Electronic Supplementary Material (ESI) for CrystEngComm

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Interpenetrated and polycatenated nets of Cd(II) coordination networks from mixed *N,N′*-dipyridyladipoamide and dicarboxylate ligands

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Table S1. Selected bond distances (Å) and angles (°) for complexes **1** - **5**.

1

Bond distances			
Cd-N(4A)	2.283(4)	Cd-O(3B)	2.391(3)
Cd-O(5)	2.294(3)	Cd-O(3)	2.481(2)
Cd-N(1)	2.306(3)	Cd-O(6)	2.572(2)
Cd-O(4)	2.357(2)		
Bond angles			
N(4A)-Cd-O(5)	90.35(13)	O(5)-Cd-O(3)	164.68(9)
N(4A)-Cd-N(1)	175.84(14)	N(1)-Cd-O(3)	85.47(10)
O(5)-Cd-N(1)	88.79(12)	O(4)-Cd-O(3)	53.83(8)
N(4A)-Cd-O(4)	89.72(12)	O(3B) -Cd-O(3)	77.02(9)
O(5)-Cd-O(4)	140.90(10)	N(4A) -Cd-O(6)	93.38(11)
N(1)-Cd-O(4)	93.52(12)	O(5)-Cd-O(6)	52.85(9)
N(4A)-Cd-O(3B)	86.37(12)	N(1)-Cd-O(6)	89.34(10)
O(5)-Cd-O(3B)	88.77(9)	O(4)-Cd-O(6)	88.13(9)
N(1)-Cd-O(3B)	89.54(11)	O(3B) -Cd-O(6)	141.61(8)
O(4)-Cd-O(3B)	130.23(8)	O(3)-Cd-O(6)	141.05(9)
N(4A)-Cd-O(3)	94.35(11)		

2

Bond distances			
Cd(1)-O(13)	2.290(5)	Cd(2)-O(12B)	2.261(4)
Cd(1)-N(4A)	2.305(4)	Cd(2)-O(11)	2.273(4)
Cd(1)-N(1)	2.325(4)	Cd(2)-N(5)	2.290(4)
Cd(1)-O(9)	2.348(4)	Cd(2)-N(8A)	2.307(5)
Cd(1)-O(5)	2.357(4)	Cd(2)-O(8C)	2.343(4)
Cd(1)-O(10)	2.427(4)	Cd(2)-O(7C)	2.545(4)
Cd(1)-O(6)	2.614(4)		
Bond angles			
O(13)-Cd(1)-N(4A)	87.00(18)	O(12B)-Cd(2)-O(11)	130.03(16)
O(13)-Cd(1)-N(1)	87.86(19)	O(12B)-Cd(2)-N(5)	88.88(16)
N(4A)-Cd(1)-N(1)	173.39(17)	O(11)-Cd(2)-N(5)	87.53(16)
O(13)-Cd(1)-O(9)	142.52(18)	O(12B)-Cd(2)-N(8A)	89.23(16)
N(4A)-Cd(1)-O(9)	97.21(16)	O(11)-Cd(2)-N(8A)	96.81(16)
N(1)-Cd(1)-O(9)	89.40(16)	N(5)-Cd(2)-N(8A)	175.50(17)
O(13)-Cd(1)-O(5)	137.40(16)	O(12B)-Cd(2)-O(8C)	145.24(15)

Table S1. Selected bond distances (Å) and angles (°) for complexes **1** - **5**. (cont.)

N(4A)-Cd(1)-O(5)	90.12(15)	O(11)-Cd(2)-O(8C)	84.68(16)
N(1)-Cd(1)-O(5)	90.84(15)	N(5)-Cd(2)-O(8C)	91.24(15)
O(9)-Cd(1)-O(5)	79.99(14)	N(8A)-Cd(2)-O(8C)	88.00(15)
O(13)-Cd(1)-O(10)	88.68(18)	O(12B)-Cd(2)-O(7C)	91.54(14)
N(4A)-Cd(1)-O(10)	87.50(15)	O(11)-Cd(2)-O(7C)	137.59(15)
N(1)-Cd(1)-O(10)	96.55(15)	N(5)-Cd(2)-O(7C)	85.00(14)
O(9)-Cd(1)-O(10)	54.55(14)	N(8A)-Cd(2)-O(7C)	90.97(14)
O(5)-Cd(1)-O(10)	133.67(14)	O(8C)-Cd(2)-O(7C)	53.90(14)
O(13)-Cd(1)-O(6)	85.17(17)	N(4A) -Cd(1)-O(6)	91.97(14)
N(1)-Cd(1)-O(6)	83.44(14)	O(9)-Cd(1)-O(6)	131.57(14)
O(5)-Cd(1)-O(6)	52.43(13)	O(10)-Cd(1)-O(6)	173.85(13)
3			
Bond distances			
Cd-N(3)	2.277(4)	Cd-N(1)	2.292(4)
Cd-O(4)	2.317(4)	Cd-O(7A)	2.330(4)
Cd-O(6A)	2.340(4)	Cd-O(3)	2.358(4)
Bond angles			
N(3)-Cd-N(1)	100.06(16)	N(3)-Cd-O(4)	145.66(15)
N(1)-Cd-O(4)	93.57(15)	N(3)-Cd-O(7A)	90.84(15)
N(1)-Cd-O(7A)	146.01(15)	O(4)-Cd-O(7A)	95.22(14)
N(3)-Cd-O(6A)	99.42(16)	N(1)-Cd-O(6A)	90.64(15)
O(4)-Cd-O(6A)	111.88(14)	O(7A)-Cd-O(6A)	55.67(13)
N(3)-Cd-O(3)	91.39(15)	N(1)-Cd-O(3)	97.48(15)
O(4)-Cd-O(3)	55.43(13)	O(7A)-Cd-O(3)	114.47(14)
O(6A)-Cd-O(3)	165.16(15)		
4			
Bond distances			
Cd-N(3)	2.270(2)	Cd-N(1)	2.281(2)
Cd-O(4)	2.291(2)	Cd-O(7A)	2.300(2)
Cd-O(8A)	2.54(2)	Cd-O(3)	2.451(5)
Bond angles			
N(3)-Cd-N(1)	95.18(8)	N(3)-Cd-O(4)	138.46(8)

Table S1. Selected bond distances (Å) and angles (°) for complexes **1** - **5**. (cont.)

N(1)-Cd-O(4)	95.04(8)	N(3)-Cd-O(7A)	101.90(8)
N(1)-Cd-O(7A)	137.54(9)	O(4)-Cd-O(7A)	97.17(9)
N(3)-Cd-O(8A)	127.7(4)	N(1)-Cd-O(8A)	85.7(6)
O(4)-Cd-O(8A)	93.1(4)	O(7A)-Cd-O(8A)	53.2(6)
N(3)-Cd-O(3)	88.18(12)	N(1)-Cd-O(3)	129.72(14)
O(4)-Cd-O(3)	55.16(12)	O(7A)-Cd-O(3)	89.75(14)
O(8A)-Cd-O(3)	129.7 (6)		
5			
Bond distances			
Cd-O(7)	2.259(2)	Cd-N(1)	2.339(2)
Cd-N(4A)	2.306(3)	Cd-O(3)	2.361(2)
Cd-O(5B)	2.325(2)	Cd-O(4)	2.385(2)
Bond angles			
O(7)-Cd-N(4A)	102.68(9)	O(5B)-Cd-O(3)	80.43(7)
O(7)-Cd-O(5B)	86.39(8)	N(1)-Cd-O(3)	98.61(7)
N(4A)-Cd-O(5B)	90.13(8)	O(7)-Cd-O(4)	164.48(9)
O(7)-Cd-N(1)	85.53(8)	N(4A)-Cd-O(4)	92.33(8)
N(4A)-Cd-N(1)	95.81(8)	O(5B)-Cd-O(4)	97.66(7)
O(5B)-Cd-N(1)	170.85(8)	N(1)-Cd-O(4)	89.07(8)
O(7)-Cd-O(3)	111.68(9)	O(3)-Cd-O(4)	54.80(7)
N(4A)-Cd-O(3)	143.53(7)		

Symmetry transformations used to generate equivalent atoms:

(A) x, y - 1, z; (B) –x + 1, y, -z + 3/2 ; (C) – x + 1, y - 1, -z + 3/2 for **1** ; (A) x - 1, y, z + 1; (B) –x + 1, -y, -z + 2; (C) -x, y + 1/2, -z + 3/2 for **2** ; (A) x, y + 1, z for **3** ; (A) -x, -y + 1,-z + 3 for **4** ; (A) x, y, z + 1; (B) –x + 1/2, y - 1/2, -z + 1/2 for **5**.

Fig. S1. TGA curves for **1** – **5**.

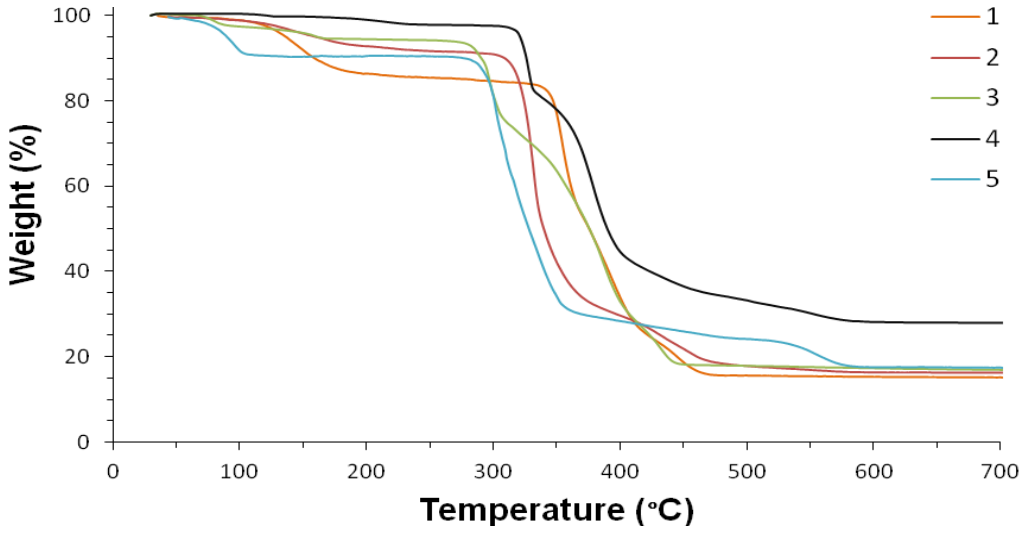

Fig. S2. Emission spectra for **1** – **5**.

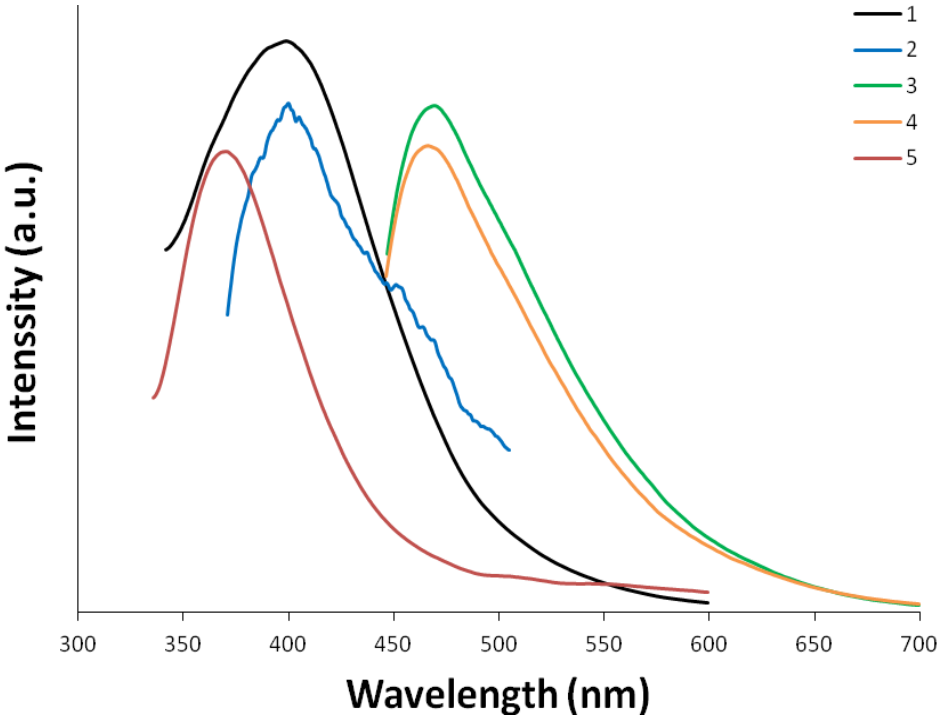

Fig. S3. The simulated and observed XRPD patterns of **1**.

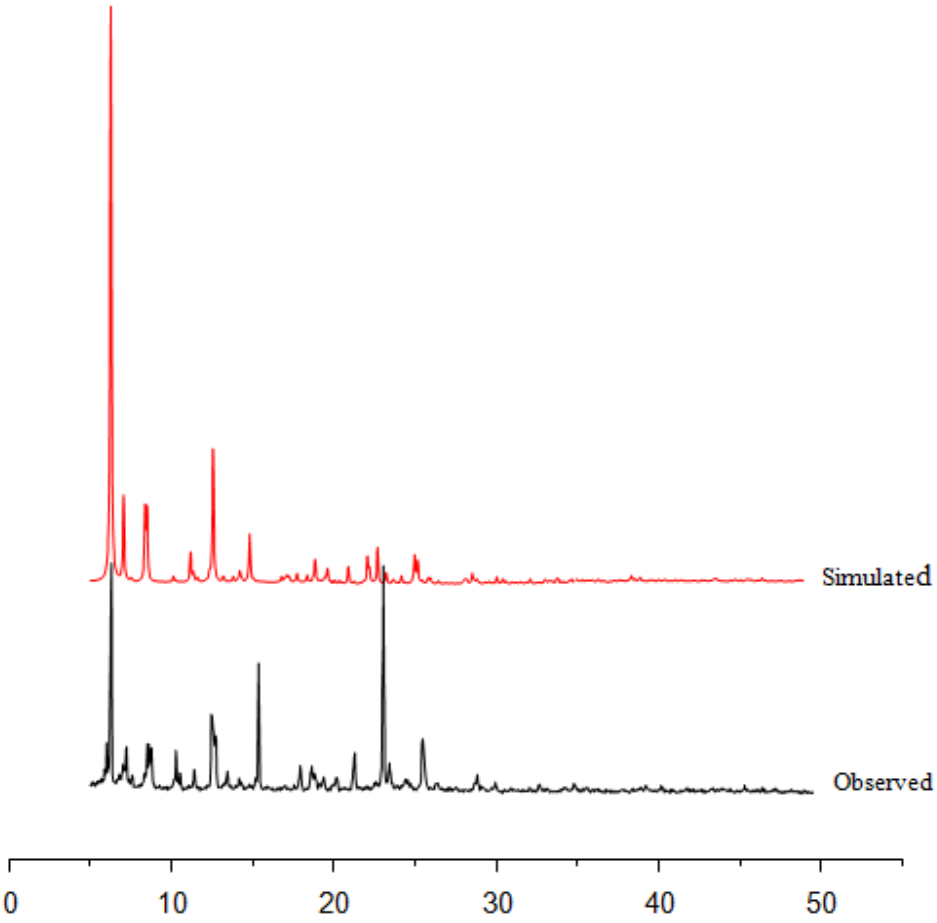

Fig. S4. The XRPD patterns of **1** at 30 - 200 ˚C.

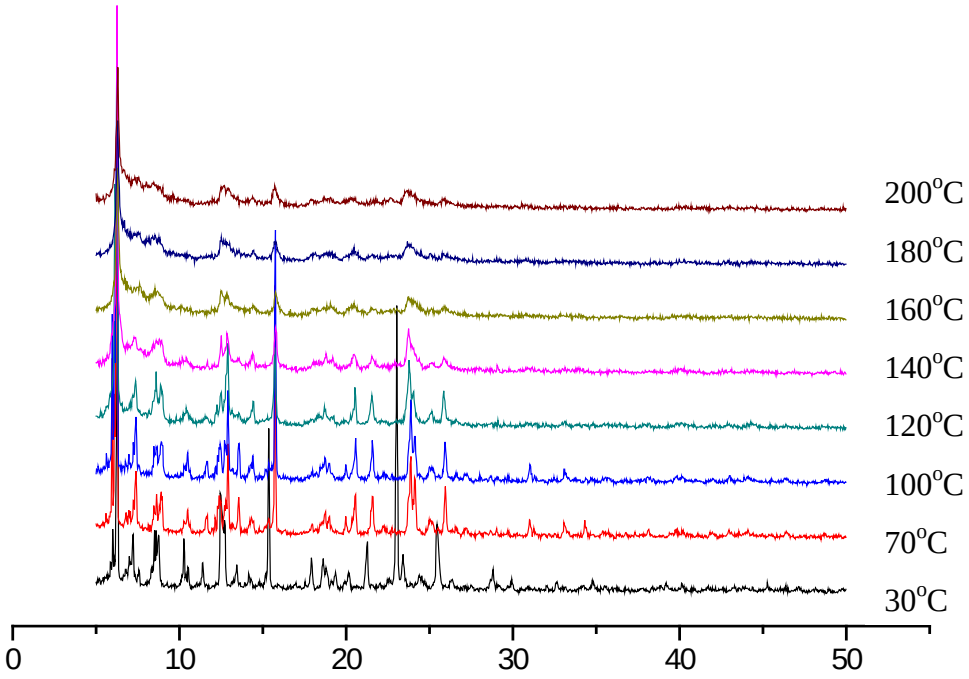

Fig. S5. N_2 adsorption/desorption isotherm of **1'** at 77K.