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Supporting Information

Two low-dimensional Schiff base copper(I/II) complexes: syntheses, characterization and catalytic activity for degradation of organic dyes

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Content

*Table **S1** Crystal data and structure refinement of three compounds **1**, **2** and **3**.*

	1	**2**	**3**
Chemical formula	$C_{40}H_{48}Cu_4I_4N_{16}O_{10}$	$C_{88}H_{108}Cu_{10}I_{10}N_{36}O_{17}$	$C_{42}H_{47}Cu_6I_6N_{17}O_8$
M	1674.70	3846.50	2060.61
Crystal system	Tetragonal	Triclinic	Monoclinic
Space group	*I*4(1)/*a*	*P*-1	*P*2(1)/*n*
a /Å	22.267(3)	11.541(3)	16.408(5)
b /Å	22.267(3)	13.901(3)	23.207(7)
c /Å	23.162(3)	20.769(4)	16.670(5)
α/°	90	91.178(3)	90
β/°	90	90.148(3)	98.473(5)
γ/°	90	107.497(3)	90
V/Å^3	11485(2)	3177.2(11)	6278(3)
Z	8	1	4
T /*K*	298(2)	298(2)	298(2)
F(000)	6464	1844	3896
D_{calcd} / gcm^{-3}	1.937	2.010	2.180
μ /mm^{-1}	3.676	4.137	5.006
λ /Å	0.71073	0.71073	0.71073
R_{int}	0.0716	0.0352	0.0806
data/restraint/parm	5220 / 6 / 361	11324 / 0 / 742	11355 / 2 / 725
GOF	1.012	0.989	1.002
R_1 [$I = 2\sigma(I)$][a]	0.0591	0.0655	0.0589
wR_2 [$I = 2\sigma(I)$][b]	0.1323	0.1614	0.1398
R_1 [all data][a]	0.0993	0.1080	0.0958
wR_2 [all data][b]	0.1712	0.1863	0.1799
Largest diff. peak and hole(e·Å^{-3})	1.170 and -0.897	0.814 and -0.759	1.114 and -1.224

[a] $R_1 = \Sigma||F_o| - |F_c||/|F_o|$, [b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$, where $w = 1/[\sigma^2(F_o^2) + (aP)_2 + bP]$. $P = (F_o^2 + 2F_c^2)/3$.

Table S2. Selected atomic distances (Å) and bond angles (°) for compounds **1**, **2** and **3**.

1			
Cu(1)-N(2)	1.926(3)	O(1)#1-Cu(1)-I(1)	160.53(7)
Cu(1)-N(4)#1	2.001(3)	N(6)-Cu(2)-O(3)	79.14(15)
Cu(1)-O(1)	2.013(3)	N(6)-Cu(2)-N(8)#2	178.31(18)
Cu(1)-N(1)	2.027(4)	O(3)-Cu(2)-N(8)#2	99.26(15)
Cu(1)-O(1)#1	2.326(3)	N(6)-Cu(2)-N(5)	80.78(17)
Cu(1)-I(1)	3.0807(8)	O(3)-Cu(2)-N(5)	159.68(15)
Cu(2)-N(6)	1.916(4)	N(8)#2-Cu(2)-N(5)	100.79(17)
Cu(2)-O(3)	2.001(3)	N(6)-Cu(2)-O(3)#2	105.34(15)
Cu(2)-N(8)#2	2.003(4)	O(3)-Cu(2)-O(3)#2	91.84(17)
Cu(2)-N(5)	2.022(4)	N(8)#2-Cu(2)-O(3)#2	74.09(14)
Cu(2)-O(3)#2	2.338(3)	N(5)-Cu(2)-O(3)#2	90.45(15)
O(1)-Cu(1)#3	2.326(3)	C(8)-O(1)-Cu(1)	109.4(3)
O(3)-Cu(2)#4	2.338(3)	C(8)-O(1)-Cu(1)#3	109.2(3)
N(4)-Cu(1)#3	2.001(3)	Cu(1)-O(1)-Cu(1)#3	141.19(13)
N(8)-Cu(2)#4	2.003(4)	C(18)-O(3)-Cu(2)	109.1(3)
N(2)-Cu(1)-N(4)#1	174.38(15)	C(18)-O(3)-Cu(2)#4	109.1(3)
N(2)-Cu(1)-O(1)	79.21(13)	Cu(2)-O(3)-Cu(2)#4	141.83(15)
N(4)#1-Cu(1)-O(1)	101.93(13)	C(1)-N(1)-Cu(1)	128.8(3)
N(2)-Cu(1)-N(1)	80.13(15)	C(5)-N(1)-Cu(1)	111.6(3)
N(4)#1-Cu(1)-N(1)	98.65(14)	C(6)-N(2)-Cu(1)	120.7(3)
O(1)-Cu(1)-N(1)	159.34(13)	N(3)-N(2)-Cu(1)	118.1(3)
N(2)-Cu(1)-O(1)#1	100.38(12)	C(9)-N(4)-Cu(1)#3	124.2(3)
N(4)#1-Cu(1)-O(1)#1	74.21(12)	O(2)-N(4)-Cu(1)#3	122.6(3)
O(1)-Cu(1)-O(1)#1	88.86(16)	C(11)-N(5)-Cu(2)	130.3(4)
N(1)-Cu(1)-O(1)#1	95.00(13)	C(15)-N(5)-Cu(2)	111.5(3)
N(2)-Cu(1)-I(1)	97.23(10)	C(16)-N(6)-Cu(2)	119.6(3)
N(4)#1-Cu(1)-I(1)	88.35(10)	N(7)-N(6)-Cu(2)	118.5(3)
O(1)-Cu(1)-I(1)	86.32(9)	C(19)-N(8)-Cu(2)#4	123.7(3)
N(1)-Cu(1)-I(1)	96.15(11)	O(4)-N(8)-Cu(2)#4	122.4(3)
2			
Cu(1)-N(2)	1.915(12)	N(14)-Cu(4)-N(12)	175.1(5)
Cu(1)-O(1)	2.003(10)	N(14)-Cu(4)-O(7)	79.6(5)
Cu(1)-N(16)	2.017(12)	N(12)-Cu(4)-O(7)	100.7(5)
Cu(1)-N(1)	2.023(12)	N(14)-Cu(4)-N(13)	80.3(6)
Cu(1)-O(7)	2.327(10)	N(12)-Cu(4)-N(13)	99.2(5)
Cu(2)-N(6)	1.912(12)	O(7)-Cu(4)-N(13)	159.8(5)
Cu(2)-O(3)	1.985(10)	N(14)-Cu(4)-O(5)	101.7(5)
Cu(2)-N(4)	1.994(13)	N(12)-Cu(4)-O(5)	73.5(4)
Cu(2)-N(5)	2.015(13)	O(7)-Cu(4)-O(5)	90.6(4)
Cu(2)-O(1)	2.326(10)	N(13)-Cu(4)-O(5)	91.8(5)
Cu(3)-N(10)	1.930(12)	N(14)-Cu(4)-I(1)	95.4(4)
Cu(3)-N(8)	1.997(14)	N(12)-Cu(4)-I(1)	89.5(4)
Cu(3)-O(5)	2.012(10)	O(7)-Cu(4)-I(1)	92.2(3)
Cu(3)-N(9)	2.039(12)	N(13)-Cu(4)-I(1)	91.3(4)
Cu(3)-O(3)	2.304(10)	O(5)-Cu(4)-I(1)	163.0(2)
Cu(4)-N(14)	1.905(13)	I(4)-Cu(5)-I(5)	139.3(3)
Cu(4)-N(12)	1.991(13)	I(4)-Cu(5)-I(5)#5	118.1(2)
Cu(4)-O(7)	2.011(10)	I(5)-Cu(5)-I(5)#5	102.5(2)
Cu(4)-N(13)	2.023(14)	Cu(5)-I(5)-Cu(5)#5	77.5(2)

Cu(4)-O(5)	2.336(10)	C(8)-O(1)-Cu(1)	108.9(9)
Cu(4)-I(1)	3.085(2)	C(8)-O(1)-Cu(2)	110.9(9)
Cu(5)-I(4)	2.475(7)	Cu(1)-O(1)-Cu(2)	140.2(5)
Cu(5)-I(5)	2.545(6)	C(18)-O(3)-Cu(2)	111.1(10)
Cu(5)-I(5)#5	2.646(6)	C(18)-O(3)-Cu(3)	109.9(10)
I(5)-Cu(5)#5	2.646(6)	Cu(2)-O(3)-Cu(3)	138.9(5)
N(2)-Cu(1)-O(1)	79.0(4)	C(28)-O(5)-Cu(3)	109.0(9)
N(2)-Cu(1)-N(16)	176.1(5)	C(28)-O(5)-Cu(4)	110.5(9)
O(1)-Cu(1)-N(16)	99.1(4)	Cu(3)-O(5)-Cu(4)	140.4(5)
N(2)-Cu(1)-N(1)	81.5(5)	C(38)-O(7)-Cu(4)	110.0(9)
O(1)-Cu(1)-N(1)	160.3(5)	C(38)-O(7)-Cu(1)	109.8(9)
N(16)-Cu(1)-N(1)	100.2(5)	Cu(4)-O(7)-Cu(1)	140.2(5)
N(2)-Cu(1)-O(7)	102.4(5)	C(1)-N(1)-Cu(1)	129.2(11)
O(1)-Cu(1)-O(7)	91.5(4)	C(5)-N(1)-Cu(1)	110.9(10)
N(16)-Cu(1)-O(7)	74.1(4)	C(6)-N(2)-Cu(1)	118.5(11)
N(1)-Cu(1)-O(7)	90.4(4)	N(3)-N(2)-Cu(1)	119.6(9)
N(6)-Cu(2)-O(3)	79.2(5)	C(9)-N(4)-Cu(2)	124.5(10)
N(6)-Cu(2)-N(4)	178.8(5)	O(2)-N(4)-Cu(2)	122.6(10)
O(3)-Cu(2)-N(4)	100.0(5)	C(11)-N(5)-Cu(2)	128.2(13)
N(6)-Cu(2)-N(5)	79.9(5)	C(15)-N(5)-Cu(2)	113.4(11)
O(3)-Cu(2)-N(5)	158.6(5)	C(16)-N(6)-Cu(2)	121.4(12)
N(4)-Cu(2)-N(5)	100.9(5)	N(7)-N(6)-Cu(2)	117.2(9)
N(6)-Cu(2)-O(1)	105.4(4)	C(19)-N(8)-Cu(3)	124.4(11)
O(3)-Cu(2)-O(1)	92.6(4)	O(4)-N(8)-Cu(3)	121.4(11)
N(4)-Cu(2)-O(1)	73.8(4)	C(21)-N(9)-Cu(3)	130.1(12)
N(5)-Cu(2)-O(1)	88.8(4)	C(25)-N(9)-Cu(3)	111.3(11)
N(10)-Cu(3)-N(8)	178.5(5)	C(26)-N(10)-Cu(3)	119.5(11)
N(10)-Cu(3)-O(5)	79.3(5)	N(11)-N(10)-Cu(3)	117.6(9)
N(8)-Cu(3)-O(5)	102.1(5)	C(29)-N(12)-Cu(4)	123.6(11)
N(10)-Cu(3)-N(9)	80.4(5)	O(6)-N(12)-Cu(4)	122.1(9)
N(8)-Cu(3)-N(9)	98.2(5)	C(31)-N(13)-Cu(4)	130.3(12)
O(5)-Cu(3)-N(9)	159.7(5)	C(35)-N(13)-Cu(4)	110.3(12)
N(10)-Cu(3)-O(3)	107.0(5)	C(36)-N(14)-Cu(4)	121.3(12)
N(8)-Cu(3)-O(3)	73.6(5)	N(15)-N(14)-Cu(4)	117.6(10)
O(5)-Cu(3)-O(3)	91.5(4)	C(39)-N(16)-Cu(1)	121.9(10)
N(9)-Cu(3)-O(3)	95.6(5)	O(8)-N(16)-Cu(1)	123.7(10)
		3	
Cu(1)-N(2)	1.934(8)	O(5)-Cu(3)-I(2)	91.8(2)
Cu(1)-O(1)	1.987(7)	N(16)-Cu(3)-I(2)	91.2(3)
Cu(1)-N(8)	2.002(8)	N(9)-Cu(3)-I(2)	93.1(2)
Cu(1)-N(1)	2.018(9)	O(7)-Cu(3)-I(2)	163.64(18)
Cu(1)-O(3)	2.333(6)	N(14)-Cu(4)-N(13)	80.7(3)
Cu(1)-I(1)	3.0182(17)	N(14)-Cu(4)-O(7)	80.1(3)
Cu(2)-N(6)	1.915(8)	N(13)-Cu(4)-O(7)	160.8(3)
Cu(2)-O(3)	1.994(6)	N(14)-Cu(4)-N(4)	176.8(4)
Cu(2)-N(5)	1.997(8)	N(13)-Cu(4)-N(4)	97.6(3)
Cu(2)-N(12)	2.035(8)	O(7)-Cu(4)-N(4)	101.5(3)
Cu(2)-O(5)	2.250(7)	N(14)-Cu(4)-O(1)	107.8(3)
Cu(3)-N(10)	1.945(9)	N(13)-Cu(4)-O(1)	92.7(3)
Cu(3)-O(5)	1.995(7)	O(7)-Cu(4)-O(1)	94.2(3)
Cu(3)-N(16)	2.006(9)	N(4)-Cu(4)-O(1)	74.8(3)
Cu(3)-N(9)	2.018(10)	I(3)-Cu(5)-I(5)	121.48(8)

Cu(3)-O(7)	2.345(6)	I(3)-Cu(5)-I(6)	120.66(8)
Cu(3)-I(2)	3.0208(17)	I(5)-Cu(5)-I(6)	117.86(8)
Cu(4)-N(14)	1.919(8)	I(3)-Cu(5)-Cu(6)	177.65(10)
Cu(4)-N(13)	1.990(9)	I(5)-Cu(5)-Cu(6)	58.92(6)
Cu(4)-O(7)	2.003(6)	I(6)-Cu(5)-Cu(6)	58.96(6)
Cu(4)-N(4)	2.008(8)	I(4)-Cu(6)-I(5)	118.77(8)
Cu(4)-O(1)	2.255(7)	I(4)-Cu(6)-I(6)	123.50(8)
Cu(5)-I(3)	2.541(2)	I(5)-Cu(6)-I(6)	117.72(8)
Cu(5)-I(5)	2.559(2)	I(4)-Cu(6)-Cu(5)	176.72(10)
Cu(5)-I(6)	2.578(2)	I(5)-Cu(6)-Cu(5)	58.70(6)
Cu(5)-Cu(6)	2.654(3)	I(6)-Cu(6)-Cu(5)	59.05(6)
Cu(6)-I(4)	2.539(2)	Cu(5)-I(5)-Cu(6)	62.38(7)
Cu(6)-I(5)	2.565(2)	Cu(6)-I(6)-Cu(5)	61.99(7)
Cu(6)-I(6)	2.575(2)	C(8)-O(1)-Cu(1)	110.2(7)
N(2)-Cu(1)-O(1)	78.5(3)	C(8)-O(1)-Cu(4)	111.4(7)
N(2)-Cu(1)-N(8)	173.7(4)	Cu(1)-O(1)-Cu(4)	138.4(3)
O(1)-Cu(1)-N(8)	99.1(3)	C(18)-O(3)-Cu(2)	108.9(6)
N(2)-Cu(1)-N(1)	80.8(4)	C(18)-O(3)-Cu(1)	109.7(6)
O(1)-Cu(1)-N(1)	159.1(3)	Cu(2)-O(3)-Cu(1)	141.3(3)
N(8)-Cu(1)-N(1)	101.2(4)	C(28)-O(5)-Cu(3)	109.1(6)
N(2)-Cu(1)-O(3)	100.3(3)	C(28)-O(5)-Cu(2)	112.4(7)
O(1)-Cu(1)-O(3)	88.2(3)	Cu(3)-O(5)-Cu(2)	138.5(3)
N(8)-Cu(1)-O(3)	73.7(3)	C(38)-O(7)-Cu(4)	108.2(6)
N(1)-Cu(1)-O(3)	92.4(3)	C(38)-O(7)-Cu(3)	110.9(6)
N(2)-Cu(1)-I(1)	94.7(2)	Cu(4)-O(7)-Cu(3)	140.8(3)
O(1)-Cu(1)-I(1)	93.24(19)	C(1)-N(1)-Cu(1)	130.0(8)
N(8)-Cu(1)-I(1)	91.2(2)	C(5)-N(1)-Cu(1)	112.0(7)
N(1)-Cu(1)-I(1)	91.6(2)	C(6)-N(2)-Cu(1)	118.4(8)
O(3)-Cu(1)-I(1)	164.94(17)	N(3)-N(2)-Cu(1)	118.9(7)
N(6)-Cu(2)-O(3)	79.7(3)	C(9)-N(4)-Cu(4)	121.9(8)
N(6)-Cu(2)-N(5)	81.1(3)	O(2)-N(4)-Cu(4)	120.5(7)
O(3)-Cu(2)-N(5)	160.4(3)	C(11)-N(5)-Cu(2)	130.4(8)
N(6)-Cu(2)-N(12)	176.2(4)	C(15)-N(5)-Cu(2)	111.5(7)
O(3)-Cu(2)-N(12)	100.4(3)	C(16)-N(6)-Cu(2)	119.6(7)
N(5)-Cu(2)-N(12)	98.5(3)	N(7)-N(6)-Cu(2)	118.1(6)
N(6)-Cu(2)-O(5)	109.8(3)	C(19)-N(8)-Cu(1)	124.1(7)
O(3)-Cu(2)-O(5)	94.3(3)	O(4)-N(8)-Cu(1)	121.7(6)
N(5)-Cu(2)-O(5)	96.0(3)	C(25)-N(9)-Cu(3)	112.8(8)
N(12)-Cu(2)-O(5)	74.0(3)	C(21)-N(9)-Cu(3)	130.8(10)
N(10)-Cu(3)-O(5)	78.7(3)	C(26)-N(10)-Cu(3)	118.2(8)
N(10)-Cu(3)-N(16)	171.8(3)	N(11)-N(10)-Cu(3)	117.7(7)
O(5)-Cu(3)-N(16)	101.2(3)	C(29)-N(12)-Cu(2)	122.8(8)
N(10)-Cu(3)-N(9)	80.4(4)	O(6)-N(12)-Cu(2)	120.3(7)
O(5)-Cu(3)-N(9)	159.0(3)	C(31)-N(13)-Cu(4)	128.7(8)
N(16)-Cu(3)-N(9)	99.1(4)	C(35)-N(13)-Cu(4)	112.8(7)
N(10)-Cu(3)-O(7)	98.8(3)	C(36)-N(14)-Cu(4)	120.2(7)
O(5)-Cu(3)-O(7)	87.3(3)	N(15)-N(14)-Cu(4)	117.5(6)
N(16)-Cu(3)-O(7)	73.0(3)	C(39)-N(16)-Cu(3)	124.9(7)
N(9)-Cu(3)-O(7)	93.6(3)	O(8)-N(16)-Cu(3)	120.9(6)
N(10)-Cu(3)-I(2)	97.0(2)		

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

Table S**3** Distances (Å) and angles (°) of hydrogen bonds for compounds **1, 2** and **3**[a].

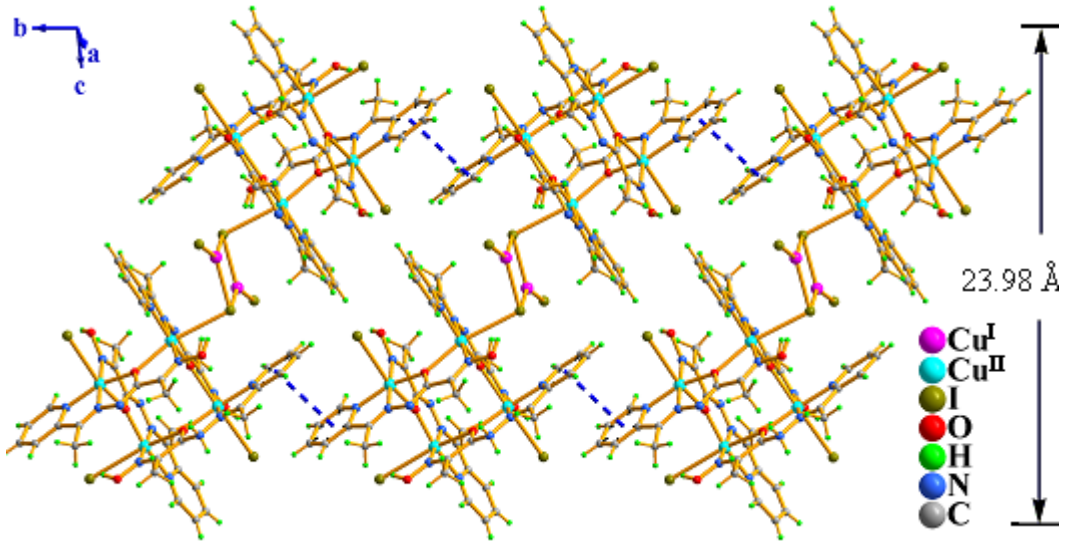
D-H…A	Distance(D-H)	Distance(H···A)	Distance(D···A)	Angle(D-H···A)
		1		
O(2)-H(2)···I(1)#1	0.82	2.592(15)	3.297(12)	144.6(2)
O(4)-H(4)···I(2)#2	0.82	2.593(15)	3.365(11)	158.3(1)
O(5)-H(5A)···O(6)#3	0.85	1.707(14)	2.498(13)	153.7(1)
O(5)-H(5B)···I(2)#4	0.85	3.035(14)	3.632(10)	129.1(2)
O(6)-H(6B)···I(1)#3	0.85	3.130(15)	3.861(10)	145.4(2)
C(13)-H(13)···I(1)#3	0.93	3.106(14)	3.869(10)	140.6(2)
C(7)-H(7B)···I(1)#3	0.93	3.122(13)	3.882(10)	137.3(2)
		2		
O(4)-H(4)···I(5)#5	0.82	2.621(10)	3.293(15)	140.3(1)
O(6)-H(6)···I(1)#6	0.82	2.592(9)	3.309(13)	147.3(2)
O(8)-H(8)···I(3)#6	0.82	2.701(10)	3.327(13)	135.1(2)
C(11)-H(11)···N(18)#7	0.93	2.643(10)	3.460(12)	146.9(2)
C(13)-H(13)···N(17)#7	0.93	2.546(10)	3.310(11)	139.6(2)
C(30)-H(30A)···N(17)#7	0.93	2.707(11)	3.529(11)	143.9(1)
C(17)-H(17B)···I(4)#8	0.93	3.009(10)	3.939(12)	163.4(2)
C(22)-H(22)···N(7)#9	0.93	2.707(11)	3.559(11)	151.9(2)
π---π[b]			3.956(11)	
		3		
C(2)-H(2A)···I(6)#10	0.93	3.198(8)	3.925(7)	143.6(1)
O(4)-H(4)···I(1)	0.82	2.621(8)	3.345(7)	148.2(1)
O(8)-H(8)···I(2)	0.82	2.652(7)	3.329(8)	148.3(2)
C(22)-H(22)···N(15)	0.93	2.603(8)	3.512(8)	166.3(1)
C(14)-H(14)···O(8)	0.93	2.668(7)	3.336(7)	129.4(2)
C(42)-H(42A)···I(4)	0.93	3.142(8)	3.988(8)	147.9(2)
C(30)-H(30C)···I(1)	0.93	3.151(8)	3.932(8)	155.7(2)
C(33)-H(33)···N(17)	0.93	2.734(7)	3.396(8)	128.9(2)
C(37)-H(37C)···O(4)	0.93	2.644(7)	3.597(7)	171.8(2)

*[a]Symmetry transformations used to generate equivalent atoms: #1 y-1/4,-x+5/4,-z+1/4; #2 y+1/4,-x+3/4,-z+3/4; #3 -y+3/4, x+1/4, z+1/4; #4 -x+1,-y+1,-z+1; #5 x+1,y+1,z; #6 –x+1,-y+1,z; #7 x,-1+y,z; #8 -1+x,-1+y,z; #9 –x,-y,2-z; #10 -0.5+x,0.5-y,0.5+z; #11.

[b] denots the centroid distance between two pyridyl rings from two adjacent molecules in **2**.

Figure S1

(a)



(b)

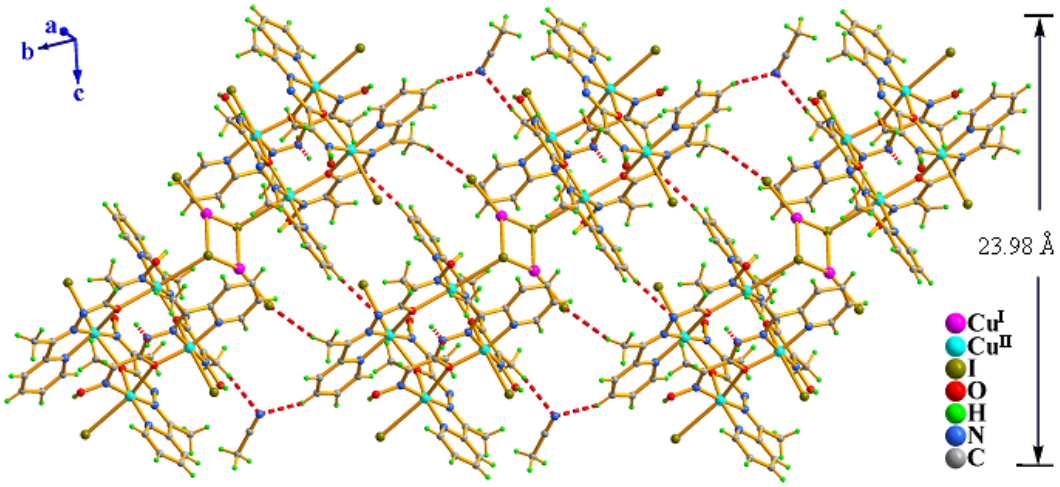
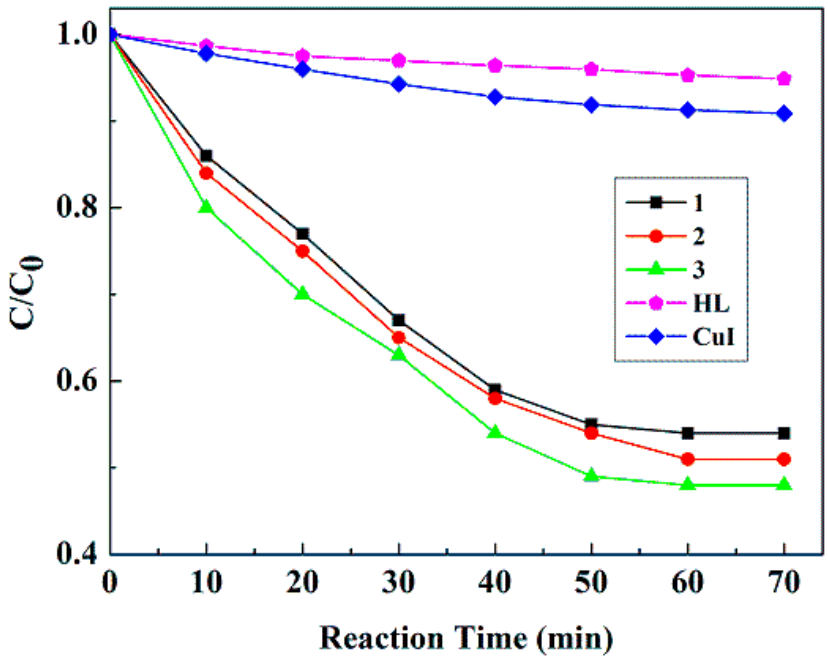


Figure S2.

(a)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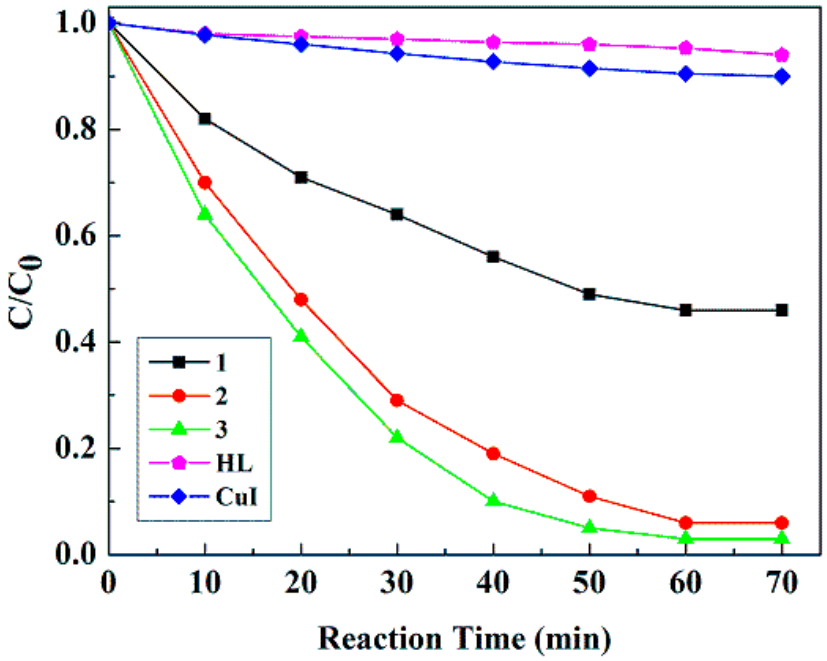
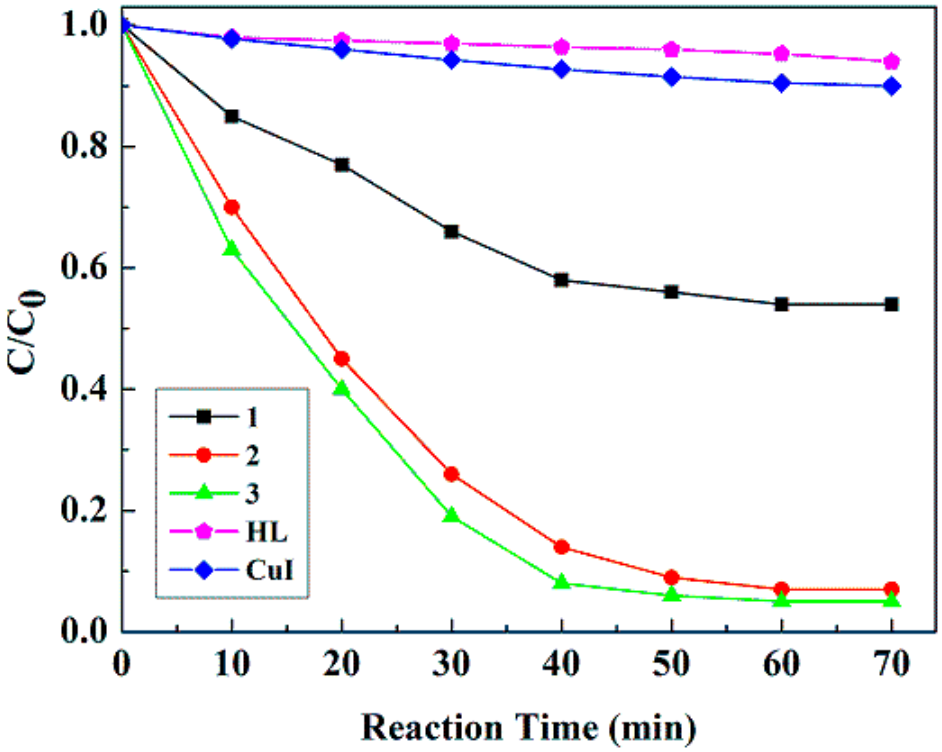
0.8
0.6
0.4
C/C0
0
10
20
30
40
50
60
70
Reaction Time (min)
1
2
3
HL
CuI

(b)


1.0
0.8
0.6
0.4
0.2
0.0
C/C0
0
10
20
30
40
50
60
70
Reaction Time (min)
1
2
3
HL
CuI

(c)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0.8
0.6
0.4
0.2
0.0
C/C0
0
10
20
30
40
50
60
70
Reaction Time (min)
1
2
3
HL
CuI

(d)

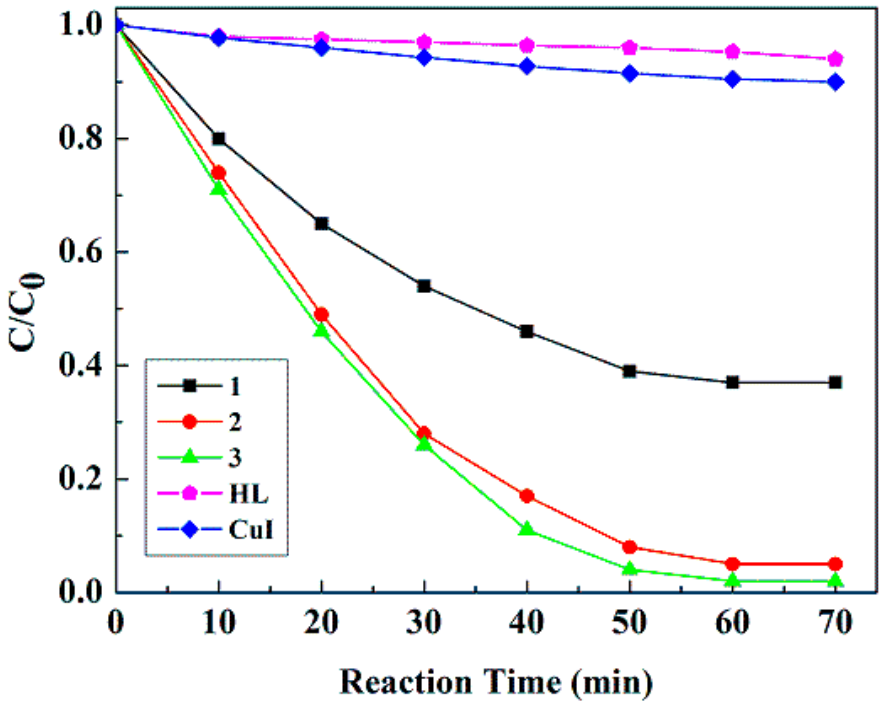
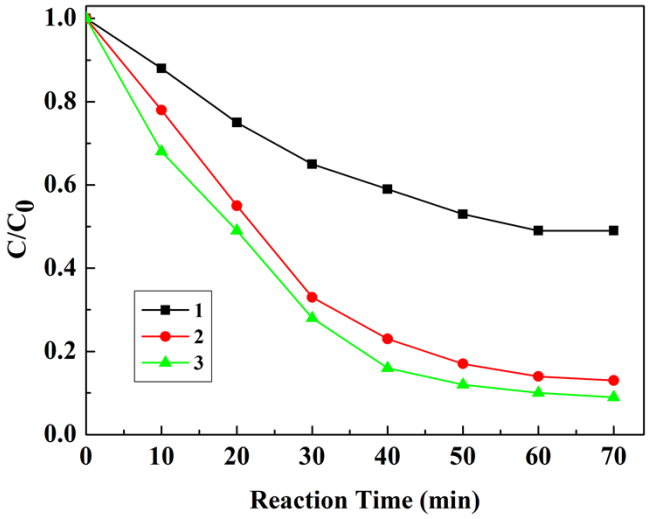
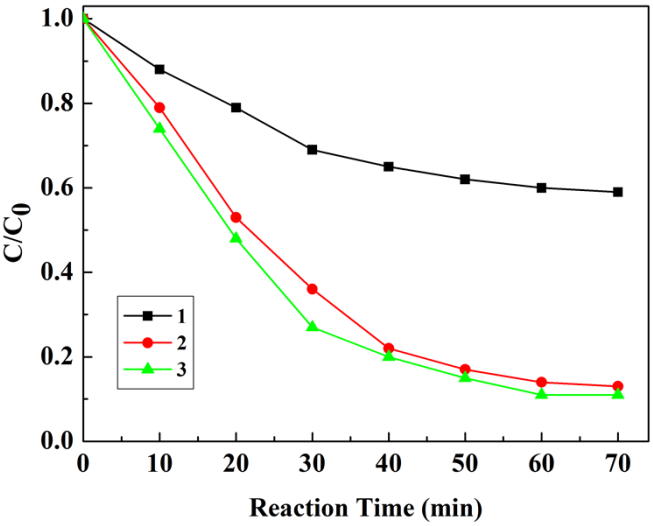

1.0
0.8
0.6
0.4
0.2
0.0
C/C0
0
10
20
30
40
50
60
70
Reaction Time (min)
1
2
3
HL
CuI

Figure S3

(a)



(b)



(c)