Metal-organic frameworks based on 1,3,5 – triazine - 2,4,6- triyltrithio-tri-acetate: Structures, topologies, photoluminescence and photocatalytic properties

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Table S1 Selected bond lengths (Å) and angles (º) for complexes **1-3**

Complex 1			
Pb(1)-O(3)	2.464(6)	Pb(1)-O(2)	2.542(6)
Pb(1)-O(8)#1	2.890(7)	Pb(1)-O(6)	2.696(6)
Pb(1)-O(2)#1	2.659(5)	Pb(2)-O(7)#3	2.415(6)
Pb(2)-O(1)#5	2.854(6)	Pb(2)-O(3)	2.646(6)
O(2)-Pb(1)-O(1)	49.86(18)	O(2)-Pb(1)-O(6)	162.0(2)
O(2)-Pb(1)-O(5)#2	124.10(17)	O(4)#4-Pb(2)-O(5)#4	48.21(19)
O(7)#3-Pb(2)-O(1)#5	168.4(2)	O(7)#3-Pb(2)-O(3)	80.0(2)
Complex 2*			
Pb(1)-O(5)#6	2.418(7)	Pb(1)-O(7)#7	2.879(8)
Pb(1)-O(2)	2.431(9)	Pb(1)-O(6)#8	2.936(7)

Pb(2)-O(6)#8	2.432(8)	Pb(2)-O(6)#9	2.897(8)
O(3)#6-Pb(1)-O(4)#6	50.1(2)	O(3)#6-Pb(1)-O(6)#8	157.3(2)
O(2)-Pb(1)-O(4)#6	131.3(2)	O(6)#8-Pb(2)-O(4)#8	71.4(2)
O(6)#8-Pb(2)-O(6)#9	146.29(11)	O(6)#8-Pb(2)-O(1)	89.0(2)
Complex 3			
Ni(1)-O(1)	2.078(3)	Ni(1)-O(7)	2.094(4)
Ni(1)-N(5)#11	2.091(5)	Ni(1)-N(4)	2.093(5)
Ni(2)-O(6)#12	2.058(3)	Ni(2)-O(3)	2.100(3)
Ni(2)-N(7)#13	2.081(4)	Ni(2)-N(6)	2.094(4)
O(1)#10-Ni(1)-O(1)	178.54(18)	O(1)-Ni(1)-O(7)	88.10(14)
N(5)#11-Ni(1)-O(7)	88.79(9)	N(4)-Ni(1)-O(7)	91.21(9)
N(5)#11-Ni(1)-N(4)	180.000(1)	O(6)#12-Ni(2)-O(3)	87.92(14)
O(6)#12-Ni(2)-O(9)	175.96(14)	N(7)#13-Ni(2)-O(8)	85.96(14)
N(6)-Ni(2)-O(8)	176.52(15)	N(7)#13-Ni(2)-N(6)	92.08(16)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1, -y+1, -z+1 #2 x-1, -y+1/2, z-1/2 #3 -x+1, -y+1, -z+2 #4 x-1, y, z

#5 x, -y+1/2, z+1/2 #6 -x+1, -y, -z+1 #7 -x+1, -y+1, -z+2 #8 x, y+1, z+1

#9 -x, -y, -z+1 #10 -x+1,y,-z+1/2 #11 x, y-1, z #12 x, -y+1, z+1/2

#13 -x+1/2, y-1/2, -z+1/2

*In complex **2**, Pb2 is found close to the inversion center rather than right on it.

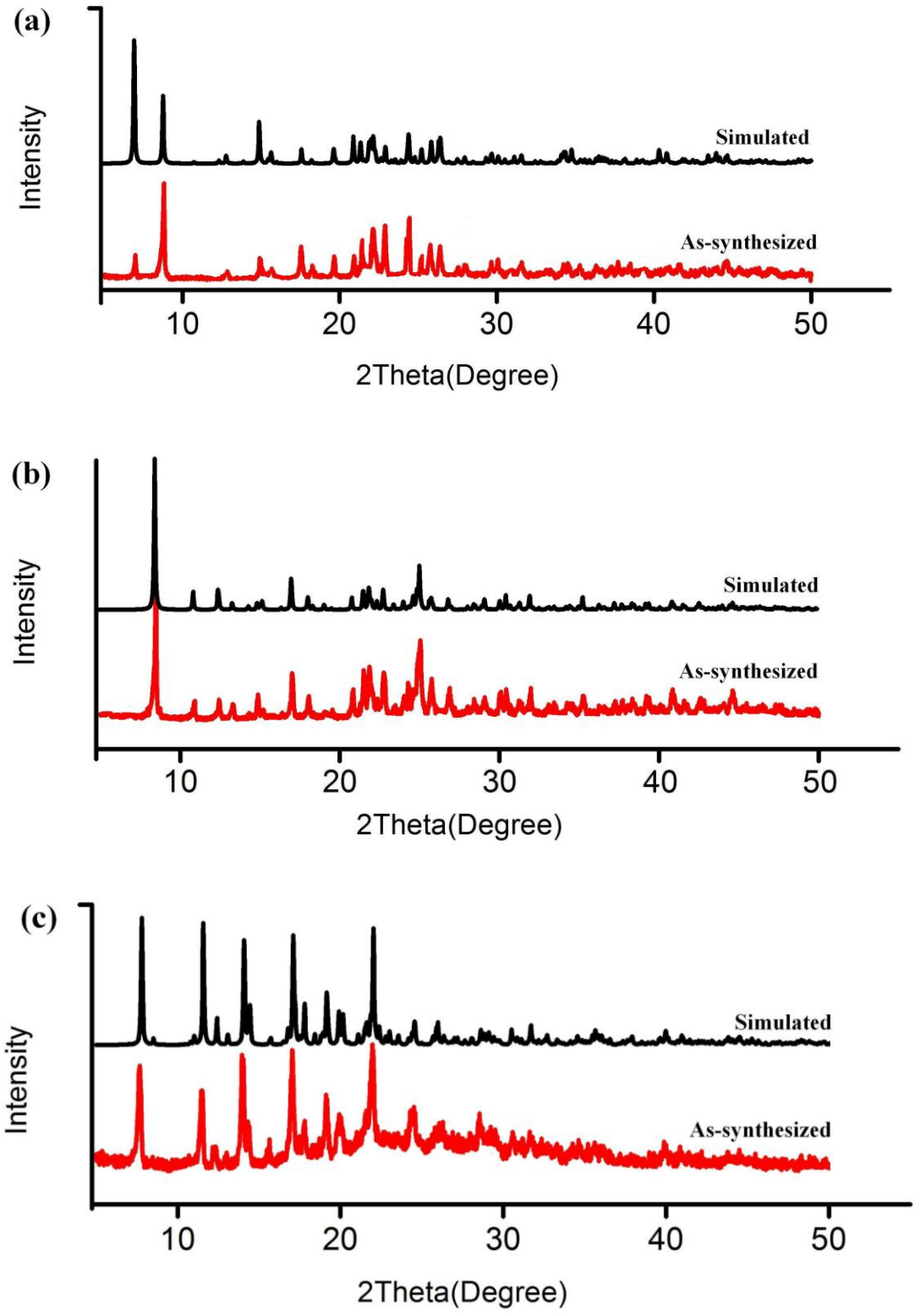


Fig.S1 The powder XRD patterns for complexes **1** (**a**), **2** (**b**) and **3** (**c**).

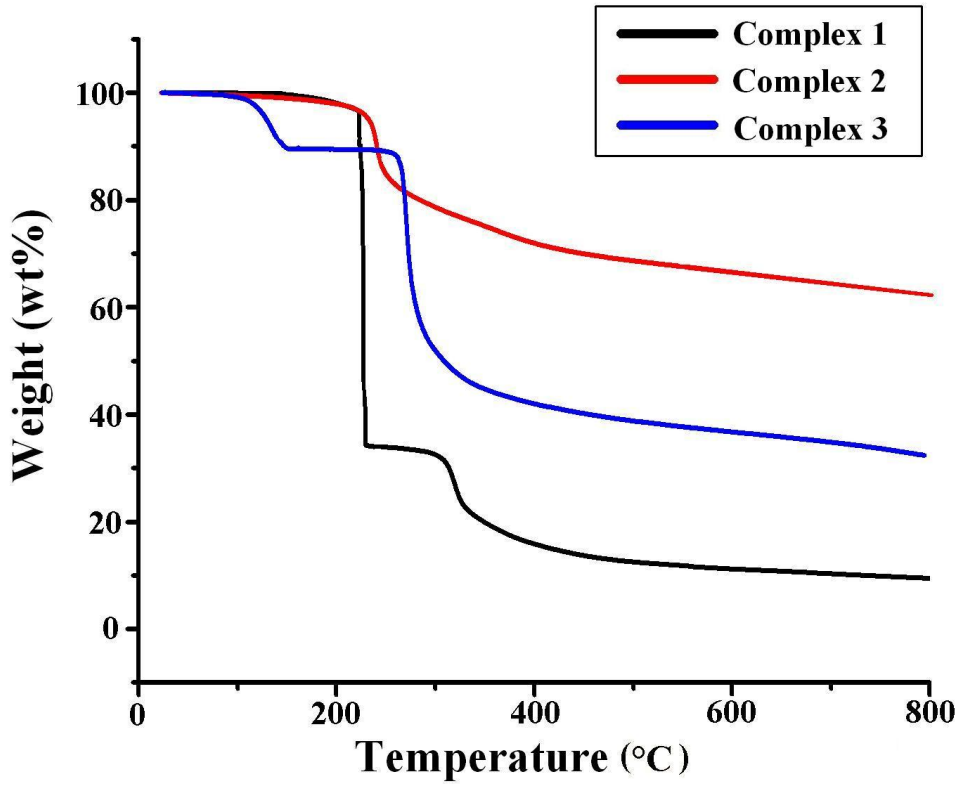


Fig. S2 Thermogravimetric curves of complexes **1** (**black**), **2** (**red**) and **3** (**blue**).

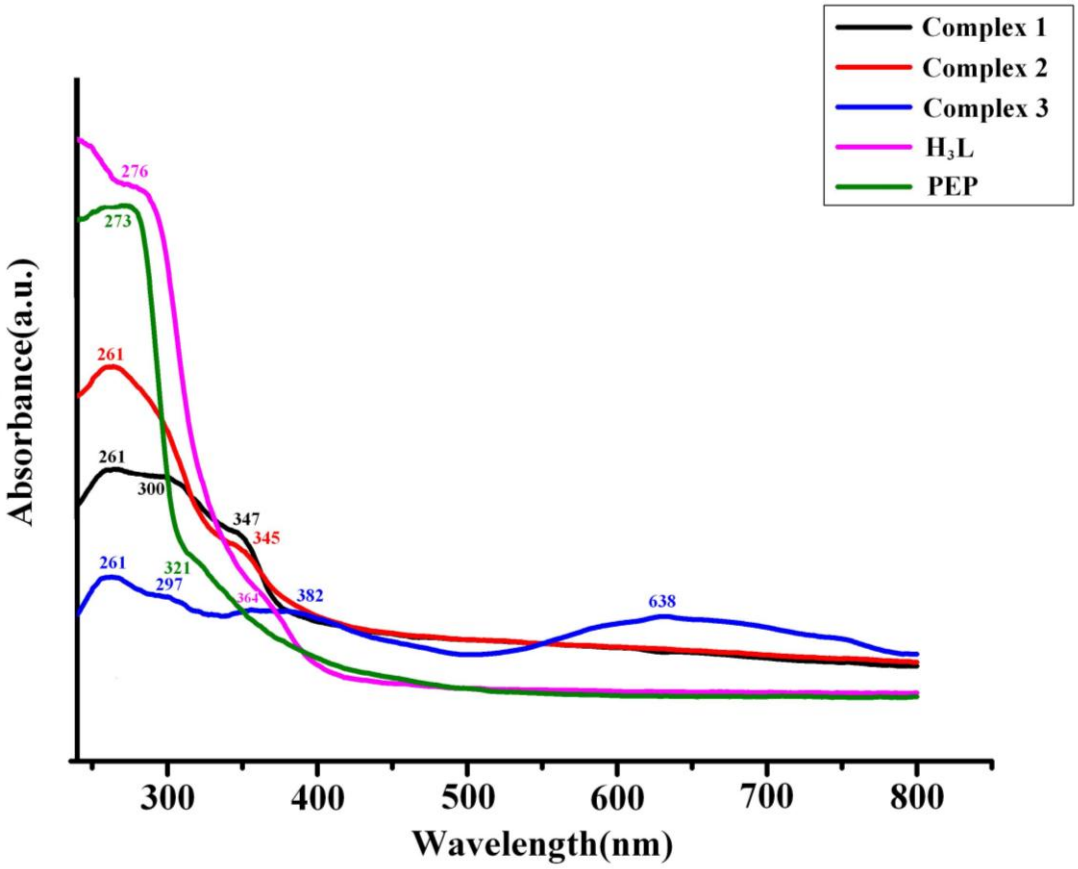


Fig. S3 UV-vis absorption spectra at room temperature for the free organic ligands and complexes **1**-**3**.

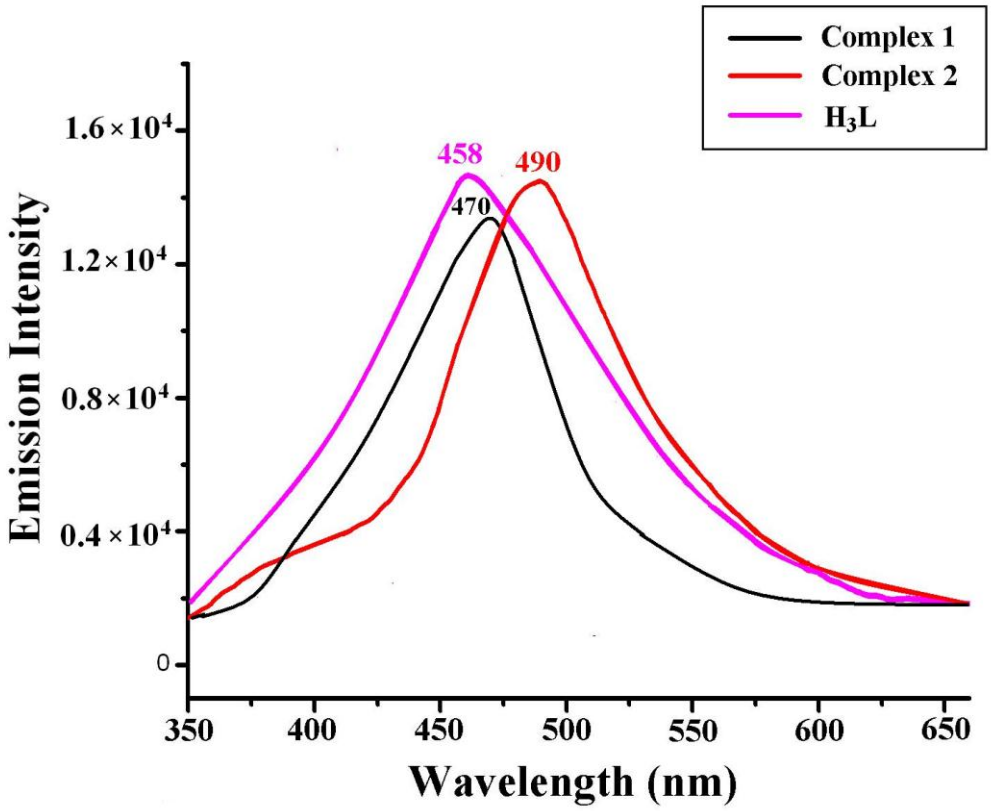
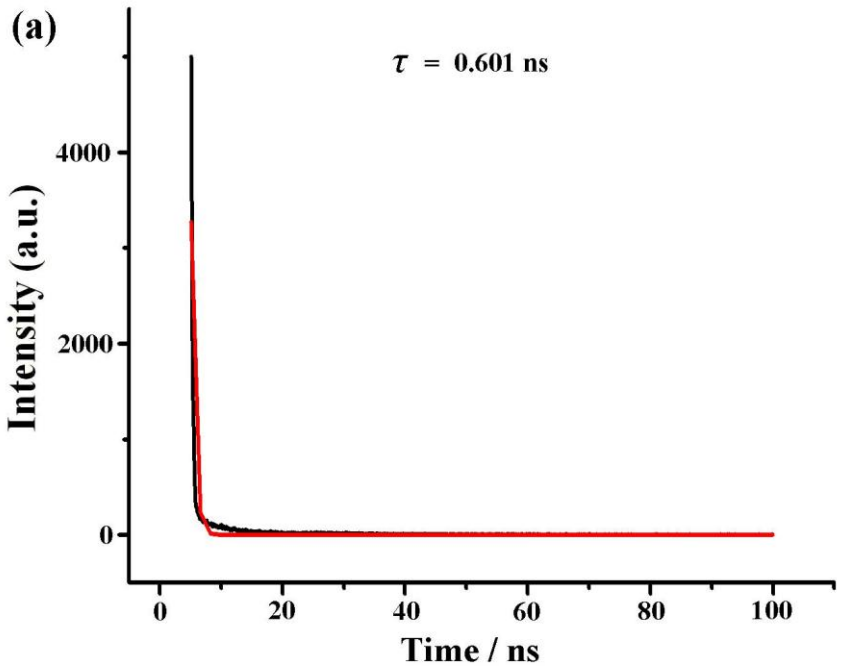
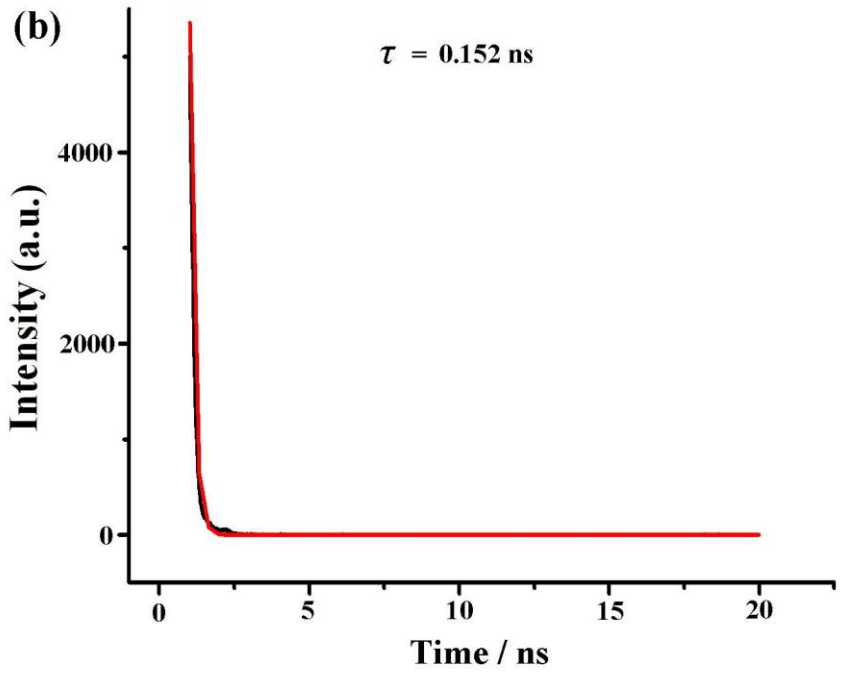


Fig. S4 Solid-state emission spectra at room temperature for the free organic ligand **H_3L** and complexes **1**-**2**.





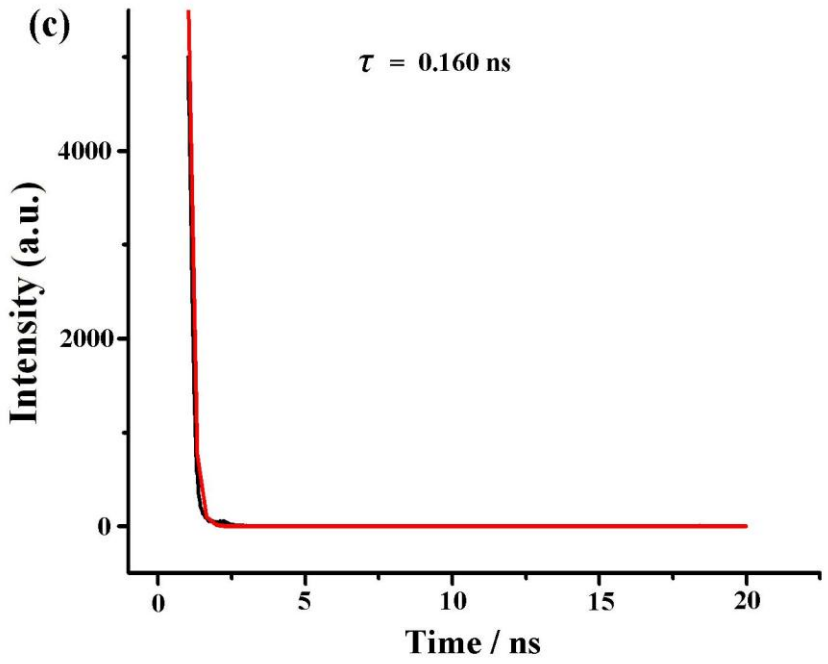


Fig. S5. Typical luminescence decay profile observed in the solid state at room temperature (black lines) and the corresponding monoexponential fits (red lines) for **H_3L** (**a**), complexes **1** (**b**) and **2** (**c**).

The equation $I_t = A \times \exp(-t/\tau)$ was utilized for fitting the fluorescence decay curves, which gave the best parameters as $A = 1.527\times10^7$ and $\tau = 0.601$ ns with an overall χ^2 of 0.9467 for **H_3L**, $A = 4.359\times10^6$ and $\tau = 0.152$ ns with an overall χ^2 of 0.9934 for complex **1**, $A = 3.343\times10^6$ and $\tau = 0.160$ ns with an overall χ^2 of 0.9852 for complex **2**.

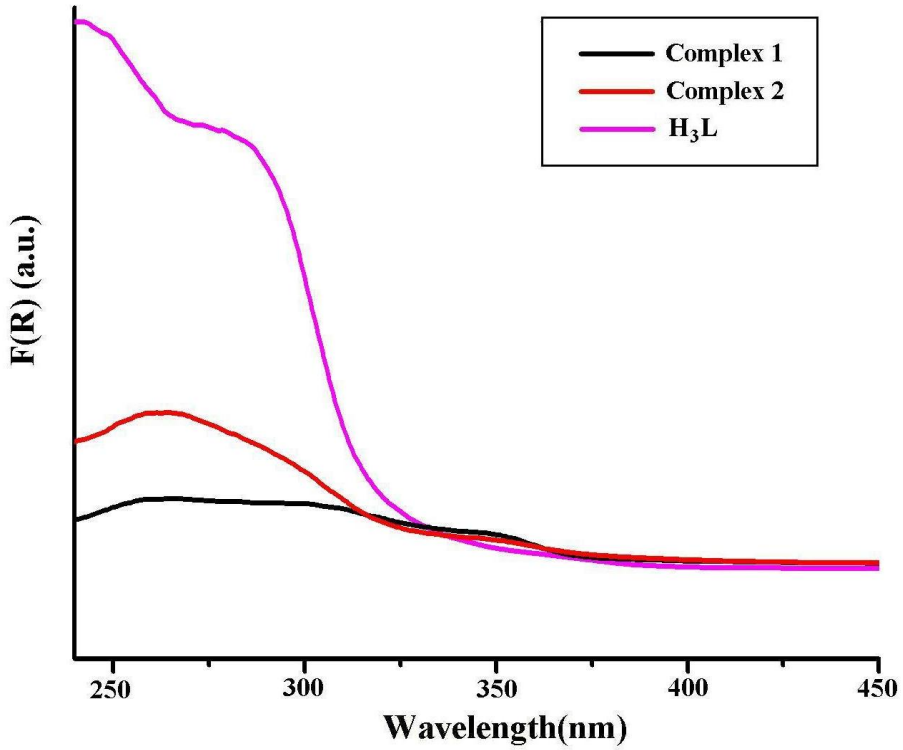


Fig. S6 The diffuse reflectance spectra of the pure ligand **H_3L** and complexes **1-2** in Kubelka–Munk units. F(R) is the Kubelka–Munk function, where $F(R) = (1-R)^2/2R$, R is the experimentally observed reflectance.

The formula for the calculation of band gap is as follows:

Band Gap energy = $hc/\lambda = 1240/\lambda$ eV

h = planks constant = 6.626×10^{-34} Joules ·sec

c = Speed of light = 3.0×10^{8} meter/sec

λ = cut off wavelength (nm)

where 1eV = 1.6×10^{-19} Joules (conversion factor)

λ, the cut off wavelength, is obtained according to the diffuse reflectance spectrum {F(R) vs. wavelength, $F(R) = (1-R)^2/2R$, R is the experimentally observed reflectance}.

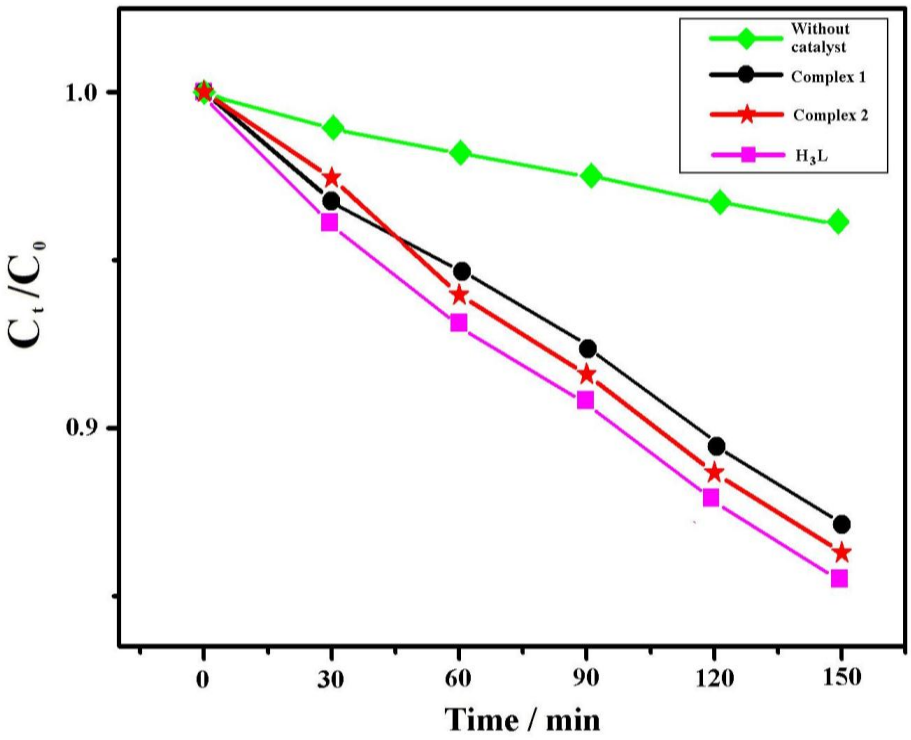


Fig. S7 Changes in C_t/C_0 plot of MO solutions (2.0×10^{-5} mol· L^{-1}) versus reaction time in the absence and presence of 50 mg free organic ligand **H_3L** or complexes **1–2**.