Two-dimensional Coordination Polymers and Metal-Organic Gels of Symmetrical and Unsymmetrical Dipyridyl β-diketones: Luminescence, Dye Absorption and Mechanical Properties

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Supporting Information:

Contents:

^{1}H NMR of the ligand.

^{1}H NMR of **L_1:**

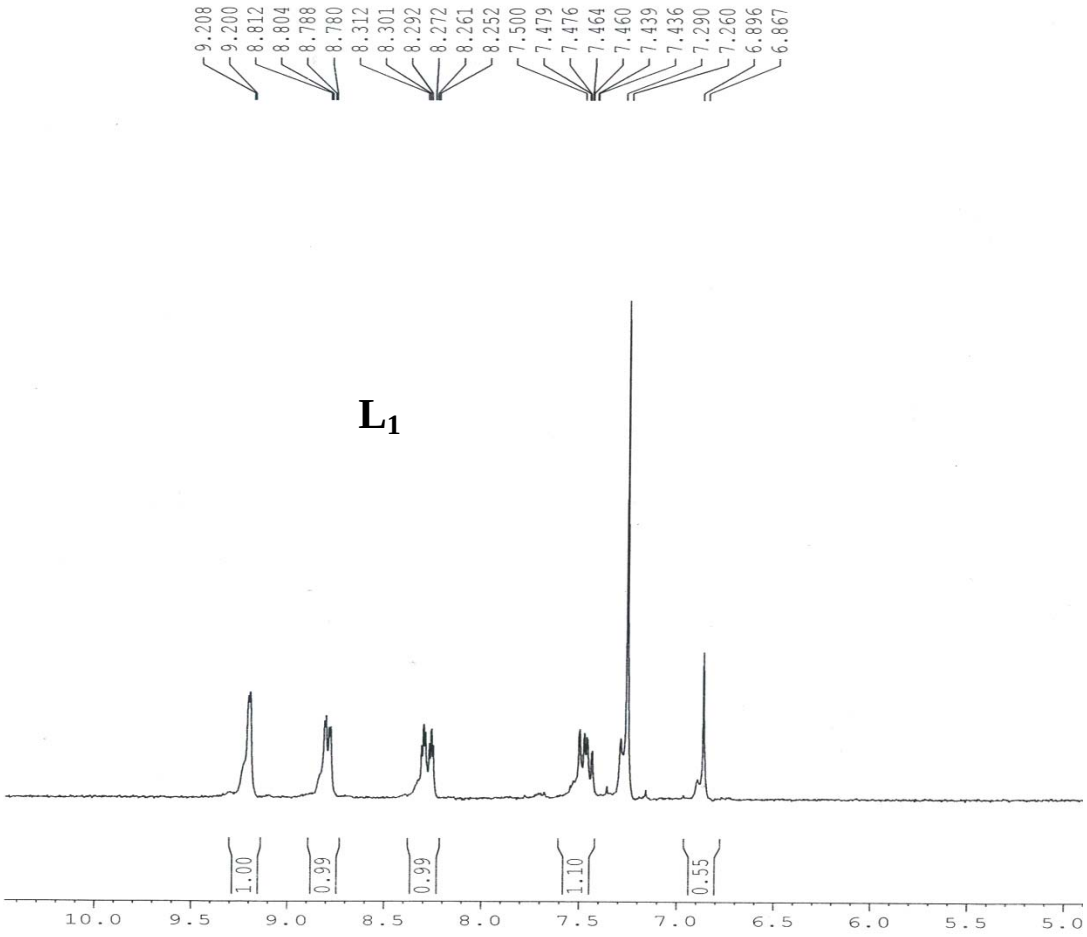

Figure-**S1:** ^{1}H NMR of **L_1**: ^{1}H NMR(200MHz,$CDCl_3$):δ=6.896(s,1H),9.204(s,2H),8.796(d,2H) 8.282(d,2H),7.465(t,2H).

^{1}H NMR of **L_2:**

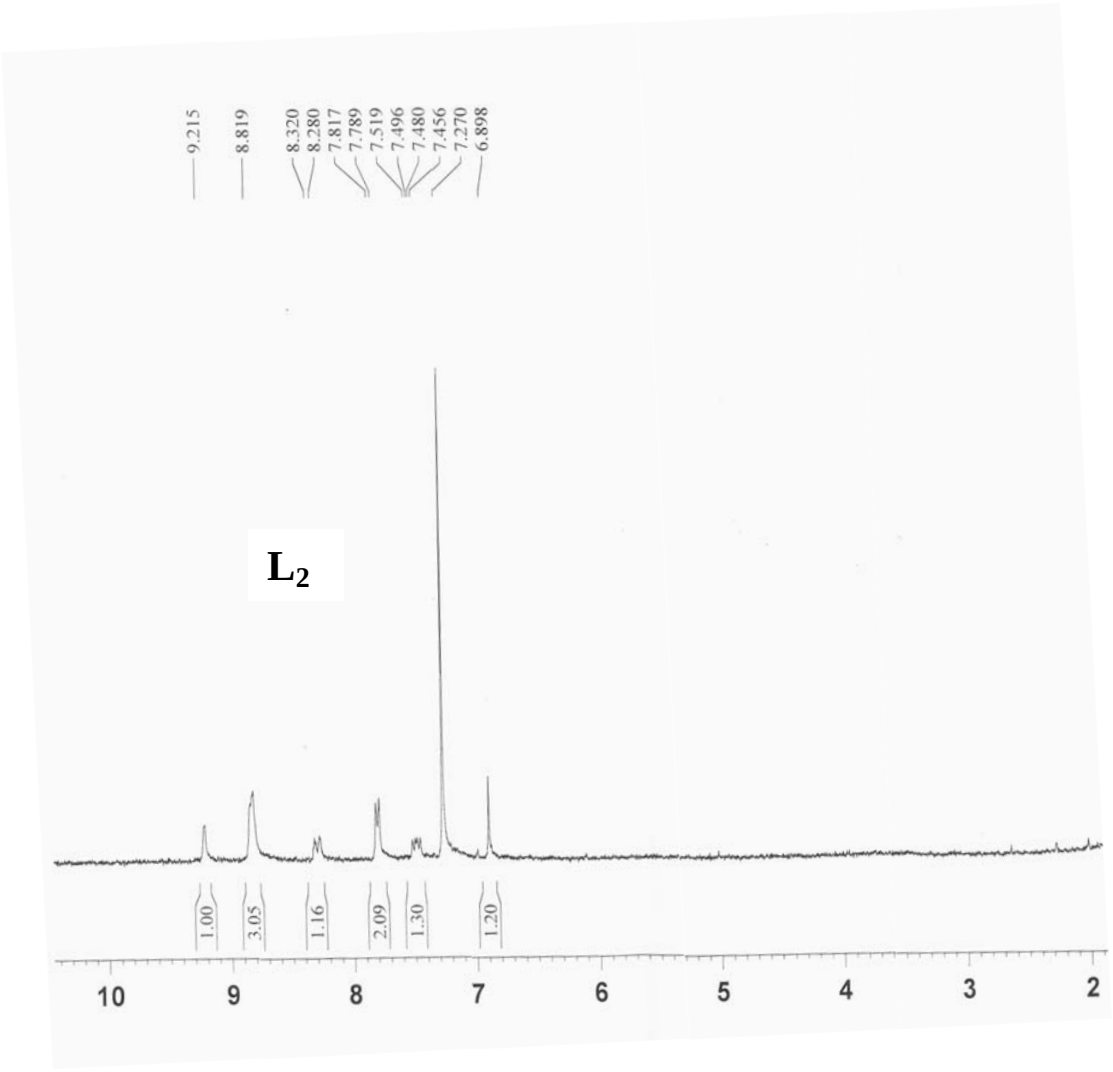

Figure-**S2**. ^{1}H NMR of **L_2:**
(400MHz,d^{6}DMSO):δ=7.495(s,1H),9.339(s,1H),8.806(d,3H),8.486(d,1H), 8.027(d,1H), 7.60 (t,1H).

IR spectra:

Ligand L_1

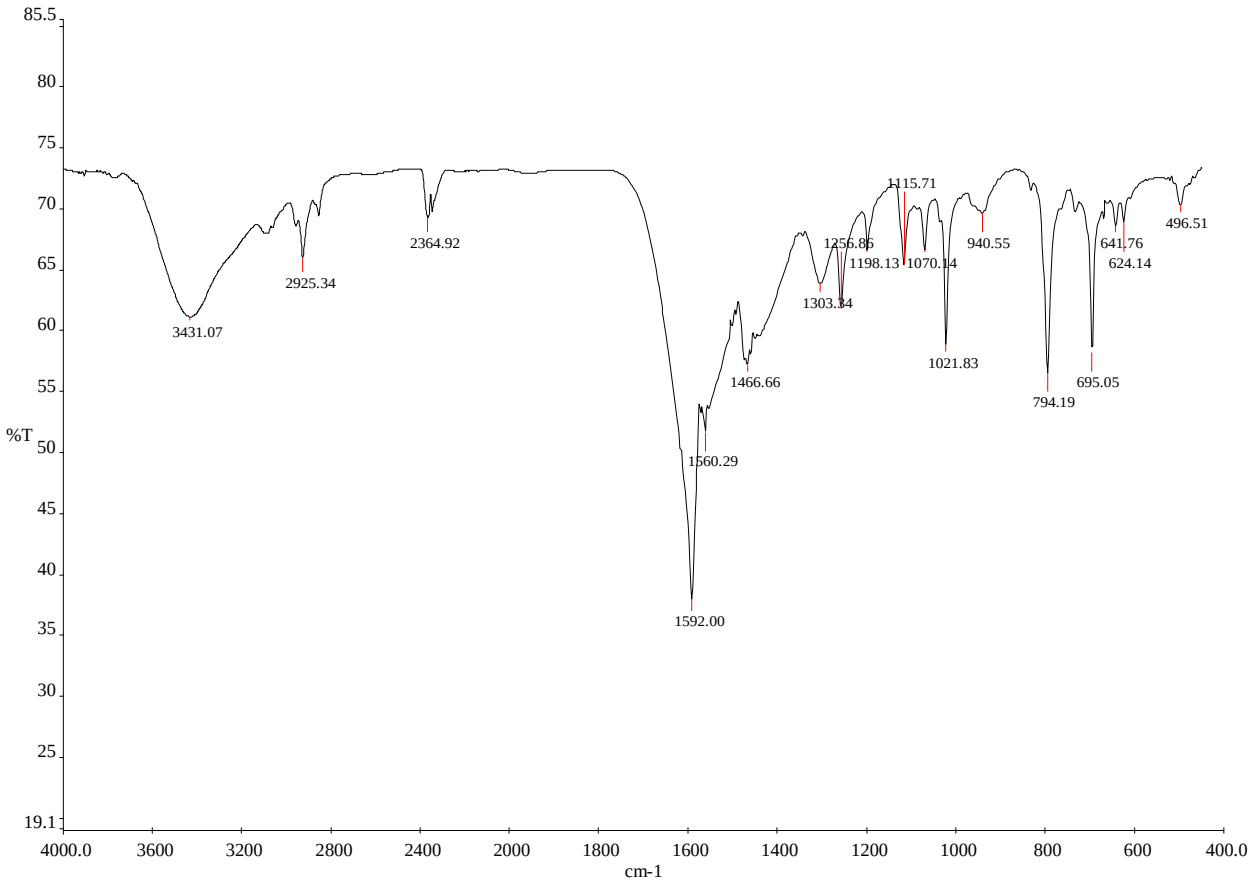

Figure-**S3**. (O-H hydrogen bond 3431.07cm^{-1}), (C=O stretch 1303.34, 1256.86, 1198.13 cm^{-1}), (C=O hydrogen bonded 1592.00 cm^{-1}), (aromatic C-H stretch 2925.34 cm^{-1})

Complex-**1**:

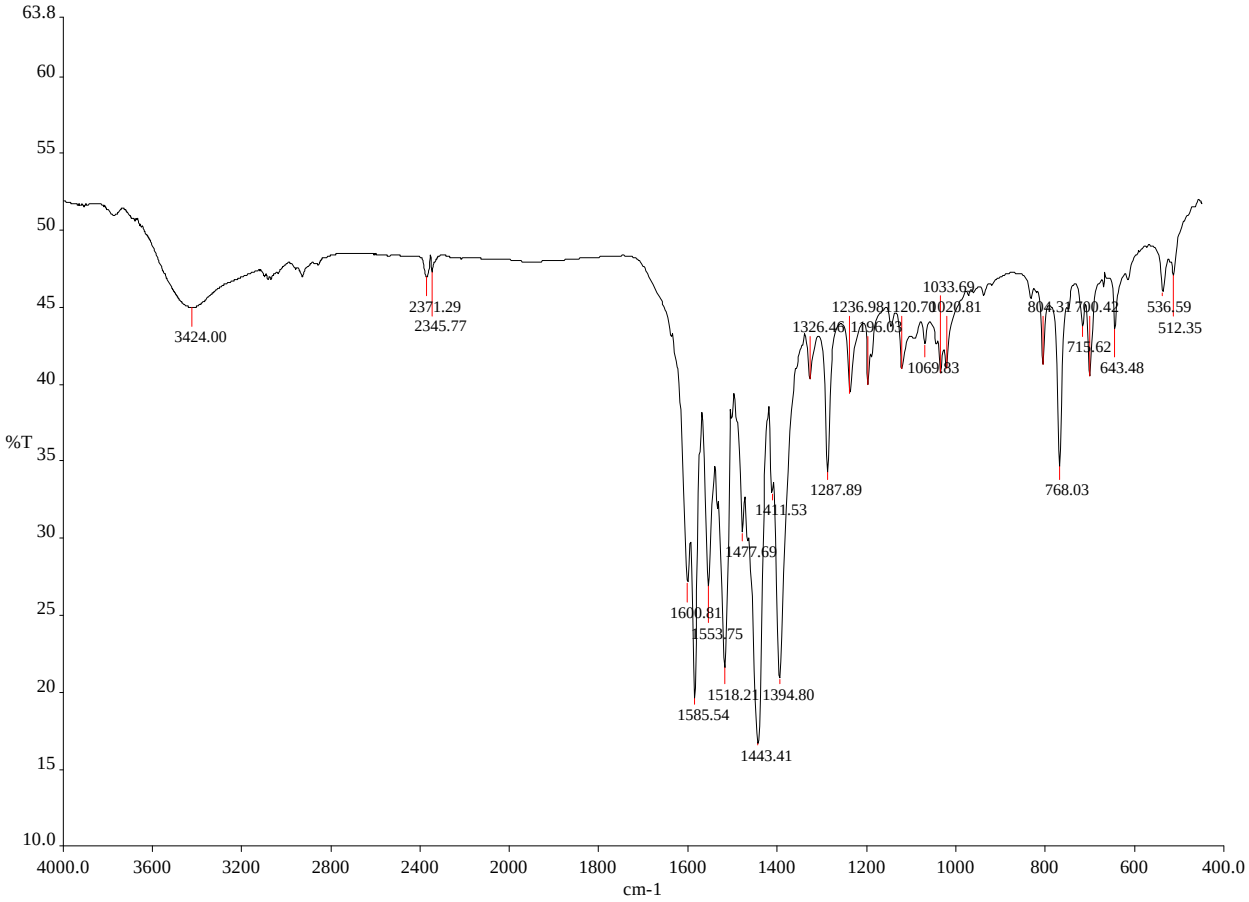

Figure-**S4**. (C-O stretch 1196.03 cm^{-1}), (M-O stretch 536.59 cm^{-1}, 512.35 cm^{-1}),

Complex-**2**:

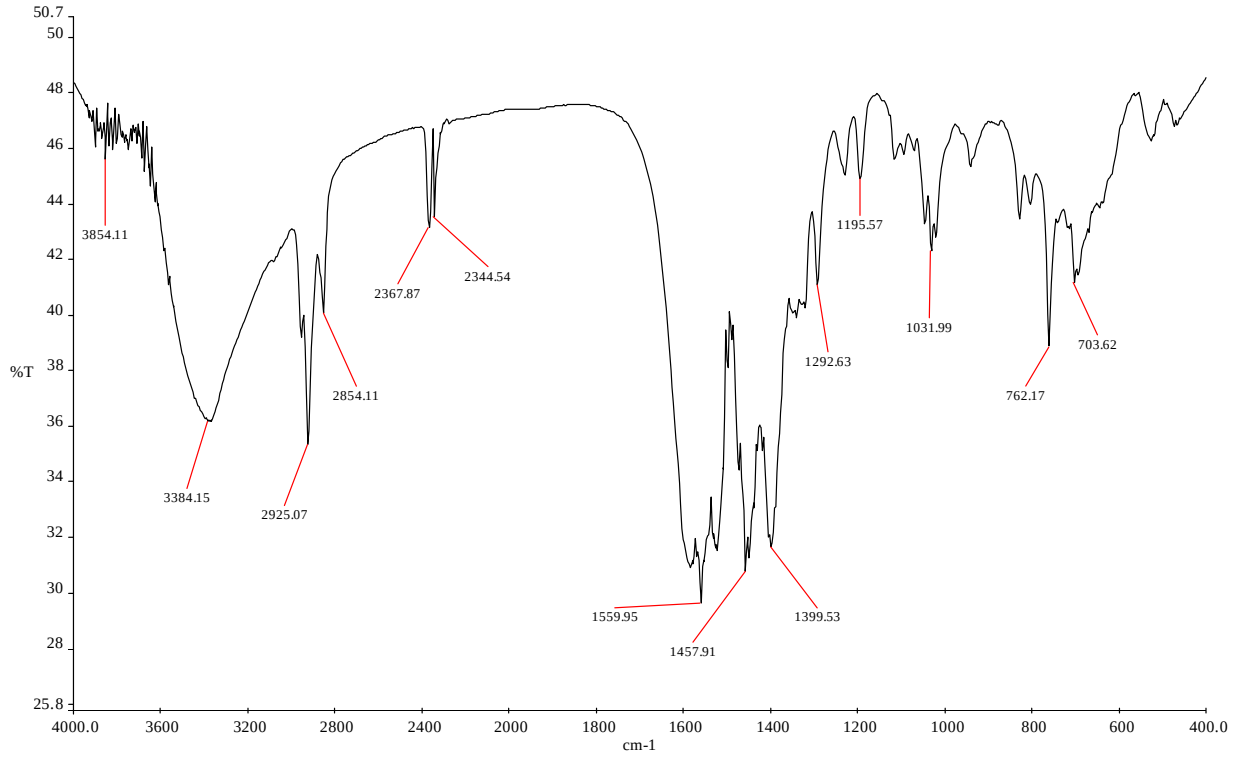

Figure-**S5** (C-O stertch 1195.57 cm^{-1}), (M-O stretch 701.62 cm^{-1}), (aromatic C-H stretch 2925.07 cm^{-1})

Complex-**3**:

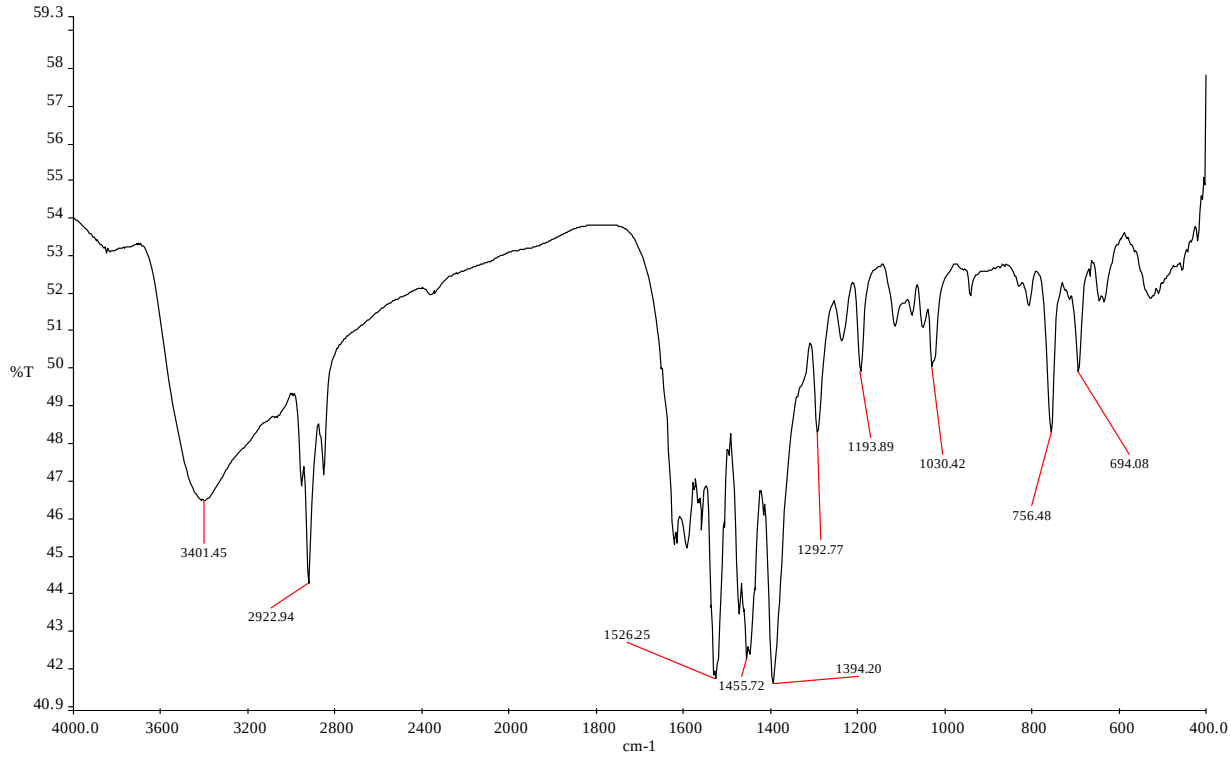

Figure-**S6**. (C-O stertch 1193.89 cm^{-1}), (M-O stretch 694.08 cm^{-1}), (aromatic C-H stretch 2922.94 cm^{-1})

Complex-**4**:

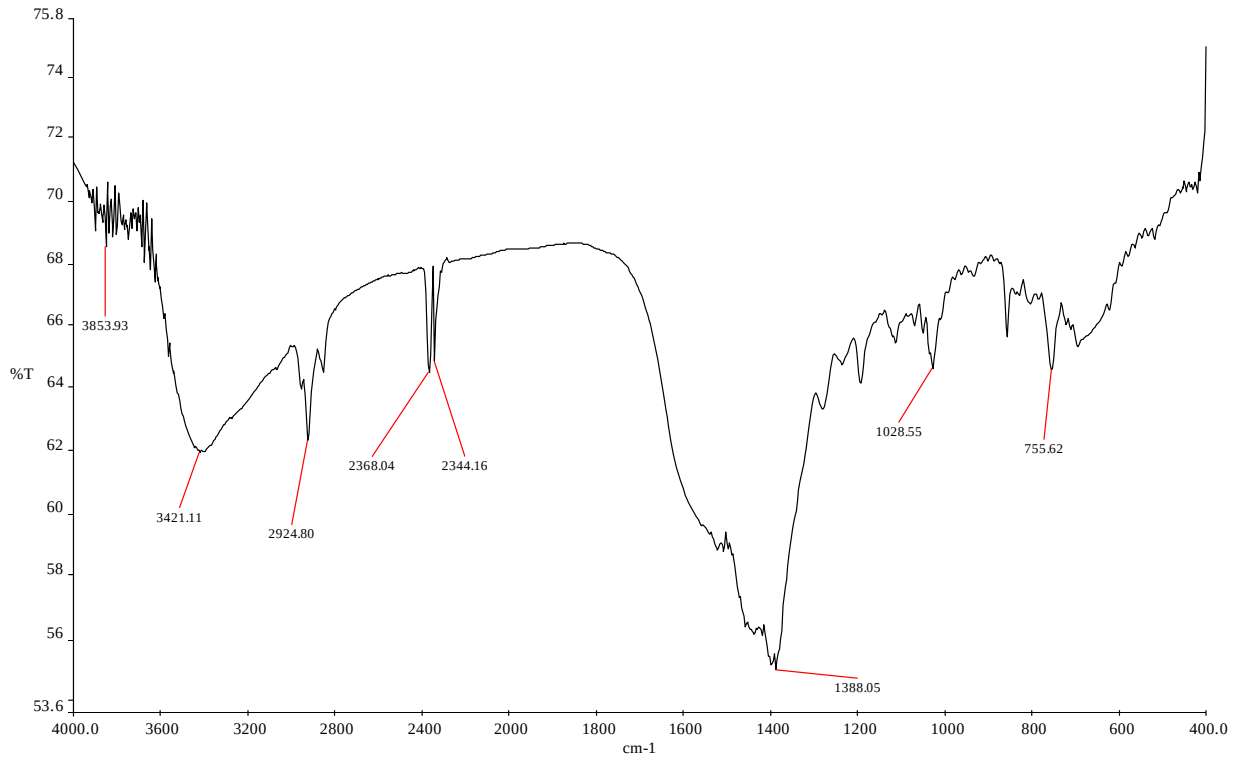

Figure-**S7**. (C-O stertch 1028.53 cm^{-1}), (M-O stretch 755.62 cm^{-1}).

MOG formed between $CdBr_2$ and L_1:

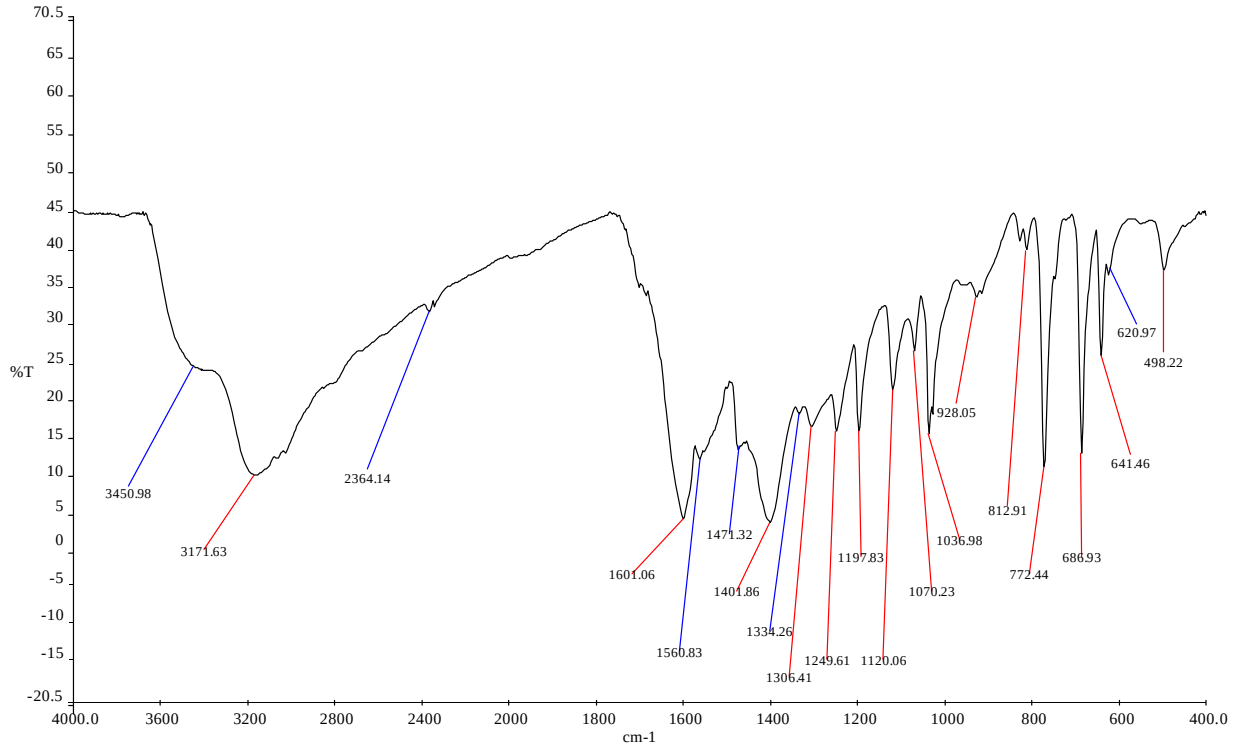

Figure-**S8**

XRPD for complexes.

$[Mn(L_1)_2]_n$ 1

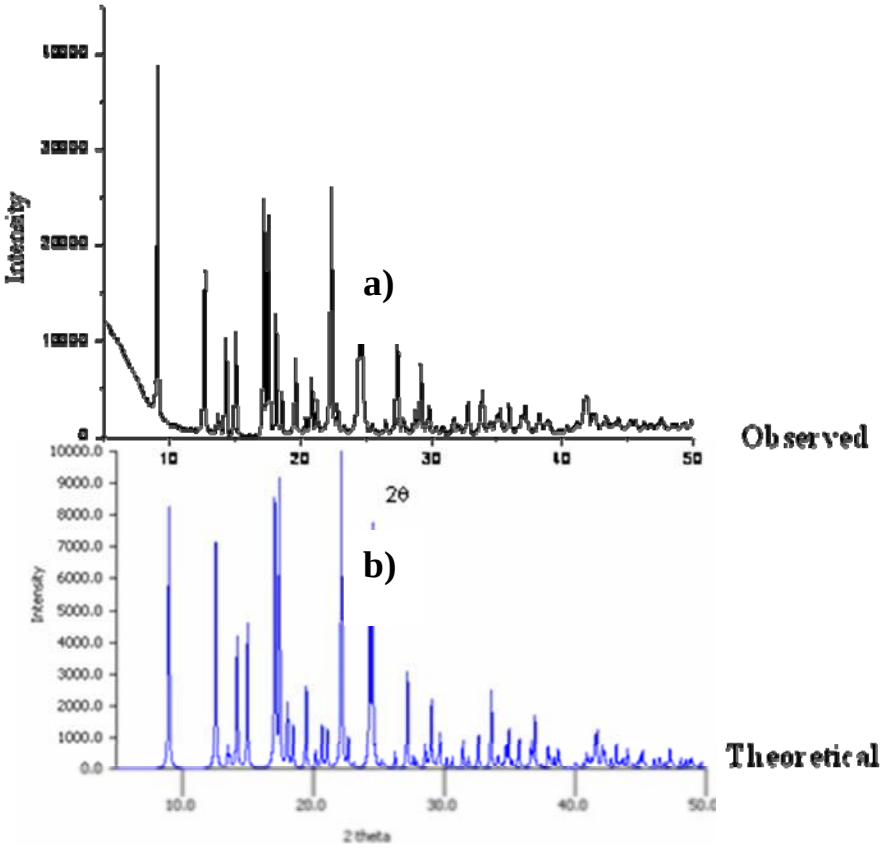

Figure-**S9**. a) Observed PXRD Pattern and b) Theoritical PXRD pattern for **1**

$[Cd(L_1)_2]_n$ 2

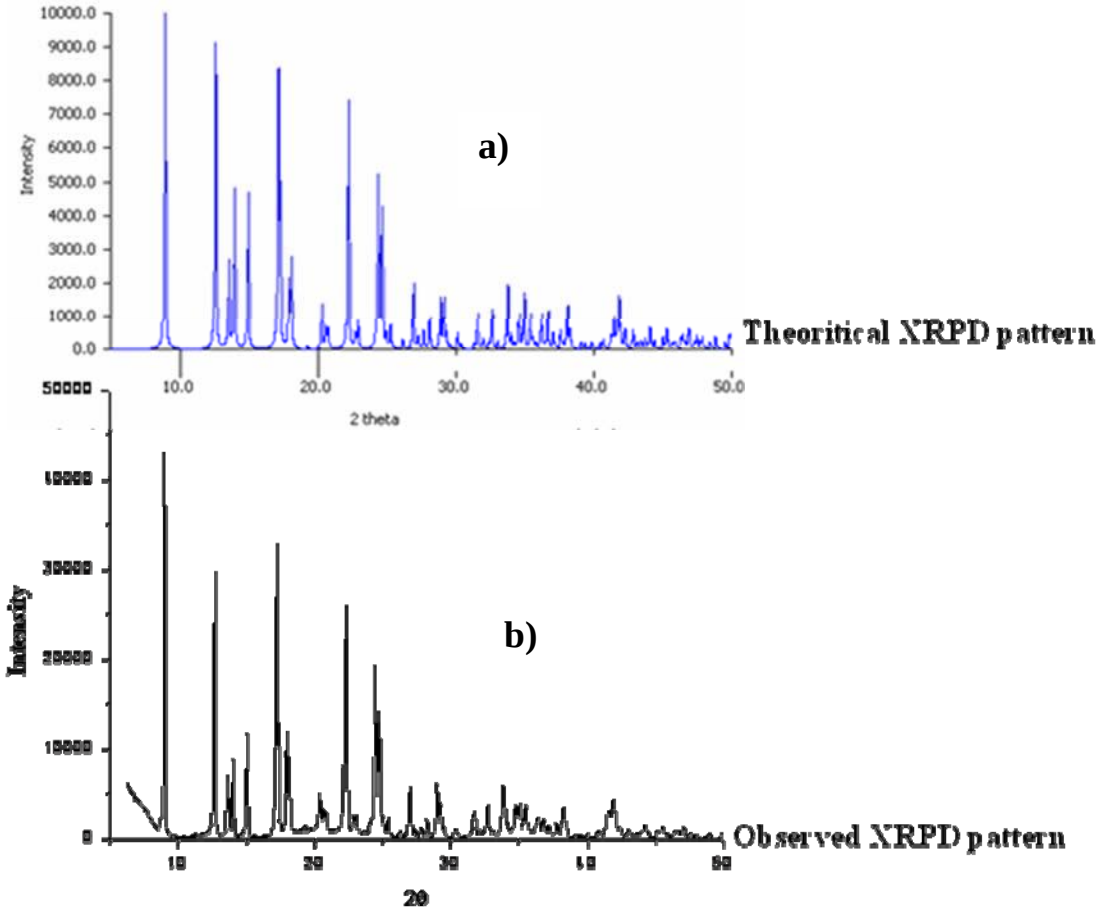

Figure- **S10**. a) Observed PXRD Pattern and b) Theoritical PXRD pattern for **2**

$[Zn(L_1)_2]_n$ 3

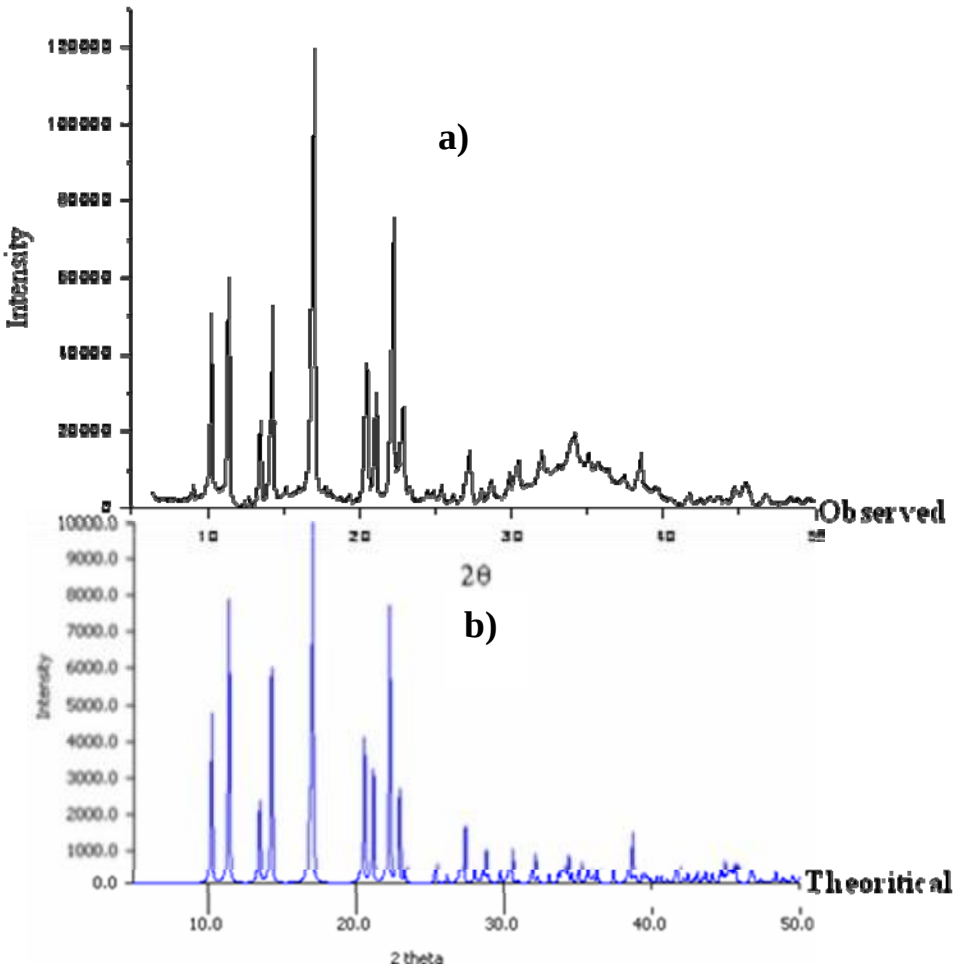

Figure- **S11**. a) Observed PXRD Pattern and b) Theoritical PXRD pattern for **3**

$[Mn(L_2)_2]_n$ 4

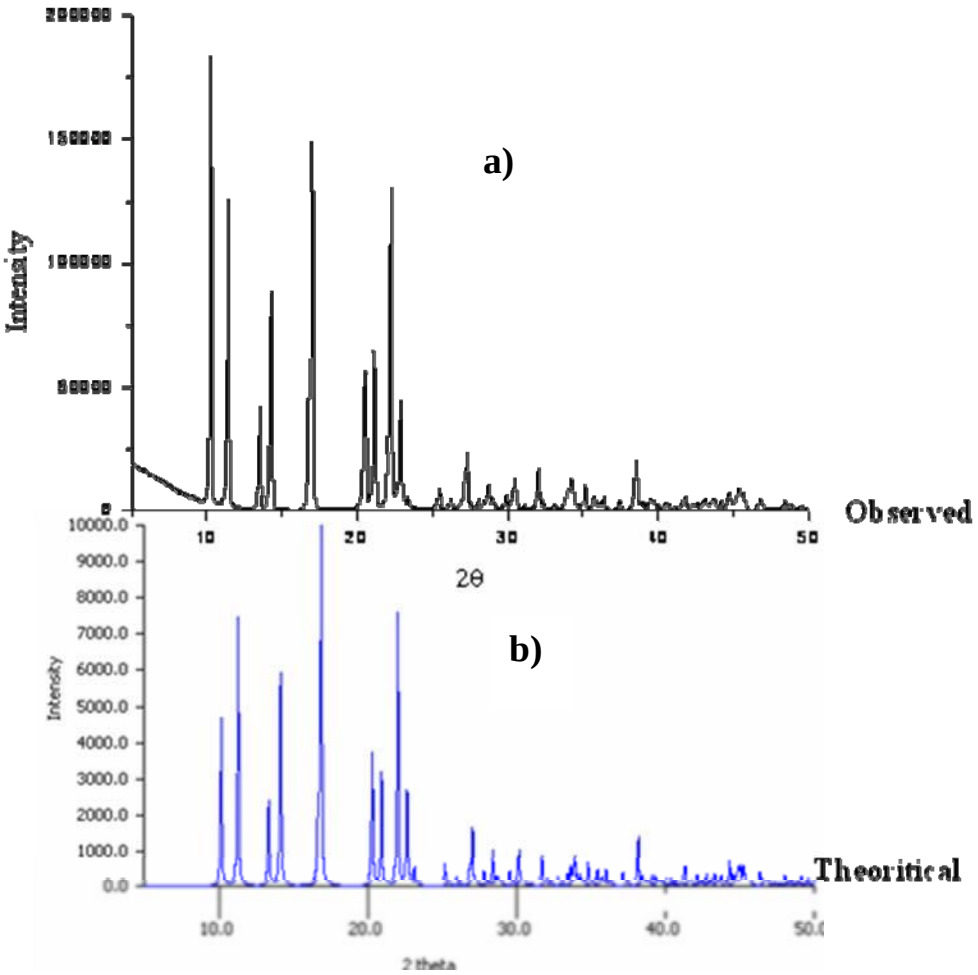

Figure- **S12**. a) Observed PXRD Pattern and b) Theoritical PXRD pattern for $[Mn(\mathbf{L_2})_2]_n$

XRPD Pattern of Xerogel of MOG

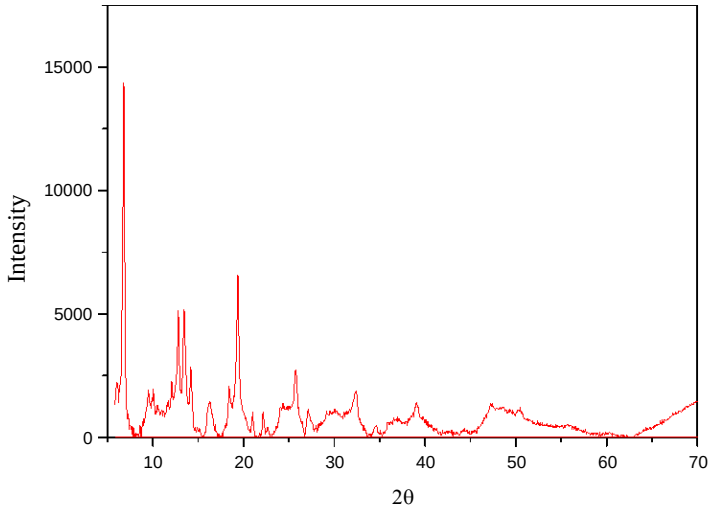

Figure- **S13**

TGA for the metallo-assemblies.

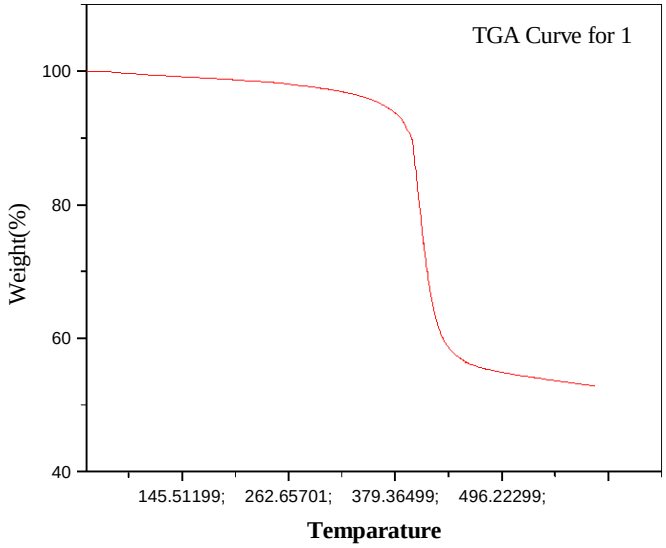

Figure- **S14**. Complete rupture of the CP assembly starts at 386.03 °C due to the breaking of all the M-L bonds from the CPs.

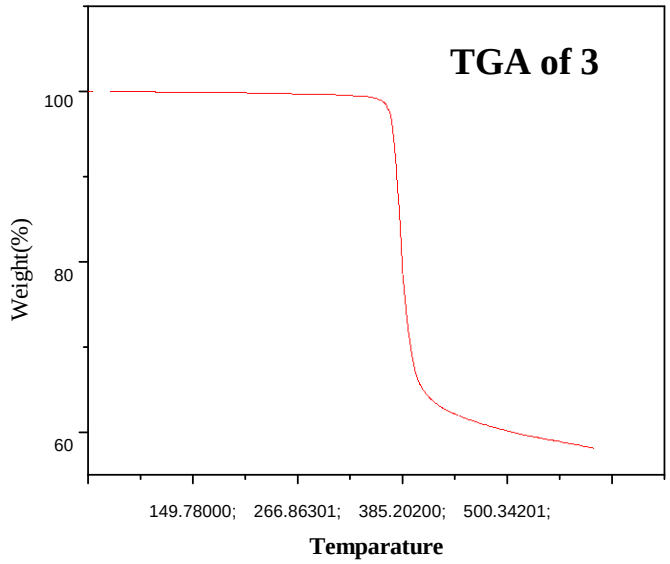

Figure- **S15**. Complete rupture of the CP assembly starts at 363.59 °C due to the breaking of all the M-L bonds from the CPs.

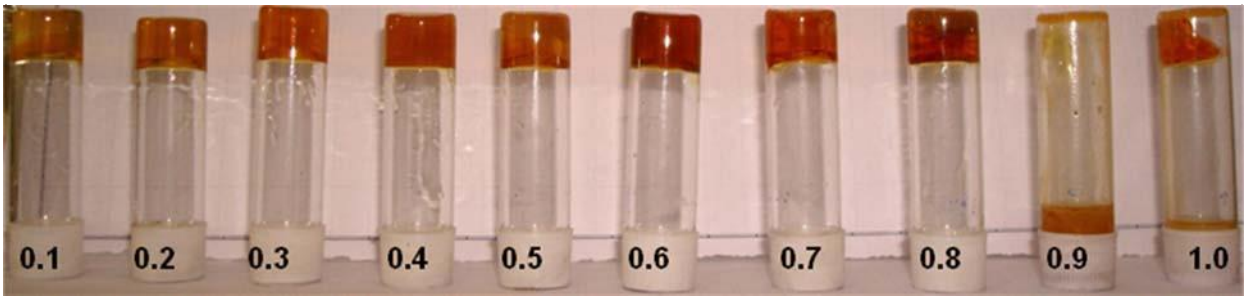

Figure- **S16**. Snapshots of inverted vials of HMOG. Numbers on the cap indicates the equivalents of $[Mn(\mathbf{L_1})_2]_n$ with respect to $AgNO_3$ present in the respective vial.

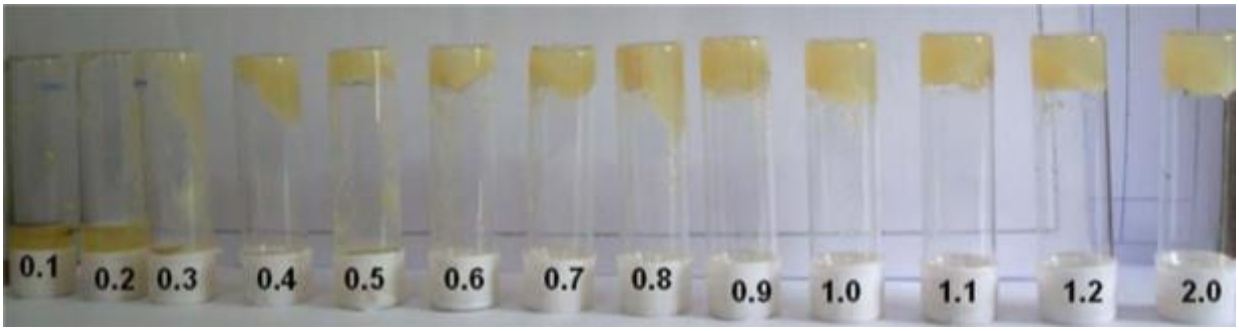

Figure- **S17**. Snapshots of inverted vials of MOG. Numbers on the cap indicates the equivalents of $CdBr_2$ with respect to HL_1 present in the respective vial.

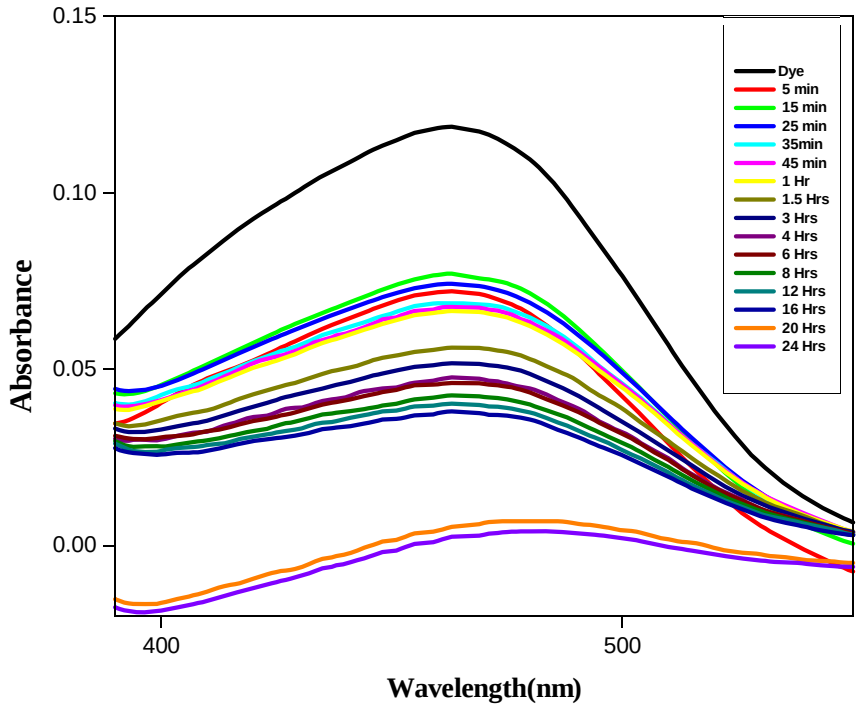

Figure-**S18**. UV−vis spectra of dye solution (black line) after the addition of MOG xerogel at various time intervals (colored lines).

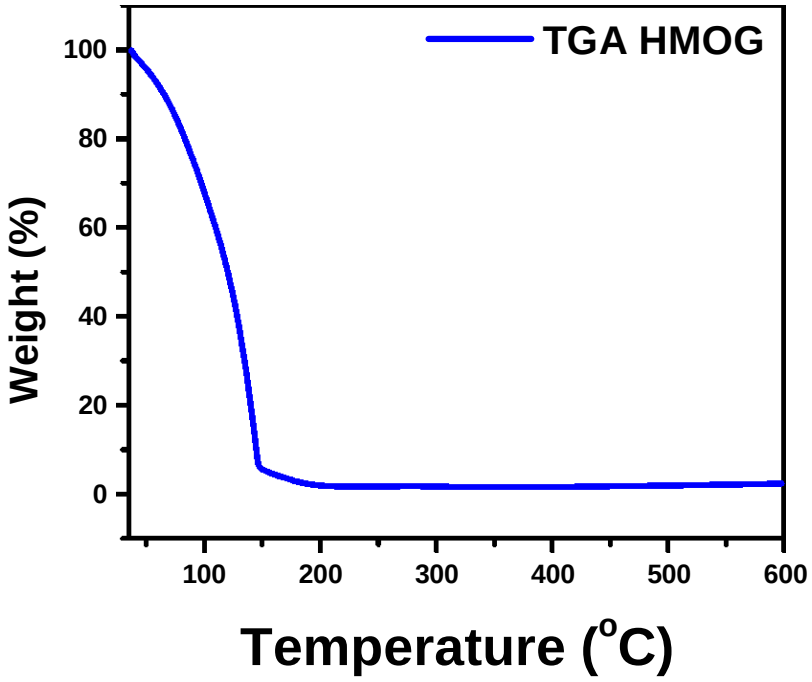

Figure-**S19** TGA for HMOG

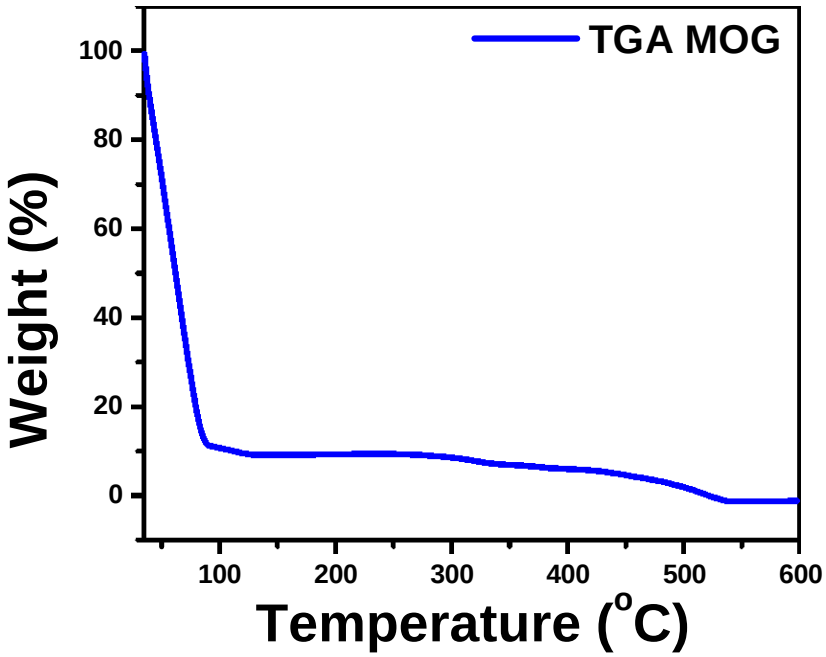

Figure-**S20** TGA for MOG

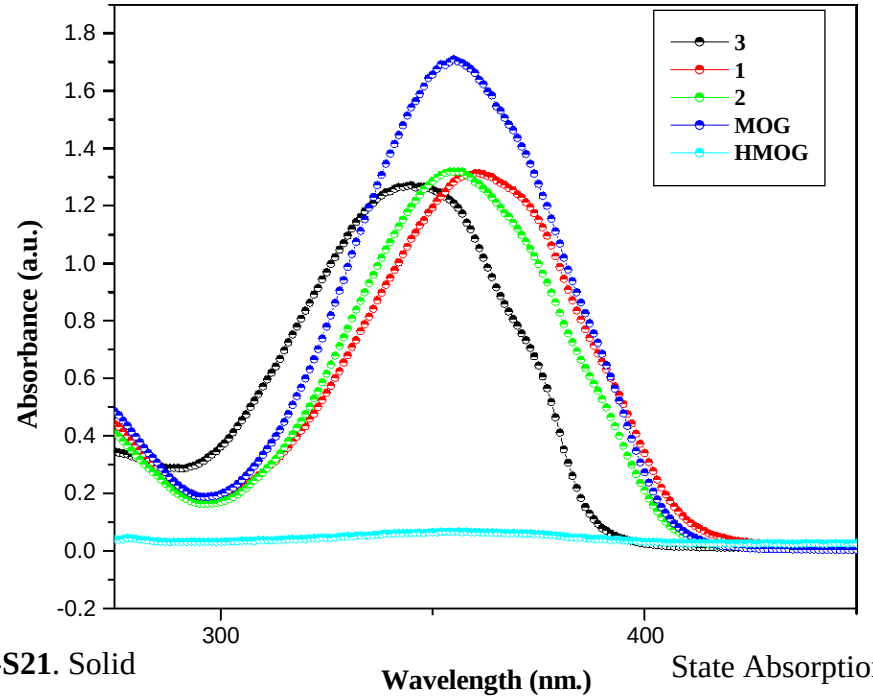

Figure-**S21**. Solid State Absorption Spectra of the CPs and HMOGs.

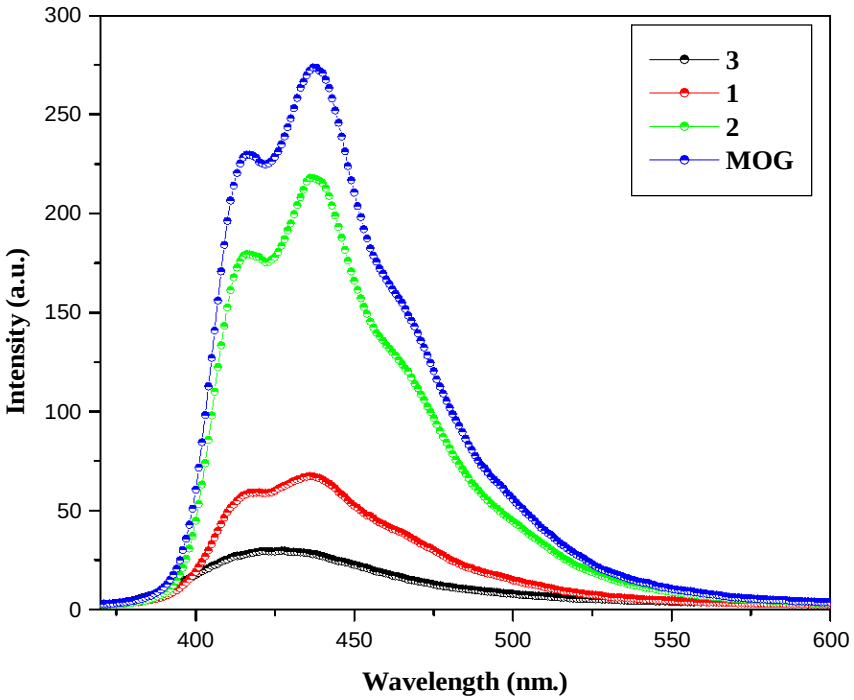

Figure-**S22**. Emission Spectra of the CPs and HMOGs in DMSO at conc. range 1.0×10^{-5}g/mL.

Table SI1. Selected bond Lengths (Å) and bond angles for complexes **1**-**5**.

Complex	M-O (Å)	M-N (Å)	O-M-O (°)	O-M-N (°)
1	2.145(4)	2.335(3)	84.92(11)	89.87(11)
	2.137(3)		95.08(11	90.13(11
2	2.275(6)	2.365(8)	97.2(2)	91.5(3)
	2.269(7)		97.2(2)	88.5(3)
3	2.0601(14)	2.1808(17)	89.23(5)	87.30(6)
	2.0694(13		90.77(5)	92.70(6)
4	2.073(4)	2.177(6)	90.99(16)	87.33(19)
	2.063(4)		89.01(16	92.67(19
5	3.018(8)	2.130(7)	119.24(2)	102.0(3)
	3.082(8)	2.140(6)		
	3.209(9)			

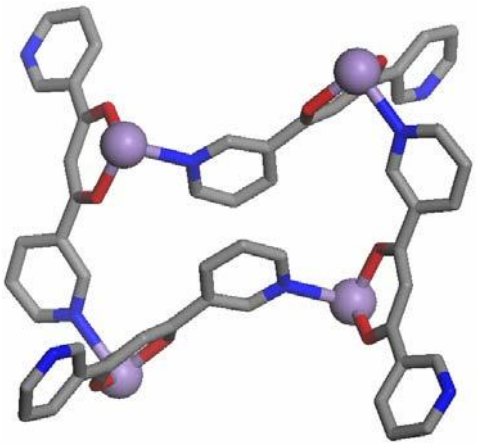

Figure-**S23** Illustrations for the crystal structures of **1** and **2**: Strong π-π interactions between the coordinated pyridines groups of the (4,4) grid.

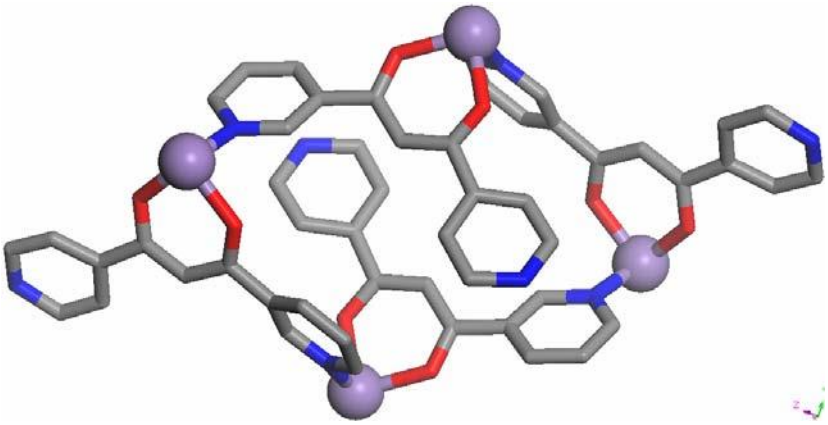

Figure-**S24** Illustrations for the crystal structures of **4**:Strong π-π interactions between the non-coordinated 4-pyridine and enolate moieties of the (4,4) grid.