Homochiral Cu(I) coordination polymer based on achiral precursors and its photocatalytic property

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Table 1. Crystal data and structural refinement for compound **1**

Compound	**1**
Formula	$C_{73}H_{50}N_{31}OCu_7$
Formula weight	1822.22
Crystal system	*C2*
Space group	Monoclinic
a (Å)	18.775(3)
b (Å)	15.626(3)
c (Å)	12.872(2)
α (º)	90
β (º)	99.973(2)
γ (º)	90
V (Å^3)	3719.2(12)
Z	2
D_c (g/cm^{-3})	1.627
F(000)	1832
μ (mm^{-1})	2.031
θ for data collection (º)	1.71 to 25.00
Reflections collected	9690
Unique reflections	6106
R_{int}	0.0498
Data/restraints/parameters	6106 / 1 / 506
Goodness-of-fit on F^2	0.968
R_1, wR_2 [I >2σ(I)]	0.0562, 0.1013
R_1, wR_2 (all data)	0.1017, 0.1158

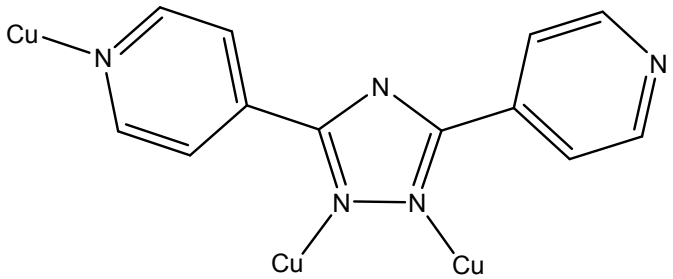
$R_1 = \sum(|F_o| - |F_c|) / \sum|F_o|$, $wR_2 = [\sum w(F_o^2 - F_c^2)^2/\sum w(F_o^2)^2]^{1/2}$.

Table 2. Selected bond distances (Å) and angles (º) for compound **1**

Compound **1**					
Cu(1)-N(9)	1.929(7)	N(9)-Cu(1)-N(13)	124.1(3)	C(37)-Cu(2)-N(15)	111.4(3)
Cu(1)-N(13)	1.941(7)	N(9)-Cu(1)-N(3)	119.2(3)	N(6)#1-Cu(2)-N(15)	102.7(3)
Cu(1)-N(3)	1.966(7)	N(13)-Cu(1)-N(3)	116.7(3)	C(37)-Cu(2)-N(1)#2	113.9(3)
Cu(2)-C(37)	1.865(6)	N(9)-Cu(1)-Cu(3)	63.70(19)	N(6)#1-Cu(2)-N(1)#2	104.1(3)

Cu(2)-N(6)#1	2.029(7)	N(13)-Cu(1)-Cu(3)	137.2(2)	N(15)-Cu(2)-N(1)#2	101.8(3)
Cu(2)-N(15)	2.079(7)	N(3)-Cu(1)-Cu(3)	72.49(19)	N(2)#3-Cu(3)-N(8)	176.1(3)
Cu(2)-N(1)#2	2.095(8)	C(37)-Cu(2)-N(6)#1	120.9(3)	N(14)-Cu(4)-N(14)#3	163.0(4)
Cu(3)-N(2)#3	1.870(7)	Cu(4)-N(14)#3	1.916(7)	N(14)-Cu(4)-O(1)	98.5(2)
Cu(3)-N(8)	1.871(7)	Cu(4)-O(1)	2.440(10)	N(14)#3-Cu(4)-O(1)	98.5(2)
Cu(4)-N(14)	1.916(7)				

Symmetry transformations used to generate equivalent atoms: #1 x+1/2, y-1/2, z+1, #2 x, y-1, z, #3 -x, y, -z+2, #4 x, y+1, z, #5 x-1/2, y+1/2, z-1, #6 -x, y, -z+3 for **1**.



Scheme 1. Coordination mode of the 4-bpt Ligand in complex **1**.

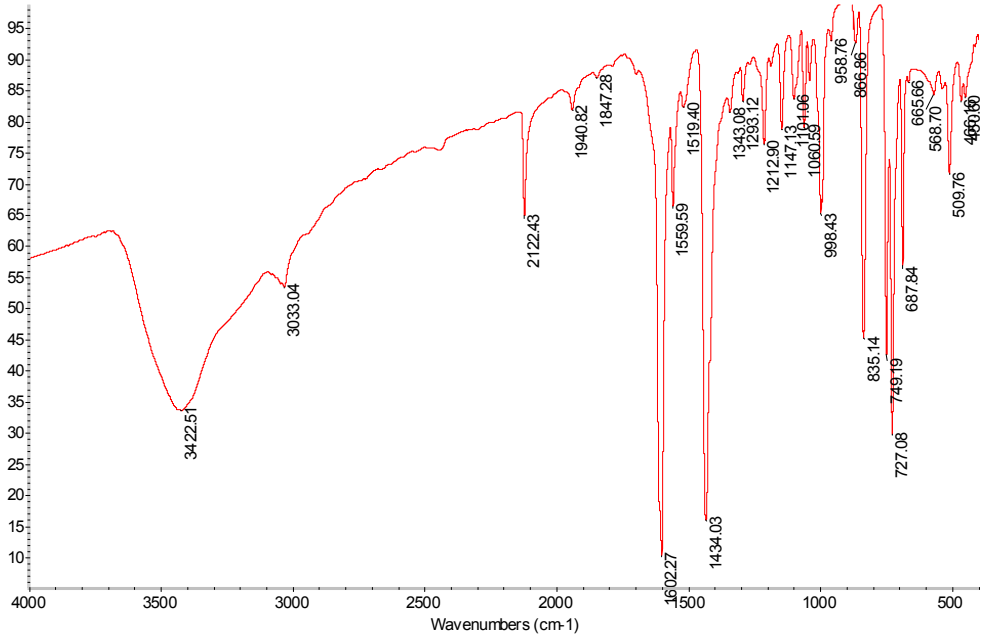


Fig. S1. IR of Complex **1**.

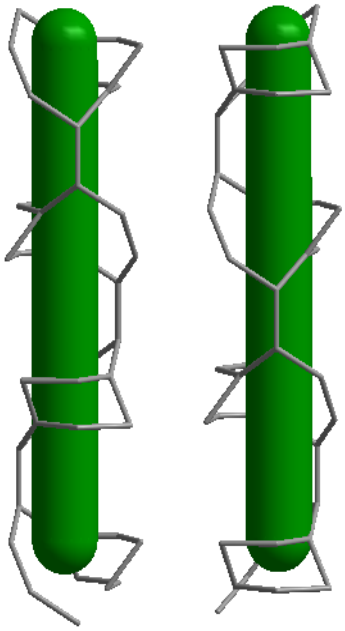


Fig. S2. The right-handed helice along the b-axis in Complex **1**.

Table S1 A summary of the 10 structure determinations of **1** with the R factors and Flack absolute structure parameters for each refinement.

序号	空间群	a	b	c	β	R_1	wR_2	Flack
1	C2	18.775(3)	15.626(3)	12.872(2)	99.973(2)	0.0562	0.1013	0.04(2)
2	C2	18.706(7)	15.538(6)	12.906(5)	99.729(5)	0.0306	0.0819	-0.016(10)
3	C2	18.766(13)	15.574(11)	12.948(9)	99.631(8)	0.0576	0.1546	0.03(2)
4	C2	18.888(13)	15.727(11)	13.003(8)	99.740(7)	0.0943	0.2343	0.02(3)
5	C2	18.756(18)	18.756(18)	12.900(12)	99.499(12)	0.0353	0.0924	0.006(13)
6	C2	18.787(13)	15.638(11)	12.919(9)	99.735(10)	0.0978	0.2466	0.05(4)
7	C2	18.715(4)	15.545(3)	12.899(3)	99.655(2)	0.0473	0.1324	0.01(2)
8	C2	18.714(18)	15.550(15)	12.943(13)	99.911(12)	0.0581	0.1560	0.06(2)
9	C2	18.714(8)	15.560(6)	12.909(5)	99.673(5)	0.0319	0.0835	0.001(11)
10	C2	18.781(12)	15.659(19)	12.943(16)	99.803(13)	0.0892	0.2583	0.80(4)

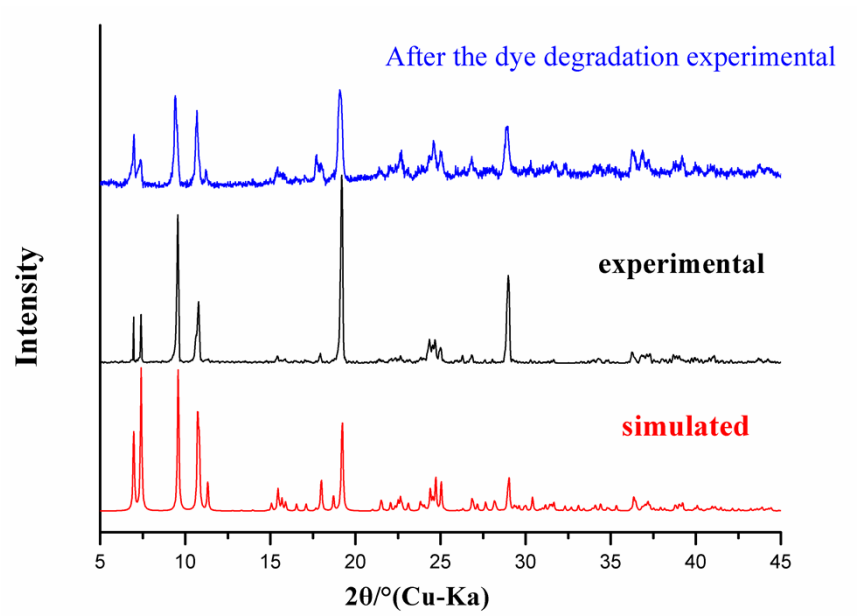


Fig. S3. XPRD patterns for **1** (top, blue) after the dye degradation experimental; (middle, black) experimental at room temperature; (bottom, red) calculated on the basis of the structure determined by single-crystal X-ray diffraction.

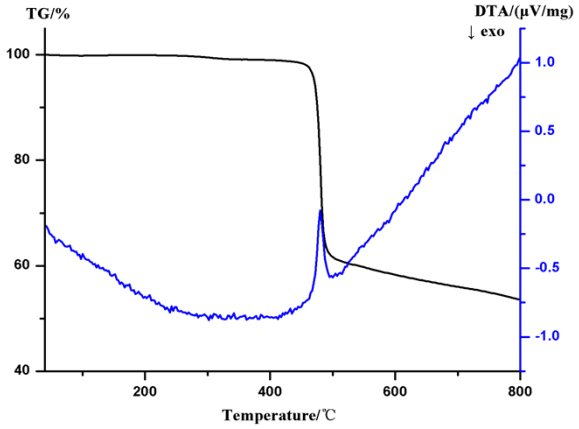


Fig. S4. The TGA diagram of **1**.

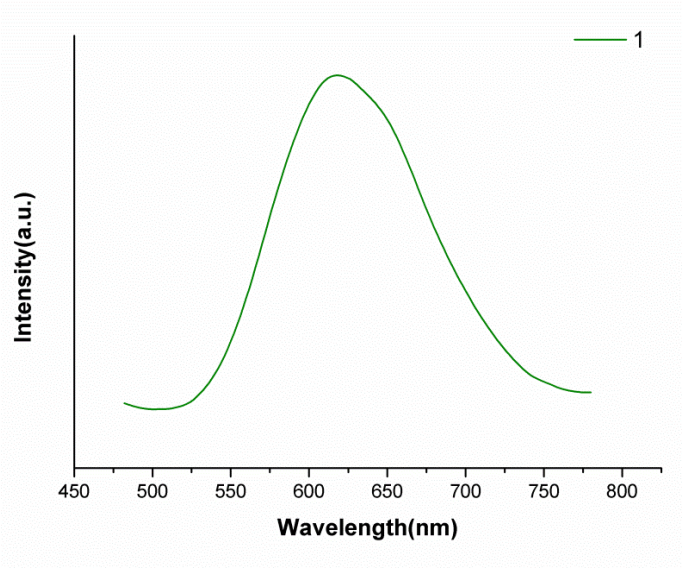


Fig. S5. Solid-state emission spectra of complex **1** (excitation at 370nm).

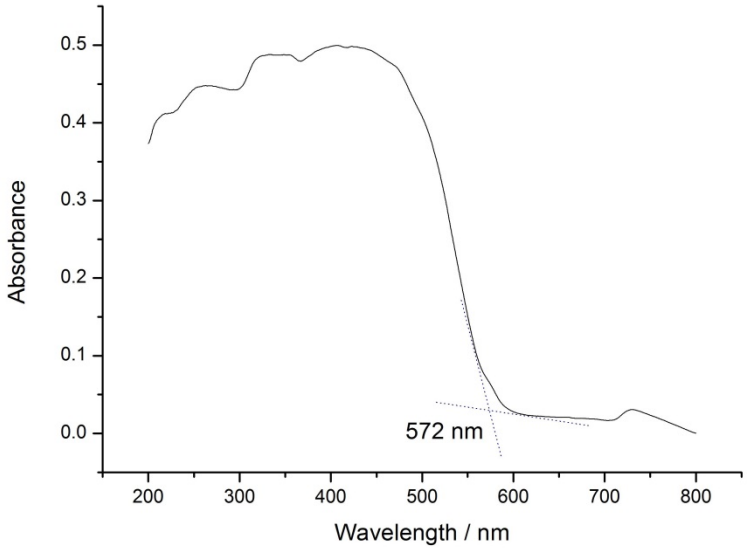


Fig. S6. UV-Vis spectrum of complex **1** in solid state.