

Supporting Information

Experimental Part

All of the starting compounds, such as diamines, aldehyde and $\text{Cu}(\text{OAc})_2 \cdot 2\text{H}_2\text{O}$ were directly used for the preparation of the ligands and complexes. A Teflon vessel inserted into a steel autoclave was utilized to carry out the reaction; the ligands (L-1 and L-2) were dissolved in ethanol and added to the ethanol-dissolved $\text{Cu}(\text{OAc})_2 \cdot 2\text{H}_2\text{O}$. The solid complexes were ultimately precipitated in microcrystalline form when the autoclave was heated at self-induced pressure for 6 hours at 70 °C. The Cu (II) complexes are sparingly soluble in acetonitrile, methanol, and other polar solvents but are highly soluble in DMF and DMSO.

Characterization techniques used for analysis of Cu (II) complexes.

A JMS-S3000 SpiralTOF™-plus Ultra-High Mass Resolution MALDI-TOFMS System (IICT, Hyderabad) was used. The FESEM images were captured on a Quanta FEG 250. The X-ray photoelectron spectroscopic (XPS) spectra were obtained by using a Shimadzu 3140 X-ray photoelectron spectrometer through an excitation energy of 1253.6 eV (Mg Ka) and with 80 eV energy. Thermograms of all samples were obtained using a Shimadzu differential thermal analyzer (DTG-60H) with a heating rate of 10°C min⁻¹ in the range from 50 to 1000 °C under a nitrogen purging rate of 20 mL/minute. Brunauer–Emmett–Teller (BET) surface areas were determined by nitrogen adsorption–desorption isotherm measurements at 77 K on a Quantachrome autosorb automated gas sorption system. All of the photoreactions were performed by using a multitube photoreactor system with tungsten visible light (Lelesil Innovative Systems, India). The UV-visible DRS spectra were measured on a JASCO V-760 UV-vis spectrophotometer. The photoluminescence (PL) spectra of the new nanomaterials were estimated on a HORIBA Fluoromax Plus with respect to their excitation with a slit width of 1.5 nm. The oxidation potentials were obtained with an electrochemical workstation (CHI 660) in a standard three-electrode system. A flexible fluorine-doped tin oxide (FTO) substrate (1 cm × 1 cm) covered with the catalyst, acted as the working electrode. An Ag/AgCl and a platinum wire were used as the reference and counter electrodes, respectively, with 0.05 M K₂SO₄ solution as the electrolyte. FTIR spectra were recorded using a Shimadzu spectrometer by applying KBr pellets with 4 cm⁻¹ resolution.

Table S1. Physicochemical and elemental data of C-1 and C-2 complexes

Complex	% of	DP	% C	% H	% X	% N	% Cu	$\Lambda_m \text{ ohm}^{-1} \text{ mol}^{-1}$
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	yield	(°C)	(calcd)	(calcd)	(calcd)	(calcd)	(calcd)	cm ²
C-1	61	386	65.58 (65.63)	3.32 (3.34)	6.89 (Cl) (6.92)	5.43 (5.47)	12.33 (12.40)	12.07
C-2	59	392	67.76 (67.80)	3.42 (3.45)	3.78 (F) (3.83)	5.62 (5.65)	12.74 (12.81)	9.17

IICT - HYDERABAD

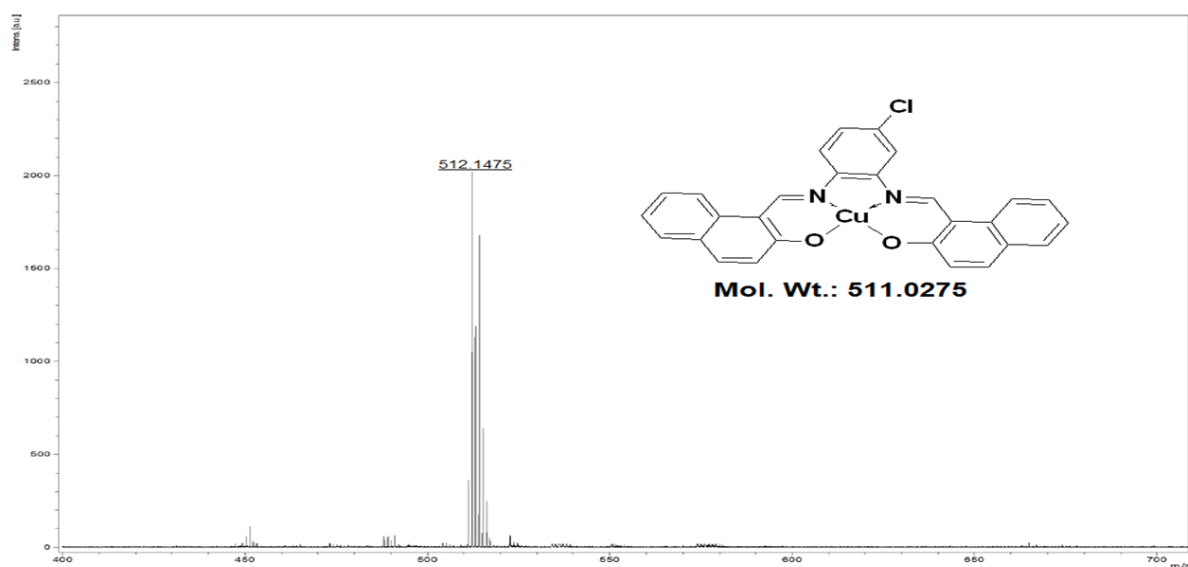


Figure S1. HR MALDI mass spectrum of the C-1 complex.

IICT - HYDERABAD

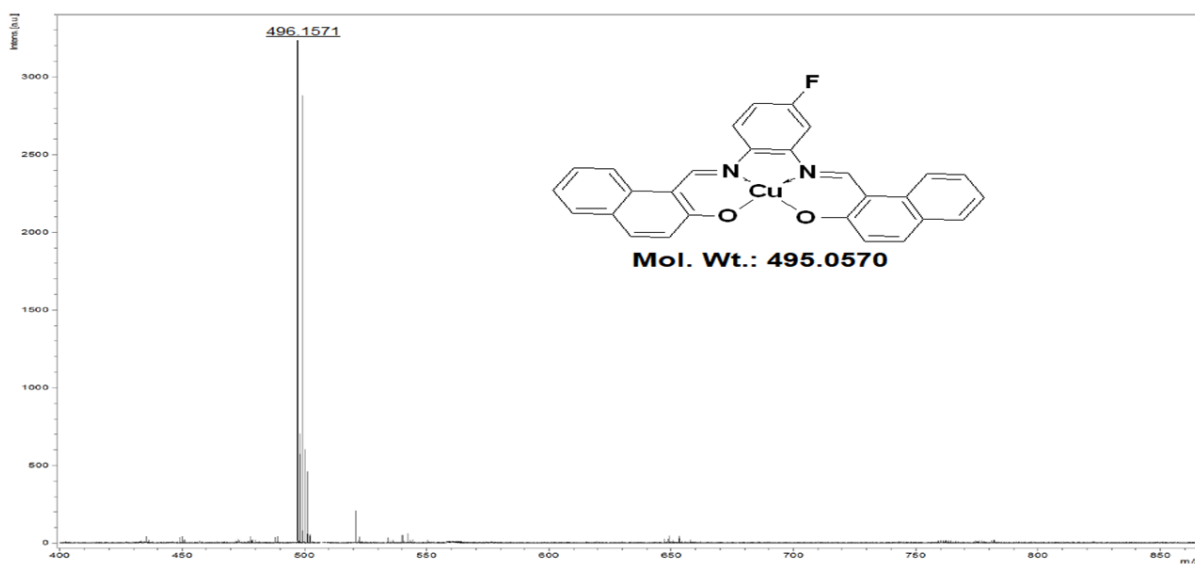


Figure S2. HR MALDI mass spectrum of the C-2 complex.

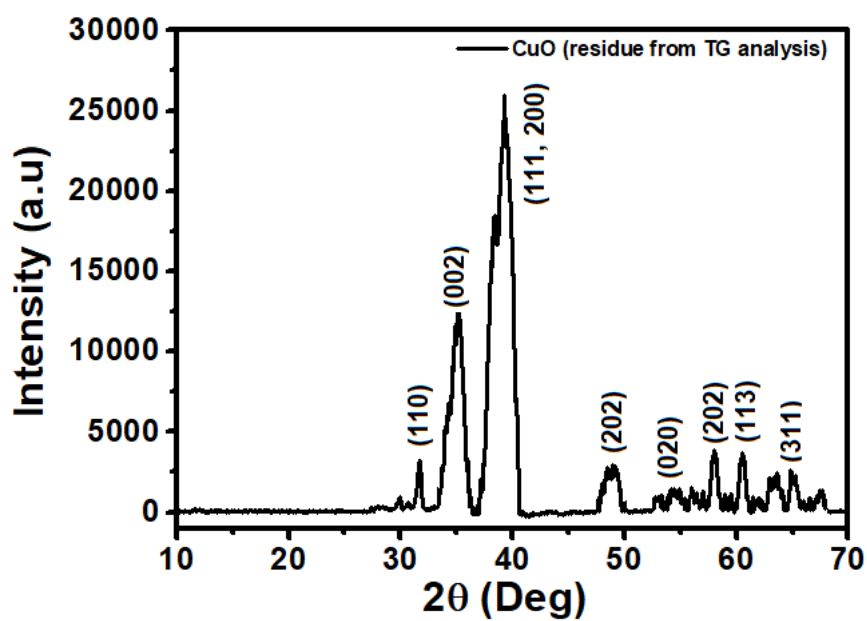
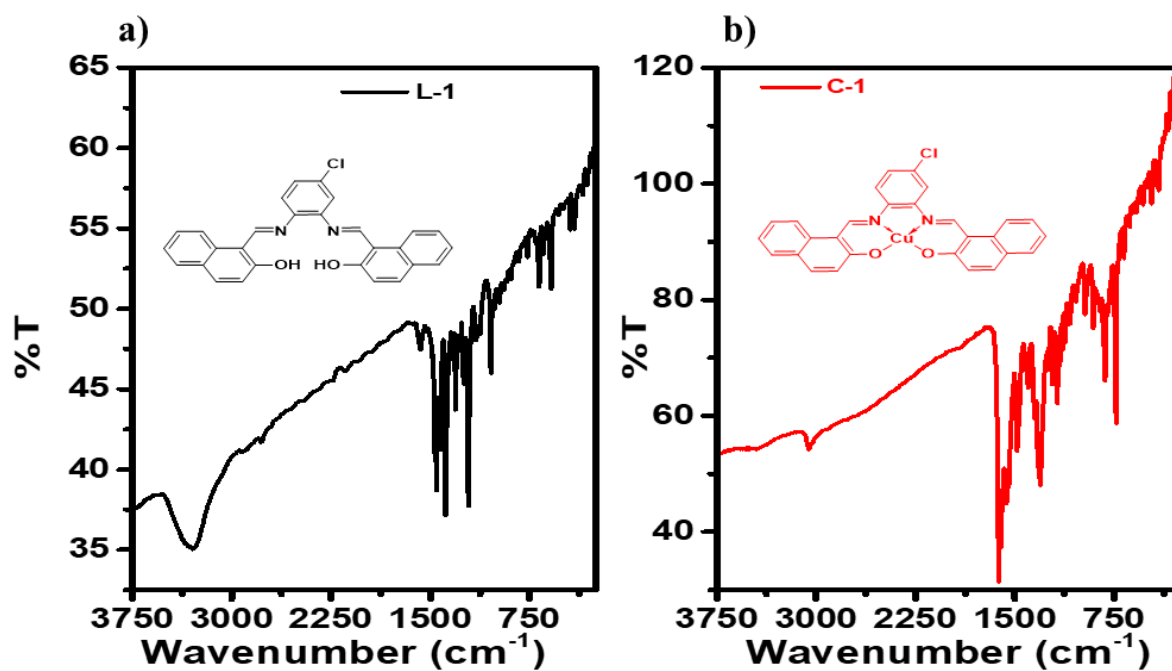


Figure S3. Powder XRD pattern of CuO residue formed from TG analysis.



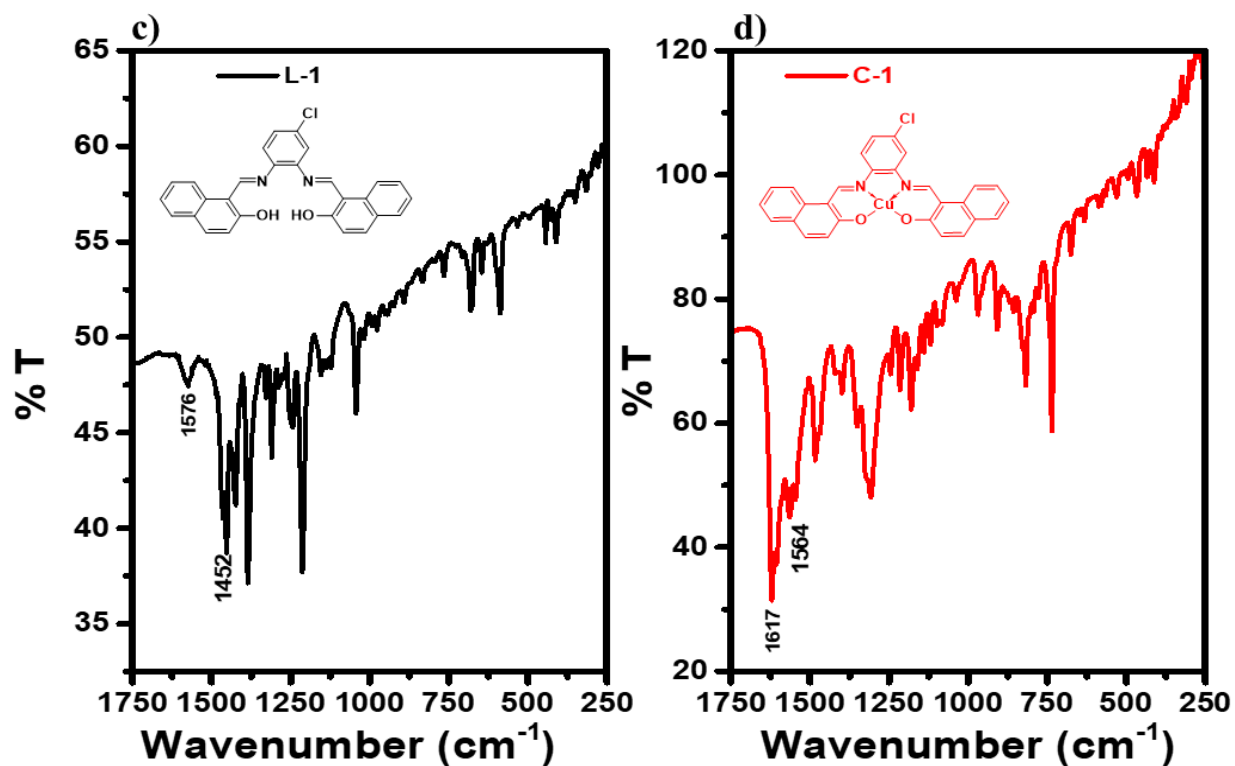
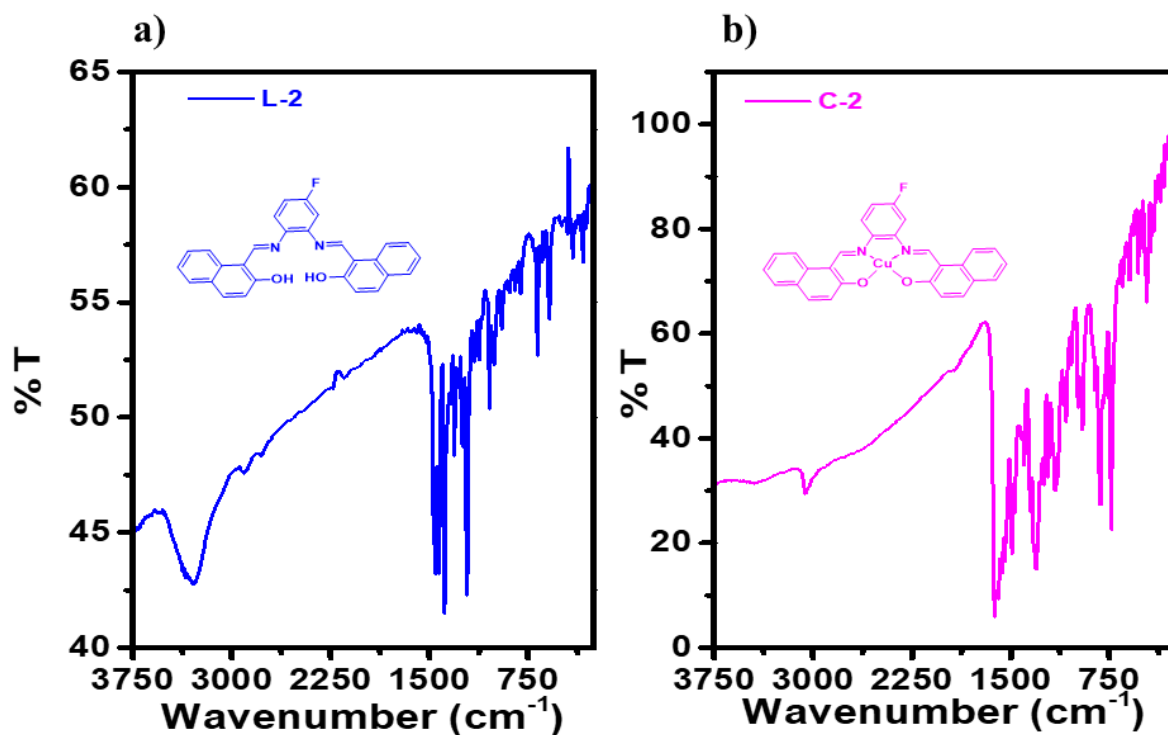


Figure S4. FTIR spectra of the L-1 ligand (a,c) and the C-1 complex (b,d).



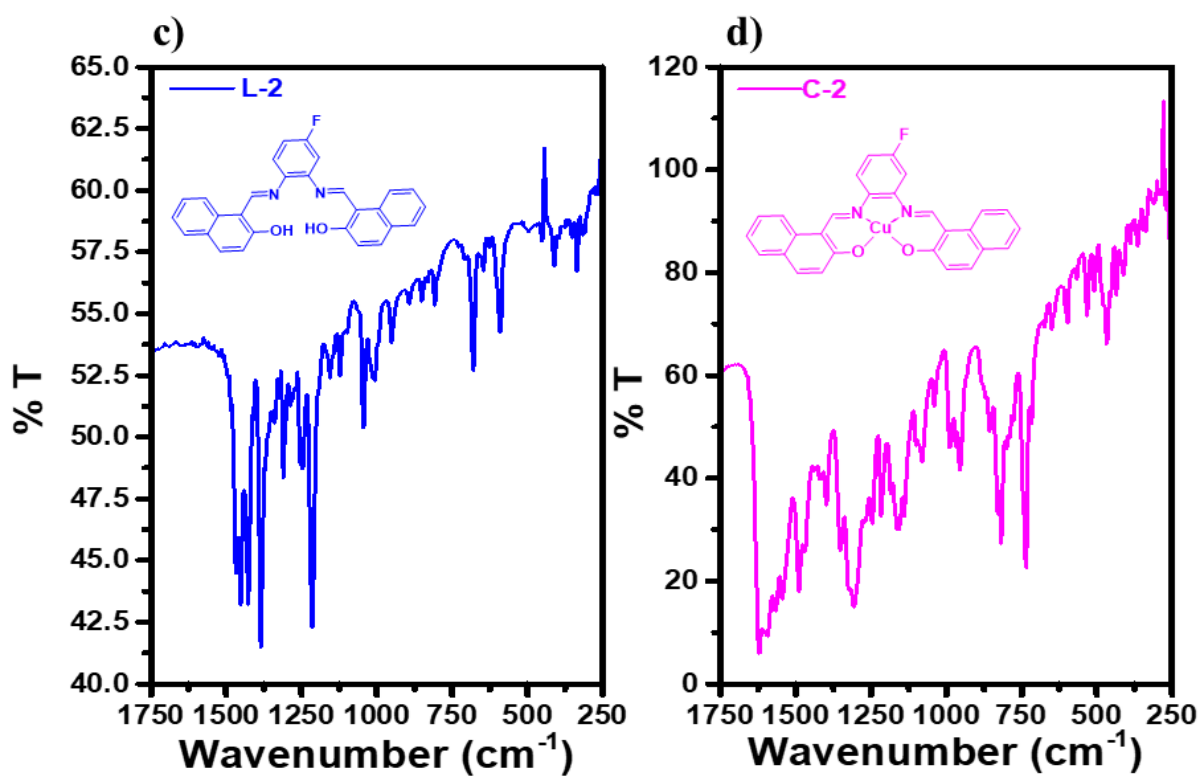


Figure S5. FTIR spectra of the L-2 ligand (a,c) and the C-2 complex (b,d).

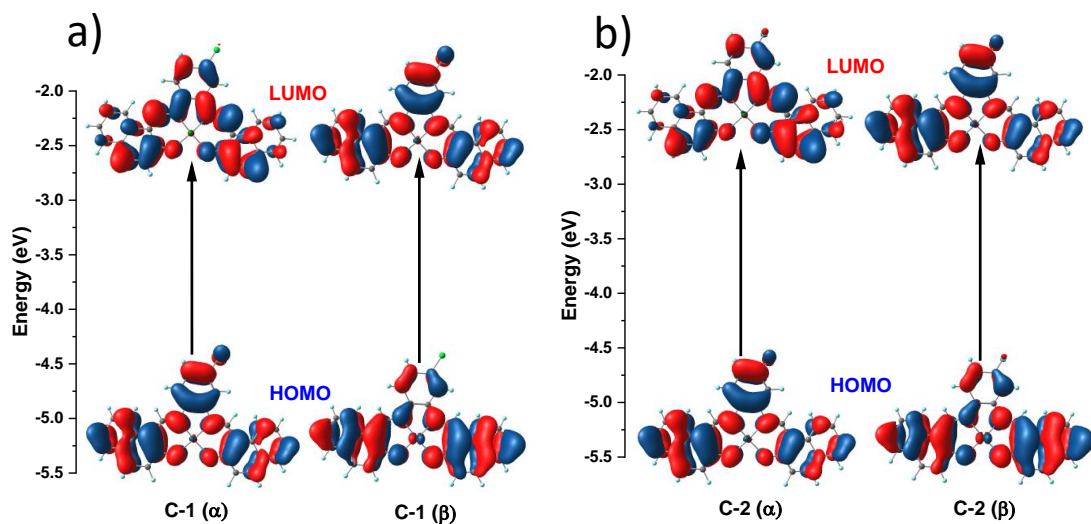


Figure S6 Frontier molecular orbitals for the C-1 (a) and C-2 complexes (b).

Table S2. Absorption energies (λ), oscillator strength (f), major transitions (MT), and percentage weight contribution for the B3LYP/6-31G (d, p) level of theory in combination with LANL2DZ basis set.

Molecules	State	λ (nm)	f	MT	%Ci
C-1	$S_0 \rightarrow S_9$	445	0.237	126A \rightarrow 127A	30
				111B \rightarrow 126B	7
				112B \rightarrow 126B	12
				113B \rightarrow 126B	8
				125B \rightarrow 127B	31
	$S_0 \rightarrow S_{10}$	439	0.162	126A \rightarrow 127A	10
				103B \rightarrow 126B	15
				109B \rightarrow 126B	7
				111B \rightarrow 126B	11
				112B \rightarrow 126B	15
				113B \rightarrow 126B	9
				120B \rightarrow 126B	5
				125B \rightarrow 127B	12
C-2	$S_0 \rightarrow S_9$	448	0.246	122A \rightarrow 123A	35
				109B \rightarrow 122B	16
				121B \rightarrow 123B	36
	$S_0 \rightarrow S_{10}$	440	0.085	122A \rightarrow 123A	5
				99B \rightarrow 122B	6
				100B \rightarrow 122B	13
				106B \rightarrow 122B	8
				109B \rightarrow 122B	45
				121B \rightarrow 123B	6

Table S3. Calculated HOMO and LUMO energies, and HLG (in eV) for the Cu (II) complexes.

Complexes	E_{HOMO} (eV)	E_{LUMO} (eV)	HLG
C-1	-5.42	-2.21	3.21
C-2	-5.36	-2.16	3.20