Electronic Supplementary Material (ESI) for CrystEngComm

Synthesis and characterization of two self-catenated networks and one case of pcu topology based on the mixed ligands

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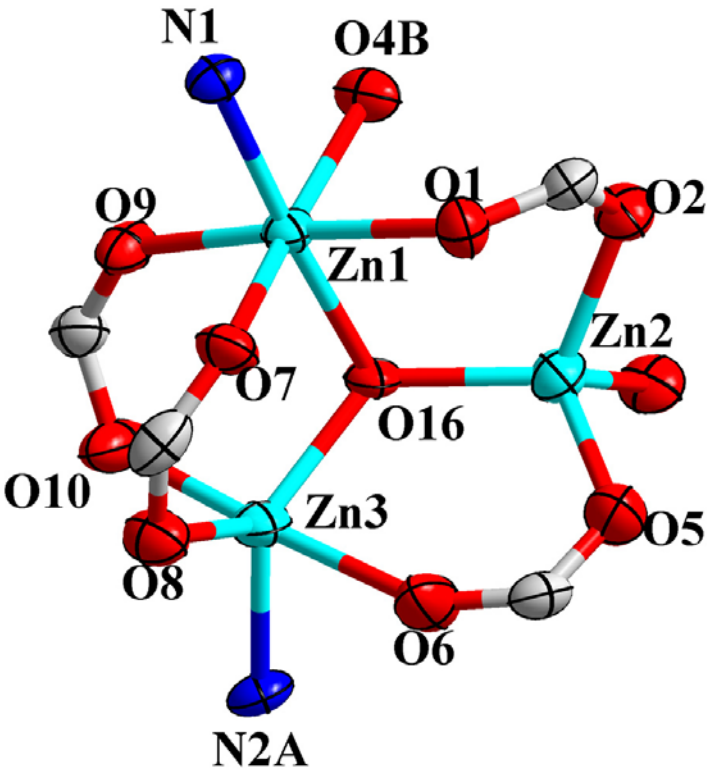

Fig. S1 Coordination environment of Zn^{II} in **1** with the ellipsoids drawn at the 30% probability level, with hydrogen atoms were omitted for clarity (Symmetry transformations used to generate equivalent atoms: A, x, y, 1 + z; B, 1 – x, 1 – y, 2 – z.).

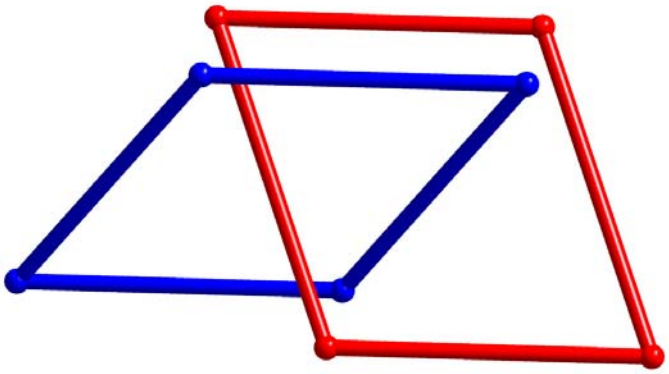

Fig. S2 Schematic representation of the (4,8)-connected net for **1**: the shortest four-membered rings are interlocked**.**

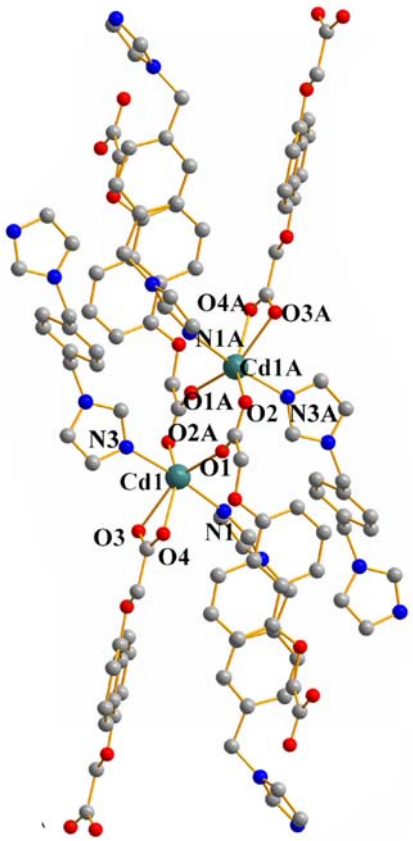

Fig. S3 Coordination environment of Cd^{II} in **2**, with hydrogen atoms were omitted for clarity (Symmetry transformations used to generate equivalent atoms: A, 1 – x, –y, 2 – z)**.**

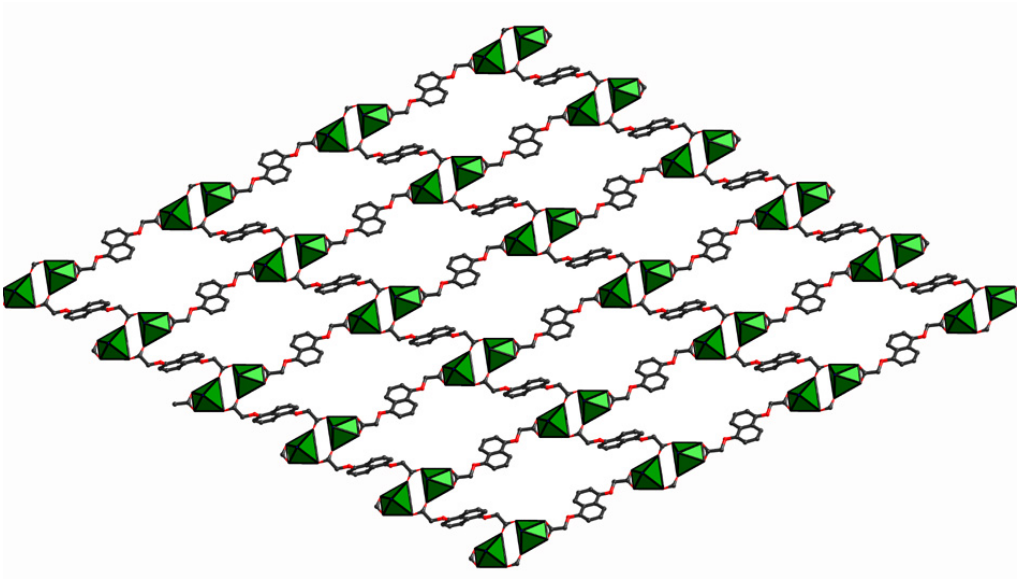

Fig. S4 Schematic view of the 2D structure is connected by **ndd** ligands for **2**.

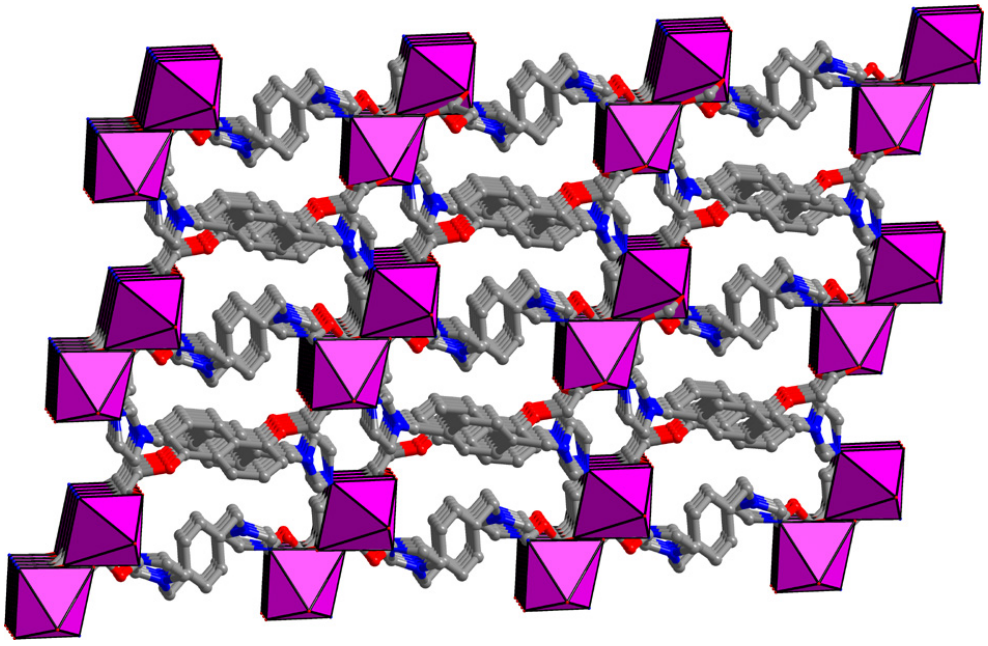

Fig. S5 Schematic view of the 3D structure is connected by **ndd** and **BIMB** ligands for **2**.

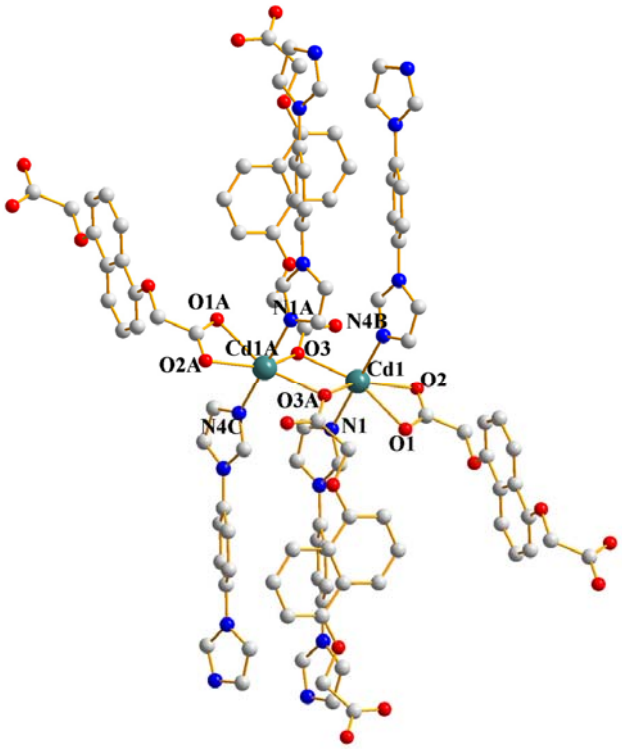

Fig. S6 Coordination environment of Cd^{II} in **3**, with hydrogen atoms were omitted for clarity (Symmetry transformations used to generate equivalent atoms: A, –x, 1 – y, 1 – z; B, –1 + x, –1 + y, –1 + z; C, 1 – x, 2 – y, 2 – z).

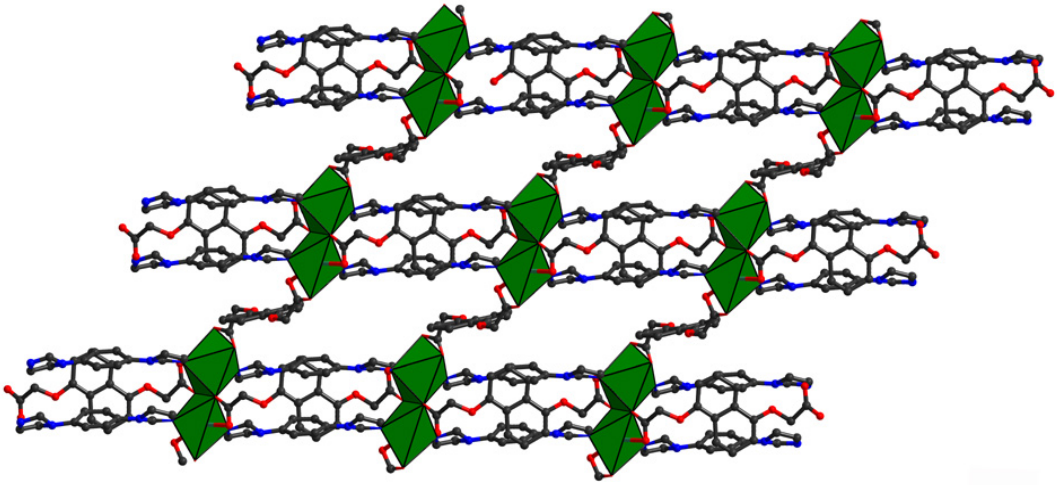

Fig. S7 Schematic view of the 3D structure is connected by **BIMB** and **ndd** ligands for **3**.

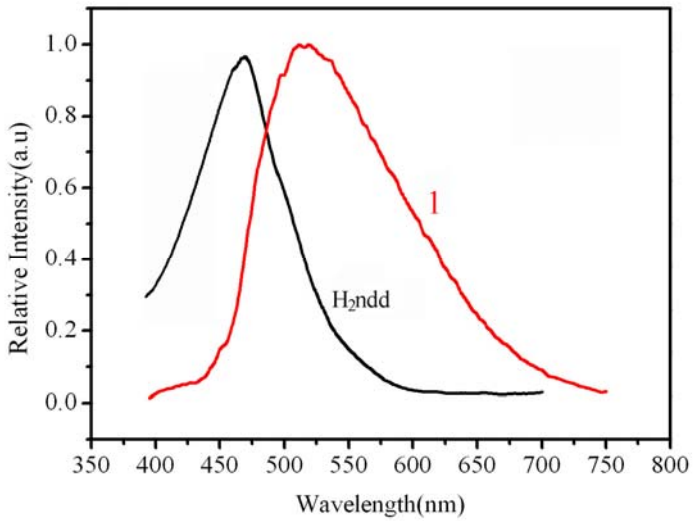

Fig. S8 Emission spectra of compound **1** and **H_2ndd** in the solid state at room temperature.

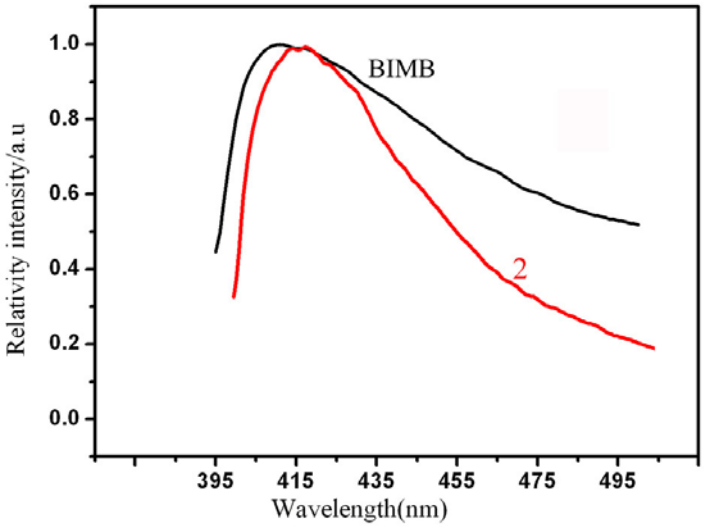

Fig. S9 Emission spectra of compound **2** and **BIMB** in the solid state at room temperature.

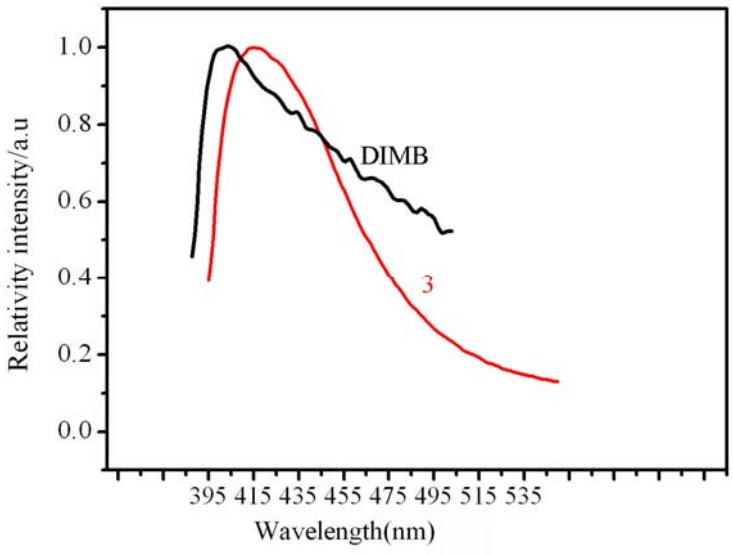

Fig. S10 Emission spectra of compound **3** and **DIMB** in the solid state at room temperature.

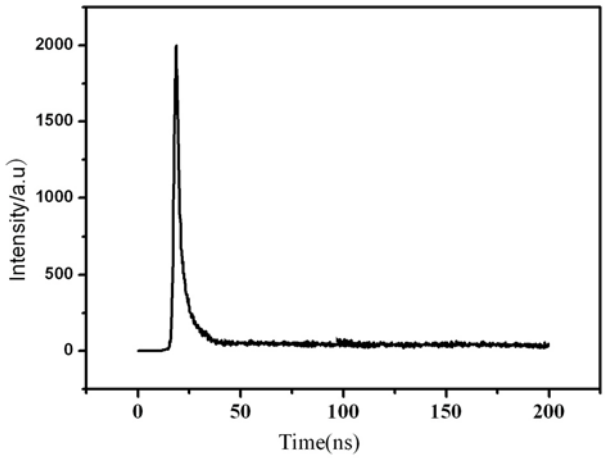

Fig. S11 Fitted decay curve monitored at 507 nm for compound **1**.

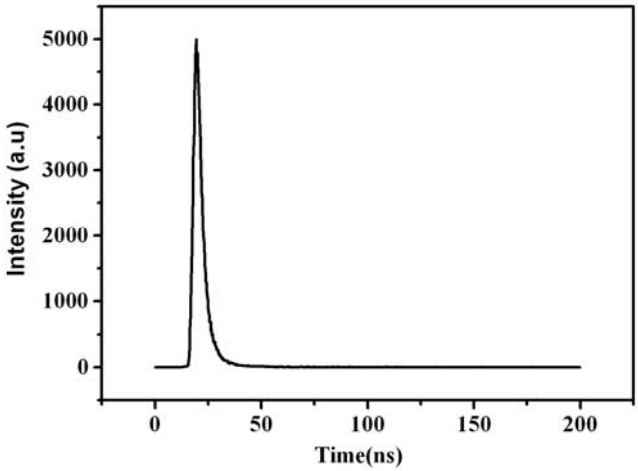

Fig. S12 Fitted decay curve monitored at 425 nm for compound **2**.

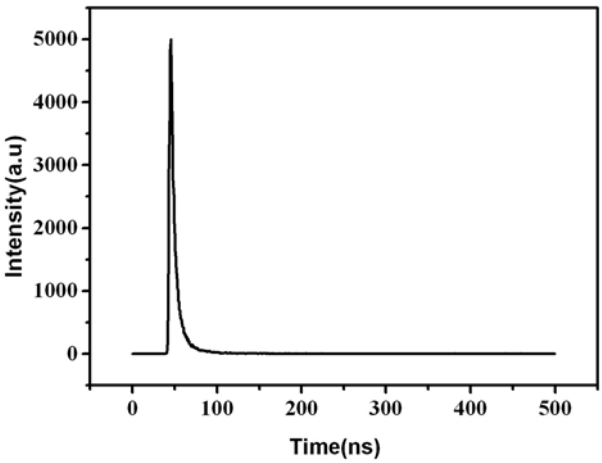

Fig. S13 Fitted decay curve monitored at 427 nm for compound **3**.

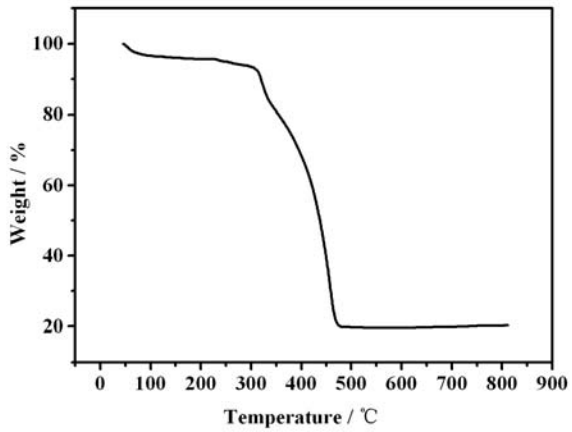

Fig. S14 The TG curves of **1**.

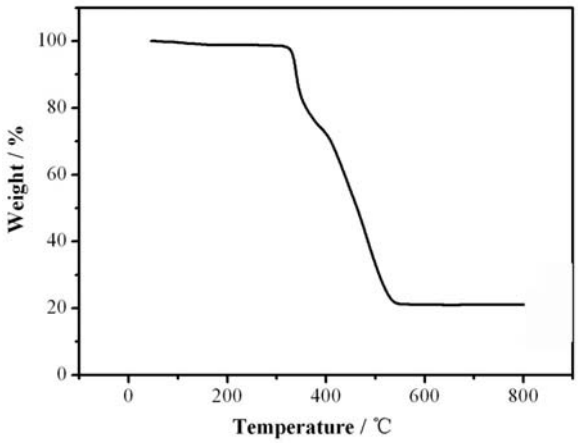

Fig. S15 The TG curves of **2**.

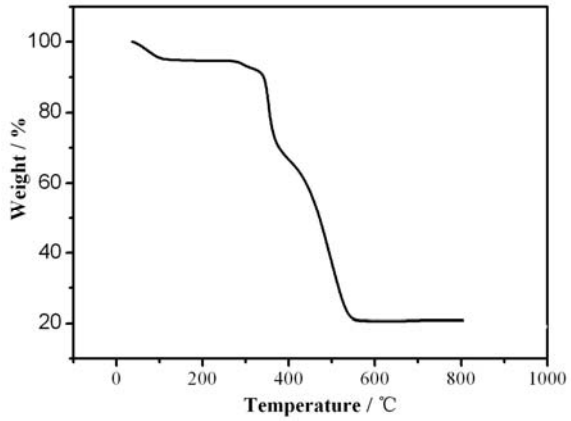

Fig. S16 The TG curves of **3**.

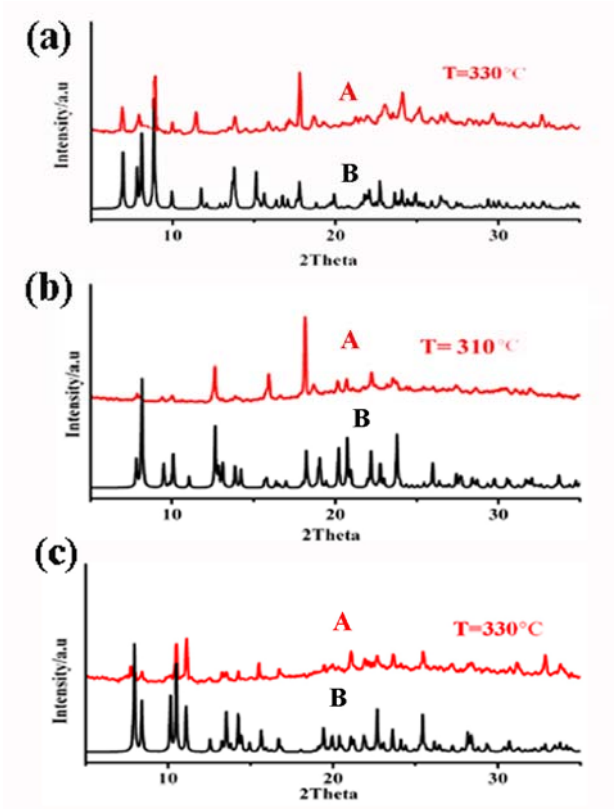

Fig. 17 (a) Simulated and experimental PXRD spectra of **1**: A as-synthesized (T = 330°C); B simulated. (b) Simulated and experimental PXRD spectra of **2**: A as-synthesized (T = 310°C); B simulated. (c) Simulated and experimental PXRD spectra of **3**: A as-synthesized (T = 330°C); B simulated.

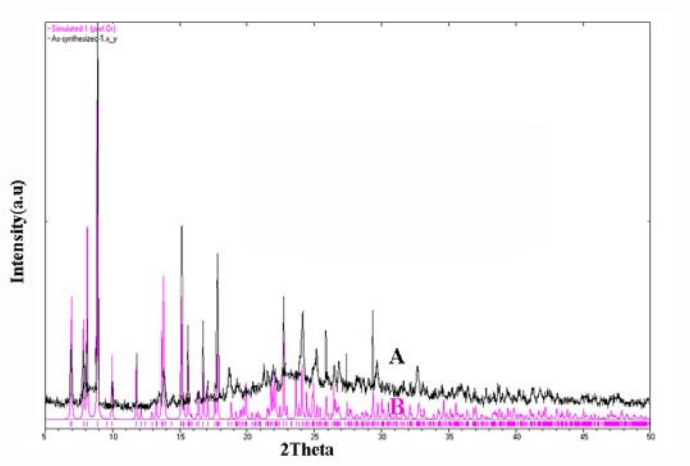

Fig. S18 Schematic representation of the simulated and experimental PXRD spectra of **1,**: (A as-synthesized; B simulated.).

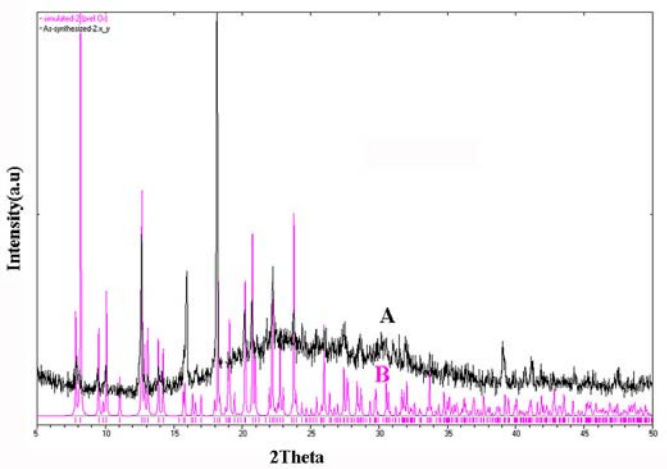

Fig. S19 Schematic representation of the simulated and experimental PXRD spectra of **2**: (A as-synthesized; B simulated.).

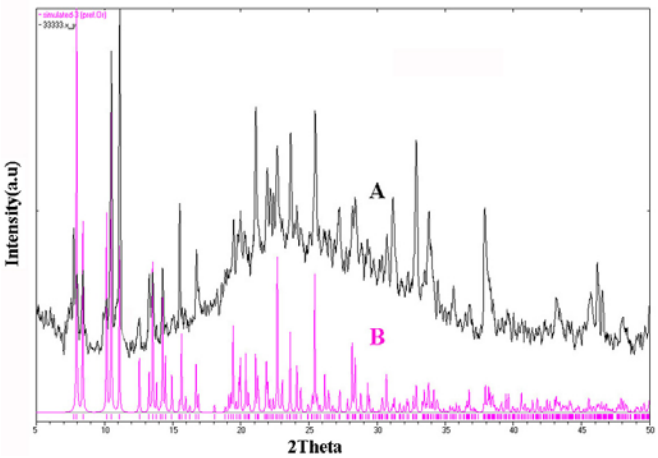

Fig. S20 Schematic representation of the simulated and experimental PXRD spectra of **3**: (A as-synthesized; B simulated.).

Table S1 Crystal data and structure refinements for complexes **1**-**3**.

Complex	**1**	**2**	**3**
Formula	$C_{45}H_{38}N_2O_{17}Zn_3$	$C_{28}H_{24}CdN_4O_6$	$C_{26}H_{24}N_4O_8Cd$
Formula weight	1090.91	624.92	632.87
Crystal system	Triclinic	Triclinic	Triclinic
Space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
a /Å	13.006(13)	10.005(2)	9.361(19)
b /Å	13.637(14)	11.303(3)	12.713(19)
c /Å	14.104(15)	12.206(3)	12.755(3)
α/°	79.971(17)	100.797(3)	111.843(2)
β/°	64.389(15)	107.308(4)	105.938(2)
γ/°	71.276(15)	98.944(4)	97.104(2)
V/Å^3	2134.5(4)	1261.3(5)	1310.7(4)
Z	2	2	2
$D_{calcd.}$[g cm^{-3}]	1.690	1.646	1.593
μ/mm^{-1}	1.756	0.918	0.890
F(000)	1102.0	632.0	632.0
reflection/unique	10810/7380	7467/5506	6646/4520
R_{int}	0.0448	0.0245	0.0502
GOF on F^2	1.065	1.002	1.007
R_1[a],wR_2[b][I>2σ(I)]	0.0629, 0.1260	0.0558, 0.1265	0.0611, 0.0947
R_1, wR_2 (all data)	0.1262, 0.1682	0.0864, 0.1411	0.1223, 0.1074

Table S2 Selected bond lengths (Å) and angles (˚) for complexes **1**-**3**[a]

Complex **1**			
Zn(1)-O(1)	2.148(5)	Zn(2)-O(2)	1.987(5)
Zn(2)-O(3)	1.970(5)	Zn(1)-O(4)B	2.088(5)
Zn(2)-O(5)	1.964(6)	Zn(3)-O(6)	2.249(6)
Zn(1)-O(7)	2.071(5)	Zn(3)-O(8)	1.975(5)
Zn(1)-O(9)	2.055(5)	Zn(3)-O(10)	2.088(5)
Zn(2)-O(16)	1.966(5)	Zn(3)-O(16)	1.995(5)
Zn(1)-O(16)	2.202(5)	Zn(1)-O(4)B	2.088(5)
Zn(3)-N(2)A	2.030(6)	O(9)-Zn(1)-N(1)	92.7(2)
O(9)-Zn(1)-O(4)B	93.1(2)	N(1)-Zn(1)-O(4)B	86.7(2)
O(9)-Zn(1)-O(7)	95.5(2)	N(1)-Zn(1)-O(7)	87.9(2)
O(4)B-Zn(1)-O(7)	170.0(2)	O(9)-Zn(1)-O(1)	175.6(2)
N(1)-Zn(1)-O(1)	91.6(2)	O(4)B-Zn(1)-O(1)	88.2(2)

O(7)-Zn(1)-O(1)	83.6(2)	O(9)-Zn(1)-O(16)	87.25(19)
N(1)-Zn(1)-O(16)	174.4(2)	O(4)B-Zn(1)-O(16)	87.71(19)
O(7)-Zn(1)-O(16)	97.8(2)	O(1)-Zn(1)-O(16)	88.61(19)
O(5)-Zn(2)-O(16)	111.8(2)	O(5)-Zn(2)-O(3)	109.1(2)
O(16)-Zn(2)-O(3)	112.3(2)	O(5)-Zn(2)-O(2)	109.0(3)
O(16)-Zn(2)-O(2)	113.8(2)	O(3)-Zn(2)-O(2)	113.8(2)
O(8)-Zn(3)-O(16)	125.6(2)	O(8)-Zn(3)-N(2)A	109.6(3)
O(16)-Zn(3)-N(2)A	124.1(2)	O(8)-Zn(3)-O(10)	94.6(2)
O(16)-Zn(3)-O(10)	90.0(2)	N(2)A-Zn(3)-O(10)	94.2(2)
O(8)-Zn(3)-O(6)	89.2(2)	O(16)-Zn(3)-O(6)	86.7(2)
N(2)A-Zn(3)-O(6)	85.7(2)	O(10)-Zn(3)-O(6)	176.0(2)
		Complex **2**	
Cd(1)-N(3)	2.276(4)	Cd(1)-O(1)	2.305(4)
Cd(1)-N(1)	2.314(4)	Cd(1)-O(2)A	2.317(4)
Cd(1)-O(4)	2.370(4)	Cd(1)-O(3)	2.463(4)
N(3)-Cd(1)-O(1)	94.29(17)	N(3)-Cd(1)-N(1)	171.87(16)
O(1)-Cd(1)-N(1)	93.83(18)	N(3)-Cd(1)-O(2)A	89.96(15)
O(1)-Cd(1)-O(2)A	114.58(18)	N(1)-Cd(1)-O(2)A	86.87(16)
N(3)-Cd(1)-O(4)	90.28(15)	O(1)-Cd(1)-O(4)	98.48(16)
O(2)A-Cd(1)-O(4)	88.30(16)	N(3)-Cd(1)-O(3)	93.32(15)
O(1)-Cd(1)-O(3)	151.35(17)	N(1)-Cd(1)-O(3)	79.33(17)
O(2)A-Cd(1)-O(3)	92.98(16)	O(4)-Cd(1)-O(3)	79.39(16)
		Complex **3**	
Cd(1)-N(4)B	2.267(6)	Cd(1)-N(1)	2.283(6)
Cd(1)-O(2)	2.350(5)	Cd(1)-O(3)	2.383(5)
Cd(1)-O(3)A	2.366(5)	Cd(1)-O(1)	2.500(5)
N(4)B-Cd(1)	2.267(6)	O(3)A-Cd(1)	2.651(5)
N(4)B-Cd(1)-O(2)	87.0(2)	N(1)-Cd(1)-O(2)	94.34(19)
O(2)-Cd(1)-O(3)	146.23(17)	N(4)B-Cd(1)-O(3)A	84.0(2)
N(1)-Cd(1)-O(3)A	93.36(19)	O(2)-Cd(1)-O(3)A	141.06(16)
O(3)-Cd(1)-O(3)A	72.51(18)	N(4)B-Cd(1)-O(1)	95.31(19)

N(1)-Cd(1)-O(1)	83.38(18)	O(2)-Cd(1)-O(1)	53.71(15)
O(3)-Cd(1)-O(1)	157.87(16)	O(3)A-Cd(1)-O(1)	89.52(16)
N(4)B-Cd(1)-O(4)	83.9(2)	N(1)-Cd(1)-O(4)	98.53(19)
O(2)-Cd(1)-O(4)	96.72(17)	O(3)-Cd(1)-O(4)	50.39(16)
O(3)A-Cd(1)-O(4)	119.73(17)	O(1)-Cd(1)-O(4)	150.35(17)

[a]Symmetry transformations used to generate equivalent atoms: for **1**: A, x, y, 1 + z; B, 1 – x, 1 – y, 2 – z. for **2**: A, 1 – x, –y, 2 – z, for **3**: A, –x, 1 – y, 1 – z; B, –1 + x, –1 + y, –1 + z.