Supporting Information

Reversible Single-Crystal-to-Single-Crystal Transformation and Highly Selective Adsorption Property of Three-Dimensional Cobalt(II) Frameworks

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Table S1. Crystal Data and Structure Refinements for Complex **1'.**

	1'
Empirical formula	$C_{36}H_{28}Co_3N_8O_{16}$
Formula weight	1005.45
Temperature / K	293
Crystal system	Triclinic
Space group	*P*-1
a /Å	8.5503(12)
b /Å	10.0700(14)
c /Å	11.2653(15)
α /°	77.638(2)
β /°	73.9210(10)
γ /°	88.716(2)
V (Å^3)	909.7(2)
Z	1
Dc (g cm^{-3})	1.835
F(000)	505
θ range /°	1.93 - 25.04
Reflns. collected	4473
Independent reflns.	2759
Goodness-of-fit	1.012
R_1[a] ($I > 2\sigma(I)$)	0.0349
wR_2[b] ($I > 2\sigma(I)$)	0.0904

Table S2. Selected Bond Lengths [Å] and Bond Angles [deg] for Complex **1'.**

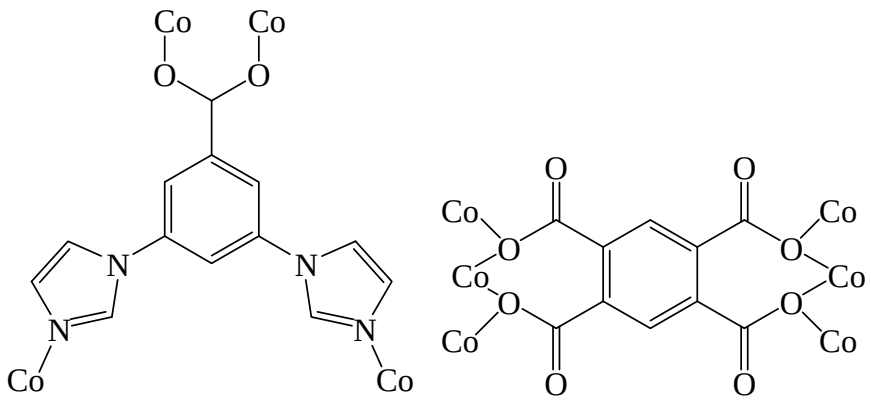
	1'		
Co1-O1	2.1071(19)	Co1-O5	2.0499(18)
Co1-O3	2.0620(19)		
Co2-O3	2.0931(19)	Co2-O6	2.0701(19)
Co2-N12#1	2.117(3)	Co2-O1#2	2.204(2)
Co2-O7	2.125(2)	Co2-N32#3	2.123(2)
O1-Co1-O3	95.54(7)	O3-Co1-O3#2	180.00
O1-Co1-O5#2	88.37(8)	O5#2-Co1-O5	180.00
O1-Co1-O1#2	180.00	O1#2-Co1-O5#2	91.63(8)
O3-Co1-O5#2	87.47(8)	O3#2-Co1-O5#2	92.53(8)
O1#2-Co1-O3	84.46(7)		
O3-Co2-N12#1	97.26(9)	O6-Co2-N12#1	88.90(9)
O3-Co2-O6	94.21(8)	O1#2-Co2-N12#1	177.67(8)
O1#2-Co2-O3	81.36(7)	N12#1-Co2-N32#3	89.59(10)
O3-Co2-N32#3	89.58(8)	O1#2-Co2-O6	89.33(8)
O6-Co2-O7	90.87(8)	O3-Co2-O7	166.25(9)
O1#2-Co2-O7	85.94(8)	O7-Co2-N12#1	95.60(10)
O7-Co2-N32#3	85.66(9)	O6-Co2-N32#3	176.07(8)
O1#2-Co2-N32#3	92.27(9)		

Symmetric transformations used to generate equivalent atoms for **1'**: #1 1-x, 1-y, 2-z; #2 -x, -y, 2-z; #3 -1+x, y, 1+z.

Table S3. Hydrogen bonding distances (Å) and angles (°) for Complex **1**

D–H···A	*d*(H ···A)	*d*(D ···A)	∠(D – H ··· A)
O8-H13····O2#1	2.13(6)	3.029(5)	172(5)
O7-H11····O6#2	2.50(3)	2.935(3)	131(4)
O7-H11····O7#1	2.31(3	2.797(3)	138(4)
O7-H12····O4	1.79(3)	2.656(3)	161(3)

Symmetry transformations used to generate equivalent atoms: #1 2-x, 1-y, -z; #2 1-x, 1-y, 1-z.



Scheme S1. The coordination modes of L^- and $BTEC^{4-}$ in **1** and **2**.

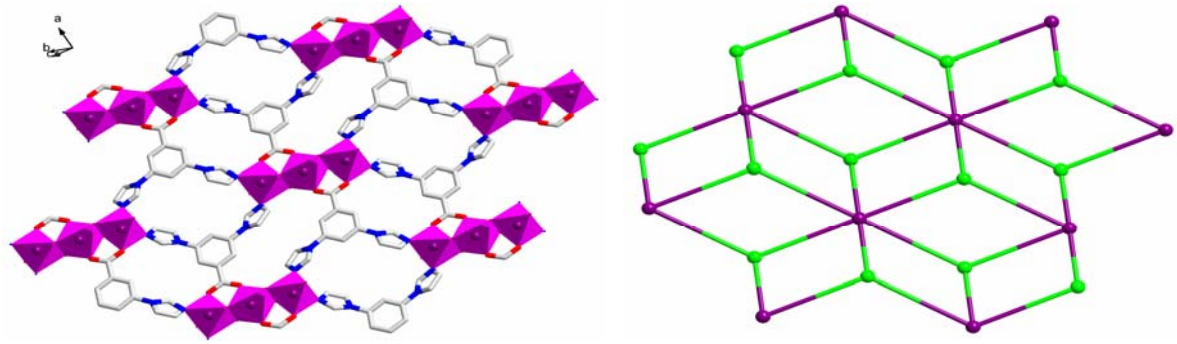


Figure S1. Polyhedral and topological views of 2D layer constructed by SBUs and L^- in **1** (Green balls: L^- ligands; Violet balls: trinuclear SBUs).

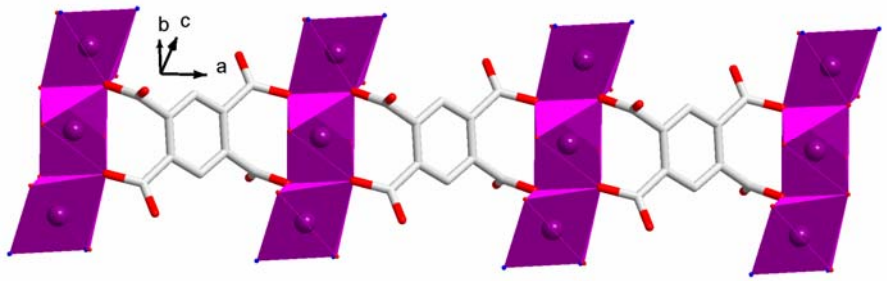


Figure S2. The 1D infinite chain constructed by SBUs and $BTEC^{4-}$ in **1**.

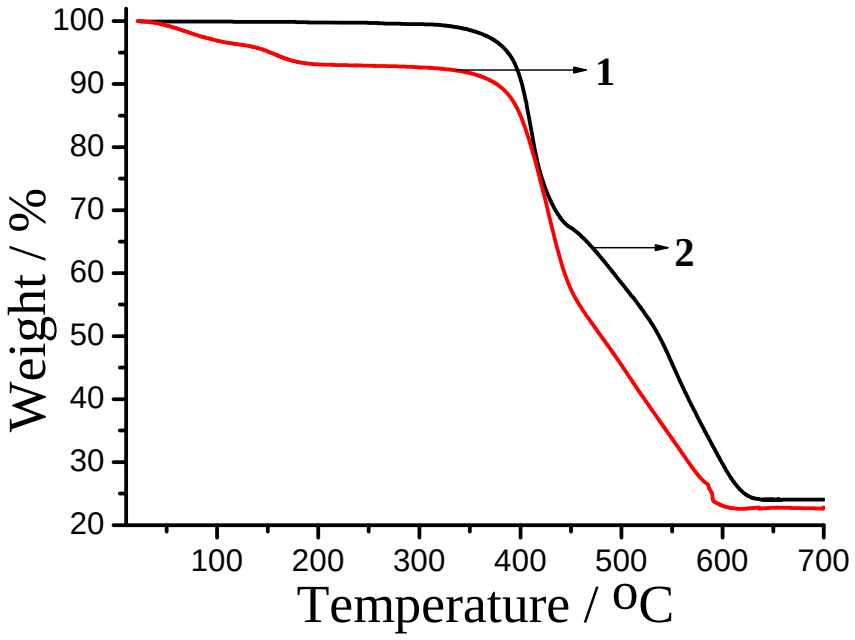


Figure S3. The TG curves of **1** and **2**.

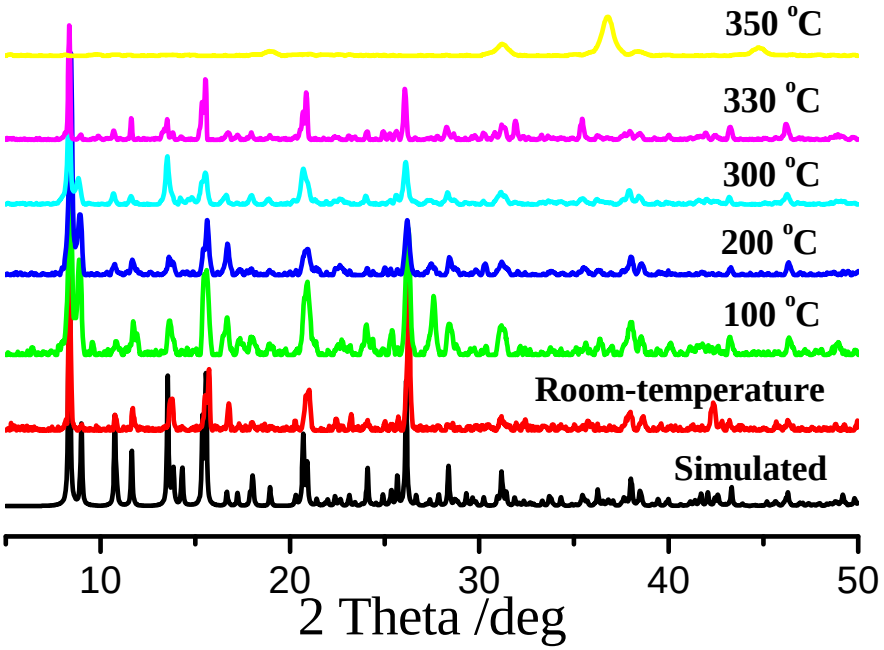


Figure S4. Variable-temperature PXRD of complex **1**.

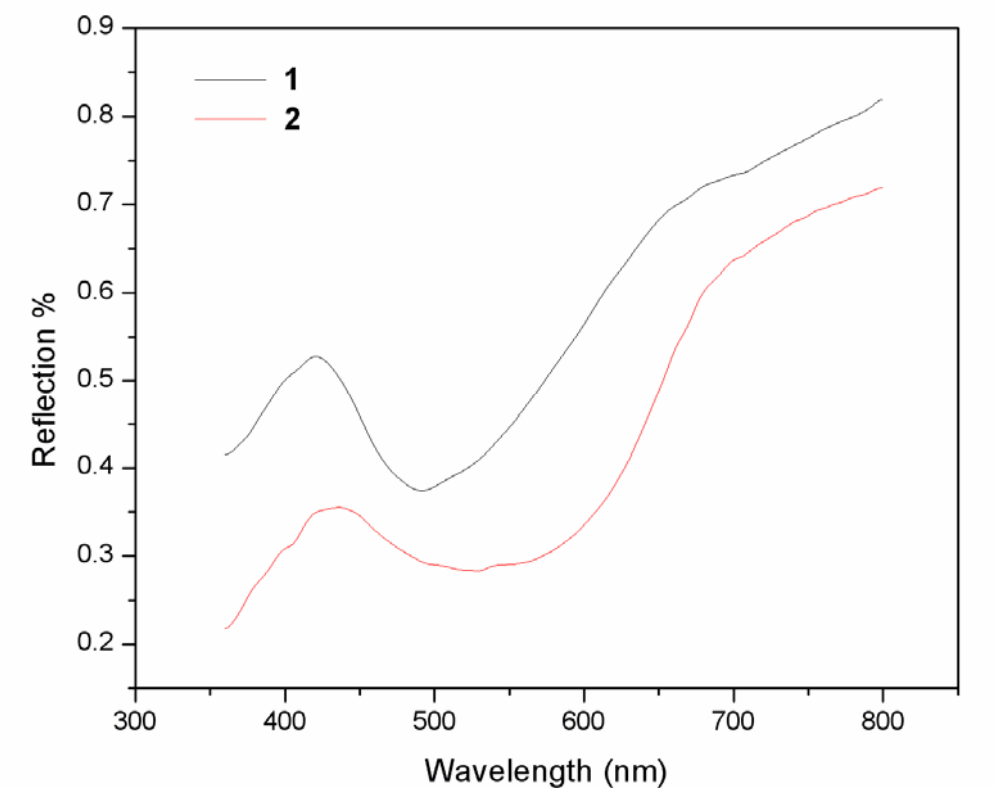


Figure S5. UV-visible spectra of **1** and **2** in the solid state at room temperature.

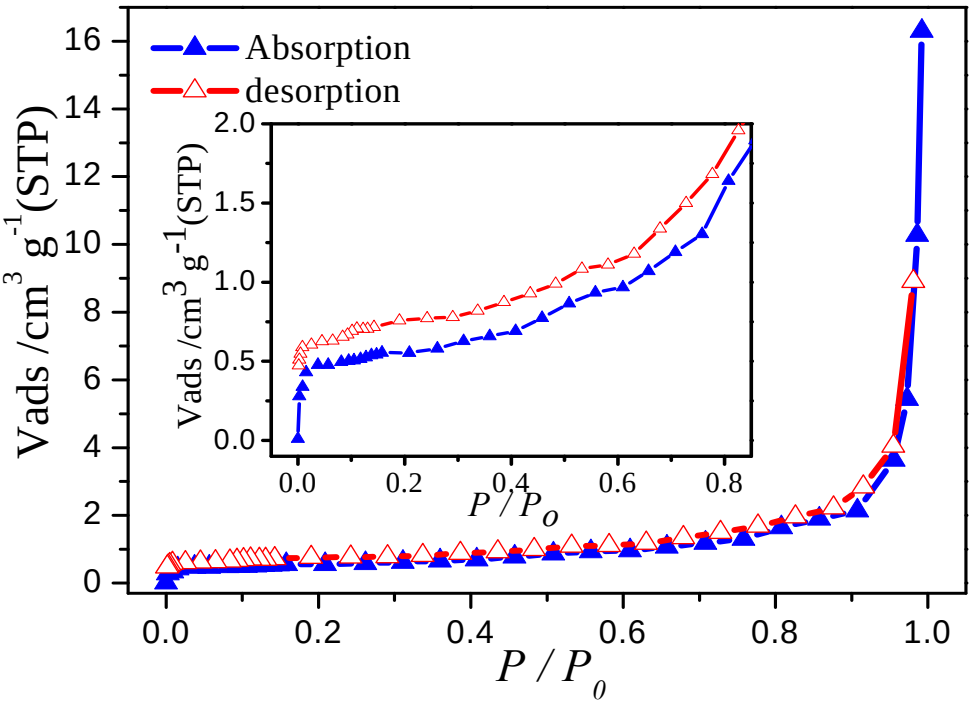


Figure S6. N_2 (77K) adsorption isotherm of **2** (Filled blue shapes: adsorption and open red ones: desorption, respectively). Insert: the enlargement data of adsorption isotherm in the range of 0 ~ 0.85 p/p_0.

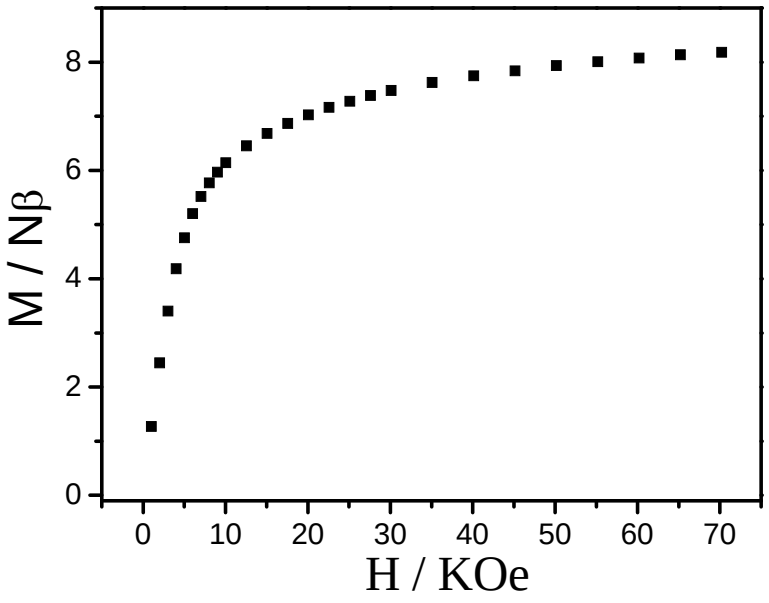


Figure S7. The plot of magnetization versus applied magnetic field of **1** at 1.8 K.

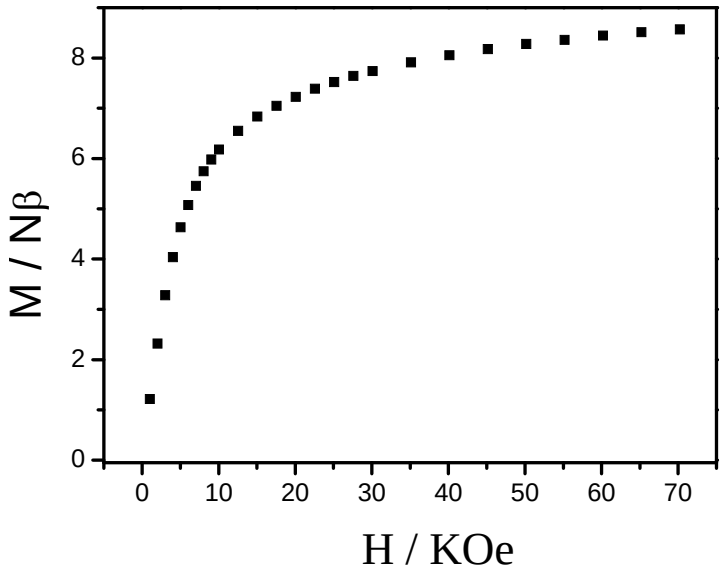


Figure S8. The plot of magnetization versus applied magnetic field of **2** at 1.8 K.