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Supporting Informatin

Five new 2D and 3D coordination polymers based on two new multifunctional pyridyl-tricarboxylate ligands: hydrothermal syntheses, structural diversity, luminescent and magnetic properties

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Table S1. The selected bond lengths (Å) and angles (◦) for compound **1**.

Zn(1)-O(6)C	1.992(5)	Zn(1)-O(3)A	2.038(6)
Zn(1)-O(4)B	2.004(5)	Zn(1)-N(1)	2.075(5)
Zn(1)-O(6)	2.118(6)	O(6)C-Zn(1)-O(4)B	102.7(2)
O(6)C-Zn(1)-O(3)A	95.8(2)	O(4)B-Zn(1)-O(3)A	87.1(2)
O(6)C-Zn(1)-N(1)	105.3(3)	O(4)B-Zn(1)-N(1)	151.6(3)
O(3)A-Zn(1)-N(1)	94.6(3)	O(6)C-Zn(1)-O(6)	108.41(18)
O(4)B-Zn(1)-O(6)	89.6(2)	O(3)A-Zn(1)-O(6)	155.7(2)
N(1)-Zn(1)-O(6)	77.3(3)		

Symmetry transformations used to generate equivalent atoms: A: 2-x, 1-y, 0.5+z; B: 0.5+x, 1-y, z; C: 2.5-x, y, 0.5+z.

Table S2. The selected bond lengths (Å) and angles (◦) for compound **2**.

Cd(1)-O(9)	2.251(5)	Cd(1)-O(9)A	2.280(5)
Cd(1)-O(2)B	2.318(4)	Cd(1)-N(1)	2.325(6)
Cd(1)-O(4)E	2.342(4)	Cd(1)-N(2)	2.405(5)
Cd(2)-O(5)	2.285(5)	Cd(2)-O(9)	2.225(4)
Cd(2)-N(4)	2.374(6)	Cd(2)-N(5)E	2.354(5)
Cd(2)-N(3)	2.441(5)	Cd(2)-O(4)E	2.418(4)
O(9)A-Cd(1)-O(2)B	81.69(17)	O(9)-Cd(1)-O(9)A	81.56(18)
O(9)A-Cd(1)-N(1)	97.36(19)	O(9)-Cd(1)-O(2)B	106.65(18)
O(2)B-Cd(1)-N(1)	92.06(19)	O(9)-Cd(1)-N(1)	160.81(18)
O(2)B-Cd(1)-O(4)E	75.03(15)	O(9)-Cd(1)-O(4)E	78.97(16)
O(9)-Cd(1)-N(2)	93.30(19)	O(9)A-Cd(1)-O(4)E	143.68(16)
O(2)B-Cd(1)-N(2)	154.73(19)	N(1)-Cd(1)-O(4)E	110.79(18)
O(9)-Cd(2)-O(5)	95.62(17)	O(9)A-Cd(1)-N(2)	117.23(18)
O(5)-Cd(2)-N(5)E	98.49(17)	N(1)-Cd(1)-N(2)	70.0(2)
O(5)-Cd(2)-N(4)	107.2(2)	O(9)-Cd(2)-N(5)E	141.83(18)
O(9)-Cd(2)-O(4)E	77.86(16)	O(9)-Cd(2)-N(4)	101.28(19)
N(5)E-Cd(2)-O(4)E	68.13(16)	N(5)E-Cd(2)-N(4)	107.98(19)

O(9)-Cd(2)-N(3)	87.85(18)	O(5)-Cd(2)-O(4)E	85.66(17)
N(5)E-Cd(2)-N(3)	80.65(18)	N(4)-Cd(2)-O(4)E	167.09(17)
O(4)E-Cd(2)-N(3)	98.35(17)	O(5)-Cd(2)-N(3)	175.19(18)
N(4)-Cd(2)-N(3)	68.75(19)		

Hydrogen bond lengths (Å) and angles (◦) for compound **2**.

D-H	A	d(D-H)	d(H..A)	<DHA	d(D..A)
O7	O8 [x, y+1, z]	0.850	2.136	162.88	2.959
O7	O10	0.850	1.982	162.72	2.805
O8	O3 [-x+1, -y+1, -z]	0.850	2.041	162.54	2.864
O8	O7 [-x+1, -y+1, -z]	0.850	2.153	137.22	2.836
O9	O1 [-x+1, -y+1, -z+1]	0.726	2.160	160.93	2.856

D : Donor; A: Acceptor

Symmetry transformations used to generate equivalent atoms: A: -x+2, -y+1, -z+1; B: x+1, y, z; E: -x+2,-y+1,-z.

Table S3. The selected bond lengths (Å) and angles (◦) for compound **3**.

Co(1)-O(5)	2.0437(16)	Co(1)-O(3)B	2.1084(13)
Co(1)-O(4)	2.0697(13)	Co(1)-O(2)A	2.1111(13)
Co(1)-N(1)A	2.1338(15)	Co(1)-O(6)	2.1459(13)
O(5)-Co(1)-O(4)	94.40(6)	O(5)-Co(1)-O(3)B	88.72(7)
O(4)-Co(1)-O(3)B	100.15(5)	O(5)-Co(1)-O(2)A	100.75(7)
O(4)-Co(1)-O(2)A	91.15(5)	O(3)B-Co(1)-O(2)A	164.71(5)
O(5)-Co(1)-N(1)A	177.48(7)	O(4)-Co(1)-N(1)A	86.88(5)
O(3)B-Co(1)-N(1)A	93.20(6)	O(2)A-Co(1)-N(1)A	77.04(5)
O(5)-Co(1)-O(6)	83.65(6)	O(4)-Co(1)-O(6)	173.30(5)
O(3)B-Co(1)-O(6)	86.23(5)	O(2)A-Co(1)-O(6)	82.95(5)
N(1)A-Co(1)-O(6)	94.84(5)		

Hydrogen bond lengths (Å) and angles (◦) for compound **3**.

D	A	d(D-H)	d(H..A)	<DHA	d(D..A)
O5	O1 [-x+1, y+1/2, -z+1/2]	0.820	1.978	158.63	2.758
O6	O1 [x, y, z-1]	0.820	1.872	166.64	2.676
O7	O8 [-x, -y+2, -z+1]	0.820	1.791	173.20	2.607
O6	O2 [-x+1, y+1/2, -z+1/2]	0.831	1.925	174.49	2.753
O5	O6 [x, -y+3/2, z+1/2]	0.775	2.020	157.07	2.750

D : Donor; A: Acceptor

Symmetry transformations used to generate equivalent atoms: A: x, 0.5-y, -0.5+z; B: x, 1.5-y, -0.5+z.

Table S4. The selected bond lengths (Å) and angles (◦) for compound **4**.

Co(1)-O(3)C	2.0718(12)	Co(1)-O(3)	2.0718(12)
Co(1)-O(1)B	2.0872(12)	Co(1)-O(1)A	2.0872(12)
Co(1)-O(4)	2.1328(12)	Co(1)-O(4)C	2.1328(12)
Co(2)-O(8)	2.0674(14)	Co(2)-O(8)E	2.0674(14)
Co(2)-O(9)	2.0779(11)	Co(2)-O(9)E	2.0779(11)
Co(2)-N(1)E	2.1073(12)	Co(2)-N(1)	2.1073(12)
Co(3)-O(5)D	2.0812(12)	Co(3)-O(5)	2.0812(12)
Co(3)-O(7)	2.1066(11)	Co(3)-O(7)D	2.1066(11)
Co(3)-O(6)	2.1045(14)	Co(3)-O(6)D	2.1045(14)
O(1)B-Co(1)-O(1)A	180.0	O(3)C-Co(1)-O(4)	84.20(5)
O(3)-Co(1)-O(4)	95.80(5)	O(1)A-Co(1)-O(4)	88.66(6)
O(1)B-Co(1)-O(4)	91.34(6)	O(3)C-Co(1)-O(4)C	95.80(5)
O(3)-Co(1)-O(4)C	84.20(5)	O(1)A-Co(1)-O(4)C	91.34(6)
O(4)-Co(1)-O(4)C	180.00(3)	O(1)B-Co(1)-O(4)C	88.66(6)
O(8)-Co(2)-O(8)E	180.0	O(8)-Co(2)-O(9)	89.90(6)
O(8)E-Co(2)-O(9)	90.10(6)	O(8)-Co(2)-O(9)E	90.10(6)
O(8)E-Co(2)-O(9)E	89.90(6)	O(9)-Co(2)-O(9)E	180.0
O(8)-Co(2)-N(1)E	88.47(5)	O(8)E-Co(2)-N(1)E	91.53(5)
O(9)-Co(2)-N(1)E	102.23(5)	O(9)E-Co(2)-N(1)E	77.77(5)
O(8)-Co(2)-N(1)	91.53(5)	O(8)E-Co(2)-N(1)	88.47(5)
O(9)-Co(2)-N(1)	77.77(5)	O(9)E-Co(2)-N(1)	102.23(5)
N(1)E-Co(2)-N(1)	180.0	O(5)D-Co(3)-O(5)	180.000(1)
O(5)D-Co(3)-O(7)	87.66(5)	O(5)-Co(3)-O(7)	92.34(5)
O(5)-Co(3)-O(7)D	87.66(5)	O(5)D-Co(3)-O(7)D	92.34(5)
O(7)-Co(3)-O(7)D	180.00(5)	O(5)D-Co(3)-O(6)	89.93(6)
O(5)-Co(3)-O(6)	90.07(6)	O(7)-Co(3)-O(6)	89.82(5)
O(7)D-Co(3)-O(6)	90.18(5)	O(5)D-Co(3)-O(6)D	90.07(6)
O(7)-Co(3)-O(6)D	90.18(5)	O(5)-Co(3)-O(6)D	89.93(6)
O(7)D-Co(3)-O(6)D	89.82(5)	O(6)-Co(3)-O(6)D	180.0

Symmetry transformations used to generate equivalent atoms: A: -x+1, -y, -z+2; B: x-1, y, z; C: -x, -y, -z+2; D: -x, -y+1, -z+2; E: -x-1, -y+1, -z+1.

Table S5. The selected bond lengths (Å) and angles (◦) for compound **5**.

Mn(1)-O(5)C	2.130(3)	Mn(1)-O(7)E	2.152(3)
Mn(1)-O(5)B	2.130(3)	Mn(1)-O(7)D	2.152(3)
Mn(1)-O(2)	2.219(3)	Mn(1)-O(2)A	2.219(3)
Mn(2)-O(1)	2.122(3)	Mn(2)-O(6)E	2.128(3)
Mn(2)-O(4)B	2.147(3)	Mn(2)-O(2)	2.188(3)
Mn(2)-N(1)	2.316(4)	O(5)C-Mn(1)-O(5)B	180.0
O(5)C-Mn(1)-O(7)D	92.89(14)	O(5)B-Mn(1)-O(7)D	87.11(14)
O(5)C-Mn(1)-O(7)E	87.11(14)	O(5)B-Mn(1)-O(7)E	92.89(14)
O(7)D-Mn(1)-O(7)E	180.0	O(5C-Mn(1)-O(2)	94.99(13)
O(5)B-Mn(1)-O(2)	85.01(13)	O(7)D-Mn(1)-O(2)	94.57(13)

O(7)E-Mn(1)-O(2)	85.43(13)	O(5)C-Mn(1)-O(2)A	85.01(13)
O(5)B-Mn(1)-O(2)A	94.99(13)	O(7)D-Mn(1)-O(2)A	85.43(13)
O(7)E-Mn(1)-O(2)A	94.57(13)	O(2)-Mn(1)-O(2)A	180.00(3)
O(1)-Mn(2)-O(6)E	92.06(14)	O(1)-Mn(2)-O(4)B	114.84(15)
O(6)E-Mn(2)-O(4)B	94.47(14)	O(1)-Mn(2)-O(2)	133.95(14)
O(6)E-Mn(2)-O(2)	98.54(13)	O(4)B-Mn(2)-O(2)	108.84(13)
O(1)-Mn(2)-N(1)	83.59(15)	O(6)E-Mn(2)-N(1)	170.36(15)
O(4)B-Mn(2)-N(1)	79.68(15)	O(2)-Mn(2)-N(1)	90.64(13)

Hydrogen bond lengths (Å) and angles (◦) for compound **5** (D : Donor; A: Acceptor).

D	A	d(D..A)	d(D-H)	d(H..A)	<DHA
O1	O3 [-x, -y+1, -z+1]	0.820	1.991	166.54	2.795
O1	N2 [x-1, y-1, z]	0.812	1.919	173.14	2.727

Symmetry transformations used to generate equivalent atoms: A: -x, 1-y, -z; B: 1+x, y, z; C: -1-x, 1-y, -z; D: -x, 2-y, -z; E: x, -1+y, z.

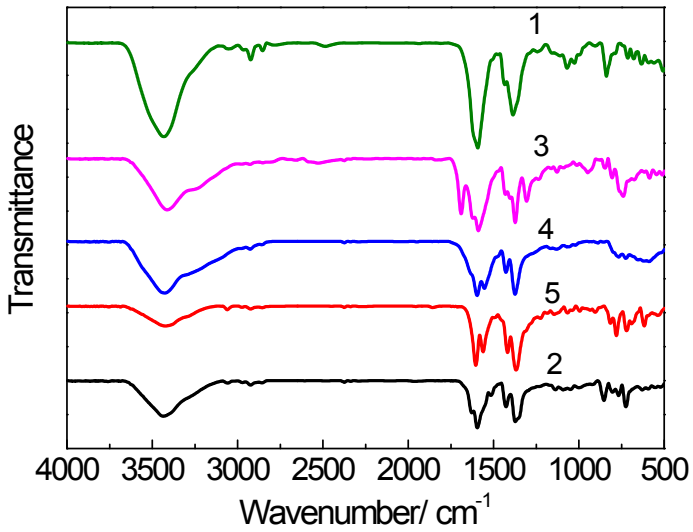

Fig. S1 The IR spectra of compounds **1-5**.

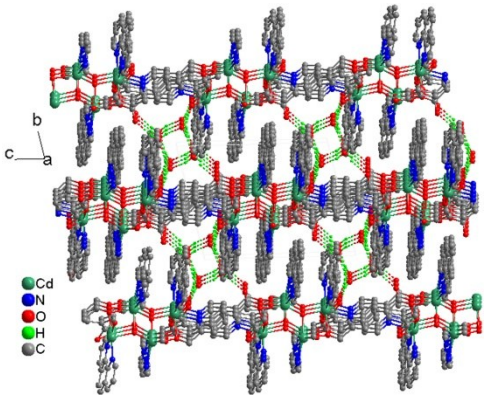

Fig. S2 The 3D structure interlinked by O-H···O hydrogen bonds in compound **2**.

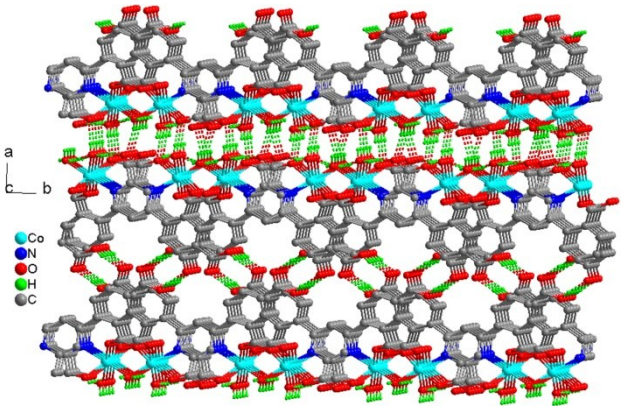

Fig. S3 The 3D structure interlinked by O-H···O hydrogen bonds in compound **3**.

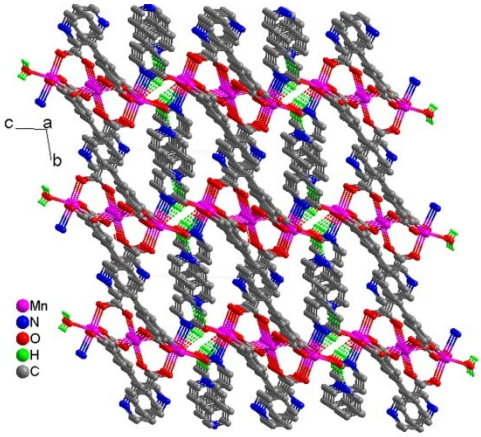

Fig. S4 The 3D structure interlinked by O-H···O and O-H···N hydrogen bonds in compound **5**.

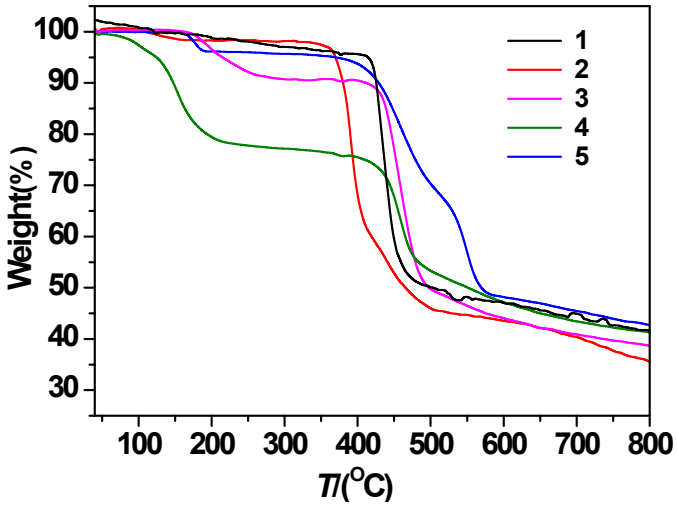

Fig. S5 The TGA curves for **1**, **2**, **3**, **4** and **5**.

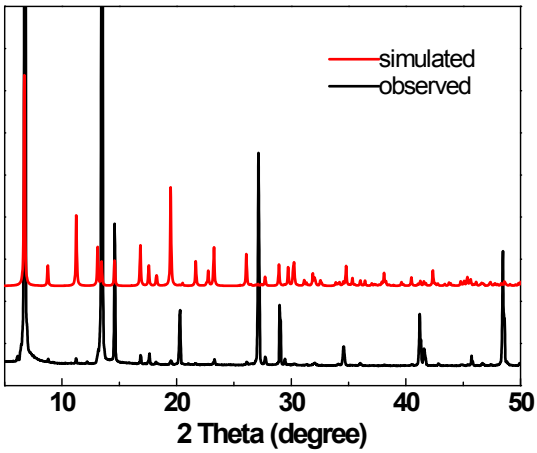

Fig. S6. PXRD patterns for **1**.

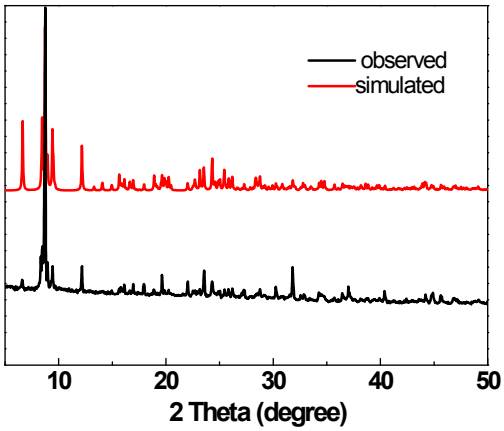

Fig. S7. PXRD patterns for **2**.

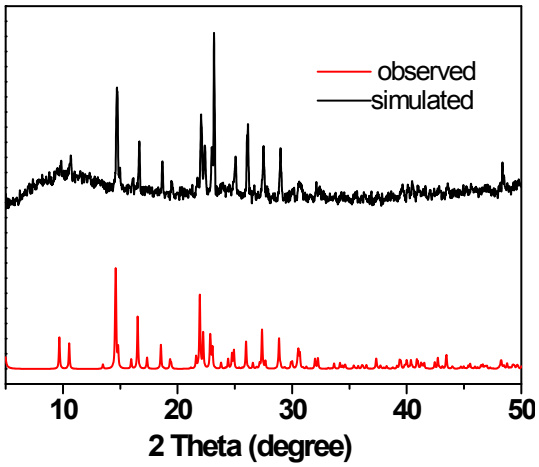

Fig. S8. PXRD patterns for **3**.

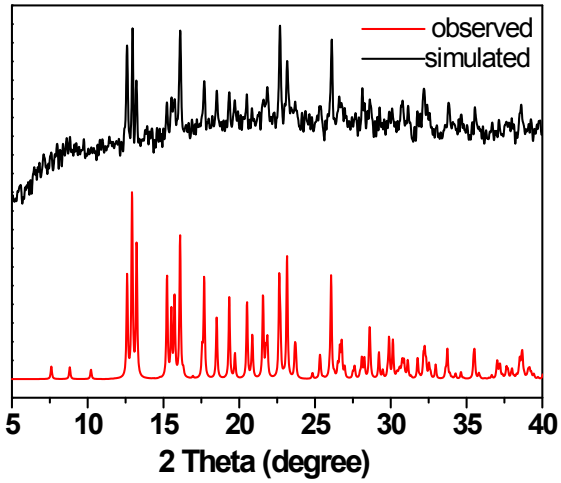

Fig. S9. PXRD patterns for **4**.

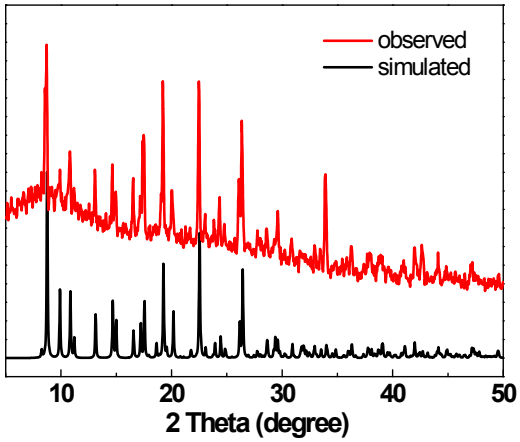

Fig. S10. PXRD patterns for **5**.

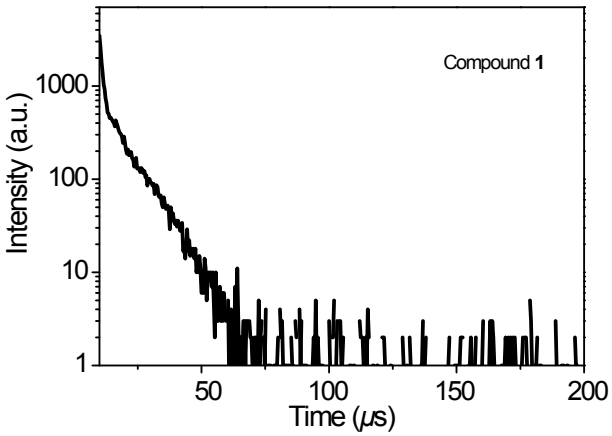

Fig. S11. Semilog plot of fluorescence decay versus time, excited and monitored at 330 nm and 534 nm for **1**.

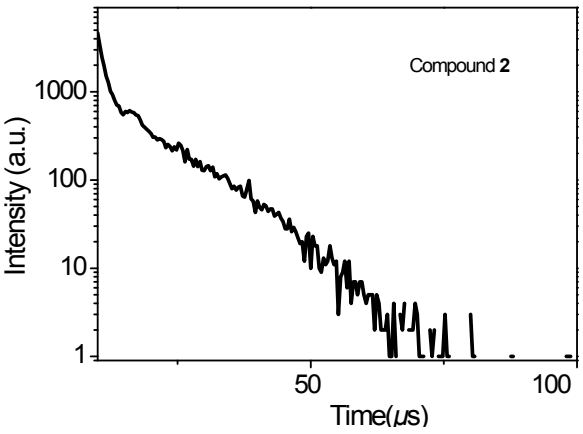

Fig. S12. Semilog plot of fluorescence decay versus time, excited and monitored at 370 nm and 429 nm for **2**.