Supporting Information Available

Hydrogen-bonded Dicubane Co^{II}_7 Single-Molecule-Magnet Coordinated by In-situ Solvothermally Generated 1,2-bis(8-hydroxyquinolin-2-yl)ethane-1,2-diol) arranged in a Trefoil

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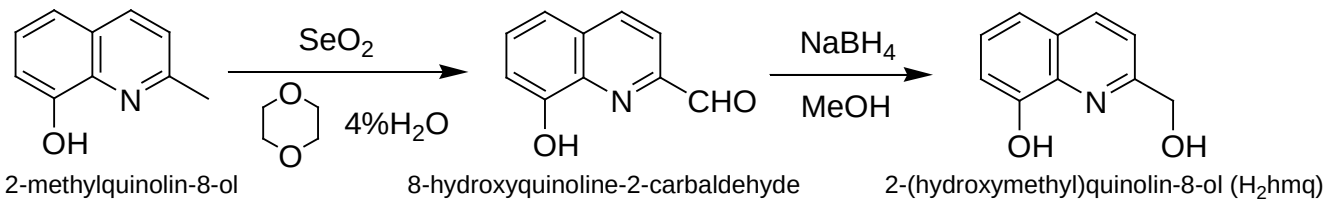
Synthesis of ligand: 2-(hydroxymethyl)-quinolin-8-ol (H_2hmq) was prepared according to literature procedure.[1] 2-methylquinolin-8-ol was first oxidized to the aldehyde by selenium dioxide in dioxane (yield 95%), followed by reduction with $NaBH_4$ in methanol to give 2-(hydroxymethyl)-quinolin-8-ol (H_2hmq) in 72% yield, M.p. 121.9-122.0 ^{o}C. The ligand was identified by ^{1}H and ^{13}C NMR spectra: ^{1}H NMR ($CDCl_3$, 500 MHz) δ(ppm): 8.09 (d, 1H, *J* = 8.49 Hz, *J* = 8.00 Hz, Ar-H), 7.46 (t, 1H, *J* = 7.93 Hz, *J* = 7.90 Hz, Ar-H), 7.33 (d, 1H, *J* = 7.19 Hz, Ar-H), 7.32(d, 1H, *J* = 6.63 Hz, Ar-H), 7.20 (d, 1H, *J* = 8.53 Hz, Ar-H), 4.89 (s, 2H, CH_2). ^{13}C NMR ($CDCl_3$, 125 MHz) δ(ppm): 157.5, 151.8, 136.9, 127.8, 127.3, 119.0, 117.9, 111.1, 64.7.



Scheme S1. Synthesis of ligand H_2hmq.

Synthesis of compound 1: A mixture of $Co(NO_3)_2 \cdot 6H_2O$ (1 mmol), H_2hmq (0.5 mmol), and triethylamine (0.25 mL) in 50% ethanol (10 mL) was sealed in a 15-mL Teflon-lined stainless steel bomb. The bomb was heated at 180 ^oC for 120 hours. After cooling to room temperature the red block crystals were separated from the liquor, washed with ethanol and dried in air (Yield of 17 % based on H_2hmq). Elemental analysis (%): found (calcd) for **1** ($Co_7C_{64}H_{64}O_{23}N_6$): C, 45.73 (45.28); H, 4.05 (3.80); N, 4.73 (4.95). Selected IR data (KBr pellet, cm^{-1}): 3407s, 1600*w*, 1565*m*, 1502*m*, 1454*s*, 1329*m*, 1272*m*, 1106*m*, 1052*m*, 898*w*, 764*m*, 494*w*.

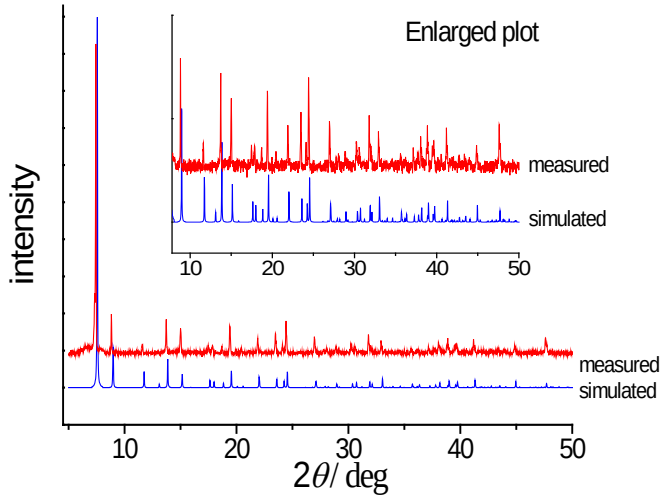


Figure. S1. Observed and simulated PXRD patterns of **1**.

Thermal Properties. The DT-TGA curves for **1** show several steps in the decomposition of the compound. The first weight loss below 120 °C, corresponding to the departure of ethanol guest molecules, is gradual and it is followed by a sharp one at 160 ^oC, corresponding to the removal of the

guest and coordinated water molecules to reach a mass percentage of 87% (calcd. 87.1%). The compound is then stable up to 330 °C where the hydroxide are removed and the pyrolysis of the organic ligand occurred leaving a mass percentage of 34.4%, which correspond to the formation of Co_2O_3 (calcd. 34.2%). The last step at 910 °C is the reduction of Co_2O_3 to CoO (remaining weight found, 31.2%; calcd. 30.9%).

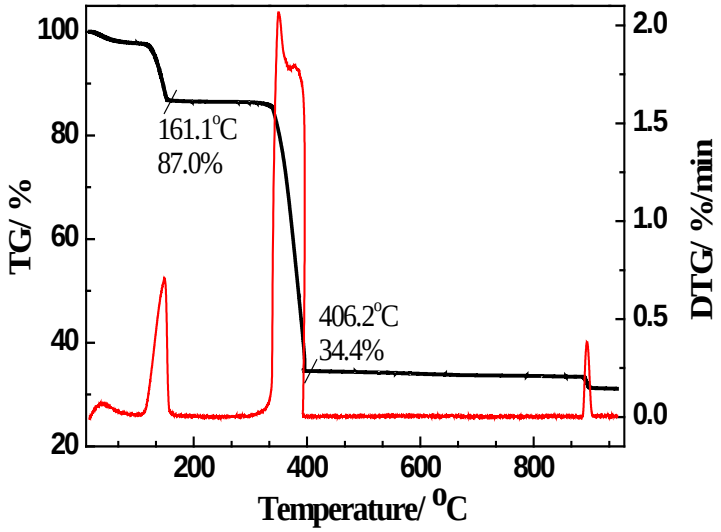


Figure S2. DT-TGA curves for **1** under N_2 atmosphere.

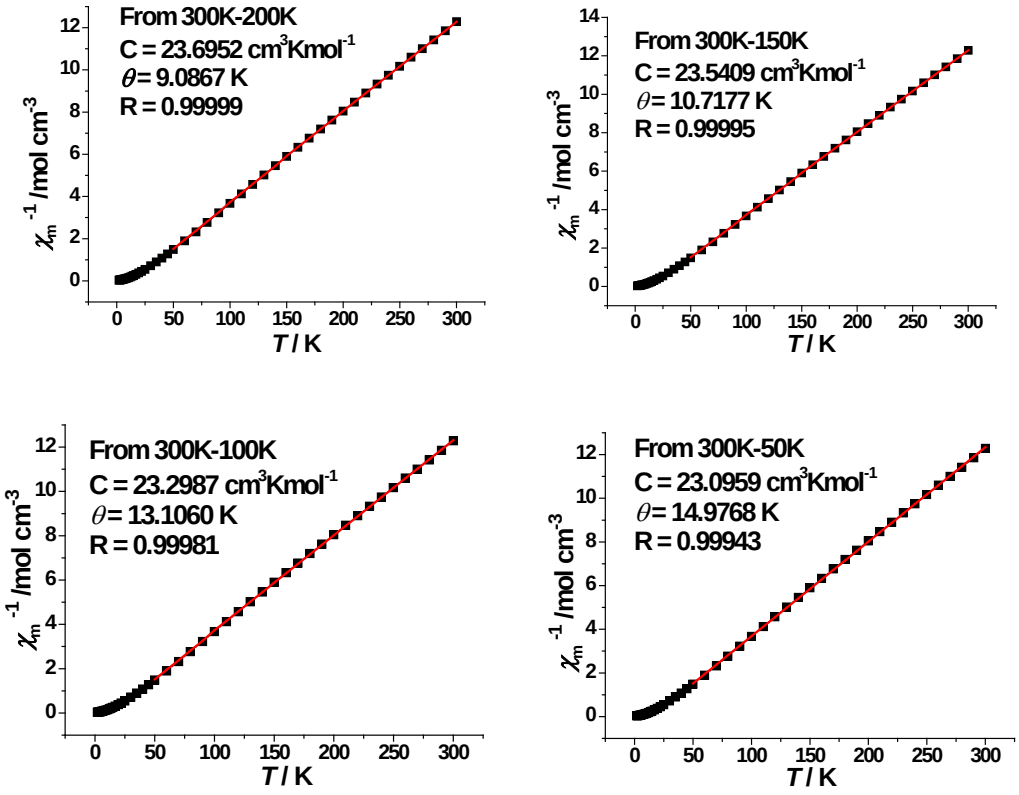


Figure S3. Plots of χ_m^{-1} and the Curie-Weiss fit (solid curve) give for different temperature ranges (50-300 K; 100-300 K; 150-300 K; 200-300 K).

References

(1) Yoneda, A.; Newkome, G. R.; Theriot, K. J. *J. Org. Chem*. **1991**. *401*. 217.

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