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A series of coordination polymers based on 5-(2-carboxybenzyloxy) isophthalic acid and bis(imidazole) ligands: syntheses, topological structures and photoluminescent properties

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Table S1a. Selected bond distances (Å) and angles (°) for **1**.

Cd(1)-N(1)	2.235(7)	Cd(1)-O(1)	2.264(5)
Cd(1)-N(4)#1	2.282(8)	Cd(1)-O(3)#2	2.383(4)
Cd(1)-O(4)#2	2.407(5)	Cd(1)-O(7)#3	2.459(6)
N(1)-Cd(1)-O(1)	127.6(2)	N(1)-Cd(1)-N(4)#1	96.1(3)
O(1)-Cd(1)-N(4)#1	89.8(3)	N(1)-Cd(1)-O(3)#2	93.3(2)
O(1)-Cd(1)-O(3)#2	137.6(2)	N(4)#1-Cd(1)-O(3)#2	97.2(2)
N(1)-Cd(1)-O(4)#2	147.36(19)	O(1)-Cd(1)-O(4)#2	84.02(19)
N(4)#1-Cd(1)-O(4)#2	91.4(2)	O(3)#2-Cd(1)-O(4)#2	54.18(17)
N(1)-Cd(1)-O(7)#3	87.6(2)	O(1)-Cd(1)-O(7)#3	87.2(2)
N(4)#1-Cd(1)-O(7)#3	176.2(3)	O(3)#2-Cd(1)-O(7)#3	83.51(18)
O(4)#2-Cd(1)-O(7)#3	85.92(19)		

Table S1b. Hydrogen bonds for **1.**

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(6)-H(6')···O(1)#3	0.82	2.02	2.837(10)	172.9

Symmetry transformations used to generate equivalent atoms: #1 -x, -y, -z + 2; #2 x - 1, y, z; #3 -x, y + 1, -z + 1.

Table S2. Selected bond distances (Å) and angles (°) for **2**.

Zn(1)-O(3)#1	1.940(4)	Zn(1)-O(1)	1.948(4)
Zn(1)-N(1)	1.976(5)	Zn(1)-N(4)#2	1.997(6)
Zn(2)-O(8)	1.955(4)	Zn(2)-O(11)#3	1.985(4)
Zn(2)-N(8)#4	1.989(5)	Zn(2)-N(5)	2.019(5)
O(3)#1-Zn(1)-O(1)	108.78(19)	O(3)#1-Zn(1)-N(1)	114.7(2)
O(1)-Zn(1)-N(1)	114.7(2)	O(3)#1-Zn(1)-N(4)#2	101.5(2)
O(1)-Zn(1)-N(4)#2	108.5(2)	N(1)-Zn(1)-N(4)#2	107.7(2)
O(8)-Zn(2)-O(11)#3	107.58(18)	O(8)-Zn(2)-N(8)#4	107.25(19)
O(11)#3-Zn(2)-N(8)#4	124.54(19)	O(8)-Zn(2)-N(5)	99.0(2)

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O(11)#3-Zn(2)-N(5)	108.87(19)	N(8)#4-Zn(2)-N(5)	106.7(2)

Symmetry transformations used to generate equivalent atoms: #1 x, -y + 1/2, z - 1/2; #2 -x, y - 1/2, -z + 1/2; #3 x, -y + 1/2, z + 1/2; #4 –x + 1, y - 1/2, -z + 3/2.

Table S3. Selected bond distances (Å) and angles (°) for **3**.

Zn(1)-O(4)#1	1.952(3)	Zn(1)-O(1)	1.958(3)
Zn(1)-N(1)	1.998(4)	Zn(1)-N(4)#2	2.008(4)
O(4)#1-Zn(1)-O(1)	111.62(15)	O(4)#1-Zn(1)-N(1)	117.79(16)
O(1)-Zn(1)-N(1)	109.67(16)	O(4)#1-Zn(1)-N(4)#2	103.16(17)
O(1)-Zn(1)-N(4)#2	100.17(17)	N(1)-Zn(1)-N(4)#2	112.90(18)

Symmetry transformations used to generate equivalent atoms: #1 –x + 1/2, y - 1/2, z - 1/2; #2 x - 1/2, -y + 1/2, z.

Table S4. Selected bond distances (Å) and angles (°) for **4**.

Co(1)-O(1)	1.969(2)	Co(1)-O(3)#1	2.025(2)
Co(1)-N(1)	2.033(3)	Co(1)-N(4)#2	2.044(3)
O(1)-Co(1)-O(3)#1	120.72(9)	O(1)-Co(1)-N(1)	123.43(10)
O(3)#1-Co(1)-N(1)	94.90(10)	O(1)-Co(1)-N(4)#2	101.62(10)
O(3)#1-Co(1)-N(4)#2	111.91(10)	N(1)-Co(1)-N(4)#2	103.43(12)

Table S4b. Hydrogen bonds for **4.**

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(6)-H(6A)···O(3)#5	0.82	2.28	2.987(4)	144.3

Symmetry transformations used to generate equivalent atoms: #1 x + 1, y, z; #2 x, y + 1, z.

Table S5a. Selected bond distances (Å) and angles (°) for **5**.

Co(1)-O(2W)	2.104(3)	Co(1)-O(1W)	2.121(3)
Co(1)-N(1)	2.144(4)	Co(1)-N(4)#1	2.147(4)
Co(1)-N(8)#2	2.155(4)	Co(1)-N(5)	2.151(4)
O(2W)-Co(1)-O(1W)	177.04(12)	O(2W)-Co(1)-N(1)	91.31(13)
O(1W)-Co(1)-N(1)	91.62(13)	O(2W)-Co(1)-N(4)#1	87.91(14)

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O(1W)-Co(1)-N(4)#1	92.27(13)	N(1)-Co(1)-N(4)#1	93.73(15)
O(2W)-Co(1)-N(8)#2	87.89(14)	O(1W)-Co(1)-N(8)#2	91.99(14)
N(1)-Co(1)-N(8)#2	85.28(14)	N(4)#1-Co(1)-N(8)#2	175.65(15)
O(2W)-Co(1)-N(5)	90.64(13)	O(1W)-Co(1)-N(5)	86.40(13)
N(1)-Co(1)-N(5)	176.07(17)	N(4)#1-Co(1)-N(5)	89.75(15)
N(8)#2-Co(1)-N(5)	91.39(14)		

Table S5b. Hydrogen bonds for **5.**

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1W)-H(1A)···O(3)#3	0.92	1.82	2.713(4)	163.1
O(1W)-H(1B)···O(4W)	0.87	1.86	2.725(4)	170.7
O(2W)-H(2B)···O(6)#4	0.86	1.90	2.691(4)	151.7
O(2W)-H(2A)···O(3W)	0.86	1.92	2.652(4)	143.4
O(3W)-H(3B)···O(6)	0.85	2.22	2.898(5)	136.1
O(3W)-H(3B)···O(3W)#4	0.85	2.33	2.835(6)	118.2
O(4W)-H(4A)···O(3)#5	0.73	2.02	2.737(4)	167.5
O(4W)-H(4B)···O(2)#3	0.81	1.98	2.781(4)	170.2
O(6W)-H(6B)···O(4)	0.84	2.30	2.705(5)	109.5
O(7)-H(7)···O(1)#4	0.82	2.16	2.969(6)	170.3

Symmetry transformations used to generate equivalent atoms: #1 x + 1, y, z; #2 x - 1, y, z; #3 x, y, z+1; #4 –x + 1, -y + 1, -z + 1; #5 –x + 1, -y, -z + 1.

Table S6a. Selected bond distances (Å) and angles (°) for **6**.

Cu(1)-N(1)	1.968(4)	Cu(1)-O(1)	1.985(3)
Cu(2)-O(3)	1.945(3)	Cu(2)-N(4)#3	1.996(5)
N(1)-Cu(1)-O(1)	89.38(17)	N(1)-Cu(1)-O(1)#1	90.62(16)
O(3)-Cu(2)-N(4)#3	88.85(18)	O(3)#2-Cu(2)-N(4)#3	91.15(18)

Table S6b. Hydrogen bonds for **6.**

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D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(6)-H(6A)···O(7)#6	0.82	2.22	3.013(7)	163.3

Symmetry transformations used to generate equivalent atoms: #1 –x + 2, -y, -z+1; #3 x+1, y, z; #6 –x + 2, -y - 1, -z + 1.

Table S7a. Selected bond distances (Å) and angles (°) for **7**.

Cu(1)-O(1)	1.934(3)	Cu(1)-N(1)	1.977(4)
Cu(1)-N(4)#1	1.991(4)	Cu(1)-O(3)#2	1.998(3)
O(1)-Cu(1)-N(1)	95.17(19)	O(1)-Cu(1)-N(4)#1	93.48(19)
N(1)-Cu(1)-N(4)#1	160.79(15)	O(1)-Cu(1)-O(3)#2	150.47(15)
N(1)-Cu(1)-O(3)#2	89.68(18)	N(4)#1-Cu(1)-O(3)#2	91.21(19)

Table S7b. Hydrogen bonds for **7.**

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(7)-H(7)···O(2)#4	0.82	2.14	2.882(7)	150.1

Symmetry transformations used to generate equivalent atoms: #1 -x, -y + 1, z; #2 x, y, z+1; #4 x + 1/2, -y + 3/2, -z + 1.

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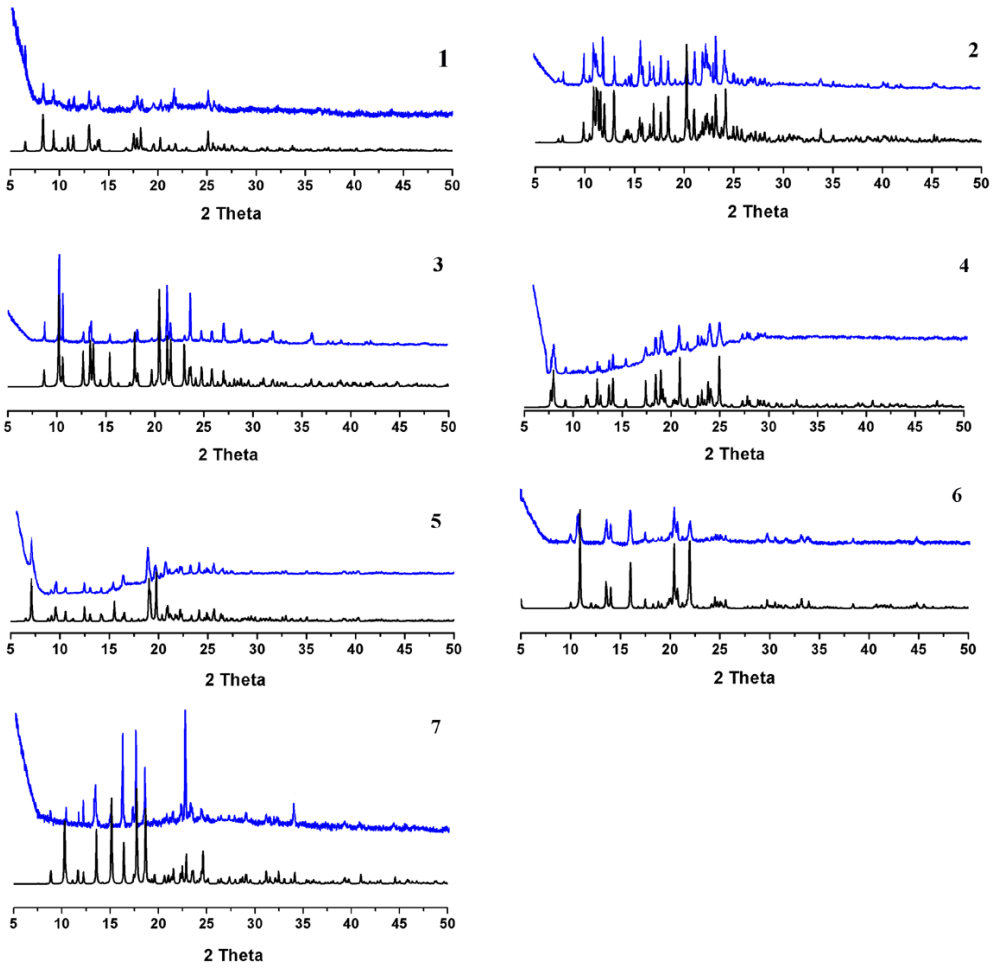

Fig. S1 The simulated (black) and experimental (blue) PXRD patterns for compounds **1**-**7**.

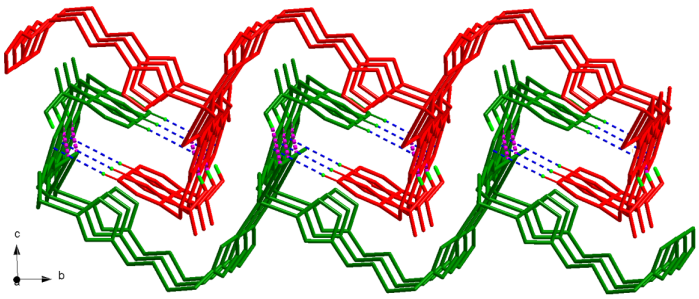

Fig. S2 View of the hydrogen bonds in compound **4** (the blue lines represent C-H···π interactions and the pink lines represent the hydrogen bonding interactions).

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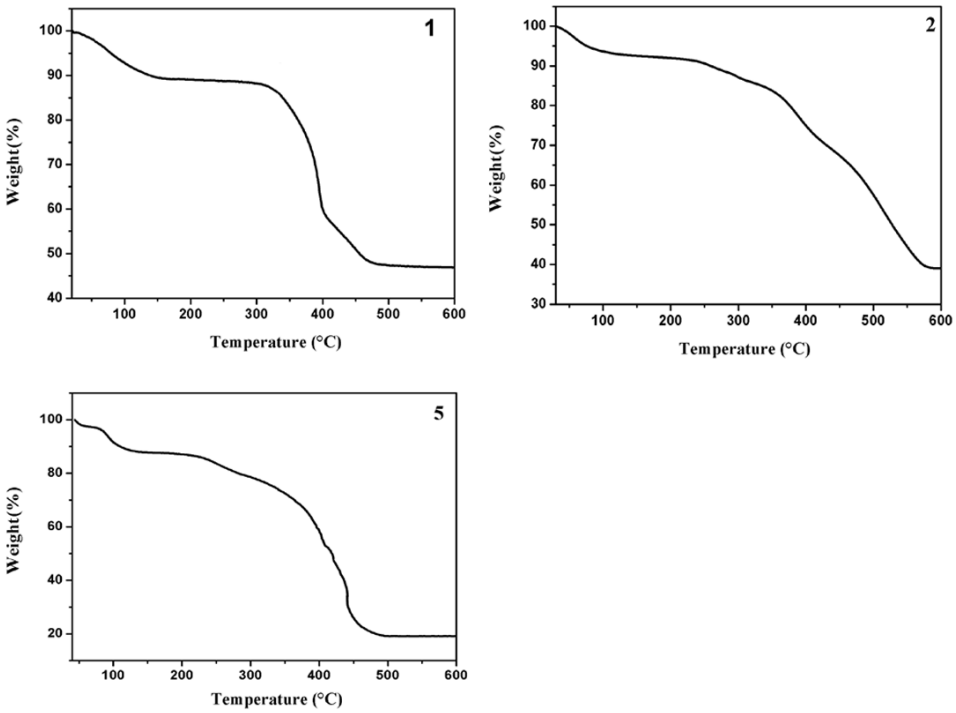

Fig. S3 TGA curves of compounds **1**, **2** and **5**.