Electronic Supplementary Information (ESI) for

Five Cd(II) Coordination Polymers Based on 2,3',5,5'-Biphenyl Tetracarboxylic Acid and N-donor Coligands: Syntheses, Structures and Fluorescent Properties

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Table S1. Crystallographic Data and Structure Refinement Details for **1**–**5**.

Complexes	**1**	**2**	**3**	**4**	**5**
Formula	$C_{41}H_{32}Cd_2N_4O_{18}$	$C_{26}H_{24}Cd_2N_4O_{10}$	$C_{30}H_{30}Cd_2N_4O_{13}$	$C_{36}H_{28}CdN_4O_9$	$C_{31}H_{20}Cd_2N_6O_9$
Formula weight	1093.51	777.29	879.38	773.02	845.33
Temperature	296(2)	296(2)	296(2)	296(2)	296(2)
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	*C*2/*c*	$P2_1$	$P2_1/n$	$P2_1/n$	$P2_1/n$
a (Å)	18.65(3)	10.3863(12)	11.128(5)	17.246(6)	13.3294(17)
b (Å)	7.982(11)	12.9737(15)	14.055(6)	17.018(6)	16.202(2)
c (Å)	27.53(4)	10.8834(13)	22.979(10)	10.945(4)	20.283(3)
β (°)	109.469(16)	113.5820(10)	103.992(5)	91.414(4)	99.496(2)
V (Å^3)	3863(9)	1344.1(3)	3488(3)	3211(2)	4320.4(9)
Z	4	2	4	4	4
D_c(g cm^{-3})	1.880	1.921	1.675	1.599	1.300
μ (mm^{-1})	1.192	1.648	1.287	0.745	1.031
F (000)	2184	768	1752	1568	1664
θ Range/^{o}	2.33-25.50	2.29-25.50	2.29-25.50	2.36-25.50	2.35-25.50
Reflns. collected	9642	6860	25105	24207	31893
Independent reflns.	3552	4185	6473	5977	8042
R_{int}	0.1172	0.0169	0.0459	0.0583	0.0799
Data/restraints/parameters	3552/99/295	4185/1/379	6473/0/442	5977/0/453	8042/21/433
GOOF	1.064	1.032	1.034	1.021	0.987
R_1[a], wR_2[b] [$I>2\sigma(I)$]	0.0806, 0.1987	0.0182, 0.0388	0.0301, 0.0617	0.0370, 0.0665	0.0590, 0.1463
R_1, wR_2 (all data)	0.1269, 0.2398	0.0191, 0.0391	0.0450, 0.0672	0.0624, 0.0753	0.1021, 0.1622
$\Delta\rho_{max}$ and $\Delta\rho_{min}$ (e Å^{-3})	1.921, -1.978	0.287, -0.369	0.597, -0.411	0.374, -0.406	2.253, -2.044

[a] $R_1 = \Sigma(|F_o| - |F_c|)/\Sigma|F_o|$; [b] $wR_2 = \{\Sigma[w(|F_o|^2-|F_c|^2)^2]/\Sigma[w(|F_o|^2)^2]\}^{1/2}$.

Table S2 Selected bond distances (Å) and angles (°) of complexes 1–5[a].

Complex 1			
Cd(1)-O(7)#1	2.221(9)	O(8)-Cd(1)-O(2)#2	146.6(3)
Cd(1)-O(1)	2.312(8)	O(7)#1-Cd(1)-O(3)#3	104.2(3)
Cd(1)-O(8)	2.322(8)	O(1)-Cd(1)-O(3)#3	93.6(3)
Cd(1)-O(2)#2	2.349(8)	O(8)-Cd(1)-O(3)#3	80.0(3)
Cd(1)-O(3)#3	2.378(8)	O(2)#2-Cd(1)-O(3)#3	131.9(3)
Cd(1)-O(2)#3	2.526(8)	O(7)#1-Cd(1)-O(2)#3	111.3(3)
O(7)#1-Cd(1)-O(1)	161.9(3)	O(1)-Cd(1)-O(2)#3	81.8(3)
O(7)#1-Cd(1)-O(8)	92.1(3)	O(8)-Cd(1)-O(2)#3	131.0(2)
O(1)-Cd(1)-O(8)	87.9(3)	O(2)#2-Cd(1)-O(2)#3	78.7(2)
O(7)#1-Cd(1)-O(2)#2	89.0(3)	O(3)#3-Cd(1)-O(2)#3	53.3(3)
O(1)-Cd(1)-O(2)#2	82.6(3)		
Complex 2			
Cd(1)-O(4)	2.223(3)	N(1)-Cd(1)-O(2)#3	93.72(11)
Cd(1)-N(1)	2.273(3)	O(8)#1-Cd(1)-O(2)#3	106.08(9)
Cd(1)-O(8)#1	2.277(2)	O(6)#2-Cd(1)-O(2)#3	124.70(9)
Cd(1)-O(6)#2	2.291(2)	O(3)-Cd(2)-O(9)	102.36(10)
Cd(1)-O(2)#3	2.314(2)	O(3)-Cd(2)-N(4)#4	165.87(11)
Cd(2)-O(3)	2.203(3)	O(9)-Cd(2)-N(4)#4	90.51(10)
Cd(2)-O(9)	2.247(2)	O(3)-Cd(2)-O(10)	81.22(10)
Cd(2)-N(4)#4	2.269(3)	O(9)-Cd(2)-O(10)	172.47(9)
Cd(2)-O(10)	2.333(2)	N(4)#4-Cd(2)-O(10)	86.70(10)
Cd(2)-O(5)#2	2.339(2)	O(3)-Cd(2)-O(5)#2	90.51(10)
Cd(2)-O(7)#5	2.400(2)	O(9)-Cd(2)-O(5)#2	82.44(9)
O(4)-Cd(1)-N(1)	179.23(11)	N(4)#4-Cd(2)-O(5)#2	97.03(10)
O(4)-Cd(1)-O(8)#1	87.94(10)	O(10)-Cd(2)-O(5)#2	90.96(8)
N(1)-Cd(1)-O(8)#1	91.32(10)	O(3)-Cd(2)-O(7)#5	87.70(10)
O(4)-Cd(1)-O(6)#2	95.28(9)	O(9)-Cd(2)-O(7)#5	82.74(9)
N(1)-Cd(1)-O(6)#2	85.37(10)	N(4)#4-Cd(2)-O(7)#5	88.17(10)
O(8)#1-Cd(1)-O(6)#2	129.21(8)	O(10)-Cd(2)-O(7)#5	104.14(9)
O(4)-Cd(1)-O(2)#3	86.27(10)	O(5)#2-Cd(2)-O(7)#5	164.32(8)
Complex 3			
Cd(1)-N(4)	2.219(3)	O(9)#2-Cd(1)-O(12)#1	96.91(9)
Cd(1)-O(13)#1	2.237(2)	N(4)-Cd(1)-O(8)#2	84.46(10)
Cd(1)-O(7)	2.252(2)	O(13)#1-Cd(1)-O(8)#2	94.97(9)
Cd(1)-O(9)#2	2.273(2)	O(7)-Cd(1)-O(8)#2	140.60(8)
Cd(1)-O(12)#1	2.471(2)	O(9)#2-Cd(1)-O(8)#2	54.21(7)
Cd(1)-O(8)#2	2.504(2)	O(12)#1-Cd(1)-O(8)#2	100.46(9)
Cd(2)-N(1)#3	2.245(3)	N(1)#3-Cd(2)-O(6)	150.82(11)
Cd(2)-O(6)	2.258(2)	N(1)#3-Cd(2)-O(10)#4	88.23(11)
Cd(2)-O(10)#4	2.296(3)	O(6)-Cd(2)-O(10)#4	117.38(10)
Cd(2)-O(4)	2.375(3)	N(1)#3-Cd(2)-O(4)	89.84(12)
Cd(2)-O(5)	2.413(3)	O(6)-Cd(2)-O(4)	82.10(10)

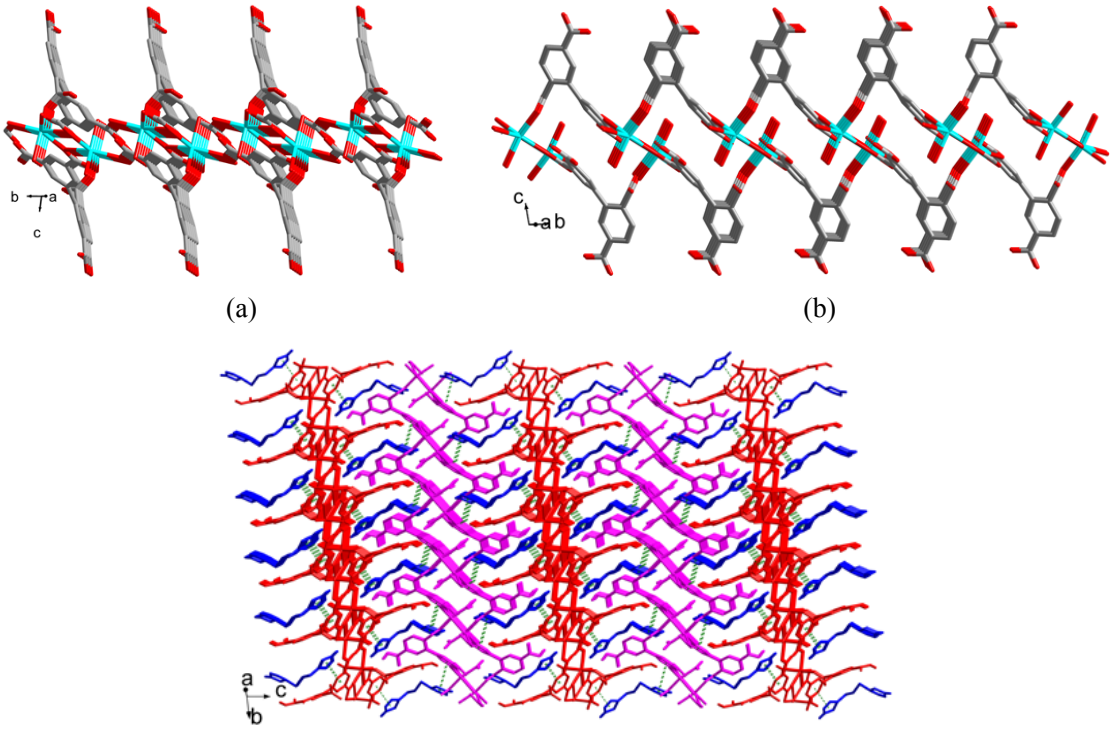
Cd(2)-O(11)#4	2.464(3)	O(10)#4-Cd(2)-O(4)	79.34(11)
N(4)-Cd(1)-O(13)#1	104.72(10)	N(1)#3-Cd(2)-O(5)	86.36(11)
N(4)-Cd(1)-O(7)	96.19(10)	O(6)-Cd(2)-O(5)	91.93(9)
O(13)#1-Cd(1)-O(7)	122.45(9)	O(10)#4-Cd(2)-O(5)	119.68(10)
N(4)-Cd(1)-O(9)#2	101.85(10)	O(4)-Cd(2)-O(5)	160.40(9)
O(13)#1-Cd(1)-O(9)#2	136.58(9)	N(1)#3-Cd(2)-O(11)#4	123.83(11)
O(7)-Cd(1)-O(9)#2	87.52(8)	O(6)-Cd(2)-O(11)#4	84.40(9)
N(4)-Cd(1)-O(12)#1	159.67(10)	O(10)#4-Cd(2)-O(11)#4	54.40(9)
O(13)#1-Cd(1)-O(12)#1	55.41(8)	O(4)-Cd(2)-O(11)#4	117.11(10)
O(7)-Cd(1)-O(12)#1	92.37(8)	O(5)-Cd(2)-O(11)#4	80.57(9)
Complex 4			
Cd(1)-N(4)#1	2.234(3)	O(8)-Cd(1)-O(1)	83.73(9)
Cd(1)-O(8)	2.277(2)	N(1)-Cd(1)-O(1)	161.70(9)
Cd(1)-N(1)	2.333(3)	O(4)#2-Cd(1)-O(1)	115.91(10)
Cd(1)-O(4)#2	2.417(2)	N(4)#1-Cd(1)-O(9)	105.85(10)
Cd(1)-O(1)	2.474(3)	O(8)-Cd(1)-O(9)	54.55(8)
Cd(1)-O(9)	2.519(2)	N(1)-Cd(1)-O(9)	79.25(9)
Cd(1)-O(5)#2	2.539(2)	O(4)#2-Cd(1)-O(9)	133.09(8)
N(4)#1-Cd(1)-O(8)	157.30(10)	O(1)-Cd(1)-O(9)	83.35(9)
N(4)#1-Cd(1)-N(1)	96.85(11)	N(4)#1-Cd(1)-O(5)#2	83.77(7)
O(8)-Cd(1)-N(1)	90.71(10)	O(8)-Cd(1)-O(5)#2	109.77(9)
N(4)#1-Cd(1)-O(4)#2	118.33(9)	N(1)-Cd(1)-O(5)#2	123.39(9)
O(8)-Cd(1)-O(4)#2	83.97(9)	O(4)#2-Cd(1)-O(5)#2	51.77(7)
N(1)-Cd(1)-O(4)#2	80.62(9)	O(1)-Cd(1)-O(5)#2	74.81(8)
N(4)#1-Cd(1)-O(1)	82.45(11)	O(9)-Cd(1)-O(5)#2	154.85(9)
Complex 5			
Cd(1)-N(1)	2.247(6)	Cd(2)-O(6)#3	2.219(6)
Cd(1)-N(6)#1	2.256(5)	Cd(2)-N(4)#4	2.234(6)
Cd(1)-O(2)	2.269(4)	Cd(2)-O(4)	2.272(6)
Cd(1)-O(8)#2	2.280(5)	Cd(2)-O(9)	2.385(9)
Cd(1)-O(1)	2.453(5)	Cd(2)-O(3)	2.482(5)
Cd(1)-O(7)#2	2.532(5)	O(2)-Cd(1)-O(7)#2	102.46(17)
N(1)-Cd(1)-N(6)#1	93.0(2)	O(8)#2-Cd(1)-O(7)#2	53.33(17)
N(1)-Cd(1)-O(2)	94.24(19)	O(1)-Cd(1)-O(7)#2	153.27(19)
N(6)#1-Cd(1)-O(2)	147.25(18)	O(6)#3-Cd(2)-N(4)#4	114.0(2)
N(1)-Cd(1)-O(8)#2	139.59(18)	O(6)#3-Cd(2)-O(4)	87.6(2)
N(6)#1-Cd(1)-O(8)#2	88.6(2)	N(4)#4-Cd(2)-O(4)	156.7(2)
O(2)-Cd(1)-O(8)#2	105.89(19)	O(6)#3-Cd(2)-O(9)	105.8(3)
N(1)-Cd(1)-O(1)	105.6(2)	N(4)#4-Cd(2)-O(9)	92.3(3)
N(6)#1-Cd(1)-O(1)	92.42(18)	O(4)-Cd(2)-O(9)	89.6(3)
O(2)-Cd(1)-O(1)	54.89(16)	O(6)#3-Cd(2)-O(3)	140.7(2)
O(8)#2-Cd(1)-O(1)	114.7(2)	N(4)#4-Cd(2)-O(3)	104.1(2)
N(1)-Cd(1)-O(7)#2	88.64(18)	O(4)-Cd(2)-O(3)	53.29(19)
N(6)#1-Cd(1)-O(7)#2	109.62(18)	O(9)-Cd(2)-O(3)	80.7(2)

Symmetry transformations used to generate equivalent atoms: #1: $x, y-1, z$; #2: $-x+1/2, -y-1/2, -z$; #3: $x-1/2, y-1/2, z$ for **1**. #1: $x, y, z-1$; #2: $x-1, y, z-1$; #3: $-x+2, y-1/2, -z+2$; #4: $x, y+1, z$; #5: $-x+2, y+1/2, -z+2$ for **2**. #1: $-x+1, -y+1, -z$; #2: $-x+3/2, y-1/2, -z+1/2$; #3: $-x+2, -y+1, -z+1$; #4: $x+1, y, z$ for **3**. #1: $x+1, -y+3/2, -z-1/2$; #2: $x, y, z-1$ for **4**. #1: $x, -y+3/2, z-1/2$; #2: $x+1, y, z-1$; #3: $x, -y+1/2, z+1/2$; #4: $-x+1, y-1/2, -z+3/2$ for **5**.

Table S3 Hydrogen bonding distances (Å) and angles (°) data for 1–5[a].

D-H···A	d(D-H)	d(H···A)	d(D···A)	∠(DHA)
Complex 1				
O(1)-H(1W)...O(5)#7	0.85	2.56	3.408(14)	179.6
O(1)-H(2W)...O(6)#8	0.85	2.25	2.706(12)	113.6
O(5)-H(5)...O(3)#9	0.82	1.96	2.731(13)	156.5
Complex 2				
O(10)-H(4W)···O(6)#5	0.85	1.96	2.783(3)	164.1
O(10)-H(3W)···O(1)#2	0.85	2.17	2.699(3)	120.5
O(9)-H(2W)···O(2)#1	0.85	1.91	2.753(4)	169.5
O(9)-H(1W)···O(8)#1	0.85	1.95	2.761(3)	159.9
Complex 3				
O(1)-H(1W)...O(5)#5	0.85	2.27	3.081(4)	160.6
O(1)-H(2W)...O(13)#9	0.85	2.19	2.938(4)	146.0
O(2)-H(3W)...O(3)#8	0.85	1.90	2.740(5)	168.7
O(2)-H(4W)...O(12)#1	0.85	2.14	2.988(4)	174.0
O(3)-H(5W)...O(11)#9	0.85	1.95	2.765(4)	159.7
O(3)-H(6W)...O(6)#3	0.85	2.22	2.869(4)	133.6
O(4)-H(7W)...N(1)#3	0.85	2.62	3.263(5)	132.8
O(4)-H(8W)...O(1)#4	0.85	1.96	2.805(4)	174.4
O(5)-H(9W)...O(9)#2	0.85	1.98	2.822(3)	173.1
O(5)-H(10W)...O(1)#2	0.85	2.26	3.081(4)	162.0
Complex 4				
O(6)-H(6)...O(5)#5	0.82	1.74	2.541(3)	165.0
O(2)-H(2)...O(4)#6	0.82	1.83	2.645(3)	172.2
O(1)-H(2W)...O(7)#7	0.85	2.09	2.923(3)	165.0
O(1)-H(1W)...O(7)	0.85	2.08	2.907(4)	163.3
Complex 5				
O(9)-H(2W) ···O(1)#9	0.85	2.22	2.850(8)	131.2

[a] Symmetry codes: #7: x – 1/2, – y + 1/2, z – 1/2; #8 –x, –y, –z; #9 – x + 1, y, – z + 1/2 for **1**. #1: *x*, *y*, *z* – 1; #2: *x* – 1, *y*, *z* – 1; #5: – *x* + 2, *y* + 1/2, – *z* + 2 for **2**. #1: – *x* + 1, - *y* + 1, – *z*; #2: – *x* + 3/2, *y* – 1/2, – *z* +1/2; #3: – *x* + 2, – *y* + 1, – *z* + 1; #4: *x* + 1, *y*, *z*; #5: – *x* + 3/2, *y* + 1/2, – *z* +1/2; #7: *x* – 1/2, – *y* + 3/2, *z* + 1/2; #8: *x*, *y*, *z* – 1; #9: – *x* + 1, – *y* + 1, – *z* + 1for **3**. #5: – x + 3, – y + 1, – z + 1; #6: – x + 2, – y + 1, – z + 1; #7:– x + 3, – y + 1, – z for **4.** #9: – *x*, – *y* + 1, – *z* + 1 for **5**.



(a) (b)

(c)

Fig. S1. (a) View of 2D layer along the crystallographic [110] direction in **1**. (b) View of 2D layer along the[100] direction in **1**. (c) π···π stacking interactions exist between benzene rings of $Hbptc^{3-}$ ligands and imidazole rings of 1,3-H_2bip ligands.

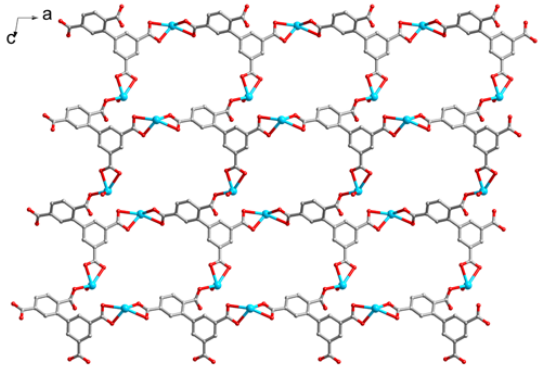


Fig. S2. View of the 2D layer constructed by Cd(II) atoms and $bptc^{4-}$ ligands.

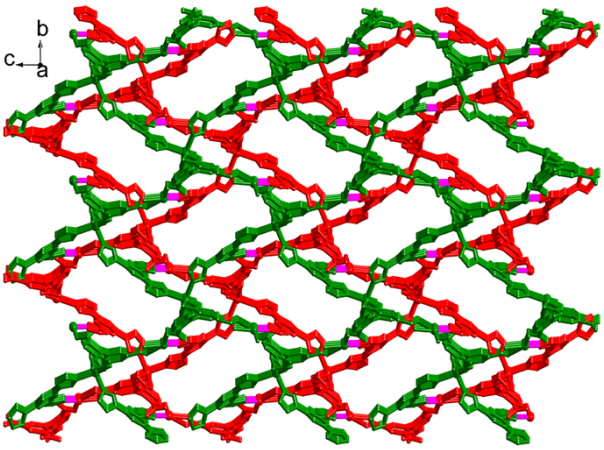


Fig. S3. View of 3D network of **5**, in which, two parts of **dia** nets (green and red) are joined together by N4-Cd2 bonds (pink).

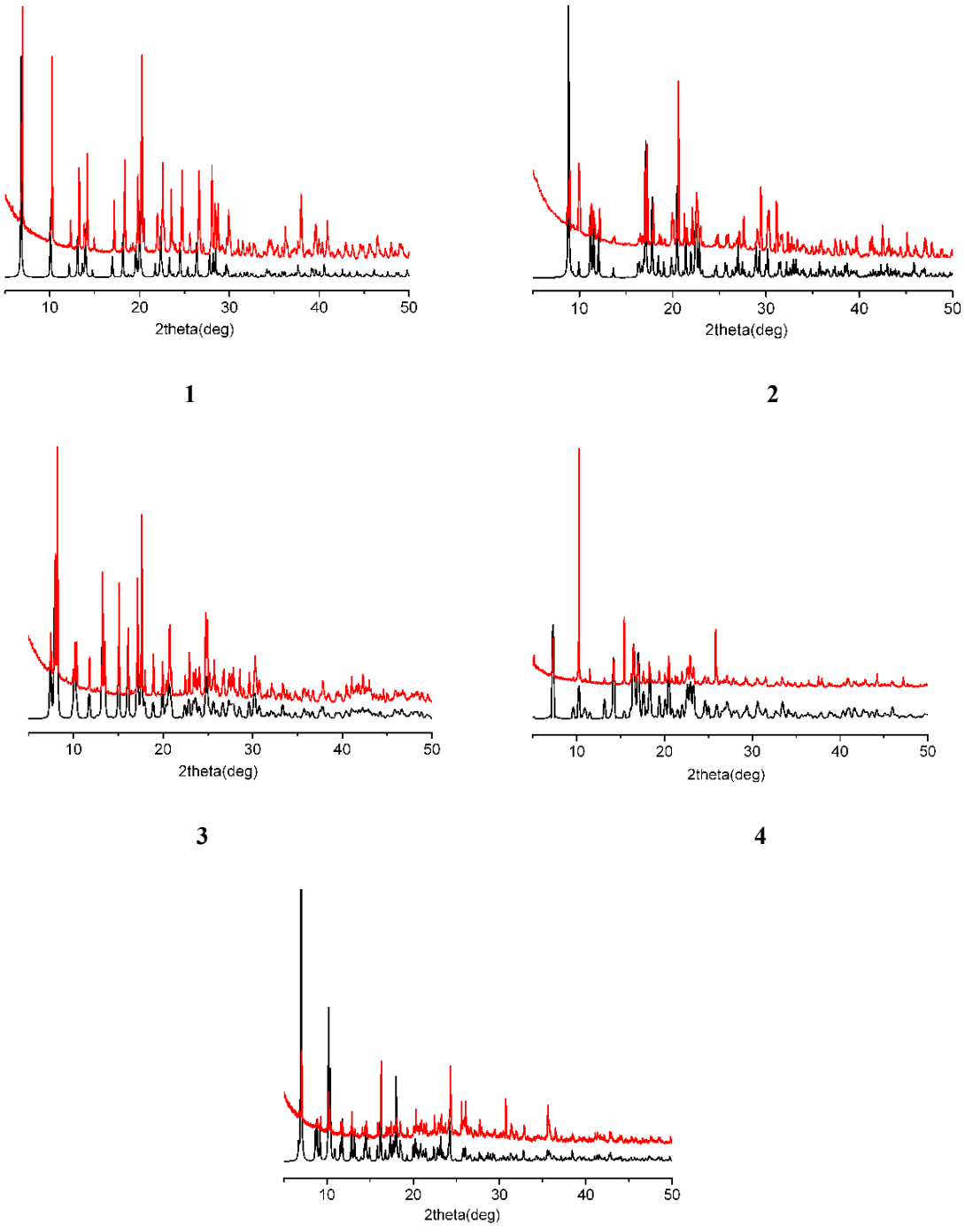


Fig. S4. Comparison of the experimental and simulated PXRD patterns. In each case, the top is the experimental pattern and the bottom is the simulated one.