Supplementary Materials

Zn(II), Cd(II) and Hg(II) Halide Coordination polymers supported by bis-pyridyl-bis-amide: structural diversity and structural transformation

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Fig. S1. The 2D layers of complex **9** are supported by the N-H---O hydrogen bonds.

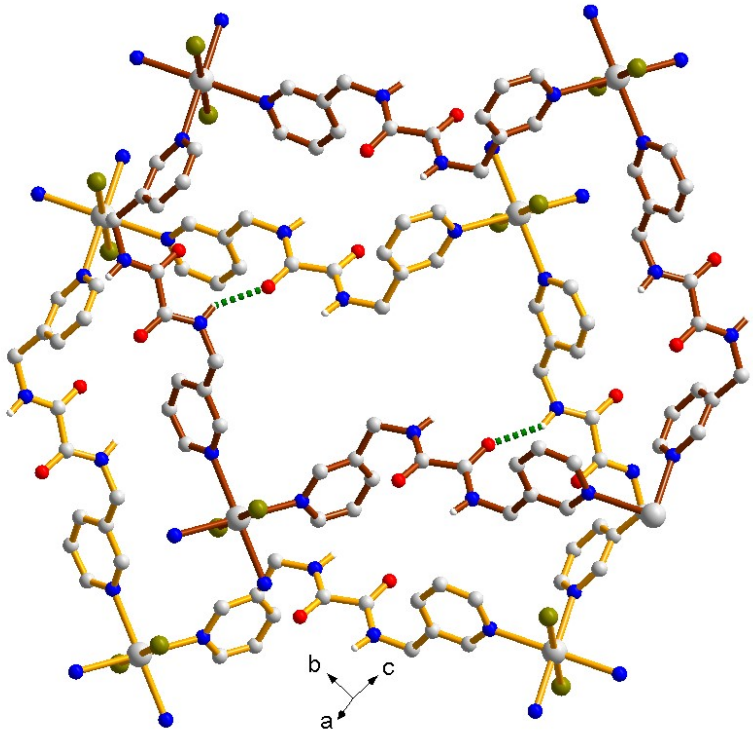

Fig. S2. The 3D framework of complex **10** is supported by the N-H---O hydrogen bonds.

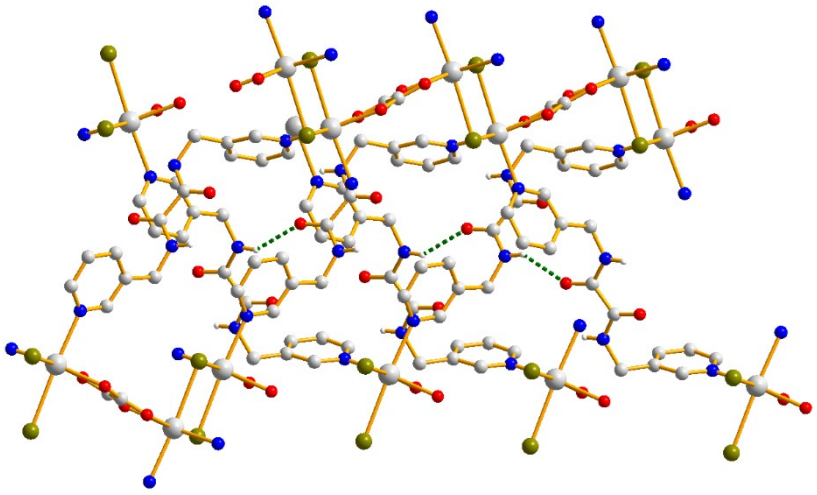

Fig. S3. The 2D layers of complex **11** are supported by the N-H---O hydrogen bonds.

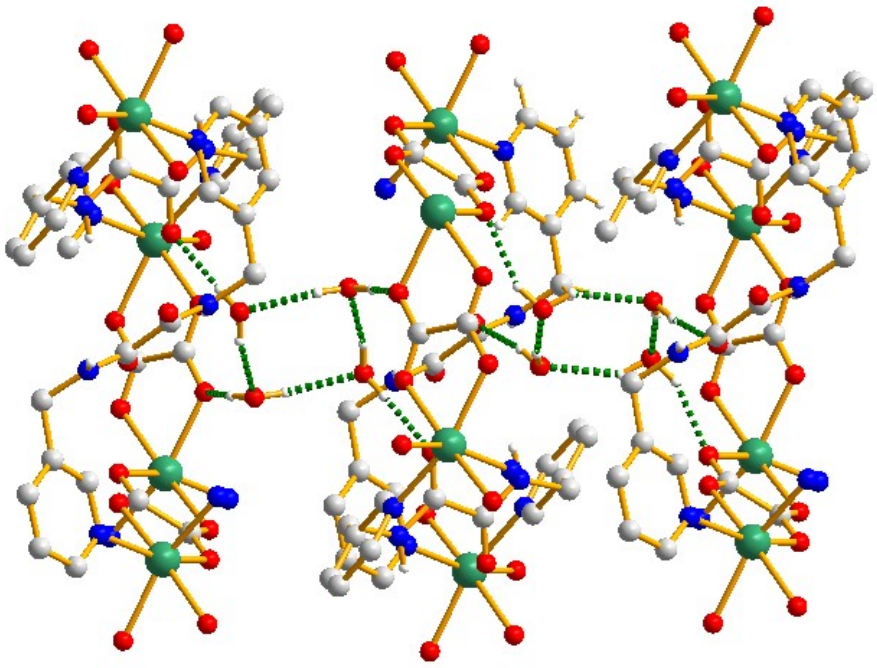

Fig. S4. (a) Simulated and (b) experimental PXRD patterns of **1**. Complex **1** has been transformed to complex **2** upon DMF removal.

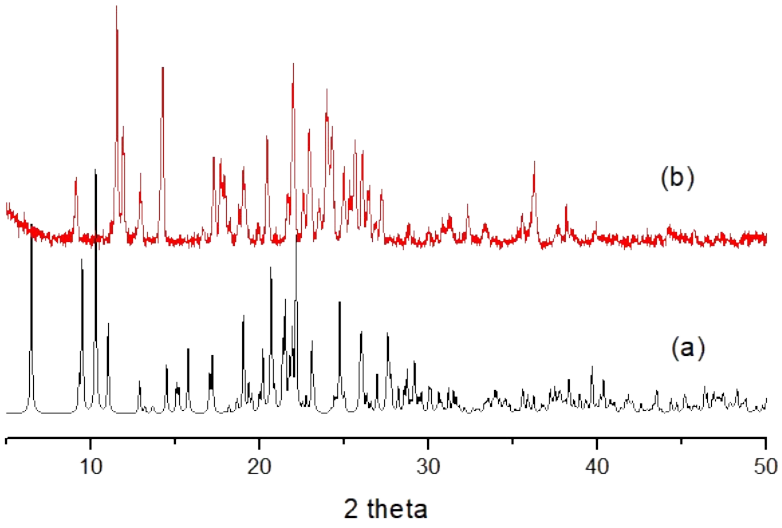

Fig. S5. (a) Simulated and (b) experimental PXRD patterns of **2**.

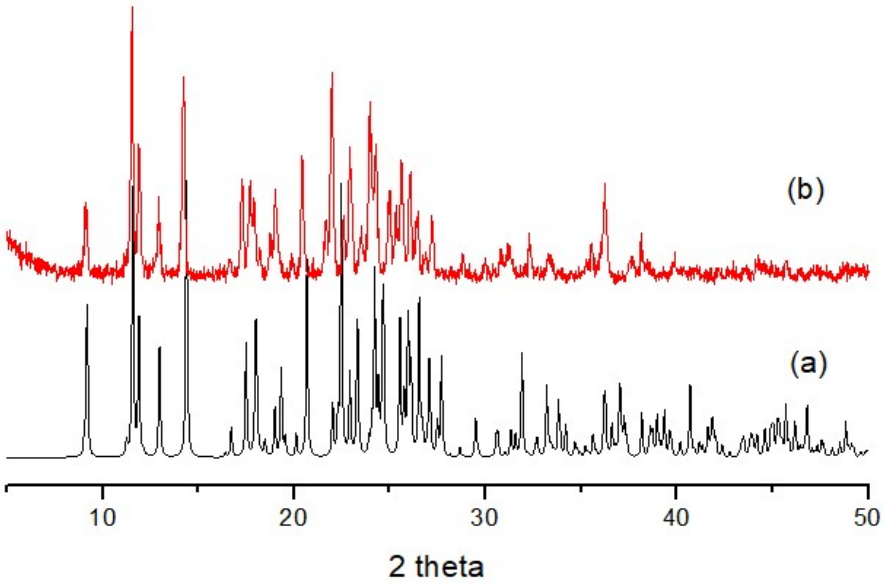

Fig. S6. (a) Simulated and (b) experimental PXRD patterns of **3**.

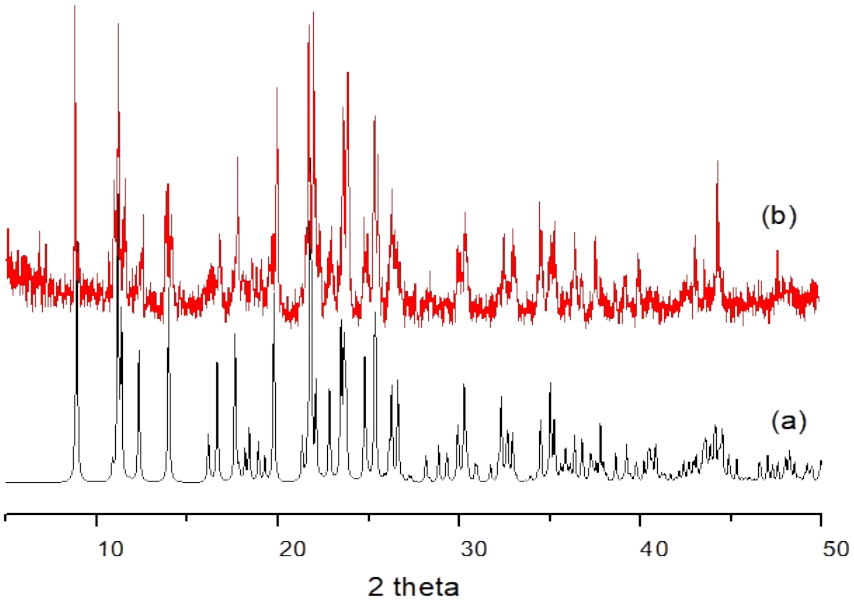

Fig. S7. (a) Simulated and (b) experimental PXRD patterns of **4**.

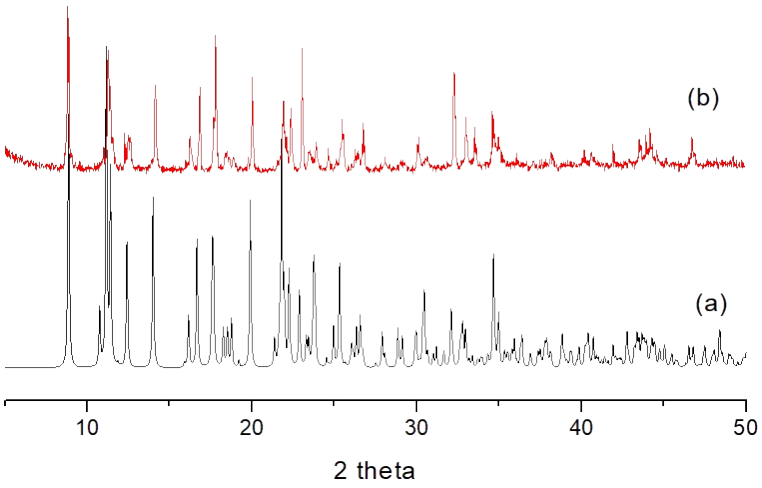

Fig. S8. (a) Simulated and (b) experimental PXRD patterns of **5**.

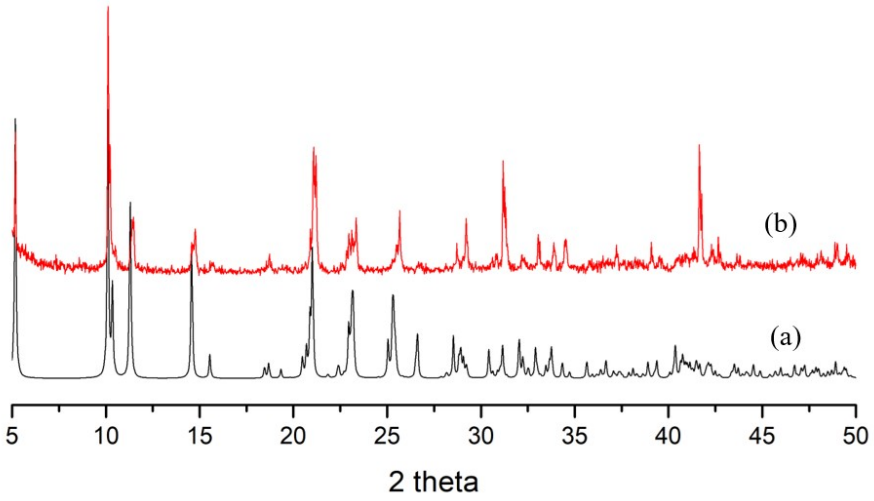

Fig. 9. (a) Simulated and (b) experimental PXRD patterns of **6**.

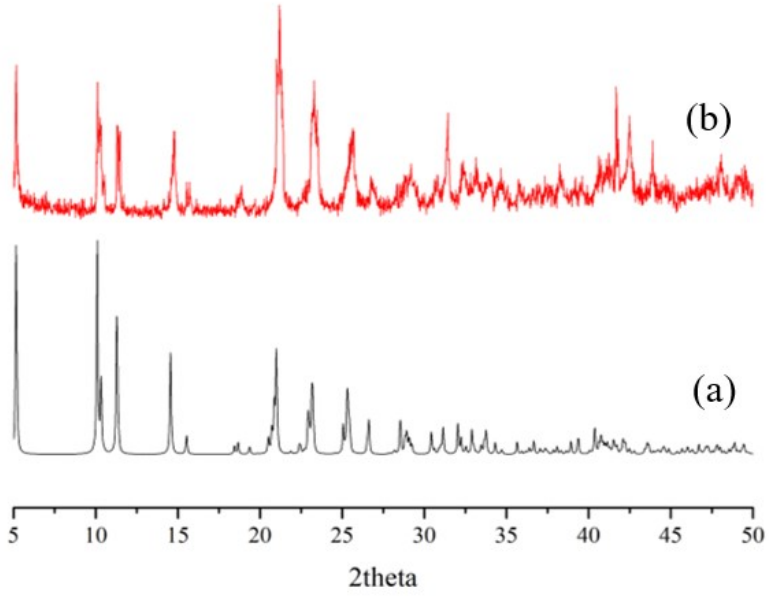

Fig. 10. (a) Simulated and (b) experimental PXRD patterns of **7**.

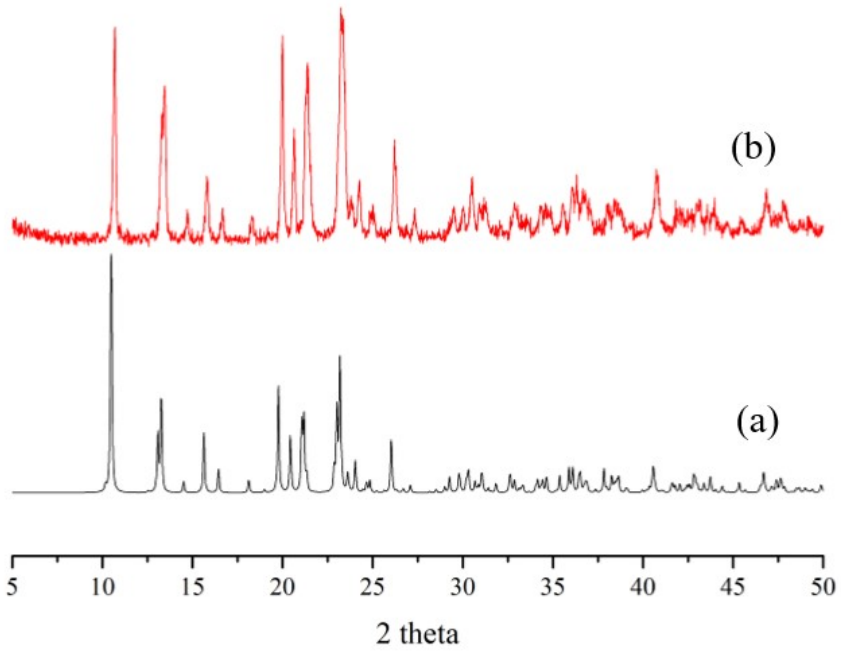

Fig. S11. (a) Simulated and (b) experimental PXRD patterns for **8**.

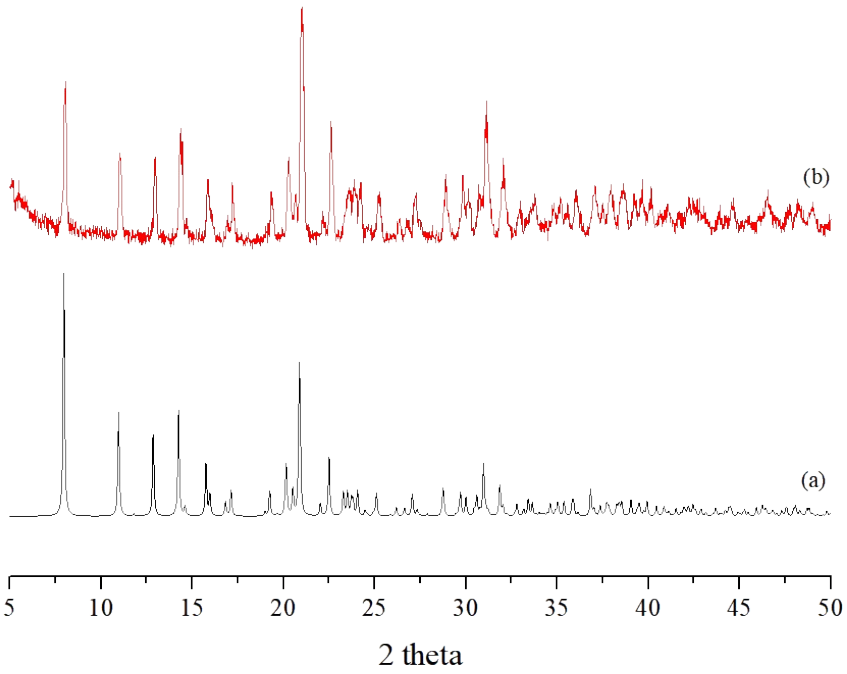

Fig. S12. (a) Simulated and (b) experimental PXRD patterns for **9**.

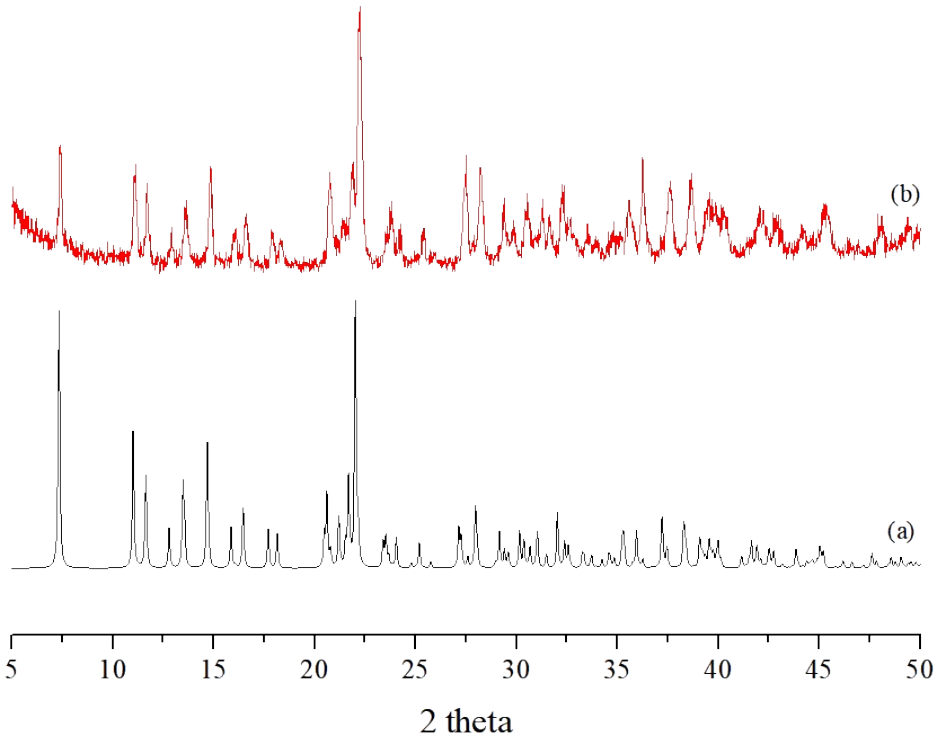

Fig. S13. (a) Simulated and (b) experimental PXRD patterns for **10**.

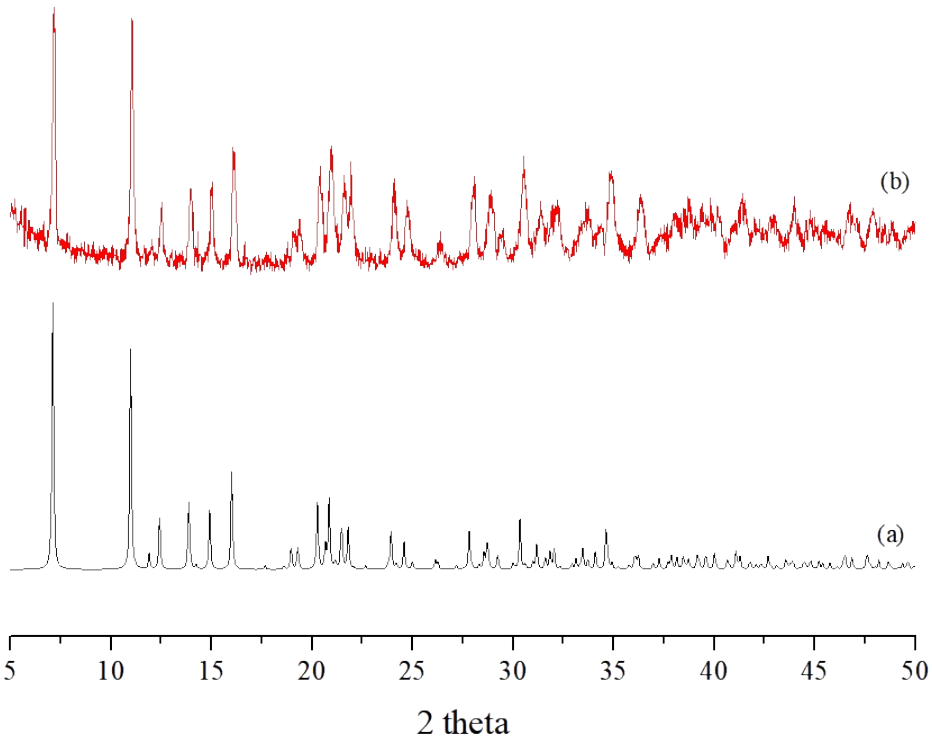

Fig. S14. (a) Simulated and (b) experimental PXRD patterns for **11**.

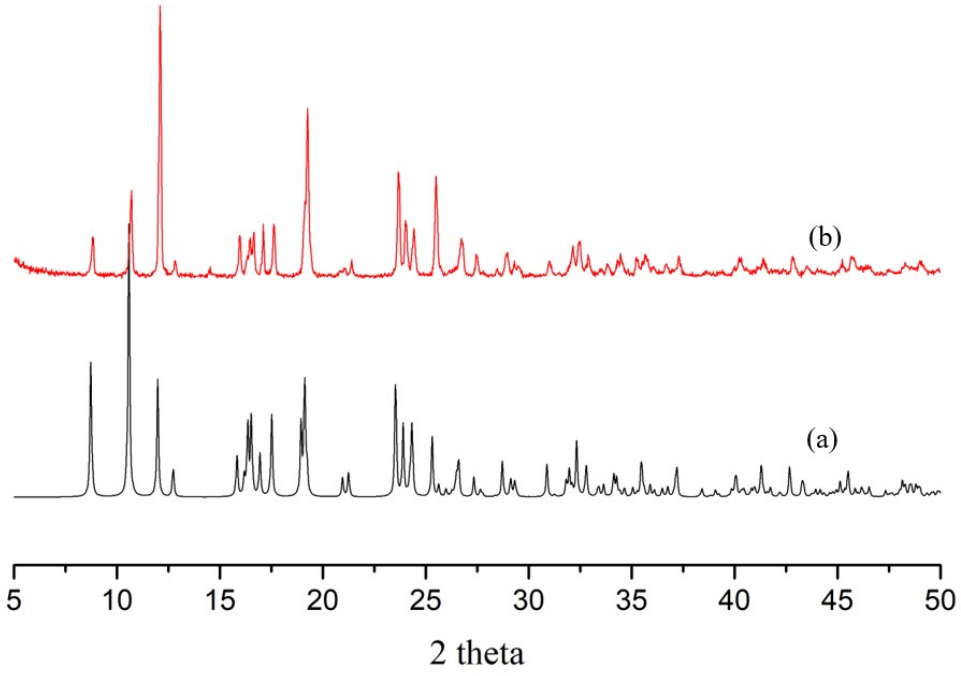

Fig. S15. (a) Simulated PXRD pattern of **8**, (b) as-synthesized PXRD pattern of **8**, (c) PXRD pattern of the sample of (b) heated in water at 120 °C for 2 days and (d) simulated PXRD pattern of **10**.

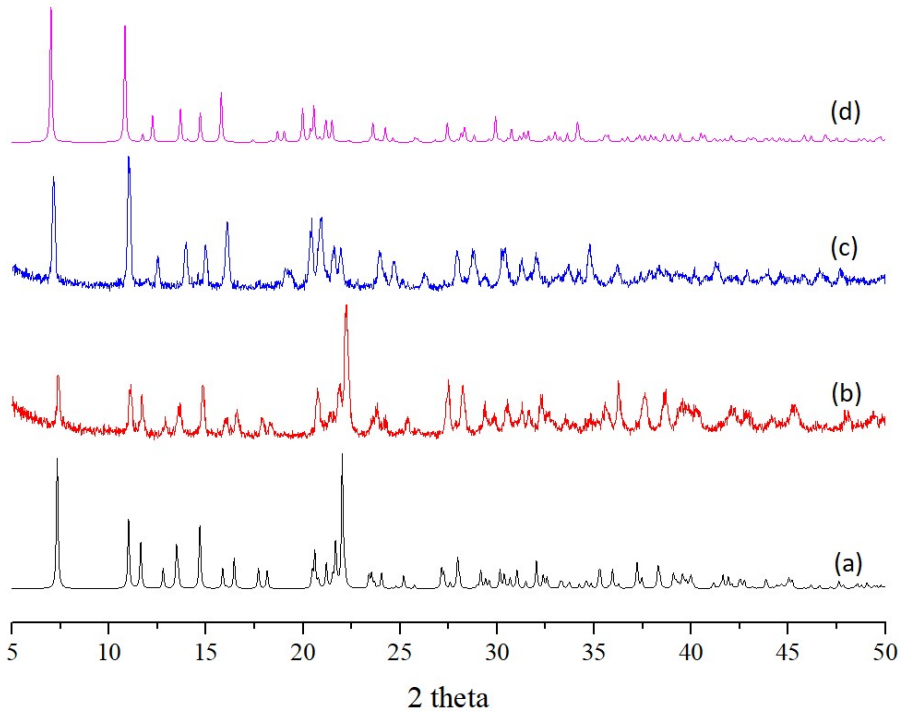

Fig. S16. (a) Simulated PXRD pattern of **9**, (b) as-synthesized PXRD pattern of **9**, (c) PXRD pattern of the sample of (b) heated in water at 140 °C for 2 days and (d) simulated PXRD pattern of **10**.

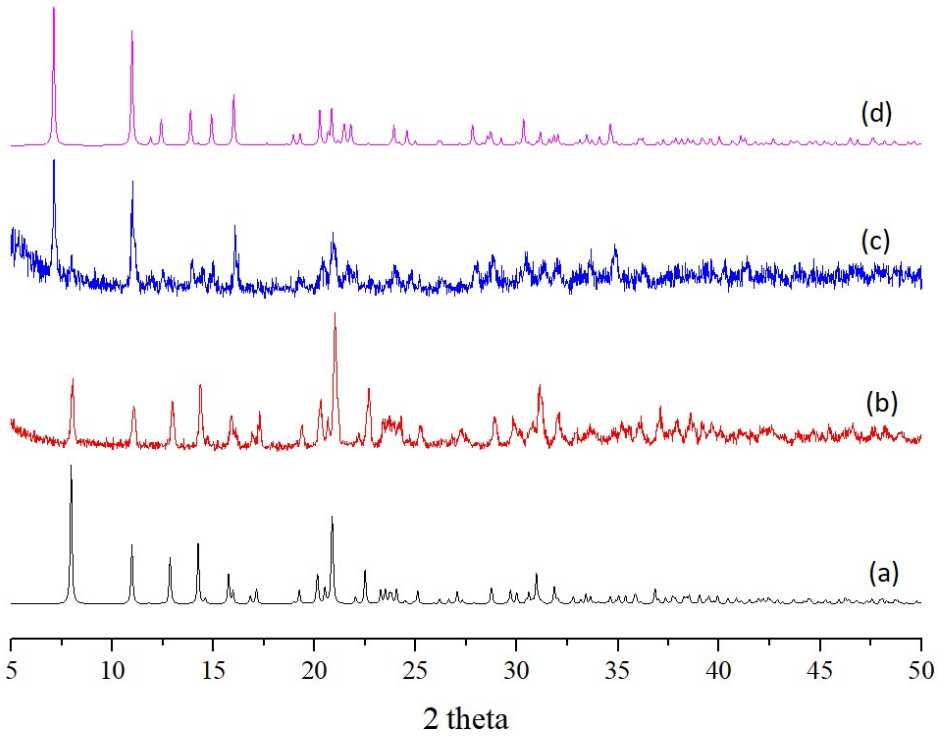

Table S1. Crystal data for complexes **1** – **11**.

Complex	**1**	**2**	**3**	**4**	**5**	**6**
Formula	$C_{20}H_{28}ZnI_2N_6O_4$	$C_{14}H_{14}ZnI_2N_4O_2$	$C_{14}H_{14}CdI_2N_4O_2$	$C_{14}H_{14}HgI_2N_4O_2$	$C_{14}H_{14}HgI_2N_4O_2$	$C_{18}H_{22}Hg_2I_4N_4O_2$
Formula weight	735.65	589.46	636.49	724.68	724.68	1235.17
Crystal system	Monoclinic	Triclinic	Triclinic	Triclinic	Monoclinic	Monoclinic
Space group	$P2_1/n$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P2/n$	$C2/c$
a, Å	9.6781(11)	8.61(2)	8.9922(8)	8.9249(10)	8.5935(6)	38.197(2)
b, Å	9.9149(11)	10.55(3)	11.0373(11)	11.0499(13)	5.1210(4)	4.6289(2)
c, Å	27.660(3)	10.87(3)	11.2843(11)	11.3056(13)	21.3841(16)	17.4981(9)
α, °	90	94.51(6)	93.850(2)	94.773(3)	90	90
β, °	99.307(3)	112.25(6)	112.8580(19)	112.746(2)	99.260(2)	116.5188(16)
γ,°	90	110.10(8)	111.5981(19)	110.951(2)	90°.	90
V, Å^3	2619.2(5)	833(4)	930.25(15)	927.96(19)	928.79(12)	2768.4(2)
Z	4	2	2	2	2	4

D_{calc}, Mg/m^3	1.866	2.349	2.272	2.594	2.591	2.964
F(000)	1432	556	592	656	656	2184
μ(Mo K_α), mm^{-1}	3.332	5.191	4.505	11.633	11.622	15.559
Range(2θ) for data collection,°	2.98≦2θ≦52.00	4.17≦2θ≦52.00	4.04≦2θ≦57.18	4.04≦2θ≦57.09	3.86≦2θ≦52.00	4.66≦2θ≦57.02
Independent reflections	5135 [R(int) = 0.0341]	3279 [R(int) = 0.2605]	4710 [R(int) = 0.0761]	4687 [R(int) = 0.1098]	1838 [R(int) = 0.0551]	3481 [R(int) = 0.0471]
Data / restraints / parameters	5135 / 8 / 271	3279/0/184	4710 / 0 / 208	4687 / 0 / 209	1838 / 0 / 105	3481 / 0 / 137
quality-of-fit indicator [c]	1.056	1.014	0.969	0.944	1.055	1.026
Final R indices[I > 2σ(I)] [a,b]	R_1 = 0.0331 wR^2 = 0.0934	R^1 = 0.0824, wR_2 = 0.1235	R^1 = 0.0488 wR_2 = 0.0608	R_1 = 0.0486 wR^2 = 0.0595	R1 = 0.0361, wR2 = 0.0914	R1 = 0.0315, wR2 = 0.0651
R indices (all data)	R_1 = 0.0405 wR_2 = 0.0979	R_1 = 0.2360 wR_2 = 0.1568	R_1 = 0.1166 wR_2 = 0.0746	R_1 = 0.1403 wR_2 = 0.0771	R1 = 0.0497, wR2 = 0.0993	R1 = 0.0465, wR2 = 0.0697

[a]$R_1 = \sum\left|\left|F_o\right| - \left|F_c\right|\right| / \sum\left|F_o\right|$.[b]$wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{1/2}$. $w = 1 / [\sigma^2(F_o^2) + (ap)^2 + (bp)]$, $p = [\max(F_o^2 \text{ or } 0) + 2(F_c^2)] / 3$. a = 0.0543, b = 5.0224 for **1**; a = 0.0183, b = 0 for **2**; a = 0.0179, b = 0 for **3**; a = 0.0122, b = 0 for **4**; a = 0.0459, b = 0 for **5**; a = 0.0300, b = 2.9329 for **6**; a = 0.0108 , b = 0 for **7**; a = 0.0282 , b = 0.0652 for **8**; a = 0.021600, b = 0.952000 for **9**; a = 0.0183, b = 1.1855 for **10**; a = 0.017200, b = 2.738500 for **11**. [c]quality-of-fit = $[\sum w(\left|F_o^2\right| - \left|F_c^2\right|)^2 / N_{observed} - N_{parameters})]^{1/2}$.

Table S1. Crystal data for complexes **1** – **11**. (cont.)

Complex	**7**	**8**	**9**	**10**	**11**
Formula	$C_{18}H_{22}CdI_2N_4O_2$	$C_{28}H_{28}Br_2CdN_8O_4$	$C_{28}H_{28}Br_2CdN_8O_4$	$C_{30}H_{28}Br_2Cd_2N_8O_8$	$C_{16}H_{22}CdN_4O_{10}$
Formula weight	692.61	812.80	812.80	1013.22	542.77
Crystal system	Monoclinic	Triclinic	Monoclinic	Monoclinic	Monoclinic
Space group	*Cc*	*P*$\bar{1}$	$P2_1/c$	$P2_1/c$	*C*2/*c*
a, Å	12.0191(15)	7.530(4)	8.1474(3)	8.2630(5)	17.859(2) Å
b, Å	13.5251(17)	8.876(5)	22.1923(8)	24.8667(15)	13.892(2) Å
c, Å	14.9707(18)	12.919(7)	9.4033(3)	9.4656(6)	10.4606(13) Å
α, °	90	71.439(13)	90	90	90
β, °	109.607(3)	74.215(13)	113.0272(9)	115.88(0)	124.251(3)
γ,°	90	68.987(12)	90	90	90
V, Å^3	2292.5(5)	751.9(8)	1564.73(10)	1749.89(18)	2145.1(5)
Z	4	1	2	2	4
D_{calc}, Mg/m^3	2.007	1.795	1.725	1.923	1.681
F(000)	1312	402	804	988	1096

μ(Mo K_α), mm^{-1}	3.665	3.432	3.298	3.559	1.078
Range(2θ) for data collection,°	4.69≦2θ≦56.71	3.38≦2θ≦52.00	3.67≦2θ≦57.10	3.28≦2θ≦52.00	4.02≦2θ≦57.33
Independent reflections	5576 [R(int) = 0.0492]	2949 [R(int) = 0.0482]	3941 [R(int) = 0.0339]	3443 [R(int) = 0.0607]	2726 [R(int) = 0.0546]
Data / restraints / parameters	5576 / 2 / 244	2949 / 0 / 196	3941 / 0 /196	3443 / 0 / 226	2726 / 0 / 141
quality-of-fit indicator [c]	1.006	1.048	1.034	1.031	1.048
Final R indices[$I > 2\sigma(I)$] [a,b]	R1 = 0.0383, wR2 = 0.0500	R1 = 0.0275, wR2 = 0.0562	R1 = 0.0272, wR2 = 0.0538	R1 = 0.0254, wR2 = 0.0564	R1 = 0.0282, wR2 = 0.0543
R indices (all data)	R1 = 0.0916, wR2 = 0.0630	R1 = 0.0466, wR2 = 0.0629	R1 = 0.0403, wR2 = 0.0574	R1 = 0.0326, wR2 = 0.0592	R1 = 0.0378 wR2 = 0.0582