(2)	85.84(17)	N(2)-Cd(1)-O(2)	79.76(16)	O(3)#1-Cd(1)-O(2)	164.29(17)
2					
Cd(1)-O(1)	2.201(5)	Cd(1)-O(1)#1	2.202(5)	Cd(1)-O(6)#2	2.644(7)
Cd(1)-O(6)#3	2.644(7)	Cd(1)-N(3)	2.373(6)	Cd(1)-N(3)#1	2.373(6)
Cd(2)-O(3)	2.362(5)	Cd(2)-O(4)	2.425(4)	Cd(2)-O(2)#4	2.350(6)
Cd(2)-O(6)#5	2.272(5)	Cd(2)-O(7)#5	2.618(6)	Cd(2)-N(1)	2.314(7)
Cd(2)-N(2)	2.366(10)				
O(1)-Cd(1)-O(1)#1	134.8(3)	O(1)-Cd(1)-N(3)	132.8(2)	N(3)#1-Cd(1)-N(3)	70.6(3)
O(6)#2-Cd(1)-N(3)	109.8(2)	N(3)#1-Cd(1)-O(6)#2	74.3(2)	O(6)#2-Cd(1)-O(1)	102.7(2)
O(6)#2-Cd(1)-O(1)#1	75.4(2)	O(6)#3-Cd(1)-O(6)#2	175.2(2)	O(6)#5-Cd(2)-N(1)	97.8(2)
O(6)#5-Cd(2)-O(2)#4	81.0(2)	N(1)-Cd(2)-O(2)#4	85.4(3)	O(6)#5-Cd(2)-O(3)	117.5(2)
N(1)-Cd(2)-O(3)	142.6(2)	O(2)#4-Cd(2)-O(3)	88.3(2)	O(6)#5-Cd(2)-N(2)	111.6(2)
N(1)-Cd(2)-N(2)	71.8(4)	O(2)#4-Cd(2)-N(2)	155.0(4)	O(3)-Cd(2)-N(2)	103.5(3)
O(6)#5-Cd(2)-O(4)	165.3(2)	N(1)-Cd(2)-O(4)	87.9(2)	O(2)#4-Cd(2)-O(4)	86.0(2)
O(3)-Cd(2)-O(4)	54.9(2)	N(2)-Cd(2)-O(4)	83.1(2)	O(6)#5-Cd(2)-O(7)#5	52.5(2)
N(1)-Cd(2)-O(7)#5	125.0(2)	O(2)#4-Cd(2)-O(7)#5	124.4(2)	O(3)-Cd(2)-O(7)#5	88.4(2)
N(2)-Cd(2)-O(7)#5	78.6(3)	O(4)-Cd(2)-O(7)#5	133.4(2)		
3					
Cd(1)-O(1)	2.466(5)	Cd(1)-O(1)#1	2.466(5)	Cd(1)-O(5)#2	2.187(4)
Cd(1)-O(5)#3	2.187(4)	Cd(1)-N(1)	2.404(6)	Cd(1)-N(1)#1	2.404(6)
Cd(2)-O(1)	2.387(5)	Cd(2)-O(2)	2.444(5)	Cd(2)-O(4)#2	2.350(5)
Cd(2)-O(6)#4	2.344(5)	Cd(2)-O(7)#4	2.426(5)	Cd(2)-N(2)	2.316(6)
Cd(2)-N(3)	2.374(6)				
O(5)#2-Cd(1)-O(5)#3	133.7(3)	O(5)#2-Cd(1)-N(1)#1	136.2(2)	O(5)#2-Cd(1)-N(1)#1	85.8(2)
N(1)#1-Cd(1)-N(1)	68.7(3)	O(5)#2-Cd(1)-O(1)	80.49(18)	O(5)#3-Cd(1)-O(1)	92.85(17)
N(1)#1-Cd(1)-O(1)	79.3(2)	N(1)-Cd(1)-O(1)	115.3(2)	O(1)-Cd(1)-O(1)#1	163.1(2)
N(2)-Cd(2)-O(6)#4	151.11(19)	N(2)-Cd(2)-O(4)#2	84.66(19)	O(4)#2-Cd(2)-O(6)#4	86.43(18)
N(2)-Cd(2)-N(3)	70.0(2)	N(3)-Cd(2)-O(6)#4	106.5(2)	N(3)-Cd(2)-O(4)#2	148.4(2)
N(2)-Cd(2)-O(1)	94.25(19)	O(6)#4-Cd(2)-O(1)	111.29(18)	O(1)-Cd(2)-O(4)#2	80.56(18)
N(3)-Cd(2)-O(1)	118.8(2)	N(2)-Cd(2)-O(7)#4	96.8(2)	O(6)#4-Cd(2)-O(7)#4	54.66(17)
O(4)#2-Cd(2)-O(7)#4	81.17(18)	N(3)-Cd(2)-O(7)#4	83.3(2)	O(1)-Cd(2)-O(7)#4	157.63(18)
N(2)-Cd(2)-O(2)	117.1(2)	O(6)#4-Cd(2)-O(2)	89.61(18)	O(4)#2-Cd(2)-O(2)	129.28(18)
N(3)-Cd(2)-O(2)	80.5(2)	O(1)-Cd(2)-O(2)	54.26(17)	O(7)#4-Cd(2)-O(2)	133.99(19)
4					
Cd(1)-O(1)	2.333(8)	Cd(1)-O(2)	2.486(5)	Cd(1)-O(3)#1	2.300(6)
Cd(1)-O(4)#1	2.554(7)	Cd(1)-O(6)#2	2.301(8)	Cd(1)-O(7)#2	2.477(9)
Cd(1)-N(1)	2.291(6)				
N(1)-Cd(1)-O(3)#1	97.0(2)	N(1)-Cd(1)-O(6)#2	128.3(3)	O(3)#1-Cd(1)-O(6)#2	84.5(3)

N(1)-Cd(1)-O(1)	133.6(2)	O(1)-Cd(1)-O(3)#1	120.4(3)	O(1)-Cd(1)-O(6)#2	84.9(3)
N(1)-Cd(1)-O(7)#2	90.0(3)	O(7)#2-Cd(1)-O(3)#1	129.0(3)	O(6)#2-Cd(1)-O(7)#2	53.6(3)
O(1)-Cd(1)-O(7)#2	86.8(4)	N(1)-Cd(1)-O(2)	80.8(2)	O(3)#1-Cd(1)-O(2)	134.9(2)
O(6)#2-Cd(1)-O(2)	131.8(3)	O(1)-Cd(1)-O(2)	53.64(19)	O(7)#2-Cd(1)-O(2)	96.1(3)
N(1)-Cd(1)-O(4)#1	101.5(3)	O(3)#1-Cd(1)-O(4)#1	52.7(2)	O(6)#2-Cd(1)-O(4)#1	118.7(3)
O(1)-Cd(1)-O(4)#1	83.4(3)	O(7)#2-Cd(1)-O(4)#1	168.2(3)	O(2)-Cd(1)-O(4)#1	83.3(2)
5					
Cd(1)-O(1)	2.535(5)	Cd(1)-O(2)	2.421(5)	Cd(1)-O(9)	2.304(5)
Cd(1)-O(20)#1	2.547(6)	Cd(1)-O(21)#1	2.285(5)	Cd(1)-O(27)#2	2.469(5)
Cd(1)-O(28)#2	2.361(6)	Cd(2)-O(22)	2.331(5)	Cd(2)-O(29)	2.243(5)
Cd(2)-O(10)#3	2.508(5)	Cd(2)-O(11)#3	2.406(5)	Cd(2)-N(1)	2.305(7)
Cd(2)-N(4)	2.375(6)	Cd(3)-O(9)	2.587(5)	Cd(3)-O(30)	2.278(5)
Cd(3)-O(27)#2	2.501(5)	Cd(3)-O(24)#4	2.308(5)	Cd(3)-N(5)	2.294(6)
Cd(3)-N(8)	2.419(7)	Cd(4)-O(15)	2.514(5)	Cd(4)-O(16)	2.383(5)
Cd(4)-O(13)#1	2.459(5)	Cd(4)-O(14)#1	2.333(5)	Cd(4)-O(6)#2	2.483(6)
Cd(4)-O(7)#2	2.299(6)	Cd(5)-O(8)	2.263(5)	Cd(5)-O(16)	2.279(6)
Cd(5)-O(31)	2.266(5)	Cd(5)-O(32)	2.331(6)	Cd(5)-O(17)#5	2.310(5)
Cd(5)-O(18)#5	2.341(5)	Cd(6)-O(1)	2.301(6)	Cd(6)-O(23)	2.327(5)
Cd(6)-O(33)	2.315(5)	Cd(6)-O(34)	2.230(5)	Cd(6)-O(3)#5	2.351(5)
Cd(6)-O(4)#5	2.306(5)				
O(21)#1-Cd(1)-O(9)	86.90(18)	O(21)#1-Cd(1)-O(28)#2	168.8(2)	O(9)-Cd(1)-O(28)#2	91.83(18)
O(21)#1-Cd(1)-O(2)	90.60(18)	O(9)-Cd(1)-O(2)	151.37(19)	O(28)#2-Cd(1)-O(2)	95.76(18)
O(21)#1-Cd(1)-O(27)#2	136.2(2)	O(9)-Cd(1)-O(27)#2	83.59(16)	O(28)#2-Cd(1)-O(27)#2	54.43(19)
O(2)-Cd(1)-O(27)#2	78.61(16)	O(21)#1-Cd(1)-O(1)	103.12(19)	O(9)-Cd(1)-O(1)	155.37(18)
O(28)#2-Cd(1)-O(1)	73.97(18)	O(1)-Cd(1)-O(2)	52.32(18)	O(27)#2-Cd(1)-O(1)	103.12(19)
O(21)#1-Cd(1)-O(20)#1	54.06(19)	O(9)-Cd(1)-O(20)#1	92.62(16)	O(28)#2-Cd(1)-O(20)#1	115.0(2)
O(2)-Cd(1)-O(20)#1	108.85(17)	O(27)#2-Cd(1)-O(20)#1	168.41(17)	O(1)-Cd(1)-O(20)#1	76.10(17)
O(29)-Cd(2)-N(1)	103.9(2)	O(29)-Cd(2)-O(22)	84.05(19)	N(1)-Cd(2)-O(22)	153.5(2)
O(29)-Cd(2)-N(4)	151.4(2)	N(1)-Cd(2)-N(4)	74.2(2)	N(4)-Cd(2)-O(22)	86.7(2)
O(29)-Cd(2)-O(11)#3	83.32(19)	N(1)-Cd(2)-O(11)#3	124.8(2)	O(22)-Cd(2)-O(11)#3	80.76(19)
N(4)-Cd(2)-O(11)#3	121.72(19)	O(29)-Cd(2)-O(10)#3	128.2(2)	N(1)-Cd(2)-O(10)#3	84.3(2)
O(22)-Cd(2)-O(10)#3	110.82(16)	N(4)-Cd(2)-O(10)#3	80.3(2)	O(10)#3-Cd(2)-O(11)#3	53.11(17)
O(30)-Cd(3)-N(5)	130.5(2)	N(5)-Cd(3)-O(24)#4	120.4(2)	O(30)-Cd(3)-O(24)#4	84.36(17)
N(8)-Cd(3)-N(5)	73.3(2)	O(30)-Cd(3)-N(8)	137.8(2)	N(8)-Cd(3)-O(24)#4	115.17(19)
N(5)-Cd(3)-O(27)#2	88.9(2)	O(30)-Cd(3)-O(27)#2	69.56(17)	O(24)#4-Cd(3)-O(27)#2	149.74(17)
N(8)-Cd(3)-O(27)#2	78.19(19)	O(9)-Cd(3)-N(5)	150.9(2)	O(30)-Cd(3)-O(9)	68.45(17)
O(24)#4-Cd(3)-O(9)	78.87(17)	O(9)-Cd(3)-N(8)	78.77(19)	O(9)-Cd(3)-O(27)#2	77.46(17)
O(7)#2-Cd(4)-O(14)#1	132.5(2)	O(7)#2-Cd(4)-O(22)	83.20(19)	O(14)#1-Cd(4)-O(22)	77.70(17)
O(7)#2-Cd(4)-O(16)	108.11(19)	O(14)#1-Cd(4)-O(16)	92.77(18)	O(16)-Cd(4)-O(22)	168.53(18)
O(7)#2-Cd(4)-O(13)#1	169.30(17)	O(14)#1-Cd(4)-O(13)#1	54.67(18)	O(13)#1-Cd(4)-O(22)	91.79(17)
O(13)#1-Cd(4)-O(16)	77.37(17)	O(7)#2-Cd(4)-O(6)#2	54.1(2)	O(14)#1-Cd(4)-O(6)#2	172.2(2)
O(22)-Cd(4)-O(6)#2	108.57(17)	O(16)-Cd(4)-O(6)#2	80.46(19)	O(13)#1-Cd(4)-O(6)#2	119.47(19)
O(7)#2-Cd(4)-O(15)	81.81(18)	O(14)#1-Cd(4)-O(15)	77.76(17)	O(22)-Cd(4)-O(15)	129.27(19)
O(16)-Cd(4)-O(15)	53.03(17)	O(13)#1-Cd(4)-O(15)	108.57(16)	O(6)#2-Cd(4)-O(15)	100.86(18)
O(8)-Cd(5)-O(31)	79.09(19)	O(8)-Cd(5)-O(16)	132.60(18)	O(31)-Cd(5)-O(16)	80.0(2)
O(8)-Cd(5)-O(17)#5	106.8(2)	O(31)-Cd(5)-O(17)#5	143.3(2)	O(16)-Cd(5)-O(17)#5	115.22(19)
O(8)-Cd(5)-O(18)#5	107.3(2)	O(31)-Cd(5)-O(18)#5	87.60(19)	O(16)-Cd(5)-O(18)#5	113.76(19)
O(17)#5-Cd(5)-O(18)#5	55.85(18)	O(8)-Cd(5)-O(32)	81.1(2)	O(31)-Cd(5)-O(32)	127.3(2)
O(16)-Cd(5)-O(32)	78.6(2)	O(32)-Cd(5)-O(17)#5	89.2(2)	O(32)-Cd(5)-O(18)#5	145.09(19)
O(34)-Cd(6)-O(1)	86.1(2)	O(34)-Cd(6)-O(4)#6	147.9(2)	O(1)-Cd(6)-O(4)#6	105.29(19)

O(34)-Cd(6)-O(23)	84.2(2)	O(1)-Cd(6)-O(23)	145.05(17)	O(23)-Cd(6)-O(4)#6	100.62(19)
O(34)-Cd(6)-O(33)	109.5(2)	O(1)-Cd(6)-O(33)	77.8(2)	O(33)-Cd(6)-O(4)#6	102.26(19)
O(23)-Cd(6)-O(33)	74.05(19)	O(34)-Cd(6)-O(3)#6	92.0(2)	O(1)-Cd(6)-O(3)#6	118.55(19)
O(3)#6-Cd(6)-O(4)#6	56.15(17)	O(23)-Cd(6)-O(3)#6	95.30(19)	O(33)-Cd(6)-O(3)#6	154.5(2)
Cd(6)-O(1)-Cd(1)	134.8(2)	Cd(3)-O(9)-Cd(1)	97.11(15)		
6					
Cd(1)-O(1)	2.321(2)	Cd(1)-O(15)	2.266(2)	Cd(1)-O(16)	2.269(2)
Cd(1)-O(10)#1	2.283(2)	Cd(1)-O(11)#1	2.413(2)	Cd(1)-N(1)	2.366(3)
Cd(2)-O(1)	2.481(2)	Cd(2)-O(2)	2.408(2)	Cd(2)-O(8)	2.285(3)
Cd(2)-O(9)	2.593(3)	Cd(2)-O(6)#3	2.436(3)	Cd(2)-O(7)#3	2.454(2)
Cd(2)-O(13)#4	2.332(2)	Cd(2)-O(14)#4	2.506(3)	Cd(3)-O(9)	2.296(3)
Cd(3)-O(17)	2.269(2)	Cd(3)-O(18)	2.245(2)	Cd(3)-O(3)#5	2.469(2)
Cd(3)-O(4)#5	2.272(2)	Cd(3)-N(2)	2.402(3)		
O(15)-Cd(1)-O(16)	111.00(10)	O(15)-Cd(1)-O(10)#1	99.47(10)	O(16)-Cd(1)-O(10)#1	149.34(9)
O(15)-Cd(1)-O(1)	78.66(9)	O(16)-Cd(1)-O(1)	81.65(9)	O(1)-Cd(1)-O(10)#1	101.68(9)
O(15)-Cd(1)-N(1)	85.11(10)	O(16)-Cd(1)-N(1)	80.69(10)	N(1)-Cd(1)-O(10)#1	105.99(10)
N(1)-Cd(1)-O(1)	149.83(9)	O(15)-Cd(1)-O(11)#1	154.68(10)	O(16)-Cd(1)-O(11)#1	93.66(9)
O(10)#1-Cd(1)-O(11)#1	55.68(8)	O(1)-Cd(1)-O(11)#1	100.18(8)	N(1)-Cd(1)-O(11)#1	105.18(10)
O(8)-Cd(2)-O(13)#4	87.31(9)	O(8)-Cd(2)-O(2)	165.59(9)	O(2)-Cd(2)-O(13)#4	81.18(9)
O(8)-Cd(2)-O(6)#3	115.94(9)	O(13)#4-Cd(2)-O(6)#3	125.50(9)	O(2)-Cd(2)-O(6)#3	78.05(9)
O(8)-Cd(2)-O(7)#3	81.58(9)	O(13)#4-Cd(2)-O(7)#3	165.50(9)	O(2)-Cd(2)-O(7)#3	111.10(8)
O(6)#3-Cd(2)-O(7)#3	53.40(8)	O(8)-Cd(2)-O(1)	127.80(9)	O(1)-Cd(2)-O(13)#4	119.59(8)
O(1)-Cd(2)-O(2)	53.38(8)	O(6)#3-Cd(2)-O(1)	85.39(8)	O(7)#3-Cd(2)-O(1)	74.80(8)
O(8)-Cd(2)-O(14)#4	79.98(10)	O(13)#4-Cd(2)-O(14)#4	53.40(9)	O(2)-Cd(2)-O(14)#4	86.18(10)
O(6)#3-Cd(2)-O(14)#4	163.98(9)	O(7)#3-Cd(2)-O(14)#4	132.53(9)	O(1)-Cd(2)-O(14)#4	82.92(8)
O(8)-Cd(2)-O(9)	52.99(9)	O(13)#4-Cd(2)-O(9)	74.67(8)	O(2)-Cd(2)-O(9)	130.54(9)
O(6)#3-Cd(2)-O(9)	81.94(8)	O(7)#3-Cd(2)-O(9)	91.15(8)	O(1)-Cd(2)-O(9)	165.01(8)
O(14)#4-Cd(2)-O(9)	110.98(9)	O(17)-Cd(3)-O(18)	100.45(10)	O(18)-Cd(3)-O(4)#5	93.61(9)
O(17)-Cd(3)-O(4)#5	165.66(9)	O(18)-Cd(3)-O(9)	89.83(9)	O(17)-Cd(3)-O(9)	77.87(9)
O(9)-Cd(3)-O(4)#5	99.58(9)	O(18)-Cd(3)-N(2)	107.66(10)	O(17)-Cd(3)-N(2)	78.20(10)
O(4)#5-Cd(3)-N(2)	100.25(10)	O(9)-Cd(3)-N(2)	152.52(9)	O(18)-Cd(3)-O(3)#5	148.28(9)
O(17)-Cd(3)-O(3)#5	110.63(9)	O(4)#5-Cd(3)-O(3)#5	55.09(8)	O(9)-Cd(3)-O(3)#5	90.63(8)
N(2)-Cd(3)-O(3)#5	85.33(9)	Cd(1)-O(1)-Cd(2)	129.86(10)		
7					
Cd(1)-O(1)	2.388(5)	Cd(1)-O(2)	2.341(4)	Cd(1)-O(9)#1	2.264(5)
Cd(1)-O(4)#2	2.358(5)	Cd(1)-N(1)	2.376(6)	Cd(1)-N(2)	2.294(6)
Cd(2)-O(7)	2.209(5)	Cd(2)-O(8)	2.282(5)	Cd(2)-O(3)#3	2.265(4)
Cd(2)-N(3)	2.314(6)	Cd(2)-N(4)	2.364(5)	Cd(3)-O(10)	2.327(5)
Cd(3)-O(11)	2.364(5)	Cd(3)-O(13)#4	2.604(5)	Cd(3)-O(14)#4	2.222(5)
Cd(3)-N(5)	2.325(7)	Cd(3)-N(6)	2.365(8)		
O(9)#1-Cd(1)-N(2)	120.39(19)	O(9)#1-Cd(1)-O(2)	90.61(18)	O(2)-Cd(1)-N(2)	138.09(18)
O(9)#1-Cd(1)-O(4)#2	85.31(18)	N(2)-Cd(1)-O(4)#2	107.76(18)	O(2)-Cd(1)-O(4)#2	101.81(16)
O(9)#1-Cd(1)-N(1)	160.82(18)	N(2)-Cd(1)-N(1)	70.8(2)	O(2)-Cd(1)-N(1)	88.74(19
N(1)-Cd(1)-O(4)#2	76.08(18)	O(9)#1-Cd(1)-O(1)	98.29(19)	N(2)-Cd(1)-O(1)	90.26(18)
O(2)-Cd(1)-O(1)	55.45(15)	O(4)#2-Cd(1)-O(1)	156.80(15)	N(1)-Cd(1)-O(1)	97.09(19)
O(7)-Cd(2)-O(3)#3	97.94(18)	O(7)-Cd(2)-O(8)	95.76(18)	O(8)-Cd(2)-O(3)#3	96.50(17)
O(7)-Cd(2)-N(3)	133.38(19)	N(3)-Cd(2)-O(3)#3	99.04(18)	N(3)-Cd(2)-O(8)	124.76(18)
O(7)-Cd(2)-N(4)	88.65(19)	N(4)-Cd(2)-O(3)#3	169.8(2)	N(4)-Cd(2)-O(8)	90.53(18)
N(4)-Cd(2)-N(3)	70.84(19)	O(14)#4-Cd(3)-O(10)	123.01(18)	O(14)#4-Cd(3)-N(5)	97.3(2)
O(10)-Cd(3)-N(5)	122.2(2)	O(14)#4-Cd(3)-O(11)	99.8(2)	O(10)-Cd(3)-O(11)	55.14(17)

N(5)-Cd(3)-O(11)	159.7(3)	O(14)#4-Cd(3)-N(6)	146.8(2)	O(10)-Cd(3)-N(6)	88.3(2)
N(5)-Cd(3)-N(6)	70.6(3)	N(6)-Cd(3)-O(11)	89.1(3)	O(14)#4-Cd(3)-O(13)#4	53.69(17)
O(10)-Cd(3)-O(13)#4	150.39(18)	N(5)-Cd(3)-O(13)#4	86.0(2)	O(11)-Cd(3)-O(13)#4	95.33(18)
N(6)-Cd(3)-O(13)#4	93.8(2)				
8					
Cd(1)-O(1)	2.380(6)	Cd(1)-O(2)	2.388(7)	Cd(1)-O(13)	2.366(10)
Cd(1)-O(14)	2.544(10)	Cd(1)-O(15)	2.355(6)	Cd(1)-N(1)	2.346(10)
Cd(1)-N(2)	2.345(9)	Cd(2)-O(3)	2.483(6)	Cd(2)-O(4)	2.324(7)
Cd(2)-O(16)	2.301(6)	Cd(2)-O(8)#1	2.402(7)	Cd(2)-O(9)#1	2.461(7)
Cd(2)-N(3)	2.345(9)	Cd(2)-N(4)	2.332(8)	Cd(3)-O(6)	2.450(7)
Cd(3)-O(7)	2.381(6)	Cd(3)-O(17)	2.244(7)	Cd(3)-O(10)#2	2.311(6)
Cd(3)-O(11)#2	2.517(6)	Cd(3)-N(5)	2.352(8)	Cd(3)-N(6)	2.347(9)
N(1)-Cd(1)-N(2)	69.7(4)	N(2)-Cd(1)-O(1)	94.9(3)	N(1)-Cd(1)-O(1)	84.4(3)
N(2)-Cd(1)-O(15)	83.9(3)	N(1)-Cd(1)-O(15)	129.7(3)	O(1)-Cd(1)-O(15)	141.7(2)
N(2)-Cd(1)-O(13)	130.6(4)	N(1)-Cd(1)-O(13)	90.2(4)	O(1)-Cd(1)-O(13)	128.5(3)
O(15)-Cd(1)-O(13)	75.2(3)	N(2)-Cd(1)-O(2)	101.7(3)	N(1)-Cd(1)-O(2)	137.6(3)
O(1)-Cd(1)-O(2)	54.3(2)	O(15)-Cd(1)-O(2)	88.3(2)	O(13)-Cd(1)-O(2)	121.4(4)
N(2)-Cd(1)-O(14)	158.8(4)	N(1)-Cd(1)-O(14)	89.5(4)	O(1)-Cd(1)-O(14)	78.3(3)
O(15)-Cd(1)-O(14)	113.9(3)	O(13)-Cd(1)-O(14)	50.5(4)	O(2)-Cd(1)-O(14)	90.7(3)
O(16)-Cd(2)-O(4)	95.2(3)	O(16)-Cd(2)-N(4)	158.7(3)	O(4)-Cd(2)-N(4)	95.3(3)
O(16)-Cd(2)-N(3)	90.5(3)	O(4)-Cd(2)-N(3)	142.6(3)	N(4)-Cd(2)-N(3)	70.1(3)
O(16)-Cd(2)-O(8)#1	79.8(2)	O(4)-Cd(2)-O(8)#1	115.8(3)	N(4)-Cd(2)-O(8)#1	111.9(3)
N(3)-Cd(2)-O(8)#1	101.6(3)	O(16)-Cd(2)-O(9)#1	120.0(3)	O(4)-Cd(2)-O(9)#1	77.7(3)
N(4)-Cd(2)-O(9)#1	80.4(3)	N(3)-Cd(2)-O(9)#1	130.0(3)	O(8)#1-Cd(2)-O(9)#1	53.4(3)
O(16)-Cd(2)-O(3)	87.7(2)	O(4)-Cd(2)-O(3)	54.2(2)	N(4)-Cd(2)-O(3)	83.6(3)
N(3)-Cd(2)-O(3)	89.3(3)	O(3)-Cd(2)-O(8)#1	163.3(3)	O(3)-Cd(2)-O(9)#1	127.2(3)
O(17)-Cd(3)-O(10)#2	99.7(3)	O(17)-Cd(3)-N(5)	94.1(3)	N(5)-Cd(3)-O(10)#2	137.7(3)
O(17)-Cd(3)-N(6)	161.5(3)	N(6)-Cd(3)-O(10)#2	98.1(3)	N(6)-Cd(3)-N(5)	69.1(4)
O(17)-Cd(3)-O(7)	101.0(3)	O(7)-Cd(3)-O(10)#2	80.0(2)	O(7)-Cd(3)-N(5)	136.1(3)
O(7)-Cd(3)-N(6)	87.0(3)	O(17)-Cd(3)-O(6)	89.0(3)	O(6)-Cd(3)-O(10)#2	133.2(2)
N(5)-Cd(3)-O(6)	86.4(3)	N(6)-Cd(3)-O(6)	82.4(3)	O(7)-Cd(3)-O(6)	53.2(2)
O(17)-Cd(3)-O(11)#2	90.0(2)	O(10)#2-Cd(3)-O(11)#2	53.5(2)	N(5)-Cd(3)-O(11)#2	86.9(3)
N(6)-Cd(3)-O(11)#2	96.5(3)	O(7)-Cd(3)-O(11)#2	133.5(2)	O(6)-Cd(3)-O(11)#2	173.2(2)

[a] Symmetry transformations used to generate equivalent atoms: #1 *x*–1/2, –*y*+1/2, *z*+1/2 for **1**; #1 –*x*+2, *y*, –*z*+3/2; #2 *x*, –*y*+1, *z*+1/2; #3 –*x*+2, –*y*+1, –*z*+1; #4 –*x*+3/2, –*y*+1/2, –*z*+1; #5 –*x*+3/2, *y*–1/2, –*z*+1/2 for **2**; #1 –*x*+1, *y*, –*z*+1/2; #2 *x*, –*y*+1, *z*+1/2; #3 –*x*+1, –*y*+1, –*z*; #4 –*x*+1/2, *y*–1/2, –*z*+1/2 for **3**; #1 –*x*+2, –*y*, –*z*+1; #2 *x*–1/2, –*y*+1/2, *z* for **4**; #1 –*x*+2, –*y*+1, –*z*+1; #2 –*x*+2, –*y*, –*z*; #3 *x*–1, *y*–1, *z*; #4 *x*+1, *y*+1, *z*; #5 –*x*+3, –*y*+1, –*z*+1; #6 –*x*+1, –*y*, –*z* for **5**; #1 *x*, *y*–1, *z*; #2 –*x*, –*y*, –*z*; #3 –*x*, –*y*,–*z*+1; #4 –*x*+2, –*y*+1, –*z*; #5 *x*, *y*+1, *z* for **6**; #1 –*x*+1, –*y*+2, –*z*; #2 –*x*+1, –*y*+3, –*z*; #3 *x*, *y*–1, *z*; #4 –*x*+1, *y*, –*z*+1/2 for **7**; #1 –*x*+1, –*y*+2, –*z*; #2 *x*–1, *y*–1, *z*–1 for **8**.

Table S2. Hydrogen bond parameters [Å, °] in **1**–**8**.

Complexes	D-H…A	*d*(D-H)	*d*(H…A)	*d*(D…A)	∠DHA	Symmetry code
1	O(6)-H(6)···O(2)	0.820	1.775	2.590	172.04	-*x*+5/2, *y*+1/2, -*z*+3/2
2	O(8)-H(1W)···O(4)	0.850	2.126	2.975	178.10	-*x*+3/2, -*y*+1/2, -*z*+1
	O(9)-H(3W)···O(3)	0.850	1.923	2.771	175.56	
3	O(8)-H(1W)···O(7)	1.034	1.978	2.985	164.10	
	O(9)-H(3W)···O(6)	0.850	2.039	2.889	179.83	
4	N(2)-H(2)···O(9)	0.860	2.075	2.909	163.24	*x*-1, *y*+1, *z*
	N(3)-H(1)···O(2)	0.860	1.958	2.751	152.69	*x*-1/2, -*y*+5/2, *z*
	O(8)-H(1W)···O(1)	0.850	2.015	2.865	179.53	
	O(8)-H(2W)···O(9)	0.740	2.165	2.890	166.66	-*x*+1, -*y*+1, *z*-1/2
	O(9)-H(3W)···O(3)	0.850	1.924	2.774	179.43	-*x*+3/2, *y*-1/2, *z*+1/2
5	N(2)-H(2)···O(10)	0.860	2.058	2.855	153.92	-*x*+2, -*y*+1, -*z*+1
	N(3)-H(3)···O(10)	0.860	2.071	2.846	149.45	-*x*+2, -*y*+1, -*z*+1
	N(6)-H(6)···O(25)	0.860	2.036	2.829	152.84	-*x*+2, -*y*, -*z*
	N(7)-H(7)···O(25)	0.860	2.070	2.851	150.65	-*x*+2, -*y*, -*z*
	O(29)-H(29A)···O(15)	0.850	1.942	2.792	179.70	-*x*+2, -*y*, -*z*
	O(29)-H(29B)···O(35)	0.746	2.163	2.845	152.61	-*x*+1, -*y*, -*z*+1
	O(30)-H(30A)···O(27)	0.850	1.918	2.768	179.28	*x*, *y*+1, *z*
	O(30)-H(30B)···O(38)	0.727	2.052	2.751	161.49	*x*+1, *y*, *z*
	O(31)-H(31A)···O(20)	0.850	1.946	2.796	179.43	-*x*+2, -*y*+1, -*z*+1
	O(31)-H(H31B)···O(13)	0.850	1.904	2.754	179.27	-*x*+2, -*y*+1, -*z*+1
	O(32)-H(32A)···O(37)	0.809	1.986	2.719	150.31	*x*+1, *y*, *z*
	O(32)-H(32B)···O(6)	0.850	1.969	2.819	178.98	-*x*+2, -*y*, -*z*
	O(33)-H(33A)···O(20)	0.850	1.922	2.771	179.03	-*x*+2, -*y*+1, -*z*+1
	O(33)-H(33B)···O(20)	0.850	2.133	2.983	179.25	-*x*+2, -*y*+1, -*z*+1
	O(34)-H(34A)···O(28)	0.850	1.822	2.672	179.42	-*x*+2, -*y*, -*z*
	O(34)-H(34B)···O(6)	0.850	1.883	2.733	178.84	-*x*+2, -*y*, -*z*
	O(35)-H(35B)···O(7)	0.850	2.005	2.855	179.55	*x*-1, *y*, *z*+1
	O(36)-H(36A)···O(17)	0.850	1.924	2.774	179.11	*x*-1, *y*, *z*
	O(36)-H(36B)···O(37)	0.723	1.924	2.640	170.10	-*x*+1, -*y*+1, -*z*+1
	O(37)-H(37B)···O(39)	0.850	1.864	2.713	176.78	-*x*+1, -*y*+1, -*z*+1
	O(38)-H(38A)···O(24)	0.843	2.122	2.925	159.14	*x*, *y*+1, *z*
	O(39)-H(39A)···O(4)	0.850	1.918	2.768	178.76	*x*, *y*+1, *z*+1
6	O(15)-H(1W)···O(2)	0.832	2.026	2.845	168.05	*x*-1, *y*, *z*
	O(15)-H(2W)···O(7)	0.840	1.949	2.776	167.88	-*x*, -*y*, -*z*+1
	O(16)-H(3W)···O(11)	0.834	1.906	2.735	172.47	-*x*+1, -*y*+1, -*z*
	O(16)-H(4W)···O(14)	0.834	1.855	2.686	173.55	-*x*+2, -*y*+1, -*z*
	O(17)-H(5W)···O(6)	0.847	1.918	2.748	166.43	-*x*, -*y*, -*z*+1
	O(17)-H(6W)···O(3)	0.843	1.855	2.684	167.29	-*x*+1, -*y*, -*z*+1
	O(18)-H(7W)···O(13)	0.837	1.811	2.645	174.32	-*x*+2, -*y*+1, -*z*
	O(18)-H(8W)···O(7)	0.833	2.039	2.862	168.95	-*x*+1, -*y*, -*z*+1
7	O(15)-H(1W)···O(2)	0.850	2.086	2.936	179.46	*x*, *y*-1, *z*
	O(15)-H(2W)···O(9)	0.850	2.149	2.998	179.48	

8	O(15)-H(1W)···O(7)	0.850	2.302	2.716	110.27	-*x*+1, -*y*+1, -*z*
	O(15)-H(2W)···O(10)	0.850	2.109	2.959	179.48	-*x*+2, -*y*+2, -*z*+1
	O(16)-H(3W)···O(18)	0.708	1.984	2.676	165.91	-*x*+1, -*y*+2, -*z*
	O(16)-H(4W)···O(3)	0.850	1.904	2.754	179.40	-*x*+1, -*y*+2, -*z*
	O(17)-H(5W)···O(19)	0.713	1.944	2.620	158.29	-*x*+1, -*y*+1, -*z*
	O(17)-H(6W)···O(11)	0.850	1.902	2.752	179.18	-*x*+1, -*y*+2, -*z*
	O(18)-H(7W)···O(1)	0.850	1.911	2.761	179.84	
	O(18)-H(8W)···O(8)	0.965	1.885	2.801	157.31	
	O(19)-H(9W)···O(4)	0.850	2.068	2.918	178.76	-*x*+1, -*y*+1, -*z*

Table S3. Emission wavelengths (nm) for compounds **1**–**8**, H_3cpta, and H_3dbba.[a]

Compound	**H_3cpta**	**H_3dbba**	**1**	**2**	**3**
λ_{em}	467	456	366, 384	365, 386	361
Compound	**4**	**5**	**6**	**7**	**8**
λ_{em}	359	398	359	401	455

[a]λ_{ex} = 323 nm for H_3cpta and **1**–**6**, and λ_{ex} = 318 nm for H_3dbba, **7** and **8**.

Table S4. Porosity and gas sorption data for compounds **2**, **3**, and **5**.[a]

Compound	Void volume (%)	Amount of adsorbed N_2 (cm^3/g)	BET surface area (m^2/g)
2	12.6	2.6	1.1
3	15.1	3.0	1.3
5	13.4	2.8	1.2

[a] Prior to gas adsorption tests, the samples were activated to remove the guest and coordinated water molecules (samples were heated under vacuum at 120 °C for 18 h). The sorption measurements were carried out on the activated samples and N_2 adsorption/desorption isotherms were measured at 77 K.

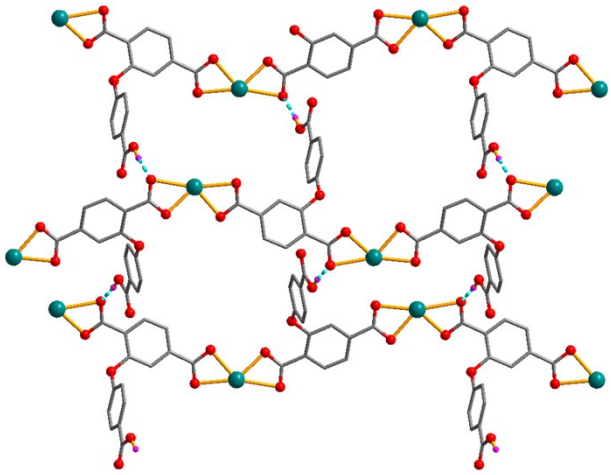

Fig. S1. 2D supramolecular network in **1** viewed along the *bc* plane (blue lines present the H-bonds).

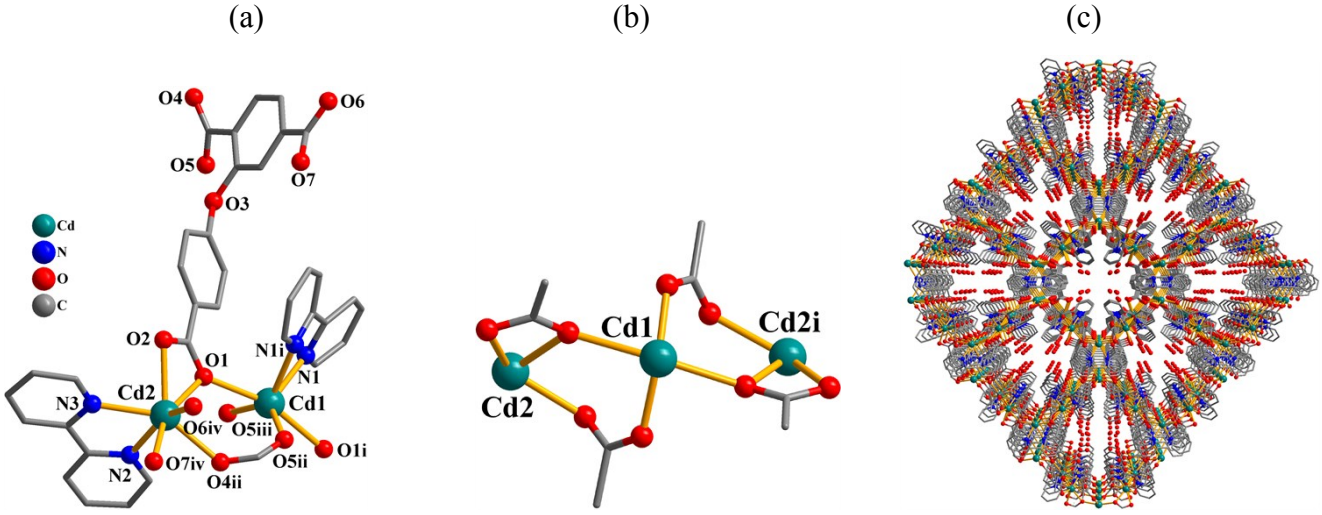

Fig. S2. Structural fragments of **3**. (a) Coordination environment around the Cd(II) atoms; H atoms are omitted for clarity. Symmetry code:i = $-x + 1, y, -z + 1/2$; ii = $x, -y + 1, z + 1/2$; iii = $-x + 1, -y + 1, -z$; iv $-x + 1/2, y - 1/2, -z + 1/2$. (b) The tricadium(II) subunit. Symmetry code: i = $-x + 1, y, -z + 1/2$. (c) 3D MOF seen along the *c* axis.

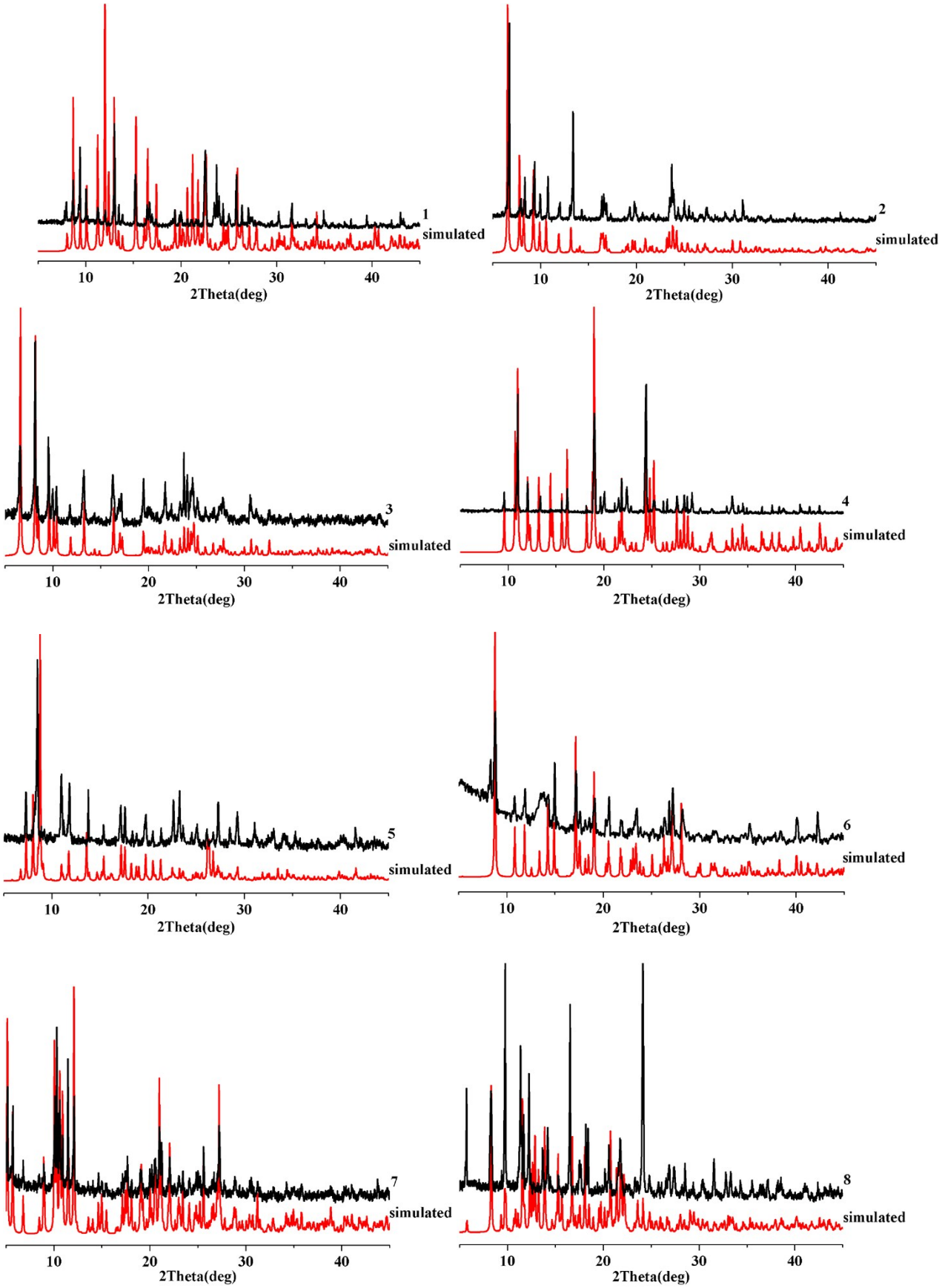

Fig. S3. PXRD patterns of compounds **1**–**8** at room temperature. Black paterns correspnond to the experimental data obtained using the as-synthesized bulk samples. Red patterns were simulated from the single crystal X-ray data.

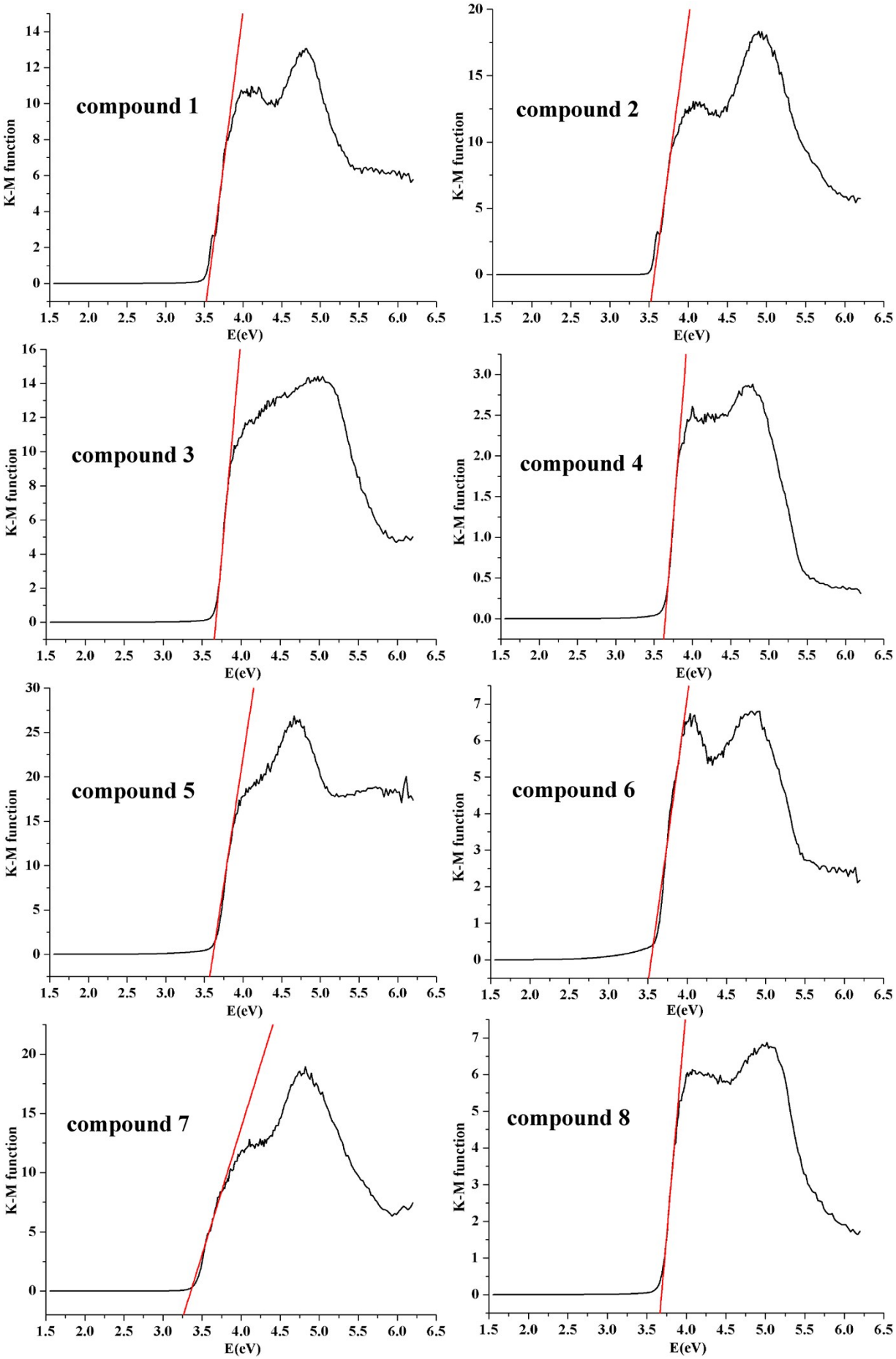

Fig. S4. Kubelka-Munk-transformed diffuse reflectance spectra of compounds **1**–**8**.

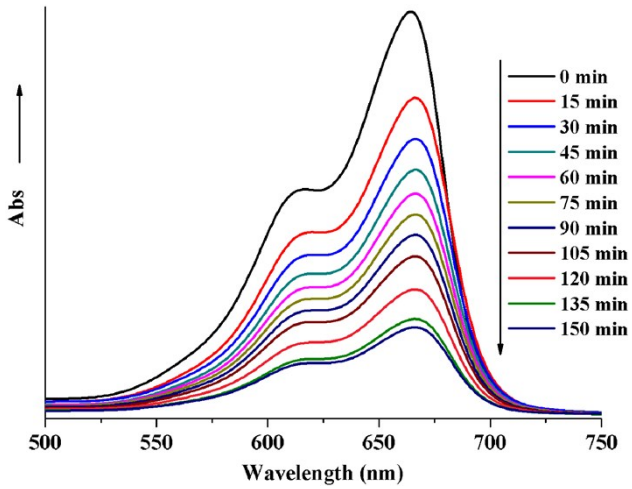

Fig. S5. Time-dependent UV-Vis spectra of the reaction mixtures in the course of the MB photodegradation catalyzed by **7**. Reaction conditions: catalyst (50 mg), 100 mL aqueous solution, MB (1 mg), under 125 W Hg lamp irradiation.

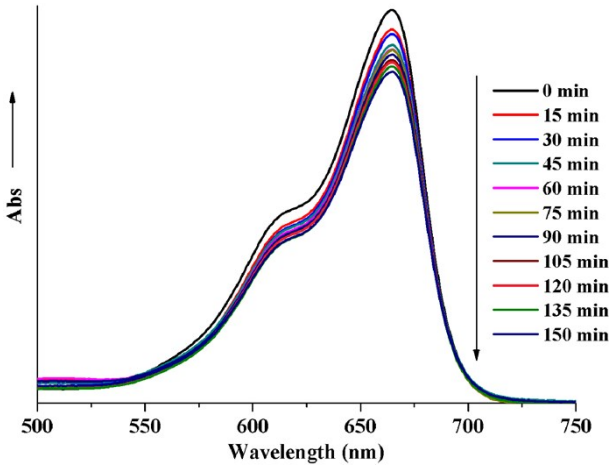

Fig. S6. Time-dependent UV-Vis spectra of the reaction mixtures in the course of the MB photodegradation catalyzed by H_3dbba (blank test). Reaction conditions: H_3dbba (50 mg), 100 mL aqueous solution, MB (1 mg), under 125 W Hg lamp irradiation.

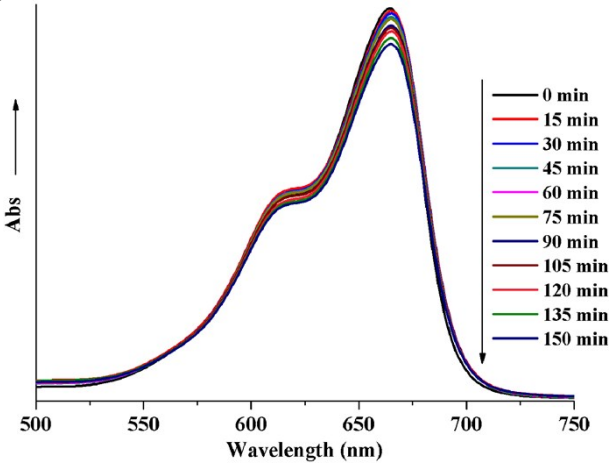

Fig. S7. Time-dependent UV-Vis spectra of the reaction mixtures in the course of the MB photodegradation catalyzed by phen (blank test). Reaction conditions: phen (50 mg), 100 mL aqueous solution, MB (1 mg), under 125 W Hg lamp irradiation.

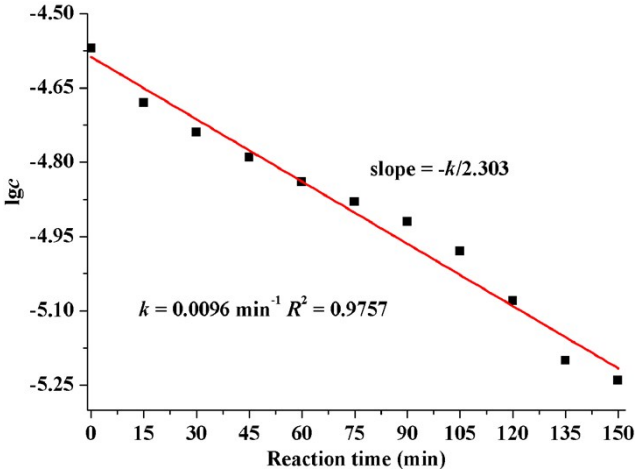

Fig. S8. Relationship between lg*c* and reaction time in the course of the MB photodegradation catalyzed by **7**. The red line corresponds to a fit to the linear relationship. Reaction conditions: catalyst (50 mg), 100 mL aqueous solution, MB (1 mg), under 125 W Hg lamp irradiation.

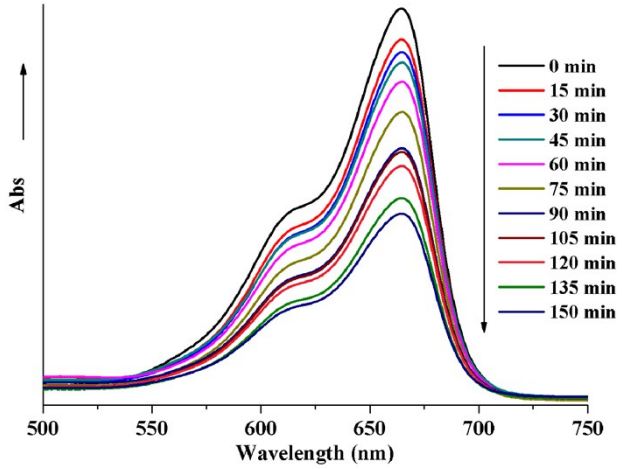

Fig. S9. Time-dependent UV-Vis spectra of the reaction mixtures in the course of the MB photodegradation with **7** in the presence of isopropanol as a radical scavenger (IPA, 0.5 mM). Reaction conditions: catalyst (50 mg), 100 mL aqueous solution, MB (1 mg), under 125 W Hg lamp irradiation.

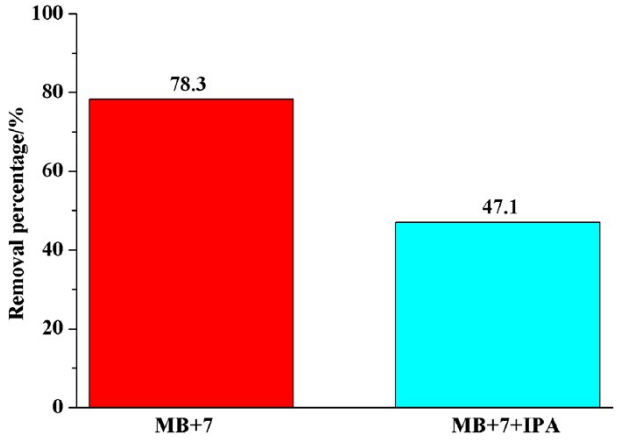

Fig. S10. MB photodegradation (removal efficiency, %) under the UV light irradiation with catalyst **7** (left bar) and in the presence of isopropanol (right bar) as a radical scavenger (IPA, 0.5 mM). Reaction conditions: catalyst (50 mg), 100 mL aqueous solution, MB (1 mg), under 125 W Hg lamp irradiation.

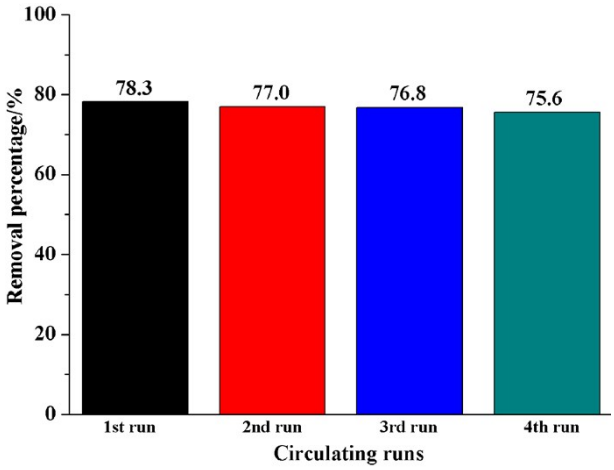

Fig. S11. Catalyst recycling experiments in the MB photodegradation (removal efficiency, %) under the UV light irradiation with catalyst **7**. Reaction conditions: catalyst (50 mg), 100 mL aqueous solution, MB (1 mg), under 125 W Hg lamp irradiation.

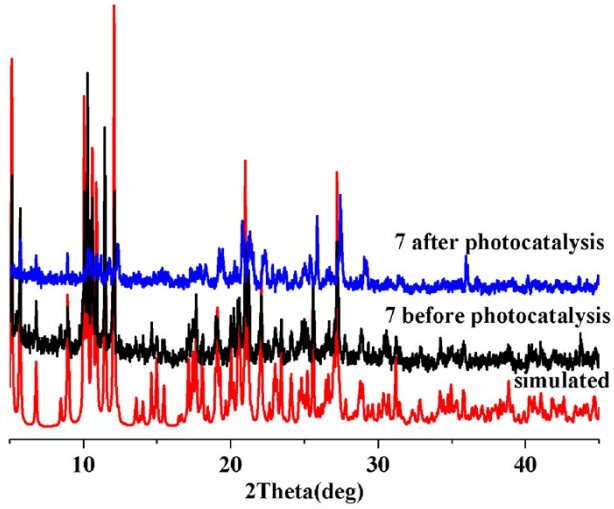

Fig. S12. PXRD patterns for **7**: simulated (red), before (black) and after (blue) photocatalysis.