Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

N-donor Auxiliary Ligands Directed Assembly of Co^{II} compounds with 2,2'-dinitro-biphenyl-4,4'-dicarboxylate ligand: Structures, and Magnetic Properties

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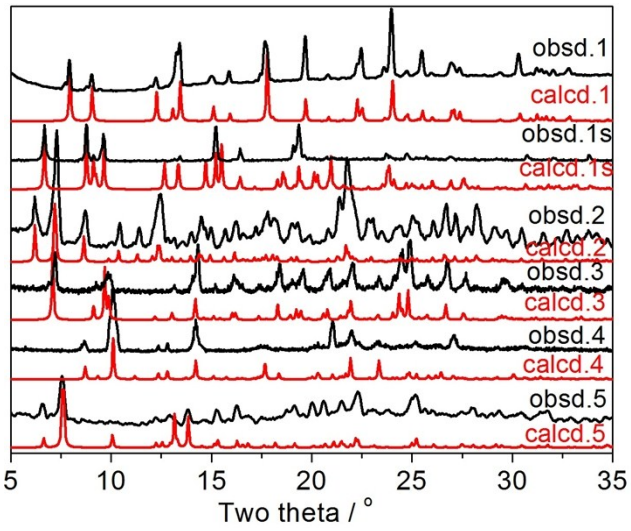

Figure S1. The comparison of the observed and calculated PXRD patterns from these reported powder compounds.

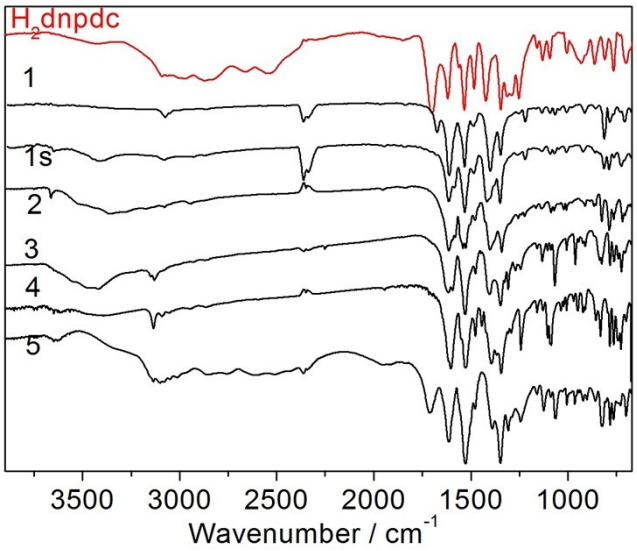

Figure S2. The FT- IR spectra of H_2dnpdc ligand and the six Co-based compounds.

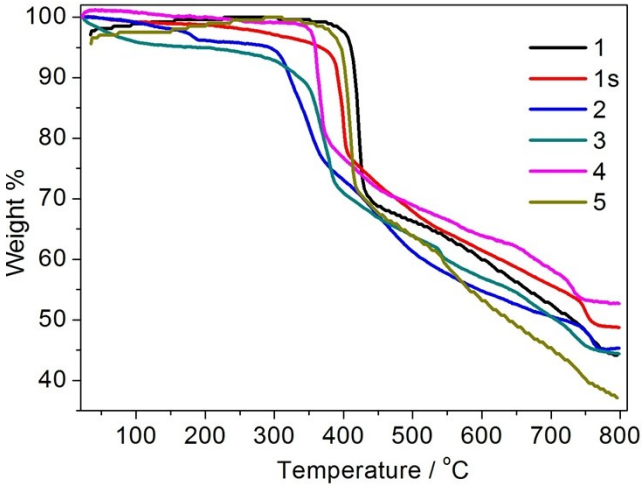

Figure S3. The TGA curves for the reported six Co-based compounds.

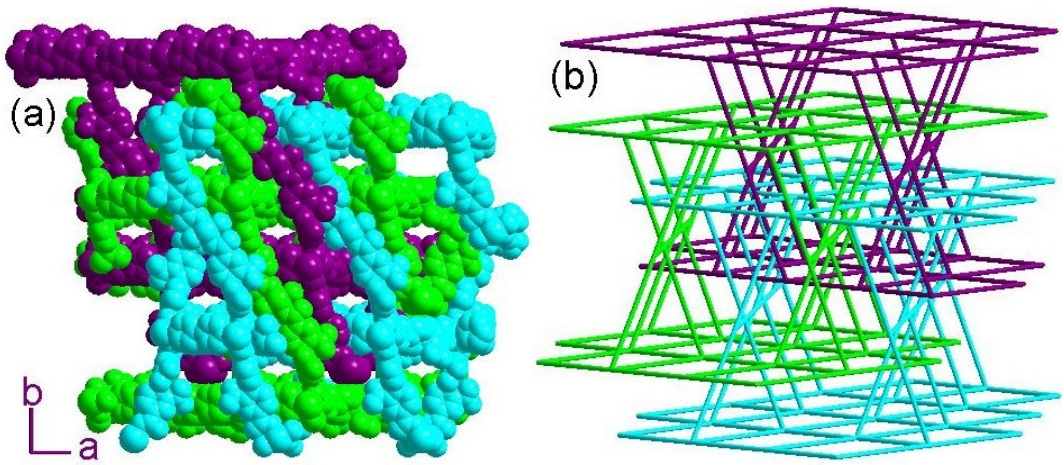

Figure S4. (a) The space-filling diagram of the 3-fold interpenetrated net in compound **1s**; (b) View of the 3-fold interpenetrated net topology.

Table S1. Selected bond [Å] and angles [º] for compound **1-5**.

Co1-N1	2.1492(16)	Co1-O1	2.0733(13)
Co1-O2#1	2.0857(14)		
O1#2-Co1-O1	172.31(8)	O1-Co1-O2#1	96.37(5)
O1-Co1-O2#3	89.26(6)	O2#1-Co1-O2#3	86.01(8)
O1- Co1-N1	84.63(6)	O2#1-Co1-N1	176.79(6)
O2#3-Co1-N1	90.96(6)	O1-Co1-N1#2	90.03(6)
N1-Co1-N1#2	92.10(9)		
Symmetry code for compound **1**: #1-x+1, -y+1, -z+2; #2 -x+1, y, -z+3/2; #3 x, -y+1, z-1/2.			
Co1-O1	2.034(3)	Co1-O2#1	2.039(3)
Co1-N1	2.163(4)	Co1-N2#2	2.176(4)
Co1-O5	2.206(3)	Co1-O6	2.223(3)
Co2-O3	2.073(3)	Co2-O7	2.104(3)
Co2-N3	2.183(3)		
O1-Co1-O2#1	112.68(13)	O1-Co1-N1	92.21(14)
O2#1-Co1-N1	95.29(13)	O1-Co1-N2#2	87.28(15)
O5-Co1-O6	59.35(12)	O2#1-Co1-N2#2	89.09(14)
N1-Co1-N2#2	175.43(15)	O1-Co1-O5	153.67(12)
O2#1-Co1-O5	93.59(12)	N1-Co1-O5	86.84(14)
N2#2-Co1-O5	91.61(15)	O1-Co1-O6	94.33(12)
O2#1-Co1-O6	152.48(13)	N1-Co1-O6	88.59(14)
N2#2-Co1-O6	86.92(14)	O3-Co2-O7#3	89.17(12)
O7#3-Co2-N3#3	91.01(13)	O3#3-Co2-O3	180.00(18)
O7#3-Co2-O7	180.00(13)	O3-Co2-O7	90.83(12)
O3#3-Co2-N3	87.91(13)	O3-Co2-N3	92.10(13)
O7-Co2-N3	91.01(13)	O7#3-Co2-N3	88.99(13)
O3#3-Co2-N3#3	92.10(12)	O3-Co2-N3#3	87.90(13)
Symmetry codes for compound **1s**: #1 -x,-y,-z; #2 x,-y,z+1/2; #3 -x+1/2,-y+3/2,-z;			
O1-Co2-O6	85.12(14)	O1#3-Co2-O6	94.88(14)
O6-Co2-O6#3	180.0(2)	O1-Co2-O2#3	85.67(15)
O6-Co2-O2#3	89.06(14)	O1-Co2-O2	94.33(15)
O2#3-Co2-O2	180.0(3)	O6-Co2-O2	90.94(14)
O1-Co3-O18	96.33(17)	O5#4-Co3-O1	167.44(17)
O5#4-Co3-O9#1	87.78(16)	O1-Co(3)-O9#1	95.85(15)
O5#4-Co3-O18	95.57(18)	O1-Co3-O2#3	81.54(15)
O9#1-Co3-O18	91.77(17)	O5#4-Co3-O7#3	89.84(15)
O1-Co3-O7#3	86.68(14)	O9#1-Co3-O7#3	177.43(16)
O18-Co3-O7#3	87.50(16)	O5#4-Co3-O2#3	86.78(16)
O18-Co3-O2#3	176.32(15)	O7#3-Co3-O2#3	95.35(14)

O9#1-Co3-O2#3	85.48(15)		
Symmetry codes for compound **2**: #1 -x-3/2, y-1/2, -z-1/2; #2 -x-1, y-1, -z-1/2; #3 -x-1, -y+1, -z; #4 x-1/2, y-1/2, z.			
Co1-N1	2.047(3)	Co1-O1	2.164(4)
Co1-O2	2.222(4)	Co2-O3	1.955(3)
Co2-N3	2.012(3)		
N1#1-Co1-N1	101.64(19)	N1-Co1-O1	147.07(15)
N1-Co1-O1#1	94.11(16)	O1-Co1-O1#1	87.7(2)
N1-Co1-O2	91.52(14)	O1-Co1-O2	57.97(14)
N1-Co1-O2#1	95.68(15)	O1-Co1-O2#1	112.78(16)
O2-Co1-O2#1	168.6(2)	O3#2-Co2-O3	100.9(2)
O3-Co2-N3#2	128.02(15)	O3-Co2-N3	97.17(14)
N3#2-Co2-N3	108.89(19)		
Symmetry code for compound **3**: #1 -x+1/2, y, -z+1/2; #2 -x+3/2, y, -z-1/2.			
Co1-N1	2.047(3)	Co1-O1	1.996(3)
Co1-O4	2.022(3)	Co1-N4	2.013(3)
O1-Co1-N4#1	129.22(12)	O1-Co1-O4#2	106.55(11)
N4#1-Co1-O4#2	110.03(11)	O1-Co1-N1	103.35(12)
N4#1-Co1-N1	105.82(13)	O4#2-Co1-N1	96.93(12)
Symmetry code for compound **4**: #1 x+1/2, y, -z+1/2; #2 -x+1/2, -y+2, z+1/2.			
Co1-O1	2.067(3)	Co1-O2#2	2.102(3)
Co1-O3#1	2.081(3)	Co1-O4#3	2.115(3)
Co1-N1	2.169(3)	Co1-N2	2.114(3)
O1-Co1-O3#1	95.30(11)	O1-Co1-O2#2	88.65(11)
O3#1-Co1-O2#2	171.17(11)	O1-Co1-N2	174.67(13)
O3#1-Co1-N2	86.48(12)	O2#2-Co1-N2	90.30(12)
O1-Co1-O4#3	83.80(11)	O3#1-Co1-O4#3	91.68(11)
O2#2-Co1-O4#3	96.61(11)	N2-Co1-O4#3	91.14(12)
O1-Co1-N1	90.66(13)	O3#1-Co1-N1	90.91(12)
O2#2-Co1-N1	81.12(12)	N2-Co1-N1	94.34(13)
O4#3-Co1-N1	174.08(12)		
Symmetry code for compound **5**: #1 x+1, -y+3/2, z+1/2; #2 x, -y+3/2, z-1/2; #3 x+1, y, z.			

Table S2. The bond valence sum (BVS) calculations for Co and O atoms in compound **2**.

	Co-O bond	Co-O bond length γ / Å	s	BVS	assignment
Co1	Co1-O1	2.0506	0.37939	1.95	Co^{2+}
	Co1-O3	2.1013	0.33081		
	Co1-O6	2.2661	0.2119		
	Co1-O8$^{\#1}$	2.0279	0.4034		
	Co1-N1	2.1261	0.30936		
	Co1-N2$^{\#2}$	2.1302	0.30595		
Co2	Co2-O1	2.0444	0.3858	2.12	Co^{2+}
	Co2-O1$^{\#3}$	2.0444	0.3858		
	Co2-O2	2.1130	0.32051		
	Co2-O2$^{\#3}$	2.1130	0.32051		
	Co2-O6	2.0763	0.35393		
	Co2-O6$^{\#3}$	2.0763	0.35393		
Co3	Co3-O1	2.0290	0.4022	1.96	Co^{2+}
	Co3-O2$^{\#3}$	2.2909	0.19817		
	Co3-O7$^{\#3}$	2.1784	0.26858		
	Co3-O5$^{\#4}$	2.0151	0.41759		
	Co3-O9$^{\#1}$	2.0676	0.36235		
	Co3-O18	2.1316	0.3048		
μ_3-O1	O1-Co1	2.0506	0.37939	1.16	OH^-
	O1-Co2	2.0444	0.3858		
	O1-Co3	2.0290	0.4022		
#1 -1.5-x, -0.5+y, -0.5-z; #2 -1-x, -1+y, -0.5-z; #3 -1-x, 1-y –z; #4 -0.5+x, -0.5+y, z.					

The computed results of the 10-connected net of **2** by TOPOS 4.0 are as follows:

Topology for V1

Atom V1 links by bridge ligands and has

Common vertex with R(A-A)

V	1	0.0000	0.0000	-0.5000	(-1 0-1)	16.639A	1
V	1	1.0000	1.0000	0.5000	(0 1 0)	16.639A	1
V	1	0.0000	1.0000	-0.5000	(-1 1-1)	16.639A	1
V	1	1.0000	0.0000	0.5000	(0 0 0)	16.639A	1
V	1	0.0000	0.0000	0.0000	(0 0 0)	16.764A	1
V	1	1.0000	1.0000	0.0000	(1 1 0)	16.764A	1
V	1	0.5000	1.5000	0.5000	(1 1 0)	17.445A	1
V	1	0.5000	-0.5000	-0.5000	(1-1-1)	17.445A	1
V	1	0.5000	-0.5000	0.5000	(1-1 0)	17.445A	1
V	1	0.5000	1.5000	-0.5000	(1 1-1)	17.445A	1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with V

Coordination sequences

V1: 1 2 3 4 5 6 7 8 9 10

Cum 11 63 185 405 751 1251 1933 2825 3955 5351

TD10=5351

Vertex symbols for selected sublattice

V1 Point (Schlafli) symbol:{3^6;4^26;5^12;6}

Extended point

symbol:[3.3.3.3.3.3.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.5.5.5(2).5(2).5(4).5(4).5(4).5(4).5(5).5(5).5(7).5(7).6(8)]

Point (Schlafli) symbol for net: {3^6;4^26;5^12;6}

10-c net; uninodal net

New topology, please, contact the authors (67371 types in 9 databases)