Electronic Supplementary Information (ESI)

A (3, 14)-connected three-dimensional metal-organic framework based on the unprecedented enneanuclear copper(II) cluster [$Cu_9(\mu_3\text{-}OH)_4(\mu_2\text{-}OH)_2$]

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Determination of the antibacterial activity

The mixed-germs-plate method was used to determine the antibacterial activity of the antibacterial substances using the Oxford plate assay system. The staphylococcus aureus and Escherichia coli strains was used as the indicating microorganisms with the concentration controlled at $2\text{-}5\times10^4$CFU/mL in the medium. Up to 250μL substance was then injected onto the Oxford cup, and the diameters of the inhibition zones were measured after being incubated at 37 °C overnight.

Table S1 Selected bond lengths [Å] and angles [°] for **1.**

Cu(1)-O(1)	2.041(5)	Cu(1)-O(1A)	2.041(5)
Cu(1)-O(15)	1.904(5)	Cu(1)-O(15A)	1.904(5)
Cu(2)-O(2)	1.968(5)	Cu(2)-O(15)	1.930(5)
Cu(2)-O(8B)	1.962(4)	Cu(2)-O(16)	1.983(5)
Cu(2)-O(12)	2.269(5)	Cu(3)-O(5E)	2.498(7)
Cu(3)-O(11C)	1.943(5)	Cu(3)-O(16)	1.981(5)
Cu(3)-O(17)	1.993(4)	Cu(3)-N(6D)	1.996(6)
Cu(4)-O(12)	2.432(5)	Cu(4)-O(17)	1.977(5)
Cu(4)-N(3)	1.978(6)	Cu(4)-O(3F)	1.921(5)
Cu(4)-O(16)	1.955(5)	Cu(5)-O(4F)	1.965(7)
Cu(5)-O(10C)	1.921(5)	Cu(5)-O(17)	1.957(5)
Cu(5)-O(18)	1.997(11)	Cu(5)-O(19)	2.226(13)
Cu(5)-O(20)	2.08(2)	Cu(5)-O(21)	2.15(2)
Cu(1)-Cu(2)	2.9793(3)	Cu(2)···Cu(3)	3.3313(3)
Cu(2)···Cu(4)	3.1987(3)	Cu(3)···Cu(4)	2.9019(3)
Cu(3)···Cu(5)	3.4256(3)	Cu(4)···Cu(5)	3.2967(4)
Cu(1)-O(15)-Cu(2)	101.993(7)	Cu(2)-O(16)-Cu(3)	114.368(5)
Cu(3)-O(16)-Cu(4)	95.016(7)	Cu(2)-O(16)-Cu(4)	108.659(7)
Cu(3)-O(17)-Cu(4)	93.926(7)	Cu(3)-O(17)-Cu(5)	120.254(7)
Cu(4)-O(17)-Cu(5)	113.877(5)		
O(1A)-Cu(1)-O(1)	180.000(1)	O(15A)-Cu(1)-O(15)	180.000(1)
O(15)-Cu(1)-O(1)	90.30(19)	O(15A)-Cu(1)-O(1)	89.70(19)
O(15)-Cu(1)-O(1A)	89.70(19)	O(15A)-Cu(1)-O(1A)	90.30(19)
O(15)-Cu(2)-O(2)	90.5(2)	O(8B)-Cu(2)-O(2)	170.2(2)
O(2)-Cu(2)-O(16)	85.0(2)	O(15)-Cu(2)-O(8B)	92.1(2)
O(15)-Cu(2)-O(16)	170.7(2)	O(8B)-Cu(2)-O(16)	91.0(2)
O(2)-Cu(2)-O(12)	93.95(19)	O(15)-Cu(2)-O(12)	104.5(2)
O(8B)-Cu(2)-O(12)	94.51(18)	O(16)-Cu(2)-O(12)	83.94(19)
O(17)-Cu(3)-O(5E)	75.8(2)	O(17)-Cu(3)-N(6D)	174.7(2)
N(6D)-Cu(3)-O(5E)	107.1(3)	O(16)-Cu(3)-O(17)	81.70(19)
O(16)-Cu(3)-O(5E)	79.27(19)	O(16)-Cu(3)-N(6D)	94.4(2)
O(11C)-Cu(3)-O(17)	97.0(2)	O(11C)-Cu(3)-O(5E)	101.2(2)
O(11C)-Cu(3)-N(6D)	86.9(2)	O(11C)-Cu(3)-O(16)	178.4(2)
O(3F)-Cu(4)-O(16)	172.7(3)	O(3F)-Cu(4)-O(17)	97.5(2)
O(3F)-Cu(4)-N(3)	83.2(3)	O(16)-Cu(4)-O(17)	82.80(19)
O(17)-Cu(4)-N(3)	164.7(3)	O(16)-Cu(4)-N(3)	98.5(2)
O(3F)-Cu(4)-O(12)	92.5(2)	O(16)-Cu(4)-O(12)	80.28(18)
O(17)-Cu(4)-O(12)	87.31(18)	N(3)-Cu(4)-O(12)	108.0(2)
O(10C)-Cu(5)-O(17)	95.2(2)	O(10C)-Cu(5)-O(4F)	167.5(2)
O(17)-Cu(5)-O(4F)	97.0(2)	O(10C)-Cu(5)-O(18)	79.3(4)
O(17)-Cu(5)-O(18)	157.1(4)	O(4F)-Cu(5)-O(18)	90.2(4)
O(10C)-Cu(5)-O(20)	89.7(6)	O(17)-Cu(5)-O(20)	157.7(6)
O(4F)-Cu(5)-O(20)	78.1(6)	O(18)-Cu(5)-O(20)	45.2(6)

O(10C)-Cu(5)-O(21)	107.9(6)	O(17)-Cu(5)-O(21)	106.0(6)
O(4F)-Cu(5)-O(21)	70.9(7)	O(18)-Cu(5)-O(21)	56.1(6)
O(20)-Cu(5)-O(21)	93.1(8)	O(10C)-Cu(5)-O(19)	84.2(4)
O(17)-Cu(5)-O(19)	92.9(4)	O(4F)-Cu(5)-O(19)	92.8(5)
O(18)-Cu(5)-O(19)	108.4(5)	O(20)-Cu(5)-O(19)	65.9(6)
O(21)-Cu(5)-O(19)	156.1(7)		

Symmetry transformations used to generate equivalent atoms: A -x+1, -y+1, -z+1; B -x, -y+1, -z+1; C x+1/2, -y+3/2, z-1/2; D x+1, y, z; E x-1/2, -y+3/2, z-1/2; F x-1, y, z.

Table S2 Hydrogen bondings for **1** (Å and °).

D-H···A	d(D-H)	d(H···A)	D(D···A)	<(DHA)
O(15)-H(1W)···N(2)^{i}	0.89(2)	2.35(6)	3.068(9)	138(7)
O(16)-H(2W)···O(23)	0.89(2)	1.85(2)	2.698(10)	158(4)
O(17)-H(3W)···O(14)	0.89(2)	2.04(4)	2.890(9)	158(8)
O(22)-H(4W)···O(15)^{ii}	0.89(2)	1.94(4)	2.778(9)	156(6)
O(22)-H(5W)···O(9)^{i}	0.90(2)	1.97(4)	2.831(8)	159(6)
O(23)-H(6W)···O(7)^{iii}	0.90(2)	1.91(3)	2.806(11)	174(8)
O(23)-H(7W)···O(25)^{iv}	0.90(2)	2.04(3)	2.892(19)	157(6)

Symmetry transformations used to generate equivalent atoms: i -x, -y+1, -z+1; ii -x+1, -y+1, -z+1; iii x-1/2, -y+3/2, z-1/2; iv -x+1/2, y-1/2, -z+1/2.

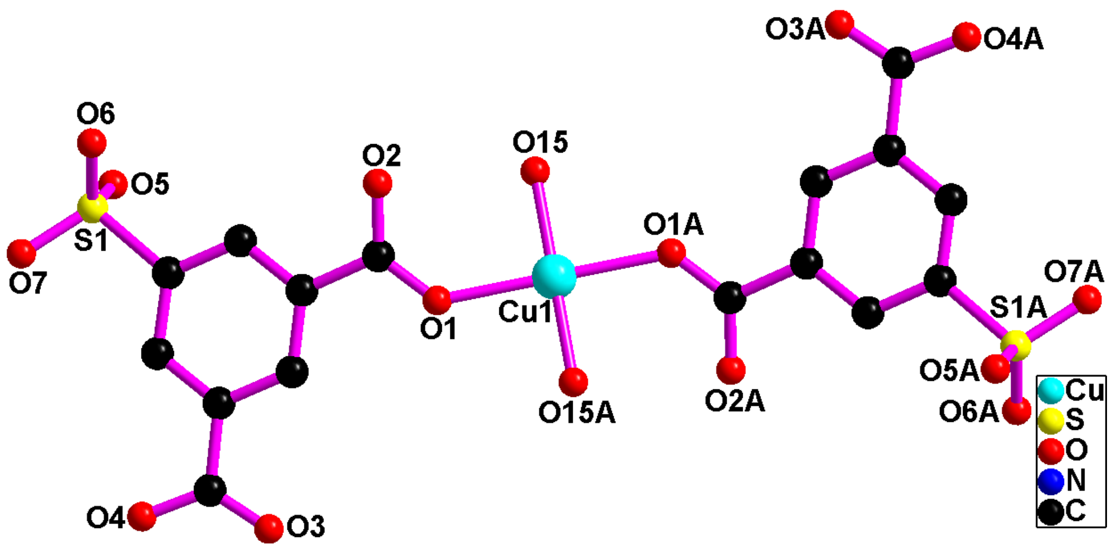

Fig. S1 The coordination environment of Cu1 atom in **1**.

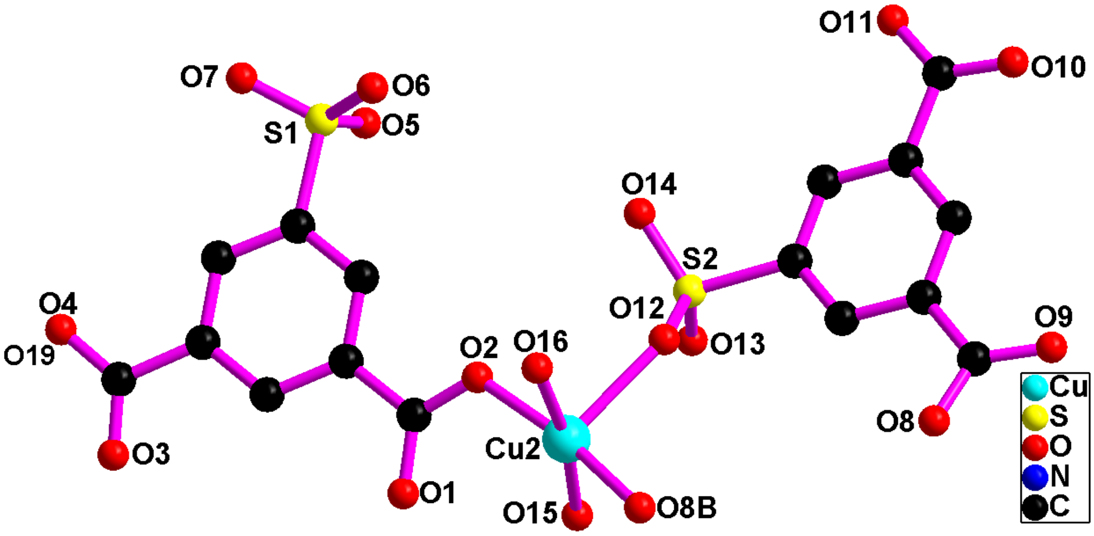

Fig. S2 The coordination environment of Cu2 atom in **1**.

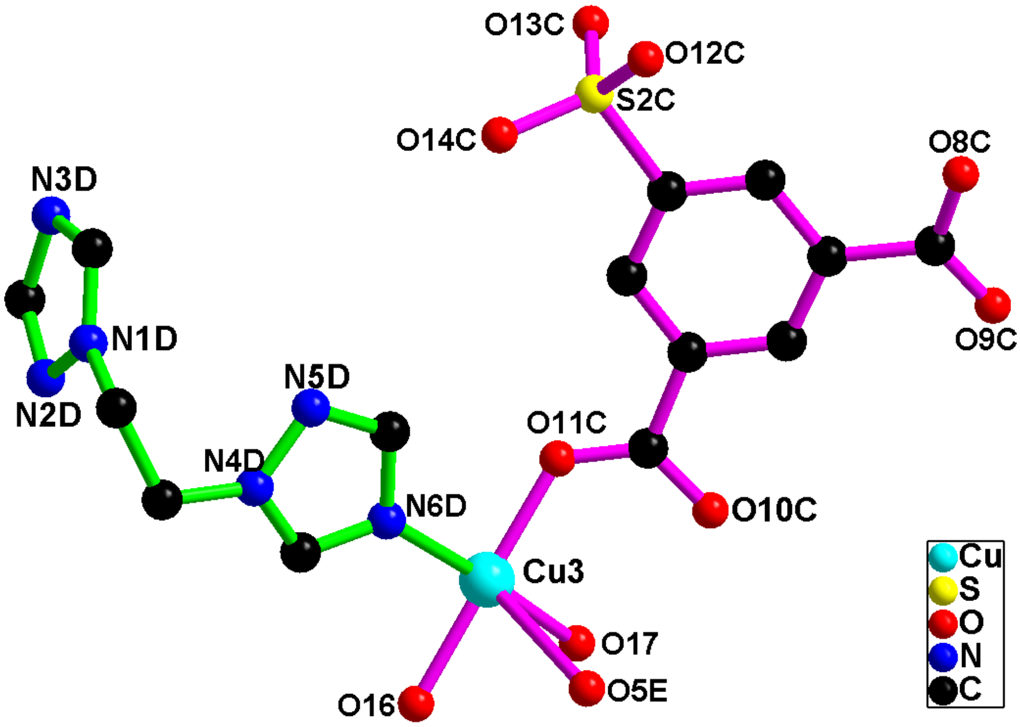

Fig. S3 The coordination environment of Cu3 atom in **1**.

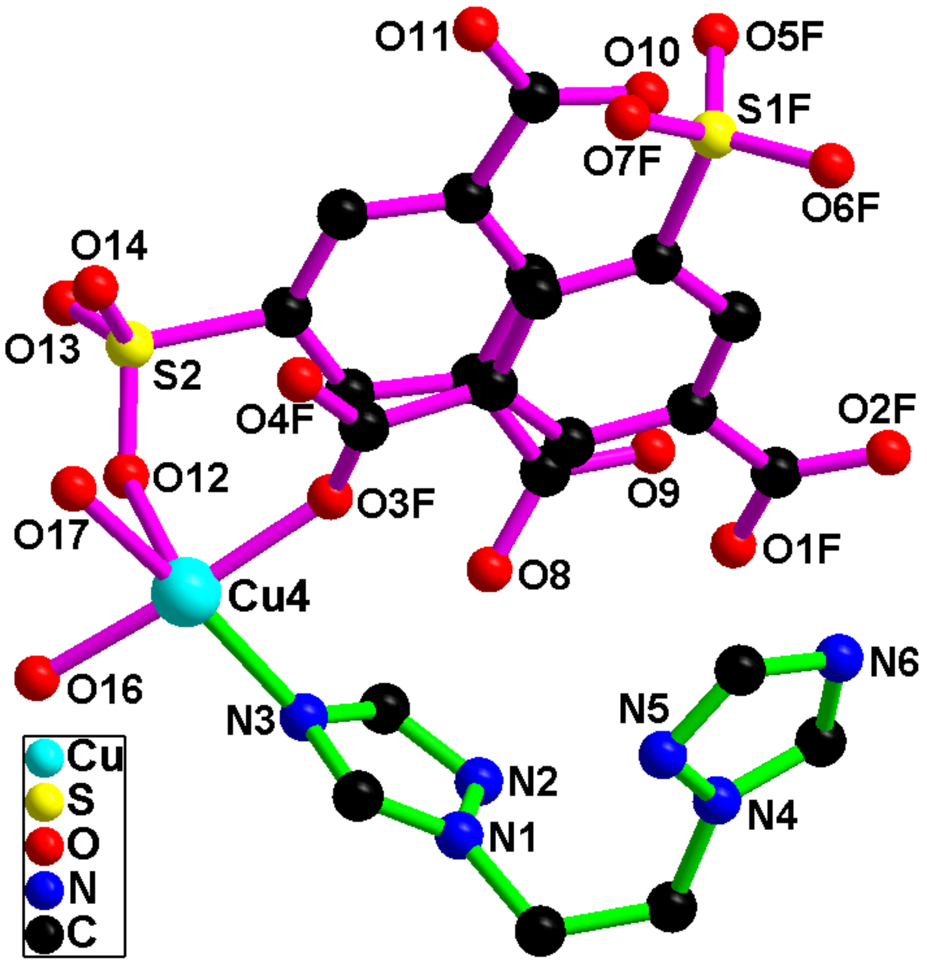

Fig. S4 The coordination environment of Cu4 atom in **1**.

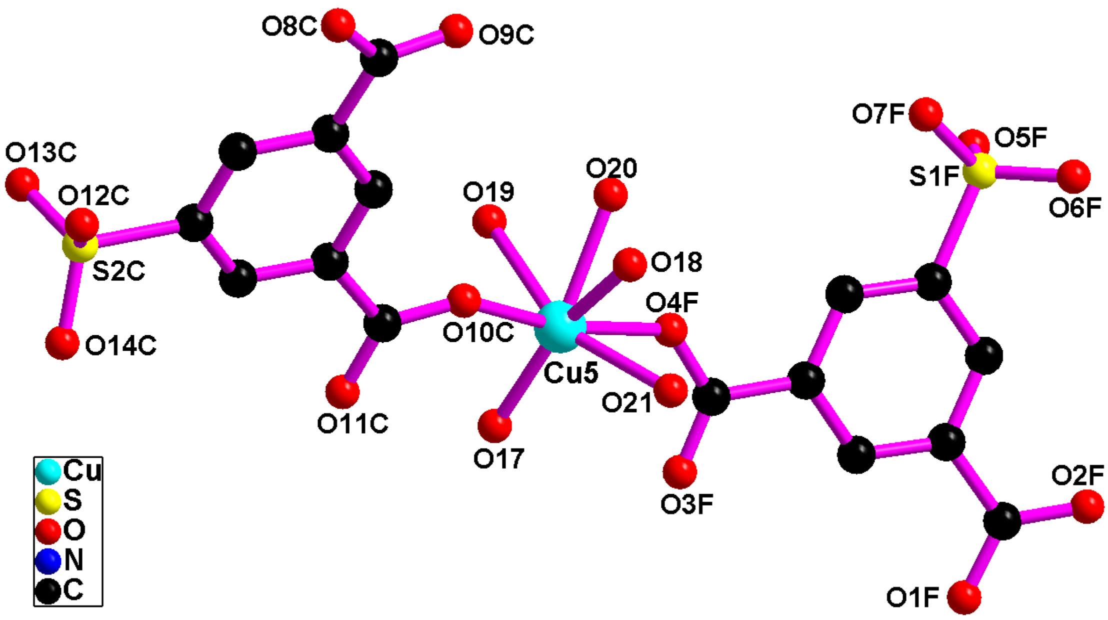

Fig. S5 The coordination environment of Cu5 atom in **1**.

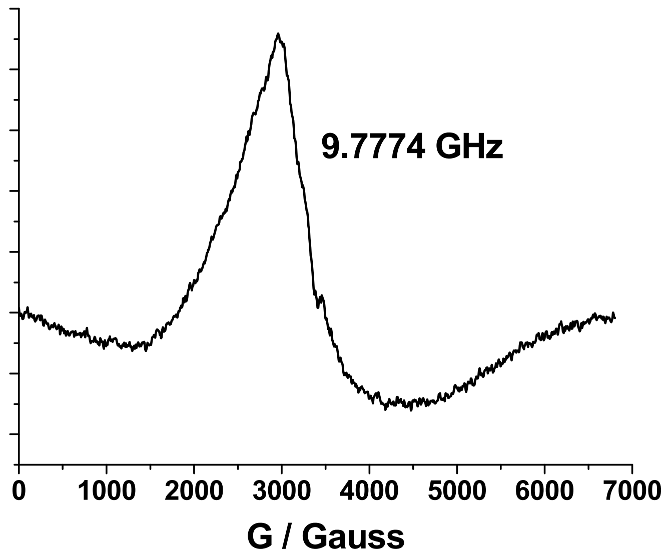

Fig. S6 X-band EPR spectra for compound **1** at room temperature.

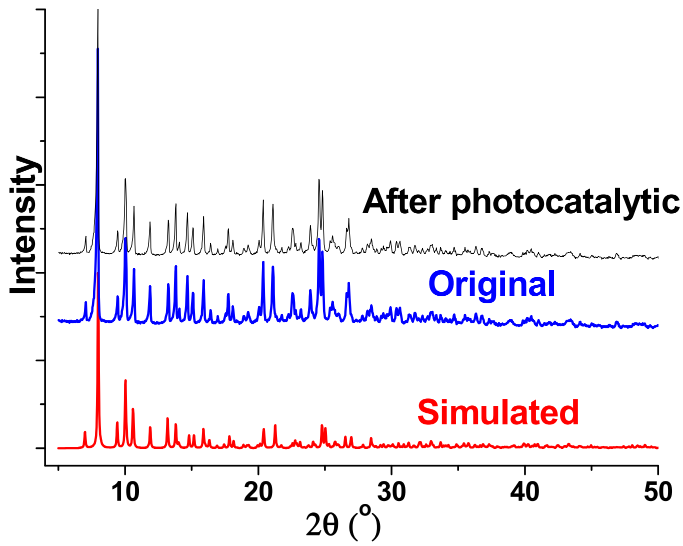

Fig. S7 Powder XRD patterns of the simulated diagram from single crystal data of compound **1** (red), **1** (blue) and **1** after a photocatalysis process (black).