Supporting Information

Significant photodegradation of carcinogenic organic dyes by 1D supramolecular heteroleptic Cu(II) complex on sunlight irradiation

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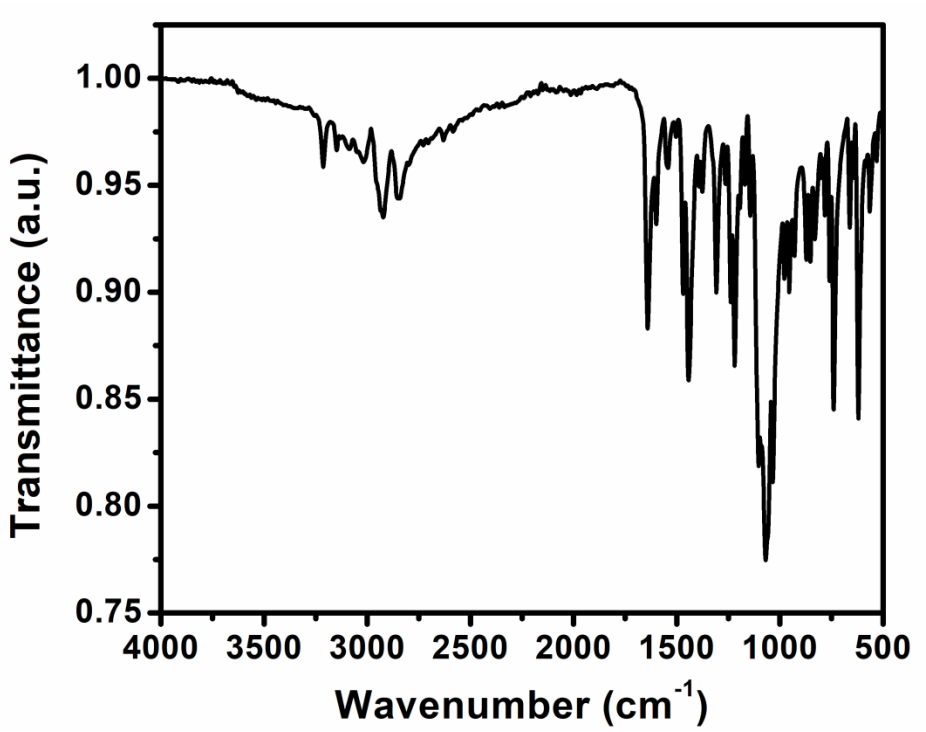


Figure S1 FTIR of the Complex

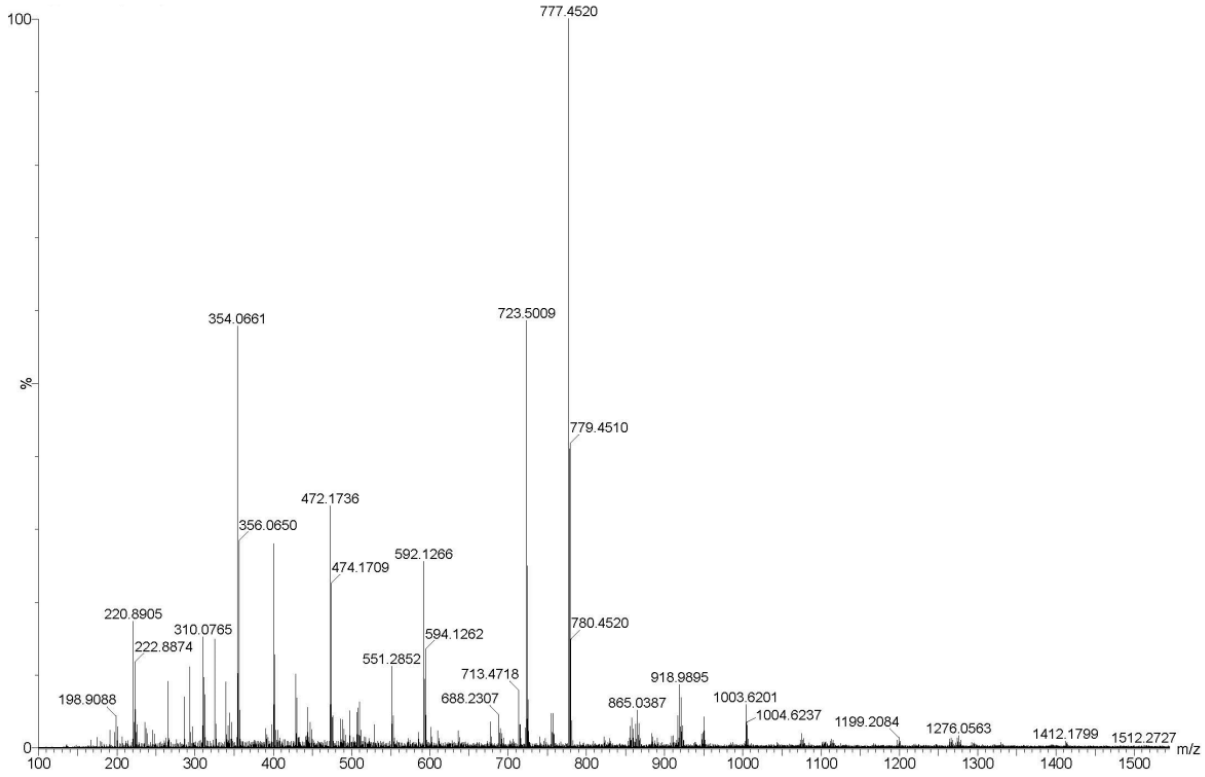


Figure S2 ESI-MS spectrum of the complex

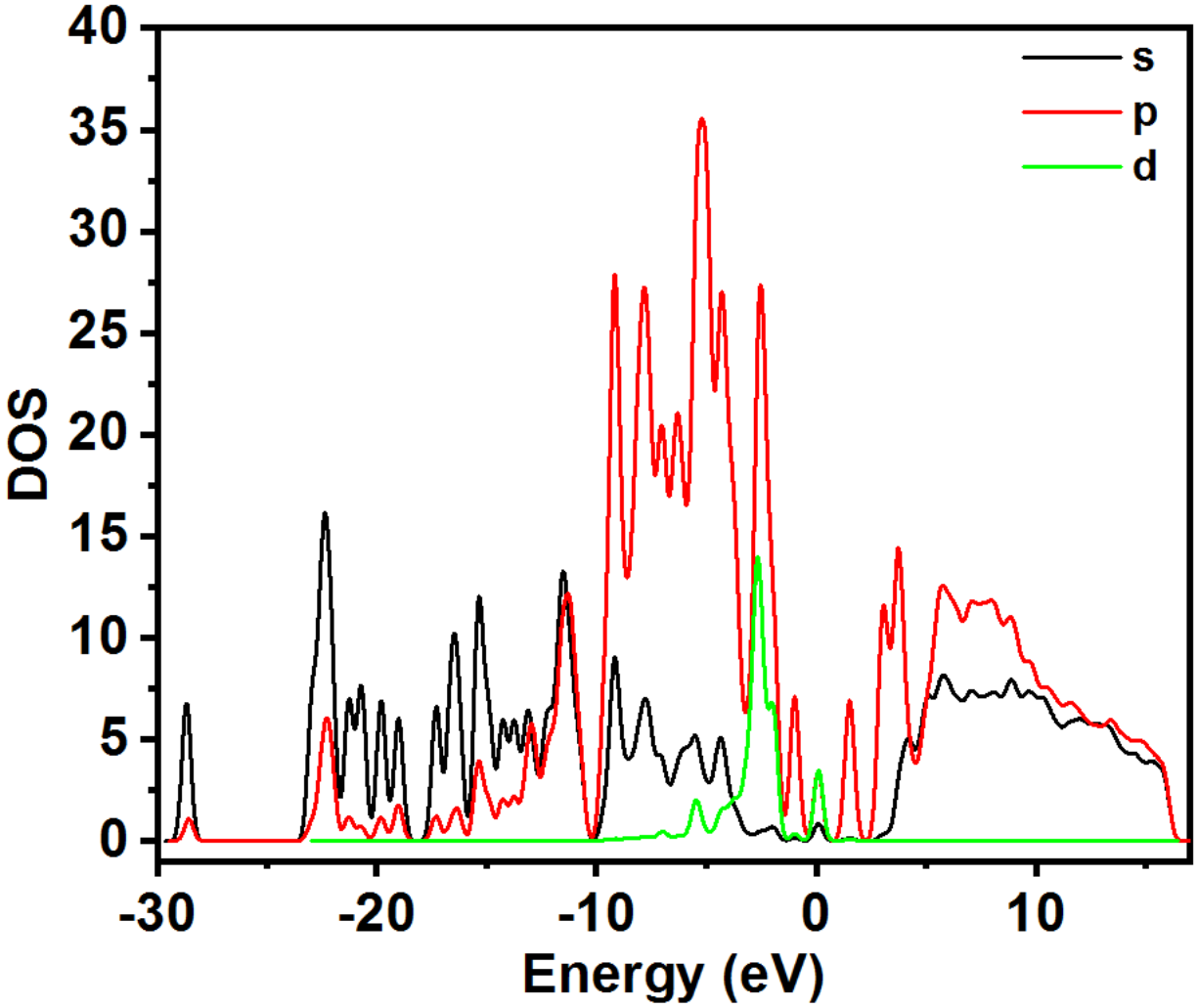


Figure S3 Partial DOS of the s, p, and d orbitals of constituents systems of the complex

Table S1 Selected peaks in ESI mass of the complex

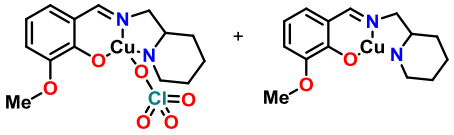
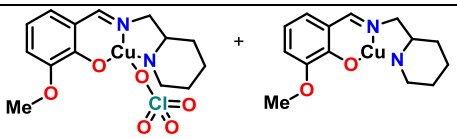
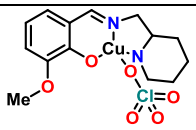
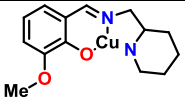
Fragments	Adduct	Peak value
 Mol. Wt. = 409.30 + Mol. Wt. = 309.86	$CH_3OH + NH_4^+ + 8H^+ = 58.15$	777.31
 Mol. Wt. = 409.30 + Mol. Wt. = 309.86	$4H^+ = 4$	723.16
 Mol. Wt. = 409.30	$CH_3CN + NH_4^+ + 4H^+ = 63.12$	472.42
 Mol. Wt. = 309.86	$CH_3CN + 3H^+ = 44.20$	354.06

Table S2 Bond Lengths

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cu1	O1	1.9236(12)	C1	C6	1.412(2)
Cu1	N1	1.9456(14)	C2	C3	1.382(2)
Cu1	N2	2.0215(14)	C3	C4	1.405(3)
Cu1	N3	1.9711(14)	C4	C5	1.371(3)
O1	C1	1.3170(19)	C5	C6	1.416(2)
O2	C2	1.372(2)	C6	C8	1.448(2)
O2	C7	1.427(2)	C9	C10	1.518(2)
N1	C8	1.282(2)	C10	C11	1.518(2)
N1	C9	1.464(2)	C11	C12	1.527(3)
N2	C10	1.494(2)	C12	C13	1.522(3)
N2	C14	1.476(2)	C13	C14	1.525(2)
N3	C15	1.326(2)	C16	C17	1.358(3)
N3	C17	1.382(2)	Cl1	O101	1.4422(14)
N4	C15	1.331(2)	Cl1	O102	1.4361(15)
N4	C16	1.371(2)	Cl1	O103	1.4461(18)
C1	C2	1.426(2)	Cl1	O104	1.4190(17)

Table S3 Bond Angles

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Cu1	N1	90.38(5)	C2	C3	C4	120.31(17)
O1	Cu1	N2	173.42(6)	C5	C4	C3	120.00(16)
O1	Cu1	N3	89.54(5)	C4	C5	C6	120.81(17)
N1	Cu1	N2	84.04(6)	C1	C6	C5	119.95(16)
N1	Cu1	N3	178.32(6)	C1	C6	C8	121.37(15)
N3	Cu1	N2	95.94(6)	C5	C6	C8	118.60(15)
C1	O1	Cu1	123.70(10)	N1	C8	C6	124.68(15)
C2	O2	C7	117.32(14)	N1	C9	C10	106.60(14)
C8	N1	Cu1	125.24(12)	N2	C10	C9	107.57(13)
C8	N1	C9	122.01(15)	N2	C10	C11	110.70(14)
C9	N1	Cu1	112.36(10)	C11	C10	C9	115.36(15)
C10	N2	Cu1	109.12(10)	C10	C11	C12	109.70(15)
C14	N2	Cu1	121.05(11)	C13	C12	C11	111.63(15)
C14	N2	C10	110.15(13)	C12	C13	C14	112.40(15)
C15	N3	Cu1	126.63(12)	N2	C14	C13	111.28(15)
C15	N3	C17	105.86(14)	N3	C15	N4	111.02(15)
C17	N3	Cu1	125.40(12)	C17	C16	N4	106.23(16)
C15	N4	C16	107.94(15)	C16	C17	N3	108.95(16)
O1	C1	C2	117.72(15)	O101	Cl1	O103	107.89(9)
O1	C1	C6	124.30(15)	O102	Cl1	O101	110.20(10)
C6	C1	C2	117.97(15)	O102	Cl1	O103	108.65(10)
O2	C2	C1	113.79(14)	O104	Cl1	O101	109.21(12)
O2	C2	C3	125.30(16)	O104	Cl1	O102	110.42(11)
C3	C2	C1	120.90(16)	O104	Cl1	O103	110.44(15)