

Topology, magnetism and dye adsorption properties of metal organic frameworks (MOFs) synthesized from bench chemicals

Khushboo Iman^a, M. Shahid,^{*a} M. Shahnawaz Khan^a, Musheer Ahmad^b, Farasha Sama^c

^aDepartment of Chemistry, Aligarh Muslim University, Aligarh 202002, India

^bDepartment of Applied Chemistry (ZHCET), Aligarh Muslim University, Aligarh 202002, India

^cDepartment of Chemistry, Indian Institute of Technology Kanpur, Kanpur 208016, India

*Corresponding author, E-mail: shahid81chem@gmail.com

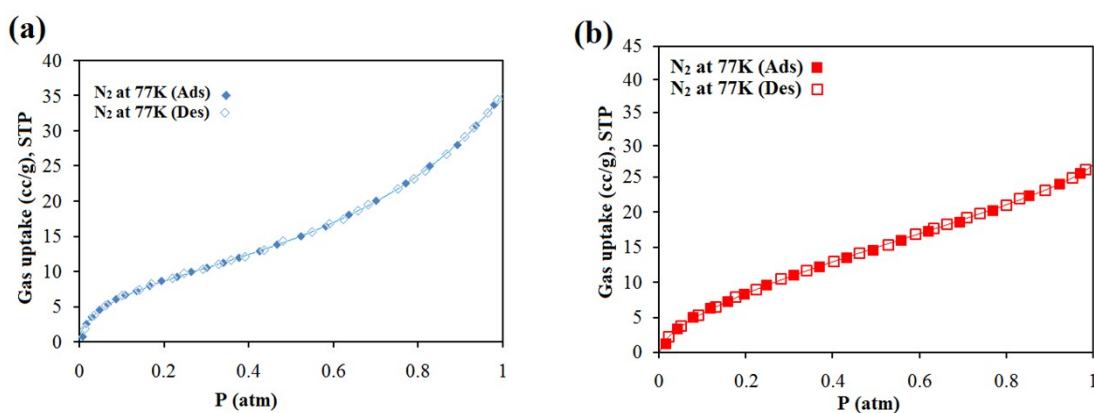


Fig. 1S. N₂ adsorption/desorption isotherms for CuMOF-1 (a) and CoMOF-2 (b) showing no noticeable porosity.

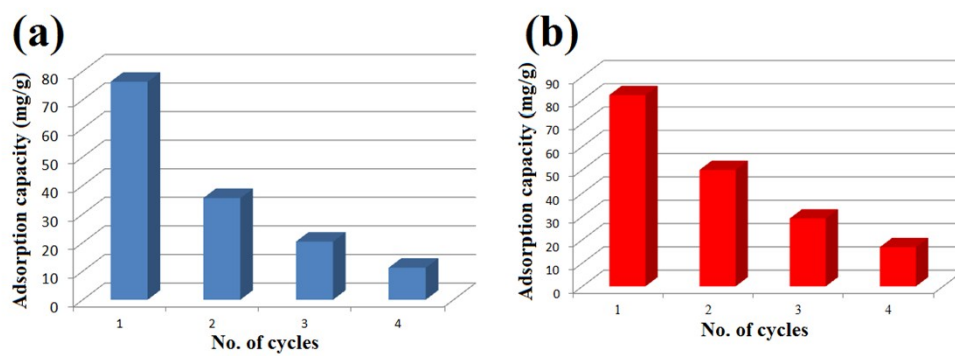


Fig 2S. Desorption plot of MB from CuMOF-1 (a) and CoMOF-2 (b) for four cycles.

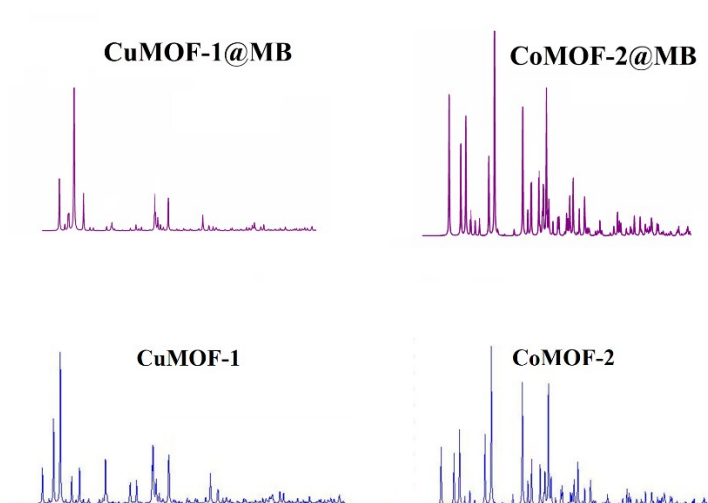


Fig 3S. PXRD patterns of CuMOF-1 and CoMOF-2 before and after the adsorption of MB.

Table 1S: Selected bond lengths for CuMOF-1 and CoMOF-2.

CuMOF-1		CoMOF-2	
Cu1 - O2	2.1327(18)	Co1- O1	2.0355(11)
Cu1 -O3	2.1711(17)	Co1- O1	2.0355(11)
Cu1 -O5	2.0007(18)	Co1- O2	2.1763(11)
Cu1 -O6	2.1375(17)	Co1- O2	2.1763(11)
Cu1 -N1	2.159(2)	Co1- N1	2.1180(13)
Cu1 -N2	2.1579(19)	Co1- N1	2.1180(13)
Cu2 -O1	2.0370(17)	Cl1- O2	1.4609(11)
Cu2 -O4	2.0752(17)	Cl1- O3	1.4408(13)
Cu2 -O5	1.9250(18)	Cl1- O4	1.4314(13)
Cu2 -N3	2.1829(19)	Cl1- O5	1.4317(12)
Cu2 -N4	2.1999(19)	O1- H1a	0.837(14)
O1- C21	1.261(3)	O1- H1b	0.815(14)
O2 -C2	1.247(3)	N1- C1	1.341(2)
O3 -C23	1.253(3)	N1- C5	1.347(2)
O4 -C23	1.280(3)	C1- H1	0.9500
O5 -H5	0.82(4)	C1- C2	1.382(2)
O6 -H6a	0.866(16)	C2- H2	0.9500
O6 -H6b	0.868(16)	C2- C3	1.394(2)
N1 -C1	1.337(3)	C3- C3	1.487(3)

Table 2S: Selected bond angles for CuMOF-1 and CoMOF-2.

CuMOF-1		CoMOF-2	
O3- Cu1-O2	89.66(14)	O1 -Co1 -O1	180.02
O5- Cu1- O2	97.15(8)	O2 -Co1- O1	82.64(4)
O5- Cu1-O3	173.15(15)	O2- Co1- O1	97.36(4)
O6 -Cu1- O2	174.60(7)	O2 -Co1- O1	82.64(4)
O6 -Cu1- O3	85.03(7)	O2- Co1 -O1	97.36(4)
O6- Cu1- O5	88.15(7)	O2- Co1 -O2	180.0
N1 -Cu1- O2	88.15(7)	N1- Co1- O1	90.39(5)
N1- Cu1- O3	88.44(7)	N1 -Co1 -O1	89.61(5)
N1- Cu1- O5	92.24(7)	N1 -Co1- O1	89.61(5)
N1- Cu1- O6	90.49(7)	N1- Co1 -O1	90.39(5)
N2- Cu1- O2	91.44(7)	N1 -Co1 -O2	90.01(5)
N2- Cu1- O3	86.79(7)	N1 -Co1- O2	89.99(5)
N2- Cu1- O5	92.52(7)	N1 -Co1- O2	90.01(5)
N2- Cu1- O6	89.25(7)	N1 -Co1 -O2	89.99(5)
N2- Cu1- N1	175.23(8)	N1- Co1 -N1	180.02
O4- Cu2- O1	149.19(7)		
O5- Cu2- O1	107.42(7)		
O5- Cu2- O4	103.38(7)		
N3- Cu2- O1	87.93(7)		
N3 -Cu2 -O4	87.78(7)		
N3- Cu2- O5	99.78(7)		
N4- Cu2- O1	87.10(7)		
N4- Cu2- O4	88.22(7)		
N4- Cu2- O5	97.17(7)		
N4- Cu2- N3	163.05(8)		

Table 3S: Summary of maximum adsorption capacity (q_{\max}) of various MOFs towards MB and/or MO.

MOF	Adsorption capacity q_{\max} (mg g ⁻¹)		References
	MB	MO	
MOF-235	187	477	a
Fe-MIL-101	124.07	505.05	b
Cu-BDC	-	86.71	c
[Cd ₂ (L)(DMF) ₃].0.5DMF _n	68.5	-	d
Ce(III)-doped UiO-66	145.1	-	e
Fe ₃ O ₄ @ZIF-8	20.2	-	f
HKUST-1	15.3	-	g
UiO-66-P composite	91.1	-	h
CuMOF-1	110	46.80	This work
CoMOF-2	158	25.50	This work

- a. E. Haque, J. W. Jun, S. H. Jhung, *J. Hazard. Mat.* 2011, **185**, 507.
- b. S. M. Hassan, A. A. Ibrahim, D. A. Mohamed, *Int. J. Mod. Chem.*, 2017, **9**, 111.
- c. R. S. Salama, S. A. El-Hakam, S. E. Samra, S. M. El-Dafrawy and A. I. Ahmed, *Int. J. Mod. Chem.*, 2018, **10**, 195.
- d. W.-P. Wu, J. Wu, J.-Q. Liu, M. Trivedi and A. Kumar, *RSC Adv.*, 2017, **7**, 54522.
- e. J.-M. Yang, R.-J. Ying, C.-X. Han, Q.-T. Hu, H.-M. Xu, J.-H. Li, Q. Wang and W. Zhang, *Dalton Trans.*, 2018, **47**, 3913.
- f. J. Zheng, C. Cheng, W. J. Fang, C. Chen, R. W. Yan, H. X. Huai and C. C. Wang, *CrystEngComm*, 2014, **16**, 3960.
- g. J. H. Qiu, Y. Feng, X. F. Zhang, M. M. Jia and J. F. Yao, *J. Colloid Interface Sci.*, 2017, **499**, 151.
- h. J. M. Yang, *J. Colloid Interface Sci.*, 2017, **505**, 178–185.