Electronic Supplementary Material (ESI) for Materials Advances.

Supporting information

Toxic Metal-Organic Gels Using a Unique Pyridine-Pyrazole Based Ligand with Pb(II), Cd(II) and Hg(II) Salts: Multi-stimuli Responsiveness and Toxic Dye Adsorption

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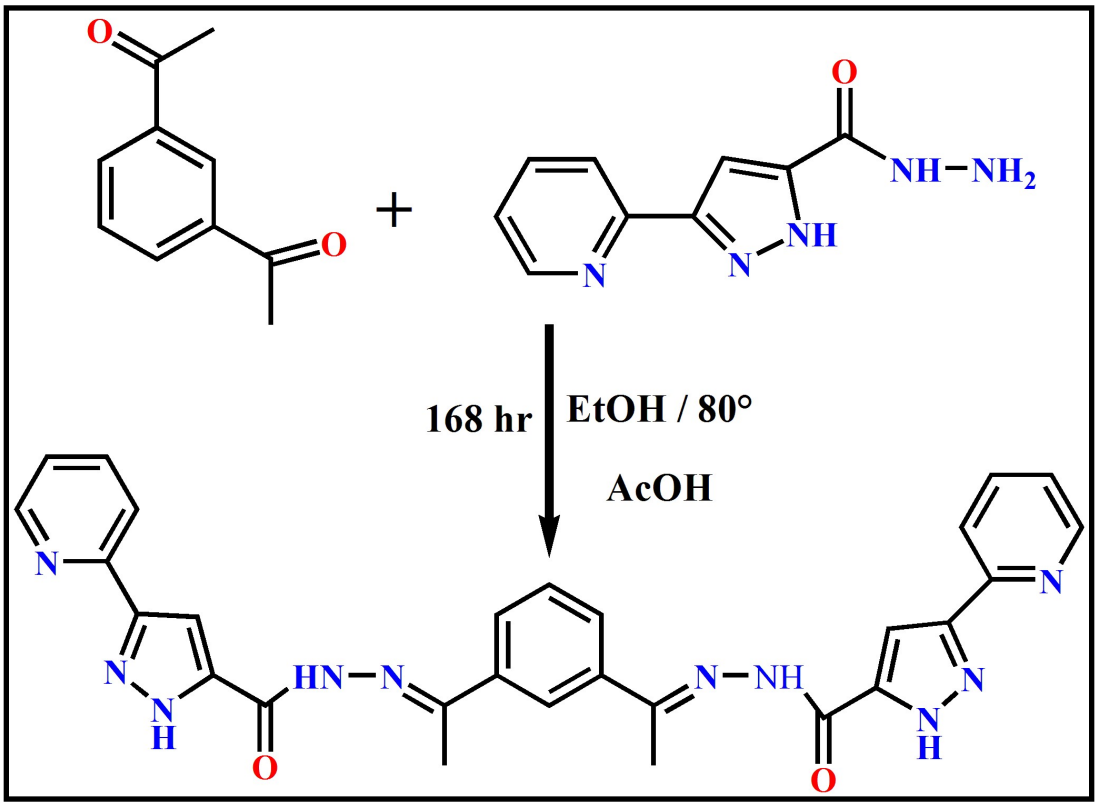
Synthesis of ligand:

1, 3 diacetyl benzene (660 mg) and pyridine pyrazole carbohydrazide (2070 mg) was taken in EtOH solution and catalytic amount of galcial acetic acetic acid was added to it, then the mixture was allowed to reflux at 80^0C, for 168 hr. After 168 hr white colour precipitate was obtained then cooled it to room temperture. Then the precipitate was filtered, washed with EtOH solvent and dried in air.Yield 85% was obtained as a schiff base.

Elemental Analysis for Ligand ($C_{28}H_{24}N_{10}O_2$): Calculated: C, 63.09; H, 4.50; N, 26.20
Found: C, 63.59; H, 4.98; N, 27.39.



Scheme S1 Schematic representation of synthesis of ligand

Thermo gravimetric Analysis:

To check the thermal stability we performed the TGA analysis. The experiment was carried out on xerogel samples of corresponding gel under N_2 atmosphere with a heating rate of 10°C/min in a platinum crucible. For Pb xerogel very small weight loss was observed initially and it shows thermal stability upto 300^0C and the steadily decreases with consequent weight loss upto 69%. Hg xerogel shows a gradual weight loss and stable upto 170^0C and then slowly complete dissociation is observed. Cd xerogel dissociates with small weight loss at 40^0C -120^0C. This intial weight loss may be attributed to the loss of solvent molecules and lastly complete dissociation is observed at higher temperature.

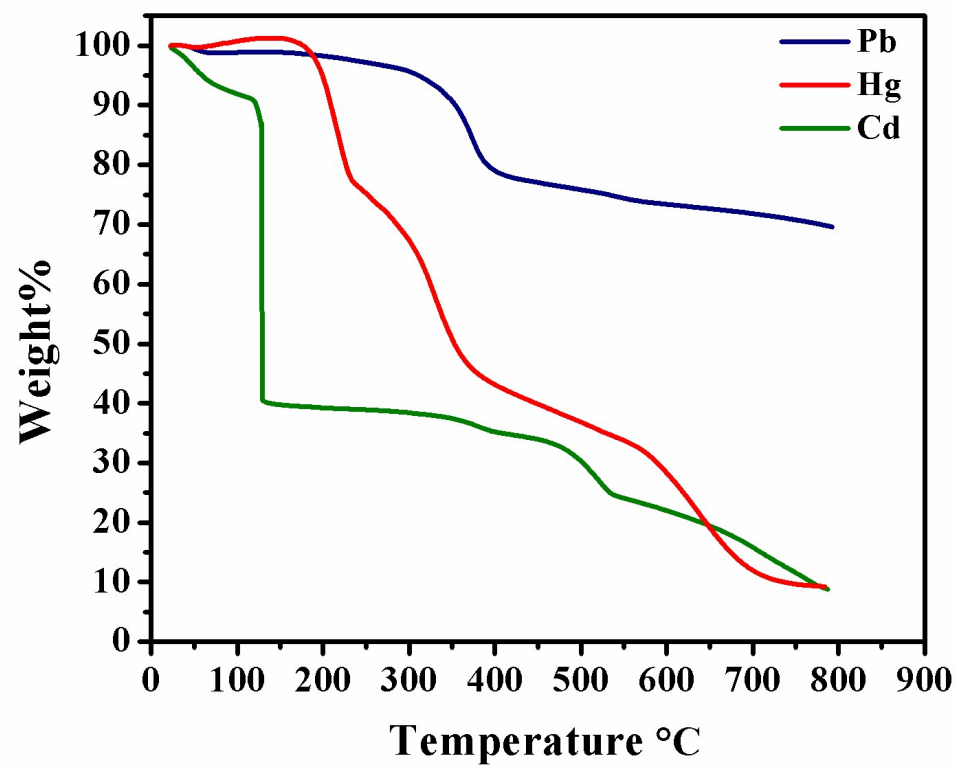


Figure S1 Thermogravimetric analysis of MOG **1-3**

PXRD analysis:

X-ray diffraction analysis has also been carried out for ligand and all the MOGs (in their gel state). X-ray diffraction pattern of free ligand shows crystalline nature. However, despite our best efforts, we were unable to get the suitable single crystal of ligand. Among all the MOGs only Pb xerogel shows crystalline natute. Crystallinity was also confirmed by nano paticle formation observed in TEM images. Whereas powder X-ray diffraction patterns of MOG**2** and MOG**3** confirms the amorphous nature. Crystaline nature of Pb MOG promped us to get a single crystal in different solvent medium and to our best efforts we were able to synthesize MOF 1. Experimental powder X-ray pattern of MOF 1 is well matched with the simulated one (Figure S3).

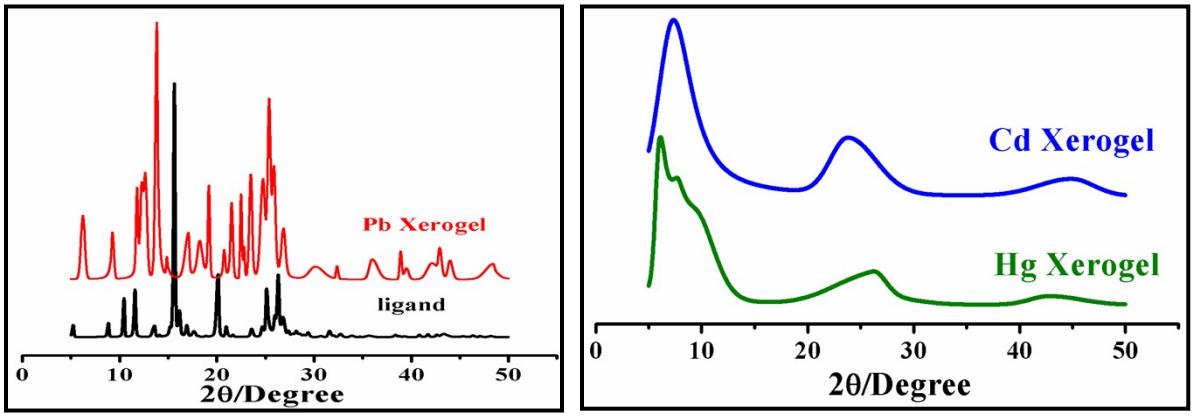
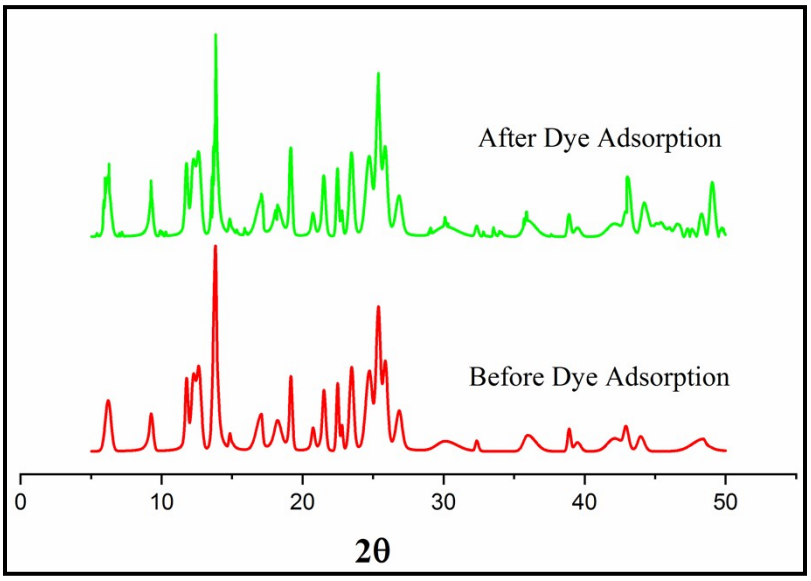


Figure S2 Powder X-ray pattern of ligand, MOG**1**, MOG **2**, and MOG**3** xerogels.



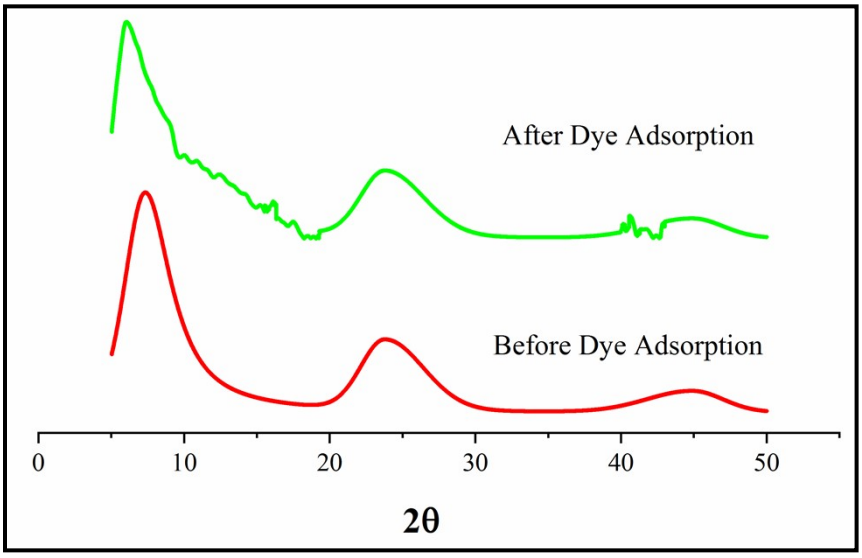


Figure S3 Comparision of PXRD pattern before & after dye adsorption of MOG1 and MOG2

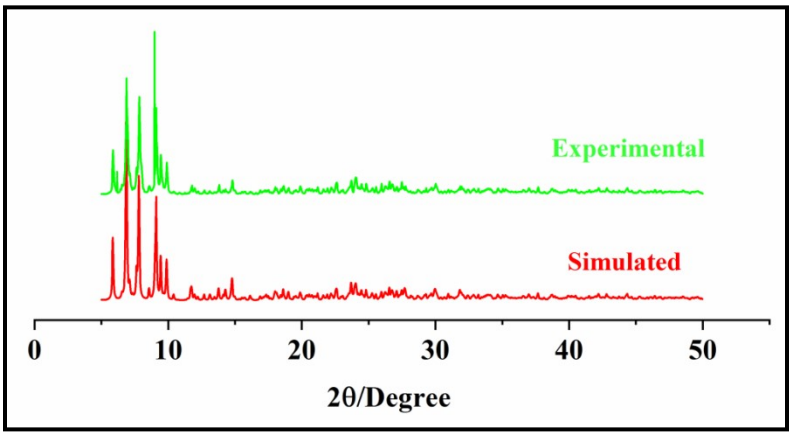


Figure S4 Simulated and experimental powder XRD patterns of MOF 1

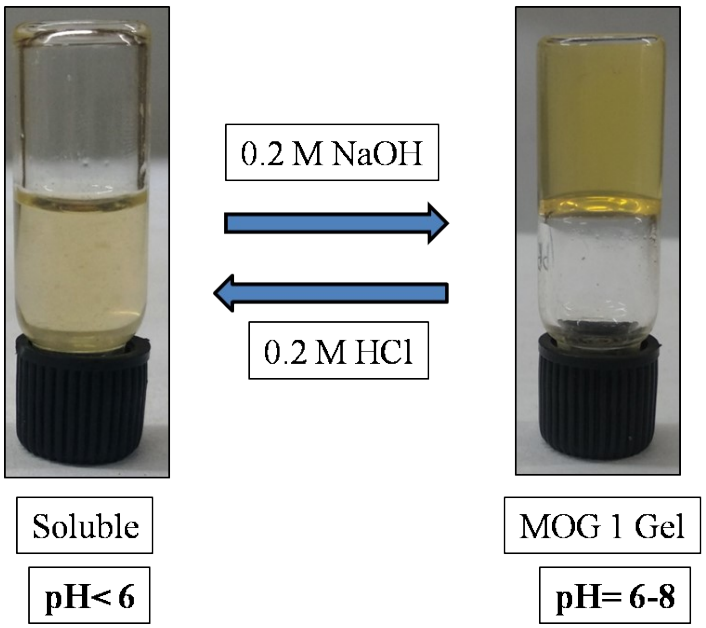


Figure S5 Effect of pH on MOG 1

Table S1: Crystallographic data file

Compound	**MOF 1**	**γ/°**	86.948(4)
Empirical formula	C_{59} H_{48} $N_{25}O_{17}Pb_5$	**V/Å3**	4690.2(8)
Crystal system	Triclinic	**Reflections collected**	12869
Formula weight	1125.88	**unique reflections**	12869
Space group	P 2_1/n	**observed reflections**	7712
a/Å	13.5047(14)	**R1**	0.1246
b/Å	15.0579(16)	**wR2**	0.3421
c/Å	23.174(2)	**CCDC no.**	2058105
α/°	87.553(4)		
β/°	85.906(4)		

Table S2: Selected bond lengths and angles of MOF 1

MOF 1			
N_{72} Pb_1 N_{29}	87.9(8)	Pb_1 -N_{72}	2.31(3)
N_{72} Pb_1 O_{31}	68.1(8)	Pb_1 -N_{29}	2.44(2)
N_{29} Pb_1 O_{31}	70.9(6)	Pb_1 -O_{31}	2.489(16)
N_{72} Pb_1 O_{7B}	78.6(8)	Pb_1-O_{7B}	2.63(3)
N_{29} Pb1 O_{7B}	143.4(7)	Pb_1 -O_{18}	2.737(17)
O_{31} Pb_1 O_{7B}	72.5(7)	Pb_2 -N_{81}	2.36(2)
N_{72} Pb_1 O_{18}	85.4(7)	Pb_2 -N_{16}	2.43(2)
N_{29} Pb_1 O_{18}	62.0(6)	Pb_2 -O_{11}	2.528(18)
O_{31} Pb1 O_{18}	126.3(6)	Pb_2 -O_{9B}	2.713(18)
O_{7B} Pb_1 O_{18}	148.0(7)	Pb_3 -N_{50}	2.47(3)
N_{81} Pb_2 N_{16}	85.6(8)	Pb_3 -N_{38}	2.51(2)
N_{81} Pb_2 O_{11}	67.3(6)	Pb_3 -N_{41}	2.52(3)
N_{16} Pb_2 O_{11}	68.7(7)	Pb_3 -N_{65}	2.65(3)
N_{81} Pb_2 O_{9B}	131.2(7)	Pb_4 -O_{31}	2.38(2)
N_{16} Pb_2 O_{9B}	82.9(7)	Pb_4 -N_{34}	2.44(2)
O_{11} Pb_2 O_{9B}	64.3(6)	Pb_4 -N_{44}	2.55(3)
N_{50} Pb_3 N_{38}	136.1(9)	Pb_4 -O_{1A1}	2.68(2)
N_{50} Pb_3 N_{41}	81.0(8)	Pb_4 -N_{54}	2.73(2)
N_{38} Pb_3 N_{41}	63.4(9)	Pb_5 -N_{35}	2.31(3)
N_{50} Pb_3 N_{65}	64.0(8)	Pb_5 -O_{11}	2.482(17)
N_{38} Pb_3 N_{65}	81.0(9)	Pb_5 -N_{67}	2.49(3)
N_{41} Pb_3 N_{65}	73.3(8)	Pb_5 -N_{46}	2.60(3)
O_{31} Pb_4 N_{34}	70.5(8)	Pb_5 -O_{9B}	2.75(2)
O_{31} Pb_4 N_{44}	64.6(7)		
N_{34} Pb_4 N_{44}	96.0(8)		
O31 Pb_4 O_{1A1}	67.6(7)		
N_{34} Pb_4 O_{1A1}	77.6(6)		
N_{44} Pb_4 O_{1A1}	131.0(7)		
O_{31} Pb_4 N_{54}	123.4(7)		
N_{34} Pb_4 N_{54}	64.1(8)		
N_{44} Pb_4 N_{54}	88.0(8)		
O_{1A1} Pb_4 N_{54}	128.5(6)		
N_{35} Pb_5 O_{11}	67.2(8)		
N_{35} Pb_5 N_{67}	85.3(10)		
O_{11} Pb_5 N_{67}	62.6(7)		
N_{35} Pb5 N_{46}	66.3(8)		
O_{11} Pb_5 N_{46}	122.0(6)		
N_{67} Pb_5 N_{46}	80.9(9)		
N_{35} Pb_5 O_{9B}	83.4(7)		
O_{11} Pb_5 O_{9B}	64.4(6)		

N_{67} Pb_5 O_{9B}	**126.0(7)**	
N_{46} Pb_5 O_{9B}	**138.3(9)**	