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

Yogendra Pratap Singh, Ram N. Patel*, Yogendra Singh, Duane Choquesillo-Lazarte, R. J. Butcher

a Department of Chemistry, A. P. S. University, Rewa (M.P.) 486003 INDIA
b Laboratorio de Estudios Cristalográficos, IACT, CSIC-Universidad de Granada, Av. de las Palmeras 4, E-18100 Armilla, Granada, Spain
c Department of Inorganic & Structural Chemistry, Howard University, Washington DC, 22031 USA

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