Electronic Supplementary Material (ESI) for New Journal of Chemistry.
This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2018

Electronic Supplementary Information

Cu(II)-based binuclear compound for the application of photosensitive electronic device

Basudeb Dutta,[a] Arka Dey,[b] Kaushik Naskar,[c] Faruk Ahmed,[a] Rakesh Purkait,[c] Sakhiul Islam,[a] Soumen Ghosh,[d] Chittaranjan Sinha,[c] Partha Pratim Ray,*[b] and Mohammad Hedayetullah Mir*[a]

[a]*Department of Chemistry, Aliah University, New Town, Kolkata 700 156, India. Email: chmmir@gmail.com*
[b]*Department of Physics, Jadavpur University, Jadavpur, Kolkata 700 032, India. Email: partha@phys.jdvu.ac.in*
[c]*Department of Chemistry, Jadavpur University, Jadavpur, Kolkata 700 032, India.*
[d]*Department of Chemistry, University of Calcutta, 92 A.P.C. Road, Kolkata 700 009, India*

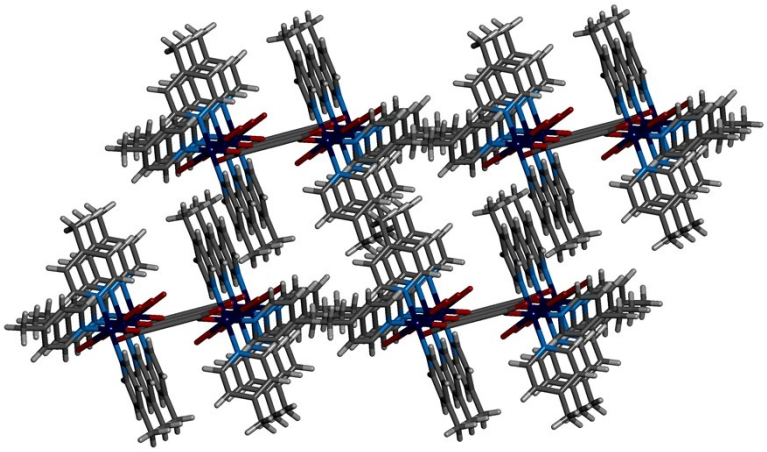


Fig. S1 A view of 3D supramolecular aggregate in compound **1** via hydrogen bonding and C-H···π interactions.

Table S1 Crystal data and refinement parameters for compound **1**

Formula	$C_{40}H_{42}Cl_2Cu_2N_6O_{16}$ (**1**)
fw	1060.77
cryst syst	triclinic
space group	$P\bar{1}$
a (Å)	8.3736(8)
b (Å)	10.9069(9)
c (Å)	14.1280(14)
α (deg)	101.860(4)
β (deg)	96.035(5)
γ (deg)	105.536(4)
V (Å^3)	1198.94(19)
Z	1
D_{calcd} (g/cm^3)	1.469
μ (mm^{-1})	1.071
λ (Å)	0.71073
data [$I > 2\sigma(I)$]/params	5960/299
GOF on F^2	1.059
final R indices [$I > 2\sigma(I)$][a,b]	$R1 = 0.0523$ $wR2 = 0.1580$

[a] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, [b] $wR2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

Table S2 Selected bond lengths and bond angles in **1**

Cu(1)-O(1)	2.006(2)	Cu(1)-O(2W)	2.587(3)
Cu(1)-N(2)	2.033(2)	Cu(1)-N(1)	2.008(2)
Cu(1)-O(1W)	2.384(2)	Cu(1)-N(3)	2.012(2)
O(1)-Cu(1)-N(3)	89.47(9)	N(2)-Cu(1)-N(3)	91.72(9)
O(1)-Cu(1)-O(1W)	86.16(8)	O(1W)-Cu(1)-N(2)	94.06(9)
O(1)-Cu(1)-N(2)	178.79(8)	O(2W)-Cu(1)-N(2)	88.38(9)
O(1W)-Cu(1)-N(1)	91.01(8)	N(1)-Cu(1)-N(3)	177.65(10)
O(2W)-Cu(1)-N(1)	93.63(9)	O(1)-Cu(1)-N(1)	88.56(9)
N(1)-Cu(1)-N(2)	90.25(9)	O(1W)-Cu(1)-O(2W)	174.75(9)
Cu(1)-O(1)-C(19)	128.68(18)	O(1W)-Cu(1)-N(3)	90.14(8)
O(1)-Cu(1)-O(2W)	91.50(8)	O(2W)-Cu(1)-N(3)	85.14(9)

Table S3 Intermolecular hydrogen bonding interactions in **1**

	D···A	D···A (Å)
Compound 1	O(1W)···O(1)	2.850

It is important to mention that the hydrogen atoms of water molecule in compound **1** could not be added even after several trials. The O-H bond may be too large and could not be refined.

Table S4 C-H···π interactions in **1**.

	C-H→ ring(j)	H···R distance (Å)	C-H···R angle(deg)	C···R distance (Å)
Compound 1	C(6)-H(6)→R(1)	3.088	160.39	4.005
	C(12)-H(12)→R(2)	3.257	157.70	4.161
	C(18)-H(18)→R(3)	2.968	157.11	3.871

R(j) denotes the j-th ring: R(1) = N(1)/C(1)/C(2)/C(3)/C(4)/C(5); R(2)= N(2)/C(7)/C(8)/C(9)/C(10)/C(11); R(3) = N(3)/C(13)/C(14)/C(15)/C(16)/C(17)

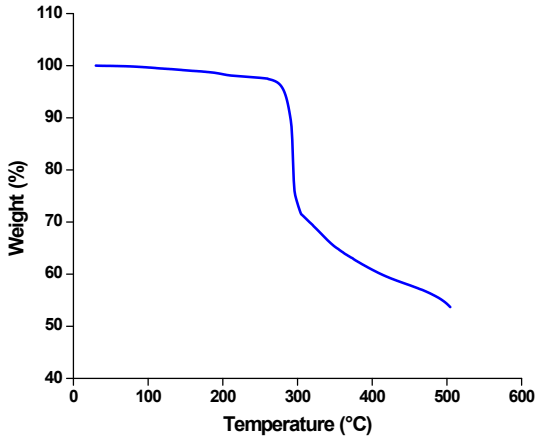


Fig. S2 TGA plot of compound **1** measured under N_2 atmosphere.

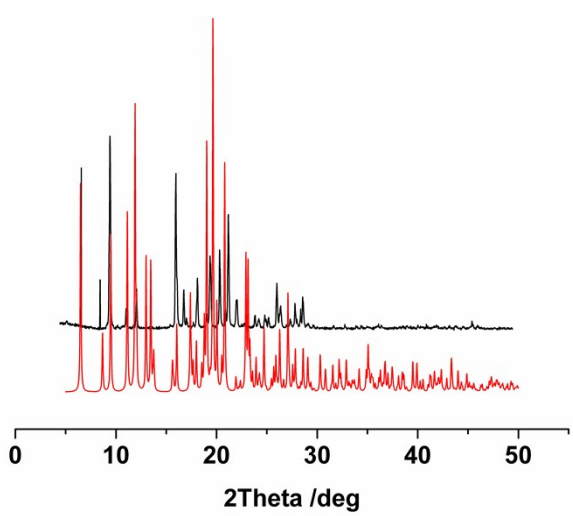


Fig. S3 Powder X-ray diffraction patterns of simulated **1** (red) and as-synthesized **1** (black).

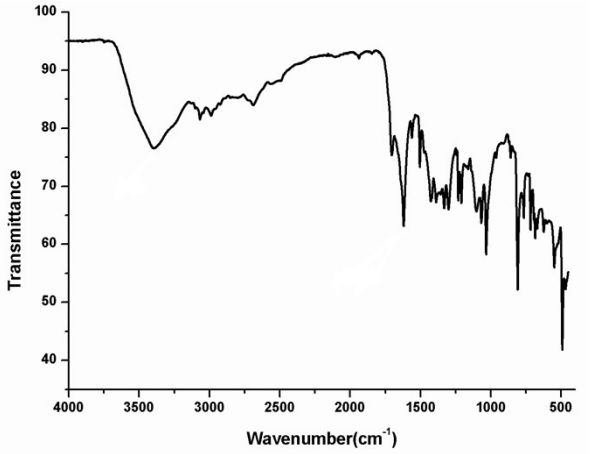
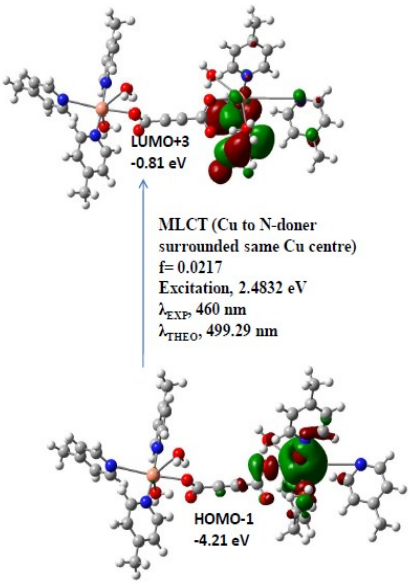
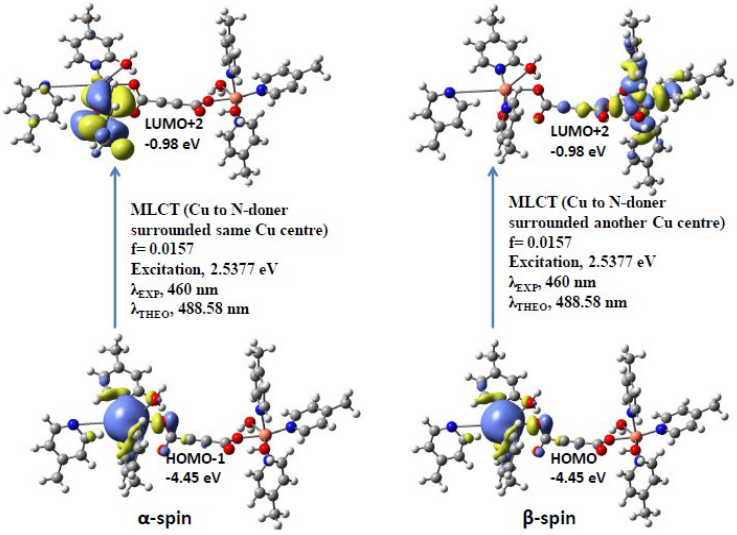


Fig. S4 FT-IR spectrum of compound **1**.



(A)



(B)

Fig. S5 Frontier molecular orbitals for (A) ground state singlet configuration and (B) ground state triplet configuration involved in theoretical electronic transition correlated with experimental values of compound **1**.