

## Supporting Information

# **A Series of Ag(I)-Cd(II) Hetero- and Ag(I) Homo-nuclear Coordination Polymers Based on 5-Iodo-Isophthalic Acid and N-Donor Ancillary Ligands**

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**Table S1.** Crystal data and structure refinement parameters for complexes **1–5**.

Compound No.	1	2	3	4	5
formula	C <sub>36</sub> H <sub>28</sub> N <sub>4</sub> O <sub>11</sub> I <sub>2</sub> CdA	C <sub>40</sub> H <sub>24</sub> N <sub>4</sub> O <sub>9</sub> I <sub>2</sub> CdAg	C <sub>14</sub> H <sub>10</sub> NO <sub>4</sub> IAg <sub>2</sub>	C <sub>20</sub> H <sub>15</sub> N <sub>2</sub> O <sub>4</sub> IAg <sub>2</sub>	C <sub>44</sub> H <sub>34</sub> N <sub>8</sub> O <sub>8</sub> I <sub>2</sub> Ag
	g <sub>2</sub>	2			4
fw	1274.58	1286.58	598.87	689.98	1488.07
crystal system	Monoclinic	Monoclinic	Monoclinic	Triclinic	Triclinic
space group	<i>P</i> 2 <sub>1</sub> / <i>c</i>	<i>P</i> 2 <sub>1</sub> / <i>c</i>	<i>C</i> 2/ <i>c</i>	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$
<i>a</i> (Å)	14.0054(3)	15.7940(5)	26.0990(17)	9.2367(9)	11.2576(4)
<i>b</i> (Å)	15.1789(3)	13.4071(6)	8.7015(3)	9.3456(8)	12.6293(4)
<i>c</i> (Å)	18.5649(3)	17.8147(8)	15.0839(9)	13.4445(11)	16.9504(3)
$\alpha$ (°)	90.00	90.00	90.00	88.897(7)	102.542(3)
$\beta$ (°)	94.108(2)	93.021(3)	116.468(8)	71.282(8)	93.087(3)
$\gamma$ (°)	90.00	90.00	90.00	67.893(8)	106.942(3)
<i>V</i> (Å <sup>3</sup> )	3936.51(13)	3767.1(3)	3066.5(4)	1011.53(16)	2232.56(14)
<i>Z</i>	4	4	8	2	2
<i>D</i> <sub>c</sub> (g·cm <sup>-3</sup> )	2.151	2.269	2.594	2.265	2.214
<i>F</i> (000)	2432	2448	2240	656	1424
reflns collected	15670	14285	6301	7642	14176
Independent reflns	6923	6616	2697	3565	7839
<i>R</i> (int)	0.0297	0.0358	0.0285	0.0338	0.0270
GOF on <i>F</i> <sup>2</sup>	1.077	1.091	1.064	1.001	1.074
<i>R</i> <sub>1</sub> <sup>a</sup> ( <i>I</i> > 2σ( <i>I</i> ))	0.0396	0.0760	0.0387	0.0332	0.0492
w <i>R</i> <sub>2</sub> <sup>b</sup> ( <i>I</i> > 2σ( <i>I</i> ))	0.0727	0.1563	0.1240	0.0665	0.1126

$$^a R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|, \quad ^b wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)]^{1/2}$$

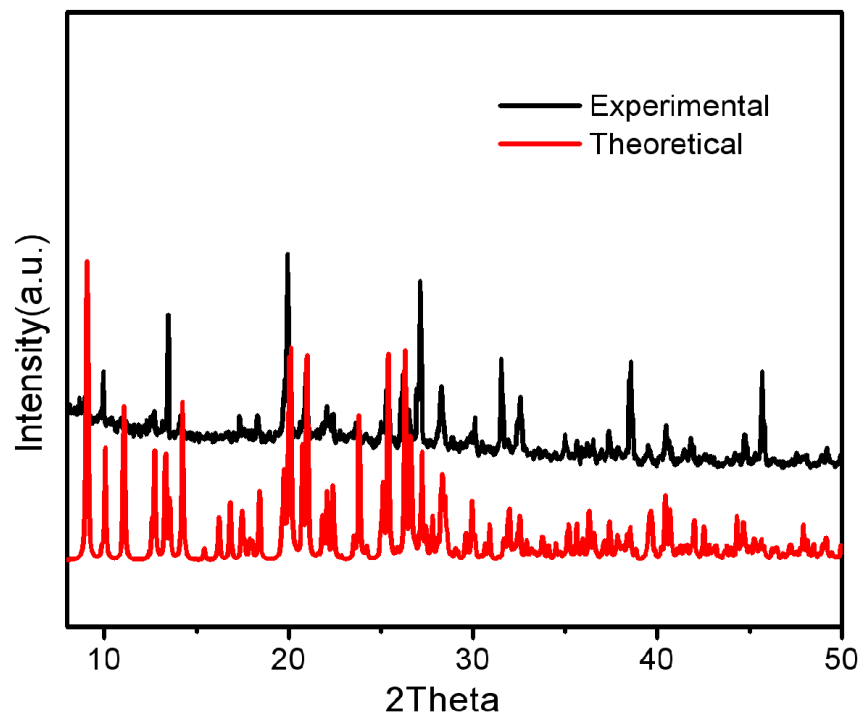
**Table S2.** Selected Bond Distances and Angles for Compounds **1–5**.

Compound 1 <sup>a</sup>			
Ag(1)–N(3)	2.175(4)	Ag(1)–N(1)	2.160(4)
Ag(2)–N(2)#3	2.172(4)	Ag(2)–N(4)	2.171(4)
Ag(2)–O(1W)	2.555(5)	Cd(1)–O(8)#2	2.325(4)
Cd(1)–O(4)#1	2.247(4)	Cd(1)–O(6)	2.295(3)
Cd(1)–O(1)	2.209(4)	N(3)–Ag(1)–N(1)	159.48(18)
N(2)#3–Ag(2)–N(4)	162.09(19)	N(4)–Ag(2)–O(1W)	104.20(18)
N(2)#3–Ag(2)–O(1W)	92.92(18)	O(1)–Cd(1)–O(4)#1	114.18(15)
O(8)#2–Cd(1)–O(4)#1	121.14(14)	O(8)#2–Cd(1)–O(1)	93.58(14)
O(6)–Cd(1)–O(1)	121.93(13)	O(8)#2–Cd(1)–O(6)	117.49(13)

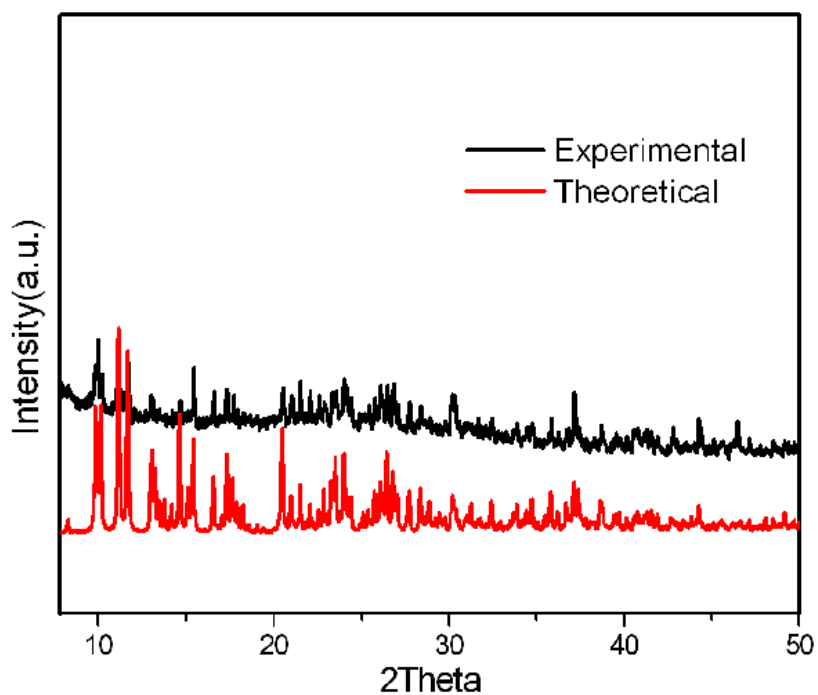
O(4)#1–Cd(1)–O(6)	91.07(14)		
Compound 2 <sup>b</sup>			
Ag(1)–N(1)	2.422(9)	Ag(1)–N(2)	2.252(9)
Ag(1)–O(4)	2.275(7)	Ag(2)–N(3)	2.286(10)
Ag(2)–N(4)	2.373(9)	Ag(2)–O(1)	2.526(8)
Cd(1)–O(3)#4	2.247(7)	Cd(1)–O(7)#5	2.259(6)
Cd(1)–O(5)	2.291(7)	Cd(1)–O(1)	2.355(7)
Cd(1)–O(2)	2.472(7)	Cd(1)–O(6)	2.581(7)
N(2)–Ag(1)–O(4)	169.3(3)	N(2)–Ag(1)–N(1)	71.2(3)
O(4)–Ag(1)–N(1)	111.2(3)	O(3)#4–Cd(1)–O(7)#5	103.1(2)
O(3)#4–Cd(1)–O(5)	109.6(3)	O(7)#5–Cd(1)–O(5)	123.9(2)
O(3)#4–Cd(1)–O(1)	118.3(2)	O(7)#5–Cd(1)–O(1)	120.8(3)
O(5)–Cd(1)–O(1)	80.8(2)	O(3)#2–Cd(1)–O(2)	85.7(3)
O(7)#1–Cd(1)–O(2)	92.7(2)	O(5)–Cd(1)–O(2)	133.1(2)
O(1)–Cd(1)–O(2)	53.8(2)	O(3)#4–Cd(1)–O(6)	89.1(2)
O(7)#5–Cd(1)–O(6)	83.7(2)	O(5)–Cd(1)–O(6)	53.5(2)
O(1)–Cd(1)–O(6)	133.3(2)	O(2)–Cd(1)–O(6)	172.8(2)
N(3)–Ag(2)–N(4)	72.1(3)	N(3)–Ag(2)–O(1)	96.6(3)
N(4)–Ag(2)–O(1)	92.6(3)		
Compound 3 <sup>c</sup>			
Ag(1)–N(1)	2.141(6)	Ag(1)–O(1)	2.227(5)
Ag(2)–O(4)#1	2.204(5)	Ag(2)–O(3)	2.207(4)
Ag(2)–O(2)#2	2.468(5)	N(1)–Ag(1)–O(1)	144.2(2)
O(4)#1–Ag(2)–O(3)	159.4(2)	O(4)#1–Ag(2)–O(2)#2	104.31(19)
O(3)–Ag(2)–O(2)#2	91.69(18)		
Compound 4 <sup>d</sup>			
Ag(1)–O(2)#1	2.194(3)	Ag(1)–O(1)	2.241(3)
Ag(1)–O(4)#2	2.486(3)	Ag(2)–N(2)	2.179(4)
Ag(2)–N(1)	2.197(4)	O(2)#1–Ag(1)–O(1)	158.62(13)
O(2)#1–Ag(1)–O(4)#2	99.81(12)	O(1)–Ag(1)–O(4)#2	96.43(12)
N(2)–Ag(2)–N(1)	165.43(15)		

Compound 5 <sup>e</sup>			
Ag(1)–O(1)	2.305(4)	Ag(1)–O(7)	2.339(4)
Ag(1)–O(8)#4	2.404(4)	Ag(2)–O(4)	2.107(4)
Ag(2)–O(4) #5	2.113(3)	Ag(5)–N(8)#6	2.097(4)
Ag(5)–N(8)	2.097(5)	Ag(3)–N(1)	2.222(5)
Ag(3)–O(6)	2.365(4)	Ag(3)–O(3) #1	2.458(4)
Ag(3)–O(5)	2.569(4)	Ag(4)–N(5)	2.121(5)
Ag(4)–N(4)	2.124(5)	O(1)–Ag(1)–O(7)	102.97(16)
O(1)–Ag(1)–O(8)#4	129.32(14)	O(7)–Ag(1)–O(8)#4	124.42(15)
O(4)–Ag(2)–O(4)#5	180.000(2)	N(8)–Ag(5)–N(8)#3	180.00(17)
N(1)–Ag(3)–O(6)	160.04(17)	N(1)–Ag(3)–O(3)#1	103.02(16)
O(6)–Ag(3)–O(3)#1	96.41(14)	N(1)–Ag(3)–O(5)	121.49(16)
O(6)–Ag(3)–O(5)	53.09(13)	O(3)#1–Ag(3)–O(5)	90.48(14)
N(5)–Ag(4)–N(4)	174.0(2)		

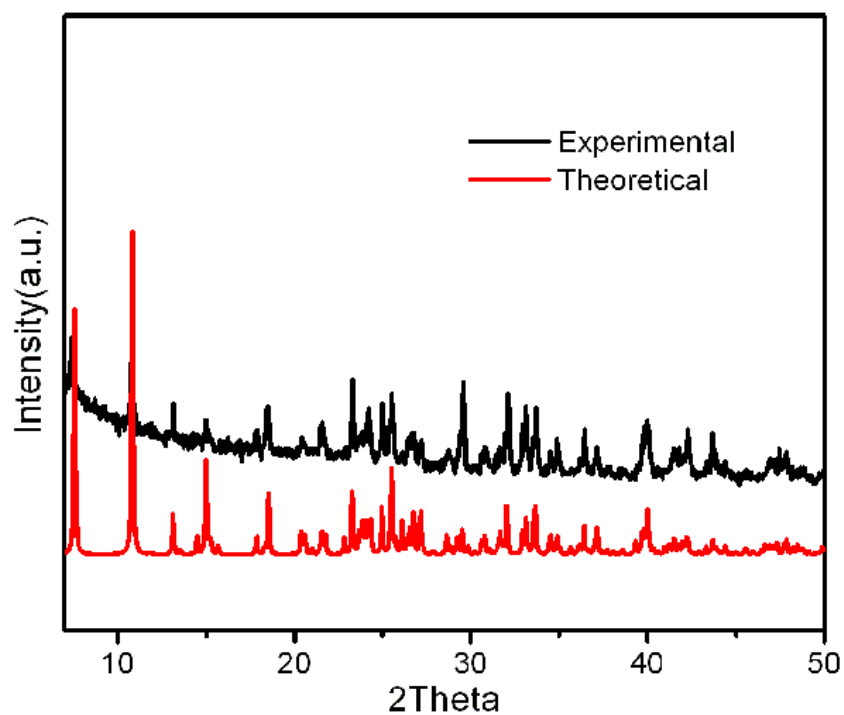
Symmetry codes: <sup>a</sup>#1 x-1, -y+1/2, z+1/2; #2 x, y-1, z; #3 x+1, y, z. <sup>b</sup>#4 1-x, y+1/2, 1/2-z; #5 -x+2, y-1/2, 1/2-z. <sup>c</sup>#1 -x+1, -y+3, -z; #2 x, y+1, z. <sup>d</sup>#1 -x+2,-y,-z; #2 -x+1,-y+1,-z. <sup>e</sup>#1 -x, -y+1, -z+1; #2 -x-1, -y+1, -z+2; #3 -x+2, -y+2, -z-1. #4 -x, -y, -z; #5 x+1, y, z-1. #6 x-1, y-1, z.



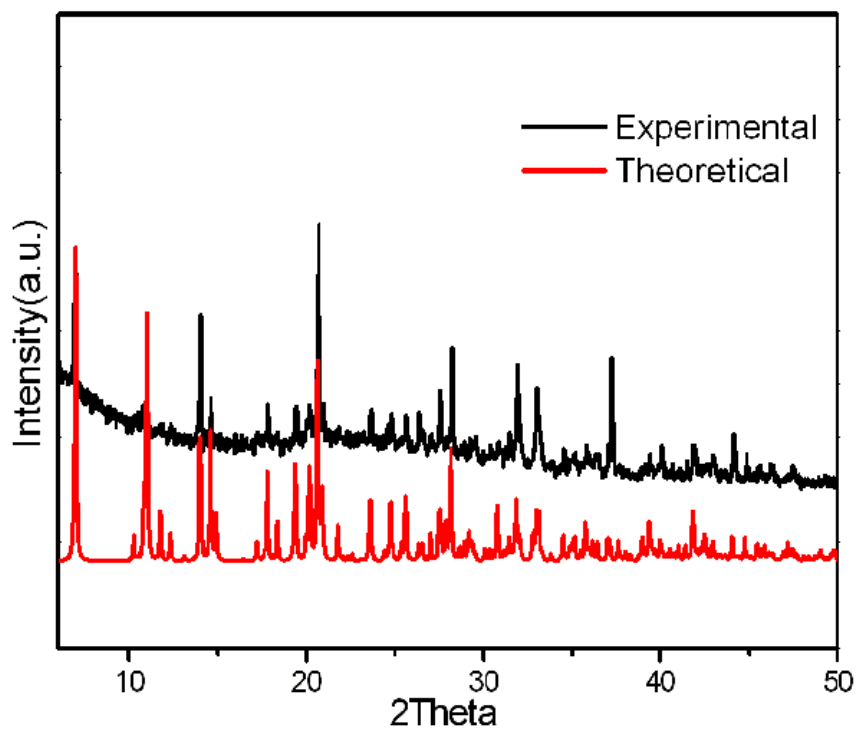
**Figure S1.** The theoretical and experimental PXR D patterns for 1.



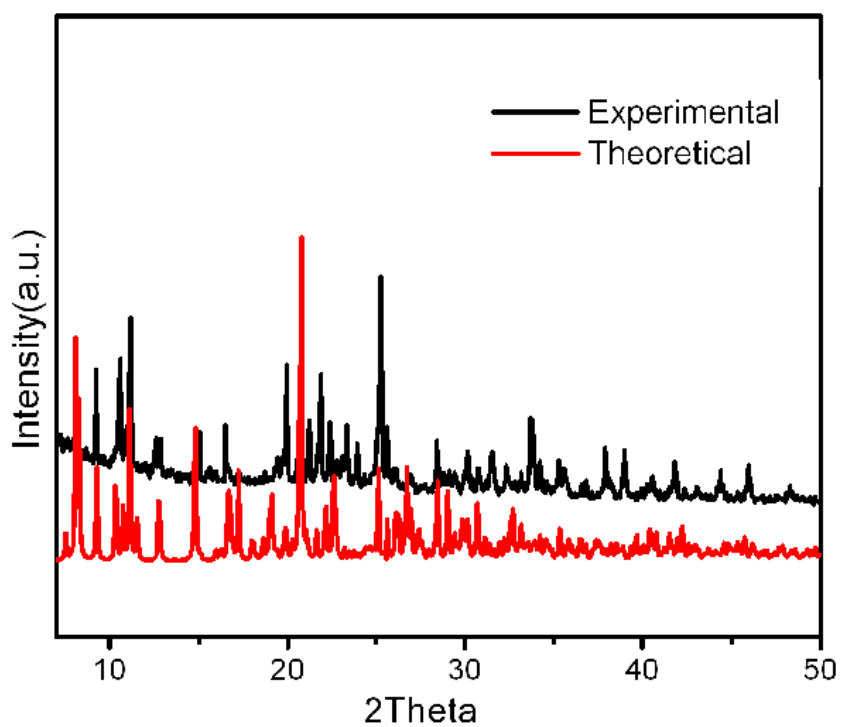
**Figure S2.** The theoretical and experimental PXR D patterns for 2.



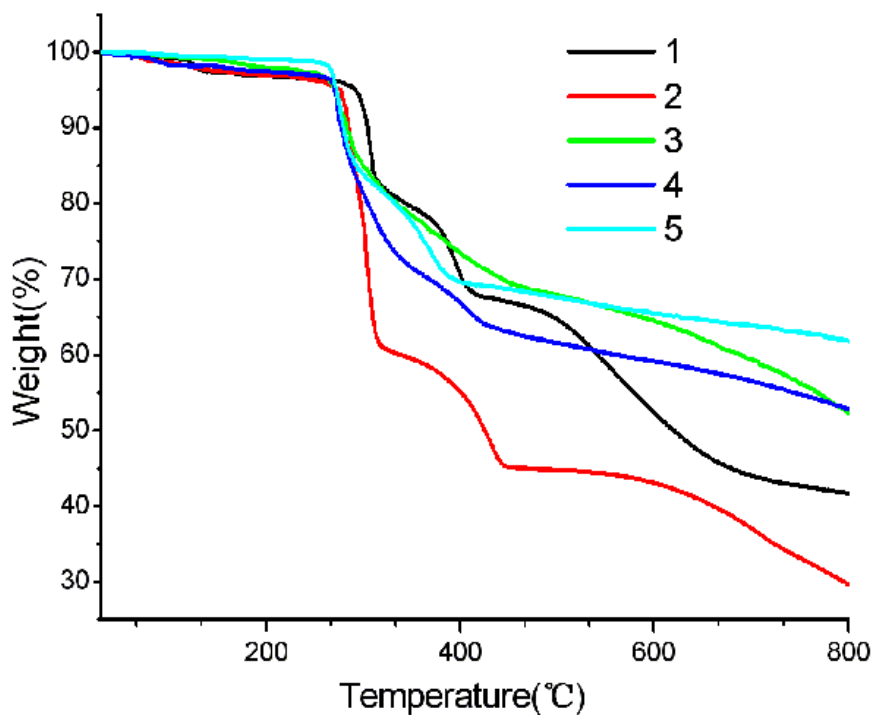
**Figure S3.** The theoretical and experimental PXR D patterns for **3**.



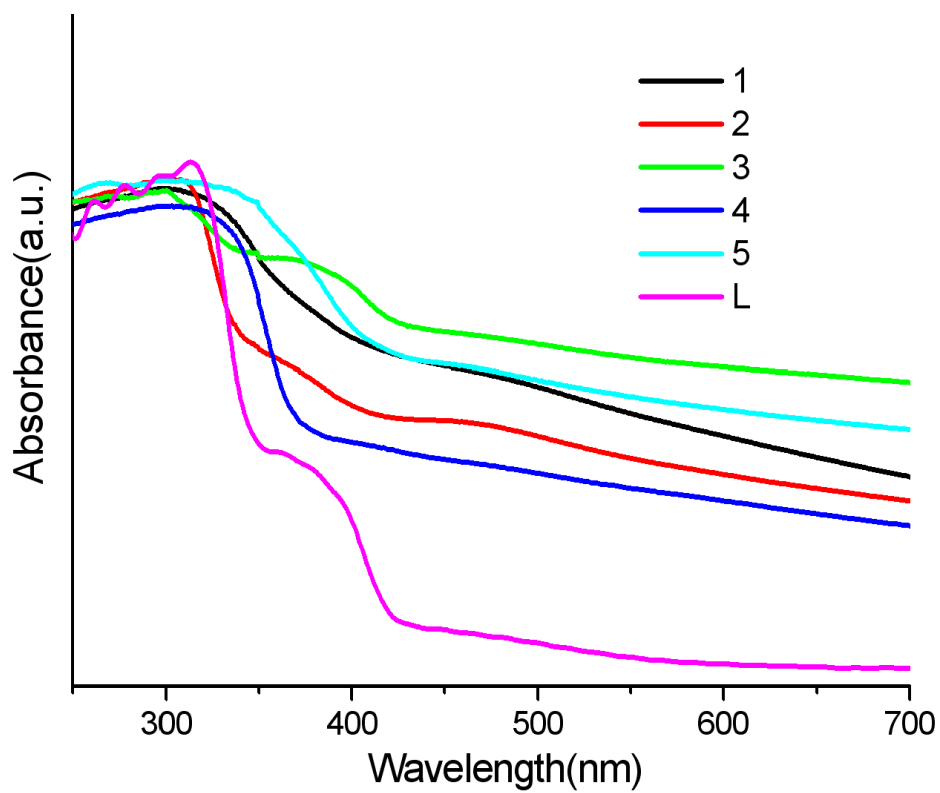
**Figure S4.** The theoretical and experimental PXR D patterns for **4**.



**Figure S5.** The theoretical and experimental PXR D patterns for 5.



**Figure S6.** TG curves for compounds 1–5.



**Figure S7.** UV-vis absorption spectre for ligand and compounds **1–5**.