Supporting Information

Structural Diversity and Catalytic Properties of Five $Co_2(COO)_4$ Cluster Based Coordination Polymers Modified by R-isophthalic acid (R=H, NO_2, CH_3, OH and ^{t}Bu):

Jian-Yong Zhang*,[a] Jun-Xia Shi[a], Peng-Hui Cui[a], Zi-Jian Yao[a], and Wei Deng*,[a]

School of Chemical and Environmental Engineering, Shanghai Institute of Technology, Shanghai 201418, China.
E-mail: jianyong1106@163.com; wdeng@sit.edu.cn.

Synthesis of 2,4,6-tris(4-pyridyl)-1,3,5-triazine (TPT) ligand: The TPT ligand was synthesized according to a modified published method. 18-crown-6 (1.0 g, 3.8 mmol), KOH (0.225 g, 4.0 mmol) and 4-cyanopyridine (10.0 g, 96.0 mmol) were mixed in methanol (3 mL). The resulting oil was stirred for 10 min at room temperature and then transferred into a 25 mL Teflon-lined stainless steel reactor and heated at 200°C for 7 h. After cooling to ambient temperature, the mixture was poured into a flask containing 30 mL pyridine. Stirring the mixture for several minutes gave the crude solid product, which was collected by filtration and washed with pyridine (25 mL) and toluene (25 mL) for twice. The collected filtrate was then dissolved in dilute hydrochloric acid (2 mol L^{-1}, 30 mL) and filtrated to remove small amount of dissolved solid, adjusting the solution to slight alkaline with concentrated NH_3 aqueous gave a pale-white solid that was filtrated, washed with water, and dried in air (Yield: 70%).

Table S1. Selected bond [Å] and angles [°] for **CPs 1-5**.

Co1-O1	2.0247(15)	Co1-O2#1	2.0309(16)
Co1-O3#2	2.1185(15)	Co1-O4#2	2.2285(17)
Co1-N1	2.1567(19)	Co1-N2#3	2.1606(19)
O1-Co1-O2#1	117.40(7)	O1-Co1-O3#2	152.58(7)
O2#1-Co1-O3#2	90.01(6)	O1-Co1-N1	91.44(7)
O2#1-Co1-N1	89.46(7)	O3#2-Co1-N1	89.43(7)
O1-Co1-N2#3	87.04(7)	O2#1-Co1-N2#3	89.20(7)
O1-Co1-O4#2	92.07(6)	O2#1-Co1-O4#2	150.34(6)
O3#2-Co1-O4#2	60.52(6)	N1-Co1-O4#2	93.26(7)
N2#3-Co1-O4#2	89.10(7)	N1-Co1-N2#3	177.24(7)
O3#2-Co1-N2#3	92.98(7)		
Symmetry code for **CP1**: #1 -x+1/2, -y+1/2, -z; #2 x-1/2, y+1/2, z; #3 x-1/2, -y+1/2, z-1/2.			
Co1-O1	1.9801(18)	Co1-O2#2	2.0052(19)
Co1-O3#1	1.963(2)	Co1-N1	2.164(2)
Co1-N2#3	2.179(2)		
O3#1-Co1-O1	137.87(12)	O3#1-Co1-O2#2	96.27(11)
O1-Co1-O2#2	125.85(9)	O3#1-Co1-N1	93.54(9)

O1-Co1-N1	87.14(8)	O2#2-Co1-N1	91.50(8)
O3#1-Co1-N2#3	88.20(9)	O1-Co1-N2#3	90.70(8)
O2#2-Co1-N2#3	89.60(8)	N1-Co1-N2#3	177.83(8)

Symmetry code for **CP2**: #1 -x+1/2, y-1/2, -z+1/2; #2 -x+1/2, -y+3/2, -z; #3 x-1/2, -y+3/2, z-1/2.

Co1-N1	2.175(3)	Co1-N2#3	2.175(3)
Co1-O1	1.999(2)	Co1-O2#1	1.999(2)
Co1-O3#2	2.106(3)	Co1-O4#2	2.315(3)
O1-Co1-O2#1	119.16(12)	O2#1-Co1-O3#2	88.36(12)
O1-Co1-O3#2	151.28(11)	O2#1-Co1-N1	93.06(11)
O1-Co1-N1	89.45(11)	O3#2-Co1-N1	97.63(11)
O2#1-Co1-N2#3	87.83(11)	O1-Co1-N2#3	86.75(11)
O3#2-Co1-N2#3	86.24(11)	N1-Co1-N2#3	176.05(12)
O2#1-Co1-O4#2	147.37(11)	O1-Co1-O4#2	92.97(10)
O3#2-Co1-O4#2	59.04(10)	N1-Co1-O4#2	92.76(11)
N2#3-Co1-O4#2	88.55(11)		

Symmetry code for **CP3**: #1 -x+3/2, -y+3/2, -z+1; #2 -x+3/2, y+1/2, -z+3/2; #3 x+1/2, -y+3/2, z+1/2.

Co1-O1	2.004(3)	Co1-O2#1	2.002(3)
Co1-O3#2	2.053(4)	Co1-N1	2.177(4)
Co1-N2#3	2.162(4)		
O2#1-Co1-O1	121.91(15)	O2#1-Co1-O3#2	89.89(17)
O1-Co1-O3#2	148.15(17)	O1-Co1-N2#3	88.17(14)
O2#1-Co1-N2#3	88.46(14)	O3#2-Co1-N2#3	91.17(15)
O2#1-Co1-N1	92.79(14)	O1-Co1-N1	88.49(14)
O3#2-Co1-N1	92.00(15)	N2#3-Co1-N1	176.60(15)

Symmetry codes for **CP4**: #1 -x+1/2, -y+3/2, -z; #2 -x+1/2, y+1/2, -z+1/2; #3 x+1/2, -y+3/2, z+1/2.

Co1-O1	2.089(2)	Co1-O2	2.310(3)
Co1-O3#2	2.035(2)	Co1-O4#1	2.015(2)
Co1-N1	2.184(3)	Co1-N2	2.152(3)
O1-Co1-O2	59.06(9)	O1-Co1-N2	95.48(10)
O1-Co1-N1	88.62(10)	N2-Co1-O2	88.56(10)
N1-Co1-O2	92.22(10)	O3#2-Co1-O2	95.34(9)
O4#1-Co1-O2	149.02(9)	O4#1-Co1-O1	89.98(10)
O4#1-Co1-O3#2	115.55(9)	O3#2-Co1-O1	153.61(9)
N2-Co1-N1	175.61(10)	O3#2-Co1-N1	85.93(10)
O4#1-Co1-N1	87.85(10)	O3#2-Co1-N2	89.69(10)
O4#1-Co1-N2	93.71(11)		

Symmetry code for **CP5**: #1 -y+2/3, x-y+1/3, z+1/3; #2 y-1/3, -x+y+1/3, -z+1/3.

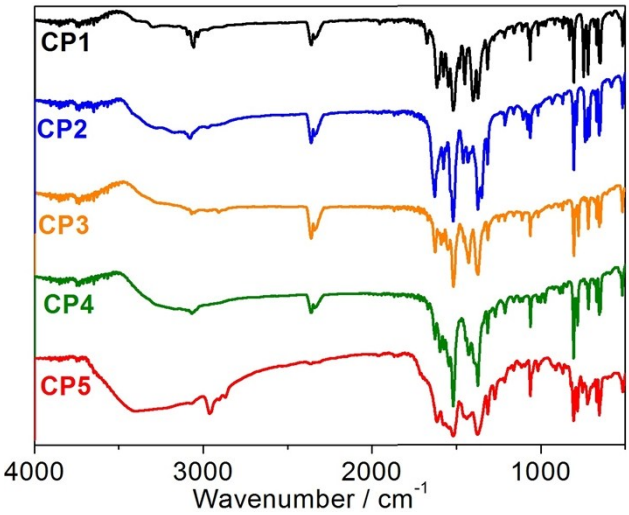


Figure S1. The FT- IR spectra of the five obtained compounds.

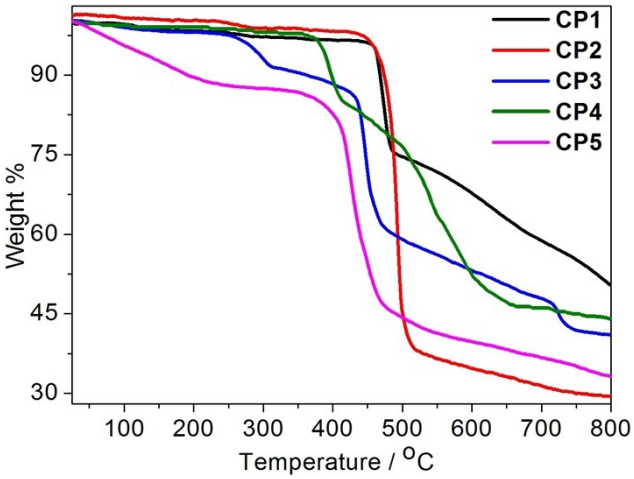
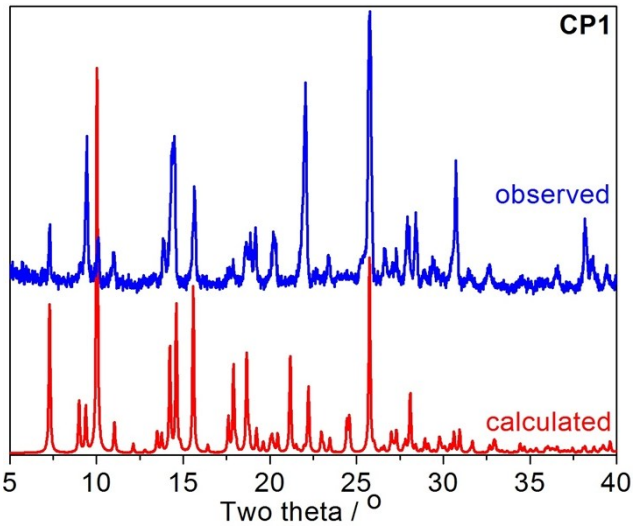
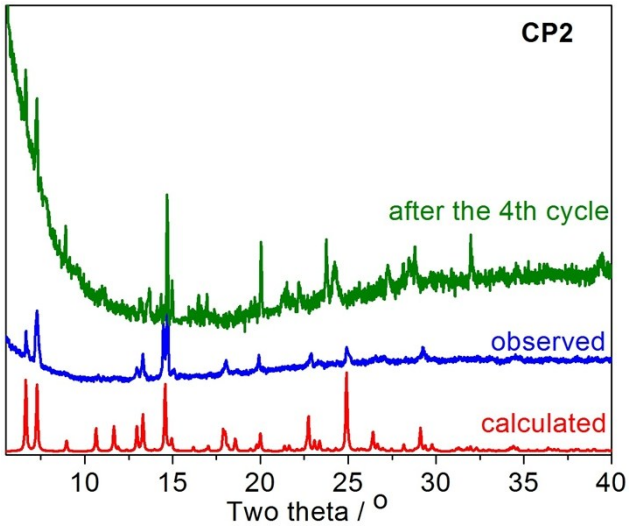
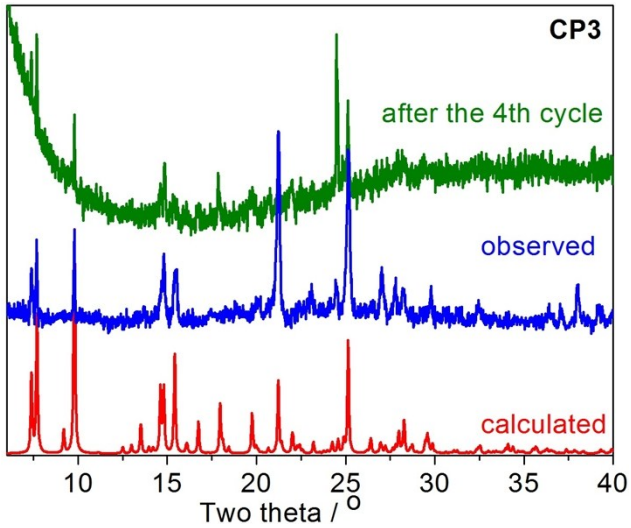
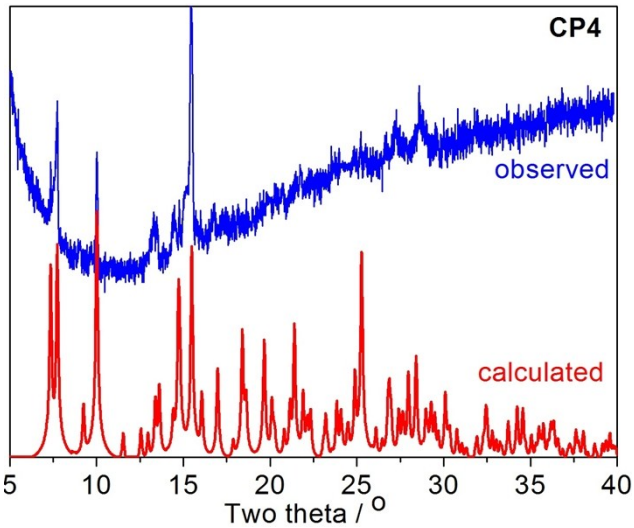


Figure S2. The TGA curves for the reported five compounds.




CP2
after the 4th cycle
observed
calculated
10
15
20
25
30
35
40
Two theta / o


CP3
after the 4th cycle
observed
calculated
10
15
20
25
30
35
40
Two theta / o


CP4
observed
calculated
5
10
15
20
25
30
35
40
Two theta / o

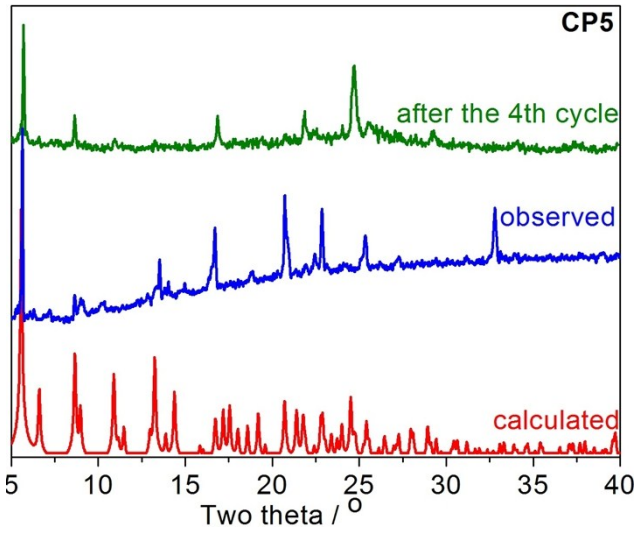


Figure S3. The comparison of the observed and calculated PXRD patterns from five powder compounds.

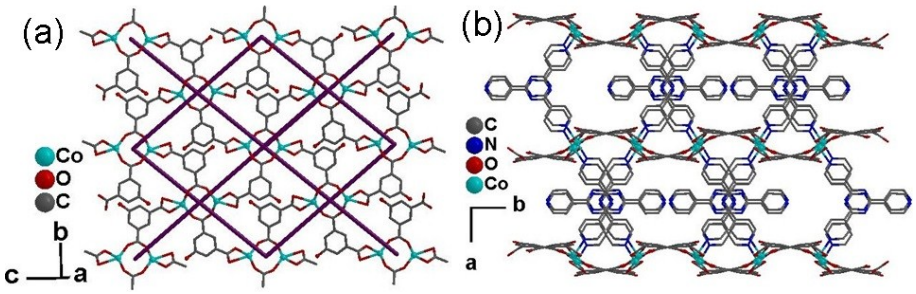


Figure. S4. (a) View of the 2D Co(OH-BDC)$_n$ sheet; (b) The 3D framework in **CP4**.

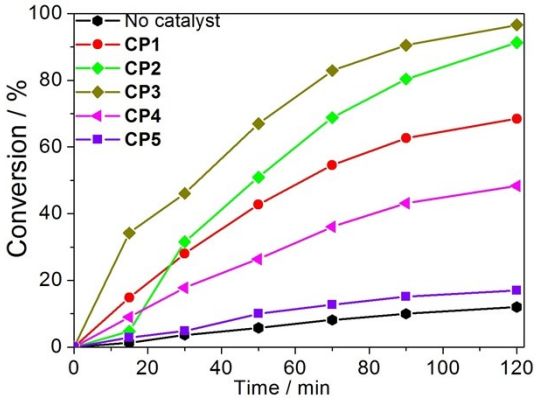


Figure S5. Conversion vs. time plots for the benzaldehyde condensation reaction with different catalysts.

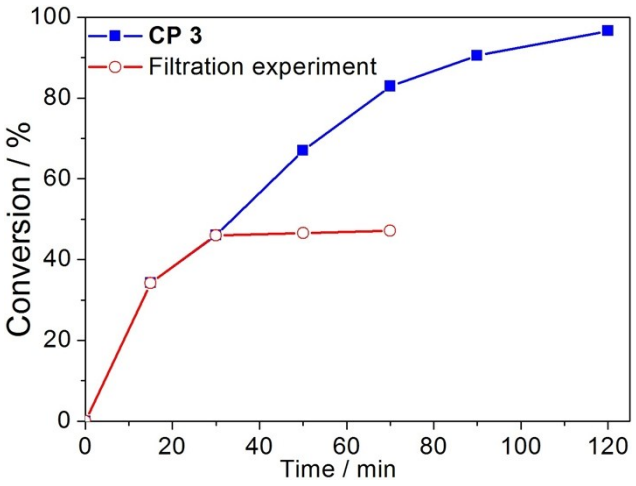


Figure S6. **CP3** catalyzed reactions with and without filtering off the catalyst.

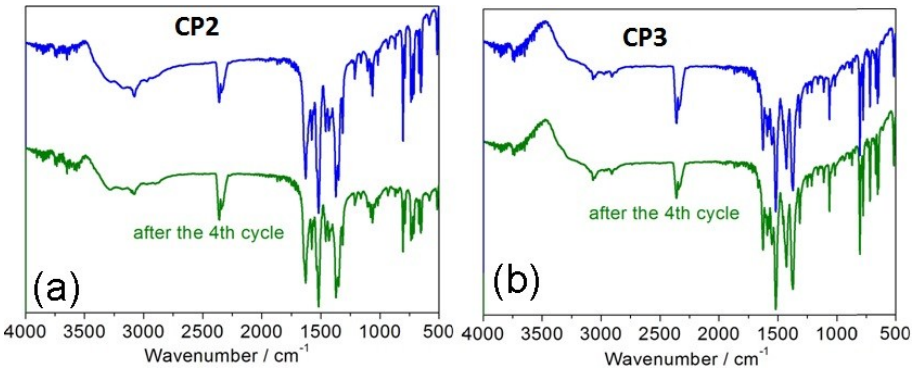


Figure S7. The FT- IR spectra of **CP2** (a) and **CP3** (b) before and after catalysis reactions.

The computed results of the (3,8)-connected net of **CP5** by TOPOS 4.0 are as follows:

Topology for Sc1

Atom Sc1 links by bridge ligands and has

Common vertex with					R(A-A)	
V	2	0.3333	0.6667	0.4161	(0 0 0)	7.920A 1
V	2	0.0000	0.0000	0.2506	(0 0 0)	7.920A 1
V	1	0.0000	0.0000	0.4281	(0-1 0)	7.984A 1
V	1	0.3333	0.6667	0.2386	(0 0 0)	7.984A 1
Sc	1	0.5000	0.5000	0.0000	(0 0-1)	10.591A 1
Sc	1	-0.1667	0.1667	0.6667	(0 0 1)	10.591A 1
Sc	1	0.3333	0.1667	0.6667	(0 0 1)	10.591A 1
Sc	1	0.0000	0.5000	0.0000	(0 0-1)	10.591A 1

Topology for V1

Atom V1 links by bridge ligands and has

Common vertex with					R(A-A)	
Sc	1	0.6667	0.8333	0.3333	(1 1 0)	7.984A 1
Sc	1	0.1667	0.8333	0.3333	(0 1 0)	7.984A 1
Sc	1	0.1667	0.3333	0.3333	(0 0 0)	7.984A 1

Topology for V2

Atom V2 links by bridge ligands and has
Common vertex with R(A-A)
Sc 1 -0.3333 -0.1667 0.3333 (0 0 0) 7.920A 1
Sc 1 0.1667 -0.1667 0.3333 (0 0 0) 7.920A 1
Sc 1 0.1667 0.3333 0.3333 (0 0 0) 7.920A 1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with V4Sc3

Coordination sequences

Sc1: 1 2 3 4 5 6 7 8 9 10
Cum 9 33 89 195 363 605 937 1371 1923 2605

V1: 1 2 3 4 5 6 7 8 9 10
Num 3 16 41 86 145 221 302 406 515 647
Cum 4 20 61 147 292 513 815 1221 1736 2383

V2: 1 2 3 4 5 6 7 8 9 10
Num 3 16 41 86 145 221 302 406 515 647
Cum 4 20 61 147 292 513 815 1221 1736 2383

TD10=2478

Vertex symbols for selected sublattice

Sc1 Point (Schlafli) symbol:{4^12;6^10;8^6}
Extended point
symbol:[4.4.4.4.4.4.4.4.4.4(2).4(2).4(2).4(2).6(3).6(3).6(3).6(3).6(3).6(3).6(3).6(3).6(3).6(6).6(6).8(12).8
(12).8(12).8(12).8(66).8(66)]

V1 Point (Schlafli) symbol:{4^3}
Extended point symbol:[4(2).4(2).4(2)]

V2 Point (Schlafli) symbol:{4^3}
Extended point symbol:[4(2).4(2).4(2)]

Point (Schlafli) symbol for net: {4^12;6^10;8^6}3{4^3}4

3,8-c net with stoichiometry (3-c)4(8-c)3; 2-nodal net
New topology, please, contact the authors (67371 types in 9 databases)