

Interweaving 3D Network with Double Helical tubes Filled by 1D

Coordination Polymer Chains

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Experimental Section

Mellitic acid (0.086g, 0.25mmol), 4,4'-bpy (0.080g, 0.50mmol) and $\text{Cu}(\text{CH}_3\text{COO})_2 \cdot \text{H}_2\text{O}$ (0.150g, 0.75mmol) in 15ml H_2O was heated at 145°C for 3 days in a Teflon-lined 23ml bomb, and blue crystals were obtained. (Anal. Calc. for $\text{C}_{32}\text{H}_{28}\text{Cu}_3\text{N}_4\text{O}_{18}$: C, 40.58; H, 2.98; N, 5.91. Found: C, 40.38; H, 2.58; N, 6.03). IR (KBr/pellet)/ cm^{-1} : 3434vs, 1634vs, 1613s, 1563ms, 1544sh, 1422vs, 1398sh, 1334ms, 1221w, 1080w, 1067w, 904m, 839m, 818s, 645s.

Crystal data were measured as follows: $\text{C}_{32}\text{H}_{28}\text{N}_4\text{O}_{18}\text{Cu}_3$, $M_r = 947.20$, blue crystal ($0.52 \times 0.32 \times 0.26\text{mm}$), Monoclinic, space group $P2_1/c$, $a = 10.173(4) \text{ \AA}$, $b = 11.1598(4) \text{ \AA}$, $c = 14.8557(5) \text{ \AA}$, $\beta = 107.0350(10)^\circ$, $V = 1613.07(10) \text{ \AA}^3$, $Z = 2$, $T = 293(2) \text{ K}$, $\rho_{\text{calcd}} = 1.950 \text{ g.cm}^{-3}$, $F(000) = 958$, $\mu = 2.057 \text{ mm}^{-1}$, $R1(wR2) = 0.0417(0.1071)$ and $S = 1.068$ for 2817 reflections with $F_o > 4\sigma(F_o)$.

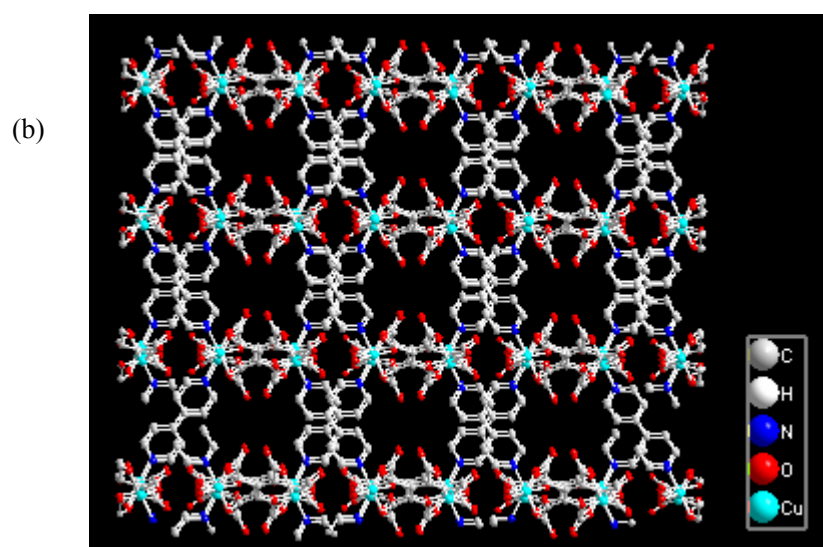
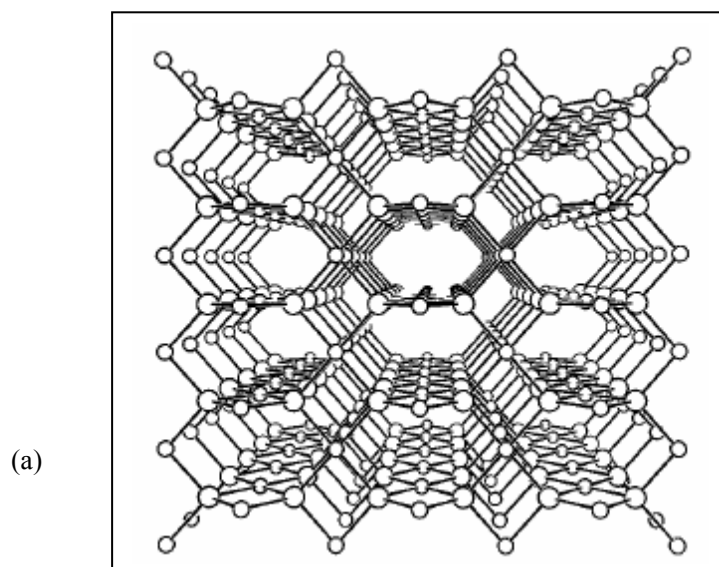


Figure S1. (a) The PtS-like net.; (b) Two interpenetrating PtS-like nets in the structure of host network, view along the [001] face.

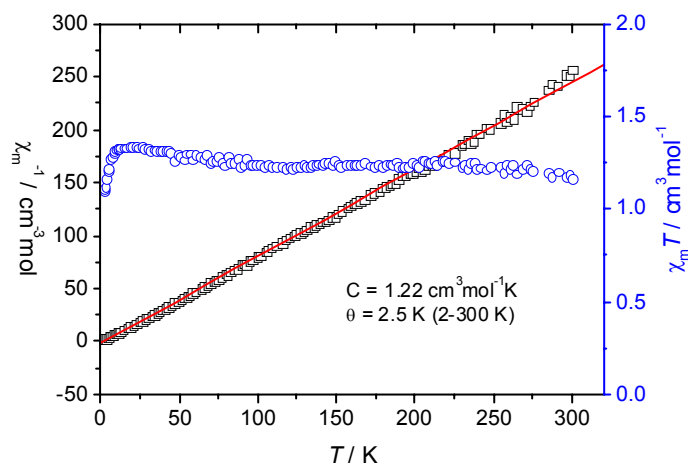


Figure S2. Experiment $\chi_M T$ versus T curves for the complex.

The temperature dependence of the magnetic susceptibility data obeys the Curie-Weiss law with $C = 1.22 \text{ cm}^3 \cdot \text{mol}^{-1} \cdot \text{K}$, and $\theta = 2.5 \text{ K}$, the C value is consistent with the expected value 1.125 for three spin-only Cu(II) ions, the small positive θ suggests a possible very weak ferromagnetic interactions between the Cu(II) ions (Figure S2).

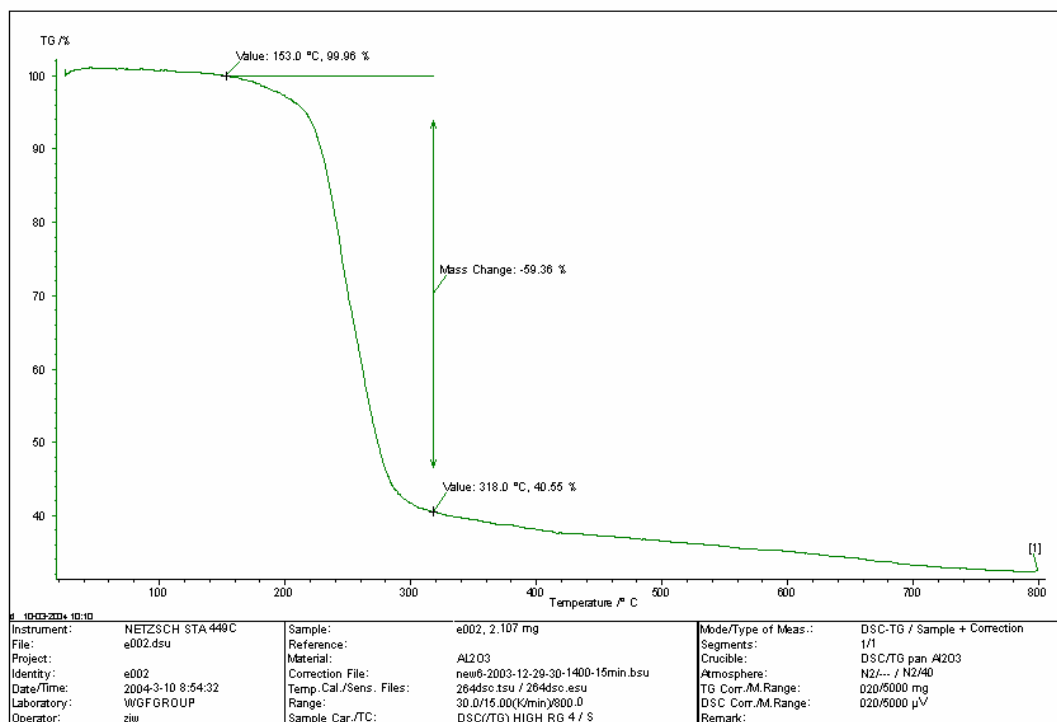


Figure S3. The thermogravimetric analysis (TGA) versus T curves for the complex.

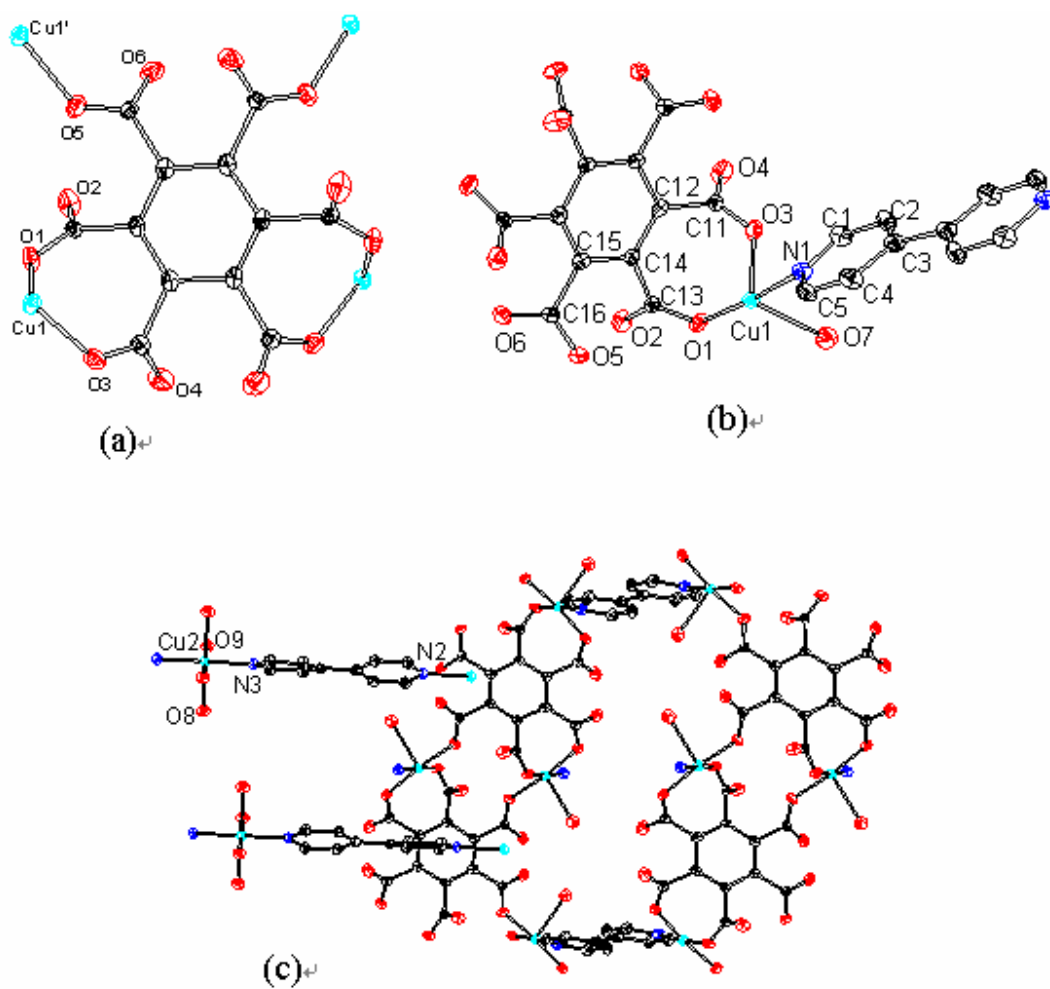


Figure S4. (a) The coordination of mellitate; (b) local coordination environment of Cu(II); (c) ORTEP representation of cell framework of the complex (only one host polymer is present), a view along the [100] direction, H atoms were omitted for clarity.

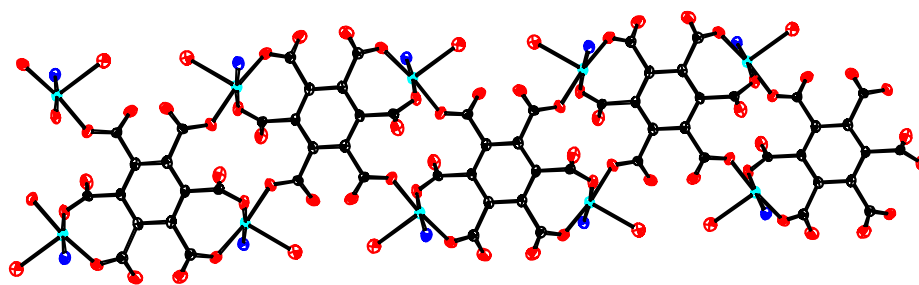


Figure S5. The mellitate zigzag chain, Cu=sky blue, O=red, N=deep blue.