Supporting Information for the Manuscript:

Metal-organic frameworks based on [1,1':3',1''-Terphenyl]-3,3'',5,5''-tetracarboxylic acid ligand: syntheses, structures and magnetic properties

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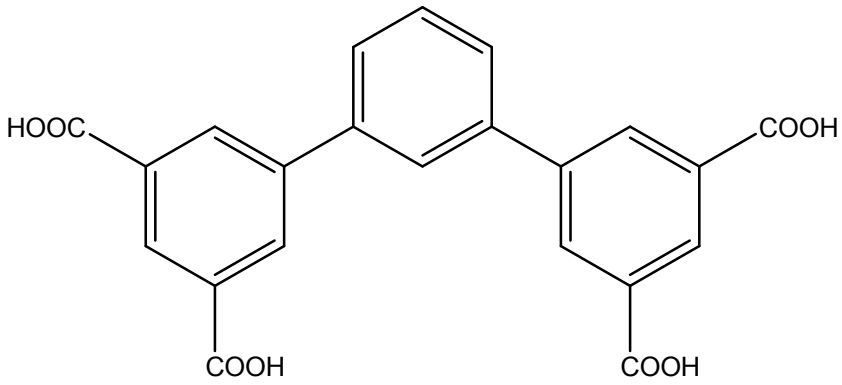


Scheme S1. Schematic Molecular Structure of H_4TPTA.

Table S1.The Crystal data and structure refinement parameters for polymers 1–5

Parameter	**1**	**2**	**3**	**4**	**5**
Empirical formula	$C_{16}H_{13}NO_6Co$	$C_{16}H_{13}NO_6Ni$	$C_{32}H_{23}N_2O_{10.5}Mn_2$	$C_{34}H_{20}N_2O_8Mn$	$C_{34}H_{20}N_2O_8Co$
Formula weight	374.20	373.98	713.40	639.46	643.45
Tempter(K)	293(2)	293(2)	293(2)	293(2)	293(2)
λ/Å	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Triclinic	Monoclinic	Monoclinic
Space group	C2/c	C2/c	P-1	C2/c	C2/c
a (Å)	18.905(4)	18.937(4)	9.7207(19)	28.507(6)	28.427(6)
b (Å)	11.646(2)	11.546(2)	10.111(2)	10.687(2)	10.685(2)
c (Å)	15.432(3)	15.385(3)	15.286(3)	18.199(4)	17.978(4)
α(°)	90	90	92.87(3)	90	90
β(°)	110.81(3)	111.08(3)	98.72(3)	97.48(3)	97.49(3)
γ(°)	90	90	96.33(3)	90	90
V (Å^3)	3176(1)	3138(1)	1472(5)	5497(2)	5414(1)
Z	8	8	2	8	8
$D_{calcd.}$(g·cm^{-3})	1.565	1.583	1.609	1.545	1.579
μ (mm^{-1})	1.113	1.268	0.924	0.542	0.696
F(000)	1528	1536	726	2616	2632
Θ range (º)	2.09~25.49	2.11~25.50	2.13~25.50	2.26 ~ 25.50	2.04~25.50
GOF	0.996	1.004	1.021	1.040	1.033
Final R indices [I > 2σ(I)]	R_1 =0.0657 wR_2 =0.1363	R_1 =0.0468 wR_2 =0.1152	R_1 =0.0524 wR_2 =0.1179	R_1 =0.0538 wR_2 =0.1061	R_1 =0.0381 wR_2 =0.0884

[a] $R_1 = \Sigma||Fo| - |Fc||/\Sigma|Fo|$, $wR_2 = [\Sigma w(Fo^2 - Fc^2)^2]/\Sigma w(Fo^2)^2]^{1/2}$.

Table S2 Selected Bond Lengths (Å) and Bond Angles (º) for compound **1**–**5**

Compound **1**

Co(1)-O(1)	2.025(3)	Co(1)-O(4)#1	2.077(3)	Co(1)-O(5)	2.152(4)
Co(1)-N(1)	2.082(4)	Co(1)-O(6)	2.146(4)	Co(1)-O(3)#1	2.232(3)
O(1)-Co(1)-O(4)#1	95.50(13)	O(1)-Co(1)-N(1)	97.55(15)	N(1)-Co(1)-O(5)	85.61(16)
O(5)-Co(1)-O(3)#1	88.51(14)	O(1)-Co(1)-O(6)	91.75(13)	N(1)-Co(1)-O(3)#1	105.80(14)
O(4)#1-Co(1)-O(6)	92.96(15)	N(1)-Co(1)-O(6)	89.72(15)	O(4)#1-Co(1)-O(3)#1	60.99(12)
O(1)-Co(1)-O(5)	89.44(14)	O(4)#1-Co(1)-O(5)	91.46(15)	O(6)-Co(1)-O(3)#1	92.22(13)

[a] Symmetry codes: #1 x,-y+1,z-1/2; #2 x,-y+1,z+1/2 ; #3 -x+1,y,-z+3/2.

Compound **2**

Ni(1)-O(1)	2.010(2)	Ni(1)-N(1)	2.033(3)	Ni(1)-O(5)	2.114(3)
Ni(1)-O(4)#1	2.051(3)	Ni(1)-O(6)	2.087(3)	Ni(1)-O(3)#1	2.178(3)
O(1)-Ni(1)-O(4)#1	94.58(11)	O(1)-Ni(1)-O(6)	93.22(11)	O(4)#1-Ni(1)-O(3)#1	62.19(10)
N(1)-Ni(1)-O(6)	90.91(13)	O(1)-Ni(1)-O(5)	87.64(12)	O(5)-Ni(1)-O(3)#1	89.26(12)
O(4)#1-Ni(1)-O(6)	91.42(12)	N(1)-Ni(1)-O(5)	86.24(13)	O(6)-Ni(1)-O(3)#1	91.04(11)
O(4)#1-Ni(1)-O(5)	91.27(12)	N(1)-Ni(1)-O(3)#1	106.00(12)		

[a] Symmetry codes: #1 x, -y+1, z-1/2; #2 x, -y+1, z+1/2; #3 -x+1, y, -z+1/2; #4 -x, -y+2, -z-1.

Compound **3**

Mn(1)-O(5)#1	2.116(3)	Mn(1)-O(4)#2	2.125(3)	Mn(2)-N(2)	2.231(3)
Mn(1)-O(9)	2.193(3)	Mn(1)-O(2)	2.193(3)	Mn(2)-O(6)#5	2.284(3)
Mn(1)-O(8)#3	2.200(3)	Mn(1)-O(1)	2.274(3)	Mn(2)-O(8)#4	2.260(3)
Mn(2)-O(3)	2.091(3)	Mn(2)-N(1)	2.232(3)	Mn(2)-O(5)#5	2.397(3)
N(1)-Mn(2)-O(8)#4	158.26(10)	O(5)#1-Mn(1)-O(4)#2	116.95(11)	O(5)#1-Mn(1)-O(2)	93.58(11)
O(4)#2-Mn(1)-O(2)	149.33(11)	O(5)#1-Mn(1)-O(1)	151.59(11)	O(3)-Mn(2)-O(5)#5	91.18(11)
O(4)#2-Mn(1)-O(1)	91.34(10)	O(2)-Mn(1)-O(1)	58.38(10)	Mn(1)#1-O(5)-Mn(2)#5	92.90(10)
O(3)-Mn(2)-N(1)	93.19(11)	O(3)-Mn(2)-N(2)	154.23(11)	N(1)-Mn(2)-O(5)#5	132.61(10)

[a] Symmetry codes: #1 -x, -y, -z+2; #2 x, y-1, z; #3 -x+1, -y, -z+2; #4 -x+1, -y+1, -z+2; #5 -x, -y+1, -z+2.

Compound **4**

Mn(1)-O(3)#1	2.109(2)	Mn(1)-O(4)#2	2.156(2)	Mn(1)-N(1)	2.267(3)
Mn(1)-O(2)	2.185(2)	Mn(1)-N(2)	2.245(2)	Mn(1)-O(1)	2.363(2)
O(3)#1-Mn(1)-O(2)	96.21 (8)	O(3)#1-Mn(1)-N(1)	120.06(9)	O(3)#1-Mn(1)-N(2)	82.04(9)
O(2)-Mn(1)-N(1)	138.89(8)	O(2)-Mn(1)-O(1)	57.15(7)	O(4)#2-Mn(1)-N(2)	172.10(9)
O(3)#1-Mn(1)-O(4)#2	98.56(9)	O(4)#2-Mn(1)-O(2)	93.23(8)		

[a] Symmetry codes: #1 -x, -y+1, -z; #2 x, -y+1, z-1/2; #3 x, -y+1, z+1/2.

Compound **5**

Co(1)-O(2)#1	2.0279(15)	Co(1)-O(1)	2.0909(14)	Co(1)-N(2)	2.1283(18)
Co(1)-O(3)#2	2.1249(15)	Co(1)-N(1)	2.1276(17)	Co(1)-O(4)#2	2.2921(17)
O(2)#1-Co(1)-O(1)	95.61(6)	O(2)#1-Co(1)-O(3)#2	93.97(6)	O(1)-Co(1)-O(4)#2	92.(6)
O(1)-Co(1)-O(3)#2	92.63(6)	O(2)#1-Co(1)-N(1)	83.08(7)	N(1)-Co(1)-O(4)#2	90.75(6)
N(1)-Co(1)-N(2)	77.81(7)	O(3)#2-Co(1)-N(1)	92.85(7)	O(3)#2-Co(1)-O(4)#2	58.86(6)
O(2)#1-Co(1)-N(2)	121.05(7)	O(1)-Co(1)-N(2)	98.39(7)	N(2)-Co(1)-O(4)#2	83.88(6)

[a] Symmetry codes : #1 -x+1, y, -z+1/2; #2 x,-y+1,z-1/2; #3 x, -y+1, z+1/2.

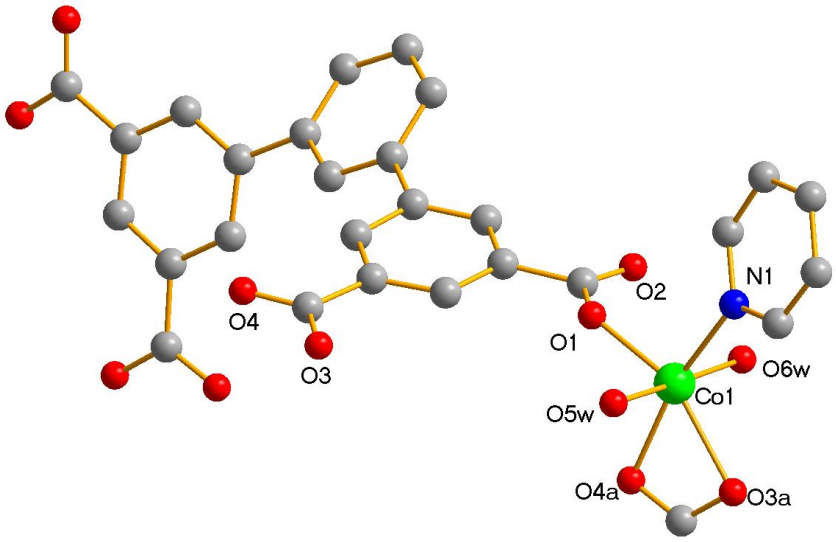
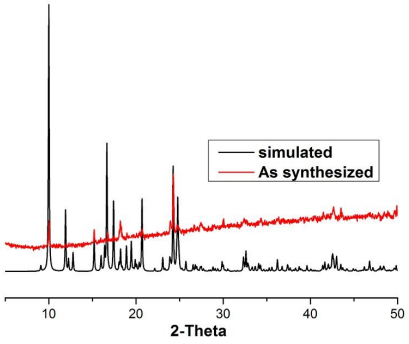
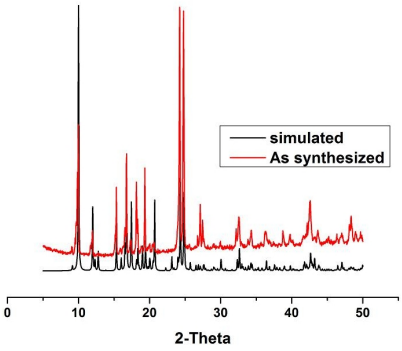


Fig. S1, The ball-and-stick drawing of the asymmetric unit in **1**, the hydrogen atoms and solvent molecules are omitted. Symmetry codes: a: x, 1-y, -1/2+z;

XRD Patterns. To confirm the phase purity of these polymers, the PXRD patterns were recorded for complexes **1**−**5**, and they were comparable to the corresponding simulated ones calculated from the single-crystal diffraction data (Figure. S7, Supporting Information), indicating a pure phase of each bulky sample.



Complex **1**



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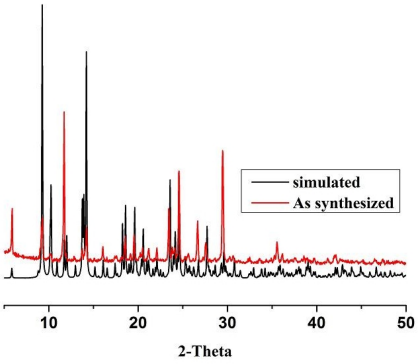

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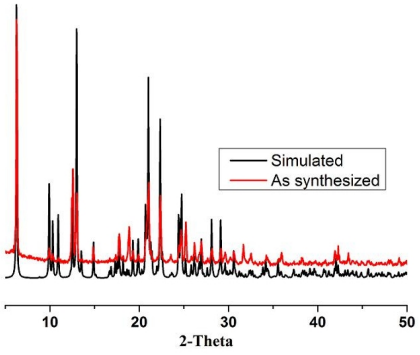

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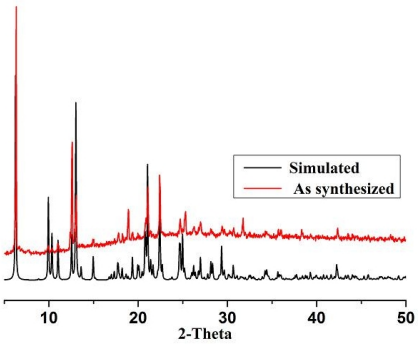

Complex **5**

Fig. S2. Experimental (red) and simulated (black) PXRD patterns of **1**−**5**.