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Supplementary Material

Synthesis, Structure, and Visible Phosphorescence Emission of Novel Cu^{I} Coordination Polymers Based on 4,4′-Bis(3-pyridyl)-2,2′-bis(hydroxylmethyl) Biphenyl

Cu^{I} Coordination Polymers with Visible Phosphorescence

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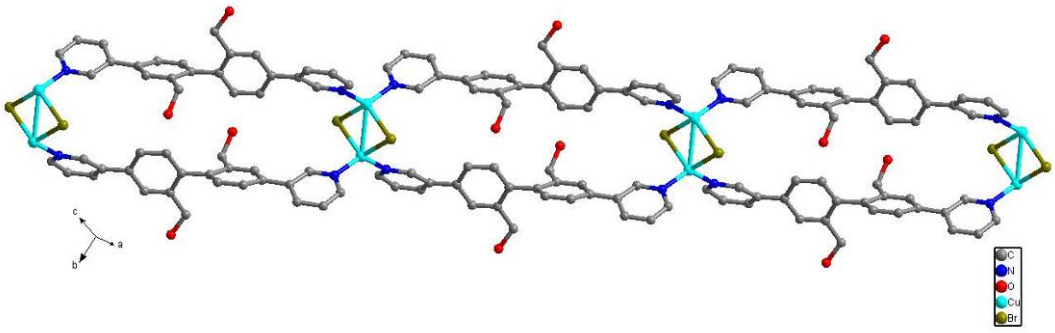


Fig. S1. 1-D double chain of **3**.

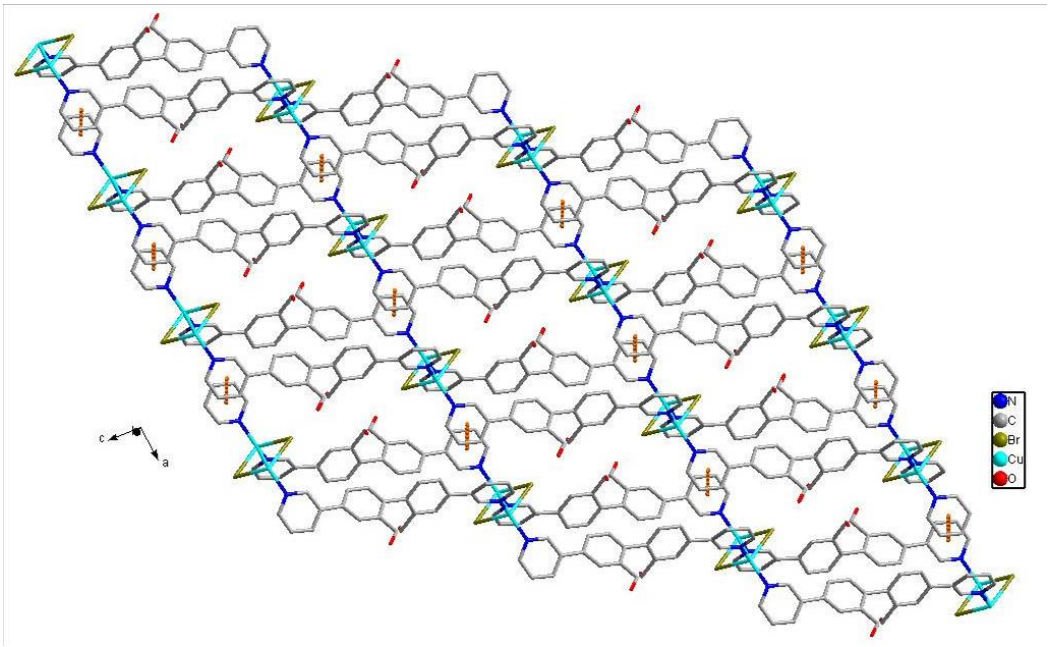


Fig. S2. Formation of 2-D sheet through π···π interactions view down *b* axis;(Disordered O1' and O2' atoms were omitted for clarity.)

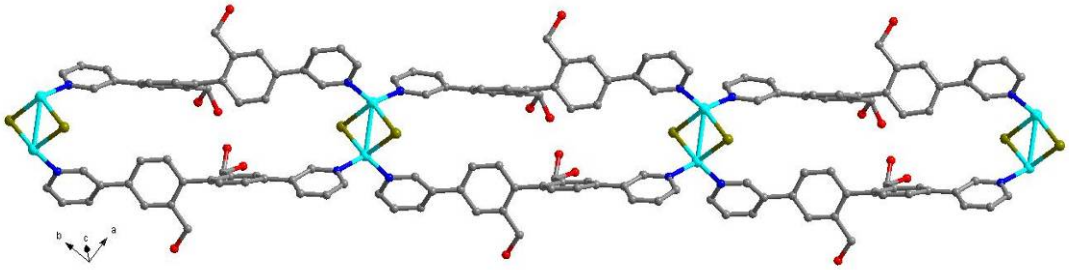


Fig. S3. 1-D double chain of **4**.

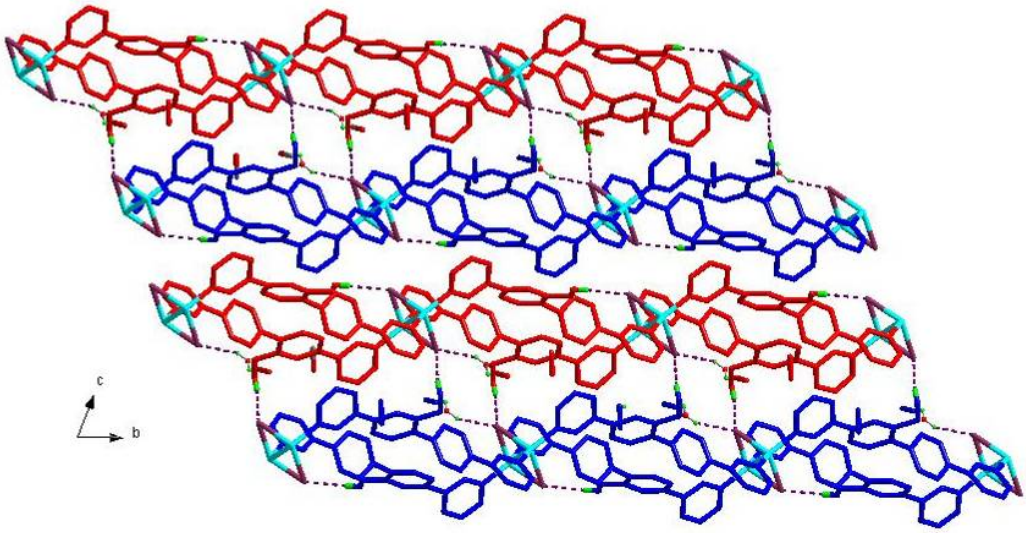
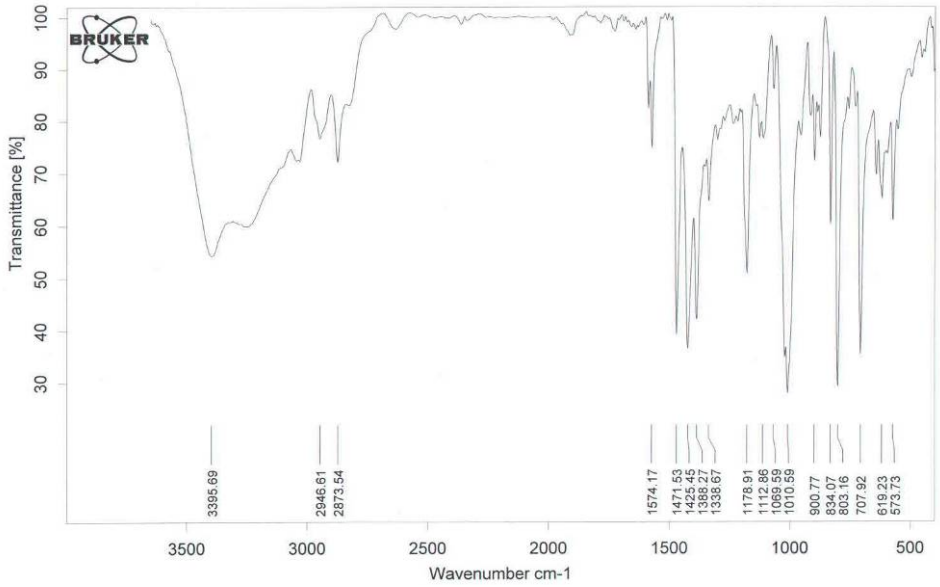
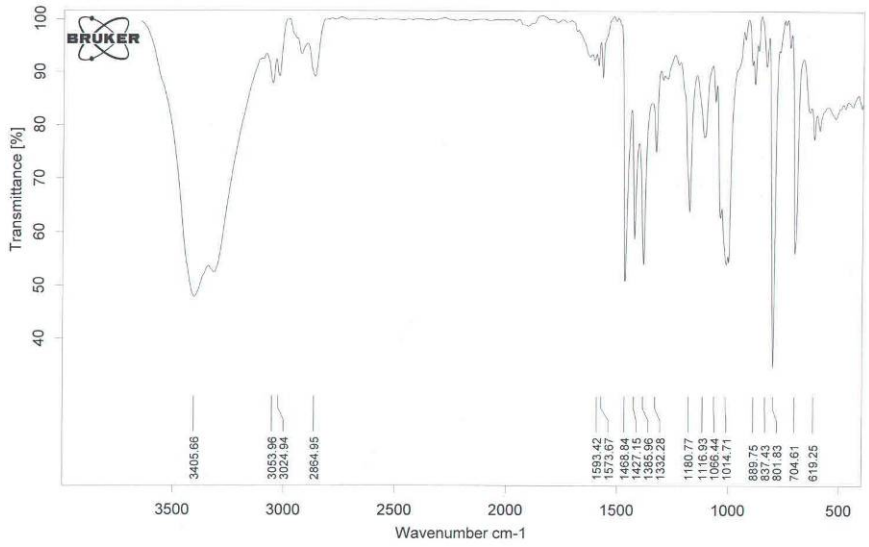


Fig. S4. 1-D chains arrangement through inter-chain H-bond interactions (O-H···Br) view down *a* axis (Disordered O1' and O3' were omitted for clarity).

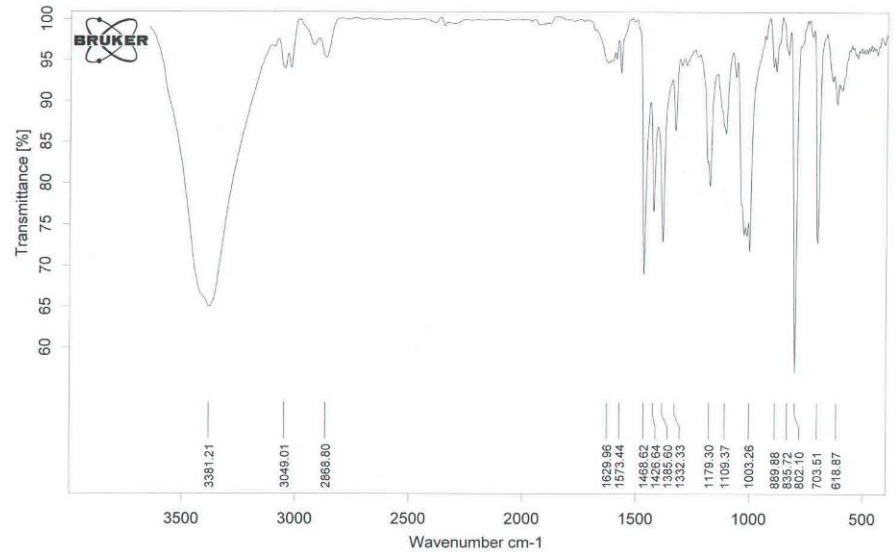
(a)



(b)



(c)



(d)

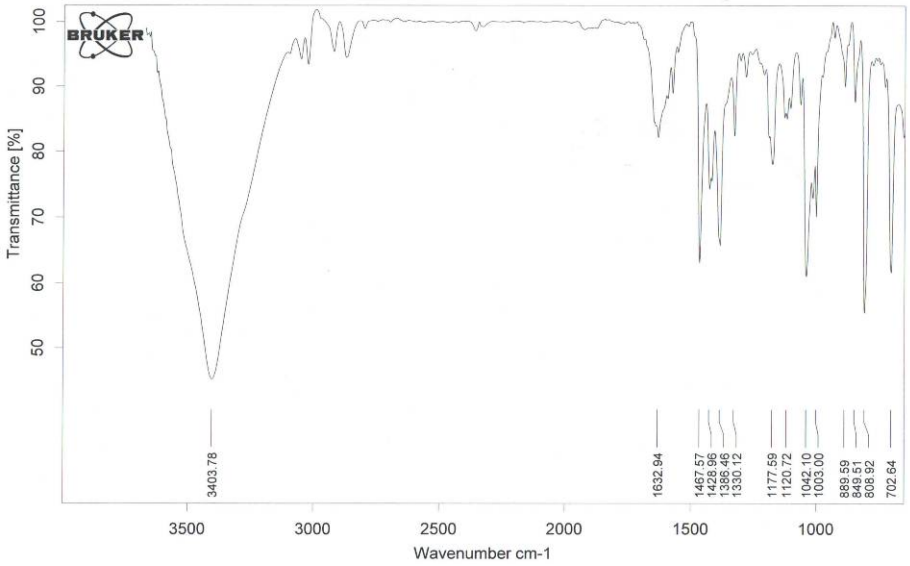
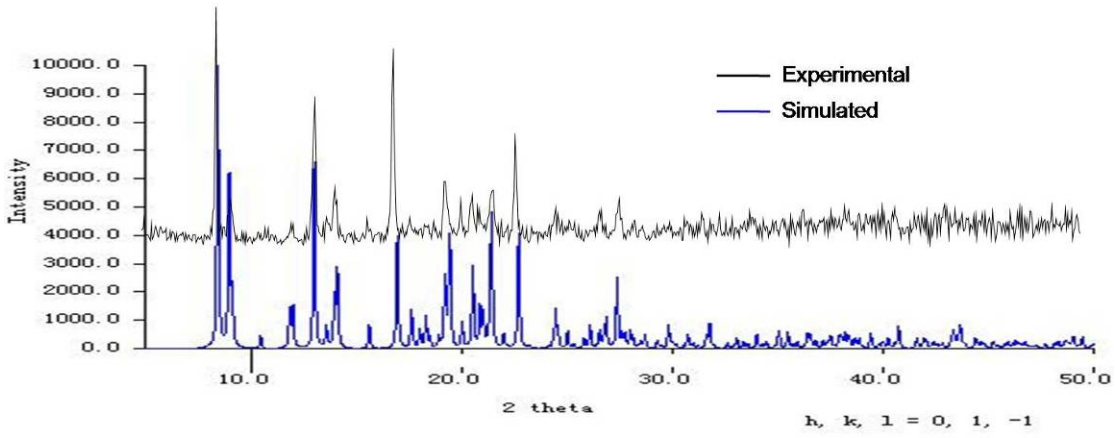
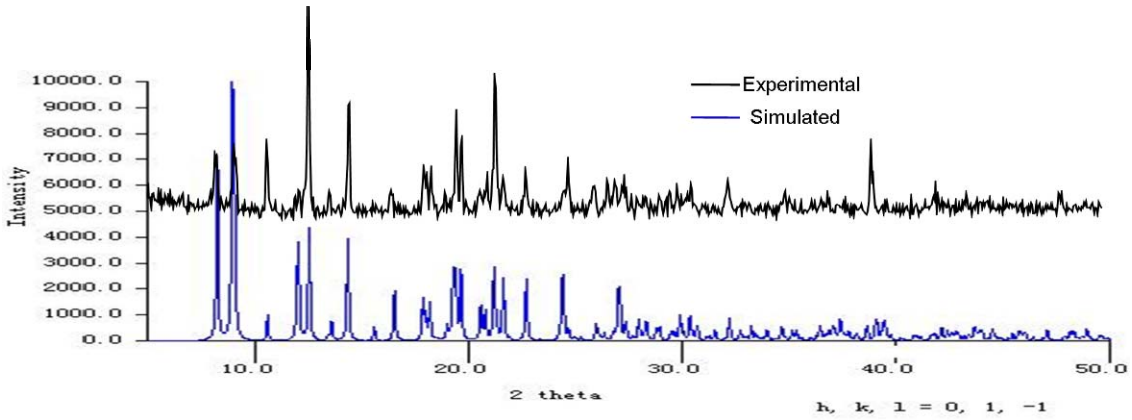


Fig. S5. IR spectra of **L**, **1, 3** and **4**.

(a)



(b)



(c)

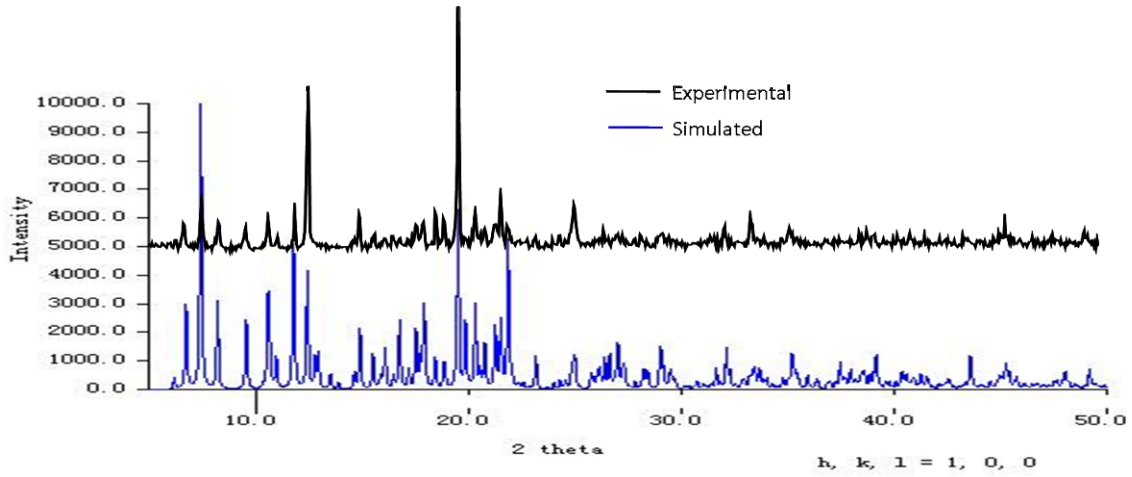


Fig. S6. The PXRD patterns of **1**, **3** and **4.**

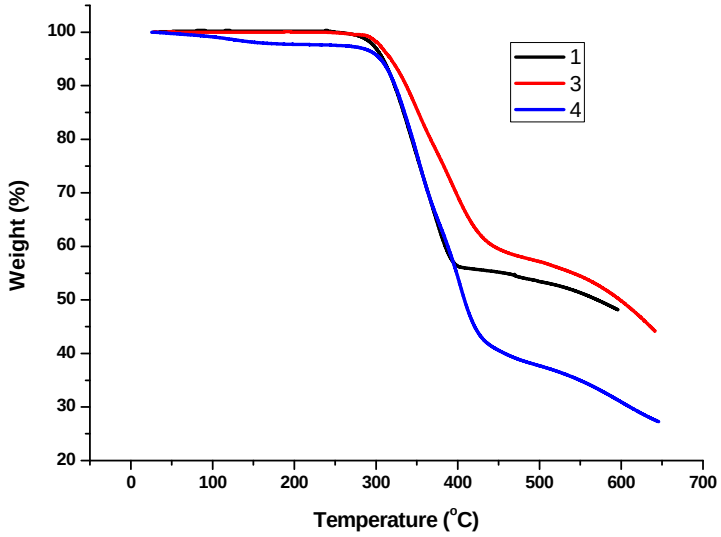


Fig. S7. TGA curves of **1**, **3** and **4.**

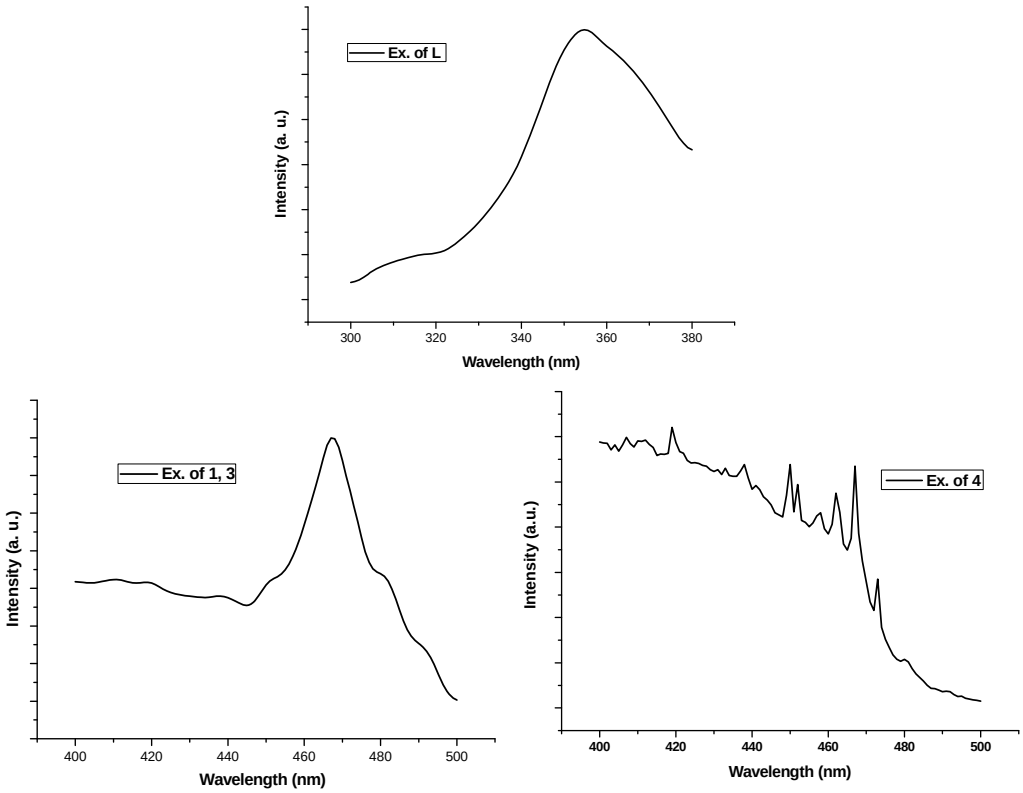
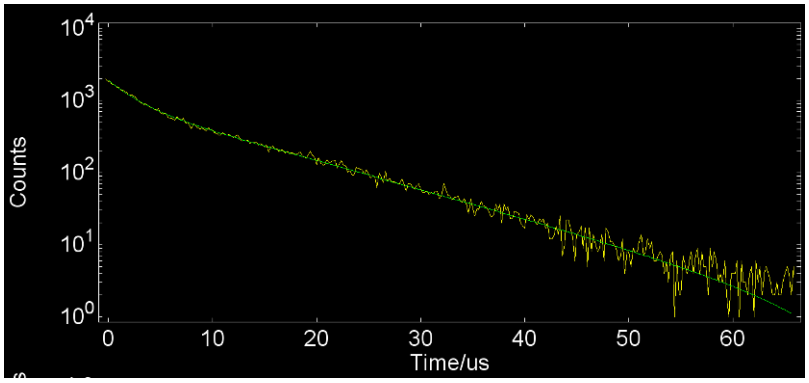
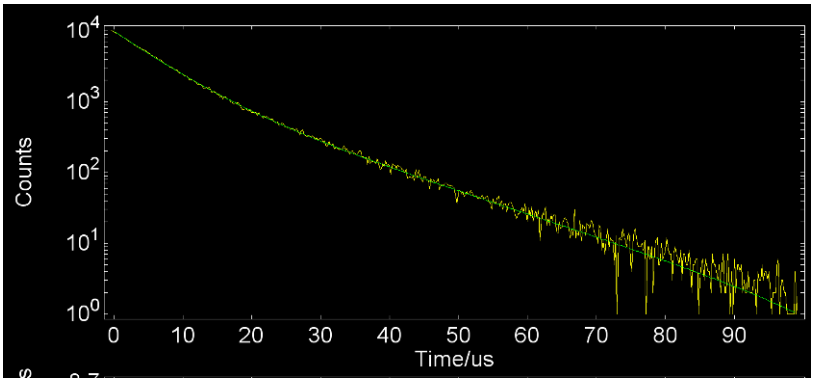


Fig.S8. Excitation spectra of **L**, **1**, **3** and **4.**

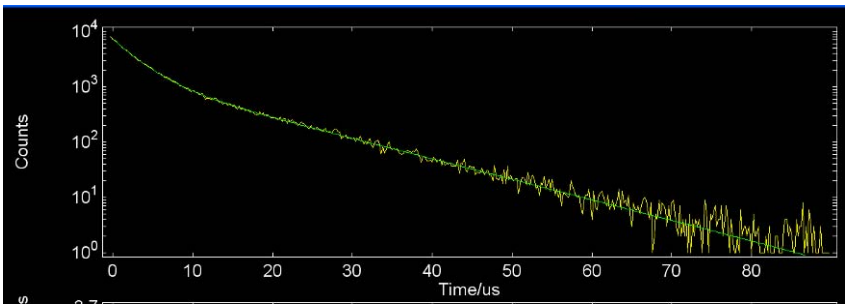
(a)



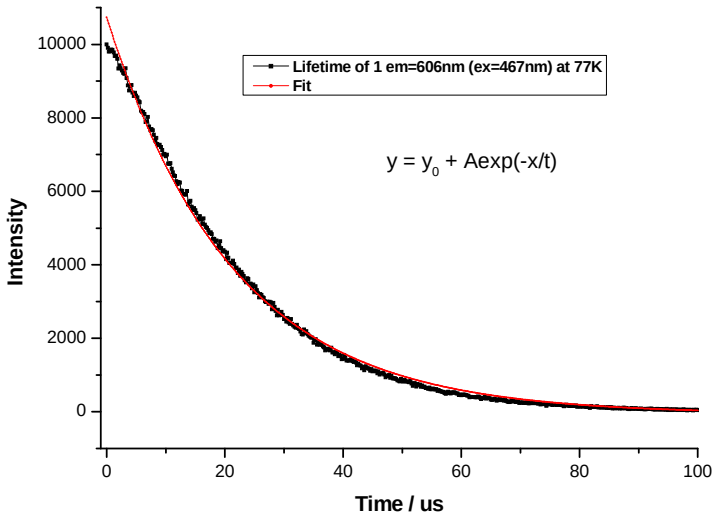
(b)



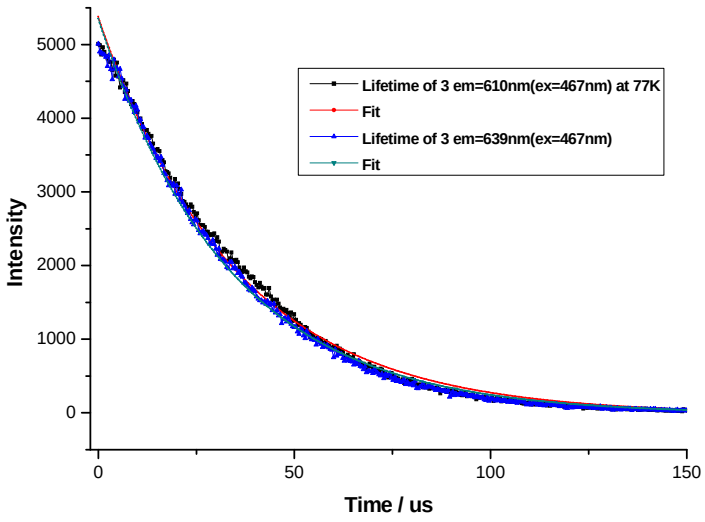
(c)


Counts
Time/us

(d)


Lifetime of 1 em=606nm (ex=467nm) at 77K
Fit
y = y0 + Aexp(-x/t)
Intensity
Time / us

(e)


Lifetime of 3 em=610nm(ex=467nm) at 77K
Fit
Lifetime of 3 em=639nm(ex=467nm)
Fit
Intensity
Time / us

(f)

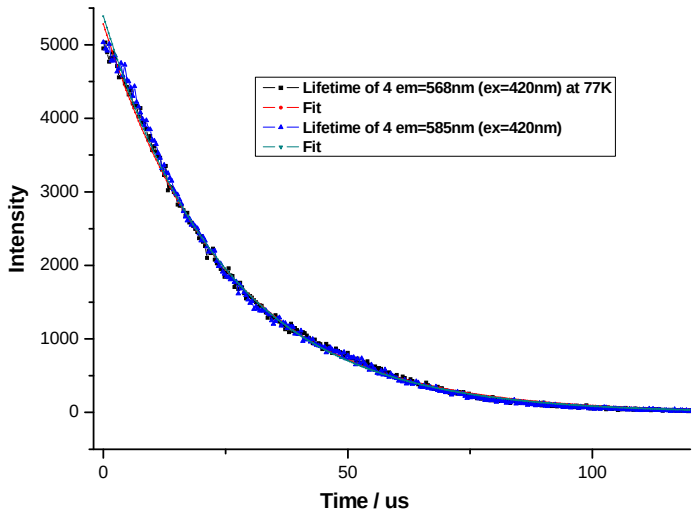


Fig. S9. Emission decay of **1**, **3** and **4** at room temperature (a-c) and 77 K (d-f) in the solid state.

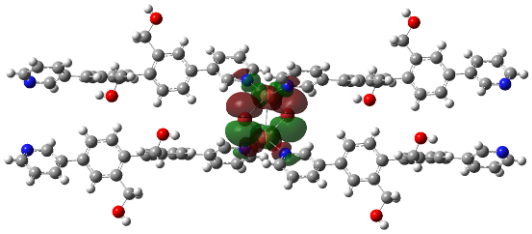
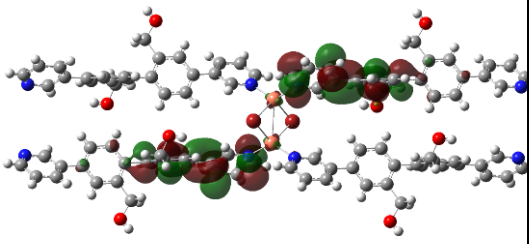
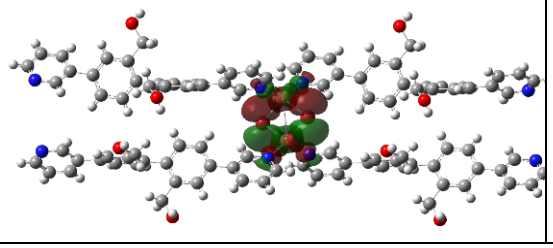
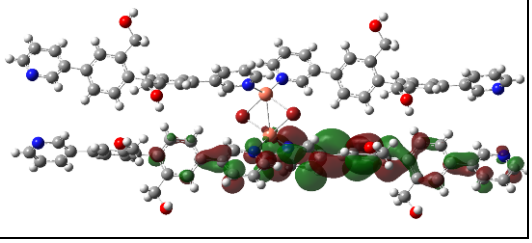
	HOMO	LUMO
3		
4		

Fig. S10. HOMO and LUMO frontier orbitals plots for **3** and **4.**

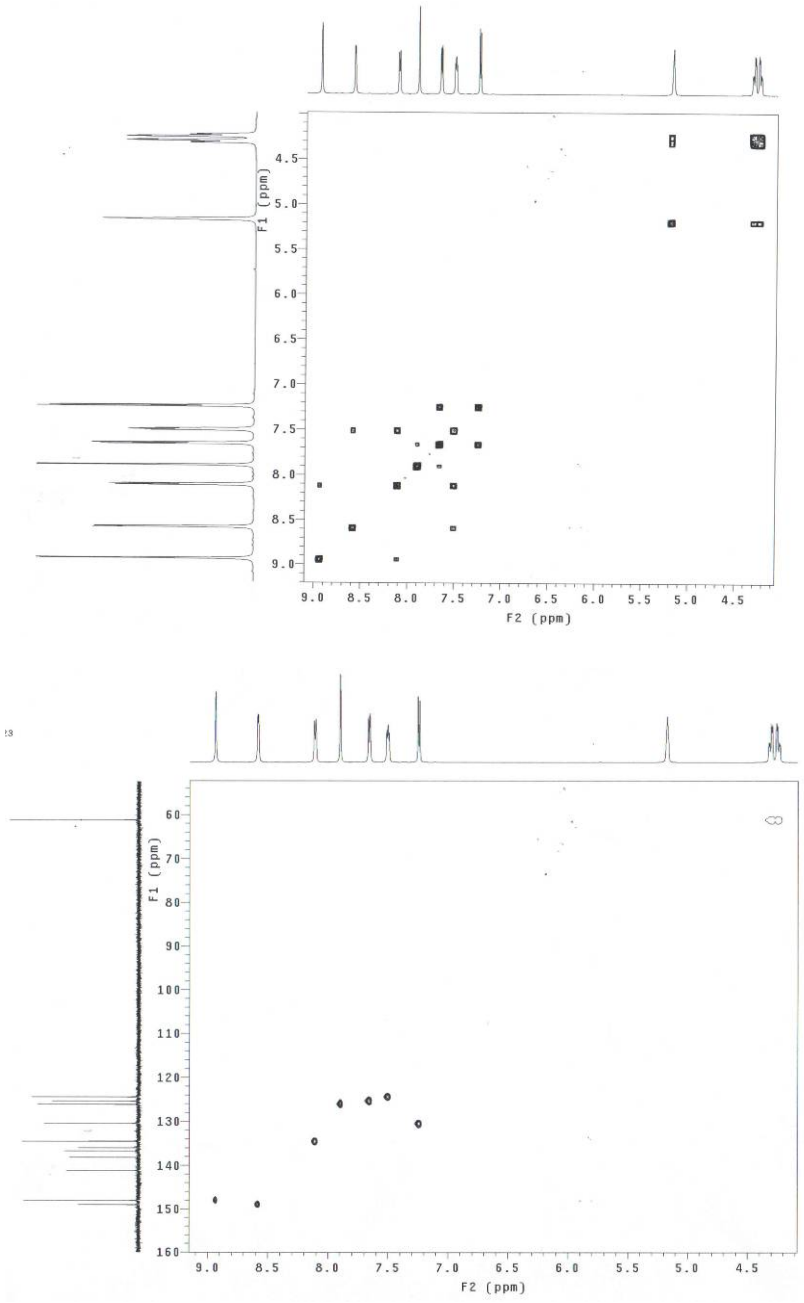


Fig. S11. gCOSY and gHSQC spectra of ligand L.

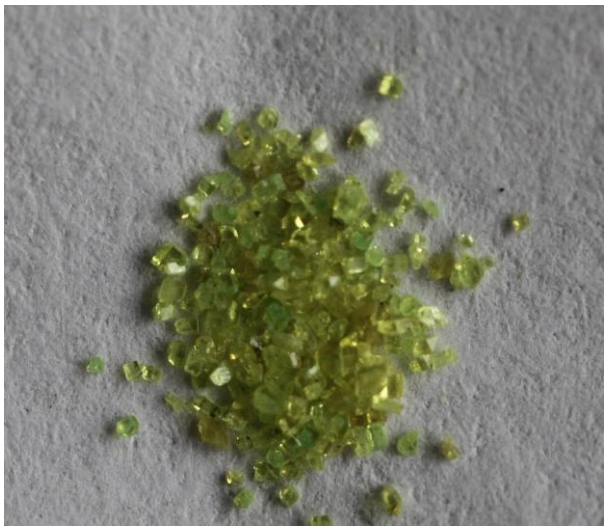


Fig. S12. Photo of **4** crystals under daylight lamp.

Table S1. Hydrogen bonds for **4** (Å and º).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(4)-H(4)...Br(2) #7	0.82	2.65	3.433(4)	160.2
O(2)-H(2A)...Br(1)#6	0.82	2.54	3.357(3)	173.6
O(5)-H(15B)...Br(2) #3	0.86	2.69	3.499(4)	157.6

Symmetry transformations used to generate equivalent atoms: #1 x+1, y-1, z. #2 x-1, y+1, z. #3 -x+1, -y, -z+1. #4 -x+1, -y+1, -z+1. #5 -x, -y+1, -z+1. #6 x-1, y, z. #7 -x+1, -y, -z+2.

Table S2. Selected Bond Length (Å) and Angles (º) for **1**.

Cl(2)-Cu(1)#1	2.4299(16)	Cu(1)-N(2)#2	1.990(3)
Cl(2)-Cu(1)	2.4636(16)	Cu(1)-Cu(1)#1	2.7707(17)
Cu(1)-N(1)	1.989(4)	C(24)-O(2)	1.369(9)
Cu(1)#1-Cl(2)-Cu(1)	68.97(5)	N(1)-Cu(1)-N(2)#2	128.53(15)
N(1)-Cu(1)-Cl(2)#1	105.47(11)	N(2)#2-Cu(1)-Cl(2)#1	104.76(11)
N(1)-Cu(1)-Cl(2)	103.35(11)	N(2)#2-Cu(1)-Cl(2)	103.30(11)
Cl(2)#1-Cu(1)-Cl(2)	111.03(5)	N(1)-Cu(1)-Cu(1)#1	116.06(11)

Symmetry transformations used to generate equivalent atoms: #1 -x+1, -y+3, -z+1. #2 x-1, y+1, z+1. #3 x+1, y-1, z-1.

Table S3. Selected Bond Length (Å) and Angles (º) for **2**.

Cu(1)-N(4)	1.963(7)	Cu(1)-N(3)#1	1.967(7)

Cu(1)-N(4)	1.963(7)	Cu(2)-N(2)#1	1.979(7)
Cu(1)-Cu(2)	2.7393(19)	Cl(3)-Cu(1)	2.404(3)
Cl(3)-Cu(2)	2.563(3)	Cl(4)-Cu(2)	2.383(3)
Cl(4)-Cu(1)	2.670(3)		
N(4)-Cu(1)-Cl(4)	97.0(2)	Cl(3)-Cu(1)-Cl(4)	111.62(9)
N(4)-Cu(1)-Cl(3)	103.7(2)	N(4)-Cu(1)-N(3)#1	132.1(3)
N(3)#1-Cu(1)-Cl(4)	100.6(2)	N(1)-Cu(2)-Cl(4)	108.6(2)
N(1)-Cu(2)-Cl(3)	101.8(2)	N(2)#1-Cu(2)-Cl(3)	102.0(2)
N(2)#1-Cu(2)-N(1)	124.5(3)	Cl(4)-Cu(2)-Cl(3)	116.17(10)

Symmetry transformations used to generate equivalent atoms: #1 x-1, y+1, z. #2 x+1, y-1, z.

Table S4. Selected Bond Length (Å) and Angles (º) for **3**.

N(2)-Cu(1)#1	2.012(6)	Cu(1)-N(1)	2.001(6)
Br(1)-Cu(1)	2.5442(18)	Cu(1)-Br(1)#2	2.5782(14)
Cu(1)-Cu(1)#2	2.781(2)		
N(1)-Cu(1)-N(2)#3	128.7(3)	N(1)-Cu(1)-Br(1)	103.34(19)
N(2)#3-Cu(1)-Br(1)	105.47(18)	N(1)-Cu(1)-Br(1)#2	103.58(17)
N(2)#3-Cu(1)-Br(1)#2	101.91(17)	Br(1)-Cu(1)-Br(1)#2	114.23(5)
Cu(1)-Br(1)-Cu(1)#2	65.77(5)		

Symmetry transformations used to generate equivalent atoms: #1 x+1, y-1, z-1. #2 -x, -y+2, -z+2. #3 x-1, y+1, z+1.

Table S5. Selected Bond Length (Å) and Angles (º) for **4**.

Br(1)-Cu(1)	2.5630(10)	Br(1)-Cu(2)	2.5996(9)
Br(2)-Cu(2)	2.5130(10)	Br(2)-Cu(1)	2.6448(9)
Cu(1)-N(1)	1.989(4)	Cu(1)-N(2)#1	1.986(4)
Cu(2)-N(4)	2.008(4)	Cu(2)-N(3)#1	2.014(4)
Cu(1)-Cu(2)	2.7233(11)		
Cu(1)-Br(1)-Cu(2)	63.67(3)	Cu(2)-Br(2)-Cu(1)	63.68(3)
Br(2)-Cu(2)-Br(1)	118.03(3)	Br(1)-Cu(1)-Br(2)	114.62(3)
N(2)#1-Cu(1)-Br(1)	104.59(11)	N(1)-Cu(1)-Br(1)	104.26(12)

N(2)#1-Cu(1)-N(1)	130.98(15)	N(1)-Cu(1)-Br(2)	99.26(11)
N(4)-Cu(2)-N(3)#1	122.53(16)	N(4)-Cu(2)-Br(2)	105.62(12)
N(3)#1-Cu(2)-Br(1)	102.61(11)	N(4)-Cu(2)-Br(1)	104.53(11)

Symmetry transformations used to generate equivalent atoms: #1 x+1, y-1, z. #2 x-1, y+1, z.