ELECTRONIC SUPPORTING INFORMATION

Diverse isostructural MOFs by postsynthetic metal node metathesis: anionic-to-cationic framework conversion, luminescence and separation of dyes

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General Aspects

¹H NMR spectra were recorded on JEOL-Lambda (400 MHz and 500 MHz) spectrometers with deuterated chloroform or DMSO as an internal standard. ¹³C NMR spectra were recorded with 125 MHz NMR spectrometer with complete proton decoupling. IR spectra were recorded with a Bruker Vector 22 FT-IR spectrophotometer. Mass spectral analyses were carried out with Waters ESI-Q^{TOF} Instrument. The melting points were determined with a JSGW melting point apparatus. Column chromatography was conducted with silica-gel 100-200 µ mesh (Souvenier Chemicals, India). All the solvents were freshly distilled prior to use. All metal salts, dyes and DMF (N,Ndimethylformamide) were obtained from Sigma-Aldrich and Alfa Aesar, and were used as received. The single crystal X-ray diffraction data were collected on a Bruker SMART/CCD diffractometer using MoKa radiation. Powder X-ray diffraction measurements were recorded on a Rigaku X-ray diffractometer. Thermal analyses (N2 atmosphere, heating rate of 10 °C/min) were carried out in a Mettler Toledo TGA equipment. Energy dispersive X-ray spectroscopy (EDX) was carried out with a JEOL-7500F Microscope equipped with an energy-dispersive spectroscopy (EDS) instrument. ICP-AES analyses were performed with ICP-9000(N+M) (USA Thermo Jarrell-Ash Corp).

X-Ray Crystal Structure Determinations

A good quality crystal in the case was chosen, mounted on a glass capillary, and the intensity data was collected at 100 K on a Bruker Nonius SMART APEX CCD detector system with Mosealed Siemens ceramic diffraction tube ($\lambda = 0.71073$) and a highly oriented graphite monochromator operating at 50 kV and 30 mA. The data were collected on a hemisphere mode and processed with Bruker SAINTPLUS. Empirical absorption correction was made using Bruker SADABS. The structures were solved by Direct Methods using SHELXTL package and refined by full matrix least squares method based on F² using SHELX97 program. All the non-hydrogen atoms were refined anisotropically. The hydrogen atoms were fixed in their ideal positions, assigned fixed isotropic U values and allowed to ride with their respective non-hydrogen atoms. The details of crystal data, structure solution and refinement are presented in Tables S3 to S6.

Synthesis of the Tetraacid Ligand H₄L.

Synthesis of 3,3',5,5'-Tetrakis(p-methylphenyl)-2,2',6,6'-tetramethoxy-1,1'-biphenyl. A two-

necked RB flask was charged with dioxane (15 mL) and water (15 mL), and the mixture was degassed and bubbled with N₂ for 15 min. Subsequently, 3,3',5,5'-tetraiodo-2,2',6,6'-tetramethoxy-1,1'-biphenyl (2.0 g; 2.56 mmol), *p*-methylphenylboronic acid (13.4 g; 25.68 mmol) and NaOH (1.0 g; 25.68 mmol) were added to the round bottom flask followed by addition of the catalyst Pd(PPh₃)₄ (0.2 g; 0.24 mmol). The entire mixture was heated at reflux for 2 d. At the end of this period, dioxane was removed in vacuo and the residue was extracted with chloroform for two times. The combined organic extract was dried with anhydrous Na₂SO₄ and the solvent was removed in vacuo to obtain the crude product, which was purified by column chromatography to obtain 1.4 g (88%) of the product, mp 230-232 °C; IR (solid) cm⁻¹ 3431, 29381462, 1060; ¹H NMR (CDCl₃, 500 MHz) δ 2.40 (s, 12H), 3.39 (s, 12H), 7.22 (d, *J* = 7.8 Hz, 8H), 7.38 (s, 2H), 7.52 (d, *J* = 7.8 Hz, 8H); ¹³C NMR (CDCl₃, 125 MHz) δ 21.2, 60.3, 124.1, 128.9, 129.0, 130.2, 132.3, 135.8, 136.5, 155.4; ESI-MS⁺ m/z Calcd for C₄₄H4₂O₄Na 657.2980 [M + Na]⁺, found 657.2986.

Synthesis of 3.3',5,5'-Tetrakis(p-carboxyphenyl)-2,2',6,6'-tetramethoxy-1,1'-biphenyl, H₄L.



3,3',5,5'-Tetrakis(*p*-tolyl)-2,2',6,6'-tetramethoxy-1,1'-biphenyl (1.0 g; 1.58 mmol) was taken in a mixture of pyridine (32 mL) and H₂O (8 mL). KMnO₄ (2.50 g; 15.8 mmol) was added to the reaction and heated

at reflux for 6 days. $KMnO_4$ was added in increments at regular intervals of time and the reaction was monitored by TLC analysis. After completion of the reaction as judged from TLC analysis, pyridine was removed in vacuo, the brown solid was filtered off and washed with water. The filtrate was acidified with conc. HCl, and the resulting precipitate was collected by filtration to afford 0.80 g (67%) of the final tetracarboxylic acid, mp (decomp) 272-274 °C; IR (solid) cm⁻¹ 3414, 2943, 2662, 1687; ¹H NMR (CD₃OD, 500 MHz) δ 3.40 (s, 12H), 7.52 (s, 2H), 7.75 (d, J = 8.5 Hz, 8H), 8.11 (d, J = 8.5 Hz, 8H); ¹³C NMR (CD₃)₂SO, 125 MHz) δ 60.5, 123.9, 128.9, 129.3, 129.6, 142.1, 155.9, 167.2; ESI-MS m/z Calcd for C₄₄H₃₃O₁₂ 753.1972 [M-H]⁻, found 753.1974.

Synthesis of Cd-MOFs

Synthesis of Cd-MOF4. The tetraacid ligand H_4L (0.01 g, 0.013 mmol) and Cd(NO₃)₂ (0.013 g, 0.053 mmol) were dissolved in 1.5 mL of DMF taken in a 5 mL culture tube. The solution was heated for 48 h in a sand-bath placed in an oven maintained at 90 °C. After this period, the temperature was allowed to slowly attain to room temperature. Colourless block-shaped crystals were isolated by filtration, washed thoroughly with DMF and allowed to air dry. (11.6 mg, 47.4%).

Cd-MOF1, Cd-MOF2, Cd-MOF8 and Cd-MOF12 were synthesized by following the same procedure used for the synthesis of Cd-MOF4, but by varying the ligand, i.e., $Cd(NO_3)_2$, mole ratio. Accordingly, H₄L and Cd(NO₃)₂ were employed in 1:1, 1:2, 1:8 and 1:12 ratios.

Typical procedure of metal exchange. The crystals of the **Cd-MOF1** (ca. 10.0 mg) were suspended in 1 mL 0.01 M solutions of different metal salts in DMF. The mother liquor in each case was replenished by a fresh solution of the metal salt every 3 days once. After 15-20 days, the crystals were filtered and washed thoroughly with DMF to remove the organic and inorganic materials adsorbed at the surface. Finally, the metal-organic materials were allowed to dry. The material thus derived was examined by ICP-AES and EDX to determine the magnitude of metal exchange in each case.

Reversibility of PSME

The reversibility of PSME was investigated for one metal ion of each of lanthanides, transition metal ions and main group metal ions; specifically, the cases for which the exchange was found to be more than 90% after soaking the crystals for 25 days were chosen for these investigations. Typically, ca. 20 mg **Cd-MOF** was soaked in 1mL each of 0.01 M solution of Tb(NO₃)₃, SrCl₂ and ZnCl₂ in DMF. The solutions were replenished by respective fresh solutions every two days. After 10 days, half of the crystals in each case were taken out, washed several times for getting rid of the excess metal ions and allowed to dry prior to ICP-AES analyses. The other parts of the crystals were subjected to the reverse exchange with 0.01 M Cd(NO₃)₂ solution in the same manner for 10 days. The ratios of the metal ions as determined from the ICP-AES analyses are collated in Table S2. The reversibility of the process in all cases and the high propensity for the exchanged metal ions to be substituted again by Cd(II) ions clearly indicates that the **Cd-MOF** is highly robust and that the exchange of the framework metal ions occurs mostly due to the flexibility of the framework as well as concentration gradient.

Code	M/Cd atomic ratio (ICP-AES)		
Tb@MOF forward	39.6: 60.4		
Tb@MOF reverse	4.5: 95.5		
Sr@MOF forward	99.8 : 0.2		
Sr@MOF reverse	0.08: 99.02		
Zn@MOF forward	56.4: 43.6		
Zn@MOF reverse	5.6: 94.4		

Table S1. M:Cd atomic ratio of the MOFs after forward and reverse metal exchange for 10 days.



Figure S1. An overlay of (a) the structures of ligand L and (b) framework structures (as a 3,8-connecting net) observed in the five Cd-MOFs, viz., Cd-MOF-1, Cd-MOF-2, Cd-MOF-4, Cd-MOF-8, and Cd-MOF-12.



Figure S2. The crystal packing diagrams of all Cd-MOFs, i.e., Cd-MOF-1, Cd-MOF-2, Cd-MOF-4, Cd-MOF-8, and Cd-MOF-12, by reducing the ligand to a pair of 3-connecting module (a-e). Note that the coordination mode and basic organization are similar in each case. Cell parameters are defined differently for each of them due to small changes in the overall structure.

Table S2. Torsional angles between the dimethoxyaryl rings (φ), and the phenylcarboxylate rings and the dimethoxyaryl rings of L⁴⁻ in the Cd-MOFs.



Cd-MOF	φ	Ψ	Cell volume (Å ³)
Cd-MOF1	72.032	43.128, 49.53, 49.194, 82.854	3731.08
Cd-MOF2	63.559	44.26, 49.363, 60.982, 49.076	3483.56
Cd-MOF4	70.601, 65.453	63.099, 50.701, 45.386, 45.722; 57.84, 55.565, 42.775, 51.803	7465.95
Cd-MOF8	72.613	47.334, 46.250, 48.803, 71.273	3844.03
Cd-MOF12	73.330, 71.752	50.792, 57.535, 48.777, 49.024; 52.197, 55.392, 43.503, 49.179	7588.83



Figure S3. TGA profile of **Cd-MOF4**. The sample was heated from 30 °C to 800 °C at a heating rate of 10 °C/min.



Figure S4. (a) PXRD profiles of Cd-MOF1, Cd-MOF2, Cd-MOF8 and Cd-MOF12 with their theoretically simulated profiles based on their single crystal structures. (b) PXRD profiles Ln@MOFs compared with the PXRD of as synthesized Cd-MOF.



Figure S5. PXRD profiles of the (a) Mm@MOFs (main group metal ions) and (b) Tm@MOFs (transition metal ions) as compared to that of the parent Cd-MOF.



Figure S6. (a) PXRD profiles of as-synthesized **Cd-MOF4**, after 1st, 2nd and 3rd cycles of dye adsorption study and their comaprison with the simulated pattern obtained from single crystal structure determination. (b) PXRD of **Eu@MOF** after the dye adsorption study as compared to that of the as-synthesized **Eu@MOF** and the simulated profile from the single crystal structure.



Figure S7. (a) Excitation and emission spectra of (a) the tetraacid ligand H_4L in the solid state and (b) the parent Cd-MOF. (c) Emission spectra of Zn-MOF, Sr-MOF and Pb-MOF, accessed by PSME of Cd-MOF (λ_{ex} = 300 nm.).



Figure S8. Adsorption (a) of the cationic dye TT in DMF with the anionic **Cd-MOF** as monitored by UV-vis spectroscopy, selective adsorption of TT by the **Cd-MOF** in the presence of negative dye XyCy (b) and neutral dye NR (c).



Figure S9. Adsorption (a) and subsequent release–upon treatment with saturated solution of NaCl–of the cationic dye Rhodamine-6G (Rh-6G) in DMF with the anionic Cd-MOF as monitored by UV-vis spectroscopy (b). (c) Competitive adsorption of Rh-6G by Cd-MOF in the presence of an anionic dye, namely, bromophenol blue.



Figure S10. Reversion of dye adsorption: (a) MB and (b) TT from the **Cd-MOF** upon treatment with a saturated solution of NaCl in DMF, as monitored by UV-vis spectroscopy.



Figure S11. Adsorption of the cationic dye Nile blue by **Cd-MOF** (a), and subsequent release upon treatment with saturated solution of NaCl in DMF, as monitored by UV-vis spectroscopy (b).



Figure S12. Adsorption of the cationic dye NB with **Cd-MOF** (a), and (b) its subsequent release upon treatment with saturated solution of NaCl in DMF, as monitored by change in the fluorescence intensity of the supernatant solution with time (b).



Figure S13. Release experiment of BB from the Eu@MOF, as monitored by UV-vis spectroscopy.

MOF	Cd-MOF1	Cd-MOF2	Cd-MOF4	Cd-MOF8
Empirical formula	$C_{88}H_{60}O_{24}Cd_3$	C ₈₈ H ₆₀ Cd ₃ O ₂₄	C ₈₈ H ₆₀ O ₂₄ Cd ₃	C ₁₁₂ H ₁₁₆ N ₈ O ₃₄ Cd ₄
Formula weight	1838.59	1838.59	1838.56	2567.72
Temperature (K)	100(2) K	100(2) K	100(2) K	100(2) K
Wavelength (Å)	0.71073 Å	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
Space group	P -1	P -1	P -1	P -1
Unit cell dimensions	a = 15.462(5) Å	a = 15.277(2) Å	a = 16.1904(18) Å	a = 15.4562(18) Å
	b = 16.063(5) Å	b = 16.131(2) Å	b = 18.127(2) Å	b = 16.278(2) Å
	c = 18.103(5) Å	c = 17.297(3) Å	c = 27.495(3) Å	c = 18.346(2) Å
	$\alpha = 107.120(5)^{\circ}$	$\alpha = 67.016(3)^{\circ}$	$\alpha = 75.967(2)^{\circ}$	$\alpha = 108.559(2)^{\circ}$
	$\beta = 102.556(5)^{\circ}$	$\beta = 81.847(3)^{\circ}$	$\beta = 88.446(2)^{\circ}$	$\beta = 103.799(2)^{\circ}$
	$\gamma = 111.229(5)^{\circ}$	$\gamma = 62.703(2)^{\circ}$	$\gamma = 72.710(2)^{\circ}$	$\gamma = 108.453(2)^{\circ}$
Volume (Å ³)	3731	3483.6(9)	7466.0(14)	3844.0(8)
Z, Calculated	1, 0.865	1, 0.876	2, 0.818	1, 1.109
density(g/cm ³)				
Absorption coefficient(mm ⁻¹)	0.604	0.499	0.465	0.607
<i>F</i> (000)	964	924	1848	1308
θ range for data collection (°)	2.291 to 28.399°	1.280 to 28.387°	0.764 to 28.348°	1.264 to 28.306°
Limiting indices	-20<=h<=20	-20<=h<=13	-21<=h<=21	-9<=h<=19
0	-21<=k<=15	-21<=k<=16	-23<=k<=23	-20<=k<=19
	-23<=1<=24	-22<=1<=14	-19<=l<=35	-24<=l<=24
Reflections collected	28367	21432	47079	23842
Independent	17923	15202	32975	16857
reflections	[R(int) = 0.0672]	[R(int) = 0.0368]	[R(int) = 0.0628]	[R(int) = 0.0338]
Completeness to θ	97.2 %	97.8 %	98.3 %	98.1 %
Refinement method	Full-matrix least-	Full-matrix least-	Full-matrix least-	Full-matrix least-
	squares on F ²	squares on F ²	squares on F ²	squares on F ²
Data / restraints / parameters	17923 / 0 / 366	15202 / 0 / 470	32975 / 0 / 976	16857 / 9 / 572
Goodness-of-fit on F^2	0.912	0.934	1.046	1.134
Final <i>R</i> indices	R1 = 0.1328	R1 = 0.0724	R1 = 0.1024	R1 = 0.1026
$[I > 2\sigma(I)]$	wR2 = 0.3375	wR2 = 0.1936	wR2 = 0.2452	wR2 = 0.2769
R indices (all data)	R1 = 0.1328	R1 = 0.1198	R1 = 0.1690	R1 = 0.1407
	wR2 = 0.3375	wR2 = 0.2286	wR2 = 0.2718	wR2 = 0.3398
Largest diff. peak and hole $(e.Å^{-3})$	2.421 and -2.549	1.155 and -2.372	5.400 and -1.638	3.684 and -3.796

 Table S3. Crystallographic parameters for Cd-MOF1, Cd-MOF2, Cd-MOF4 and Cd-MOF8.

MOF	Cd-MOF12	Ca@MOF	La@MOF	Pr@MOF
Empirical formula	C ₉₇ H ₈₂ N ₃ O ₃₀ Cd ₄	C ₈₈ H ₆₀ O ₂₉ Ca _{1.75} C	C ₉₁ H ₆₇ NO ₂₆ Cd _{1.46}	C ₉₇ H ₈₁ N ₃ O ₂₇ Cd _{1.43}
		d _{2.25}	La _{1.54}	Pr _{1.57}
Formula weight	2219.3	1904.32	1968.53	2102.71
Temperature (K)	100(2) K	100(2) K	100(2) K	100(2) K
Wavelength (Å)	0.71073 Å	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
Space group	P -1	P -1	P -1	P -1
Unit cell dimensions	a = 15.6469(17) Å	a = 15.631(5) Å	a = 15.744(3) Å	a = 15.890(5) Å
	b = 18.471(2) Å	b = 18.456(6) Å	b = 18.343(3) Å	b = 18.596(6) Å
	c = 27.450(3) Å	c = 27.517(10) Å	c = 28.121(5) Å	c = 28.500(10) Å
	$\alpha = 99.525(2)^{\circ}$	$\alpha = 80.164(7)^{\circ}$	$\alpha = 104.422(3)^{\circ}$	$\alpha = 101.979(6)^{\circ}$
	$\beta = 90.063(2)^{\circ}$	$\beta = 89.994(7)^{\circ}$	$\beta = 92.252(3)^{\circ}$	$\beta = 94.414(6)^{\circ}$
	$\gamma = 103.876(2)^{\circ}$	$\gamma = 76.264(6)^{\circ}$	$\gamma = 108.122(3)^{\circ}$	$\gamma = 108.931(5)^{\circ}$
Volume (Å ³)	7588.8(14)	7591(4)	7415(2)	7697(4)
Z, Calculated	2, 0.966	2, 0.907	2, 0.899	8, 0.925
density(g/cm ³)	,	,	,	,
Absorption	0.604	0.499	0.894	0.982
coefficient(mm ⁻¹)				
<i>F</i> (000)	2222	2096	1996	2154
θ range for data	0.753 to 28.367°	1.154 to 28.401°	0.754 to 28.325°	1.194 to 28.297°
collection (°)				
Limiting indices	-20<=h<=20	-20<=h<=19	-19<=h<=20	-20<=h<=13
	-24<=k<=12	-23<=k<=24	-22<=k<=23	-24<=k<=23
	-33<=l<=35	-35<=l<=30	-25<=l<=37	-33<=l<=37
Reflections	47106	46096	44502	42687
collected			44302	
Independent	33384	33043	31902	32008
reflections	[R(int) = 0.0582]	[R(int) = 0.0917]	[R(int) = 0.0427]	[R(int) = 0.0577]
	[()]	[()		
Completeness to θ	97.9 %	97.7 %	97.6 %	95.8 %
Refinement method	Full-matrix least-	Full-matrix least-	Full-matrix least-	Full-matrix least-
	squares on F ²	squares on F ²	squares on F ²	squares on F ²
Data / restraints /	33384 / 0 / 1105	33043 / 0 / 1077	31902 / 0 / 1016	32008 / 0 / 835
parameters				
Goodness-of-fit on	0.949	0.803	0.981	0.932
F^2				
Final R indices	R1 = 0.0903	R1 = 0.1094	R1 = 0.0823	R1 = 0.1115
$[I > 2\sigma(I)]$	wR2 = 0.2242	wR2 = 0.2623	wR2 = 0.2128	wR2 = 0.2906
<i>R</i> indices (all data)	R1 = 0.1528	R1 = 0.2188	R1 = 0.1254	R1 = 0.1687
` '	wR2 = 0.2730	wR2 = 0.2992	wR2 = 0.2548	wR2 = 0.3365
Largest diff. peak	3.268 and -2.815	2.147 and -1.638	1.749 and -2.213	3.419 and -3.001
and hole (e.Å ⁻³)				

Table S4. Crystallographic parameters for Cd-MOF12, Ca@MOF, La@MOF and Pr@MOF.

$ \begin{array}{c} b = 18.275(3) \ \dot{A} & b = 18.213(4) \ \dot{A} & b = 18.597(3) \ \dot{A} & c = 28.066(4) \ \dot{A} & c = 27.961(6) \ \dot{A} & c = 28.43(4) \ \dot{A} & c = 28.06(4) \ \dot{A} & c = 27.961(6) \ \dot{A} & c = 28.43(4) \ \dot{A} & c = 28.064(14) \ \dot{A} & c = 100.536(2)^{\circ} & \mu = 103.419(9) \ \beta = 92.048(3)^{\circ} & \beta = 91.538(4)^{\circ} & \beta = 95.130(2)^{\circ} & \beta = 91.978(7)^{\circ} \\ \gamma = 107.860(3)^{\circ} & \gamma = 107.955(4)^{\circ} & \gamma = 109.615(2)^{\circ} & \gamma = 108.705(8) \\ Volume \left(\dot{A}^3 \right) & 7405.6(19) & 7360(3) & 7716.2(19) & 7442(6) \\ Z, Calculated & 2, 0.969 & 2, 1.061 & 2, 0.936 & 2, 0.906 \\ density(g/cm^3) & \\ Absorption & 1.086 & 1.237 & 1.252 & 1.454 \\ coefficient(mm^{-1}) & & \\ F(000) & 2158 & 2374 & 2174 & 2006 \\ \partial range for data & 0.755 to 28.331^{\circ} & 0.758 to 28.373^{\circ} & 2.04 to 21.20^{\circ} & 1.211 to 28.29 \\ collection (^{\circ}) & \\ Limiting indices & -18<=h<=20 & -21<=h<=9 & -16<=h<=16 & -19<=h<=20 \\ -23<=k<=2 & -21<=k<=23 & -16<=k<=18 & -24<=k<=24 \\ -36<=1<=26 & -37<=1<=35 & -28<=1<8 & -20<= <=37 \\ -23<=k<=2 & -21<=k<=23 & -16<=k<=18 & -24<=k<=24 \\ -36<=1<<26 & -37<= <=35 & -28<=1<28 & -20<= <=37 \\ collected & \\ Independent & 32513 & 32018 & 16735 & 31641 \\ reflections & (R(int) = 0.0339] & [R(int) = 0.0462] & [R(int) = 0.0385] & [R(int) = 0.191 \\ \hline Completeness to \theta & 98.0 \% & 97.8 \% & 98.2 \% \\ Refinement method & 52513 / 0 / 977 & 32018 / 0 / 1175 & 16735 / 0 / 1041 & 31641 / 0 / 410 \\ parameters & gquares on F^2 & squares on F^2 \\ squares on F^2 & squares on F^2 \\ squares on F^2 & squares on F^2 \\ squares on F^2 & squares on F^2 \\ radia t restraints / & 32513 / 0 / 977 & 32018 / 0 / 1175 & 16735 / 0 / 1041 & 31641 / 0 / 410 \\ parameters & Goodness-of-fit on & 1.168 & 1.025 & 1.091 & 1.014 \\ f^2 & Final R indices & R1 = 0.1061 & R1 = 0.1014 & R1 = 0.0972 & R1 = 0.2057 \\ I > 20(I) & R2 = 0.2928 & R2 = 0.2695 & R2 = 0.2590 & R2 = 0.4744 \\ R indices (all data) & R1 = 0.1427 & R1 = 0.1648 & R1 = 0.1123 & R1 = 0.4734 \\ R R2 = 0.3546 & R2 = 0.3159 & R2 = 0.2695 & R2 = 0.2695 & R2 = 0.2695 \\ \end{array}$	MOF	Nd@MOF	Sm@MOF	Eu@MOF	Tb@MOF
Formula weight Temperature (K)2127.13 100(2) K2287.86 2110.182110.18 2010.152010.15 100(2) KTemperature (K) Wavelength (Å)100(2) K100(2) K100(2) K100(2) K100(2) KCrystal system Space groupP-1 a = 15.785(2) Å b = 18.275(3) Å c = 28.066(4) Å c = 27.961(6) Å c = 28.041(4) Å c = 28.064(4) Å c = 28.066(4) Å c = 28.06(4) Å c = 0.353m = 15.779(8) Å c = 28.06(4) Å c = 28.06(4)	Empirical formula				C ₈₈ H ₆₀ O ₂₆ Tb ₃
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$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Wavelength (Å)				
$ \begin{array}{llllllllllllllllllllllllllllllllllll$					
$ \begin{array}{c} \mbox{Unit cell dimensions} & a = 15.785(2) \mbox{Å} & a = 15.813(4) \mbox{Å} & a = 15.970(2) \mbox{Å} & b = 18.275(3) \mbox{Å} & b = 18.275(3) \mbox{Å} & b = 18.275(3) \mbox{Å} & c = 28.066(4) \mbox{Å} & c = 27.961(6) \mbox{Å} & c = 28.434(4) \mbox{Å} & a = 104.736(4)^\circ & \alpha = 100.536(2)^\circ & \alpha = 103.419(9) \\ \mbox{$\alpha = 104.478(3)^\circ & \alpha = 104.736(4)^\circ & \alpha = 100.536(2)^\circ & \alpha = 103.419(9) \\ \mbox{$\beta = 92.048(3)^\circ & \gamma = 107.955(4)^\circ & \gamma = 109.615(2)^\circ & \gamma = 108.705(8) \\ \mbox{$\gamma = 107.860(3)^\circ & \gamma = 107.955(4)^\circ & \gamma = 109.615(2)^\circ & \gamma = 108.705(8) \\ \mbox{Z_c Calculated} & 2, 0.969 & 2, 1.061 & 2, 0.936 & 2, 0.906 \\ \mbox{$density(g/cm^3)$ & Absorption & 1.086 & 1.237 & 1.252 & 1.454 \\ \mbox{$coefficient(mm^{-1})$ \\ $F(000) $ $2158 $ $2374 $ $2174 $ $2006 & 1.211 to $28.29 \\ $Collection (°)$ & 1.8< & $2374 $ $21.454 $ $2006 & $1.211 to $28.29 \\ \mbox{$collection (°)$ & $1.8< $ $2374 $ $21.454 $ $2006 & $1.211 to $28.29 \\ \mbox{$collection (°)$ & $1.8< $ $2374 $ $21.454 $ $2006 & $1.211 to $28.29 \\ \mbox{$collection (°)$ & $1.8< $ $23.74 $ $21.454 $ $2006 & $1.211 to $28.29 \\ \mbox{$collection (°)$ & $1.8< $ $23.74 $ $2.04 to $21.20^\circ $ $1.211 to $28.29 \\ \mbox{$collection (°)$ & $1.8< $ $23.74 $ $2.04 to $21.20^\circ $ $1.211 to $28.29 \\ \mbox{$collection (°)$ & $1.8< $ $23.74 $ $2.04 to $21.20^\circ $ $1.211 to $28.29 \\ \mbox{$collection (°)$ & $1.8< $ $2.374 $ $2.84 $ $28.723 $ $2.04 $ $1.228 $ $2.04 $ $21.20^\circ $ $1.211 to $28.29 \\ \mbox{$collected $ $1.44824 $ $28723 $ $43102 $ $2.06 $ $2.02 $ $2.06 $ $2.02 $ $2.06 $ $2.00 $ $					
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		a = 15.785(2) Å	a = 15.813(4) Å	a = 15.970(2) Å	a = 15.779(8) Å
$\begin{array}{cccccccccccccccccccccccccccccccccccc$					b = 18.369(9) Å
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$\begin{array}{c ccccccccccccccccccccccccccccccccccc$					$\alpha = 103.419(9)^{\circ}$
$\begin{array}{c} \gamma = 107.800(3)^{\circ} \qquad \gamma = 107.953(4)^{\circ} \qquad \gamma = 109.613(2)^{\circ} \qquad \gamma = 108.705(8)^{\circ} \\ \gamma = 108.705(8)^{\circ} \qquad \gamma = 108.705(8)^{\circ} \\ \gamma = 108.705(100,100,100,100,100,100,100,100,100,100$		•	•	•	
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$ \begin{bmatrix} I > 2\sigma(I) \end{bmatrix} & \text{wR2} = 0.2928 & \text{wR2} = 0.2695 & \text{wR2} = 0.2590 & \text{wR2} = 0.4474 \\ \text{R indices (all data)} & \text{R1} = 0.1427 & \text{R1} = 0.1648 & \text{R1} = 0.1123 & \text{R1} = 0.4734 \\ \text{wR2} = 0.3546 & \text{wR2} = 0.3159 & \text{wR2} = 0.2695 & \text{wR2} = 0.5884 \\ \end{array} $					
$ \begin{bmatrix} I > 2\sigma(I) \end{bmatrix} & \text{wR2} = 0.2928 & \text{wR2} = 0.2695 & \text{wR2} = 0.2590 & \text{wR2} = 0.4474 \\ \text{R indices (all data)} & \text{R1} = 0.1427 & \text{R1} = 0.1648 & \text{R1} = 0.1123 & \text{R1} = 0.4734 \\ \text{wR2} = 0.3546 & \text{wR2} = 0.3159 & \text{wR2} = 0.2695 & \text{wR2} = 0.5884 \\ \end{array} $	Final R indices	R1 = 0.1061	R1 = 0.1014	R1 = 0.0972	R1 = 0.2057
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wR2 = 0.3546 $wR2 = 0.3159$ $wR2 = 0.2695$ $wR2 = 0.5884$					
	n marcos (an aara)				
	Largest diff. peak	4.580 and -2.909	2.313 and -2.489	3.113 and -3.224	2.663 and -0.936
and hole $(e.Å^{-3})$		7.300 and -2.909	2.315 and -2.409	5.115 and -5.224	2.005 and -0.950

Table S5. Crystallographic parameters for Nd@MOF, Sm@MOF, Eu@MOF and Tb@MOF.

MOF	Mn@MOF	Co@MOF	Cu@MOF	Zn@MOF
Empirical formula	C44H30 O12Mn0.63	C ₄₄ H ₃₀ O ₁₂ Co _{1.21}	$C_{94}H_{74}N_2O_{30}Cu_{3.3}$	C44H30O12Zn1.46Cd0.04
	$Cd_{0.87}$	Cd _{0.29}	Cd _{0.69}	
Formula weight	833.15	3749(2)	1999.37	850.74
Temperature (K)	100(2) K	100(2) K	100(2) K	100(2) K
Wavelength (Å)	0.71073 Å	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
Space group	P -1	P -1	P -1	P -1
Unit cell	a = 15.957(4) Å	a = 15.468(5)	a = 15.508(3) Å	a = 15.116(5) Å
dimensions	b = 16.460(4) Å	b = 15.785(5)	b = 16.241(3) Å	b = 15.393(5) Å
	c = 17.300(5) Å	c = 18.038(6)	c = 18.383(4) Å	c = 18.225(6) Å
	$\alpha = 106.070(6)^{\circ}$	$\alpha = 107.270(6)^{\circ}$	$\alpha = 108.709(4)^{\circ}$	$\alpha = 105.732(6)^{\circ}$
	$\beta = 100.850 (5)^{\circ}$	$\beta = 103.949(6)^{\circ}$	$\beta = 104.279(4)^{\circ}$	$\beta = 106.553(6)^{\circ}$
	$\gamma = 113.408(5)^{\circ}$	$\gamma = 107.163(5)^{\circ}$	$\gamma = 107.160(4)^{\circ}$	$\gamma = 104.405(7)^{\circ}$
	$\gamma = 113.408(3)$	$\gamma = 107.103(3)$	$\gamma = 107.100(4)$	$\gamma = 104.403(7)$
Volume (Å ³)	3770.9(17)	3749(2)	3880.8(13)	3660(2)
Z, Calculated	2, 0.734	2, 0.743	1, 0.842	2, 0.770
density(g/cm ³)	,	,	,	,
Absorption	0.289	0.370	0.589	0.530
coefficient(mm ⁻¹)				
F(000)	855	861	1010	870
θ range for data collection (°)	1.464 to 28.249°.	1.471 to 28.159°	1.450 to 28.240°	1.254 to 28.371°.
Limiting indices	-18<=h<=20	-14<=h<=20	-11<=h<=20	-20<=h<=19
-	-21<=k<=21	-19<=k<=19	-21<=k<=20	-8<=k<=20
	-22<=l<=15	-23<=l<=14	-23<=l<=18	-24<=l<=24
Reflections	19658	19883	23659	22314
collected	1 4 5 1 4	15420	1 (00)	1 (0.0.2
ndependent	14714	15439	16824	16003
reflections	[R(int) = 0.1442]	[R(int) = 0.0577]	[R(int) = 0.0397]	[R(int) = 0.0768]
Completeness to θ	91.4 %	95.8 %	97.6 %	
Refinement method	Full-matrix least-	Full-matrix least-	Full-matrix least-	Full-matrix least-
	squares on F ²	squares on F ²	squares on F ²	squares on F ²
Data / restraints /	14714 / 0 / 231	15439 / 0 / 501	16824 / 0 / 513	16003 / 0 / 513
parameters	14/14/0/231	154577 07 501	10024707515	10005707515
Goodness-of-fit on	1.917		1.300	0.836
F ²	1.917	0.734	1.500	0.050
Final R indices	R1 = 0.4089	R1 = 0.0933	R1 = 0.1456	R1 = 0.1016
$[I > 2\sigma(I)]$	wR2 = 0.6100	wR2 = 0.2232	wR2 = 0.3555	wR2 = 0.2376
R indices (all data)	R1 = 0.4768	R1 = 0.1840	R1 = 0.1791	R1 = 0.2061
. /	wR2 = 0.6778	wR2 = 0.2603	wR2 = 0.4066	wR2 = 0.2719
Largest diff. peak	5.440 and -1.294	0.682 and -0.941	4.434 and -2.691	0.727 and -1.297
and hole (e.Å ⁻³)				

Table S6. Crystallographic parameters for Mn@MOF, Co@MOF, Cu@MOF and Zn@MOF.



Figure S14. ¹H NMR spectrum (500 MHz) of 2-iodo-1,3-dimethoxybenzene in CDCl₃.



Figure S15. ¹H NMR spectrum (500 MHz) of 2,2',6,6'-tetramethoxy-1,1'-biphenyl in CDCl₃.



Figure S16. ¹H NMR spectrum (500 MHz) of 3,3',5,5'-tetraiodo-2,2',6,6'-tetramethoxy-1,1'-biphenyl in CDCl₃.



Figure 17. ¹H (500 MHz) and ¹³C NMR (125 MHz) spectra of 3,3',5,5'-tetrakis(*p*-methylphenyl)-2,2',6,6'-tetramethoxy-1,1'-biphenyl in CDCl₃.



Figure 18. ¹H (500 MHz) and ¹³C (125 MHz) NMR spectra of 3.3', 5, 5'-tetrakis(*p*-carboxyphenyl)-2,2',6,6'-tetramethoxy-1,1'-biphenyl in CD₃OD and DMSO-d₆, respectively.