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Synthesis of an electrically conductive square planar copper(II) complex and its utilization in the fabrication of a photosensitive Schottky diode device and DFT study

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Supporting Information

Table S1: Crystal data and refinement details of the complex.

Formula	$C_{19}H_{23}CuN_3OS$
Formula weight	405.02
Temperature(K)	293(2)
Crystal system	Monoclinic
Space group	$P2_1/a$
a(Å)	14.659(4)
b(Å)	7.247(2)
c(Å)	18.776(6)
β(°)	106.108(5)
Z	4
d_{calc}(g cm^{-3})	1.404
μ(mm^{-1})	1.260
F(000)	844
Total reflections	8292
Unique reflections	3312
Observed data [I > 2σ(I)]	2564
R(int)	0.034
R1, wR2 (all data)	0.0547, 0.1119
R1, wR2 [I > 2σ(I)]	0.0407, 0.1045

Table S2: Selected bond lengths (Å) and bond angles (^{0}) of the complex.

bond lengths (Å)			
Cu(1)- O(1)	1.880(3)	Cu(1)-N(2)	2.054(3)
Cu(1)-N(1)	1.943(3)	Cu(1)-N(3)	1.935(2)
bond angles (^{0})			
O(1)- Cu(1)-N(1)	90.5(1)	N(1)-Cu(1)-N(2)	92.4(1)
O(1)-Cu(1)-N(2)	169.2(1)	N(1)-Cu(1)-N(3)	178.6(1)
O(1)-Cu(1)-N(3)	90.9 (1)	N(2)-Cu(1)-N(3)	86.1(1)

Table S3: Geometric features (distances in Å and angles in °) of the C-H···π interactions obtained of the complex.

C-H···Cg(Ring)	**H···Cg**	**C-H···Cg (°)**	**C···Cg (Å)**
C(9)–H(9A)···Cg(4)[a]	2.95	154.27	3.845(5)
C(14)–H(14)···Cg(3)[b]	2.97	140.15	3.732(6)
C(15)–H(15)···Cg(4)[b]	2.69	158.53	3.574(5)

Symmetry transformations: [a]= x,-1+y,z; [b]= -1/2-x,1/2+y,-z

Cg(3) = Centre of gravity of the ring [C(10)-C(11)-C(16)-C(17)-C(18)-C(19)]; Cg(4) = Centre of gravity of the ring [C(11)-C(12)-C(13)-C(14)-C(15-C(16)] of the complex.

Table S4: Frontier molecular orbital energies (eV) and compositions (%) in the ground state of the complex.

MO (α orbitals)	Energy (eV)	Contribution (%)	
		Cu	Ligands
LUMO+10	2.27	33	67
LUMO+9	1.4	91	9
LUMO+8	1.0	20	80
LUMO+7	0.87	30	70
LUMO+6	0.8	26	74
LUMO+5	0.77	64	36
LUMO+4	0.41	67	33
LUMO+3	0.36	72	28
LUMO+2	-0.08	2	98
LUMO+1	-0.72	2	98
LUMO	-1.92	1	99
HOMO	-4.91	11	89
HOMO-1	-5.54	2	98
HOMO-2	-5.85	3	97
HOMO-3	-6.13	14	86
HOMO-4	-6.24	2	98
HOMO-5	-7.36	7	93
HOMO-6	-7.71	4	96
HOMO-7	-7.76	7	93
HOMO-8	-8.04	5	95
HOMO-9	-8.28	6	94
HOMO-10	-8.37	7	93

Table S5: Frontier molecular orbital energies (eV) and compositions (%) in the ground state of the complex.

MO (β orbitals)	Energy (eV)	Contribution (%)	
		Cu	Ligands
LUMO+10	1.46	82	18
LUMO+9	1.08	25	75
LUMO+8	0.93	21	79
LUMO+7	0.87	32	68
LUMO+6	0.78	66	34
LUMO+5	0.46	76	24
LUMO+4	0.37	73	27
LUMO+3	-0.07	3	97
LUMO+2	-0.71	2	98
LUMO+1	-1.82	21	79
LUMO	-1.99	26	74
HOMO	-5.39	5	95
HOMO-1	-5.47	2	98
HOMO-2	-5.82	3	97
HOMO-3	-6.2	2	98
HOMO-4	-6.89	8	92
HOMO-5	-7.63	6	94
HOMO-6	-7.69	7	93
HOMO-7	-7.96	9	91
HOMO-8	-8.2	16	84
HOMO-9	-8.28	45	55
HOMO-10	-8.35	23	77

Table S6: Calculated transitions and their assignments for the complex.

Excitation energy (eV)	Wavelength Thro. (nm)	Oscillation frequency (f)	Key transitions	Nature of transitions
2.5035	495.25	0.0724	(60%) HOMO-1→LUMO B	MLCT
2.6551	466.97	0.0134	(70%) HOMO-2→LUMO B	MLCT
3.0798	402.58	0.0213	(74%) HOMO-1→LUMO A	MLCT
3.5265	351.58	0.0509	(66%) HOMO-2→LUMO+1 B	MLCT
3.7492	330.70	0.0514	(25%) HOMO-3 →LUMO B	MLCT
3.8156	324.94	0.1225	(47%) HOMO-4→LUMO A	MLCT

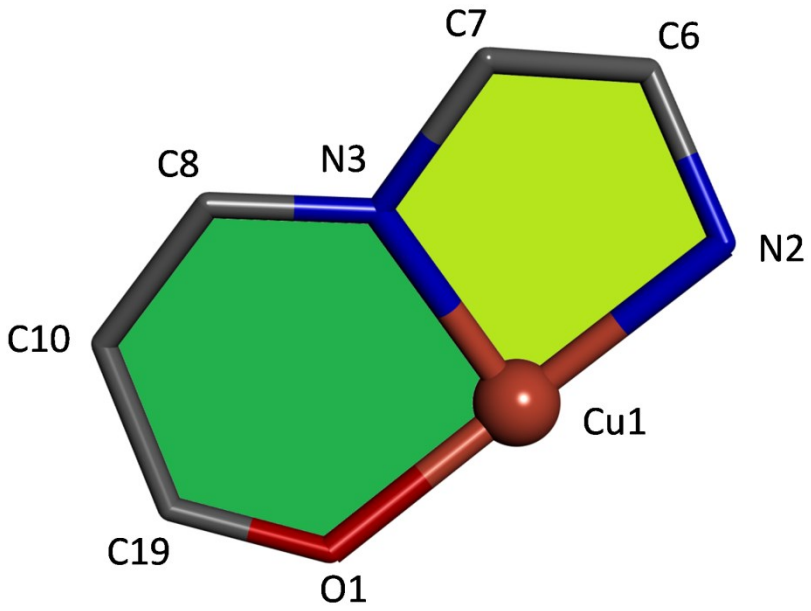

Fig. S1: A perspective view of the five member {Cu(1)-N(2)-C(6)-C(7)-N(3)} and six member {Cu(1)-N(3)-C(8)-C(10)-C(19)-O(1)} chelate rings with the copper(II) of the complex.

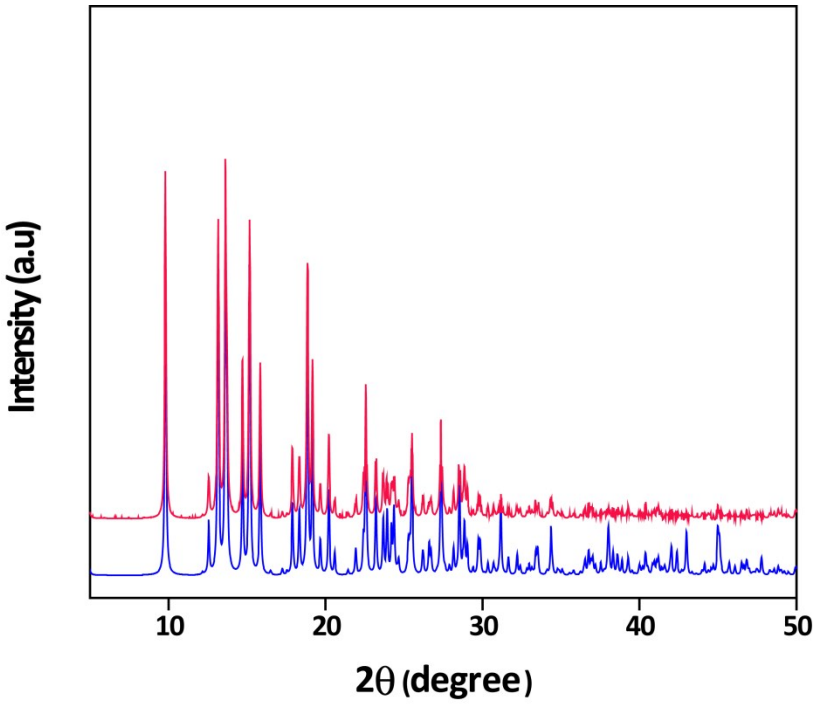

Fig. S2: Experimental (red) and simulated (blue) powder XRD patterns of the complex confirming the purity of bulk material.

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