

SUPPLEMENTARY MATERIAL

Hydrogen Bonding in the crystal lattice of $[\text{Cu}_2(\text{diep})(\text{H}_2\text{O})_4](\text{ClO}_4)_4 \cdot 2\text{H}_2\text{O}$

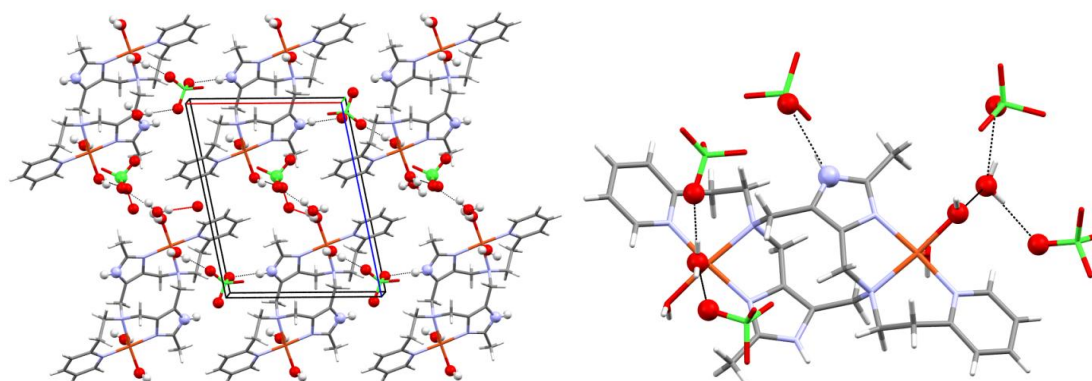


Figure S1 Hydrogen bonding for $[\text{Cu}_2(\text{diep})(\text{H}_2\text{O})_4](\text{ClO}_4)_4 \cdot 2\text{H}_2\text{O}$

Table S1. Hydrogen bonds for cu2diep [\AA and $^\circ$].

D-H...A	d(D-H)	d(H...A)	d(D...A)	$\angle(\text{DHA})$
N(4)-H(4N)...O(3)#2	0.88(6)	2.10(6)	2.973(4)	168(6)
O(3W)-H(3E)...O(6)#2	0.87(2)	2.09(4)	2.905(5)	156(7)
O(3W)-H(3E)...O(6)#2	0.87(2)	2.09(4)	2.905(5)	156(7)
O(1W)-H(1E)...O(3W)#3	0.85(2)	1.87(3)	2.678(5)	160(7)
O(2W)-H(2D)...O(4)#4	0.84(2)	1.93(2)	2.765(4)	176(7)
O(2W)-H(2E)...O(7)#5	0.85(2)	2.08(3)	2.911(5)	165(7)
O(3W)-H(3D)...O(1)#6	0.86(7)	2.14(7)	2.997(5)	174(7)

Symmetry transformations used to generate equivalent atoms:

#2 x, y, z #3 $-x+1, -y+1, -z+1$ #4 $x+1, y, z$ #5 $-x+1, y+1/2, -z+1/2$ #6 $-x, y-1/2, -z+1/2$

Fluorimetric detection of H₂O₂

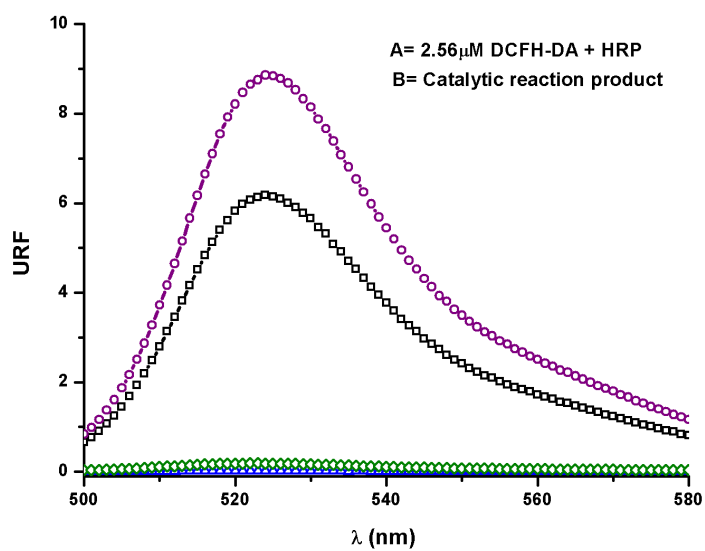


Figure S2 Fluorimetric detection of H₂O₂ (□) A+ 0.5 μM H₂O₂ (control), (○) A + 40 μL B, (◇) DCFH-DA + 40 μL B, (△) DCFH-DA + 0.2 μM Cu₂L.

EPR detection of radical intermediates DTBSQ and $O_2^{\cdot -}$

Solution 1: 5 mM solution of Cu_2diep in a 1:1 MeOH:H₂O at 298 K.

Solution 2: 5 mM solution of Cu_2diep in a 1:1 MeOH:H₂O mixture in the presence of one stoichiometric equivalent of substrate DTBC was obtained in the absence of O_2 at 298 K.

Solution 3: (Solution 2) + 6 equivalents of aqueous spin trap DMPO, after bubbling O_2 for 5 minutes.

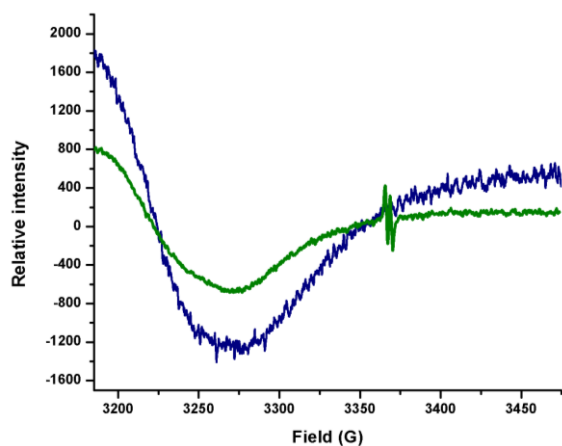


Figure S3. Blue: EPR of solution 1. Green EPR spectrum of solution 2

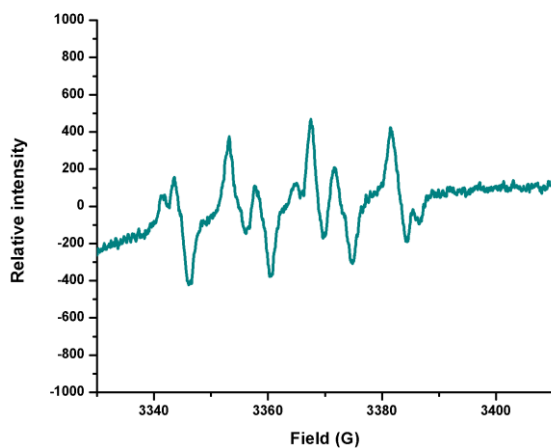


Figure S4. EPR spectrum of solution 3.