Classical hydrogen bondings and stacking of chelate rings in new copper(II) complexes

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Supplaymentary Information

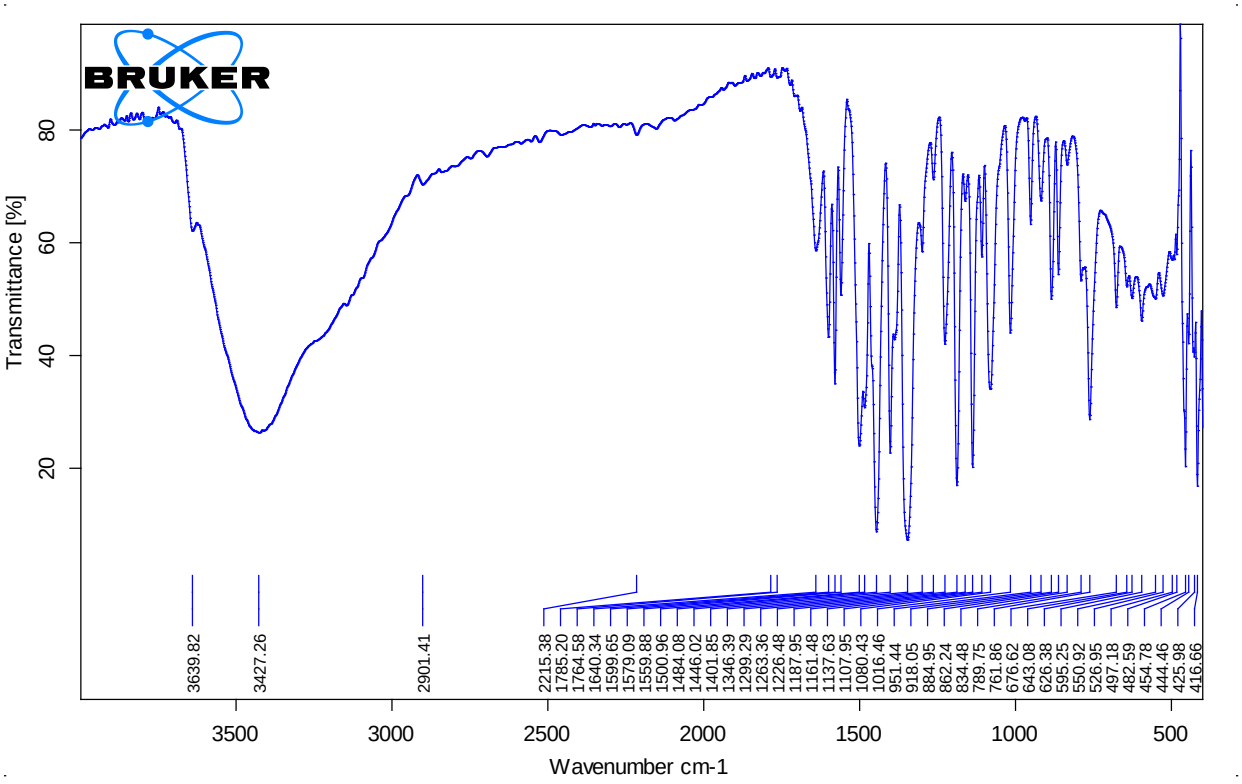


Fig. S1 IR spectrum of **HL**.

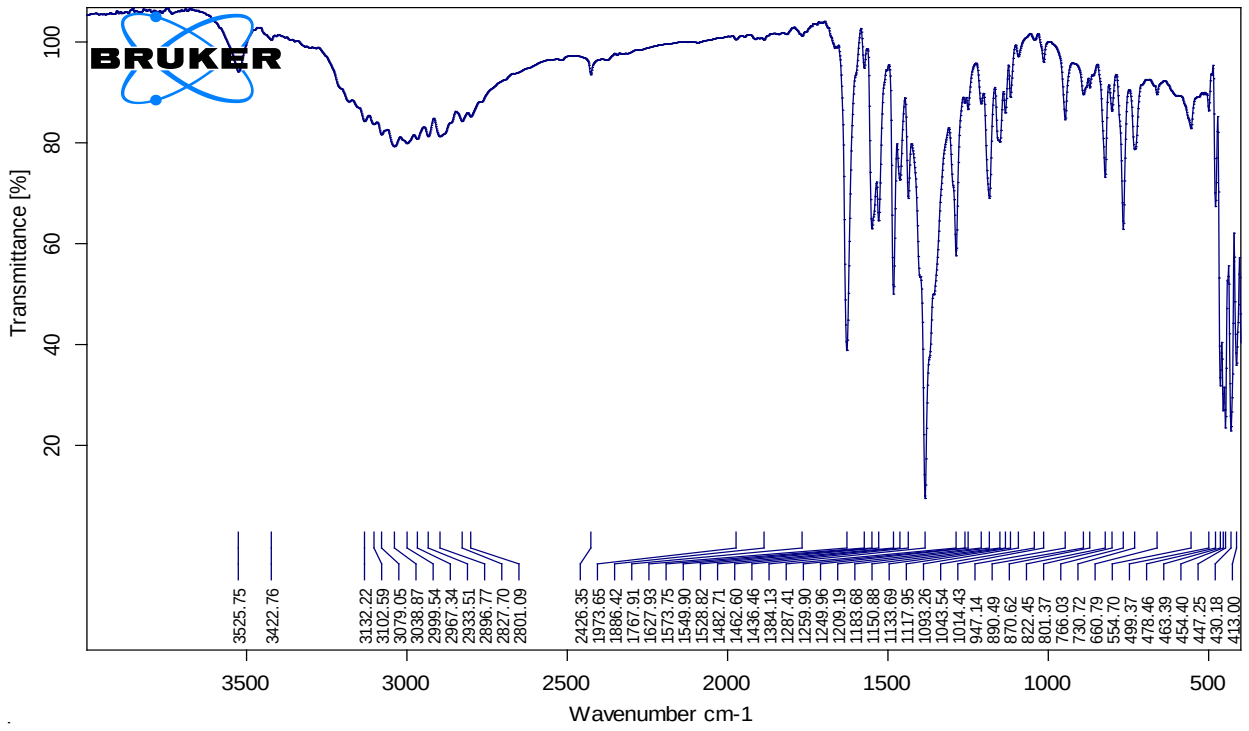


Fig. S2 IR spectrum of Complex **1**.

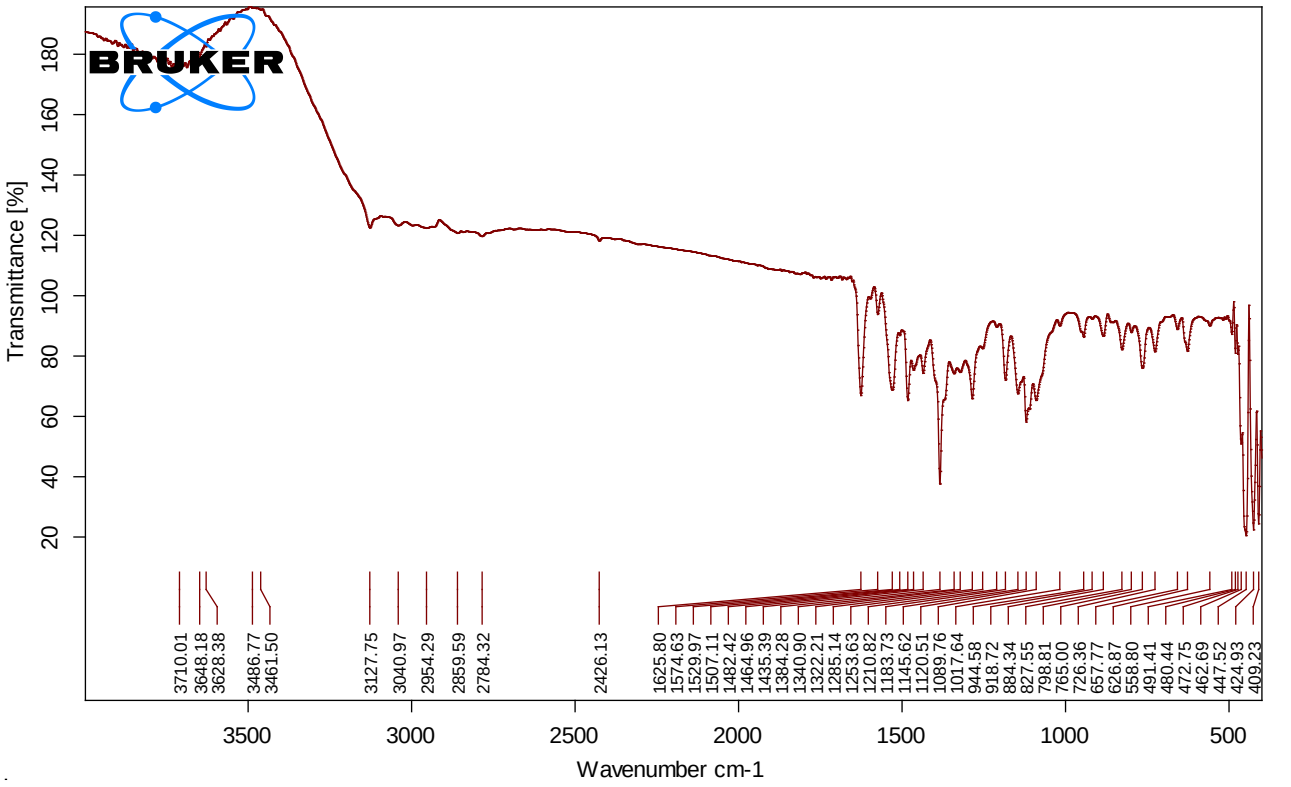


Fig. S3 IR spectrum of complex **2**.

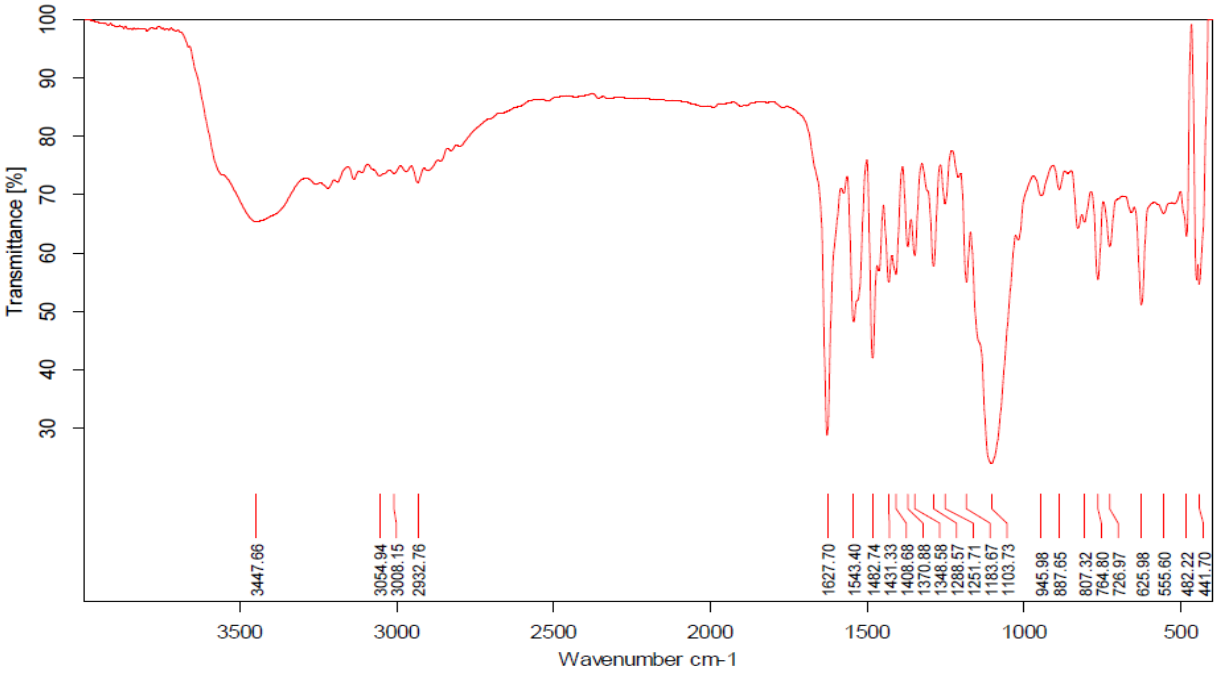


Fig. S4 IR spectrum of complex **3**.

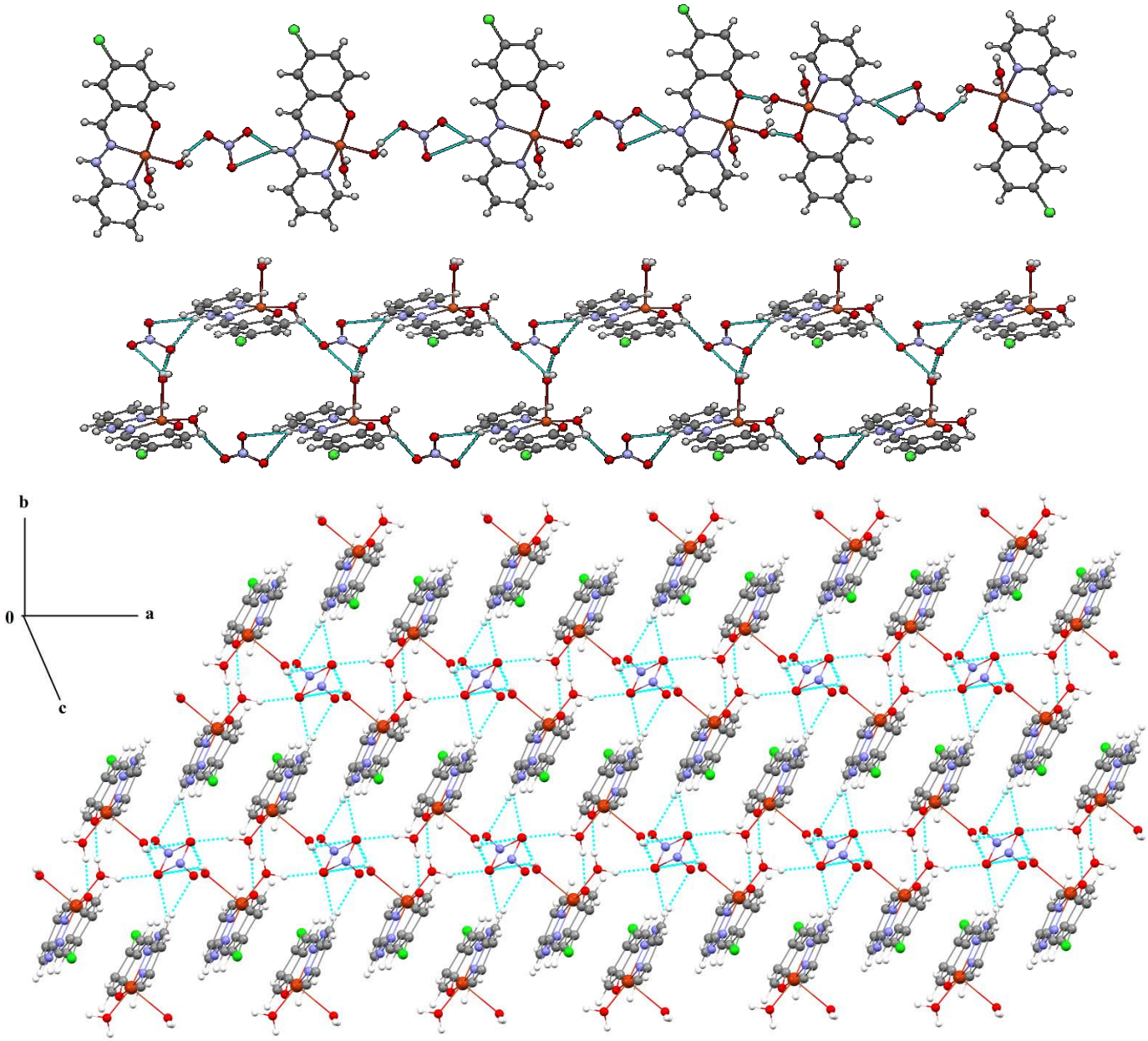


Fig. S5 Supramolecular structure of complex **2**. Top: 1D Middle: 2D and Bottom: 3D layer.

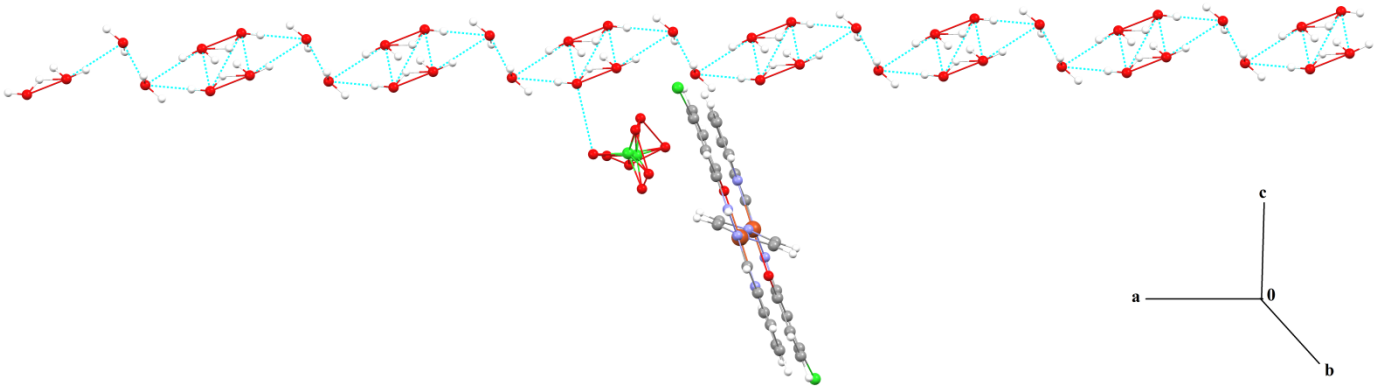
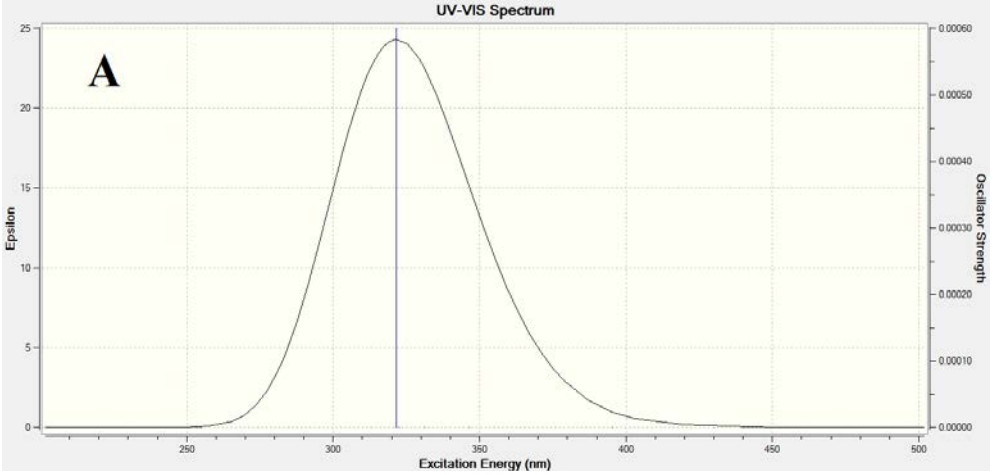
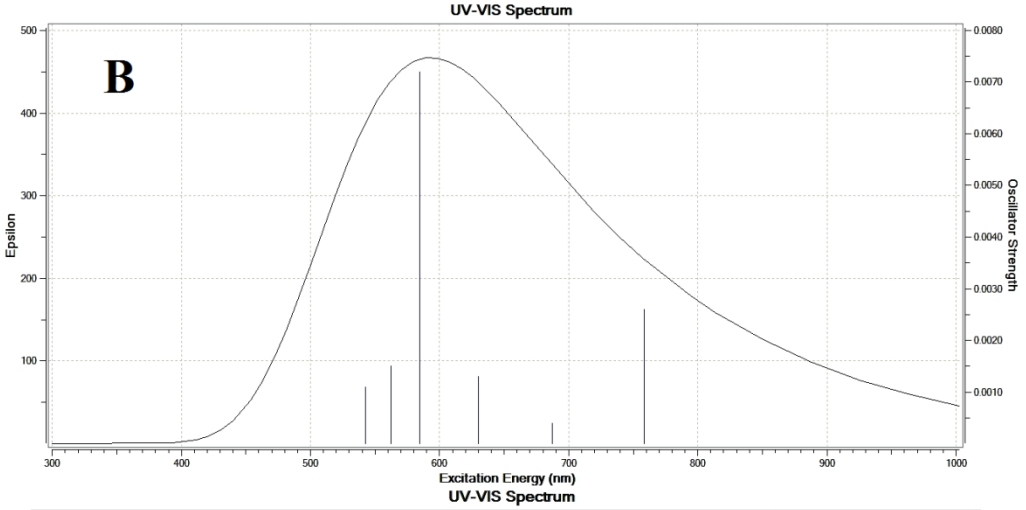
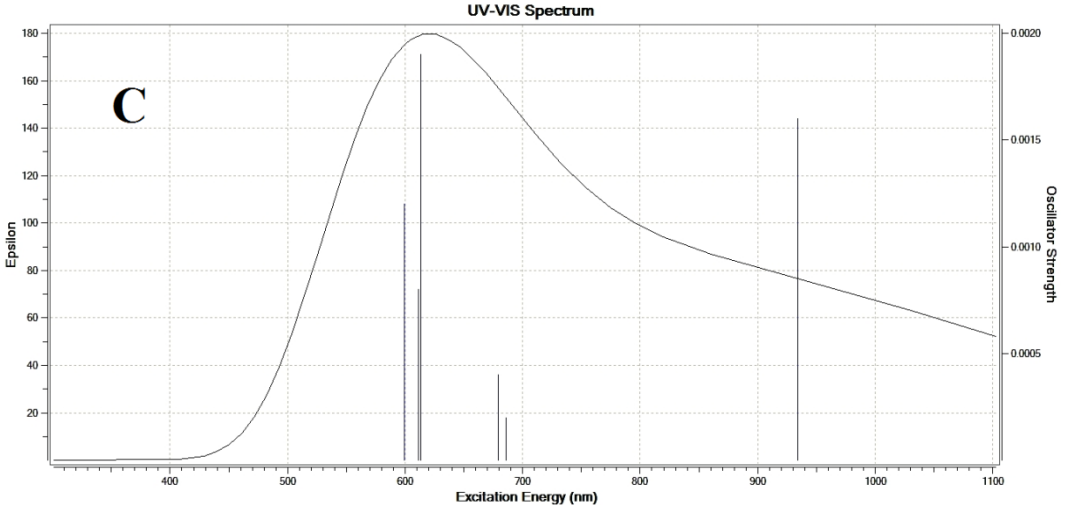


Fig. S6 1D polymeric chain bifurcated hydrogen bonding as well as oxygen-oxygen interaction of complex **3**.


UV-VIS Spectrum
A
Epsilon
Oscillator Strength
Excitation Energy (nm)


UV-VIS Spectrum
B
Epsilon
Oscillator Strength
Excitation Energy (nm)


UV-VIS Spectrum
C
Epsilon
Oscillator Strength
Excitation Energy (nm)

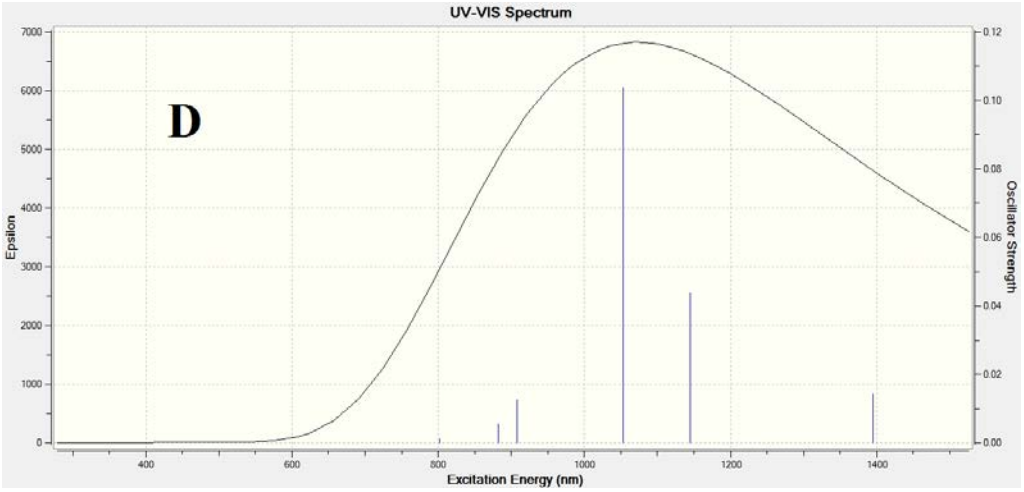
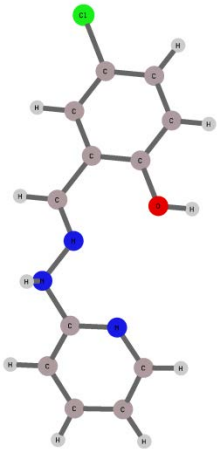
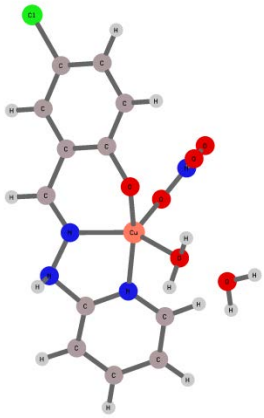


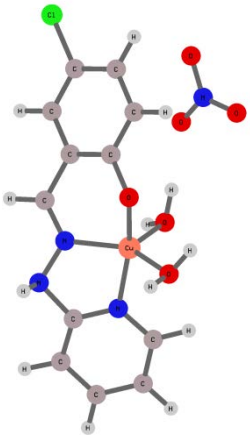
Fig. S7 DFT calculated UV-visible spectrum A Ligand, B Complex **1**, C Complex **2**, D Complex **3**.



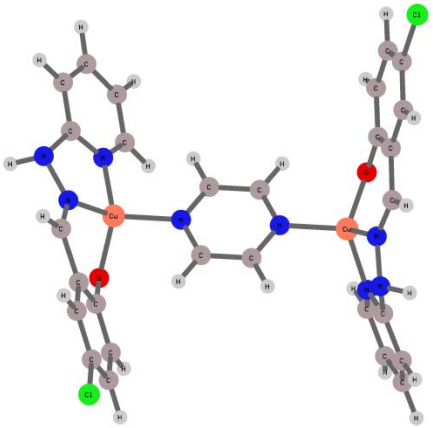
HL



Complex **1**



Complex **2**



Complex **3**

Fig. S8 DFT calculated optimized structure of **HL** and copper(II) complexes **1-3**.

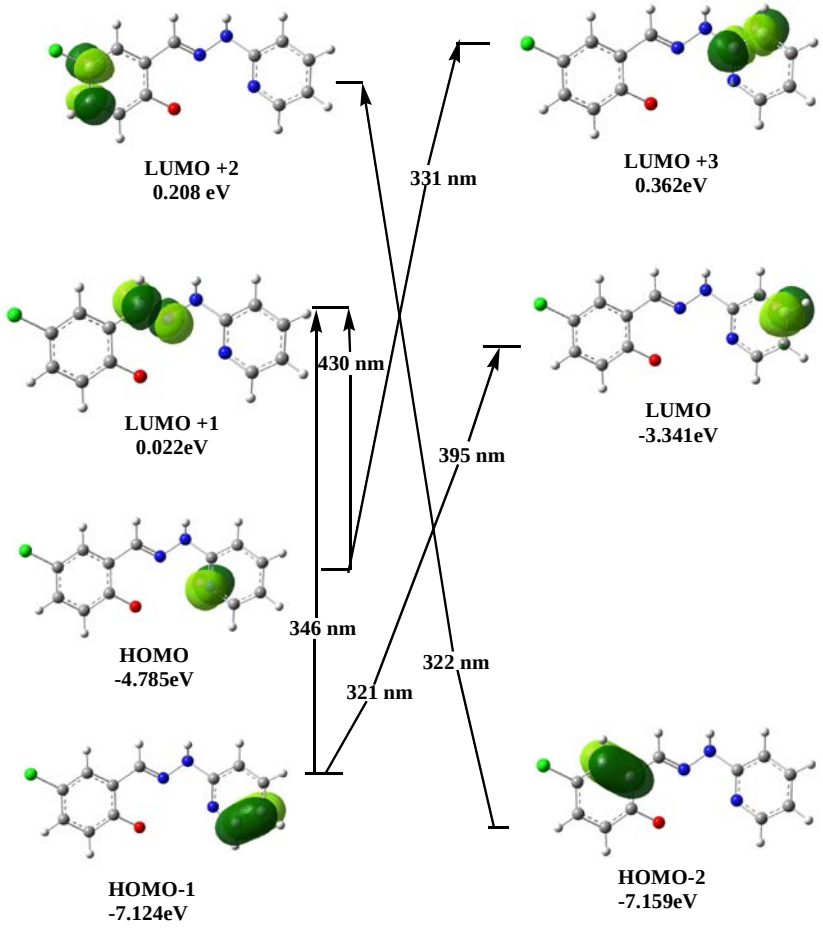


Fig. S9 DFT calculated HOMO-LUMO molecular orbital energy level diagram for **HL**.

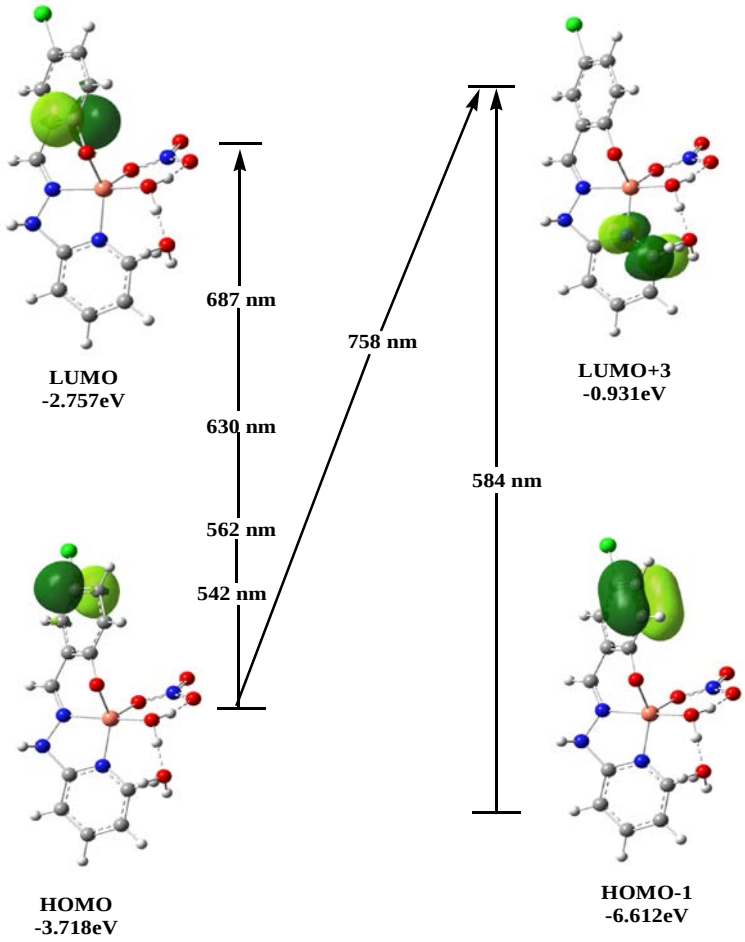


Fig. S10 DFT calculated HOMO-LUMO molecular orbital energy level diagram for complex **1**.

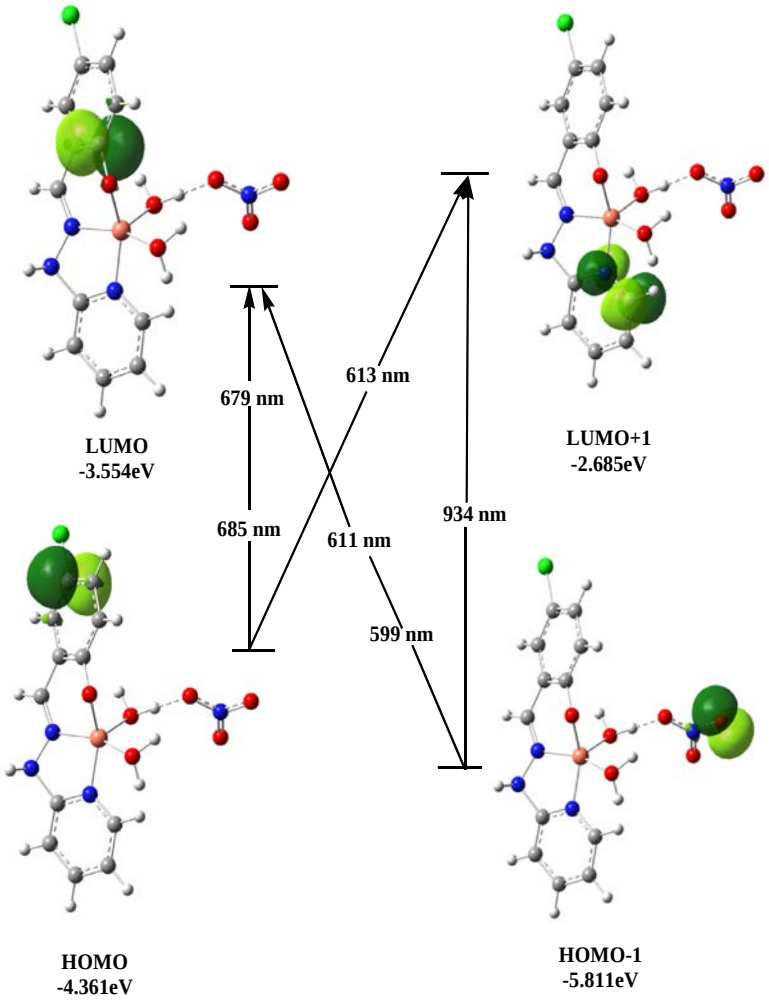


Fig. S11 DFT calculated HOMO-LUMO molecular orbital energy level diagram for complex **2**.

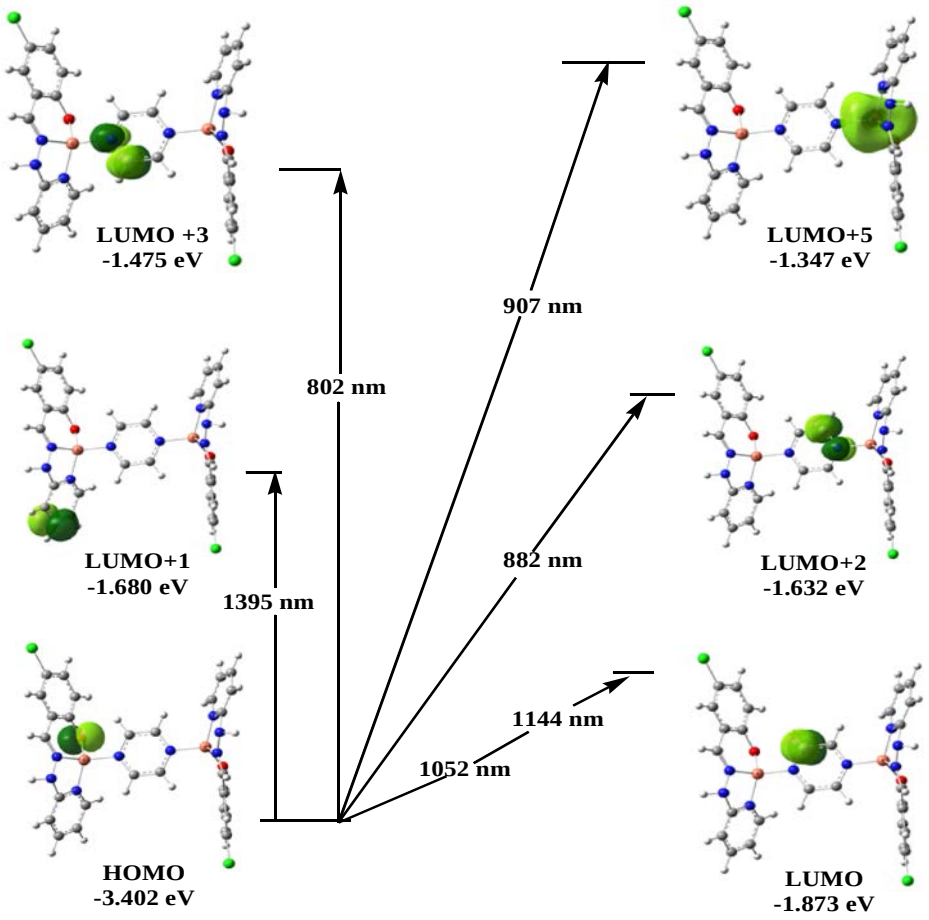


Fig. S12 DFT calculated HOMO-LUMO molecular orbital energy level diagram for complex **3**.