Electronic Supplementary Material (ESI) for Dalton Transactions

Doubly chloro bridged dimeric copper(II) complex: magneto-structural correlation and anticancer activity

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Table S1 Crystallographic data and structure refinement for **1**

CCDC no.	**1038199**
Empirical formula	$C_{22}H_{32}Cl_4Cu_2N_4O_2$
Formula mass	653.42
Crystal system	monoclinic
Space group	P 21/c
a (Å)	9.1653(5)
b (Å)	7.2194(4)
c (Å)	20.4311(11)
α (°)	90.00
β (°)	93.455(2)
γ (°)	90.00
V (Å^3)	1349.43(13)
Z	2
T (K)	296(2)
μ (mm-1)	1.999
D_{calc} (Mg/m^3)	1.608
Crystal size (mm)	0.38×0.26×0.14
θ max (°)	28.57
Data collected	20059
Unique refl. / Rint	3444/0.029
Parameters / Restraints	155/1
Goodness-of-Fit on F^2	1.072
R1 / wR2 (all data)	0.0441/0.1584
Residual peak(e/Å^3)	1.332

Table S2 Selected bond distance (Å) and bond angle (°)

Cu1 − Cl1	**2.2704(8)**	**Cl1−Cu1−Cl2**	**93.48(3)**
Cu1 – Cl2	2.2723(7)	Cl1−Cu1−N1	93.49(8)
Cu1 − N1	2.042(2)	Cl1−Cu1−N2	165.58(7)
Cu1 − N1	2.035(3)	Cl1−Cu1−Cl2#	102.21(3)
Cu1 – Cl2#	2.8270(8)	Cu1 −Cl1−Cu1#	91.64(3)
		Cu−Cl2−Cu1#	92.66(2)

Symmetry operator: # (1-x, 1-y, 1-z)

Table S3. Selected MPA atomic charges, corresponding spin densities; for atom numbering see Figure 5

		singlet		triplet	
		charges	spindensity	charges	spindensity
Cu1	1	0.1320	0.5415	0.1318	0.5391
Cl1	2	-0.4644	0.1662	-0.4642	0.1665
Cl2	3	-0.4095	0.1424	-0.4093	0.1434
N1	4	0.0369	0.0863	0.0367	0.0850
N2	5	0.0173	0.0682	0.0174	0.0684
Cu2	34	0.1319	-0.5415	0.1318	0.5391
Cl1'(Cl3)	35	-0.4643	-0.1663	-0.4642	0.1665
Cl2'(Cl4)	36	-0.4095	-0.1424	-0.4093	0.1434
N1'	37	0.0369	-0.0860	0.0367	0.0850
N2'	38	0.0174	-0.0684	0.0174	0.0684

Table S4. Selected bond lengths (Å) and angles (°) for complex **1**.

		experimental	B3LYP-D3	B3LYP
Distances				
R(1,2)	R(Cu1-Cl1)	2.270	2.320	2.328
R(1,3)	R(Cu1-CL2)	2.272	2.376	2.390
R(1,4)	R(Cu1-N1)	2.036	2.071	2.089
R(1,5)	R(Cu1-N2)	2.040	2.080	2.085
R(1,36)	R(Cu1-Cl2')	2.827	2.761	2.737
R(3,34)	R(Cl2-Cu2)	2.827	2.761	2.737
R(34,35)	R(Cu2-Cl1')	2.270	2.320	2.328
R(34,36)	R(Cu2-Cl2')	2.272	2.376	2.390
R(34,37)	R(Cu2-N1')	2.040	2.071	2.089
R(34,38)	R(Cu2-N2')	2.036	2.080	2.085
Angles				
A(2,1,3)	A(Cl1-Cu1-Cl2)	93.50	93.08	93.12
A(2,1,4)	A(Cl1-Cu1-N1)	93.39	93.82	92.94
A(2,1,36)	A(Cl1-Cu1-Cl2')	102.19	106.43	103.55
A(3,1,5)	A(Cl2-Cu1-N2)	93.11	92.02	92.29
A(3,1,36)	A(Cl2-Cu1-Cl2')	93.50	93.60	92.18
A(4,1,5)	A(N1-Cu1-N2)	80.26	80.10	79.78
A(1,3,34)	A(Cu1-Cl2-Cu2)	92.65	86.40	87.82
A(35,34,36)	A(Cl1'-Cu2-Cl2')	93.50	93.08	93.12
A(35,34,37)	A(Cl1'-Cu2-N1')	93.11	93.81	92.93
A(36,34,38)	A(Cl2'-Cu2-N2')	93.39	92.02	92.29
A(37,34,38)	A(N1'-Cu2-N2')	80.26	80.10	79.78

A(1,36,34)	A(Cu1-Cl2'-Cu2)	92.65	86.38	87.82
D(2,1,3,34)	D(Cl1-Cu1-Cl2-Cu2)	102.06	106.69	103.70
D(5,1,3,34)	D(N2-Cu1-Cl2-Cu2)	-90.74	-83.99	-90.02
D(36,1,3,34)	D(Cl2'-Cu1-Cl2-Cu2)	0.00	0.00	0.00
D(3,1,36,34)	D(Cl2-Cu1-Cl2'-Cu2)	0.00	0.00	0.00
D(4,1,36,34)	D(N1-Cu1-Cl2'-Cu2)	173.34	171.67	172.03
D(5,1,36,34)	D(N2-Cu1-Cl2'-Cu2)	90.74	91.65	92.29

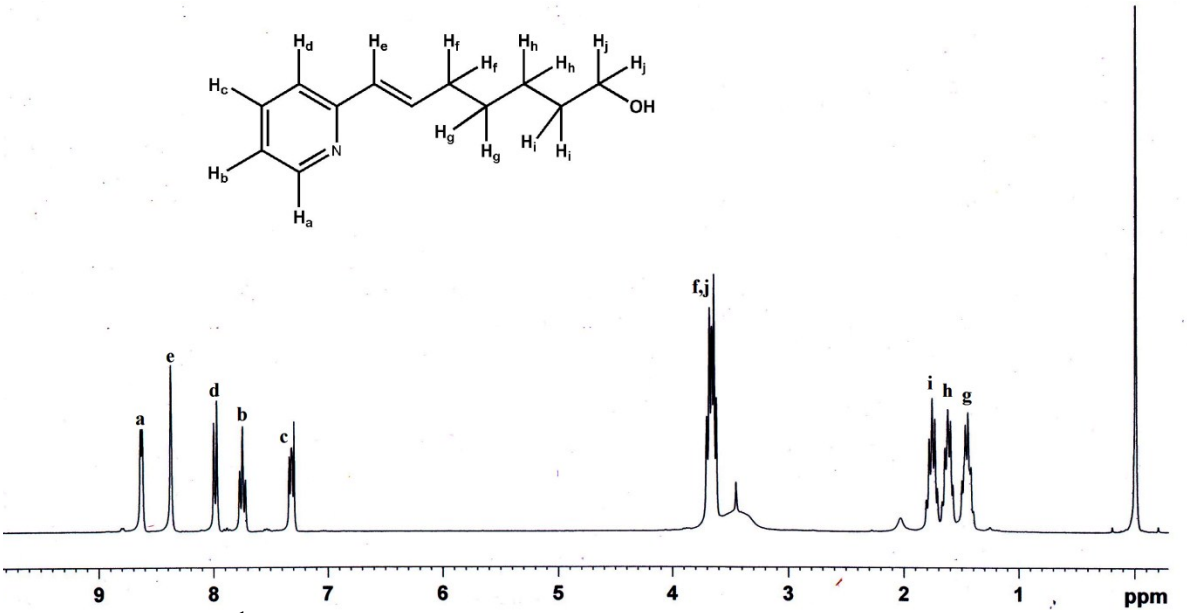

Figure S1 ^{1}H NMR of Ligand in $CDCl_3$ along with atom numbering

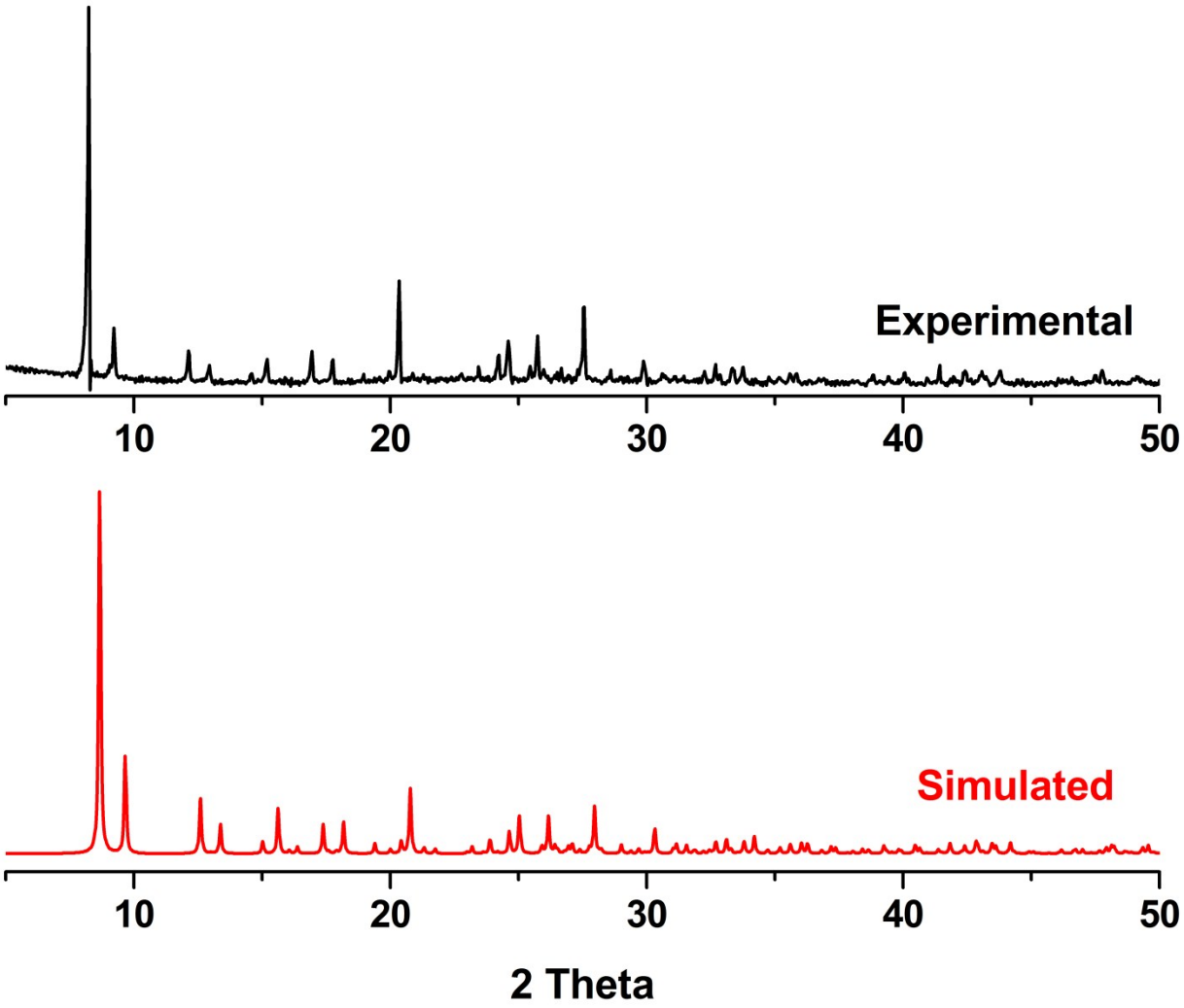

Figure S2 Experimental(Black) and Simulated(red) Powder X-ray diffraction spectrum of complex **1** to determine the phase purity.

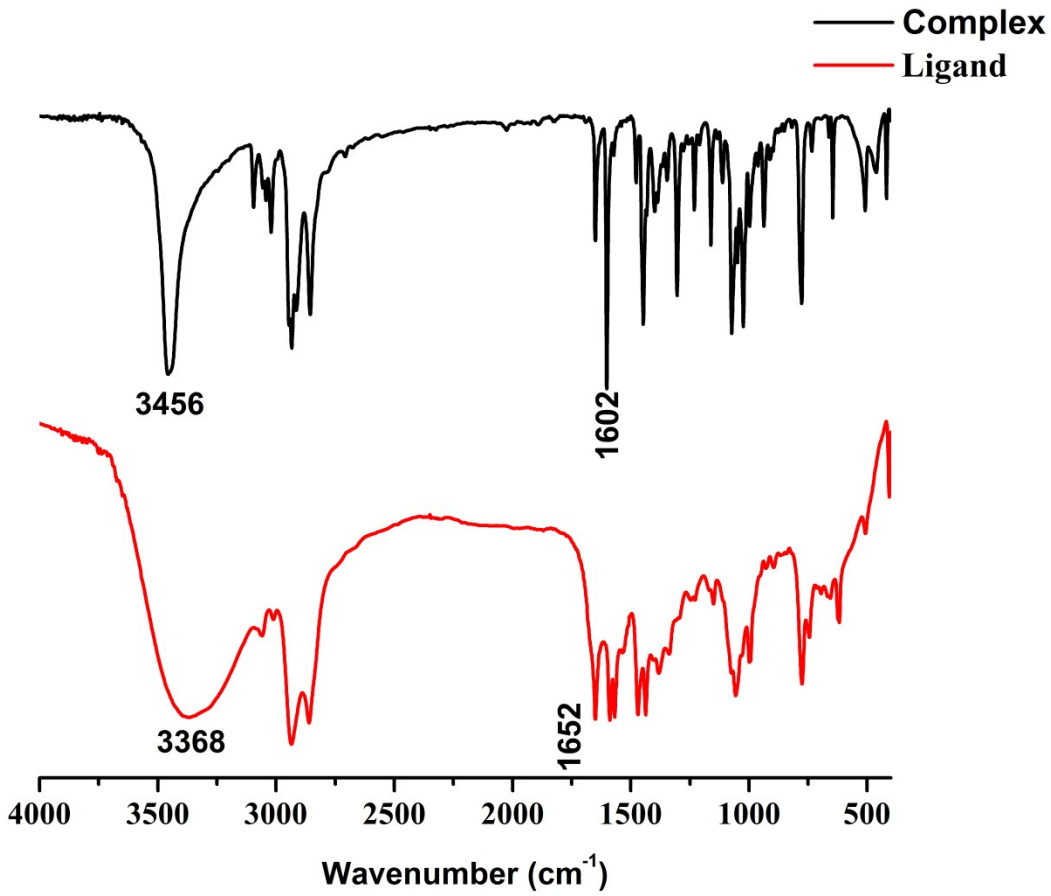

Figure S3 FT−IR spectrum of ligand and complex (**1**)

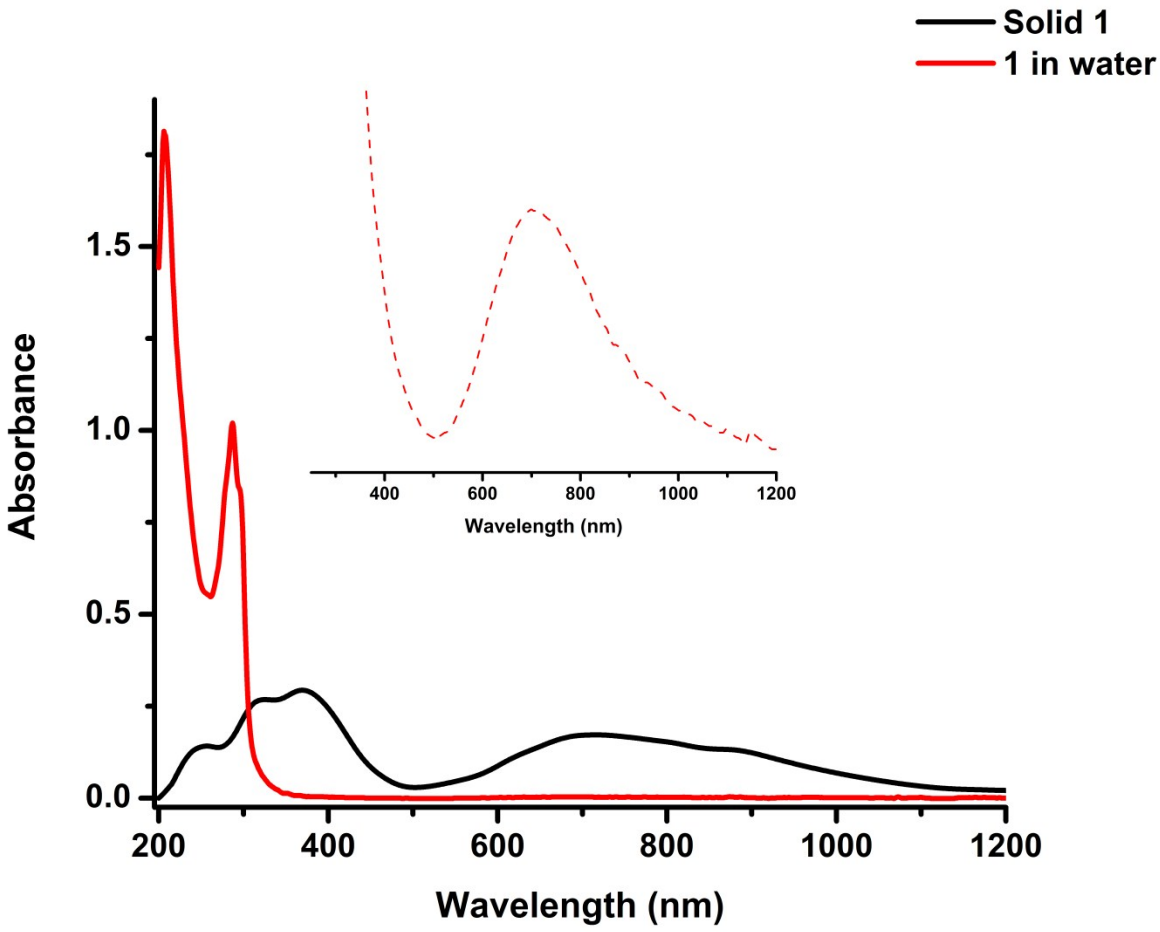

Figure S4 UV-Vis spectra of complex in solid state and in solution. (Inset shows the d−d band of the solution state)

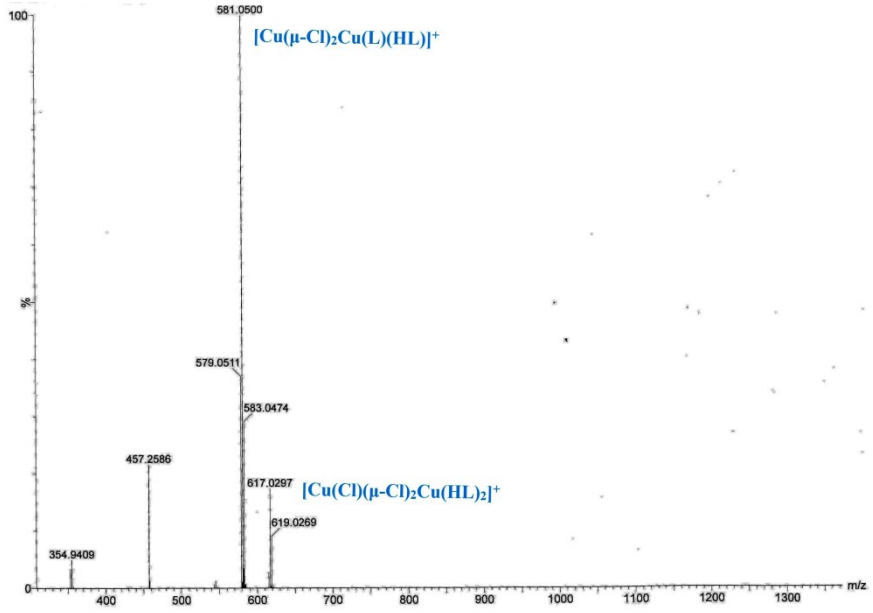

Figure S5 ESI-MS of complex **1** in methanol.

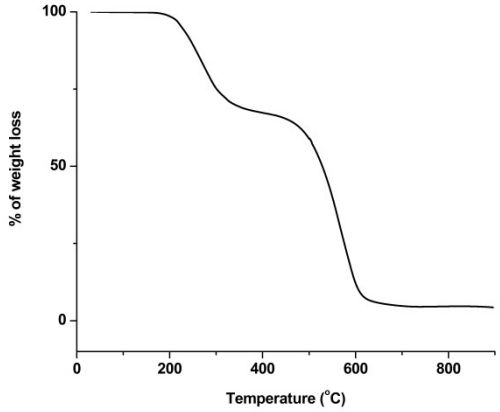

Figure S6 TGA thermograms of complex **1** under N_2 atmosphere (heating rate 10°C min^{-1})

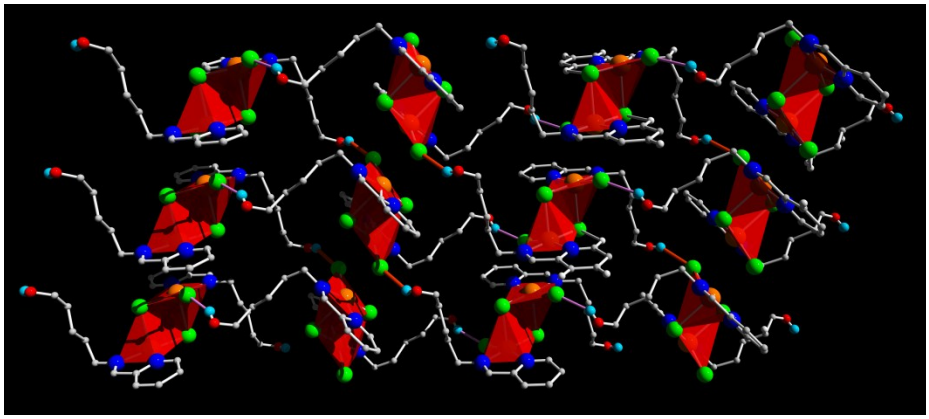

Figure S7 A three dimensional network formed in complex **1**, viewed through bc plane