Supplementary information

The influence of different coordination environments on one-dimensional Cu(II) coordination polymers for the photo-degradation of organic dyes

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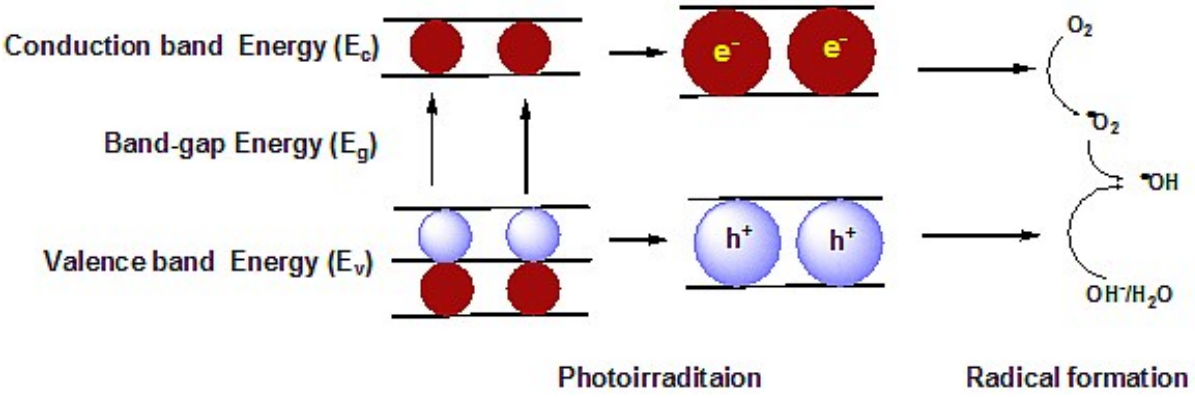

Scheme S1. Schematic diagram showing photo-catalytic mechanism

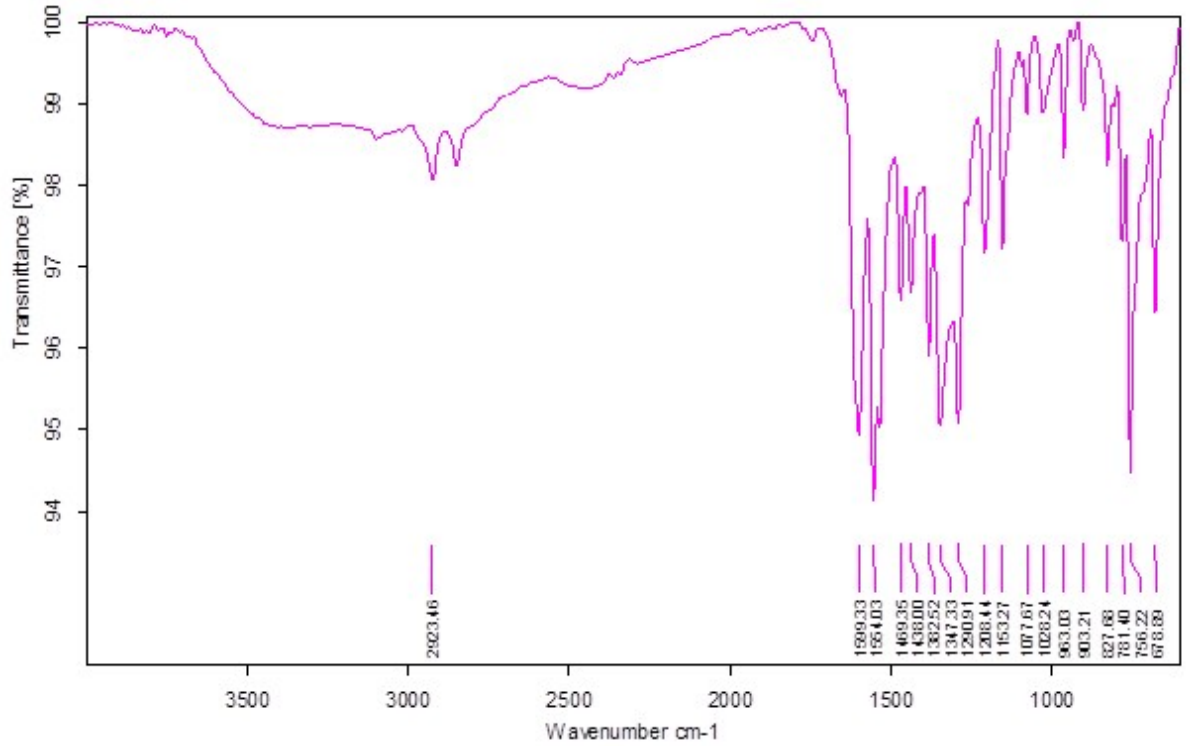

Figure S1. I.R. spectrum of complex **1**

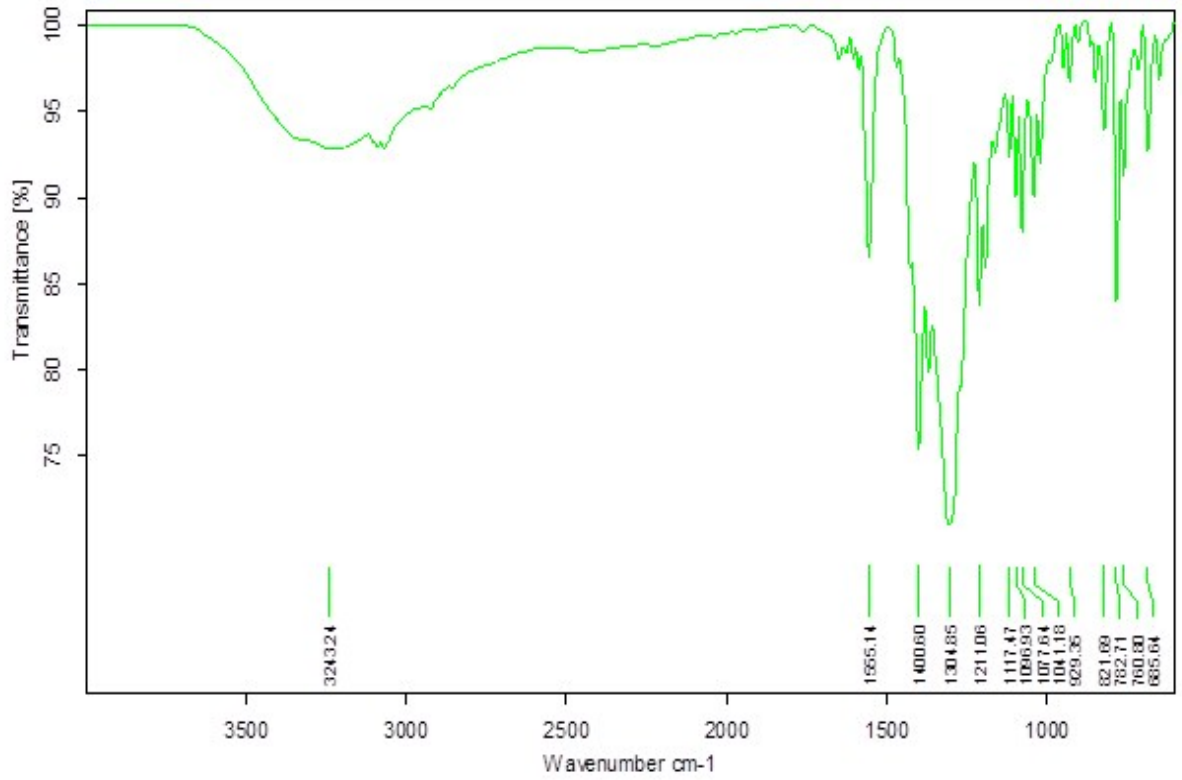

Figure S2. I.R. spectrum of complex **2**

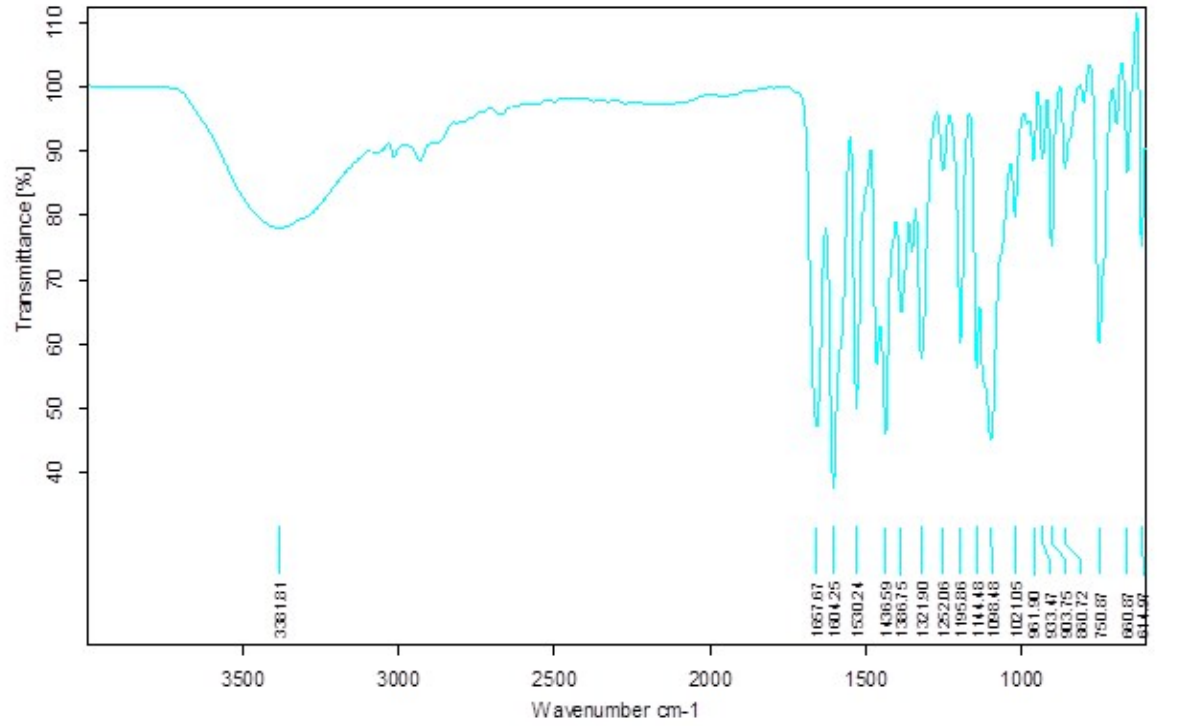

Figure S3. I.R. spectrum of complex **3**

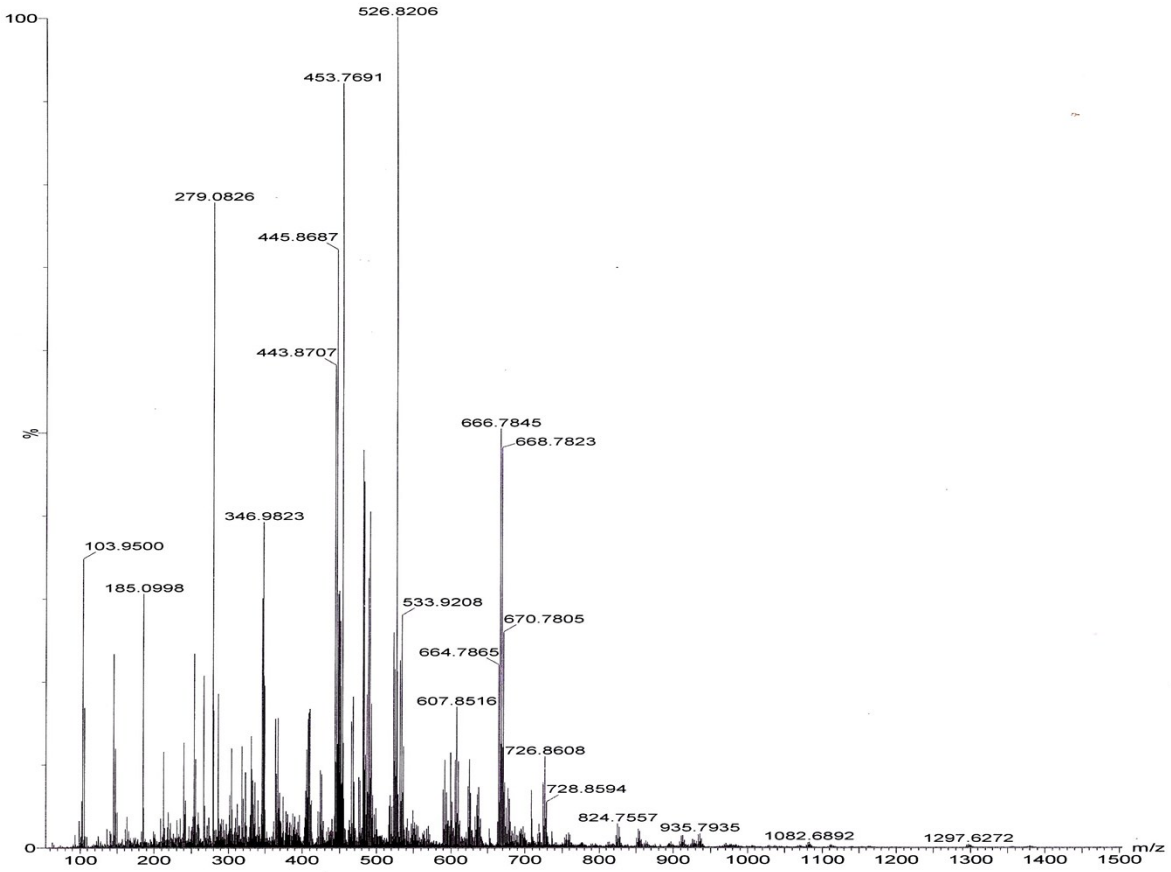

Figure S4. ESI-MS spectrum of complex **1**

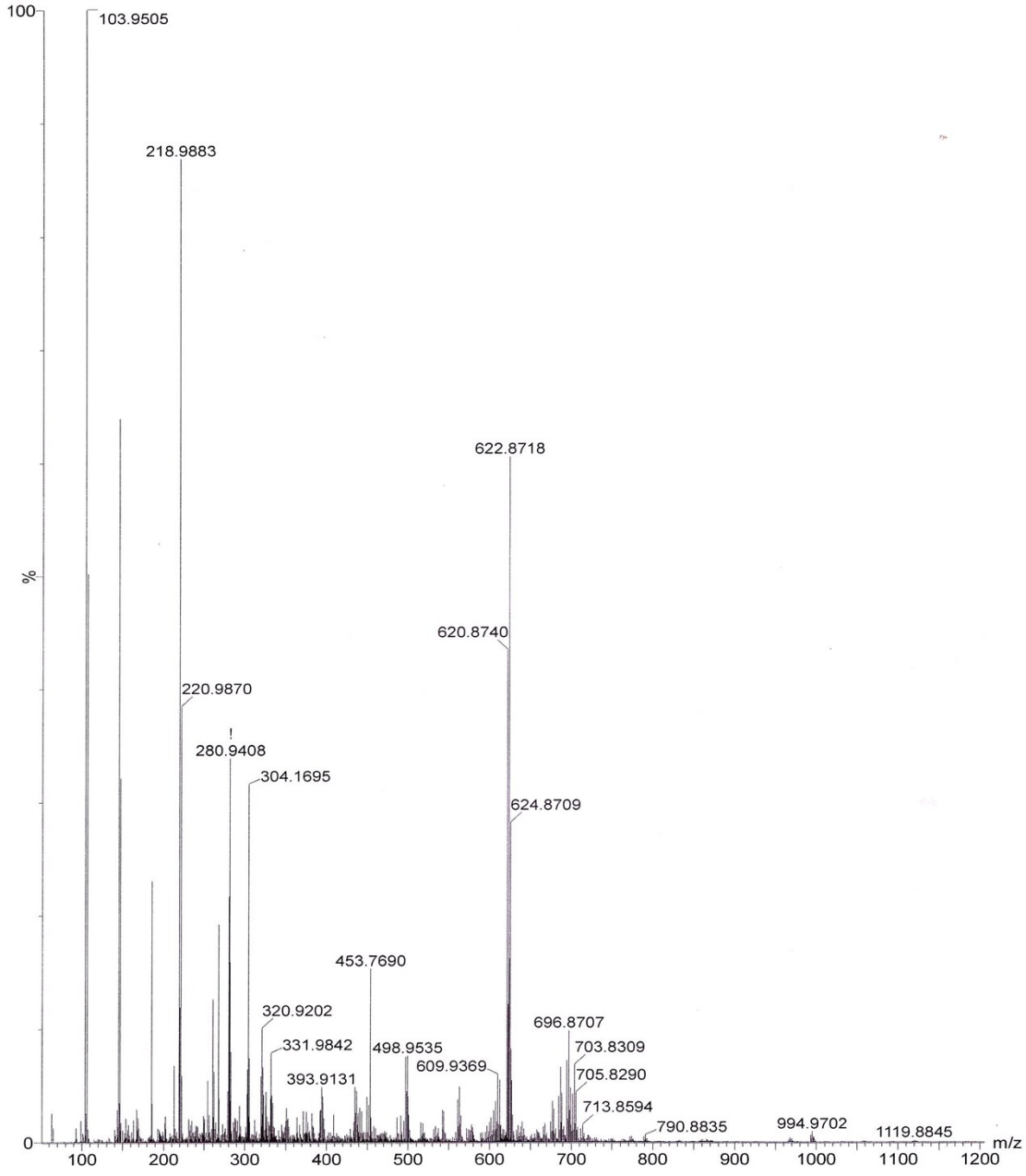

Figure S5. ESI-MS spectrum of complex **2**

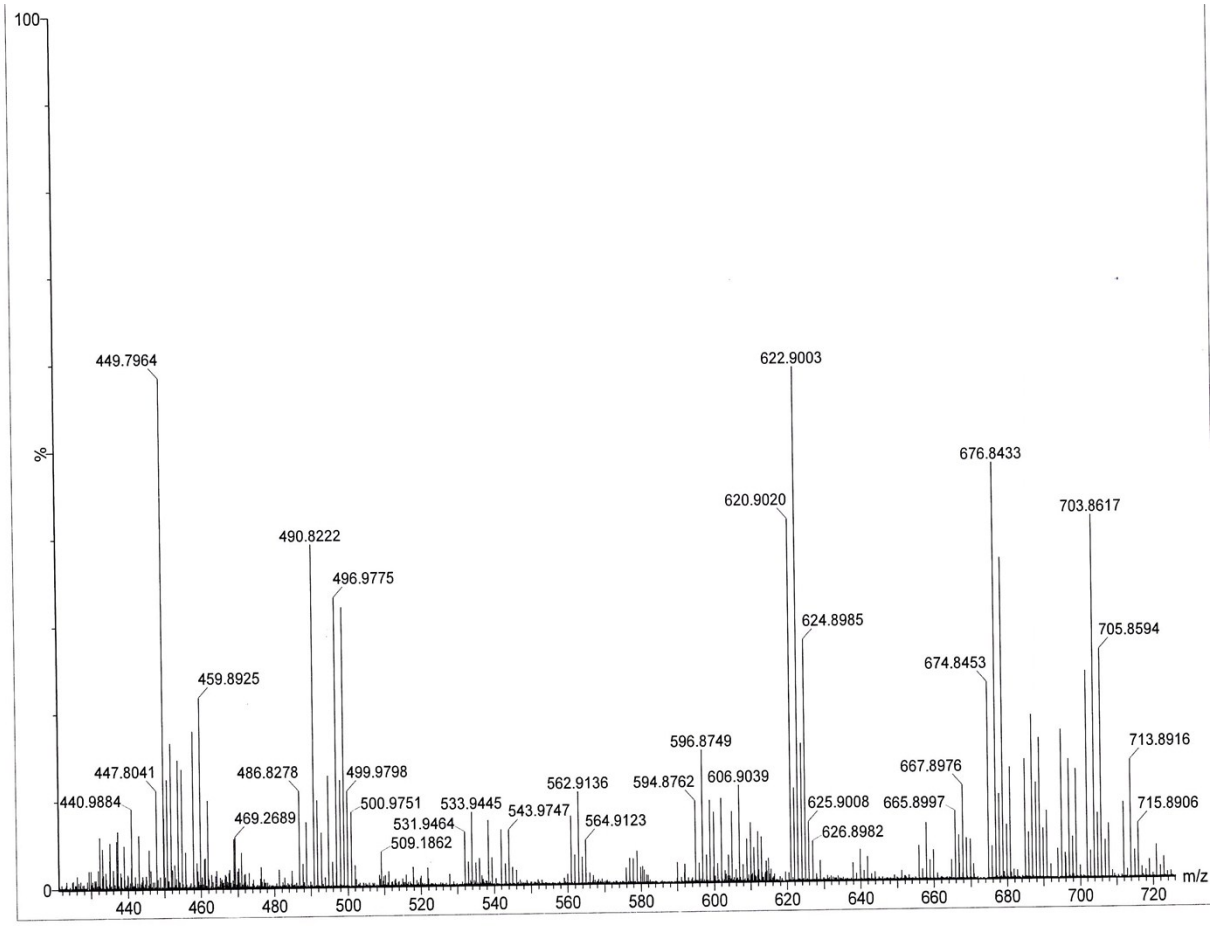

Figure S6. ESI-MS spectrum of complex **3**

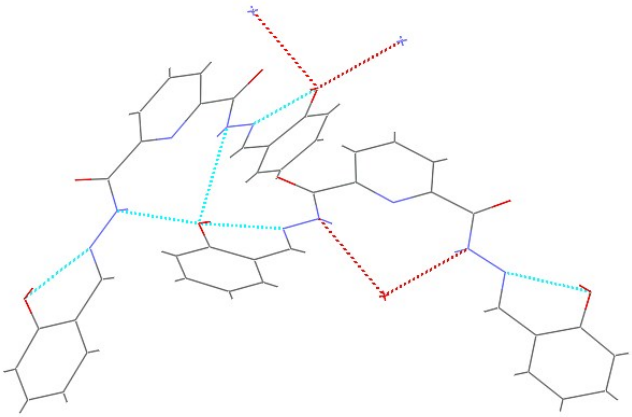

Figure S7. Packing diagram of ligand $\mathbf{H_4L^1}$

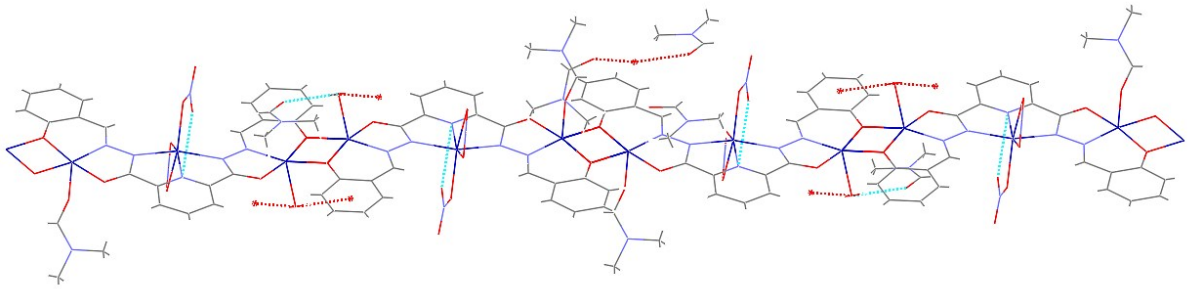

Figure S8. Hydrogen bonded pattern of compound **1** showing the chains of molecules running along along b–axis.

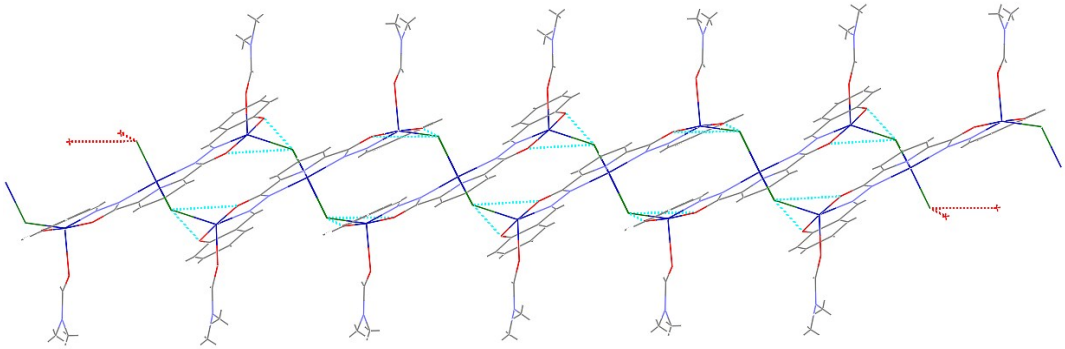

Figure S9. Non-bonding interactions of compound **2**, along c–axis showing the chains like arrangement of molecules.

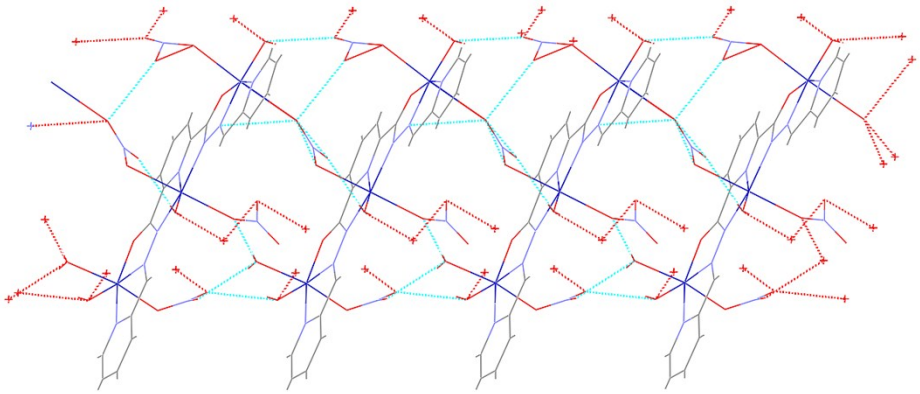

Figure S10. Hydrogen bonded pattern of compound **3** showing the chains of molecules running along along a–axis.

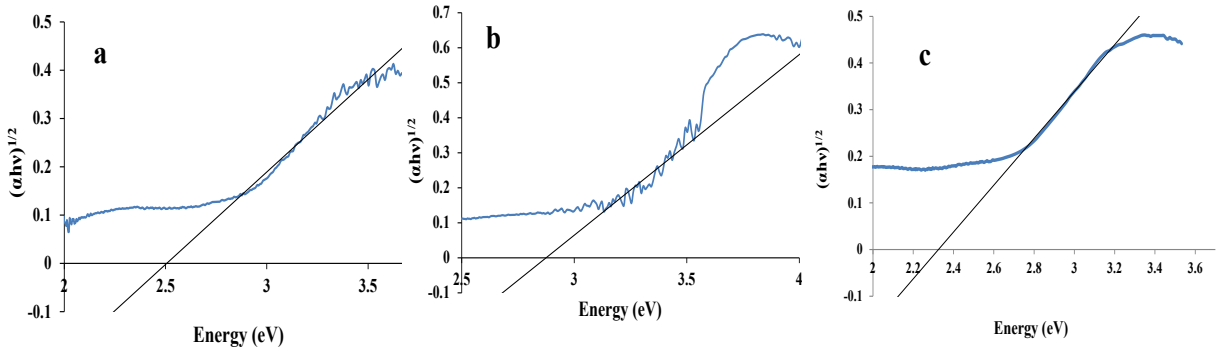

Figure S11. Tauc plot *(α hv)²* versus photon energy *(hv)* for complex (a) **1,** (b) **2** and (c) **3.**

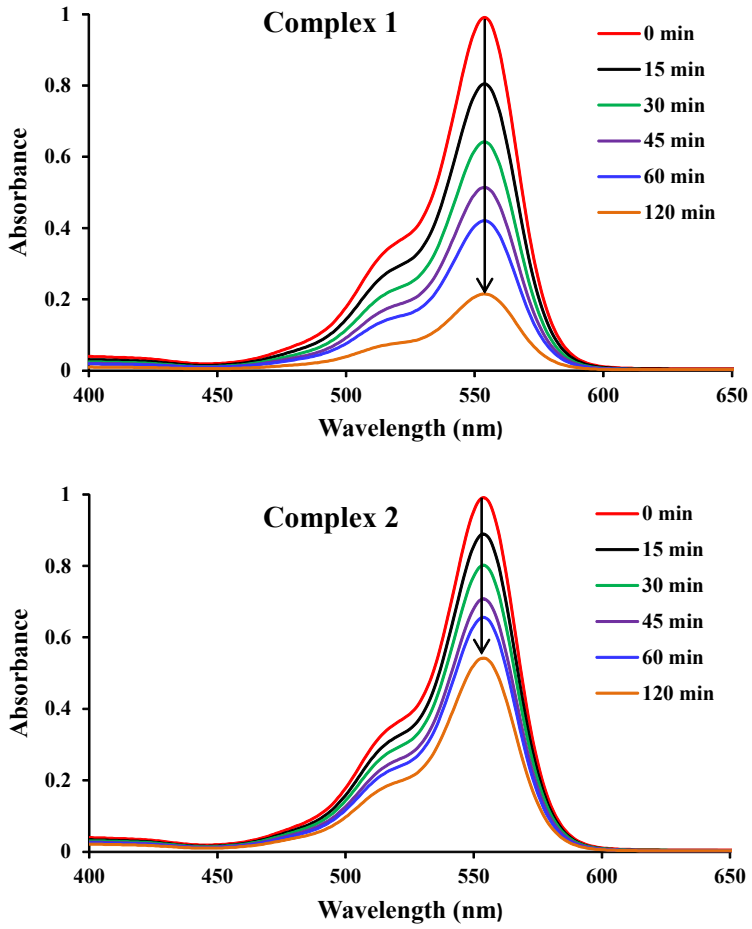

Figure S12. Changes of the UV-Vis spectra of RB in the presence of complex **1** and **2** after light illumination from 0 to 120 min.

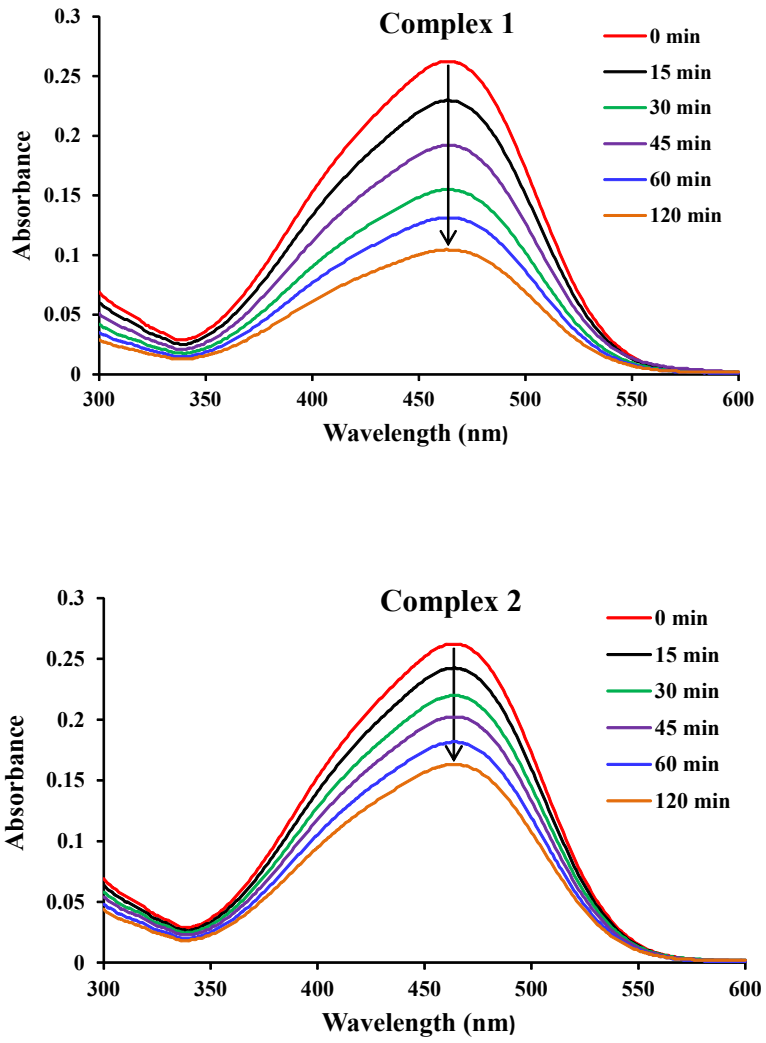

Figure S13. Changes of the UV-Vis spectra of MO in the presence of complex **1** and **2** after light illumination from 0 to 120 min.

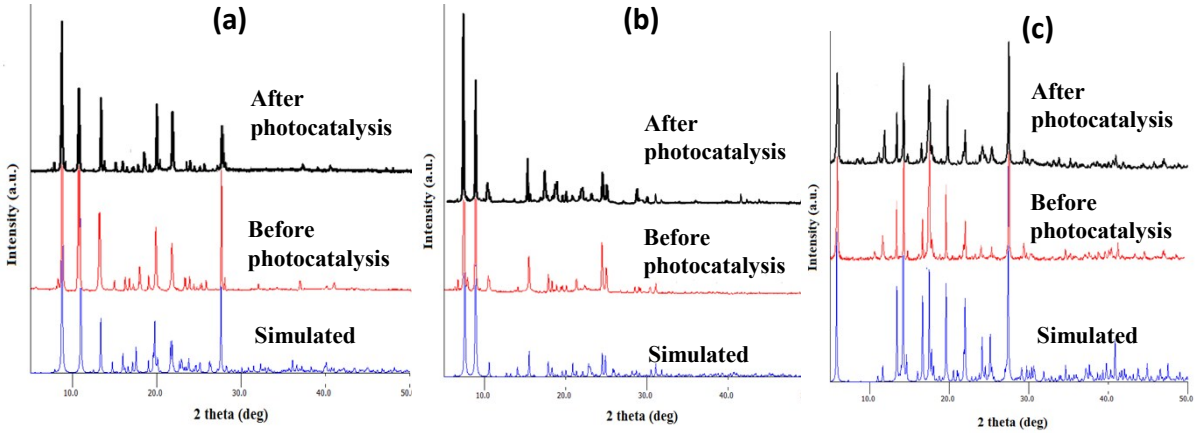

Figure S14. PXD patterns of (a) **1** (b) **2** (c) **3** simulated, before and after the photocatalytic RhB degradation.

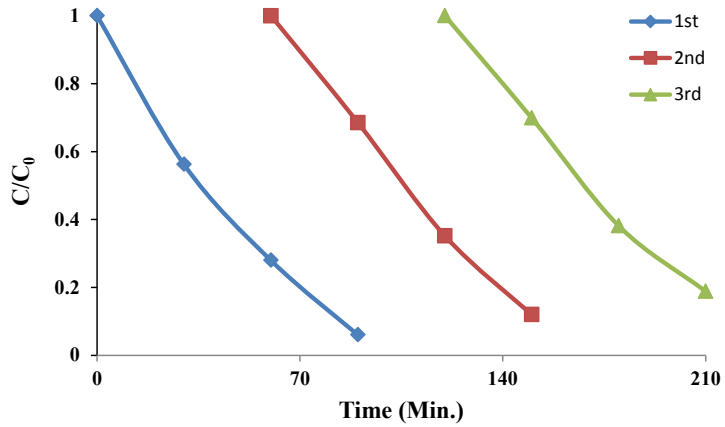

Figure S15. Recycling test on **3** for RB photo-degradation under light irradiation.

Table S1(a). Selected bond lengths and angles (Å,°) for {[$Cu_3(L^1)(NO_3)_2(DMF)(H_2O)$]•3(DMF)•}$_n$ **(1)**

Bond lengths (Å)					
Cu1-O6	2.0207(14)	Cu1-O7	2.6529(16)	Cu1-O9	2.1880(15)
Cu1-O10	2.830(2)	Cu1-N2	2.0499(15)	Cu1-N3	1.9438(16)
Cu1-N4	2.0352(16)	Cu2-O3	1.9618(13)	Cu2-O4	1.9460(13)
Cu2-O5	2.2669(18)	Cu2-N5	1.9369(15)	Cu3-O1	1.9533(14)
Cu3-O2	1.9700(14)	Cu3-O12	2.2696(16)	Cu3-N1	1.9350(15)

Bond angles(°)					
O6-Cu1-O7	53.38(5)	O6-Cu1-O9	82.15(6)	O6-Cu1-O10	131.31(6)
O6-Cu1-N2	99.09(6)	O1-Cu3-O2	169.63(6)	O6-Cu1-N3	154.13(6)
O6-Cu1-N4	99.81(6)	O7-Cu1-O9	135.50(5)	O7-Cu1-O10	74.24(5)
O7-Cu1-N2	92.68(6)	O7-Cu1-N3	100.79(6)	O7-Cu1-N4	89.23(6)
O9-Cu1-O10	49.24(5)	O9-Cu1-N2	93.18(6)	O9-Cu1-N4	100.94(6)
O10-Cu1-N2	83.38(6)	O10-Cu1-N3	74.36(6)	O10-Cu1-N4	92.85(6)
N2-Cu1-N3	78.64(6)	N2-Cu1-N4	157.75(6)	O9-Cu1-N3	123.60(6)
N3-Cu1-N4	79.22(6)	O3-Cu2-O4	172.29(6)	O3-Cu2-O5	93.99(6)
O3-Cu2-N5	81.55(6)	O4-Cu2-O5	91.09(6)	O4-Cu2-N5	92.67(6)
O5-Cu2-N5	90.01(6)	O1-Cu3-O12	95.17(6)	O1-Cu3-N1	92.29(6)
O2-Cu3-O12	94.43(6)	O2-Cu3-N1	81.25(6)	O12 -Cu3-N1	106.37(6)

Table S1(b). Selected bond lengths and angles (Å,°) for [$Cu_3(L^1)(Cl)_2(DMF)_2]_n$ **(2)**

Bond lengths (Å)					
Cu1-N2	2.027(3)	Cu1-N3	1.948(3)	Cu1-N4	2.023(3)
Cu1-Cl1_a	2.4120(9)	Cu1-Cl2_b	2.4039(9)	Cu2-Cl1	2.3242(9)

Cu2-O1	1.896(2)	Cu2-O2	1.988(2)	Cu2-O6	2.240(2)
Cu2-N1	1.953(3)	Cu3-Cl2	2.3777(9)	Cu3-O3	1.982(2)
Cu3-O4	1.889(3)	Cu3-O5	2.182(3)	Cu3-N5	1.958(3)

Bond angles(°)					
N2-Cu1-N3	78.51(12)	N2-Cu1-N4	157.29(13)	Cl1_a-Cu1-N2	97.96(8)
Cl2_b-Cu1-N2	97.90(8)	N3-Cu1-N4	78.79(12)	Cl1_a-Cu1-N3	129.76(8)
Cl2_b-Cu1-N3	131.84(8)	Cl1_a-Cu1-N4	96.06(8)	Cl2_b-Cu1-N4	97.62(8)
Cl1-Cu2-O1	91.64(7)	Cl1-Cu2-O2	93.10(7)	Cl1-Cu2-O6	98.35(8)
Cl1-Cu2-N1	149.46(8)	O1-Cu2-O2	173.21(10)	O1-Cu2-O6	91.77(11)
O1-Cu2-N1	92.75(11)	O2-Cu2-O6	92.35(10)	O2-Cu2-N1	80.72(11)
O6-Cu2-N1	111.70(10)	Cl2-Cu3-O3	92.88(7)	Cl2-Cu3-O4	92.74(8)
Cl2-Cu3-O5	96.12(8)	Cl2-Cu3-N5	143.01(8)	O3-Cu3-O4	173.27(11)
O3-Cu3-O5	90.21(10)	O3-Cu3-N5	81.02(11)	O4-Cu3-O5	92.88(11)
O4-Cu3-N5	92.25(12)	O5-Cu3-N5	120.19(11)	Cu3-O4-C21	128.5(3)

Table S1(c). Selected bond lengths and angles (Å,°) for **$[Cu_3(L^2)(NO_3)_4(H_2O)_4]_n$ (3)**

Bond lengths (Å)					
Cu1-O3	2.312(4)	Cu1-O6	2.413(4)	Cu1-O9	1.937(4)
Cu1-N3	2.126(4)	Cu1-N4	1.936(4)	Cu1-N5	2.095(4)
Cu2-O2	1.985(4)	Cu2-O10	2.291(4)	Cu2-O11	1.974(4)
Cu2-O16	2.632(4)	Cu2-N6	1.950(4)	Cu2-N7	2.011(4)
Cu3-O1	1.968(4)	Cu3-O12	1.932(4)	Cu3-O13	2.340(11)
Cu3-N1	1.996(4)	Cu3-N2	1.938(4)	Cu3-O19	2.433(13)

Bond angles(°)					
O3-Cu1-O6	173.68(14)	O16-Cu2-N7	98.69(16)	O3-Cu1-O9	91.97(16)
N6-Cu2-N7	80.64(17)	O3-Cu1-N3	92.99(15)	O1-Cu3-O12	96.68(16)
O3-Cu1-N4	97.04(15)	O1-Cu3-O13	85.2(3)	O3-Cu1-N5	90.29(14)
O1-Cu3-N1	161.44(17)	O6-Cu1-O9	82.09(16)	O1-Cu3-N2	80.01(16)
O6-Cu1-N3	86.53(15)	O1-Cu3-O19	100.4(4)	O6-Cu1-N4	89.04(15)
O6-Cu1-N5	92.66(14)	O12-Cu3-O13	81.1(3)	O9-Cu1-N3	104.99(17)
O12-Cu3-N1	101.67(17)	O9-Cu1-N4	170.16(17)	O12-Cu3-N2	172.17(17)
O9-Cu1-N5	98.10(17)	O12-Cu3-O19	90.8(4)	N3-Cu1-N4	78.56(16)
N3-Cu1-N5	156.54(16)	O13-Cu3-N1	100.3(3)	N4-Cu1-N5	77.98(16)
O13-Cu3-N2	105.5(3)	O2-Cu2-O10	97.42(15)	O2-Cu2-O11	97.26(16)
N1-Cu3-N2	81.44(17)	O2-Cu2-O16	80.49(15)	O19-Cu3-N1	82.2(4)
O2-Cu2-N6	79.86(16)	O2-Cu2-N7	158.72(17)	O19-Cu3-N2	96.8(4)
O10-Cu2-O11	85.92(15)	O10-Cu2-O16	156.54(14)	O10-Cu2-N6	91.51(15)
O3-Cu1-H9B	108.8(15)	O10-Cu2-N7	91.52(16)	O6-Cu1-H9B	65.0(15)
O11-Cu2-O16	71.30(14)	O9-Cu1-H9B	19.8(15)	O11-Cu2-N6	175.87(16)
N3-Cu1-H9B	93.3(15)	O11-Cu2-N7	102.63(16)	N4-Cu1-H9B	153.4(15)
O16-Cu2-N6	110.91(15)	N5-Cu1-H9B	107.6(15)		

Table S2 : Photocatalytic activities from reported complexes

Complex	Substrate	Conditions	Dye Degradation rate (%)	Reference
[Cd(btec)0.5(bimb)0.5]n	X3B anionic organic dye	aqueous solution, 25° C	94.1 % in 5 h	S1
$[Ag_7(4,4'\text{-tmbpt})(HL)_2(L)(H_2O)]$	Methyl Blue	aqueous solution, 25° C	73 % in 1.5 h	S2
[Ag(bpy)]4V4O12 · 2H2O	Methyl Blue	aqueous solution, 25° C	80% in 3 h	S3
[Cu(hfipbb)(2,2'-bipy)(H2O)2]n	Rhodamine B	aqueous	43% in 0.5 h	S4
[Cu(3-dpyh)0.5(1,4-NDC)]·H2O	Methyl Blue	aqueous	67% in 2h	S5
$[Cu_3(L^2)(NO_3)_4(H_2O)_4]_n$ (3).	**Rhodamine B**	**aqueous solution, 25° C**	**73 % in 1 h**	**Present Work**

References

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