Electronic Supplementary Material (ESI) for RSC Advances.

A novel 3D Cd (II) coordination polymer generated *via in situ* ligand synthesis involving C-O ester bond formation

Supplementary Material

Table S1. Crystal data and structure refinement for 1-3

Compound	**1**	**2**	**3**
Empirical formula	$C_{26}H_{14}CdN_2O_9$	$C_{40}H_{24}Cd_2N_6O_{14}$	$C_{36}H_{22}Cu_2N_6O_{13}$
Formula weight	610.79	1037.45	873.68
Crystal system	Monoclinic	Triclinic	Triclinic
Space group	*C*2/*c*	$P\bar{1}$	$P\bar{1}$
a /Å	25.8426(10)	12.140(4)	9.5425(11)
b /Å	12.5139(5)	12.715(4)	9.9857(12)
c /Å	7.1398(3)	13.939(4)	20.978(2)
α /°	90	110.148(4)	88.645(2)
β /°	95.8950(10)	112.543(4)	83.015(2)
γ /°	90	92.070(4)	64.759(2)
V/Å^3	2296.74(16)	1830.1(9)	1793.8(3)
Z	4	2	2
D calc/Mg/m^3	1.766	1.883	1.618
μ (mm^{-1})	1.014	1.247	1.263
T/K	293(2)	296(2)	293(2)
F (000)	1216	1028	884
θ Range /°	2.88 to 5.49	1.72 to 25.50	1.96 to 25.50
λ (Mo-K$_\alpha$) / Å	0.71073	0.71073	0.71073
Reflections collected	5886	9667	9504
Unique reflections	213	6750	6614
Parameters	176	575	516
S on F^2	1.08	1.095	1.049
R_1, wR_2 [$I>2\sigma(I)$] [a], [b]	0.0201, 0.0607	0.0273, 0.0697	0.0541, 0.1546
R_1, wR_2 (all data) [a], [b]	0.0207, 0.0610	0.0398, 0.0867	0.0872, 0.1720
Δ*ρ* min and max (e Å^{-3})	0.972 and -0.482	0.490 and -0.557	0.954 and -0.462

[a] $R_1 = \Sigma||F_0|-|F_C||/\Sigma|F_0|$; [b] $wR_2 = [\Sigma[w(F_0^2-F_C^2)^2]/\Sigma[(F_0^2)^2]]^{1/2}$

Table S2. Select bond lengths (Å) and angles (deg) for 1-3 [a]

Compound **1**					
Cd(1)-O(1)#1	2.2072(15)	Cd(1)-N(1)	2.3543(18)	Cd(1)-O(2)#2	2.3759(16)
Cd(1)-O(1)	2.2072(15)	Cd(1)-N(1)#1	2.3543(18)	Cd(1)-O(2)#3	2.3759(16)
O(1)#1-Cd(1)-O(1)	120.96(9)	N(1)-Cd(1)-N(1)#1	70.16(9)	O(1)#1-Cd(1)-O(2)#3	105.44(6)
O(1)#1-Cd(1)-N(1)	151.36(7)	O(1)#1-Cd(1)-O(2)#2	81.50(6)	O(1)-Cd(1)-O(2)#3	81.50(6)
O(1)-Cd(1)-N(1)	85.92(7)	O(1)-Cd(1)-O(2)#2	105.44(6)	N(1)-Cd(1)-O(2)#3	86.97(6)
O(1)#1-Cd(1)-N(1)#1	85.92(7)	N(1)-Cd(1)-O(2)#2	81.73(6)	N(1)#1-Cd(1)-O(2)#3	81.73(6)
O(1)-Cd(1)-N(1)#1	151.36(7)	N(1)#1-Cd(1)-O(2)#2	86.97(6)	O(2)#2-Cd(1)-O(2)#3	166.20(8)
Compound **2**					
Cd(1)-O(7)	2.220(3)	Cd(1)-N(4)	2.346(3)	Cd(2)-O(2)	2.326(2)
Cd(1)-O(1)	2.314(3)	Cd(1)-O(10)#1	2.527(3)	Cd(2)-N(5)	2.342(3)
Cd(1)-O(9)#1	2.324(3)	Cd(2)-O(13)	2.234(3)	Cd(2)-N(6)	2.383(3)
Cd(1)-N(3)	2.332(3)	Cd(2)-O(3)#2	2.251(2)	O(7)-Cd(1)-O(1)	96.89(9)
O(7)-Cd(1)-O(9)#1	99.76(10)	N(3)-Cd(1)-N(4)	71.27(10)	O(3)#2-Cd(2)-O(2)	80.15(9)
O(1)-Cd(1)-O(9)#1	76.45(9)	O(7)-Cd(1)-O(10)#1	94.74(10)	O(13)-Cd(2)-N(5)	91.41(11)
O(7)-Cd(1)-N(3)	87.59(10)	O(1)-Cd(1)-O(10)#1	129.81(9)	O(3)#2-Cd(2)-N(5)	140.39(11)
O(1)-Cd(1)-N(3)	151.08(10)	O(9)#1-Cd(1)-O(10)#1	53.47(9)	O(2)-Cd(2)-N(5)	84.14(10)
O(9)#1-Cd(1)-N(3)	131.08(10)	N(3)-Cd(1)-O(10)#1	77.84(10)	O(13)-Cd(2)-N(6)	116.37(11)
O(7)-Cd(1)-N(4)	126.12(10)	N(4)-Cd(1)-O(10)#1	125.97(10)	O(3)#2-Cd(2)-N(6)	93.50(10)
O(1)-Cd(1)-N(4)	83.29(10)	O(13)-Cd(2)-O(3)#2	127.65(10)	O(2)-Cd(2)-N(6)	131.72(10)
O(9)#1-Cd(1)-N(4)	131.73(10)	O(13)-Cd(2)-O(2)	104.44(11)	N(5)-Cd(2)-N(6)	70.76(10)
Compound **3**					
Cu(1)-O(2)	1.958(3)	Cu(1)-N(4)	1.985(4)	Cu(2)-O(9)#2	1.975(3)
Cu(1)-N(3)	1.970(4)	Cu(2)-O(5)	1.936(4)	Cu(2)-N(6)	1.986(4)
Cu(1)-O(12)#1	1.971(3)	Cu(2)-N(5)	1.962(4)	N(5)-Cu(2)-O(9)#2	168.18(18)
O(2)-Cu(1)-N(3)	163.15(16)	N(3)-Cu(1)-N(4)	81.88(17)	O(5)-Cu(2)-N(6)	167.15(19)
O(2)-Cu(1)-O(12)#1	92.45(15)	O(12)#1-Cu(1)-N(4)	150.19(17)	N(5)-Cu(2)-N(6)	81.39(19)
N(3)-Cu(1)-O(12)#1	98.45(16)	O(5)-Cu(2)-N(5)	94.78(18)	O(9)#2-Cu(2)-N(6)	96.33(17)
O(2)-Cu(1)-N(4)	95.00(15)	O(5)-Cu(2)-O(9)#2	89.83(17)		

[a] Symmetry codes for **1**: #1: *-x ,y, -z*+1/2; #2: *-x, -y, -z*+1; #3: *x, -y, z*-1/2; for **2**:#1:*-x*+1, *-y*+1, *-z*+1; #2: *-x*+2, *-y*+2, *-z*+2; for **3**: #1: *x*+1, *y*-1, z ; #2: *x* +1, *y*, *z*.

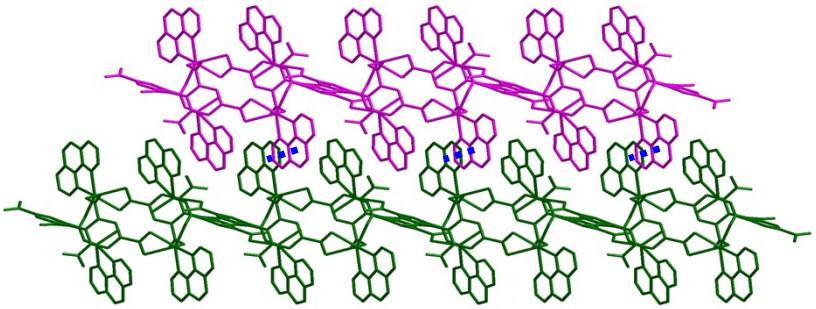

Fig.S1 The 2D supramolecular network of **2** *via* π–π stacking interactions. All hydrogen atoms are omitted for clarity.

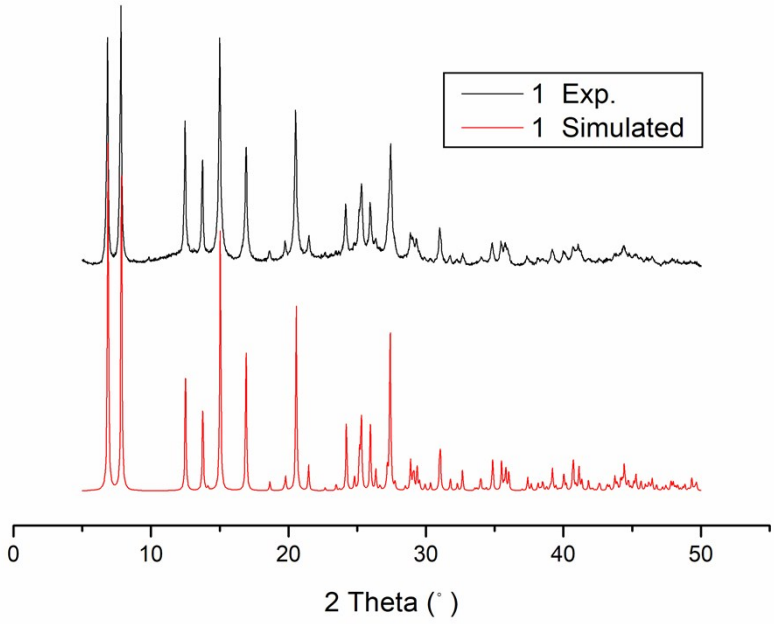

Fig.S2 PXRD patterns for **1**.

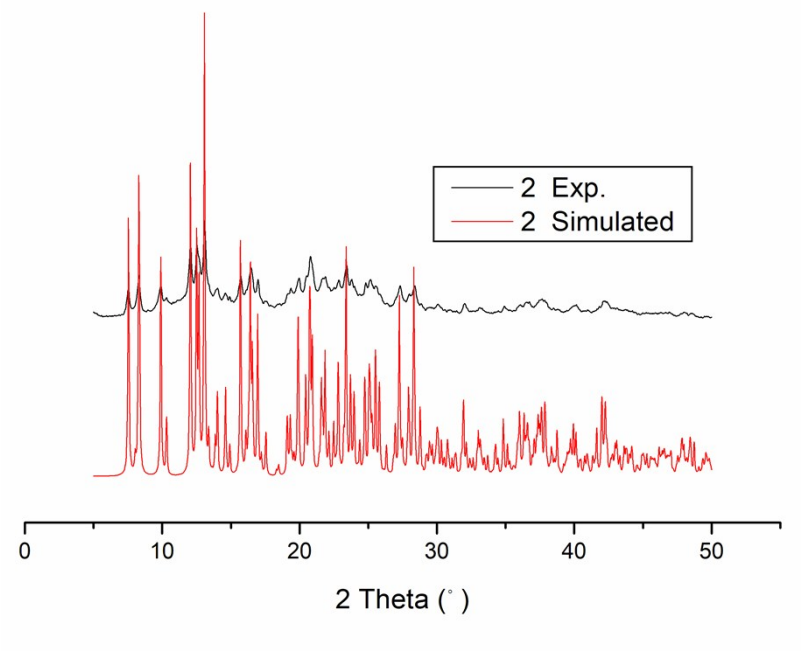

Fig.S3 PXRD patterns for **2**.

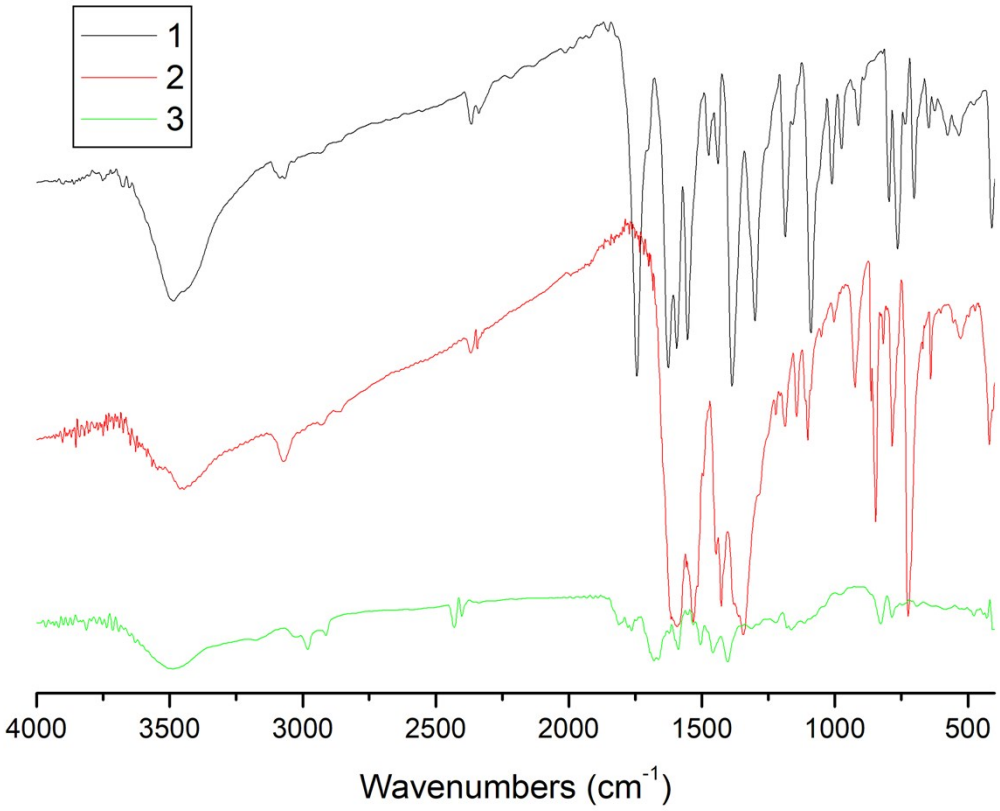

Fig.S4 IR spectra of **1**-**3**.

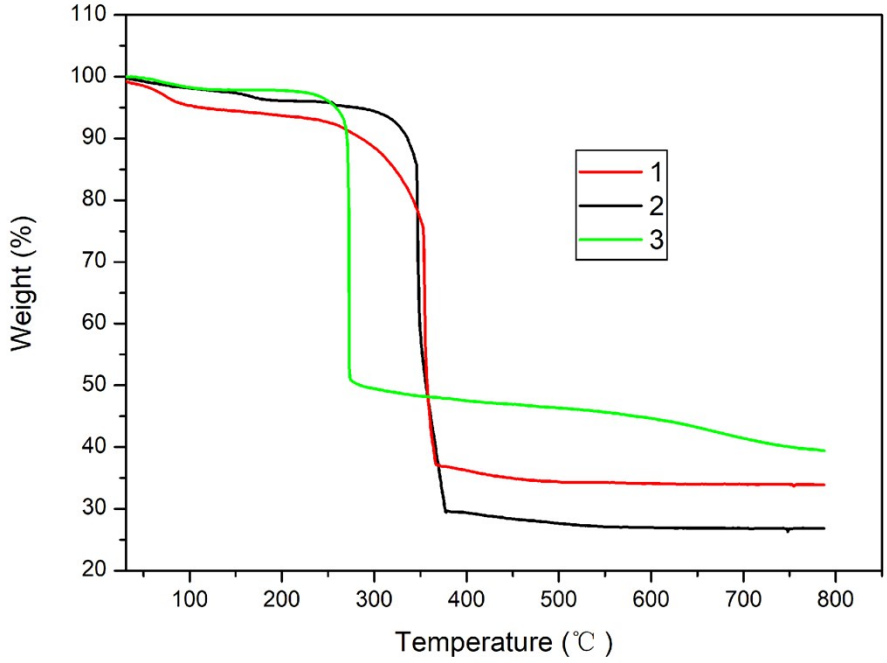

Fig.S5 Thermogravimetric analysis of **1**-**3**.