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Flexible and rigid dicarboxylic acid enabled the assembly of achiral and chiral 3D Co(II) metal-organic frameworks

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Table S1 Selected bond distances (Å) and angles (°) for compounds 1 and 2.

Compound **1**			
Co1–O1	2.057(6)	Co2–O1W	2.119(6)
Co1–O1W	2.071(3)	Co2–N2	2.180(6)
Co1–N1	2.190(6)	Co2–N8	2.098(11)
Co1–N3	2.142(7)	Co2–O2	2.084(9)
Co1–N6	2.228(8)		
O1–Co1–O1W	95.8(2)	N3– Co1– N6	92.0(3)
O1–Co1–N1	86.83(14)	N2#2–Co2–N2	81.6(3)
O1–Co1–N3	87.4(3)	N8–Co2–O1W	170.5(4)
O1–Co1–N6	179.4(3)	N8–Co2–N2	97.7(3)
O1W–Co1– N1	88.25(14)	O1W–Co2– N2	89.49(19)
O1W–Co1– N3	176.7(3)	O2–Co2–O1W	89.3(3)
O1W–Co1– N6	84.8(3)	O2–Co2–N2#2	171.9(3)
N1– Co1– N1#1	172.4(3)	O2–Co2–N2	90.4(3)
N1– Co1– N6	93.20(14)	O2–Co2–N8	84.4(3)
N3– Co1– N1	91.94(14)	O2–Co2–O2#2	97.5(5)
Symmetry code: #1 1 – *x*, + *y*, + *z*; #2 + *x*, + *y*, 1/2 – *z*.			
Compound **2**			
Co1–O1W	2.076(4)	Co2–O1W	2.077(5)
Co1–N5	2.089(5)	Co2–O3	2.086(5)
Co1–O1	2.123(5)	Co2–O1W#5	2.090(5)
Co1–O2	2.134(4)	Co2–O4	2.115(5)
Co1–N3	2.221(5)	Co2–N2	2.139(6)
Co1–N1	2.283(5)	Co2–N4	2.140(6)

N5–Co1–O1	155.1(2)	O2–Co1–C10	30.7(2)
O1W–Co1–O2	155.01(17)	O1W–Co2–O3	87.58(18)
N5–Co1–O2	93.8(2)	O1W–Co2–O1W#5	178.95(9)
O1–Co1–O2	61.63(19)	O3–Co2–O1W#5	93.45(18)
O1W–Co1–N3	87.1(2)	O1W–Co2–O4	94.44(17)
N5–Co1–N3	90.9(2)	O3–Co2–O4	178.0(2)
O1–Co1–N3	88.8(2)	O1W#5–Co2–O4	84.52(17)
O2–Co1–N3	98.2(2)	O1W–Co2–N2	86.76(18)
O1W–Co1–N1	86.5(2)	O3–Co2–N2	85.0(2)
N5–Co1–N1	87.2(2)	O1W#5–Co2–N2	93.18(19)
O1–Co1–N1	96.2(2)	O4–Co2–N2	95.3(2)
O2–Co1–N1	89.5(2)	O1W–Co2–N4	92.79(19)
N3–Co1–N1	172.18(17)	O3–Co2–N4	94.57(19)
O1W–Co1–C10	125.0(2)	O1W#5–Co2–N4	87.27(18)
N5–Co1–C10	124.4(2)	O4–Co2–N4	85.1(2)
O1–Co1–C10	30.9(2)	N2–Co2–N4	179.4(2)

Symmetrycode: #5 1/2 + *x*, 3/2 – *y*, 1 – *z*.

Table S2. The structure determinations of three randomly selected crystals of **2** from the same batch crystals.

Compounds	**2-1**	**2-2**	**2-3**
Empirical formula	$C_{23}H_{14}N_7O_5Co_2$	$C_{23}H_{14}N_7O_5Co_2$	$C_{23}H_{14}N_7O_5Co_2$
Formula weight	586.27	586.27	586.27
Crystal system	orthorhombic	orthorhombic	orthorhombic
Space group	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$
a (Å)	6.69441(19)	6.6979(2)	6.70332(17)
b (Å)	17.0072(4)	17.0039(5)	17.0078(4)
c (Å)	19.9883(9)	20.0050(8)	19.9071(6)
α (°)	90	90	90
β (°)	90	90	90
γ (°)	90	90	90
V (Å ^{3})	2275.73(13)	2278.36(13)	2269.58(11)
Z	4	4	4
D_c(g cm^{-3})	1.711	1.709	1.716
μ (mm^{-1})	11.883	11.870	11.915
F (000)	1180.0	1180.0	1180.0
Reflection collected	5734	5540	5501
Unique reflections	3937	3619	3807
R_{int}	0.0728	0.0570	0.0530
GOF	1.042	1.041	1.070
$R_1{}^a$ [I> 2σ(I)]	0.0961	0.0715	0.0769
$wR_2{}^b$ (all data)	0.2949	0.2072	0.2345
Flack parameter	-0.027(14)	-0.029(9)	-0.021(12)

$^aR_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, $^bwR_2 = \Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]^{1/2}$.

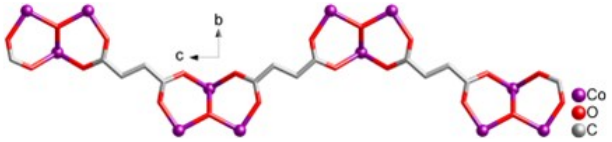


Fig. S1 1D zig-zag chain formed by succinic acid ligand and Co ions.

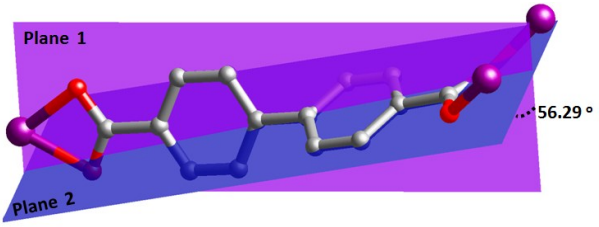
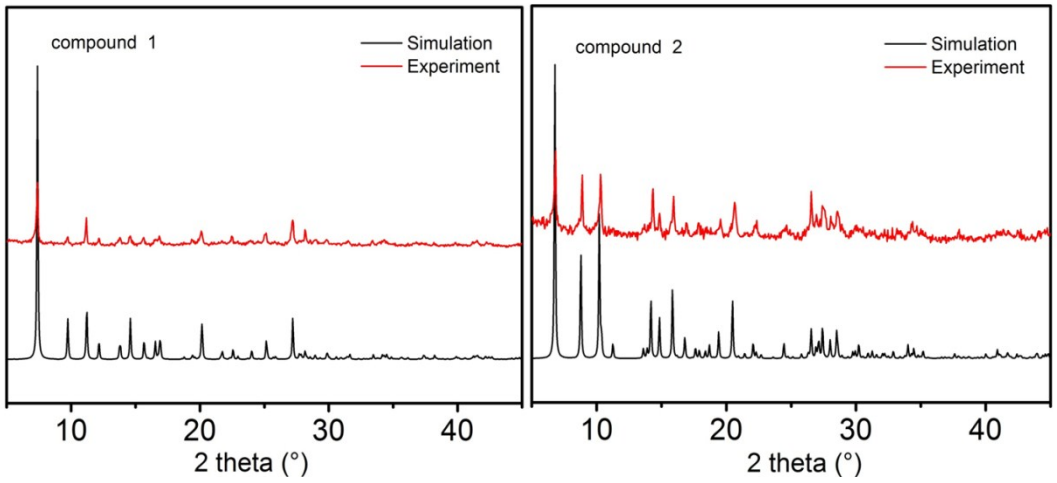
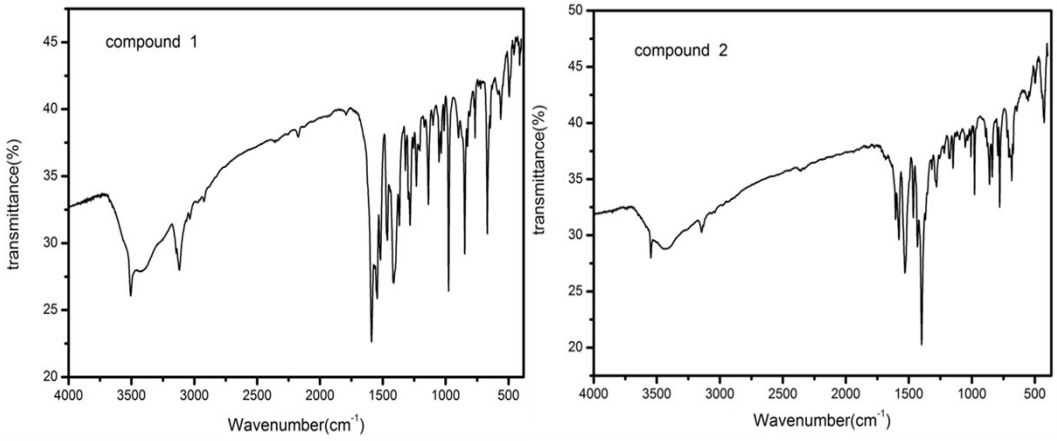


Fig. S2 The dihedral angle of two phenyl rings is 56.29° in the 4,4'-bpdc ligand.



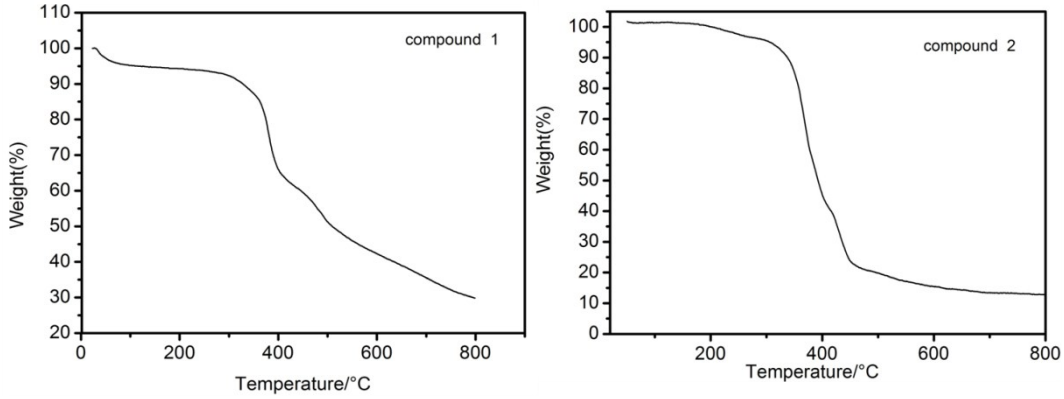
(a) (b)

Fig. S3 The Powder X–ray diffraction of compounds **1** (a) and **2** (b).



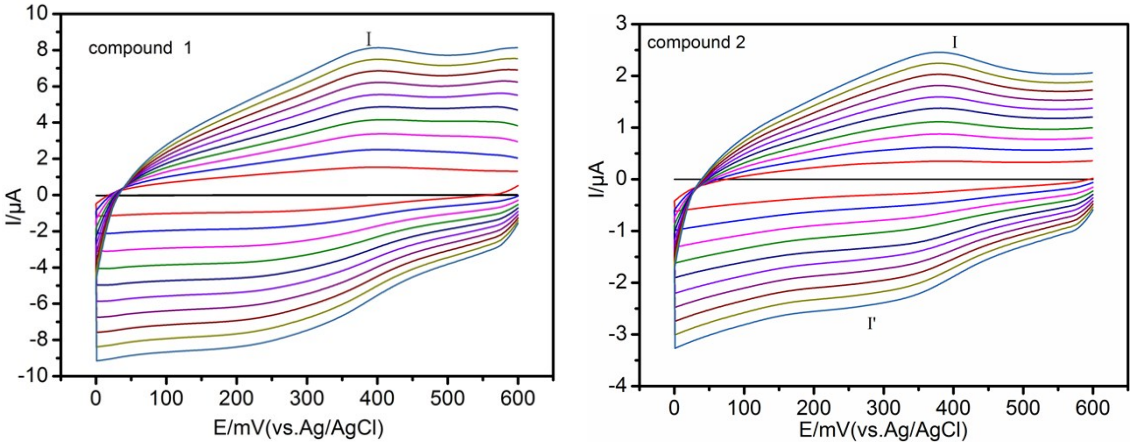
(a) (b)

Fig. S4 The IR spectra of compounds **1** (a) and **2** (b).



(a) (b)

Fig. S5 The TG curves of compounds **1** (a) and **2** (b).



(a) (b)

Fig. S6 Cyclic voltammograms of **1**-CPE (a) and **2**-CPE (b) in 0.5 M Na_2SO_4 + 0.1 M H_2SO_4 aqueous solution. Potentials measured vs. Ag/AgCl (From inside to out: 50, 100, 150, 200, 250, 300, 350, 400, 450, 500 mV s^{-1}).