Supporting Informations

Mononuclear copper (II) Schiff base complex: synthesis, structure, electrical analysis and protein binding study

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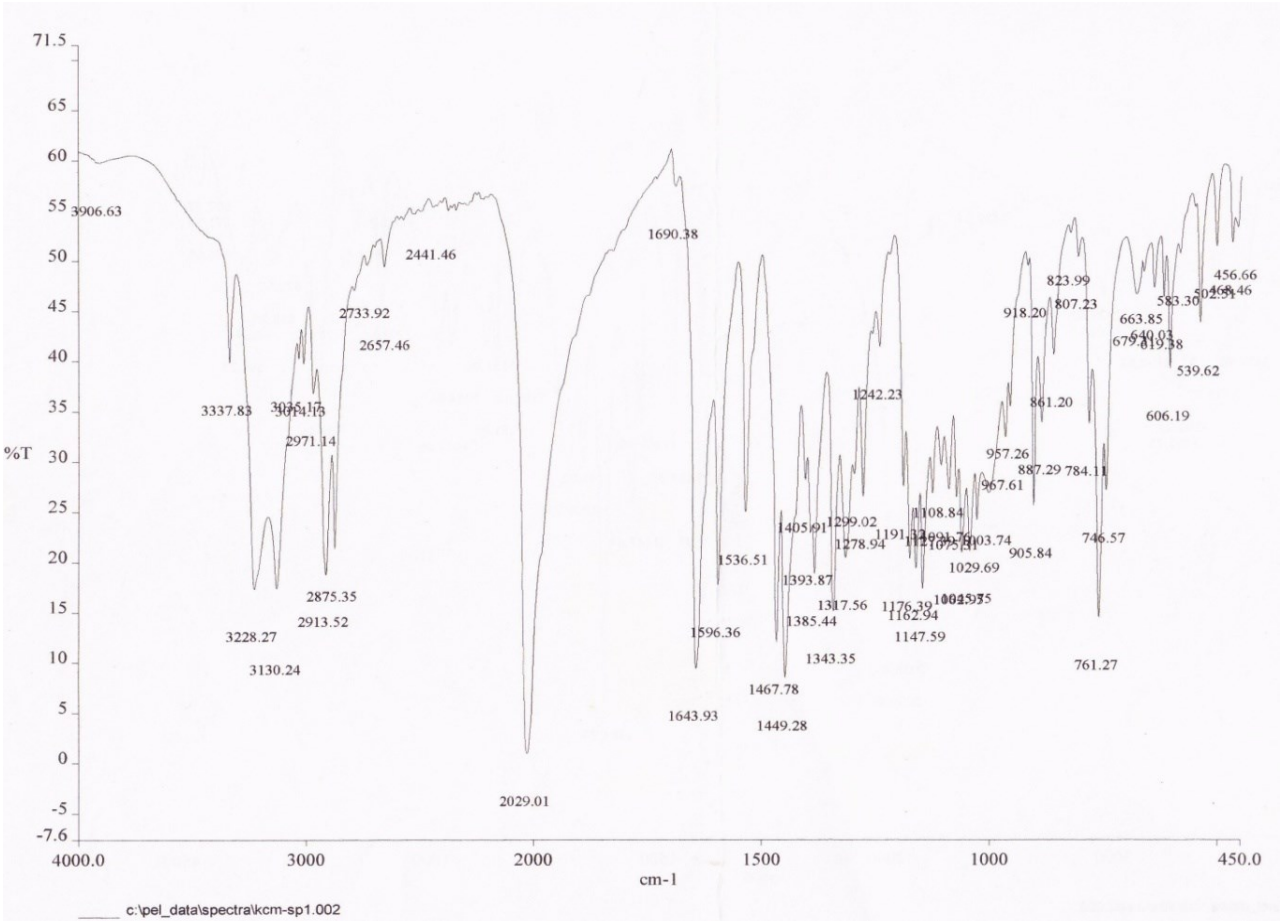
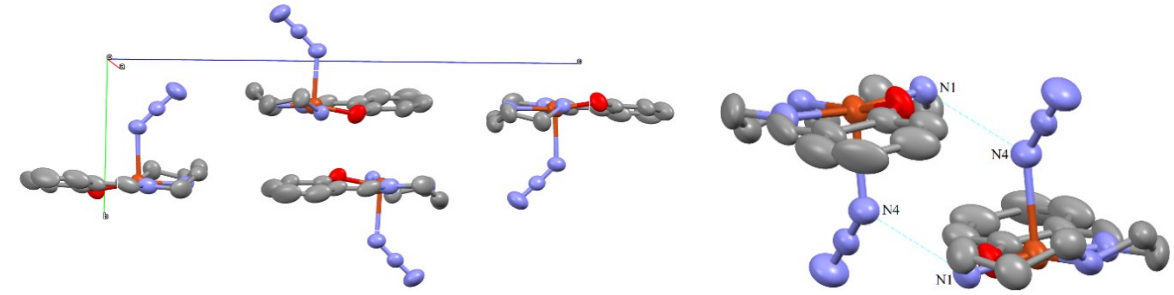
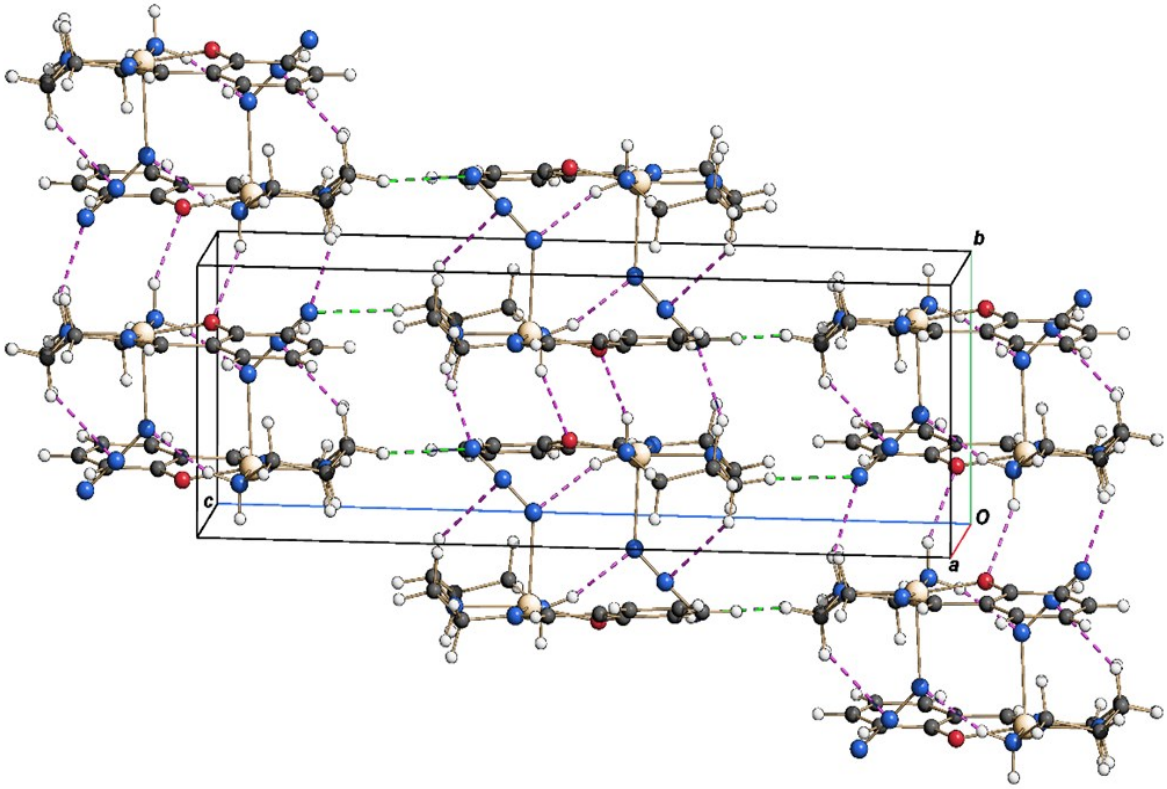


Fig. S1 FT-IR spectrum of complex **1**



(a) **(b)**



(c)

Fig. S2 (a) Inner view of unit cell. **(b)** Intermolecular hydrogen bonds between two antiparallel mononuclear units [The symmetry code is 1-x, -y, -z]. **(c)**packing diagram of **1** showing the formation of one-dimensional chains parallel to the *b* axis through N−H…N and N−H…O hydrogen bonds (purple dashed lines), linked into a layer parallel to the (1 0 1) plane via C−H…N hydrogen bonds (green dashed lines).

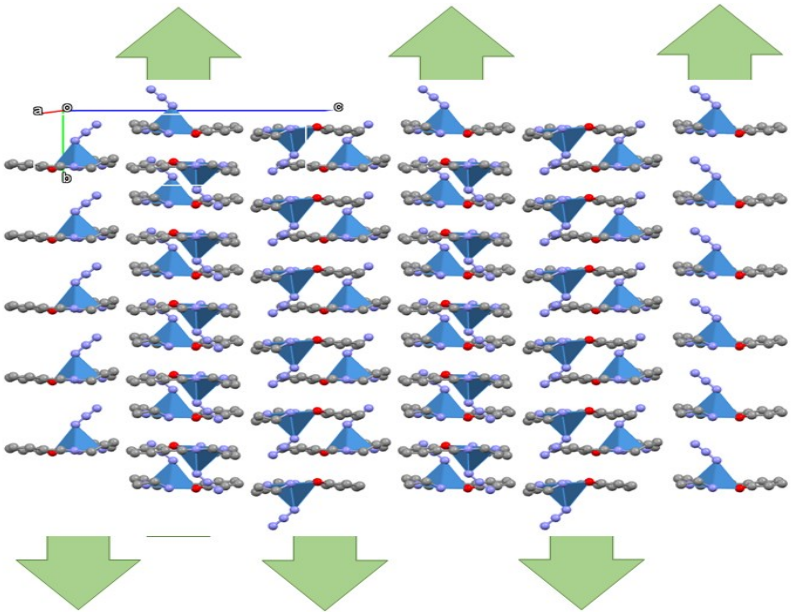


Fig. S3 Antiparallel 1D chains propagates along the c direction of unit cell and the green arrows indicates the relative direction of different 1D chains to form 2D sheet like frameworks.

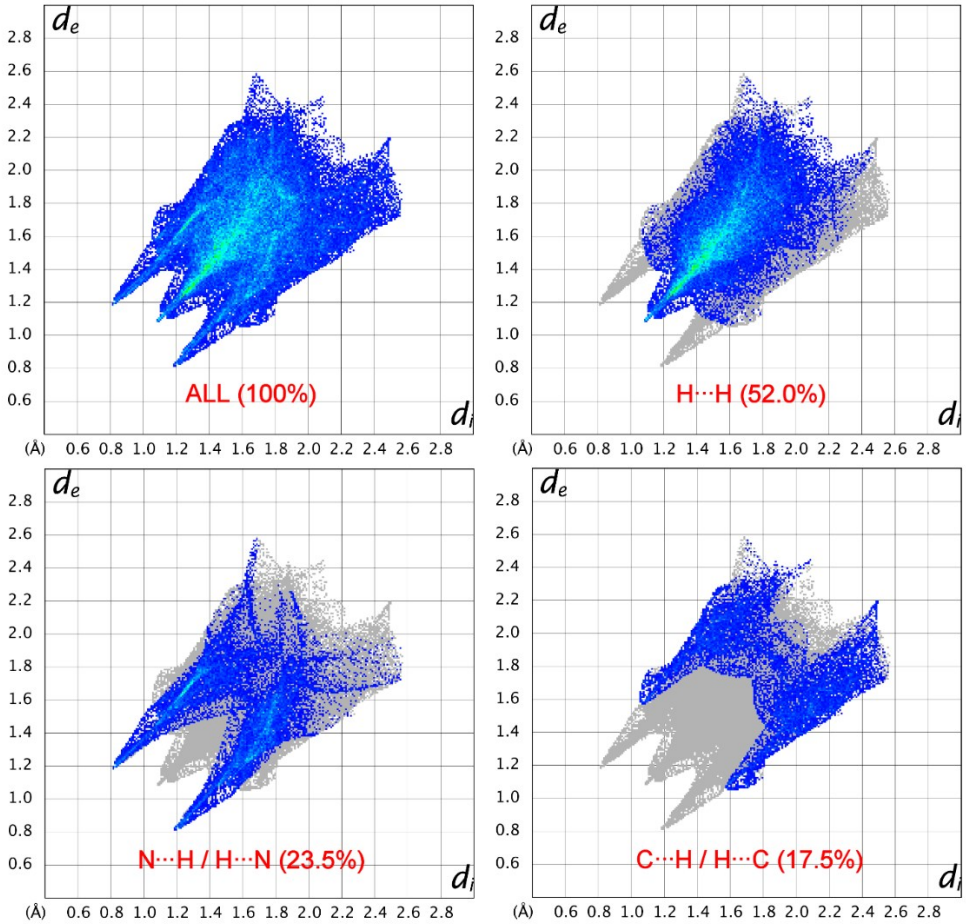


Fig. S4. The two-dimensional fingerprint plot of **1** showing the main interactions and their percentage contributions (d_i is the closest internal distance from a given point on the Hirshfeld surface, d_e is the closest external contact).

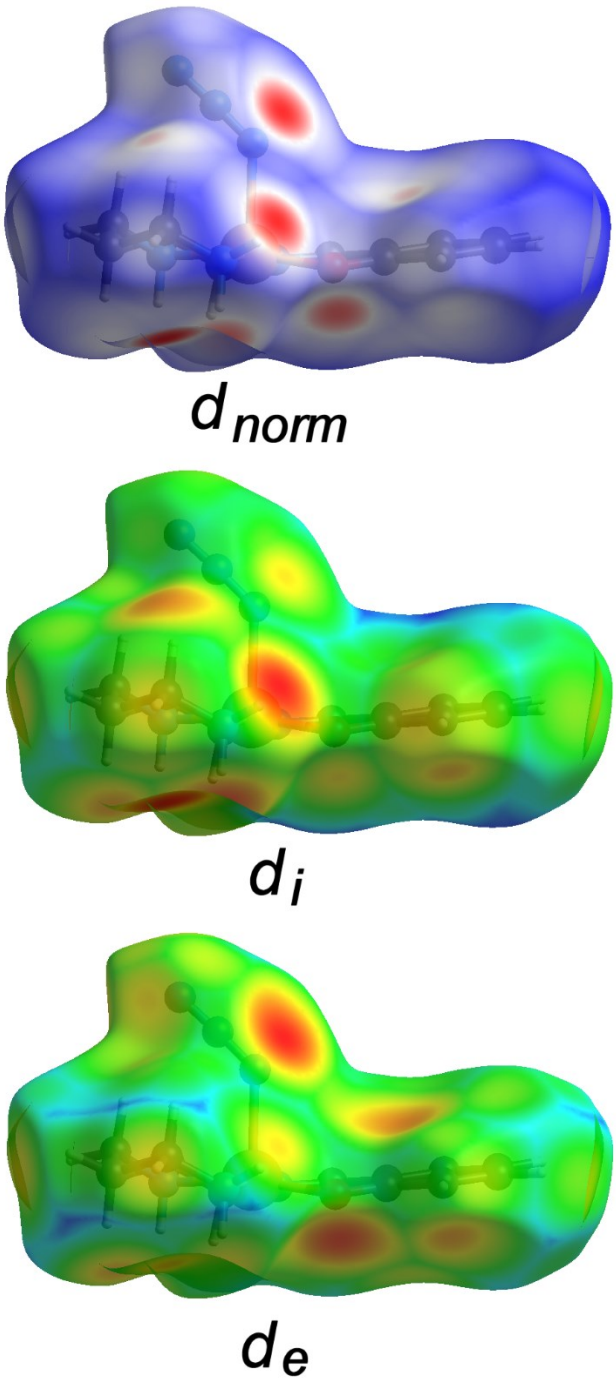


Fig. S5. The Hirshfeld surface of **1** mapped over d_{norm}, d_i and d_e. The d_{norm} surface is mapped over a fixed colour scale of -0.4853 (red) to 1.2778 (blue) arbitrary units.

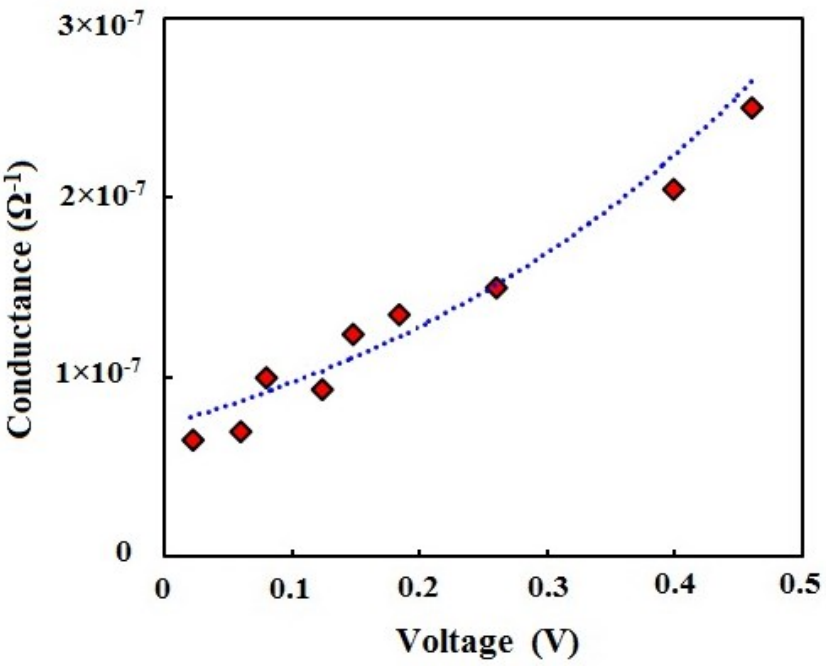


Figure S6. Conductance Vs Voltage plot.

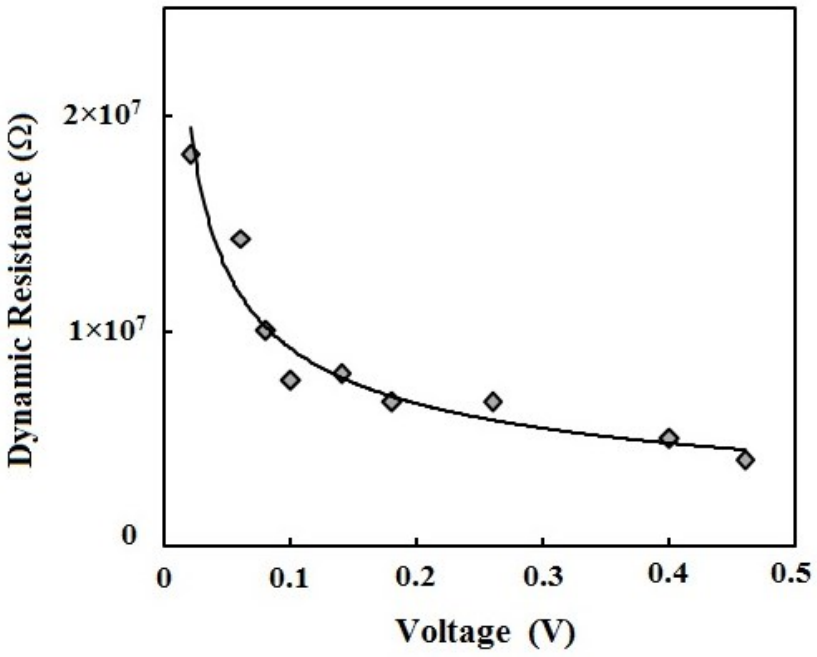


Fig. S7. Dynamic resistance Vs Voltage plot.

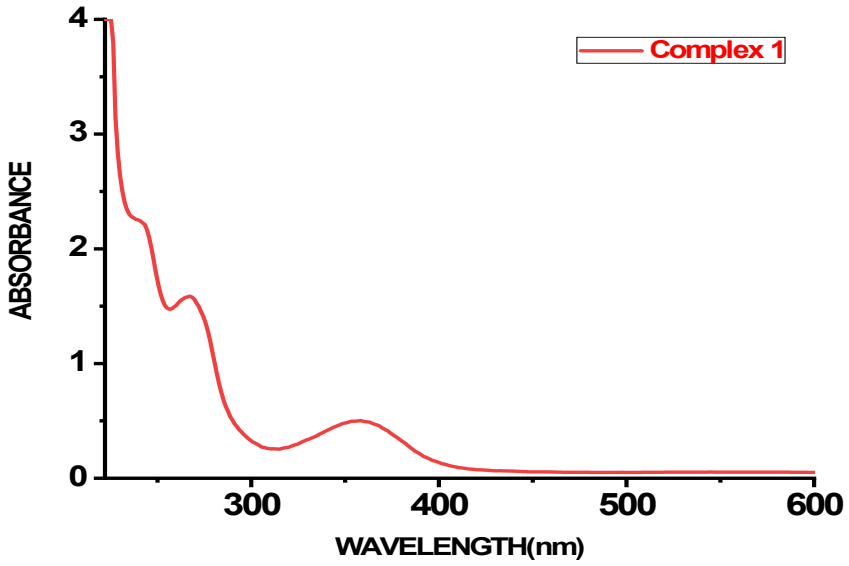


Fig. S8. Uv-vis spectrum of Complex **1**

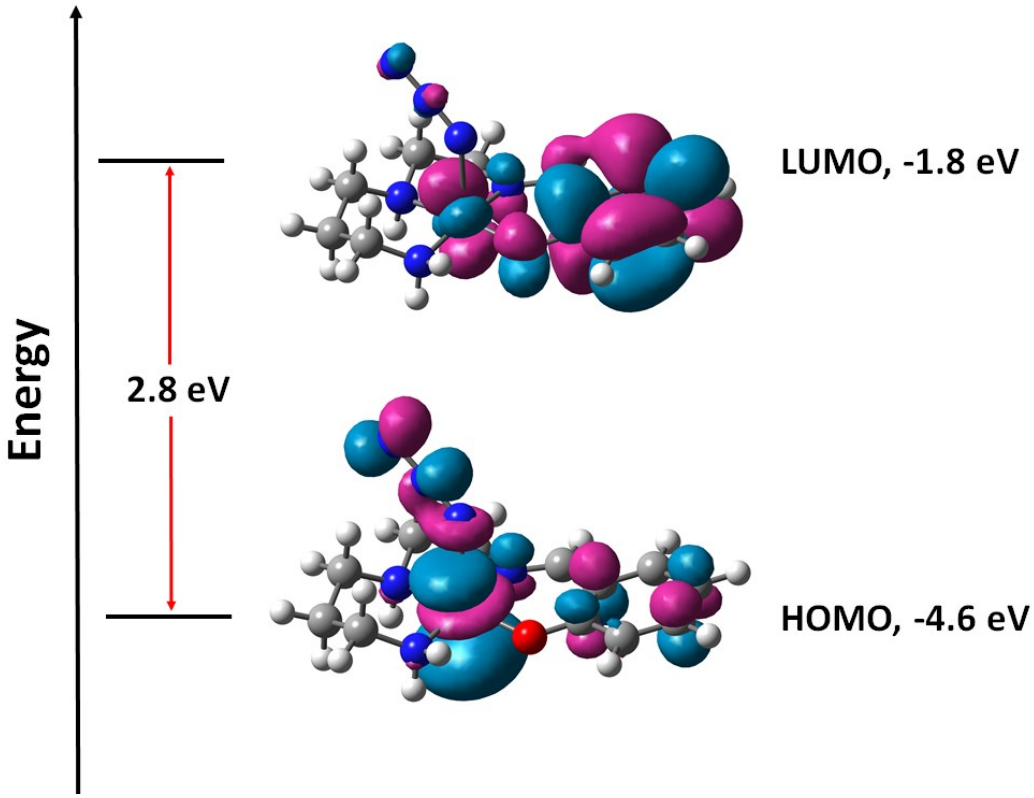


Fig. S9. The HOMO-LUMO gap of **1** in discreet state.

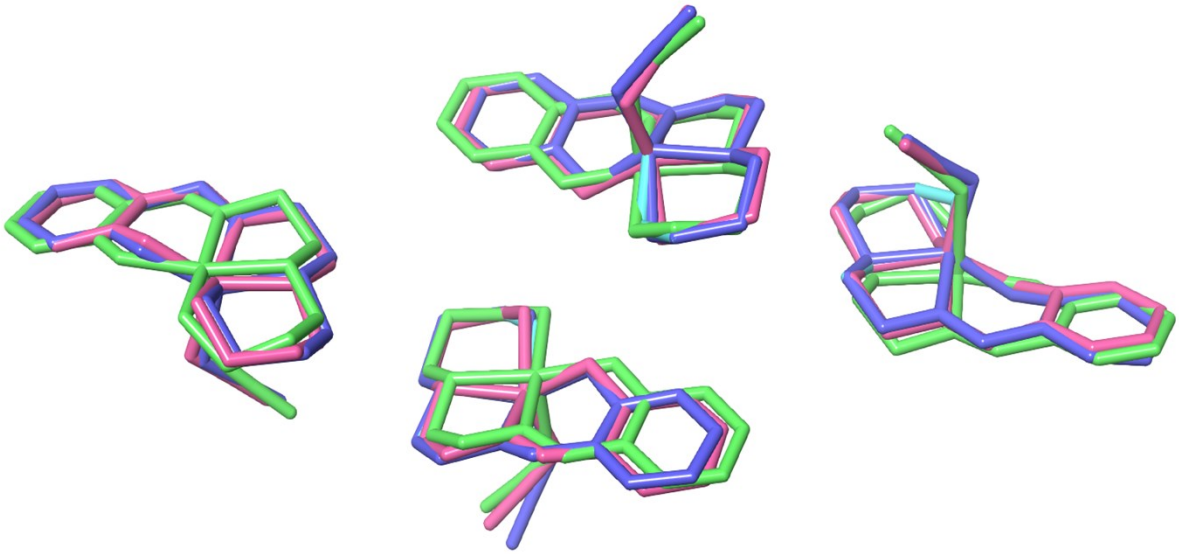


Fig. S10. Change ofthe structures of complex **1** in the unit cell of each steps obtained from the simulation and temperatures are 300 K (green), 320 K (cyan), 340 K (blue) and 360 K (red).

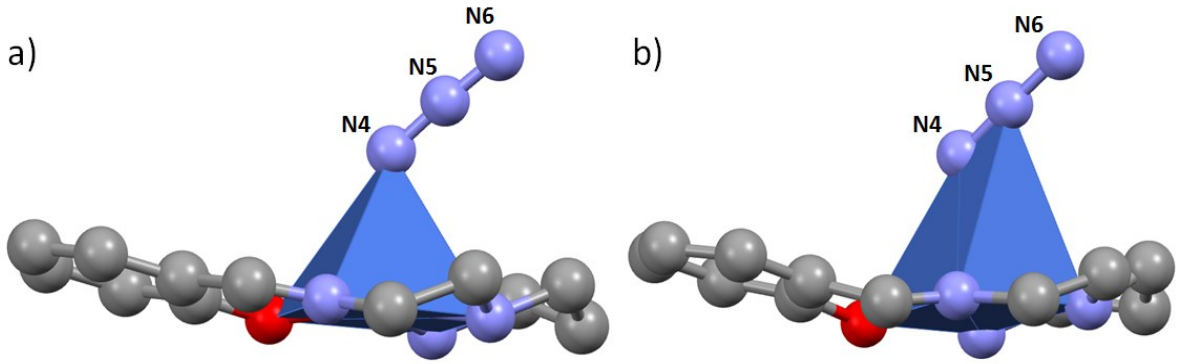
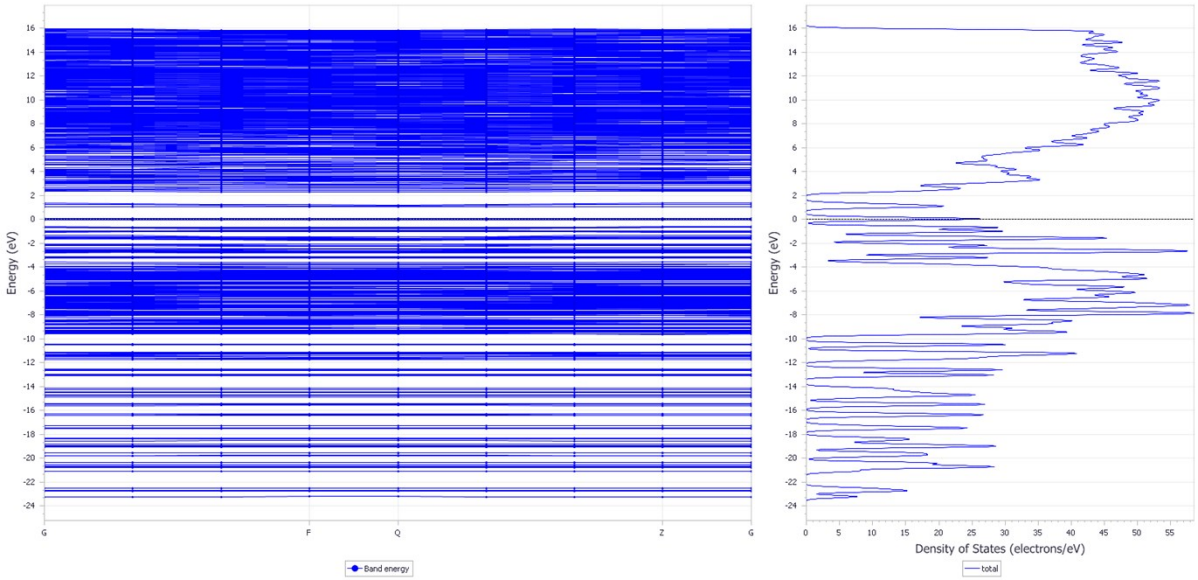
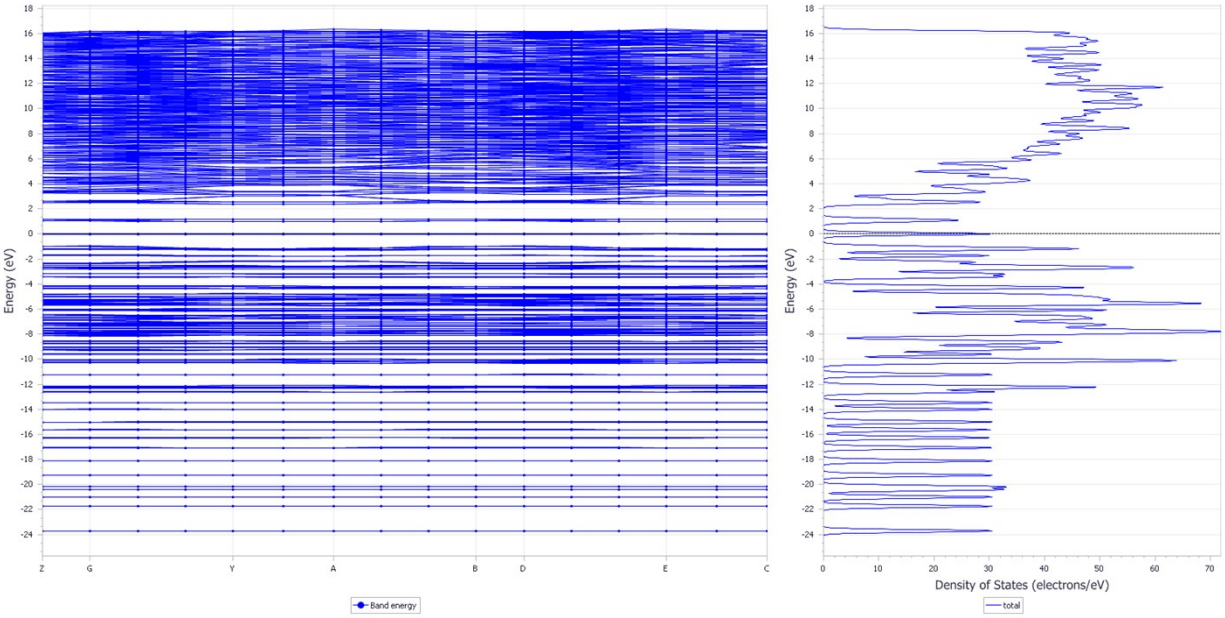


Fig. S11. The distorted square pyramidal geometry of Cu atom at a) 300 K [the bond length of Cu1-N4 is 2.37 Å] and b) 360 K [the bond length of Cu1-N4 and Cu1-N5 are 1.91 and 2.62 respectively].



(a)



(b)

Fig. S12. Band structure and density of state of the complex **1** at (a) 300K and (b)360K.

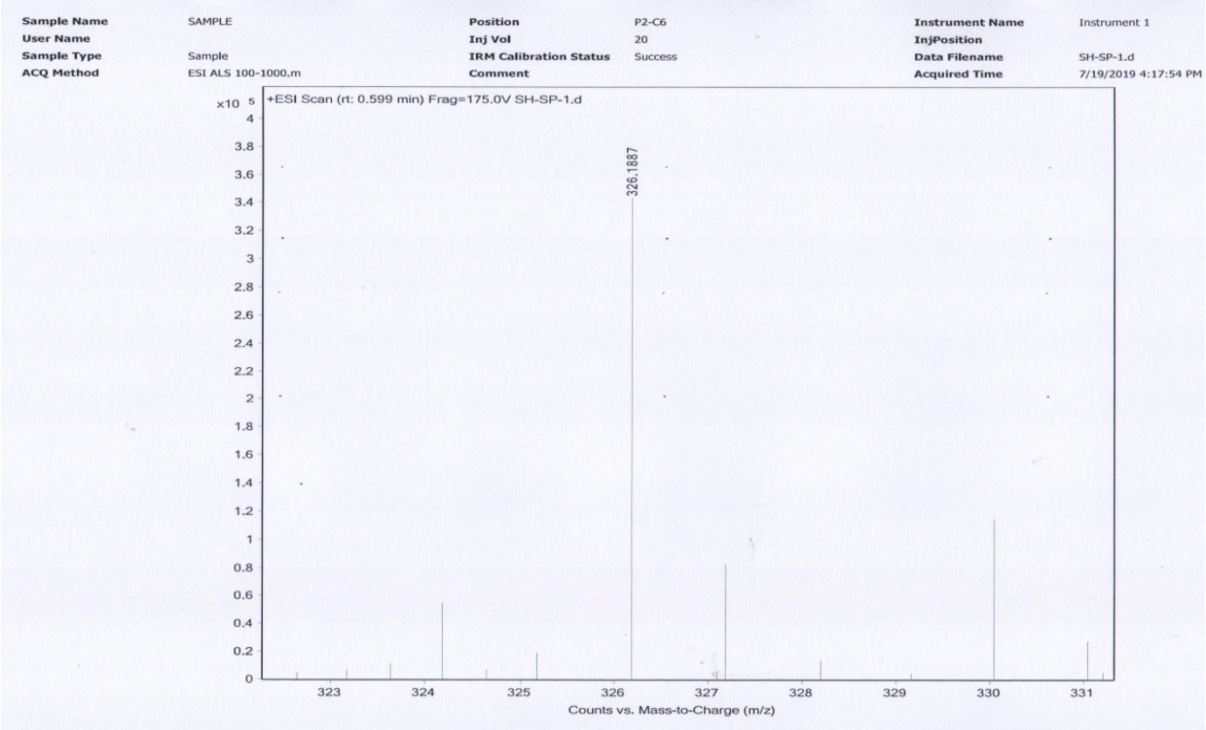


Fig. S13. ESIMSplot of complex**1** in acetonitrile.

Table S1. Selected bond lengths (Å) and bond angles (◦) for complex **1**

Bond distances					
Bond	**X-ray(Å)**	**DFT (Å)**	**Bond**	**X-ray(Å)**	**DFT(Å)**
Cu1-O1	1.914(4)	1.973	N2-C3	1.443(9)	1.387
Cu1-N1	1.975(5)	2.059	N2-C4	1.475(8)	1.430
Cu1-N2	2.028(6)	2.143	N3-C5	1.481(9)	1.474
Cu1-N3	1.952(5)	1.991	N3-C6	1.249(9)	1.225
Cu1-N4	2.379(5)	2.278	N4-N5	1.171(7)	1.232
N1-C1	1.447(8)	1.426	N5-N6	1.133(7)	1.232
Bond angles					
Angle	**X-ray (◦)**	**DFT (◦)**	**Angle**	**X-ray (◦)**	**DFT (◦)**
O1-Cu1-N1	88.09(19)	88.1	C12-O1-Cu1	126.5(4)	124.3
O1-Cu1-N2	169.3(2)	169.2	C1-N1-Cu1	118.6(4)	116.5
O1-Cu1-N3	92.0(2)	91.5	C3-N2-Cu1	118.3(4)	113.8
O1-Cu1-N4	97.64(19)	97.5	C4-N2-Cu1	106.4(4)	103.2
N1-Cu1-N2	93.8(2)	94.0	C5-N3-Cu1	112.3(5)	110.7

N1-Cu1-N4	95.6(2)	95.7	C6-N3-Cu1	124.8(5)	123.9
N2-Cu1-N4	92.7(2)	92.9	N5-N4-Cu1	132.3(4)	132.2
N3-Cu1-N1	171.3(2)	171.3	N6-N5-N4	177.3(7)	177.8
N3-Cu1-N2	84.6(2)	84.8	C3-N2-C4	113.5(6)	116.8
N3-Cu1-N4	93.0(2)	92.9	C6-N3-C5	122.8(6)	125.3

Table S2. Hydrogen bond distances (Å) and angles (°) for complex **1**

D−H…A	**D−H**	**H…A**	**D…A**	**D−H…A**
N1−H1AN…O1^{i}	0.85(6)	2.26(6)	3.053(7)	154(6)
N1−H1BN…N4^{ii}	0.90(6)	2.14(6)	3.017(8)	164(5)
N2−H2N…N6^{iii}	0.85(7)	2.15(7)	2.958(8)	158(6)
C3−H3A…N6^{iv}	0.97	2.63	3.527(9)	154
Symmetry codes: (i) 1-x, 1-y, 1-z; (ii) 1-x, -y, 1-z; (iii) x, 1+y, z; (iv) 0.5-x, 0.5+y, 0.5-z				

Table S3. Percentage contributions from interatomic contacts to the Hirshfeld surface as observed in Complex **1**.

Contact	**Percentage**
H···H	52.0
N···H/H···N	23.5
C···H/H···C	17.5
O···H/H···O	5.3
Cu···N/N···Cu	0.7
C···C	0.5
O···N/N···O	0.3
N···N	0.1