Supplementary Information

Metal ions and solvents ratio co-regulate four new magnetic coordination polymers based upon unsymmetric tricarboxylate acid ligand

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Table S1 Crystal and structure refinement data for 1–4

Compound	1	2	3	4
empirical formula	$C_{70}H_{54}Co_3O_{16}N_{12}$	$C_{54}H_{50}Mn_3N_8O_{20}$	$C_{27}H_{24}NiN_4O_9$	$C_{78}H_{74}Ni_3N_{16}O_{34}$
formula mass	1494.06	1295.84	607.21	1955.66
Crystal system	Triclinic	Triclinic	Orthorhombic	Monoclinic
Space group	$P\bar{1}$	$P\bar{1}$	$P2_12_12_1$	$P2_1/c$
a (Å)	10.193(4)	10.125(8)	11.6286(16)	13.683(2)
b (Å)	13.722(5)	10.7664(9)	13.6585(18)	23.839(4)
c (Å)	14.606(6)	13.2928(12)	15.944(2)	14.576(2)
α(°)	107.685(6)	86.521(10)	90	90
β(°)	102.170(7)	73.151(2)	90	90.745(4)
γ(°)	111.188(6)	85.317(10)	90	90
V (Å^3)	1692.5(11)	1381.2(2)	2532.4(6)	4685.8(12)
Z	1	1	4	2
D_{calcd} (mg/cm^3)	1.468	1.558	1.593	1.386
μ(mm^{-1})	0.805	0.762	0.832	0.686
F(000)	767	665	1256	2020
Θ (°)	25.10	26.24	26.27	25.10
GOF	1.044	1.012	1.009	1.153
R1[a]	0.0745	0.0514	0.0533	0.0890
wR_2[b]	0.2073	0.1315	0.1086	0.2193

[a] $R_1=\sum||F_0|-|F_c||/\sum|F_0|$. [b] $wR_2=\{\sum[w(F_0^2-F_c^2)^2]/\sum(F_0^2)^2\}^{1/2}$

Table S2 Selected bond lengths (Å) and bond angles (°) for CPs 1-4.

Compound 1			
Co(1)-O(6)	2.094(5)	N(4)-Co(2)-N(1)	177.7(2)
Co(1)-O(6)#1	2.094(5)	O(1)-Co(2)-O(4)#3	93.85(17)
Co(1)-O(7)	2.119(6)	O(2)#2-Co(2)-O(4)#3	153.21(18)
Co(1)-O(7)#1	2.119(6)	N(4)-Co(2)-O(4)#3	89.9(2)
Co(1)-N(5)	2.149(5)	N(1)-Co(2)-O(4)#3	90.20(19)
Co(1)-N(5)#1	2.149(5)	O(1)-Co(2)-O(3)#3	153.13(16)
Co(2)-O(1)	2.047(5)	O(2)#2-Co(2)-O(3)#3	93.44(16)
Co(2)-O(2)#2	2.070(4)	N(4)-Co(2)-O(3)#3	95.4(2)
Co(2)-N(4)	2.122(6)	N(1)-Co(2)-O(3)#3	86.65(19)
Co(2)-N(1)	2.148(5)	O(4)#3-Co(2)-O(3)#3	59.92(16)
Co(2)-O(4)#3	2.168(4)	C(25)-N(1)-C(26)	106.4(5)
Co(2)-O(3)#3	2.256(5)	C(25)-N(1)-Co(2)	125.9(5)
O(2)-Co(2)#2	2.070(4)	C(26)-N(1)-Co(2)	127.4(4)
O(3)-Co(2)#3	2.256(5)	C(25)-N(2)-C(27)	108.3(5)
O(4)-Co(2)#3	2.168(4)	C(25)-N(2)-C(17)#6	126.1(6)
O(6)-Co(1)-O(6)#1	180.000(1)	C(27)-N(2)-C(17)#6	125.5(6)
O(6)-Co(1)-O(7)	86.4(2)	C(23)-N(3)-C(22)	106.6(5)
O(6)#1-Co(1)-O(7)	93.6(2)	C(23)-N(3)-C(20)	128.8(6)
O(6)-Co(1)-O(7)#1	93.6(2)	C(22)-N(3)-C(20)	124.6(5)
O(6)#1-Co(1)-O(7)#1	86.4(2)	C(23)-N(4)-C(24)	104.3(5)
O(7)-Co(1)-O(7)#1	180.000(1)	C(23)-N(4)-Co(2)	125.6(5)
O(6)-Co(1)-N(5)	90.2(2)	C(24)-N(4)-Co(2)	129.7(4)
O(6)#1-Co(1)-N(5)	89.8(2)	C(33)-N(5)-C(31)	107.4(5)
O(7)-Co(1)-N(5)	89.6(2)	C(33)-N(5)-Co(1)	129.5(5)
O(7)#1-Co(1)-N(5)	90.4(3)	C(31)-N(5)-Co(1)	122.9(4)
O(6)-Co(1)-N(5)#1	89.8(2)	C(33)-N(6)-C(32)	106.3(5)
O(6)#1-Co(1)-N(5)#1	90.2(2)	C(33)-N(6)-C(30)	125.8(6)
O(7)-Co(1)-N(5)#1	90.4(3)	C(32)-N(6)-C(30)	127.9(5)
O(7)#1-Co(1)-N(5)#1	89.6(2)	C(21)-O(1)-Co(2)	145.3(4)
N(5)-Co(1)-N(5)#1	180.0(3)	C(21)-O(2)-Co(2)#2	124.3(4)
O(1)-Co(2)-O(2)#2	112.27(17)	C(13)-O(3)-Co(2)#3	87.1(4)
O(1)-Co(2)-N(4)	89.8(2)	C(13)-O(4)-Co(2)#3	91.4(3)
O(2)#2-Co(2)-N(4)	95.8(2)	C(14)-O(6)-Co(1)	131.1(5)
O(1)-Co(2)-N(1)	87.87(19)	C(34)-O(7)-Co(1)	128.3(6)
Compound 2			
Mn(1)-O(6)	2.0967	O(8)-Mn(1)-O(3)#1	92.3
Mn(1)-O(8)	2.1888(11)	N(1)-Mn(1)-O(3)#1	144.2
Mn(1)-N(1)	2.1902	O(7)-Mn(1)-O(3)#1	92.1
Mn(1)-O(7)	2.2539(11)	O(4)#1-Mn(1)-O(3)#1	56.3
Mn(1)-O(4)#1	2.2643	O(2)#2-Mn(2)-O(2)	180
Mn(1)-O(3)#1	2.3301	O(2)#2-Mn(2)-N(3)	90.5

Mn(2)-O(2)#2	2.1118	O(2)-Mn(2)-N(3)	89.5
Mn(2)-O(2)	2.1118	O(2)#2-Mn(2)-N(3)#2	89.5
Mn(2)-N(3)	2.2438	O(2)-Mn(2)-N(3)#2	90.5
Mn(2)-N(3)#2	2.2438	N(3)-Mn(2)-N(3)#2	180
Mn(2)-O(9)#2	2.3228	O(2)#2-Mn(2)-O(9)#2	96.2
Mn(2)-O(9)	2.3228	O(2)-Mn(2)-O(9)#2	83.8
O(3)-Mn(1)#5	2.3301	N(3)-Mn(2)-O(9)#2	86.7
O(4)-Mn(1)#5	2.2643	N(3)#2-Mn(2)-O(9)#2	93.3
O(6)-Mn(1)-O(8)	88.2	O(2)#2-Mn(2)-O(9)	83.8
O(6)-Mn(1)-N(1)	126.3	O(2)-Mn(2)-O(9)	96.2
O(8)-Mn(1)-N(1)	84.8	N(3)-Mn(2)-O(9)	93.3
O(6)-Mn(1)-O(7)	93.6	N(3)#2-Mn(2)-O(9)	86.7
O(8)-Mn(1)-O(7)	175.2	O(9)#2-Mn(2)-O(9)	180
N(1)-Mn(1)-O(7)	90.5	C(18)-N(1)-Mn(1)	126.67(19)
O(6)-Mn(1)-O(4)#1	145.4	C(16)-N(1)-Mn(1)	127.93(18)
O(8)-Mn(1)-O(4)#1	94.9	C(1)-O(2)-Mn(2)	168.56(18)
N(1)-Mn(1)-O(4)#1	88.3	C(11)-O(3)-Mn(1)#5	90.09(19)
O(7)-Mn(1)-O(4)#1	86.2	C(11)-O(4)-Mn(1)#5	93.28(19)
O(6)-Mn(1)-O(3)#1	89.1	C(14)-O(6)-Mn(1)	113.88(18)
Compound 3			
Ni(1)-O(1)	2.030(4)	O(1)-Ni(1)-O(7)	88.42(15)
Ni(1)-N(4)#1	2.066(5)	N(4)#1-Ni(1)-O(7)	88.58(17)
Ni(1)-N(1)	2.065(4)	N(1)-Ni(1)-O(7)	176.20(17)
Ni(1)-O(8)	2.074(4)	O(8)-Ni(1)-O(7)	85.65(15)
Ni(1)-O(7)	2.104(4)	O(1)-Ni(1)-O(9)	175.86(17)
Ni(1)-O(9)	2.106(4)	N(4)#1-Ni(1)-O(9)	93.55(18)
N(4)-Ni(1)#2	2.066(5)	N(1)-Ni(1)-O(9)	89.64(17)
O(1)-Ni(1)-N(4)#1	87.49(16)	O(8)-Ni(1)-O(9)	86.62(17)
O(1)-Ni(1)-N(1)	94.28(17)	O(7)-Ni(1)-O(9)	87.60(16)
N(4)#1-Ni(1)-N(1)	94.20(18)	C(18)-N(1)-Ni(1)	127.2(4)
O(1)-Ni(1)-O(8)	91.94(15)	C(16)-N(1)-Ni(1)	127.3(4)
N(4)#1-Ni(1)-O(8)	174.21(17)	C(25)-N(4)-Ni(1)#2	131.9(4)
N(1)-Ni(1)-O(8)	91.59(16)	C(26)-N(4)-Ni(1)#2	123.5(4)
		C(1)-O(1)-Ni(1)	132.8(4)
Compound 4			
Ni(1)-N(4)	2.053(7)	O(5)-Ni(1)-O(4)#1	90.5(2)
Ni(1)-N(4)#1	2.053(7)	O(5)#1-Ni(1)-O(4)#1	89.5(2)
Ni(1)-O(5)	2.069(6)	O(4)-Ni(1)-O(4)#1	179.999(1)
Ni(1)-O(5)#1	2.069(6)	N(7)#2-Ni(2)-O(1)	86.5(3)
Ni(1)-O(4)	2.082(5)	N(7)#2-Ni(2)-N(2)	91.0(3)
Ni(1)-O(4)#1	2.082(5)	O(1)-Ni(2)-N(2)	90.0(3)
Ni(2)-N(7)#2	2.054(7)	N(7)#2-Ni(2)-N(5)	176.7(3)
Ni(2)-O(1)	2.079(6)	O(1)-Ni(2)-N(5)	93.7(3)
Ni(2)-N(2)	2.079(7)	N(2)-Ni(2)-N(5)	92.2(3)

Ni(2)-N(5)	2.084(7)	N(7)#2-Ni(2)-O(3)	88.1(3)
Ni(2)-O(3)	2.100(6)	O(1)-Ni(2)-O(3)	172.5(2)
Ni(2)-O(2)	2.109(6)	N(2)-Ni(2)-O(3)	95.3(3)
N(7)-Ni(2)#3	2.054(7)	N(5)-Ni(2)-O(3)	91.4(3)
N(4)-Ni(1)-N(4)#1	179.997(2)	N(7)#2-Ni(2)-O(2)	89.4(3)
N(4)-Ni(1)-O(5)	89.8(3)	O(1)-Ni(2)-O(2)	88.3(2)
N(4)#1-Ni(1)-O(5)	90.2(3)	N(2)-Ni(2)-O(2)	178.2(3)
N(4)-Ni(1)-O(5)#1	90.2(3)	N(5)-Ni(2)-O(2)	87.4(3)
N(4)#1-Ni(1)-O(5)#1	89.8(3)	O(3)-Ni(2)-O(2)	86.5(2)
O(5)-Ni(1)-O(5)#1	179.999(2)	C(3)-N(2)-Ni(2)	124.2(6)
N(4)-Ni(1)-O(4)	90.4(3)	C(1)-N(2)-Ni(2)	130.9(6)
N(4)#1-Ni(1)-O(4)	89.6(3)	C(12)-N(4)-Ni(1)	127.4(6)
O(5)-Ni(1)-O(4)	89.5(2)	C(11)-N(4)-Ni(1)	127.8(6)
O(5)#1-Ni(1)-O(4)	90.5(2)	C(15)-N(5)-Ni(2)	128.7(6)
N(4)-Ni(1)-O(4)#1	89.6(3)	C(13)-N(5)-Ni(2)	127.1(6)
N(4)#1-Ni(1)-O(4)#1	90.4(3)	C(24)-N(7)-Ni(2)#3	129.7(6)
C(23)-N(7)-Ni(2)#3	124.1(6)		

Symmetry Codes: **Compound 1**: #1 = -x, -y, -z + 1; #2 = -x, -y + 2, -z + 2; #3 = -x + 1, -y + 2, -z + 2; #4 = x, y - 1, z; #5 = -x - 1, -y - 1, -z + 1; #6 = x, y + 1, z.

Compound 2: #1= x - 1, y, z; #2=-x, -y + 2, -z; #3= -x - 1, -y + 3, -z; #4= -x, -y, -z + 1; #5= x + 1, y, z.

Compound 3: #1 = -x + 5/2, -y + 1, z + 1/2; #2 = -x + 5/2, -y + 1, z-1/2.

Compound 4: #1 = -x, -y + 1, -z + 2; #2 = x - 1, y, z; #3= x + 1, y, z.

Table S3 Hydrogen bond distances and bond angles (Å, °) for 3

Donor–H···Acceptor	D – H	H···A	D···A	D – H···A
O(3)–H(3)···O(6)	0.82	1.88	2.661(5)	160
O(7)–H(7B)···O(5)	0.85	1.88	2.726(5)	173
O(8)–H(8A)···O(2)	0.82	1.99	2.718(5)	148
O(8)–H(8B)···O(6)	0.85	1.86	2.709(5)	179
O(9)–H(9A)···O(5)	0.82	1.98	2.793(6)	172
O(9)–H(9B)···O(2)	0.85	2.15	2.999(6)	174

Hydrogen bond distances and bond angles (Å, °) for 4

Donor–H···Acceptor	D – H	H···A	D···A	D – H···A
O(1)–H(1A)···O(6)	0.82	2.03	2.694(8)	138
O(1)–H(1B)···O(9)	0.82	1.88	2.651(9)	157

O(2)–H(2A)···O(4W)	0.82	2.07	2.795(11)	147
O(3)–H(3A)···O(6)	0.82	2.05	2.769(8)	146
O(3)–H(3B)···O(2)	1.07	2.21	2.882(8)	119
O(4)–H(4A)···O(10)	0.82	1.94	2.747(8)	168
O(5)–H(5A)···O(6)	0.82	2.30	2.710(7)	111
O(5)–H(5B)···O(4)	0.85	2.57	2.922(7)	106
O(5)–H(5B)···O(10)	0.85	1.89	2.743(8)	179

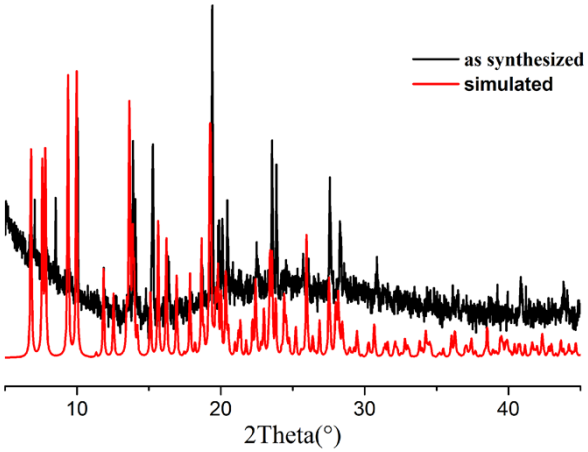

Figure S1. The Powder X-ray diffraction (PXRD) patterns of **1.**

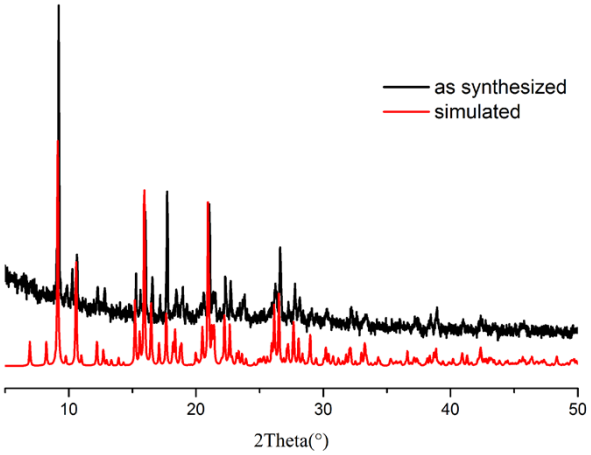

Figure S2. The Powder X-ray diffraction (PXRD) patterns of **2**.

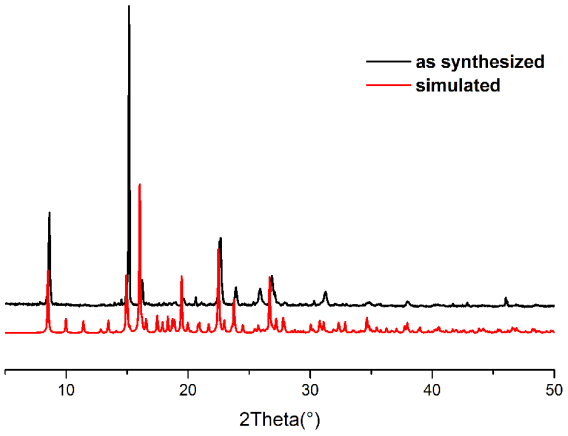

Figure S3. The Powder X-ray diffraction (PXRD) patterns of **3**.

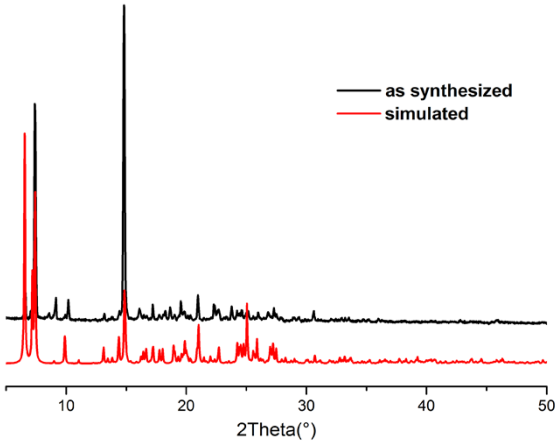

Figure S4. The Powder X-ray diffraction (PXRD) patterns of **4.**

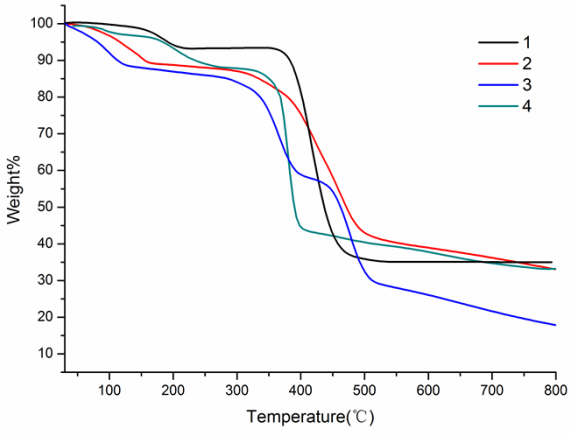

Figure S5. The TGA analyses of the compound **1** − **4**.

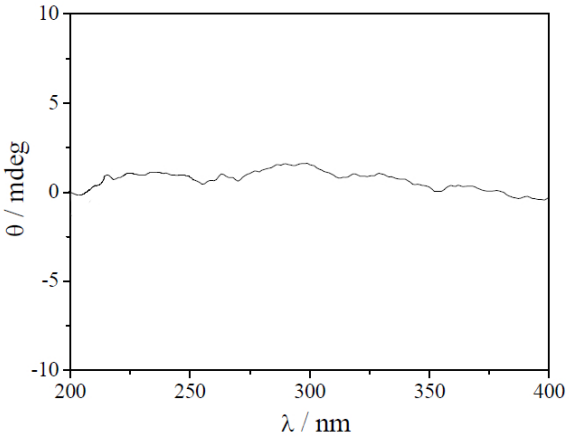

Figure S6. Solid-state CD spectra of bulk sample of compound **3** at room temperature.