Unprecedented copper(II) mediated in situ formation of *gem*-diol binuclear complexes: A combined experimental and computational study

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supplementary information

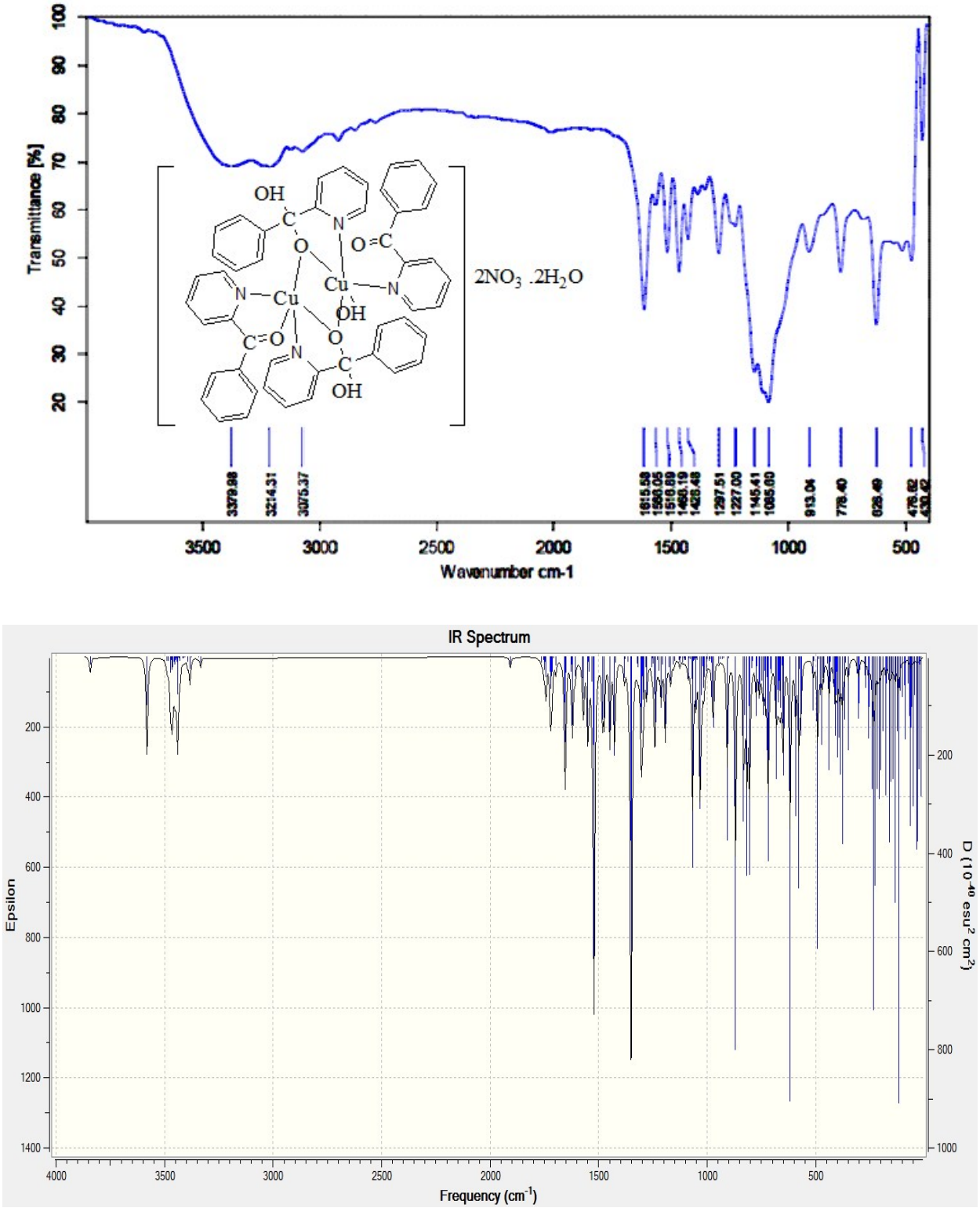


Fig. S1 FT-IR spectra of complex **1** Top: Experimental Bottom: Theoretical

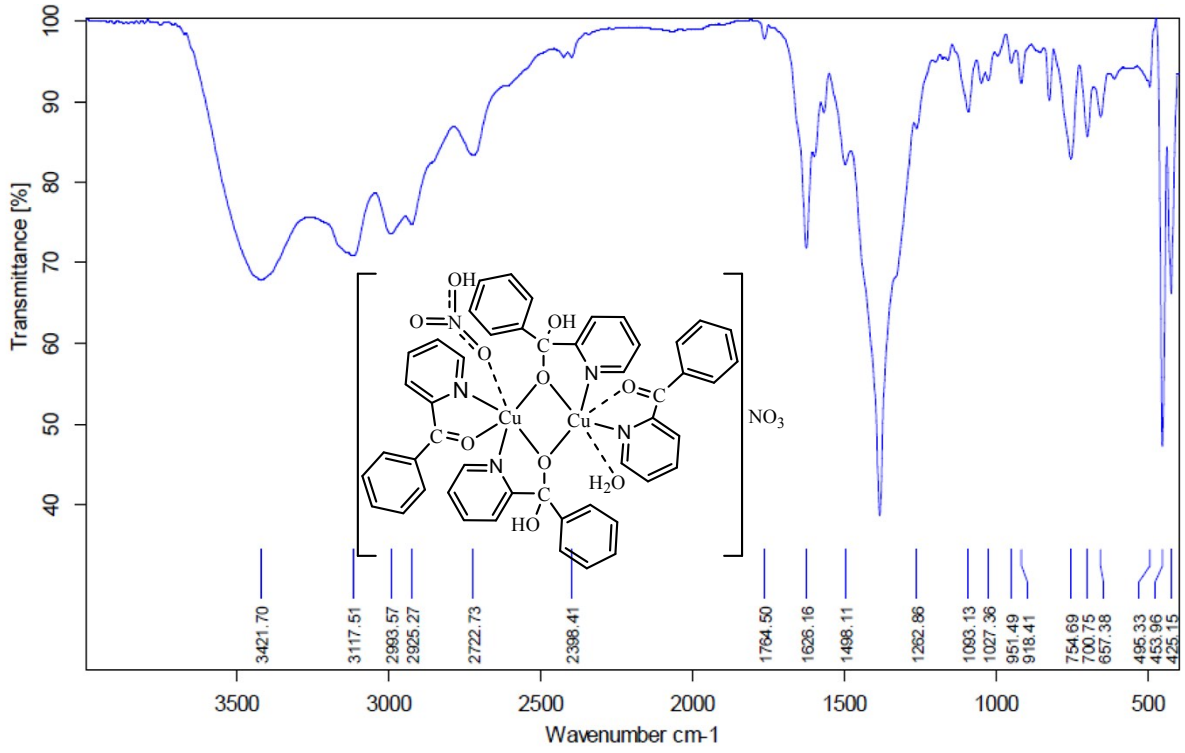


Fig. S2 FTIR spectra of complex **2.**

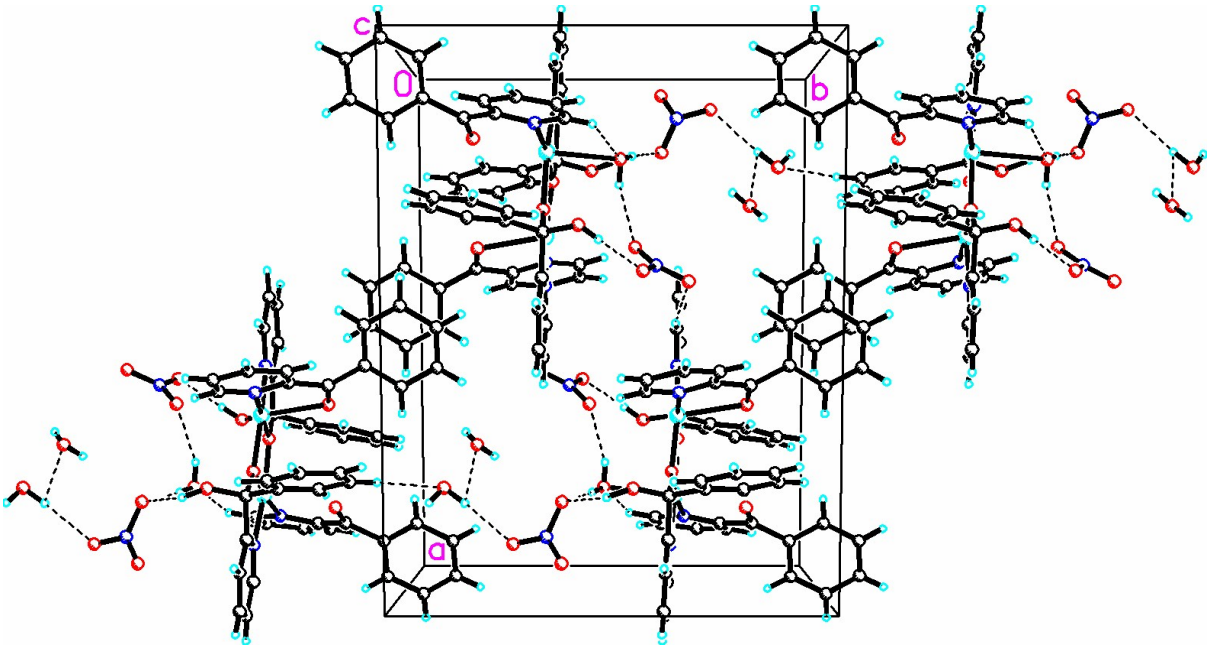


Fig. S3 Unit cell diagram with hydrogen bonding scheme of complex $[Cu_2(L^1)_2(HL^2)_2(H_2O)](NO_3)_2{\cdot}2H_2O$ 1.

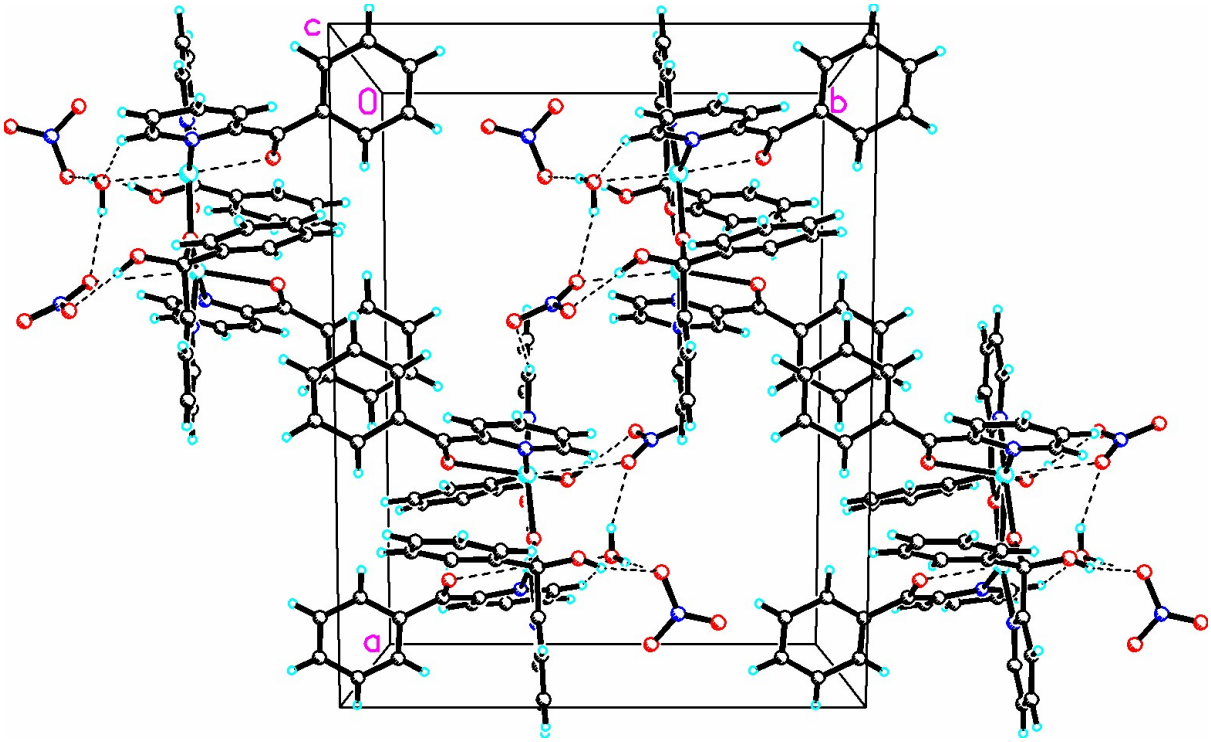
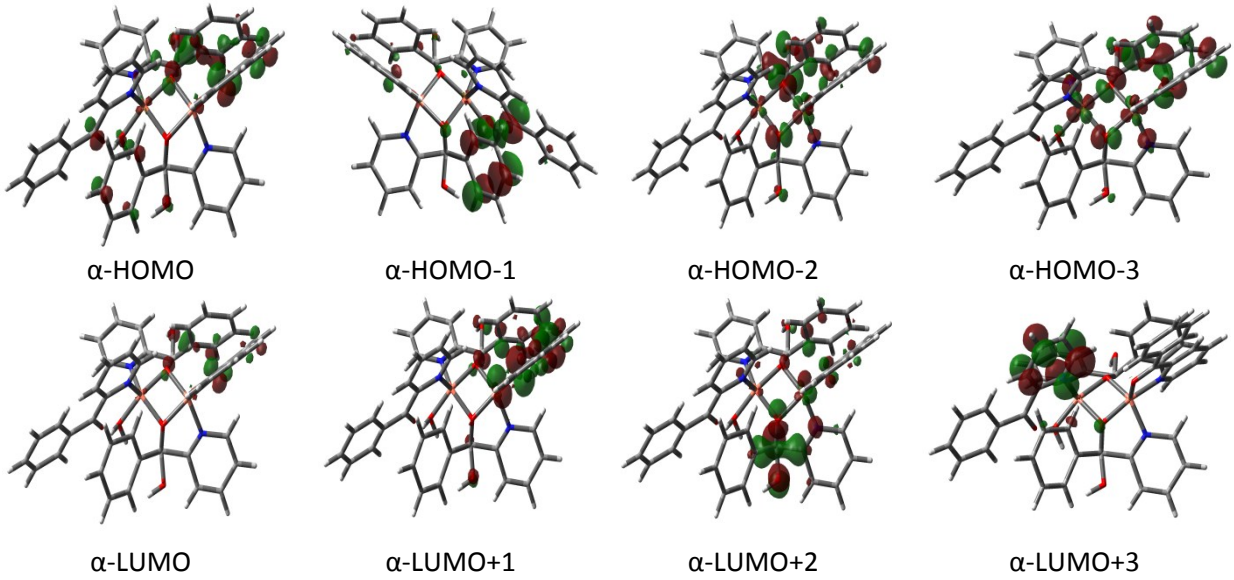


Fig. S4 Unit cell diagram with hydrogen bonding scheme of complex $[Cu_2(L^1)_2(HL^2)_2](NO_3)_2 \cdot H_2O$ **2**.

(a)



(b)

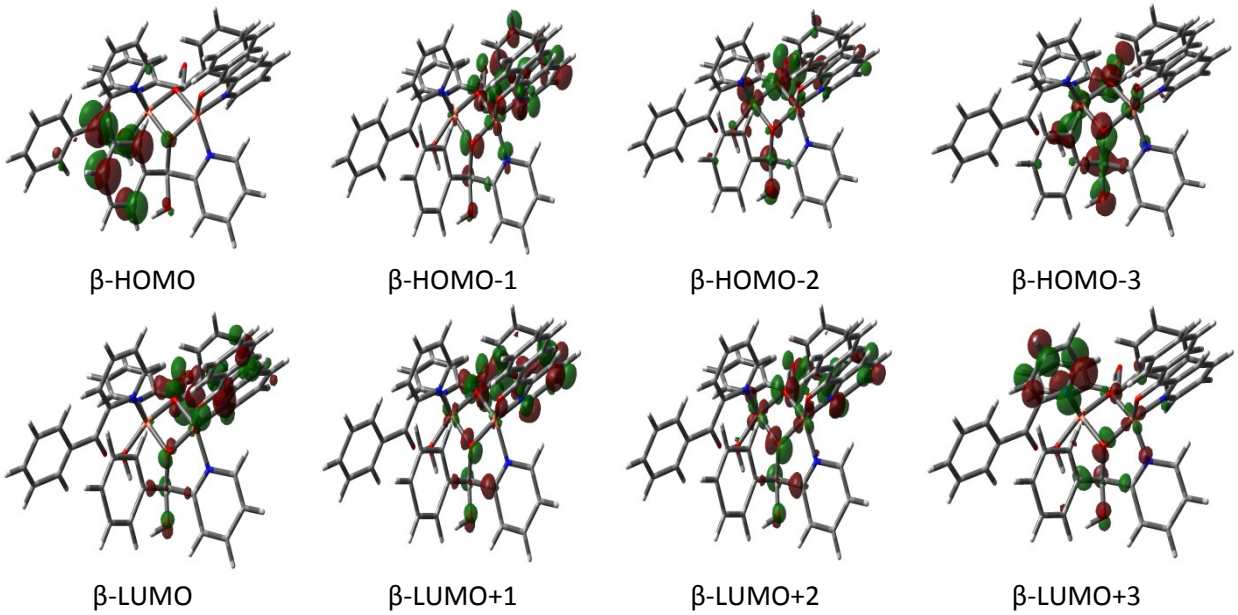
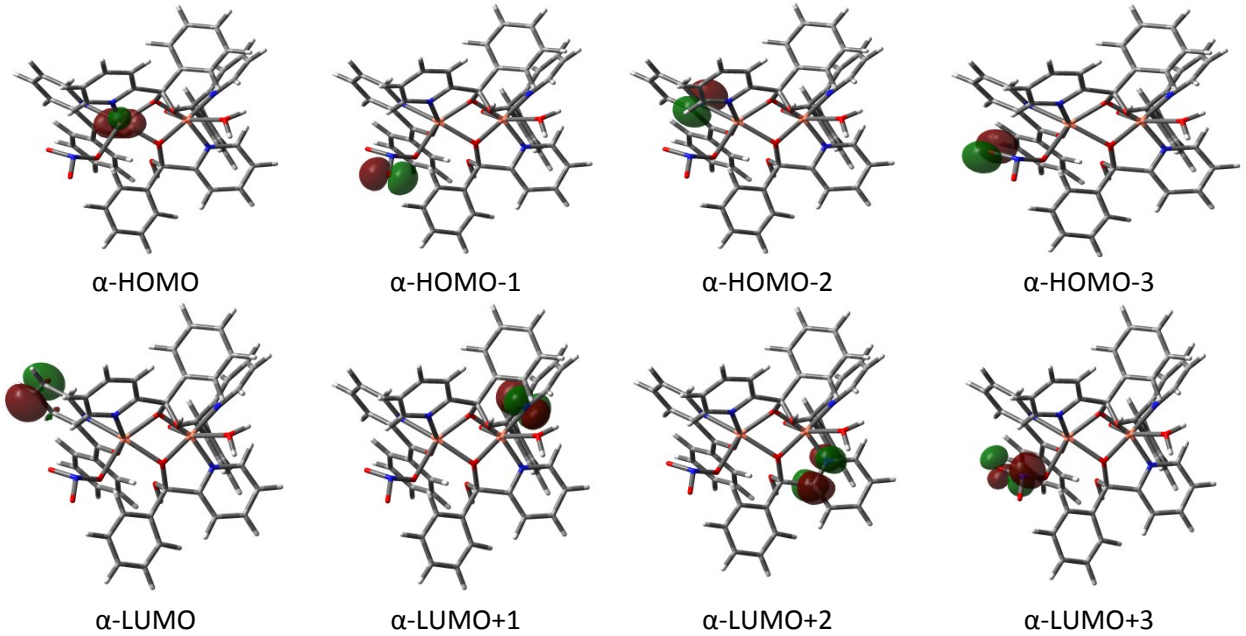


Fig. S3.(a) 3D plot of some selected MOs (α-spin) of **1** (b) 3D plot of some selected MOs (β-spin) of **1.**

(a)



(b)

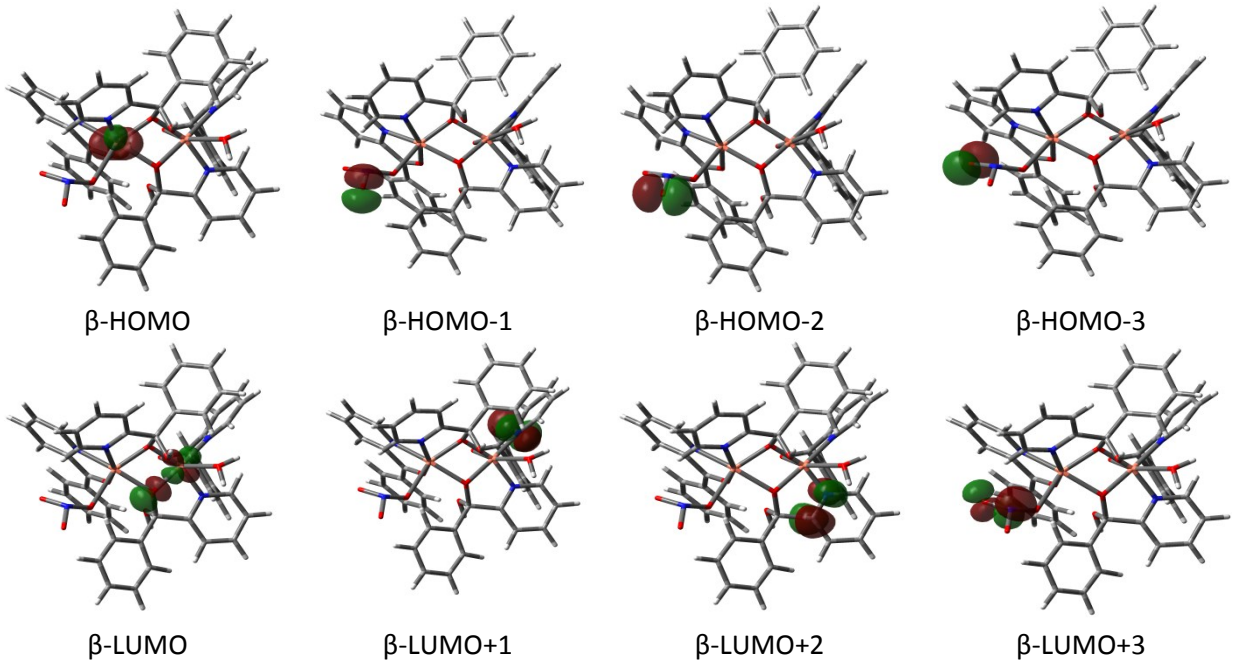


Fig. S4.(a) 3D plot of some selected MOs (α-spin) of **1** (b) 3D plot of some selected MOs (β-spin) of **2.**

Table S1 Computed and experimental infrared frequencies for compounds **1** and **2**

Vibration	Complex **1** (cm^{-1})		Complex **2** (cm^{-1})
	Computed	Experimental	Experimental
υ(OH_2) free	3370	3379	3421
υ(OH_2) bonded	3180	3214	
υ(C-OH)	3078	3075	3117
υ(C=O)	1627	1615	1764
υ(Cu-N)	435	430	425
υ(Cu-O)	480	475	453

Table S2. Molecular orbital energies and compositions of some selected orbital's for complex **1**

Orbital	Energy (eV)		% of Metal		% of ligand	
	α-spin	β-spin	α-spin	β-spin	α-spin	β-spin
LUMO+9	1.8545	1.7421	0	0	100	100
LUMO+8	1.6888	1.6199	2	6	98	94
LUMO+7	1.5793	1.4787	2	2	98	98
LUMO+6	1.4727	1.3348	1	28	99	72
LUMO+5	1.3099	1.3053	0	1	100	99
LUMO+4	0.9434	0.8814	12	23	88	77
LUMO+3	0.7627	0.6968	1	21	99	79
LUMO+2	0.5866	0.4022	13	40	87	60
LUMO+1	-0.0277	0.0223	5	14	95	86
LUMO	-0.7507	0.0329	2	5	98	95
HOMO	-1.1067	-1.2210	8	1	92	99
HOMO-1	-1.2417	-1.5108	3	22	97	78
HOMO-2	-1.8591	-1.7690	15	35	85	65
HOMO-3	-2.1268	-2.5026	20	40	80	60
HOMO-4	-2.3762	-2.7489	28	42	72	58
HOMO-5	-2.6542	-3.0828	25	13	75	87
HOMO-6	-3.1135	-3.1968	22	24	78	76
HOMO-7	-3.1770	-3.2833	18	2	82	98
HOMO-8	-3.3085	-3.5555	8	43	92	57
HOMO-9	-3.3563	-3.7133	14	38	86	62

Table S3. Molecular orbital energies and compositions of some selected orbital's for complex **2**

Orbital	Energy (eV)		% of Metal		% of ligand	
	α-spin	β-spin	α-spin	β-spin	α-spin	β-spin
LUMO+9	-0.1603	-0.3630	0	0	100	100
LUMO+8	-0.1848	-0.4666	0	0	100	100
LUMO+7	-0.2844	-0.5252	0	0	100	100
LUMO+6	-0.3347	-0.5374	0	0	100	100
LUMO+5	-0.4898	-0.6816	0	0	100	100
LUMO+4	-0.5262	-0.7469	0	0	100	100
LUMO+3	-0.9823	-1.0454	0	0	100	100
LUMO+2	-1.3091	-1.2917	0	0	100	100
LUMO+1	-1.5720	-1.8898	0	0	100	100
LUMO	-3.2061	-2.5035	0	0	100	100
HOMO	-4.6684	-4.2624	100	100	0	0
HOMO-1	-5.1259	-4.6908	0	80	100	20
HOMO-2	-5.3077	-5.1275	0	0	100	100
HOMO-3	-5.3531	-5.3526	0	0	100	100
HOMO-4	-5.5625	-5.4593	0	0	100	100
HOMO-5	-5.6146	-5.6152	0	0	100	100
HOMO-6	-5.6421	-5.6233	0	0	100	100
HOMO-7	-6.1133	-6.1539	0	0	100	100
HOMO-8	-6.1643	-6.1643	0	0	100	100
HOMO-9	-6.3442	-6.3700	0	0	100	100