Unprecedented Copper(II) Coordination Induced Nucleophilic Cleavage of Quinoxaline Heterocycle: Structural and Computational Studies†

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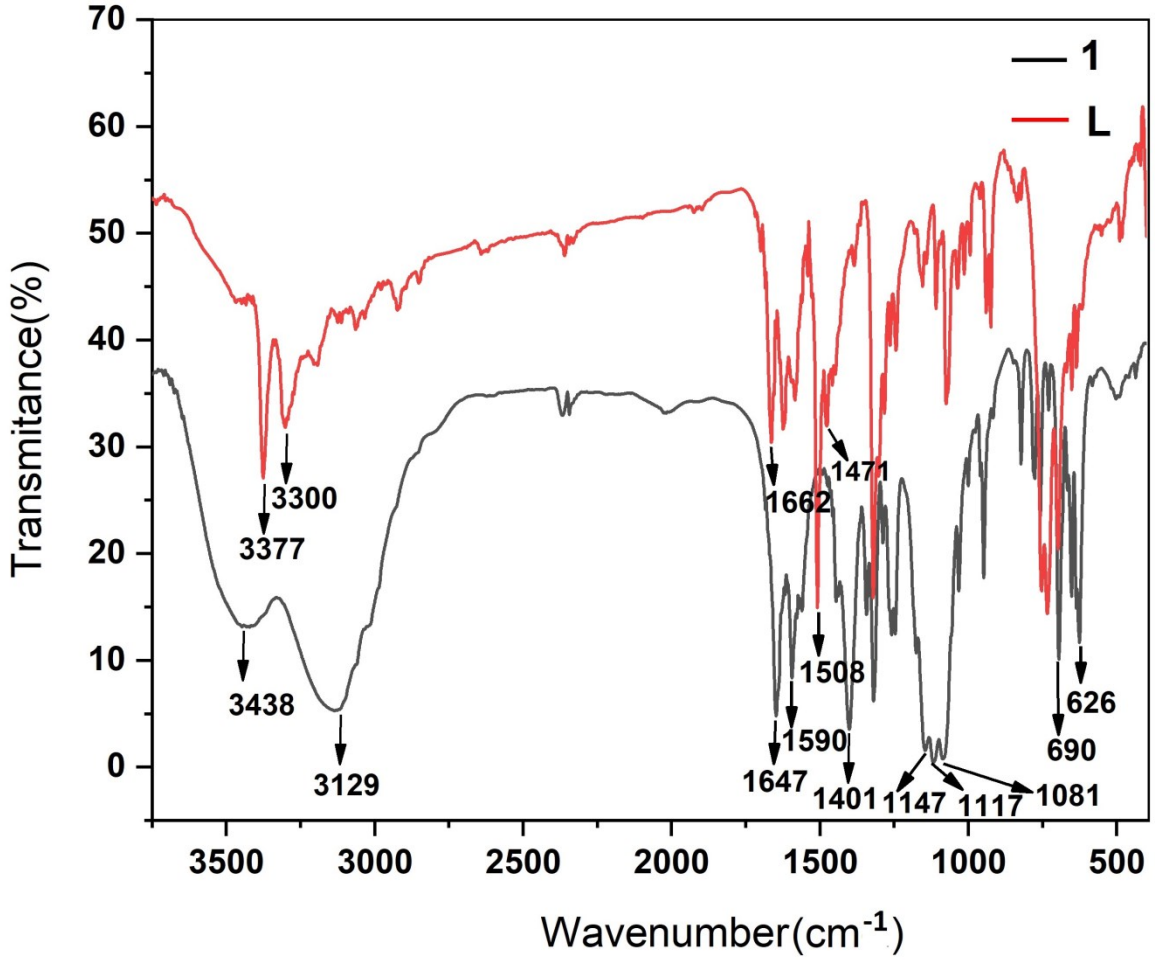

Fig. S1. FT-IR spectra of the ligand, **L** and copper(II) complex **1**

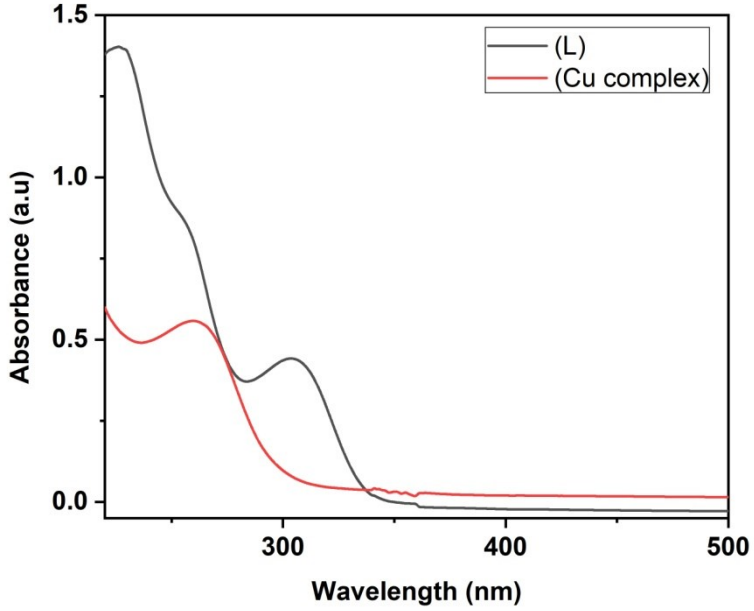

Fig. S2. UV-Vis spectra of the ligand, **L** and complex **1** in methanol

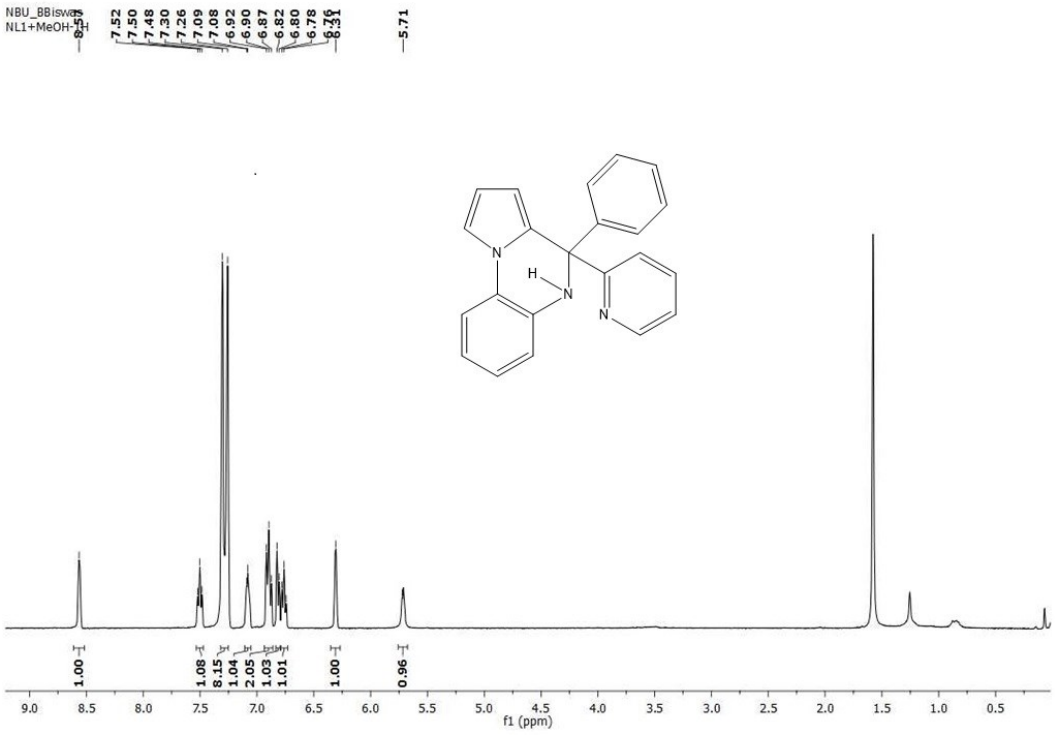

Fig. S3. ^{1}H NMR spectrum of the ligand, **L**

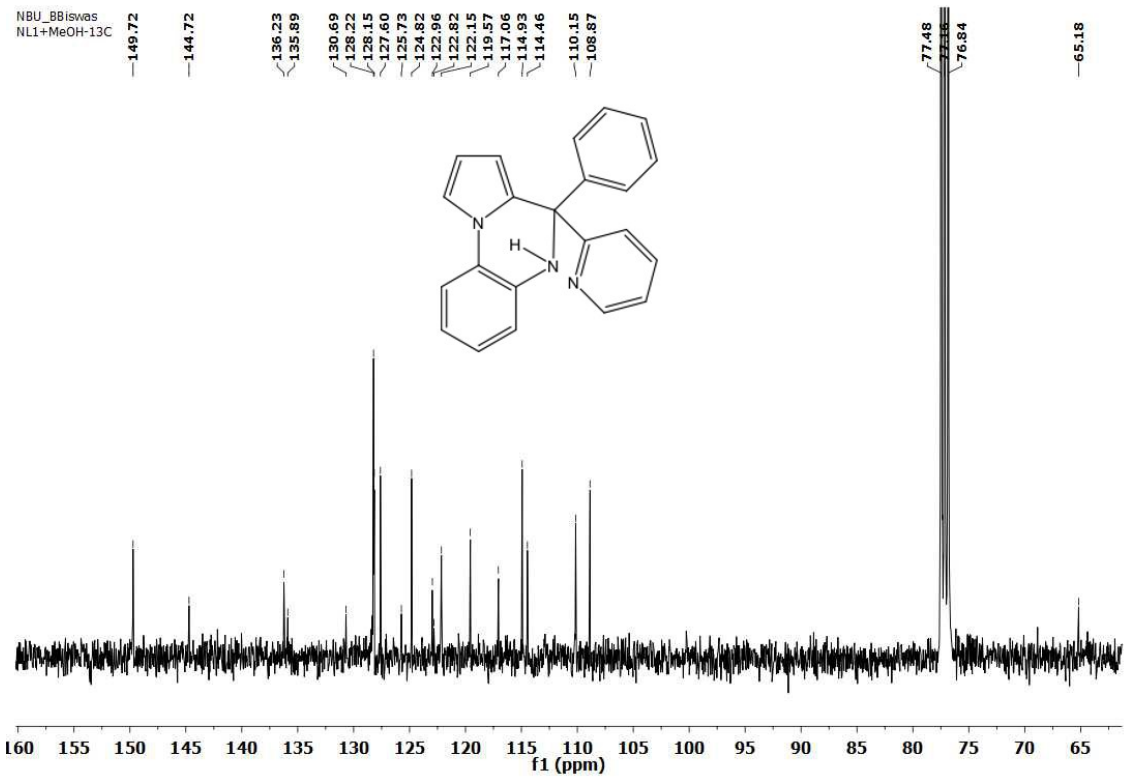

Fig. S4. Proton decoupled ^{13}C NMR spectrum of the ligand, **L**

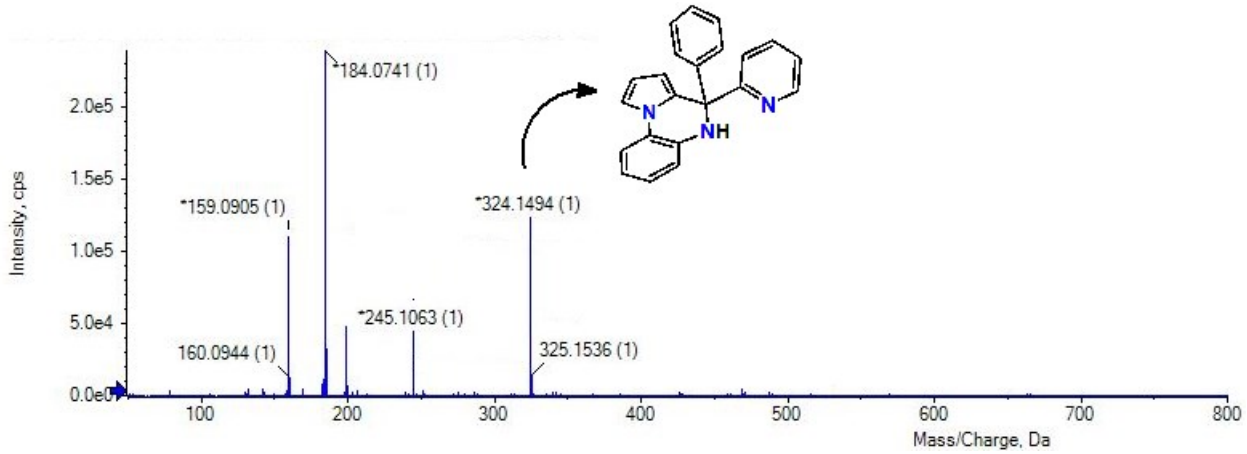

Fig. S5. ESI-MS spectrum of **L** in methanol

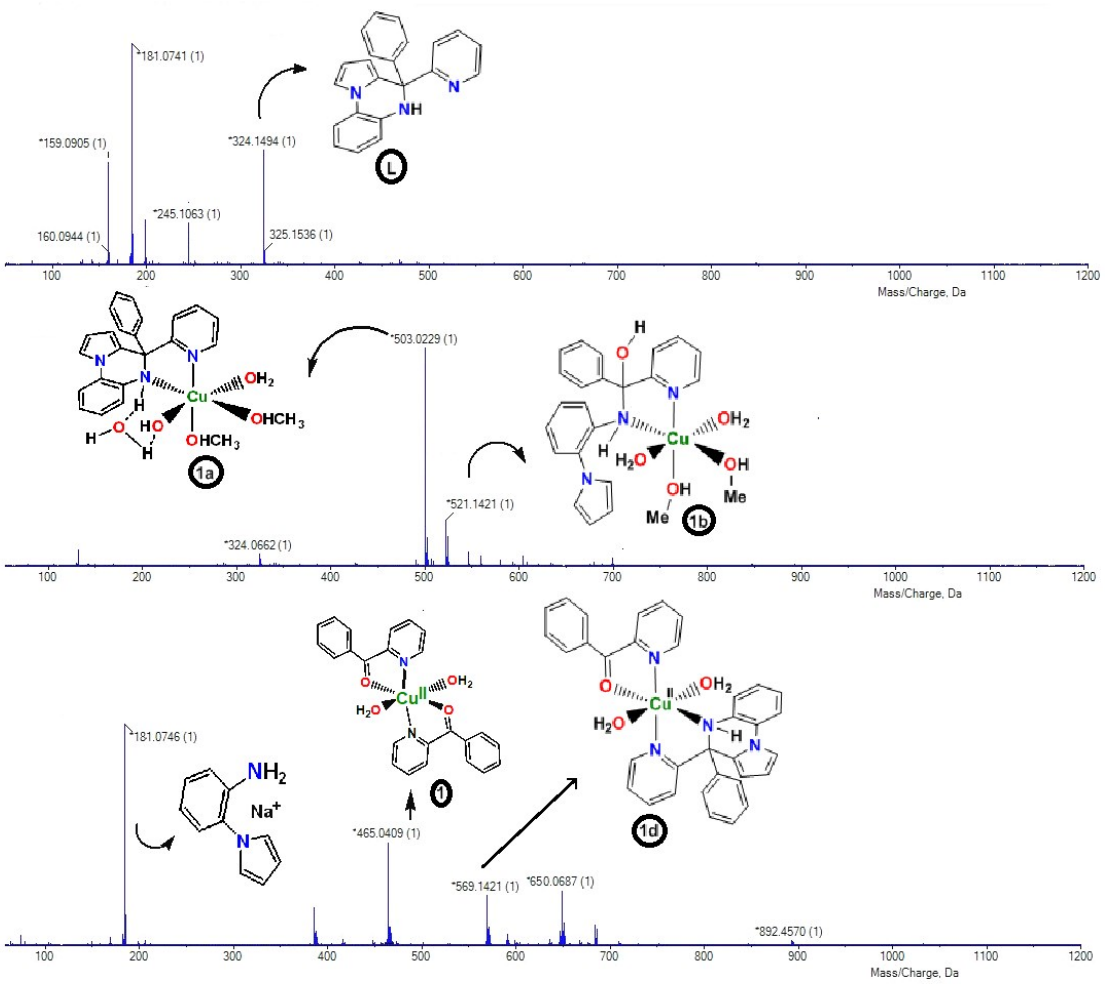

Fig. S6. Time-dependent ESI-MS spectral titration of **L** upon addition of Cu(II) ion in methanol

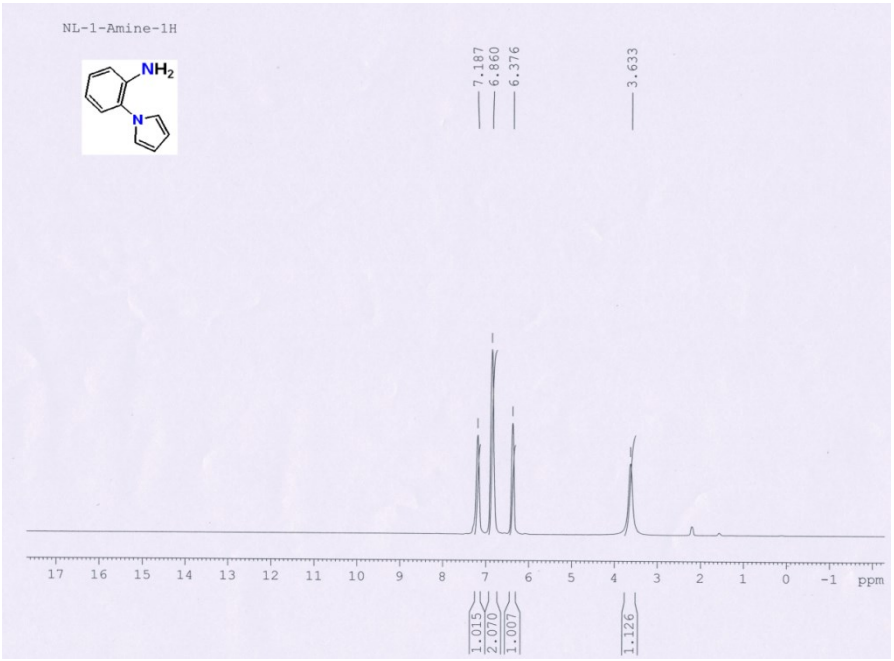

Fig. S7. ^{1}H NMR spectrum of 2-(1H-pyrrol-1-yl)aniline

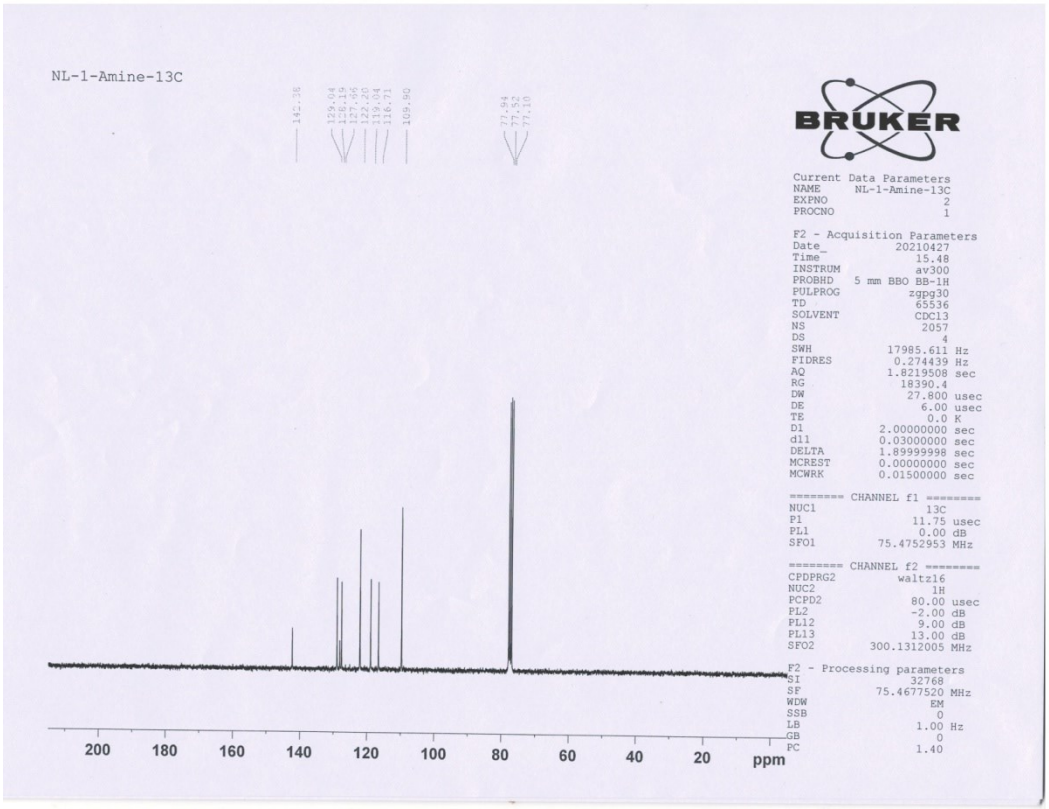

Fig. S8. ^{13}C NMR spectrum of 2-(1H-pyrrol-1-yl)aniline

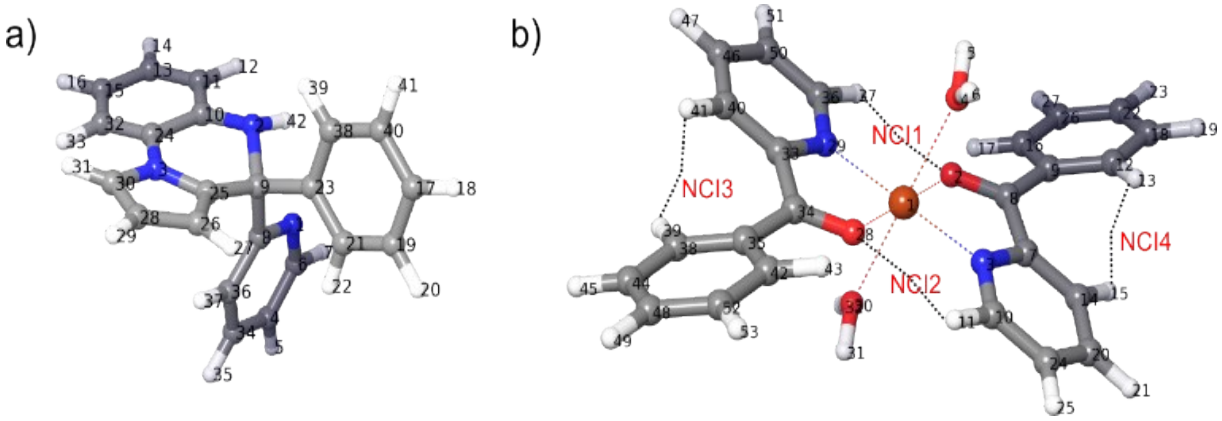

Fig. S9. Optimized geometries of a) Ligand and b) Complex (colored dashed lines denote coordination bonds, black dashed lines denote noncovalent interactions)

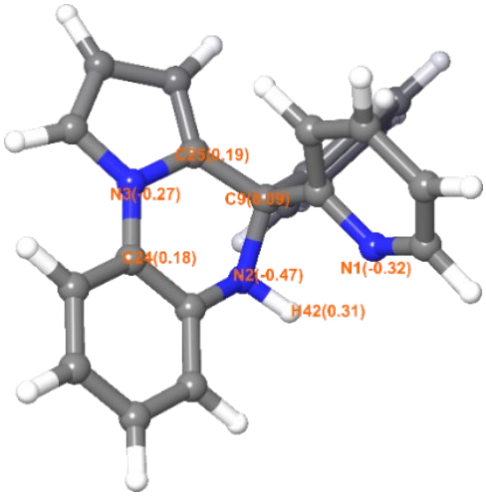

Fig. S10. Atom charges (numbers in parenthesis) of the selected atoms of Ligand.

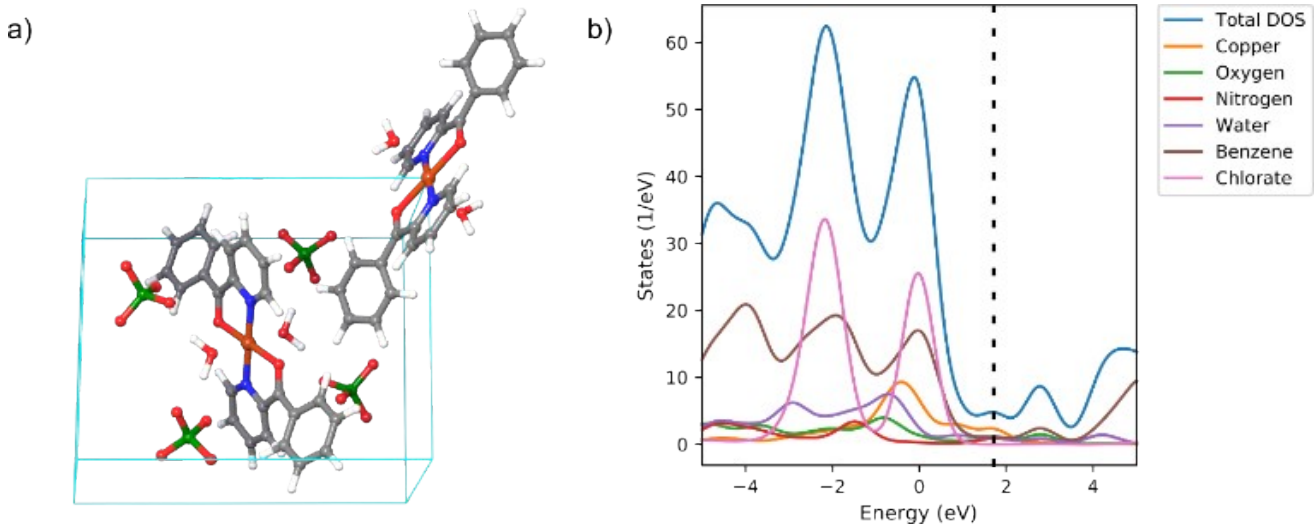

Fig. S11. a) Optimized crystal structure and b) PDOS of the crystal structure of complex.

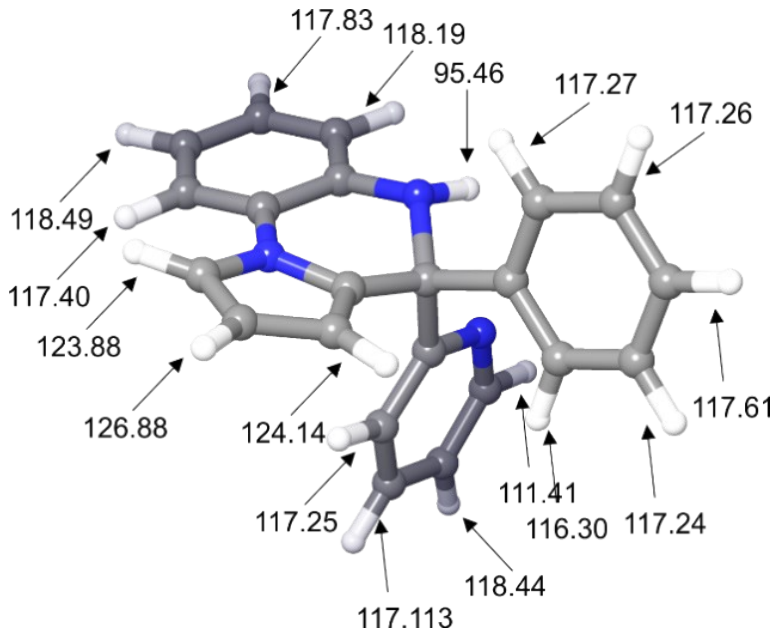

Fig. S12. H-BDE values of the Ligand.

Table S1. Selected bond lengths (Å) and bond angles (°) for **L**.

	Bond lengths		
C1-N1	1.3396(17)	C18-N2	1.3998(16)
C5-N1	1.3353(18)	C13–N3	1.3764(16)
C6-N2	1.4754(16)	C16-N3	1.376(2)
C17-N3	1.4070(18)		
	Bond angles		
N1-C1-C6	114.89(11)	N2-C6-C7	109.77(10)
N2-C6–C1	109.56(10)	N3-C13-C6	118.27(12)
N2-C6–C13	106.84(10)	N3-C17-C18	116.69(11)
N3-C16-C15	107.83(14)	N3-C17-C22	122.53(13)
N2-C18-C17	119.72(12)	N2-C18-C19	122.04(12)
C6-N2-C18	116.31(10)	C13-N3-C16	108.60(12)

Table S2. Selected bond lengths (Å) and bond angles (°) for **1** obtained from X-ray structure & theoretical calculation [theoretical values are in parenthesis].

	Bond lengths		
Cu1-O1	2.013(2) [2.007]	Cu1-O2	1.963(2) [2.105]
Cu1-N1	2.377(3) [2.052]		
	Bond angles		
O1-Cu1-O2	85.79(9) [71.996]	O2-Cu1-N1	94.33(10)[88.986]
O1-Cu1-N1	81.08(9) [128.826]	O2-Cu1-O2*	180.0 [161.548]
O1-Cu1-O1*	180.0 [86.664]	O2-Cu1-N1*	85.67(10)[89.125]
O1-Cu1-O2*	94.21(9) [99.962]	N1-Cu1-N1*	180.0 [108.378]
O1-Cu1-N1*	98.92(9) [92.365]		
	Torsion angle, benzimidazole···Ph		
N1–C5–C6–O1	10.24	C4–C5–C6–C7	13
C5–C6–C7–C8	32.06		

Table S3. Solubility parameter,δ [$MPa^{1/2}$], for Ligand and frequently used excipients.

Molecules	δ [$MPa^{1/2}$]
Ligand	20.660
PVP	18.515
Maltose	28.564
Sorbitol	32.425