Electronic supplementary information

A series of coordination polymers constructed by semi-rigid bifunctional ligand 5-((1H-1,2,4-triazol-1-yl)methoxy) isophthalic acid: syntheses, structures and role of solvents

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

Cu(1)-O(1)	1.9219(16)	Cu(1)-N(3)$^{\#2}$	2.016(2)
O(1)$^{\#1}$-Cu(1)-N(3)$^{\#2}$	91.33(8)	O(1)-Cu(1)-N(3)$^{\#2}$	88.67(8)

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ -x, -y+1, -z+1; $^{\#2}$ -x+1, -y+1, -z+1.

Table S1b. Hydrogen bonds for **1** (Å and °).

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(3)-H(3)...O(2)$^{\#5}$	0.82	1.83	2.625(2)	162.1

Symmetry transformations used to generate equivalent atoms: $^{\#5}$ -x, y+1/2, -z+1/2.

Table S2a. Selected bond distances (Å) and angles (°) for **2**.

Cu(1)-O(1)	1.9402(16)	Cu(1)-N(3)$^{\#2}$	1.983(2)
O(1)-Cu(1)-N(3)$^{\#3}$	88.91(8)	O(1)-Cu(1)-N(3)$^{\#2}$	91.09(8)

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

Table S2b. Hydrogen bonds for **2** (Å and °).

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(4)-H(4A)...O(6)$^{\#5}$	0.82	1.77	2.550(3)	158.0
C(9)-H(9A)...O(3)$^{\#6}$	0.97	2.28	3.143(3)	148.2

Symmetry transformations used to generate equivalent atoms: $^{\#5}$ -x+2, -y-1, -z+1; $^{\#6}$ x-1, y+1, z.

Table S3a. Selected bond distances (Å) and angles (°) for **3**.

Co(1)-O(1)	2.024(3)	Co(1)-O(9)$^{\#1}$	2.065(3)
Co(1)-O(6)	2.095(3)	Co(1)-O(4)$^{\#2}$	2.155(3)
Co(1)-O(3)$^{\#2}$	2.156(2)	Co(1)-N(3)$^{\#3}$	2.162(4)
Co(2)-O(2)	2.017(3)	Co(2)-O(8)$^{\#1}$	2.031(3)
Co(2)-O(11)	2.051(3)	Co(2)-O(6)	2.098(3)
Co(2)-N(6)$^{\#4}$	2.124(4)		
O(1)-Co(1)-O(9)$^{\#1}$	94.44(13)	O(1)-Co(1)-O(6)	97.12(12)
O(9)$^{\#1}$-Co(1)-O(6)	86.71(13)	O(1)-Co(1)-O(4)$^{\#2}$	103.92(12)
O(9)$^{\#1}$-Co(1)-O(4)$^{\#2}$	89.31(13)	O(6)-Co(1)-O(4)$^{\#2}$	158.82(10)
O(1)-Co(1)-O(3)$^{\#2}$	165.12(13)	O(9)$^{\#1}$-Co(1)-O(3)$^{\#2}$	84.22(12)

O(6)-Co(1)-O(3)$^{\#2}$	97.60(11)	O(4)$^{\#2}$-Co(1)-O(3)$^{\#2}$	61.29(11)
O(1)-Co(1)-N(3)$^{\#3}$	90.49(13)	O(9)$^{\#1}$-Co(1)-N(3)$^{\#3}$	175.03(13)
O(6)-Co(1)-N(3)$^{\#3}$	93.36(13)	O(4)$^{\#2}$-Co(1)-N(3)$^{\#3}$	88.85(13)
O(3)$^{\#2}$-Co(1)-N(3)$^{\#3}$	90.85(12)	O(2)-Co(2)-O(8)$^{\#1}$	94.30(14)
O(2)-Co(2)-O(11)	87.97(14)	O(8)$^{\#1}$-Co(2)-O(11)	96.46(14)
O(2)-Co(2)-O(6)	92.98(12)	O(8)$^{\#1}$-Co(2)-O(6)	103.17(12)
O(11)-Co(2)-O(6)	160.22(14)	O(2)-Co(2)-N(6)$^{\#4}$	174.71(15)
O(8)$^{\#1}$-Co(2)-N(6)$^{\#4}$	90.85(15)	O(11)-Co(2)-N(6)$^{\#4}$	90.28(14)
O(6)-Co(2)-N(6)$^{\#4}$	86.98(12)		

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ x-1, y, z; $^{\#2}$ x, y-1, z; $^{\#3}$ -x+2, -y+1, -z+1; $^{\#4}$ -x+2, -y, -z+2.

Table S4a. Selected bond distances (Å) and angles (°) for **4**.

Co(1)-N(3)$^{\#1}$	2.1023(19)	Co(1)-O(1W)	2.1162(17)
Co(1)-O(1)	2.1379(13)	Co(2)-O(2W)	2.0399(17)
Co(2)-O(4)	2.1079(15)	Co(2)-O(3)	2.1641(14)
N(3)$^{\#1}$-Co(1)-O(1W)$^{\#3}$	93.69(8)	N(3)$^{\#1}$-Co(1)-O(1W)	86.31(8)
N(3)$^{\#1}$-Co(1)-O(1)	89.01(6)	O(1W)-Co(1)-O(1)	87.76(6)
N(3)$^{\#2}$-Co(1)-O(1)	90.99(6)	O(1W)$^{\#3}$-Co(1)-O(1)	92.24(6)
O(2W)$^{\#4}$-Co(2)-O(4)	90.15(7)	O(2W)-Co(2)-O(4)	89.85(7)
O(2W)$^{\#4}$-Co(2)-O(3)	92.68(7)	O(4)-Co(2)-O(3)$^{\#4}$	118.45(6)
O(2W)-Co(2)-O(3)	87.32(7)	O(4)-Co(2)-O(3)	61.55(6)

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ -x, -y, -z+1; $^{\#2}$ x+1, y, z; $^{\#3}$ -x+1, -y, -z+1; $^{\#4}$ -x+1, -y+2, -z+2.

Table S4b. Hydrogen bonds for **4** (Å and °).

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1W)-H(1A)...O(2)$^{\#3}$	0.851(9)	1.798(11)	2.629(2)	165(3)
O(1W)-H(1B)...O(3)$^{\#6}$	0.856(9)	2.007(10)	2.856(2)	171(3)
O(2W)-H(2A)...O(1)$^{\#7}$	0.854(10)	1.935(11)	2.786(2)	174(3)
O(2W)-H(2B)...O(6)	0.853(10)	1.795(10)	2.643(3)	173(3)

Symmetry transformations used to generate equivalent atoms: $^{\#3}$ -x+1, -y, -z+1; $^{\#6}$ x, y-1, z; $^{\#7}$ x, y+1, z.

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

Co(1)-O(7)	2.049(3)	Co(1)-O(11)$^{\#1}$	2.052(3)
Co(1)-O(2)	2.057(3)	Co(1)-N(3)$^{\#2}$	2.141(3)
Co(1)-O(1W)	2.172(4)	Co(1)-O(8)$^{\#3}$	2.209(3)
Co(2)-O(11)	2.017(3)	Co(2)-O(1)	2.108(3)
Co(2)-O(8)$^{\#4}$	2.204(3)	Co(3)-O(4)$^{\#5}$	1.987(3)
Co(3)-O(6)$^{\#1}$	2.027(3)	Co(3)-O(11)	2.031(3)
Co(3)-N(6)$^{\#6}$	2.126(4)	Co(3)-O(9)$^{\#3}$	2.162(3)
Co(3)-O(1)	2.333(3)		
O(7)-Co(1)-O(11)$^{\#1}$	95.67(11)	O(7)-Co(1)-O(2)	173.83(11)
O(11)$^{\#1}$-Co(1)-O(2)	90.49(11)	O(7)-Co(1)-N(3)$^{\#2}$	84.85(12)
O(11)$^{\#1}$-Co(1)-N(3)$^{\#2}$	173.60(13)	O(2)-Co(1)-N(3)$^{\#2}$	89.00(12)
O(7)-Co(1)-O(1W)	89.90(14)	O(11)$^{\#1}$-Co(1)-O(1W)	88.52(13)
O(2)-Co(1)-O(1W)	90.00(14)	N(3)$^{\#2}$-Co(1)-O(1W)	85.10(14)
O(7)-Co(1)-O(8)$^{\#3}$	94.76(12)	O(11)$^{\#1}$-Co(1)-O(8)$^{\#3}$	80.76(10)
O(2)-Co(1)-O(8)$^{\#3}$	86.46(11)	N(3)$^{\#2}$-Co(1)-O(8)$^{\#3}$	105.57(12)
O(1W)-Co(1)-O(8)$^{\#3}$	168.67(12)	O(11)$^{\#1}$-Co(2)-O(1)	93.70(11)
O(11)-Co(2)-O(1)	86.30(11)	O(11)-Co(2)-O(8)$^{\#4}$	81.63(10)
O(1)-Co(2)-O(8)$^{\#4}$	93.20(10)	O(11)-Co(2)-O(8)$^{\#3}$	98.37(10)
O(1)-Co(2)-O(8)$^{\#3}$	86.80(10)	O(4)$^{\#5}$-Co(3)-O(6)$^{\#1}$	101.82(12)
O(4)$^{\#5}$-Co(3)-O(11)	160.52(12)	O(6)$^{\#1}$-Co(3)-O(11)	93.32(11)
O(4)$^{\#5}$-Co(3)-N(6)$^{\#6}$	93.27(13)	O(6)$^{\#1}$-Co(3)-N(6)$^{\#6}$	92.21(14)
O(11)-Co(3)-N(6)$^{\#6}$	98.37(13)	O(4)$^{\#5}$-Co(3)-O(9)$^{\#3}$	81.73(12)
O(6)$^{\#1}$-Co(3)-O(9)$^{\#3}$	176.33(11)	O(11)-Co(3)-O(9)$^{\#3}$	83.41(10)
N(6)$^{\#6}$-Co(3)-O(9)$^{\#3}$	86.64(13)	O(4)$^{\#5}$-Co(3)-O(1)	87.36(11)
O(6)$^{\#1}$-Co(3)-O(1)	90.59(12)	O(11)-Co(3)-O(1)	80.24(10)
N(6)$^{\#6}$-Co(3)-O(1)	176.94(12)	O(9)$^{\#3}$-Co(3)-O(1)	90.49(10)

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ -x+2, -y, -z+2; $^{\#2}$ x-1, y, z; $^{\#3}$ -x+1, -y, -z+2; $^{\#4}$ x+1, y, z; $^{\#5}$ -x+2, -y, -z+3; $^{\#6}$ x+1, y-1, z+1.

Table S5b. Hydrogen bonds for **5** (Å and °).

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(11)-H(11A)...O(12)$^{\#1}$	0.847(11)	2.137(18)	2.957(5)	163(4)
O(1W)-H(1A)...O(12)	0.846(11)	1.860(15)	2.691(6)	167(5)

O(1W)-H(1B)...O(13)	0.845(10)	1.96(2)	2.788(11)	166(6)

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

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

Cd(1)-O(1)	2.235(2)	Cd(1)-O(2)#1	2.278(2)
Cd(1)-N(3)#2	2.285(3)	Cd(1)-O(4)#3	2.353(2)
Cd(1)-O(3)#3	2.376(2)	Cd(1)-O(6)	2.383(3)
O(1)-Cd(1)-O(2)#1	114.99(9)	O(1)-Cd(1)-N(3)#2	98.05(10)
O(2)#1-Cd(1)-N(3)#2	91.41(10)	O(1)-Cd(1)-O(4)#3	90.69(8)
O(2)#1-Cd(1)-O(4)#3	149.46(8)	N(3)#2-Cd(1)-O(4)#3	101.49(10)
O(1)-Cd(1)-O(3)#3	145.85(8)	O(2)#1-Cd(1)-O(3)#3	97.94(8)
N(3)#2-Cd(1)-O(3)#3	89.54(9)	O(4)#3-Cd(1)-O(3)#3	55.16(7)
O(1)-Cd(1)-O(6)	91.53(10)	O(2)#1-Cd(1)-O(6)	82.20(10)
N(3)#2-Cd(1)-O(6)	170.10(10)	O(4)#3-Cd(1)-O(6)	80.80(10)
O(3)#3-Cd(1)-O(6)	83.88(9)		

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

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

Cd(1)-O(3)#1	2.289(4)	Cd(1)-O(4)#2	2.298(3)
Cd(1)-O(6)	2.320(4)	Cd(1)-N(3)#3	2.340(5)
Cd(1)-O(1)	2.362(4)	Cd(1)-O(2)	2.401(4)
O(3)#1-Cd(1)-O(4)#2	102.43(13)	O(3)#1-Cd(1)-O(6)	129.09(16)
O(4)#2-Cd(1)-O(6)	83.12(14)	O(3)#1-Cd(1)-N(3)#3	82.32(16)
O(4)#2-Cd(1)-N(3)#3	158.20(15)	O(6)-Cd(1)-N(3)#3	77.64(17)
O(3)#1-Cd(1)-O(1)	84.51(14)	O(4)#2-Cd(1)-O(1)	102.85(15)
O(6)-Cd(1)-O(1)	144.35(16)	N(3)#3-Cd(1)-O(1)	98.77(17)
O(3)#1-Cd(1)-O(2)	136.89(13)	O(4)#2-Cd(1)-O(2)	98.94(13)
O(6)-Cd(1)-O(2)	90.17(16)	N(3)#3-Cd(1)-O(2)	91.33(16)
O(1)-Cd(1)-O(2)	54.25(13)		

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

Table S8a. Selected bond distances (Å) and angles (°) for **8**.

Cd(1)-O(2W)	2.297(3)	Cd(1)-O(1)	2.342(2)

Cd(1)-N(3)$^{\#1}$	2.346(3)	Cd(1)-O(1W)	2.348(3)
Cd(1)-O(3)$^{\#2}$	2.362(2)	Cd(1)-O(2)	2.408(2)
Cd(1)-O(4)$^{\#2}$	2.433(2)		
O(2W)-Cd(1)-O(1)	100.71(9)	O(2W)-Cd(1)-N(3)$^{\#1}$	84.02(10)
O(1)-Cd(1)-N(3)$^{\#1}$	86.10(8)	O(2W)-Cd(1)-O(1W)	171.72(11)
O(1)-Cd(1)-O(1W)	84.65(9)	N(3)$^{\#1}$-Cd(1)-O(1W)	90.11(11)
O(2W)-Cd(1)-O(3)$^{\#2}$	91.10(9)	O(1)-Cd(1)-O(3)$^{\#2}$	166.24(8)
N(3)$^{\#1}$-Cd(1)-O(3)$^{\#2}$	88.16(8)	O(1W)-Cd(1)-O(3)$^{\#2}$	82.86(9)
O(2W)-Cd(1)-O(2)	93.92(10)	O(1)-Cd(1)-O(2)	54.78(7)
N(3)$^{\#1}$-Cd(1)-O(2)	139.85(9)	O(1W)-Cd(1)-O(2)	94.33(10)
O(3)$^{\#2}$-Cd(1)-O(2)	131.99(8)	O(2W)-Cd(1)-O(4)$^{\#2}$	88.20(9)
O(1)-Cd(1)-O(4)$^{\#2}$	132.19(7)	N(3)$^{\#1}$-Cd(1)-O(4)$^{\#2}$	141.71(8)
O(1W)-Cd(1)-O(4)$^{\#2}$	92.85(9)	O(3)$^{\#2}$-Cd(1)-O(4)$^{\#2}$	54.48(7)
O(2)-Cd(1)-O(4)$^{\#2}$	77.97(7)		

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ -x, y-1/2, -z+1/2; $^{\#2}$ -x+1, y-1/2, -z+3/2.

Table S8b. Hydrogen bonds for **8** (Å and °).

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1W)-H(1A)...O(4W)$^{\#6}$	0.846(10)	2.17(2)	2.960(9)	156(4)
O(1W)-H(1B)...O(4)$^{\#7}$	0.842(10)	2.071(14)	2.900(3)	168(5)
O(2W)-H(2A)...O(3W)$^{\#8}$	0.77(4)	1.97(5)	2.698(4)	156(5)
O(2W)-H(2B)...O(1)$^{\#9}$	0.73(4)	1.97(4)	2.702(3)	177(5)
O(3W)-H(3A)...O(5)$^{\#7}$	0.849(10)	2.25(2)	3.000(3)	148(4)
O(3W)-H(3B)...O(4)$^{\#2}$	0.851(10)	1.992(12)	2.840(4)	175(5)
O(4W)-H(4A)...O(3)$^{\#7}$	0.849(10)	2.12(3)	2.904(10)	153(6)

Symmetry transformations used to generate equivalent atoms: $^{\#2}$ -x+1, y-1/2, -z+3/2; $^{\#6}$ -x+1, y-1/2, -z+1/2; $^{\#7}$ -x+1, -y+1, -z+1; $^{\#8}$ x-1, y, z; $^{\#9}$ x, -y+1/2, z+1/2.

Table S9a. Selected bond distances (Å) and angles (°) for **9**.

Mn(1)-O(1W)	2.1712(18)	Mn(1)-O(2W)	2.215(2)
Mn(1)-O(4)$^{\#1}$	2.2580(16)	Mn(1)-O(2)	2.2918(17)
Mn(1)-N(3)$^{\#2}$	2.2931(19)	Mn(1)-O(3)$^{\#1}$	2.3351(18)
Mn(1)-O(1)	2.3523(16)		
O(1W)-Mn(1)-O(2W)	174.33(9)	O(1W)-Mn(1)-O(4)$^{\#1}$	98.49(7)

O(2W)-Mn(1)-O(4)$^{\#1}$	85.08(7)	O(1W)-Mn(1)-O(2)	92.34(7)
O(2W)-Mn(1)-O(2)	83.42(8)	O(4)$^{\#1}$-Mn(1)-O(2)	165.45(6)
O(1W)-Mn(1)-N(3)$^{\#2}$	85.11(7)	O(2W)-Mn(1)-N(3)$^{\#2}$	90.83(9)
O(4)$^{\#1}$-Mn(1)-N(3)$^{\#2}$	85.13(7)	O(2)-Mn(1)-N(3)$^{\#2}$	86.15(7)
O(1W)-Mn(1)-O(3)$^{\#1}$	92.44(7)	O(2W)-Mn(1)-O(3)$^{\#1}$	93.20(9)
O(4)$^{\#1}$-Mn(1)-O(3)$^{\#1}$	56.70(6)	O(2)-Mn(1)-O(3)$^{\#1}$	132.84(6)
N(3)$^{\#2}$-Mn(1)-O(3)$^{\#1}$	141.01(7)	O(1W)-Mn(1)-O(1)	87.38(6)
O(2W)-Mn(1)-O(1)	93.34(8)	O(4)$^{\#1}$-Mn(1)-O(1)	133.77(6)
O(2)-Mn(1)-O(1)	56.05(6)	N(3)$^{\#2}$-Mn(1)-O(1)	141.09(6)
O(3)$^{\#1}$-Mn(1)-O(1)	77.35(6)		

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ -x+1, y+1/2, -z+3/2; $^{\#2}$ x-1, y, z-1.

Table S9b. Hydrogen bonds for **9** (Å and °).

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(2W)-H(2B)...O(4W)	0.79(4)	2.21(4)	2.950(7)	156(4)
O(3W)-H(3A)...O(1)	0.849(10)	1.982(10)	2.830(3)	178(4)
O(1W)-H(1A)...O(4)$^{\#6}$	0.851(10)	1.853(10)	2.703(2)	177(3)
O(1W)-H(1B)...O(3W)$^{\#7}$	0.849(10)	1.863(12)	2.698(3)	167(3)
O(2W)-H(2A)...O(1)$^{\#8}$	0.76(4)	2.12(4)	2.876(3)	173(4)
O(3W)-H(3B)...O(5)$^{\#8}$	0.842(10)	2.22(2)	2.974(3)	149(3)
O(4W)-H(4A)...O(2)$^{\#5}$	0.88(6)	2.07(6)	2.924(8)	162(6)

Symmetry transformations used to generate equivalent atoms: $^{\#5}$ -x+1, -y+1, -z+1; $^{\#6}$ -x+1, -y+1, -z+2; $^{\#7}$ x-1, y, z; $^{\#8}$ x, -y+3/2, z-1/2.

Table S10a. Selected bond distances (Å) and angles (°) for **10**.

Mn(1)-O(4)$^{\#1}$	2.0821(19)	Mn(1)-O(3)$^{\#2}$	2.1005(18)
Mn(1)-O(7)	2.142(3)	Mn(1)-O(6)	2.208(2)
Mn(1)-O(1)	2.2085(18)	Mn(1)-O(2)	2.3546(18)
O(4)$^{\#1}$-Mn(1)-O(3)$^{\#2}$	113.03(7)	O(4)$^{\#1}$-Mn(1)-O(7)	90.89(13)
O(3)$^{\#2}$-Mn(1)-O(7)	95.23(13)	O(4)$^{\#1}$-Mn(1)-O(6)	86.12(9)
O(3)$^{\#2}$-Mn(1)-O(6)	93.48(9)	O(7)-Mn(1)-O(6)	171.28(13)
O(4)$^{\#1}$-Mn(1)-O(1)	153.63(7)	O(3)$^{\#2}$-Mn(1)-O(1)	93.22(6)
O(7)-Mn(1)-O(1)	89.04(13)	O(6)-Mn(1)-O(1)	90.01(8)
O(4)$^{\#1}$-Mn(1)-O(2)	96.35(7)	O(3)$^{\#2}$-Mn(1)-O(2)	150.60(7)

O(7)-Mn(1)-O(2)	84.88(13)	O(6)-Mn(1)-O(2)	87.31(9)
O(1)-Mn(1)-O(2)	57.38(6)		

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

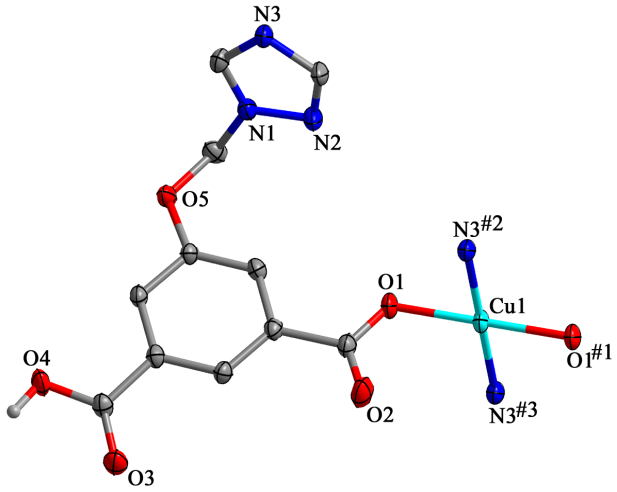

Fig. **S1.** ORTEP view of **2** showing the local coordination environment of Cu(II) atom with DMA molecule omitted for clarity (30% probability displacement ellipsoids). Symmetry codes: [#1] -x+2, -y, -z+2; [#2] -x+1, -y, -z+2; [#3] x+1, y, z.

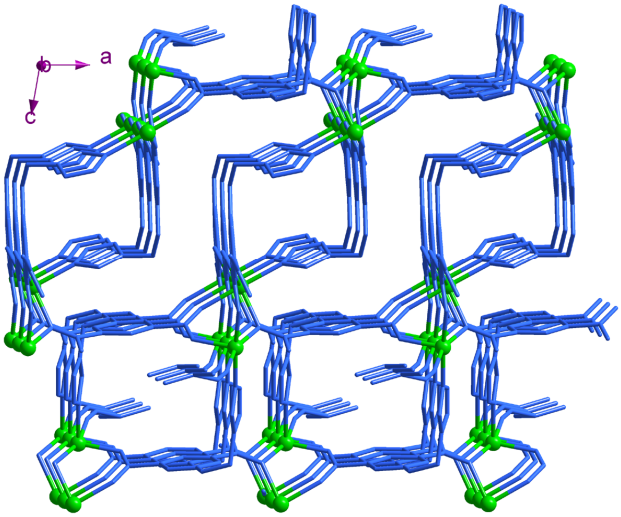

Fig. S2. View of the 3D framework of **3**.

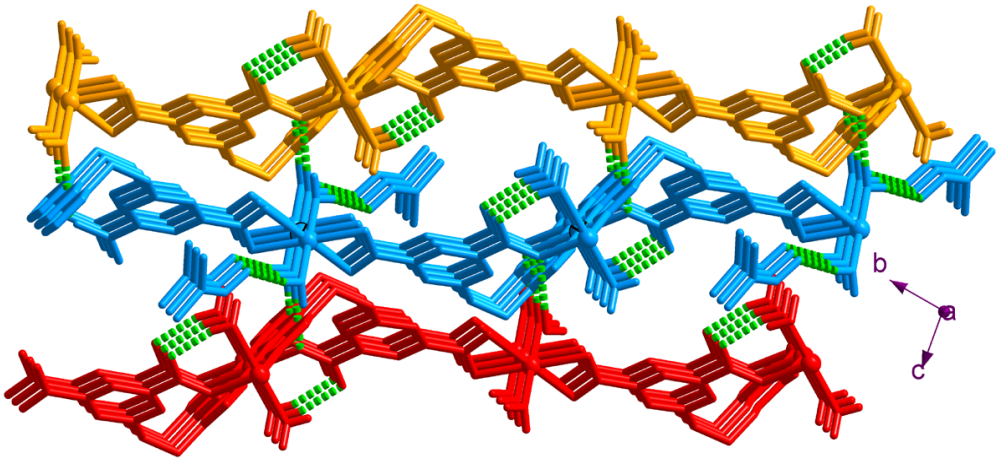

Fig. S3. The 3D supramolecular architecture formed through hydrogen bonds in **4**.

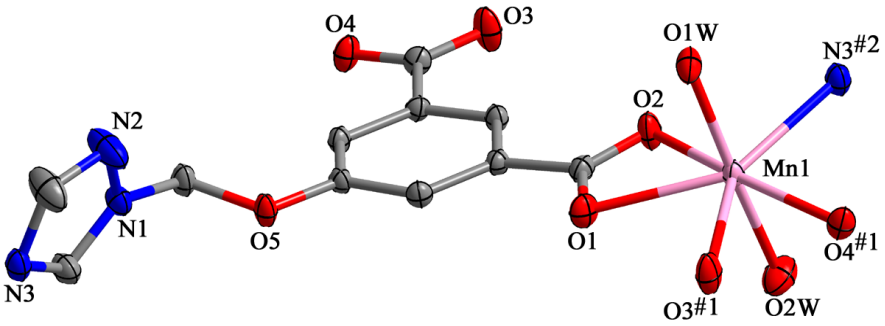

Fig. S4. ORTEP view of **9** showing the local coordination environment of Mn(II) atom with hydrogen atoms and free water molecules omitted for clarity (30% probability displacement ellipsoids). Symmetry codes: #1 -x+1, y+1/2, -z+3/2; #2 x-1, y, z-1.

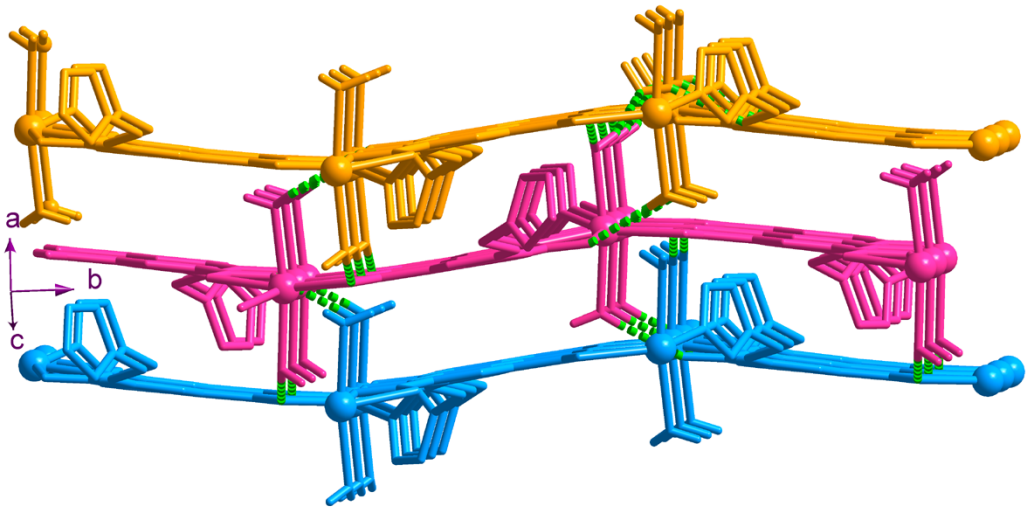

Fig. S5. The 3D supramolecular architecture formed by hydrogen bonding interactions in **8**.

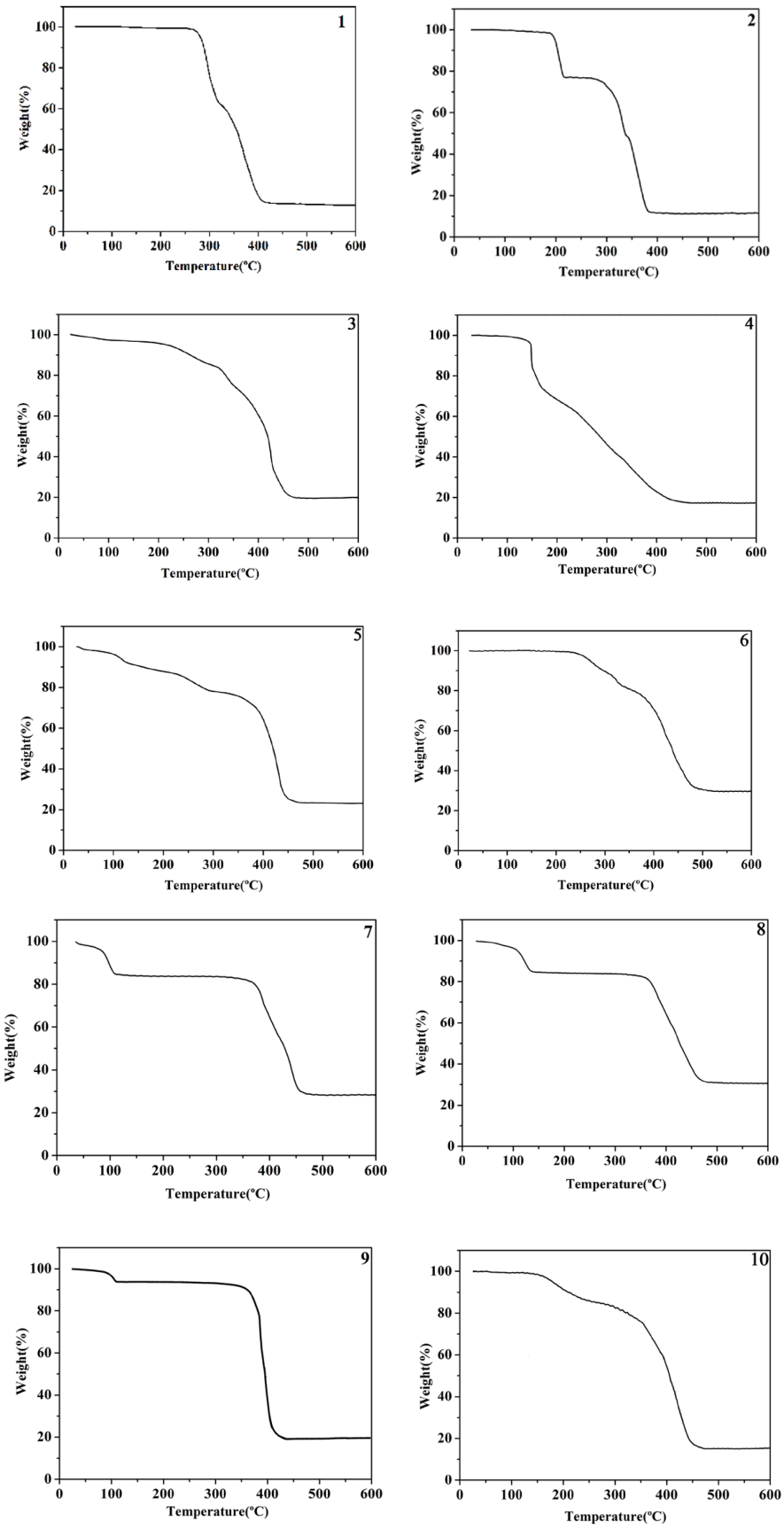

Fig. S6. TGA curves of compounds **1**–**10**.

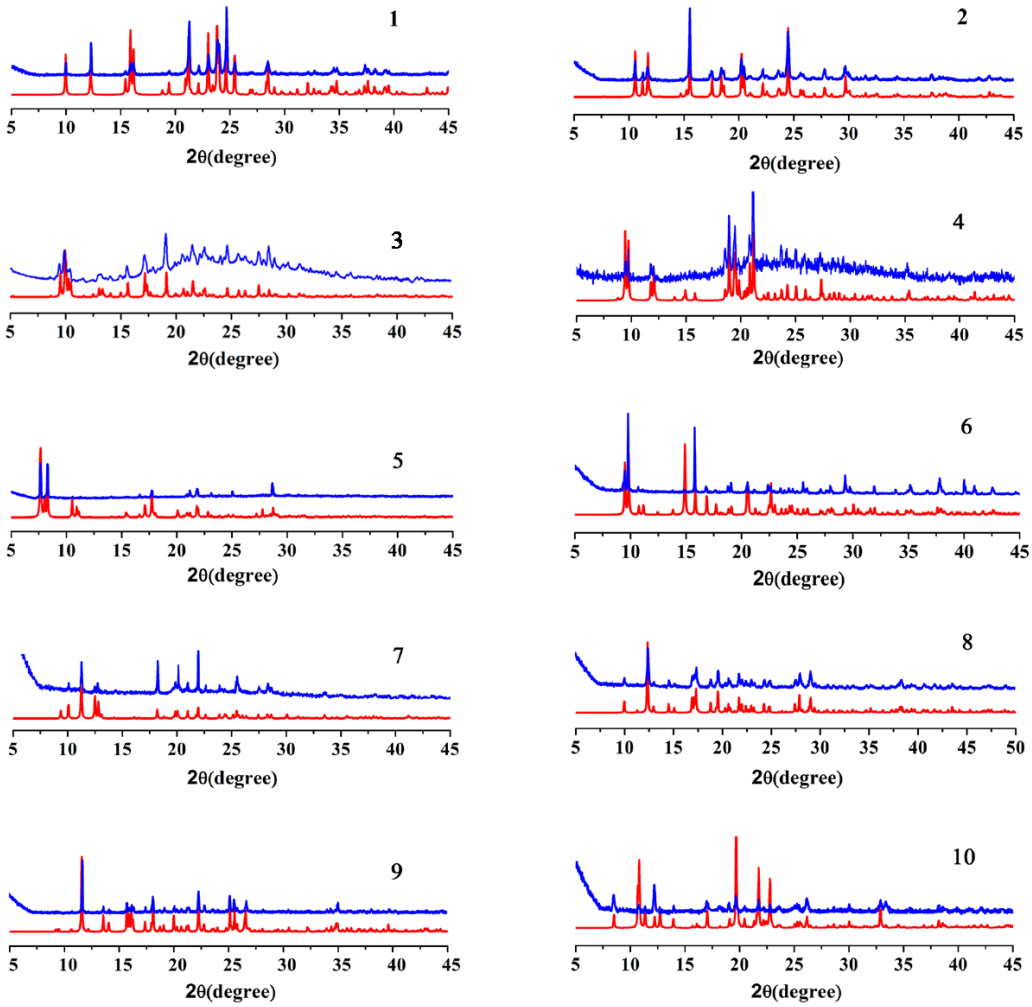

Fig. S7. Simulated (red) and experimental (blue) PXRD patterns of **1**–**10**.