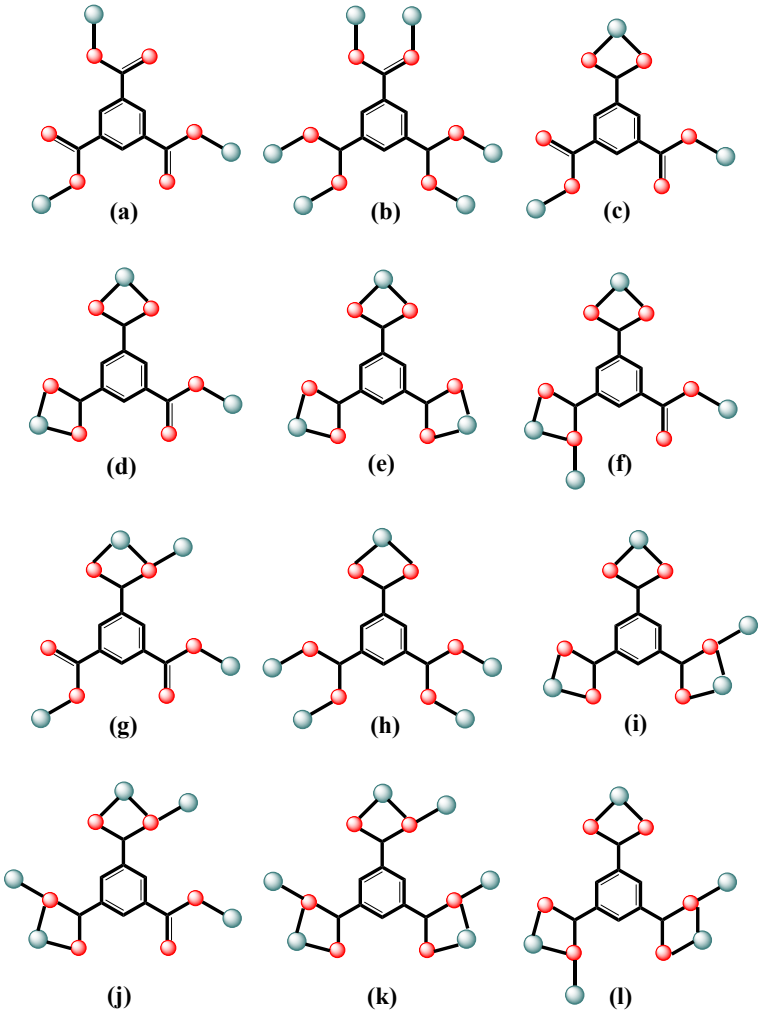
ESI

Metal organic frameworks decorated with free carboxylic acid groups: topology, metal capture and dye adsorption properties

M. Naqi Ahamad[a], M. Shahnawaz Khan[a], M. Shahid*[a], Musheer Ahmad[b]

[a]*Functional Inorganic Materials Lab (FIML), Department of Chemistry, Aligarh Muslim University, Aligarh 202002, India.*
[b]*Department of Applied Chemistry (ZHCET), Aligarh Muslim University, Aligarh 202002, India.*
*Corresponding author, E-mail: shahid81chem@gmail.com



Scheme 1S. Selected binding modes of 1,3,5-benzenetricarboxylic acid.

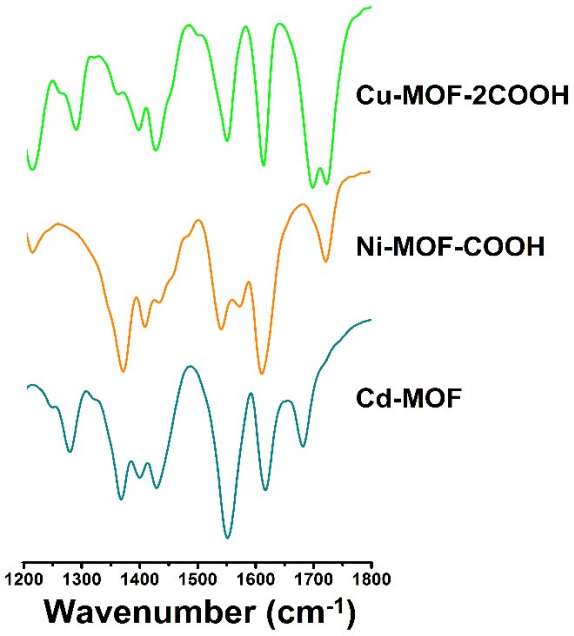


Fig 1S. FTIR spectra of the MOFs in the carboxylate frequency region.

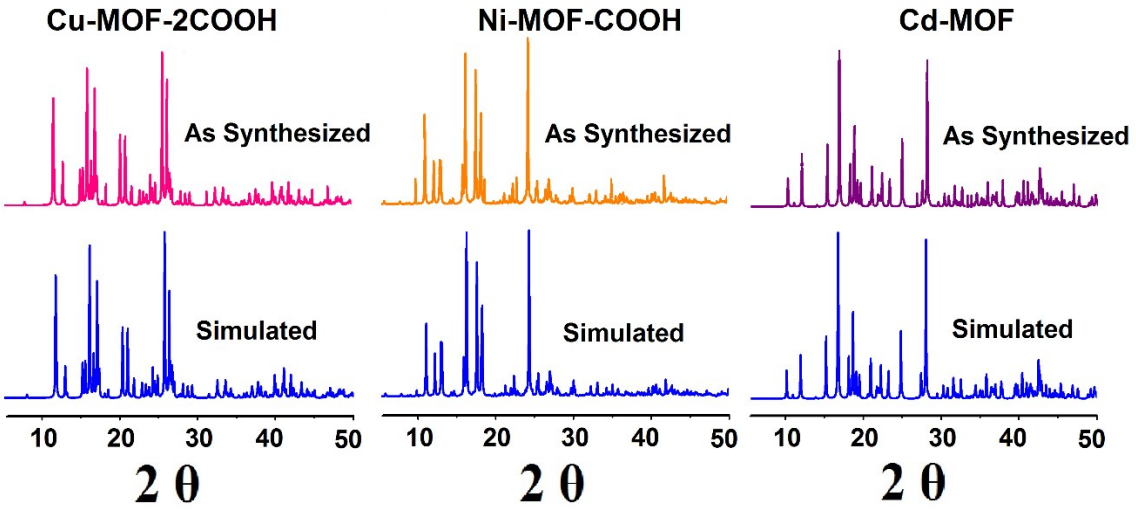


Fig 2S**.** As synthesized and simulated PXRD patterns of **Cu-MOF-2COOH**, **Ni-MOF-COOH** and **Cd-MOF.**

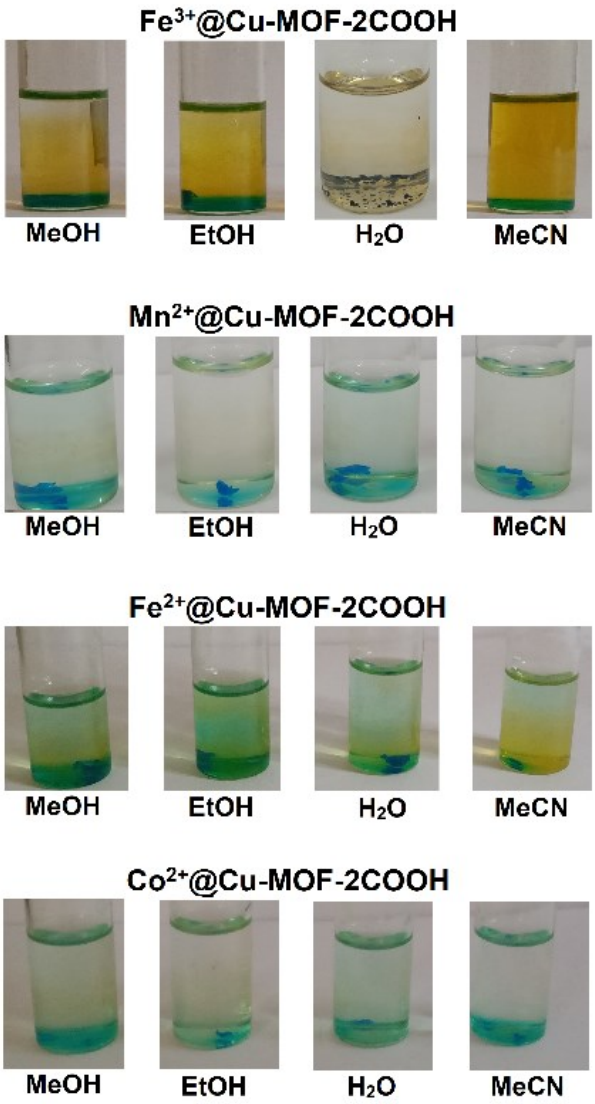


Fig 3S. Colour changes observed in the crystals after soaking Cu-MOF-2COOH in various cationic solutions in different solvents after 24 h.

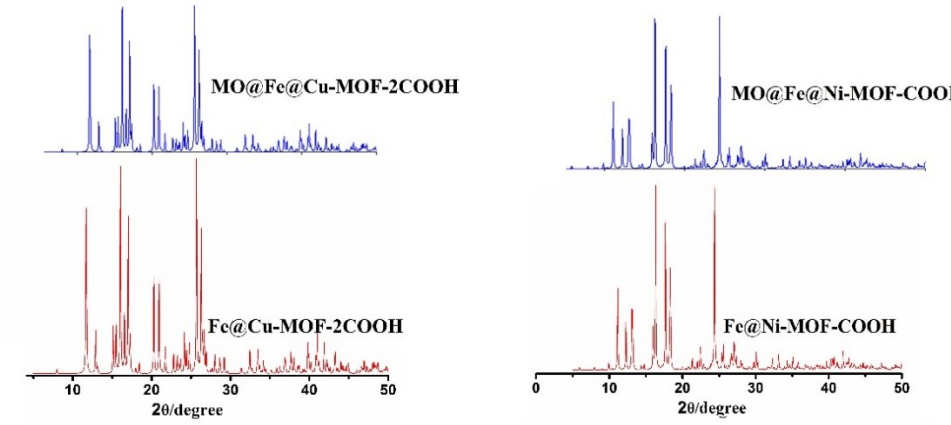


Fig. 4S. PXRD patterns recorded for both the post synthetically modified MOFs before and after adsorption of dye.

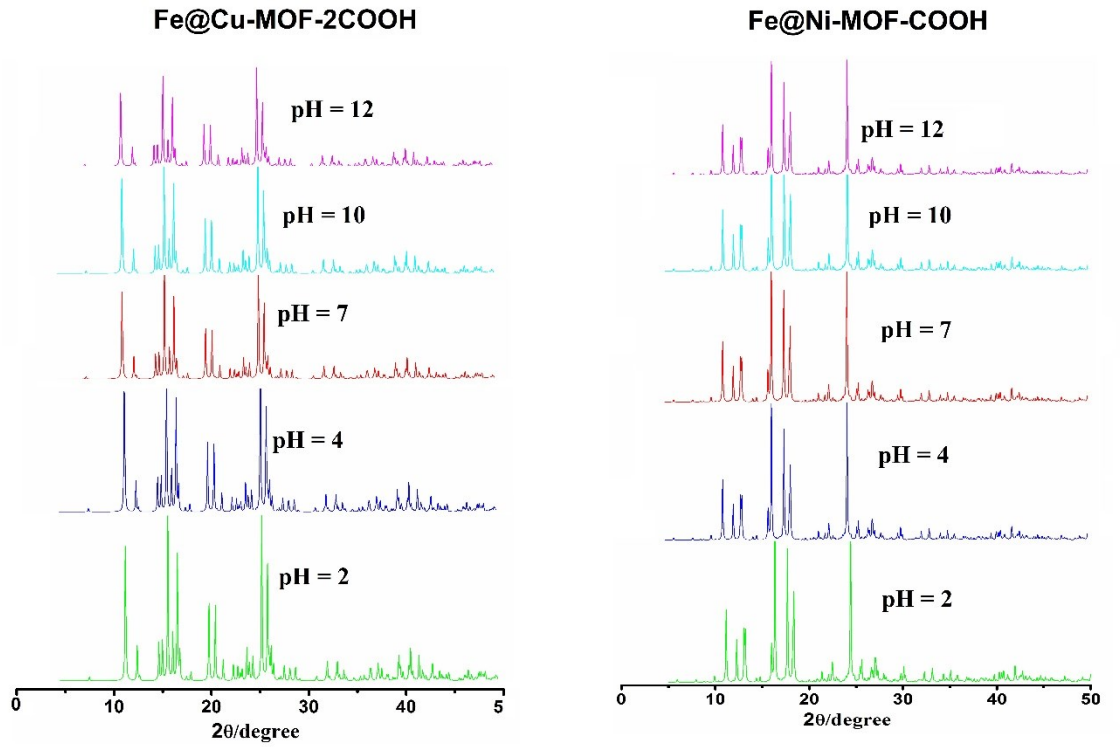


Fig. 5S. PXRD patterns recorded for both the post synthetically modified MOFs at varying pH.

Table 1S. Selected bond lengths (Å) and angles (°) for **Cu-MOF-2COOH**, **Ni-MOF-COOH** and **Cd-MOF**.

$[Cu(H_2\text{-}BTC)_2(4,4'\text{-}bipy)]_n$ (Cu-MOF-2COOH)						
Atom	**Atom**	**Length (Å)**	**Atom**	**Atom**	**Atom**	**Angle (°)**
Cu1	O1^{i}	2.4297(18)	O1^{i}	Cu1	O1	175.46(9)
Cu1	O1	2.4297(18)	O2^{i}	Cu1	O1^{i}	58.56(7)
Cu1	O2^{i}	2.0162(18)	O2	Cu1	O1^{i}	121.45(7)
Cu1	O2	2.0162(18)	N1	Cu1	O2^{i}	89.97(5)
Cu1	N1	1.976(3)	O2	Cu1	O1	58.56(7)
Cu1	N2^{ii}	1.979(3)	O2	Cu1	O2^{i}	179.94(10)
O1	C1	1.259(3)	N1	Cu1	O1^{i}	92.27(4)
O2	C1	1.272(3)	C1	Cu1	O1	29.13(7)
O3	H3	0.8400	N2^{ii}	Cu1	N1	180.000
O3	C5	1.334(3)	N2^{ii}	Cu1	O1^{i}	87.73(4)
N1	C10^{i}	1.338(3)	N2^{ii}	Cu1	O2	90.03(5)
N1	C10	1.338(3)	C1^{i}	Cu1	O2^{i}	29.43(8)
N2	C15	1.335(3)	C1^{i}	Cu1	O2	150.58(8)
N2	C15^{i}	1.335(3)	C1^{i}	Cu1	N1	91.14(6)
C1	C2	1.493(4)	C1	Cu1	N2^{ii}	88.86(6)
$[Cd(H\text{-}BTC)(H_2O)_2]_n$						
Cd1	O1	2.2768(16)	O2	Cd1	O1	53.52(6)
Cd1	O2	2.5674(17)	O3	Cd1	O1	159.00(6)
Cd1	O3	2.5354(18)	O3	Cd1	O2	146.48(6)
Cd1	O4	2.2350(17)	O4	Cd1	O1	146.07(6)
Cd1	O5	2.2871(17)	O4	Cd1	O2	92.59(6)
Cd1	O7	2.3808(19)	O4	Cd1	O3	54.64(6)
Cd1	O8	2.297(2)	O5	Cd1	O1	80.42(6)
O1	C1	1.275(3)	O5	Cd1	O2	133.94(6)
O2	C1	1.248(3)	O5	Cd1	O3	79.31(6)
O3	C8	1.248(3)	O5	Cd1	O4	133.42(6)
O4	C8	1.279(3)	O7	Cd1	O1	91.52(6)
O5	C9	1.228(3)	O7	Cd1	O2	92.34(6)
O6	C9	1.307(3)	O7	Cd1	O3	93.18(6)
C1	C2	1.489(3)	O7	Cd1	O4	88.01(7)
C2	C3	1.391(3)	O7	Cd1	O5	87.87(7)
C2	C7	1.395(3)	O8	Cd1	O1	88.74(7)
C3	C4	1.385(3)	O8	Cd1	O2	84.10(7)
C4	C5	1.393(3)	O8	Cd1	O3	88.21(7)
C4	C9^{i}	1.479(3)	O8	Cd1	O4	89.21(7)
C5	C6	1.393(3)	O8	Cd1	O5	96.73(7)
C6	C7	1.391(3)	O8	Cd1	O7	175.38(7)
$\{[Ni_2(H\text{-}BTC)_2(4,4'\text{-}bipy)_3(H_2O)]\cdot H_2O\}_n$						
Ni1	O1	2.183(3)	O2	Ni1	O1	62.18(10)
Ni1	O2	2.084(3)	O8	Ni1	O1	97.42(11)
Ni1	O8	2.008(3)	O8	Ni1	O2	159.57(12)
Ni1	N1	2.101(3)	N1	Ni1	O1	156.85(12)
Ni1	N3	2.081(3)	N1	Ni1	O2	95.05(12)
Ni1	N6^{i}	2.089(3)	N1	Ni1	O8	105.21(13)
Ni1	C1	2.450(4)	N3	Ni1	O1	85.76(12)
Ni2	O6	2.027(3)	N3	Ni1	O2	88.43(12)
Ni2	O11^{ii}	2.128(3)	N3	Ni1	O8	91.18(13)
Ni2	O12^{ii}	2.118(3)	N3	Ni1	N1	98.41(13)
Ni2	O13	2.072(3)	N6^{i}	Ni1	O1	87.89(12)
Ni2	N4^{iii}	2.078(4)	N6^{i}	Ni1	O2	88.92(12)
Ni2	N5	2.073(4)	N6^{i}	Ni1	O8	89.29(13)
Ni2	C37^{ii}	2.439(4)	O11^{ii}	Ni2	O6	96.46(11)

O1	C1	1.265(5)	O12^{ii}	Ni2	O6	158.74(11)
O2	C1	1.270(5)	O12^{ii}	Ni2	O11^{ii}	62.46(11)
O3	C8	1.197(6)	O13	Ni2	O6	95.59(13)
O4	H4	0.8400	O13	Ni2	O11^{ii}	166.11(12)
O4	C8	1.327(6)	O13	Ni2	O12^{ii}	105.03(12)
O5	C5	1.258(5)	N4^{iii}	Ni2	O6	91.22(12)
N1	C10	1.338(6)	N4^{iii}	Ni2	O11^{ii}	91.83(12)
N1	C14	1.336(5)	N4^{iii}	Ni2	O12^{ii}	92.13(12)
N2	C17	1.327(6)	N4^{iii}	Ni2	O13	94.80(12)
N2	C18	1.342(6)	N5	Ni2	O6	89.97(12)
N3	C20	1.342(5)	N5	Ni2	O11^{ii}	87.33(12)
N3	C24	1.332(6)	N5	Ni2	O12^{ii}	86.50(12)