

Supporting Information

A 3D Cu(II) Tetrazolate Coordination Polymer Based on Pentanuclear Units with Large Coercive Field

Table S1 Crystallographic data and structure refinement of (1)

Empirical formula	$C_6H_{21}Cu_{4.5}N_{12}O_{13.5}S$
Formula weight (g/mol)	794.75
Crystal system	Orthorhombic
Space group	<i>Pnma</i>
<i>a</i> (Å)	10.4983
<i>b</i> (Å)	30.2025
<i>c</i> (Å)	16.5890
α (°)	90
β (°)	90
γ (°)	90
<i>V</i> (Å ³)	5259.96
<i>Z</i>	4
ρ (g cm ⁻³)	1.976
<i>T</i> (K)	296(2)
μ (mm ⁻¹)	2.747
<i>F</i> (000)	3060
Reflections collected/unique	9507 / 1941
<i>R</i> (int)	0.00053(14)
Final <i>R</i> indices [<i>I</i> > 2 σ (<i>I</i>)]	<i>R</i> ₁ =0.0482, <i>wR</i> ₂ =0.1320

Table S2 Bond lengths(Å) and angles(°) of (**1**)

Cu(1)-O(7)#1	1.904(4)	Cu(1)-O(5)	1.986(4)
Cu(1)-N(1)	1.989(4)	Cu(1)-N(5)	2.082(4)
Cu(2)-O(5)	1.916(4)	Cu(2)-N(2)	1.981(4)
Cu(2)-O(6)	1.983(3)	Cu(2)-N(7)#2	2.001(5)
Cu(2)-O(1)	2.348(4)	Cu(3)-O(7)	1.917(4)
Cu(3)-N(6)#2	1.971(4)	Cu(3)-N(11)	1.986(4)
Cu(3)-O(6)	2.016(4)	Cu(3)-O(2)	2.283(4)
Cu(4)-O(8)	1.886(4)	Cu(4)-N(10)	1.974(4)
Cu(4)-O(6)	1.996(4)	Cu(4)-N(3)	1.999(4)
Cu(4)-O(3)	2.297(4)	Cu(5)-O(8)#3	1.913(4)
Cu(5)-O(8)	1.913(4)	Cu(5)-N(9)#3	2.020(5)
Cu(5)-N(9)	2.020(5)		
O(7)C-Cu(1)-O(5)	93.98(15)	O(7)#1-Cu(1)-N(1)	175.79(18)
O(5)-Cu(1)-N(1)	88.19(16)	O(7)#1-Cu(1)-N(5)	87.49(16)
O(5)-Cu(1)-N(5)	162.35(18)	N(1)-Cu(1)-N(5)	91.53(17)
O(5)-Cu(2)-N(2)	86.76(16)	O(5)-Cu(2)-O(6)	164.72(16)
N(2)-Cu(2)-O(6)	87.16(16)	O(5)-Cu(2)-N(7)#2	96.63(17)
N(2)-Cu(2)-N(7)#2	175.1(2)	O(6)-Cu(2)-N(7)#2	90.39(17)
O(5)-Cu(2)-O(1)	104.75(16)	N(2)-Cu(2)-O(1)	89.50(17)
O(6)-Cu(2)-O(1)	89.19(14)	N(7)#2-Cu(2)-O(1)	86.2(2)
O(7)-Cu(3)-N(6)#2	85.91(16)	O(7)-Cu(3)-N(11)	96.44(17)
N(6)#2-Cu(3)-N(11)	177.61(18)	O(7)-Cu(3)-O(6)	174.82(15)
N(6)#2-Cu(3)-O(6)	89.20(16)	N(11)-Cu(3)-O(6)	88.47(16)
O(7)-Cu(3)-O(2)	93.89(16)	N(6)#2-Cu(3)-O(2)	92.00(17)
N(11)-Cu(3)-O(2)	87.42(18)	O(6)-Cu(3)-O(2)	87.98(14)
O(8)-Cu(4)-N(10)	84.27(17)	O(8)-Cu(4)-O(6)	166.98(17)
N(10)-Cu(4)-O(6)	87.15(16)	O(8)-Cu(4)-N(3)	97.98(17)
N(10)-Cu(4)-N(3)	173.79(19)	O(6)-Cu(4)-N(3)	89.60(16)
O(8)-Cu(4)-O(3)	99.16(18)	N(10)-Cu(4)-O(3)	99.05(18)
O(6)-Cu(4)-O(3)	91.84(15)	N(3)-Cu(4)-O(3)	86.34(18)
O(8)C-Cu(5)-O(8)	92.3(2)	O(8)#3-Cu(5)-N(9)#3	86.62(17)
O(8)-Cu(5)-N(9)#3	173.6(2)	O(8)#3-Cu(5)-N(9)	173.6(2)
O(8)-Cu(5)-N(9)	86.62(17)	N(9)#3-Cu(5)-N(9)	93.7(3)

对称操作: #1 -x+3/2, -y+1, z-1/2; #2 -x+3/2, -y+1, z+1/2; #3 x, -y+1/2, z

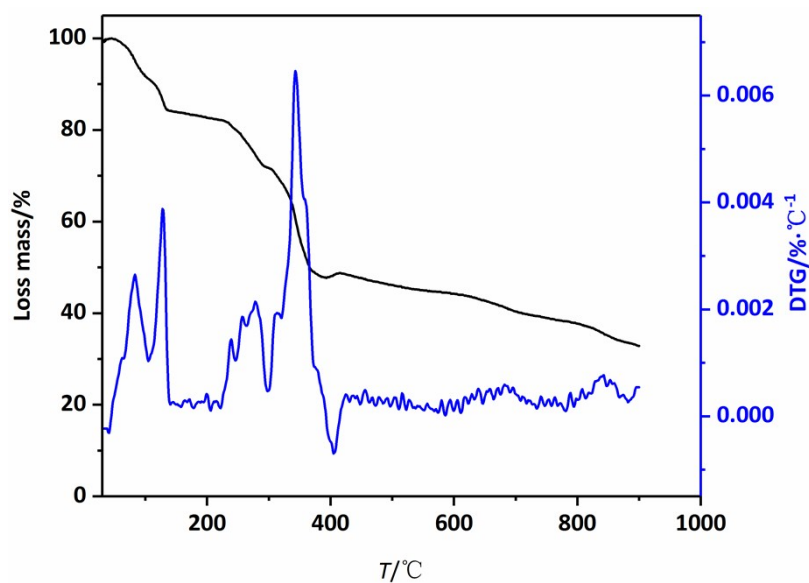


Fig. S1 TG and DTG profiles.

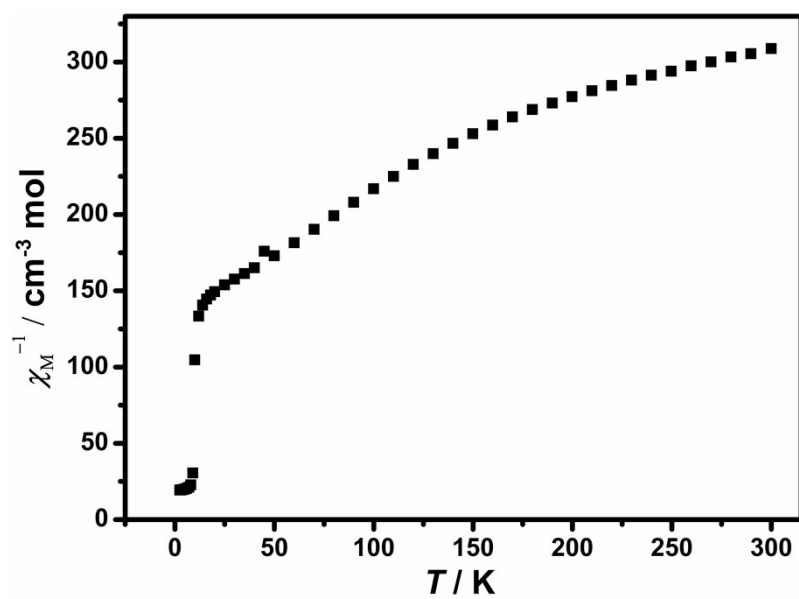


Fig.S2 Plot of χ_M^{-1} vs. T for (1) under 1000 Oe dc field.