Supporting Information

for

On the importance of CH⋯X (X=O, π) interaction of a new mixed ligand Cu(II) coordination polymer: Structure, Hirshfeld surface and theoretical studies
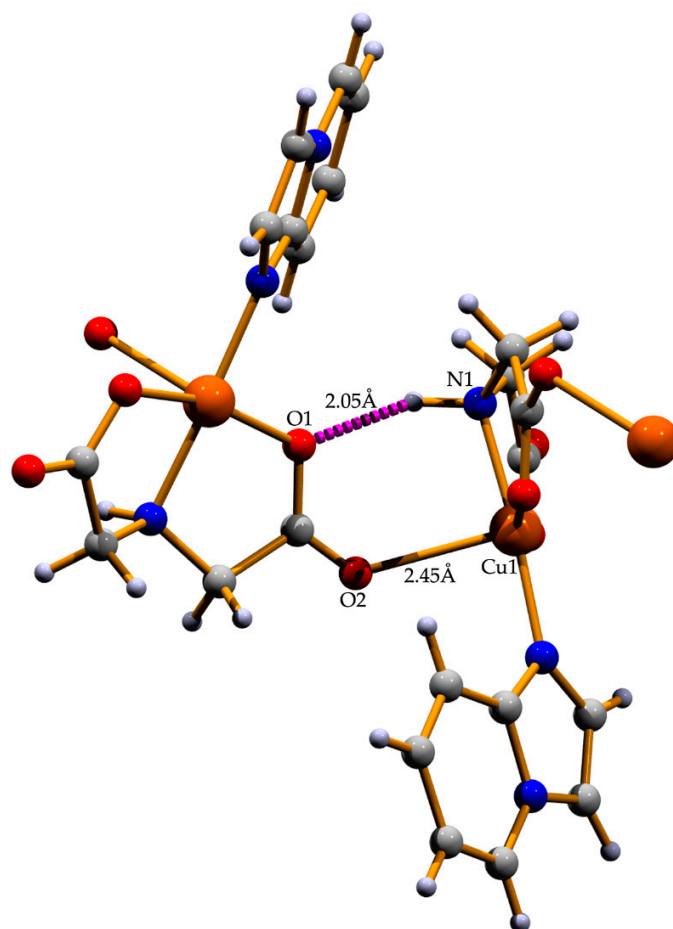
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Table S1. Selected Bond-lengths (Å) and angles (°).

|			
Cu(1)-N(1)	1.968(3)	Cu(1)-O(1)	1.956(2)
Cu(1)-N(2)	1.957(3)	Cu(1)-O(4)	1.949(2)
Cu(1)-O(2)	2.455(2)		
O(4)-Cu(1)-O(1)	163.90(10)	O(4)-Cu(1)-N(1)	84.84(11)
O(4)-Cu(1)-N(2)	96.73(11)	O(1)-Cu(1)-N(1)	84.66(10)
O(1)-Cu(1)-N(2)	94.64(11)	N(2)-Cu(1)-N(1)	175.60(12)

Figure S1. Perspective view of the N–H···O bonded motif and the symmetry generated coordination bond that forms chain network.
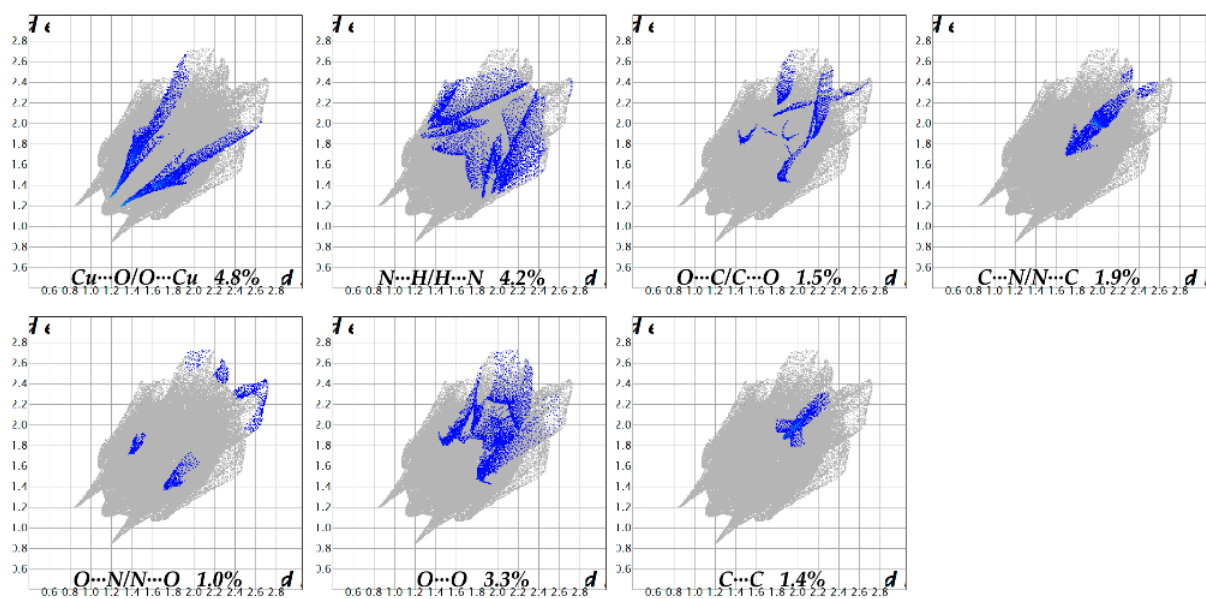
Figure S2. Fingerprint plots that resolved into diverse interactions within the compound showing percentages of contacts contributed less than 5% to the total Hirshfeld surface area of the molecules.
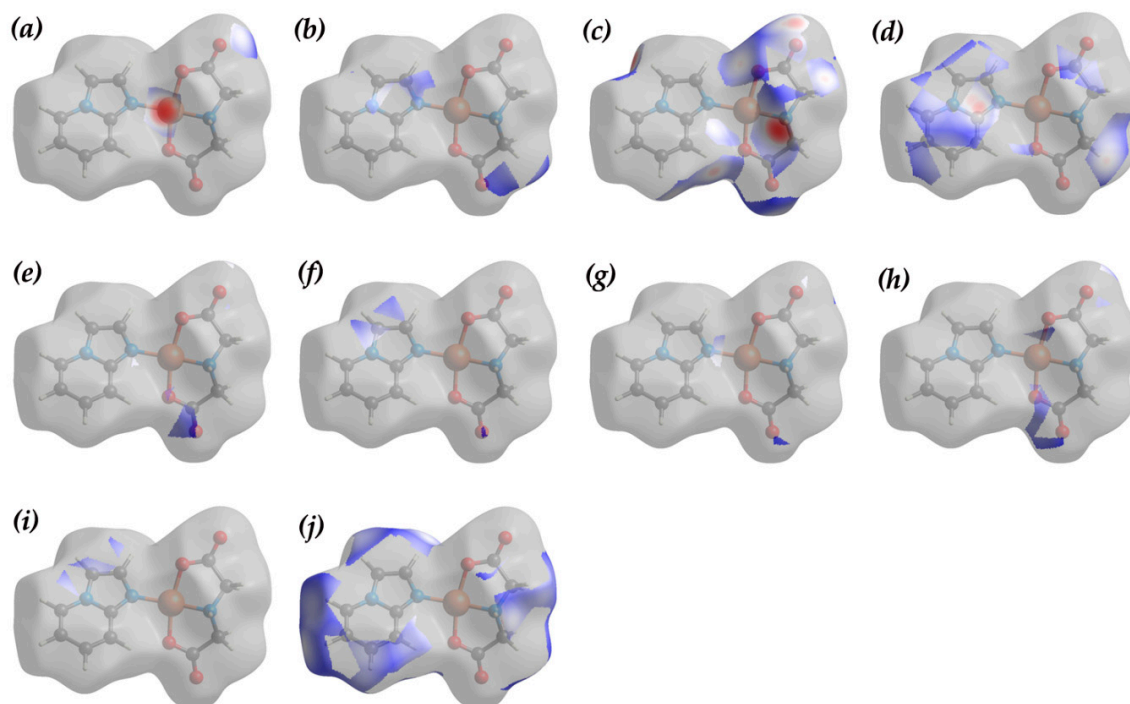
Figure S3. Decomposed d_{norm} plots for Cu···O/O···Cu (a); N···H/H···N (b); O···H/H···O (c); C···H/H···C (d); O···C/C···O (e); C···N/N···C (f); O···N/N···O (g); O···O (h); C···C (i) and H···H (j) contacts contributed to the total Hirshfeld surface area of the molecules.
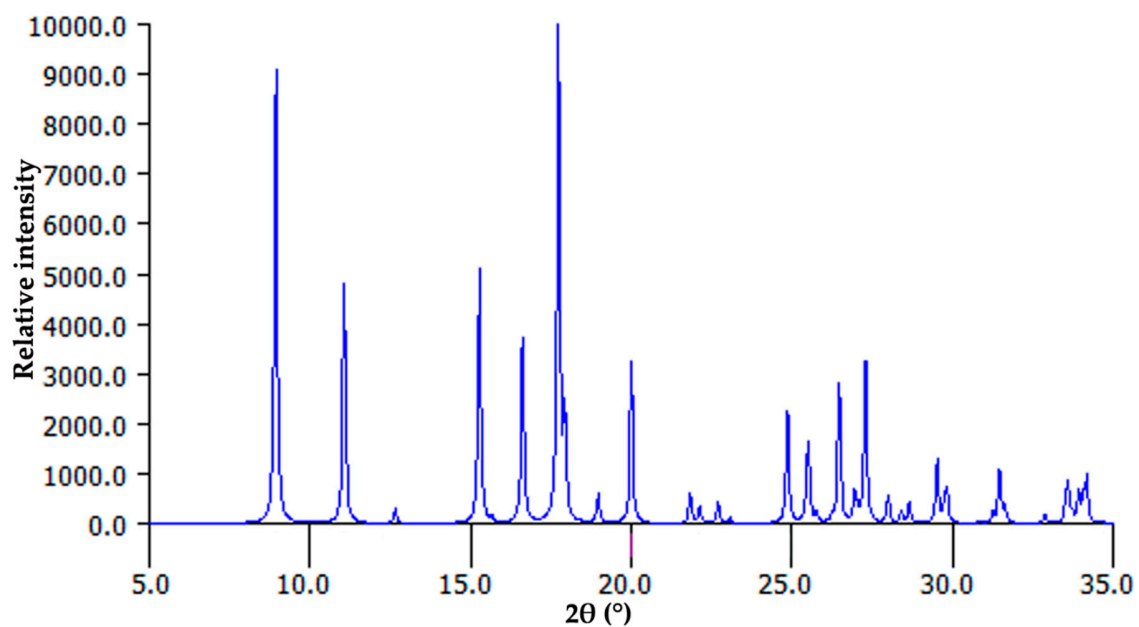
Figure S4. Calculated powder diffraction pattern of the title compound.