

Water adsorption and proton conduction of cobalt(II) complex assembled by triazine-based polycarboxylate

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Supporting Information

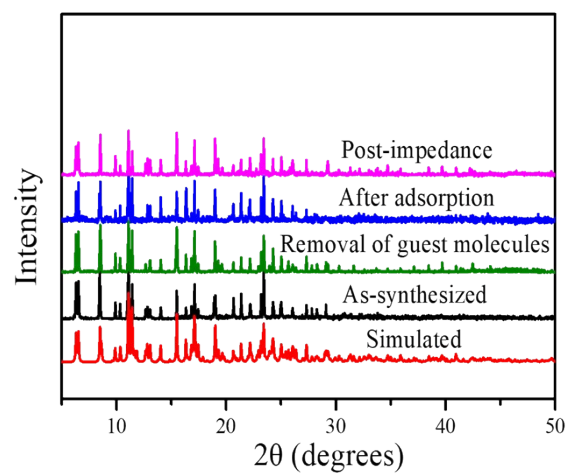


Fig. S1 The XRD patterns of **1** under different conditions.

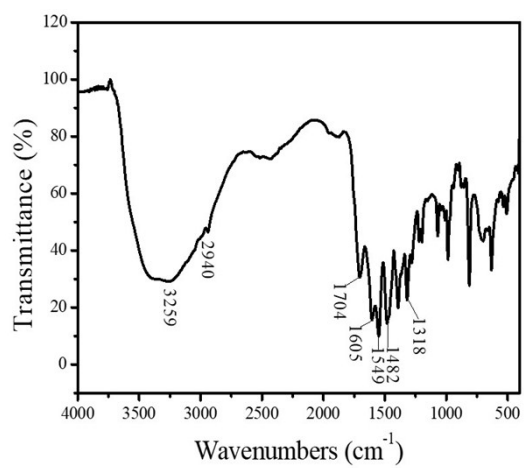


Fig. S2 The IR spectrum of **1**.

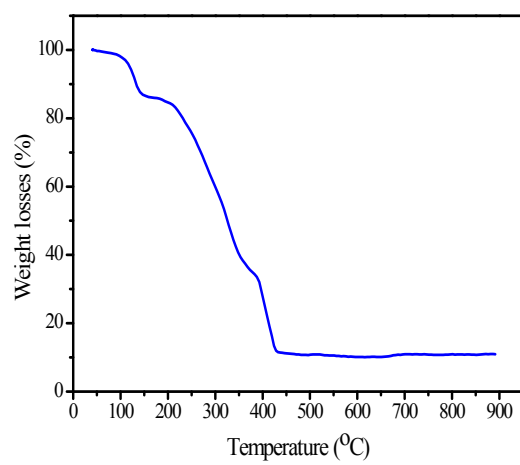


Fig. S3 TGA plot of **1**.

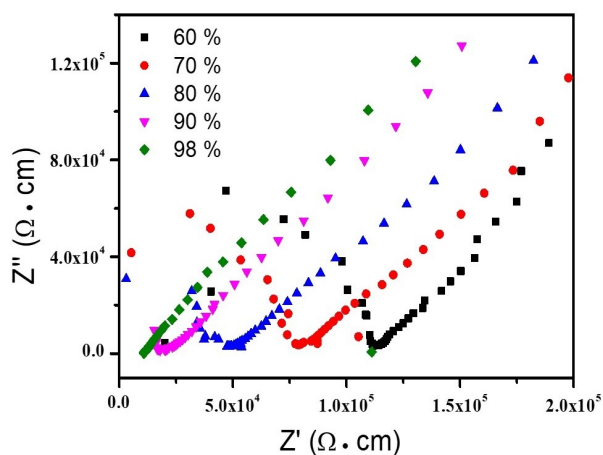


Fig. S4 Plots of the impedance plane for **1** at different relative humidity and 298 K.

Table 1 Crystallographic data and refinement parameters of **1**.

1	
CCDC number	1814876
Empirical formula	$C_{80}H_{110}N_{22}O_{44}CO_3$
Formula weigh	2260.68
Temperature/K	173
Crystal system	monoclinic
Space group	$P 2_1/n$
$a/\text{\AA}$	11.4850(6)
$b/\text{\AA}$	15.4909(9)
$c/\text{\AA}$	28.1342(16)
$\alpha/^\circ$	90
$\beta/^\circ$	95.484(2)
$\gamma/^\circ$	90
Unit cell volume/ $\text{\AA}^3$	4982.5(5)
Z	2
$D_{\text{calc}}/\text{g cm}^{-3}$	1.507
μ/mm^{-1}	0.597
$F(000)$	2354.0
h, k, l max	13, 18, 33
No. of parameters	677
S	1.042
$R_1, wR_2 [I > 2\sigma(I)]$	0.0573, 0.1524
$\Delta\rho_{\text{max}}/\text{e \AA}^{-3}$	0.745
$\Delta\rho_{\text{min}}/\text{e \AA}^{-3}$	0.644

Table S2 Selected bond lengths (Å) of **1**.

1			
Co1-O13	2.055(3)	Co1-O14	2.068(3)
Co1-O1	2.136(3)	Co1-N7	2.192(2)
Co1-N8	2.207(4)	Co1-N9	2.113(3)
Co2-O16	2.058(3)	Co2-O15	2.093(3)
Co2-N10	2.158(3)		

Table S3 Hydrogen-bond geometry (Å, °) of **1**.

D-H...A	D-H	H...A	D-H...A
O2-H2...O3	0.839(3)	1.680(3)	162.1(2)
O6-H6...O7	0.840(3)	1.635(3)	163.8(2)
O10-H10...O11	0.841(4)	1.717(5)	157.6(3)
O13-H13A...O4	0.840(3)	1.889(3)	158.0(2)
O14-H14A...O21	0.840(3)	2.145(5)	120.9(2)
O14-H14B...O5	0.849(3)	1.930(3)	168.2(2)
O15-H15A...O11	0.840(3)	2.138(5)	168.2(2)
O16-H16A...O3	0.840(3)	1.876(3)	165.3(2)
O16-H16B...O17	0.845(3)	1.830(6)	142.5(2)
O17-H17B...O20	0.849(8)	1.803(9)	179.4(6)
O18-H18A...O12	0.849(4)	1.976(5)	171.8(3)
O18-H18B...O19	0.850(5)	1.932(5)	171.5(3)
O19-H19A...O6	0.851(4)	2.048(3)	162.0(3)
O19-H19B...O9	0.851(4)	1.995(5)	161.4(3)
O20-H20A...O12	0.850(7)	1.962(5)	162.1(5)
O20-H20B...O17	0.849(8)	1.830(8)	162.5(6)
O21-H21A...O8	0.851(5)	1.924(3)	161.0(3)
O21-H21B...O14	0.848(5)	1.859(3)	160.9(4)
O22-H22A...O18	0.850(3)	2.356(5)	107.6(3)
O22-H22B...O13	0.850(4)	1.928(3)	141.4(2)

Table S4 The resistance (R) and conductivity (σ) of **1** under different temperature and 98% relative humidity. The values of pellet dimensions including sample thickness (*l*) and diameter are 500 μ m and 2 mm, respectively.

Temperature (K)	R (Ω)	σ (S/cm)
293	13426	1.19×10^{-4}
298	11066	1.44×10^{-4}
303	9141	1.74×10^{-4}
308	7391	2.15×10^{-4}
313	5184	3.07×10^{-4}
318	4859	3.28×10^{-4}
323	4219	3.78×10^{-4}
333	3175	5.02×10^{-4}
343	2492	6.39×10^{-4}
353	1813	8.79×10^{-4}

Table S5 The resistance (R) and conductivity (σ) of **1** under different relative humidity (RH) and 298 K.

RH (%)	R (Ω)	σ (S/cm)
60	113081	1.41×10^{-5}
70	81584	1.96×10^{-5}
80	51121	3.12×10^{-5}
90	23661	6.73×10^{-5}
98	11066	1.44×10^{-4}