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# A channel-type mesoporous In(III)–carboxylate coordination framework with high physicochemical stability for electrode material of supercapacitor

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#### General materials and methods

With the exception of the organic ligand 4,4',4"-(benzene-1,3,5-triyl-tris(oxy))tribenzoic acid (H<sub>3</sub>BTTB), which was prepared according to the literature method,<sup>S42</sup> all of the starting reagents and solvents were obtained commercially and used as received. Elemental analysis of C, H, and N was performed on a Vario EL III Elementar analyzer. IR spectrum was measured on a Bruker Tensor 27 OPUS FT-IR spectrometer (KBr pellet) in 4000–400 cm<sup>-1</sup> range. Powder X-ray diffraction (PXRD) patterns were recorded on a Bruker D8 Advance diffractometer (Cu-K $\alpha$ ,  $\lambda = 1.5406$  Å) at 40 kV and 100 mA, and the intensity data were recorded by continuous scans in a 2 $\theta/\theta$  mode with a scan speed of 2 s/step and a step size of 0.02°. Simulation of the PXRD patterns was performed by the single-crystal data and diffraction-crystal module of the *Mercury* (Hg) program. Thermogravimetric analysis (TGA) experiments were carried out on a Perkin-Elmer Diamond SII thermal analyzer (from 25 to 800 °C) with a heating rate of 5 °C min<sup>-1</sup> under nitrogen atmosphere. The morphologies of 437-MOF samples with different treatments were characterized by using a JEOL-JSM-7001F field-emission scanning electron microscope (SEM) at an acceleration voltage of 10 kV.

The gas sorption isotherms were collected on a Micromeritics 3Flex surface area and pore size analyzer under ultrahigh vacuum in a clean system, with a diaphragm and turbo pumping system. Ultrahigh-purity-grade (> 99.999%) N<sub>2</sub>, Ar, O<sub>2</sub>, CO<sub>2</sub>, and He gases were applied in all adsorption measurements. The experimental temperatures were maintained by liquid nitrogen (77 K), liquid argon (87 K), and dry ice-acetone baths (195 K).

#### X-ray data collection and structure determination

Single-crystal X-ray diffraction data for 437-MOF, 437-MOF-CH<sub>2</sub>Cl<sub>2</sub> (after solvent-exchange with CH<sub>2</sub>Cl<sub>2</sub> for three times), and 437-MOF-boiling water (after treatment in boiling water for one hour) were collected on an Oxford Xcalibur Gemini Eos diffractometer by using graphite-monochromated Cu-K $\alpha$  radiation ( $\lambda = 1.54178$  Å) at 294(2) K. Multi-scan absorption corrections were performed with the *CrysAlisPro* program.<sup>S43</sup> Empirical absorption corrections were carried out using spherical harmonics, implemented in *SCALE3 ABSPACK* scaling algorithm. The final structures were solved by direct methods, and all non-H atoms were refined anisotropically by full-matrix least-squares method with the SHELXTL software package.<sup>S44</sup> H atoms of the hydroxyl anions were located in the difference maps and then allowed to ride on the parent atoms for refinements [with  $U_{iso}(H) = 1.2U_{eq}(O)$ ]. H atoms of benzene ring were located in calculated sites and treated in the subsequent refinement as riding atoms [C–H = 0.93 Å and  $U_{iso}(H) = 1.2U_{eq}(C)$ ]. Attempts to locate and model the highly disordered solvent molecules (H<sub>2</sub>O, NMF, or CH<sub>2</sub>Cl<sub>2</sub> molecules) in the pores were unsuccessful. Therefore, the SQUEEZE routine, a part of the PLATON package of crystallographic software<sup>S45</sup> was used to calculate the solvent disorder area and remove the diffraction contribution from these solvents to give a set of solvent free diffraction intensity. Crystal data and structural refinement details for 437-MOF, 437-MOF-CH<sub>2</sub>Cl<sub>2</sub>, and 437-MOF-boiling water were listed in Table S3. A comparison of the selected bond parameters was given in Table S4.

#### Formula determination of 437-MOF

According to the result of single crystal X-ray determination, the framework of 437-MOF can be formulated as {[In(BTTB)<sub>2/3</sub>(OH)](solvent)}<sub>n</sub> with Z = 6 in the unit cell. As the highly disorder guest solvents cannot be determined by the current X-ray diffraction data, the identification of these included molecules was further taken by elemental analysis and thermogravimetric analysis (TGA). The TGA curve (see Fig. S1) of 437-MOF indicates that the exclusion of solvent molecules occurs in the temperature range of 25–180 °C, with no further weight loss up to ca. 400 °C. After that, the host framework will be destroyed with ligand decomposition upon heating. Since 437-MOF was prepared in NMF solvent, the excluded solvent molecules should be NMF and/or H<sub>2</sub>O (coming from the starting reagents). Also, according to the result of elemental analyses (observed: C, 40.69%; H, 5.23%; N, 8.50%), the formula of 437-MOF can be determined as {[In(BTTB)<sub>2/3</sub>(OH)](NMF)<sub>5</sub>(H<sub>2</sub>O)<sub>4</sub>}<sub>n</sub> in which the C, H, and N contents (calculated: 40.94%, 5.40%, 8.53%) are well consistent with the observed values. In addition, the observed weight loss of solvents (44.65%) in TGA curve also agrees well with the calculated value (44.73%), which further confirms this formula.

#### Calculation of BET surface area of 437-MOF samples

BET equation: 
$$V = \frac{CVmx}{(1-x)[1+(c-1)x]}$$

where  $x = P/P_0$ , *V* is the volume of gas adsorbed per gram of sample at standard temperature and pressure (STP), *Vm* is the monolayer capacity, and *C* is related to the heat of adsorption.

The equation can be rewritten in the form:

$$\frac{P}{V(P_0 - P)} = \frac{1}{VmC} + \frac{C - 1}{VmC} \times \frac{P}{P_0}$$

The BET analysis was performed by plotting  $P/[V(P_0 - P)]$  vs.  $P/P_0$ . The slope ([C - 1]/VmC) and y intercept (1/VmC) of this linear region give the monolayer capacity. Vm is used to calculate the surface area from  $A = Vm\sigma_0 N_{AV}$ , in which  $\sigma_0$  is the cross-sectional area of the adsorbate at solid or liquid density (16.2 Å<sup>2</sup> for N<sub>2</sub>). Two major criteria were established to aid the choice of pressure range for the BET analysis:<sup>S94</sup> (1) The pressure range selected should have values of  $V(P_0 - P)$  increasing with  $P/P_0$ . (2) The y intercept of the linear region must be positive to yield a meaningful value of the C parameter, which should be greater than zero. A BET surface area was obtained by using the data points on the sorption branch of N<sub>2</sub> isotherm at 77 K in the Micromeritics 3Flex 1.01.01 software package.

#### Pore size distribution of MOFs

Pore size distribution (PSD) data for all 437-MOF samples were determined by analyzing the  $N_2$  isotherms at 77 K using the non-local density functional theory (DFT) and implementing a hybrid kernel based on a zeolite/silica model containing the cylindrical pores, as implemented in the 3Flex 1.01.01 software package.



**Fig. S1** TGA curves of 437-MOF: (black curve) as-synthesized fresh crystal sample and (red curve) crystal sample placed in air overnight.



Scheme S1 Selected trigonal carboxylic ligands derived from trimesic acid.



Fig. S2 A fragment of 437-MOF with the ellipsoids drawn at the 50% probability level.



Fig. S3 View of the local coordination geometry of In(III) in 437-MOF. The BTTB ligands are distinguished by different colors for clarity.



**Fig. S4** Coordination mode of the BTTB ligand (A = -x + 1, -y + 2, z + 1/2; B = -y + 1, x - y + 1, z; C = y - 1, -x + y, z + 1/2; D = x - y + 1, x, z + 1/2, and E = -x + y, -x + 1, z).



Fig. S5 View of the 1-D rod-shaped SBU.



Fig. S6 View of the perpendicular arrangement between the benzene core and the three benzene arms or the attached carboxylates ( $\alpha$  is the dihedral angle between benzene arms and benzene core;  $\beta$  is the dihedral angle between carboxylate groups and benzene core).



**Fig. S7** View of the equilateral triangle constituted by three carboxylate carbon atoms, the centroid of which is just the center of benzene core ( $\gamma$  is the obtuse angle between two adjacent lines linked by the center of benzene core and the carboxylate carbon atom).



**Fig. S8** Strong  $\pi \cdots \pi$  stacking interaction between two parallel benzene cores.



Fig. S9 (top) Stick and (bottom) schematic views of the 1-D organic supramolecular array.



**Fig. S10** The augmented version of two-nodal six-connected 3-D network of 437-MOF. (BTTB and metal nodes are shown by triangular prism and hexagon, respectively).



**Fig. S11** Schematic representation of the (3,4)-connected topological network of 437-MOF, according to the concept of infinite rod-shaped SBUs.



**Fig. S12** Hybrid nanotube-like structure of 437-MOF viewed from different sides (Carbon: grey, Oxygen: red, and Indium: green).

#### Physicochemical stability of 437-MOF

**Thermal stability of 437-MOF.** The as-synthesized sample (ca. 10 mg) was placed inside a pre-weighed 12-mm quartz sample tube and then evacuated upon heating under different conditions for PXRD measurement (see Fig. S13). The final product, upon a long-term heating at 400 °C in vacuum, can be properly indexed to cubic  $In_2O_3$  (JCPDS No. 65-3170).



Fig. S13 PXRD patterns for heat-resistance investigation of 437-MOF.

**Chemical stability of 437-MOF.** The as-synthesized sample (ca. 30 mg) was suspended in 15 mL water and left at room temperature. After immersion, the sample was filtered and dried in air at room temperature for PXRD measurement (see Fig. S14).

The as-synthesized sample (ca. 30 mg) was dispersed into 30 mL water in a vial and then sealed into a Teflon-lined stainless steel vessel, which was heated at 100 °C in an oven. After heating, the sample was cooled down, filtered, and dried in air at room temperature for PXRD measurement (see Fig. S15).

The as-synthesized sample (ca. 10 mg) was suspended in 5 mL common organic solvent,  $H_2O_2$  (30%, aq.), HCl water solution, or NaOH water solution, at ambient temperature for at least 12 hours. Then, the sample was filtered and dried in air at room temperature for PXRD measurement (see Fig. S16 and Fig. S17).



Fig. S14 PXRD patterns of 437-MOF via treating in water at room temperature for various durations from 1 day to 30 days.



Fig. S15 PXRD patterns of 437-MOF via treating in water at 100 °C for various durations from 1 day to 30 days.



Fig. S16 PXRD patterns of 437-MOF via treating in common organic solvents and hydrogen peroxide (aq. 30%) overnight.



Fig. S17 PXRD patterns of 437-MOF via treating in HCl and NaOH water solutions of pH = 1, 3, 5, 9, and 11 for various durations from 1 hour to 7 days.



**(a)** 



**(b)** 

Fig. S18 TGA curves of (a) the as-synthesized 437-MOF, 437-MOF-80, 437-MOF-240, and 437-MOF-360, and (b) the as-synthesized 437-MOF, 437-MOF-boiling water, and 437-MOF-boiling water-3h.



Fig. S19 PXRD patterns of 437-MOF-80 before and after gas sorption.



Fig. S20 PXRD patterns of 437-MOF-240 before and after gas sorption.



Fig. S21 PXRD patterns of 437-MOF-360 before and after gas sorption.



Fig. S22 PXRD patterns of 437-MOF-boiling water before and after gas sorption.



Fig. S23 PXRD patterns of 437-MOF-boiling water-3h before and after gas sorption.



**Fig. S24** Ar sorption isotherms at 87 K for 437-MOFs activated at different conditions (filled/open circles: adsorption/desorption).



**Fig. S25** O<sub>2</sub> sorption isotherms at 77 K for 437-MOFs activated at different conditions (filled/open circles: adsorption/desorption).



**Fig. S26** CO<sub>2</sub> sorption isotherms at 195 K for 437-MOFs activated at different conditions (filled/open circles: adsorption/desorption).

#### Vapor adsorption analyses of 437-MOF

The sorption isotherms of  $H_2O$  and  $C_6H_6$  in vapor state were measured for 437-MOF-80 with Micromeritics 3Flex surface area and pore size analyzer. The temperature was maintained by temperature-programmed water bath (298 K). The adsorption isotherm of water indicates only surface sorption on the material (Fig. S27), while  $C_6H_6$  vapor can be gradually adsorbed onto the sample in the lower pressure. The  $C_6H_6$  uptake will increase as the vapor pressure raises. The adsorption features of  $H_2O$  and  $C_6H_6$  should be attributed to hydrophobization of the pore walls for 1-D channels in 437-MOF.



Fig. S27  $H_2O$  and  $C_6H_6$  adsorption isotherms of 437-MOF-80.

# Table S1 The structural features of reported mesoMOFs.

Publish Time	mesoMOF Code	<i>meso</i> MOF Formula <sup>[a]</sup>	Structural Type	Cavity-/ Channel- diameters (Å) <sup>[b]</sup>	SBUs and/or SBBs	Topology symbol <sup>[c]</sup>	Ref.
2004	MIL-100	$[Cr_{3}F(H_{2}O)_{3}O(\textbf{BTC})_{2}](H_{2}O)_{n}~(n\approx28)$	Cage	$25.0 \times 25.0$ 29.0 × 29.0	Cr <sub>3</sub> O, Super tetrahedron	MTN	S1
2005 2006	MIL-101	$[Cr_{3}F(H_{2}O)_{2}O(\textbf{BDC})_{3}](H_{2}O)_{n}~(n\approx25)$	Cage	$29.0 \times 29.0$ $29.0 \times 29.0$ $34.0 \times 34.0$	Cr <sub>3</sub> O, Super tetrahedron	MTN	S2 S3
2007	N.A. <sup>[d]</sup>	$[Tb_{16}(\textbf{TATB})_{16}(\text{DMA})_{24}](\text{DMA})_{91}(\text{H}_2\text{O})_{108}$	Cage	$\begin{array}{c} {\bf 39.1 \times 39.1} \\ {\bf 47.1 \times 47.1} \end{array}$	Tb₄ cluster, Truncated super tetrahedron	dia	<b>S</b> 4
2008	N.A. <sup>[d]</sup>	$[{\rm Cu}_6{\rm O}({\bf TZI})_3({\rm H_2O})_9({\rm NO}_3)]({\rm H_2O})_{15}$	Cage	$15.9 \times 15.9$ $22.0 \times 22.6$ $23.3 \times 23.3$	Paddle-wheel, Cu <sub>3</sub> O(N <sub>4</sub> CR) <sub>3</sub> , Truncated cuboctahedron	rht	S5
2008	ZIF-95	$[Zn(CBIM)_2]$	Cage	25.1  imes 14.3 30.1  imes 20.0	N.A. <sup>[d]</sup>	poz	S6
2009	ZIF-100 UMCM-2	$[Zn_{20}(CBIM)_{39}(OH)]$ $[Zn_4O(T^2DC)(BTB)_{4/3}]$	Cage	$35.6 \times 35.6$ $14.0 \times 17.0$ $23.9 \times 23.9$ $26.0 \times 32.0$	N.A. <sup><math>[0]</math></sup> Zn <sub>4</sub> O	moz N.A. <sup>[d]</sup>	S7
2000	PCN-61	$[Cu_3(BTEI)(H_2O)_3](DMF)_5(H_2O)_4$	Caga	$13.0 \times 13.0$ $15.0 \times 15.0$ $23.0 \times 23.0$	Paddle-wheel, Cuboctahedron	N.A. <sup>[d]</sup>	ço
2009	PCN-66	[Cu <sub>3</sub> (NTEI)(H <sub>2</sub> O) <sub>3</sub> ](DMA) <sub>21</sub> (H <sub>2</sub> O) <sub>10</sub>	Cage	$13.0 \times 13.0$ $16.0 \times 16.0$ $26.0 \times 26.0$	Paddle-wheel, Cuboctahedron	N.A. <sup>[d]</sup>	50

Publish Time	mesoMOF Code	mesoMOF Formula <sup>[a]</sup>	Structural Type	Cavity-/ Channel- diameters (Å) <sup>[b]</sup>	SBUs and/or SBBs	Topology symbol <sup>[c]</sup>	Ref.
2009	MIL-101-NDC	$[Cr_3(OH)(H_2O)_2(\mu_3-O)(2,6-NDC)_3](guest)$ $(guest = H_2O, EtOH)$	Cage	$39.0 \times 39.0$ $46.0 \times 46.0$	Cr <sub>3</sub> O, Super tetrahedron	MTN	S9
2009	NOTT-112	$[Cu_3({\bf L^1})({\rm H_2O})_3](DMSO)_8(DMF)_{15}({\rm H_2O})_3$	Cage	$13.0 \times 13.0$ $13.9 \times 13.9$ $20.0 \times 20.0$	Paddle-wheel	N.A. <sup>[d]</sup>	S10
2009	DUT-6	$[Zn_4O(2,6\text{-NDC})(\textbf{BTB})_{4/3}](\text{DEF})_{16}(\text{H}_2\text{O})_{9/2}$	Cage	$\begin{array}{c} 25.0\times25.0\\ 30.0\times30.0 \end{array}$	$Zn_4O$	pto	S11
	MOF-180	$[Zn_4O(BTE)_2](DMF)_{14.8}(NMP)_{15.6}$		15.0  imes 23.0	Zn <sub>4</sub> O	qom	
2010	MOF-200	$[Zn_4O(\textbf{BBC})_2(H_2O)_3](DEF)_{29.4}(NMP)_{32.2}$	Cage	$18.0\times28.0$	Zn <sub>4</sub> O	qom	S12
	MOF-210	$[{\rm Zn_4O}({\rm BTE})_{4/3}({\rm BPDC})]({\rm DMF})_{25.7}({\rm NMP})_{24.6}$		26.9  imes 48.3	Zn <sub>4</sub> O	toz	
2010 2010	NOTT-116 PCN-68	$\label{eq:cu_3} \begin{split} & [\mathrm{Cu_3}(\mathbf{PTEI})(\mathrm{H_2O})_3](\mathrm{DMF})_{16}(\mathrm{H_2O})_{26} \\ & [\mathrm{Cu_3}(\mathbf{PTEI})(\mathrm{H_2O})_3](\mathrm{DMF})_{33}(\mathrm{H_2O})_{13} \end{split}$	Cage	$\begin{array}{l} 12.0\times12.0^{[e]}\\ 14.8\times14.8^{[e]}\\ 23.2\times23.2^{[e]} \end{array}$	Paddle-wheel, Cuboctahedra	rht	S13 S14
2010 2010	PCN-610 NU-100	$[{\rm Cu}_3({\rm TTEI})({\rm H_2O})_3]({\rm DMF})_{22}({\rm H_2O})_{19}{}^{[e]}$	Cage	$\begin{array}{c} 12.0\times 12.0^{[e]}\\ 18.6\times 18.6^{[e]}\\ 26.0\times 26.0^{[e]} \end{array}$	Paddle-wheel, Cuboctahedra	rht	S14 S15
2010	PCN-100 PCN-101	$\label{eq:2.1} \begin{split} & [Zn_4O(\textbf{TATAB})_2](DEF)_{17}(H_2O)_3 \\ & [Zn_4O(\textbf{BTATB})_2](DEF)_{16}(H_2O)_5 \end{split}$	Cage	$27.3 \times 27.3$ $27.3 \times 27.3$	Zn <sub>4</sub> O	pyr	S16
2010	N.A. <sup>[d]</sup>	$[({\rm In_3O})({\rm OH})({\rm ADC})_2({\rm IN})_2]({\rm H_2O})_{4.67}$	Cage	9.5 × 33.9	In <sub>3</sub> O(O <sub>2</sub> CR) <sub>6</sub> X <sub>3</sub>	$(3^2.4^{17}.5^7.6^2)$	S17
	JT-1	$[\{Cu_7(OH)_2(\textbf{L}^2)_3\}\{Cu_6(OH)_2(SO_4)_3(S_3O_{10})_2\}](H_2O)_{10}$		23.6  imes 23.6	Cu <sub>6</sub> , Cu <sub>7</sub> cluster	N.A. <sup>[d]</sup>	
2011	JT-2	$\begin{split} & [\{\mathrm{Cu}_7(\mathrm{OH})_2(\mathbf{L}^2)_3\}_2\{\mathrm{Cu}_6(\mathrm{OH})_2(\mathrm{SO}_4)_6(\mathrm{S}_2\mathrm{O}_7)\} \\ & \{\mathrm{Cu}_3(\mathrm{SO}_4)(\mathrm{H}_2\mathrm{O})_6\}](\mathrm{H}_2\mathrm{O})_{18} \end{split}$	Cage	$18.0 \times 18.0$ $23.0 \times 23.0$	Cu <sub>6</sub> , Cu <sub>7</sub> cluster	N.A. <sup>[d]</sup>	S18

Publish Time	mesoMOF Code	<i>meso</i> MOF Formula <sup>[a]</sup>	Structural Type	Cavity-/ Channel- diameters (Å) <sup>[b]</sup>	SBUs and/or SBBs	Topology symbol <sup>[c]</sup>	Ref.
2011 2011	PCN-69 NOTT-119	$\label{eq:cu_3} \begin{split} & [Cu_3(\textbf{BTTI})(H_2O)_3](DMF)_{20}(H_2O)_{16} \\ & [Cu_3(\textbf{BTTI})(H_2O)_3](DMF)_{35}(H_2O)_{35} \end{split}$	Cage	$\begin{array}{c} 13.0 \times 13.0^{[f]} \\ 24.1 \times 24.1^{[f]} \\ 25.0 \times 25.0^{[f]} \end{array}$	Paddle-wheel, Cuboctahedra	ubt	S19 S20
		$[Zn_4O(L^3)_{1.5}]$		$31.0\times31.0$			
2011	N.A. <sup>[d]</sup>	$[Zn_4O(L^4)_{1.5}]$	Cage	$37.4 \times 37.4$	$Zn_4O(CO_2)_6$	cor	S21
		$[Zn_4O(L^5)_{1.5}]$		$38.4 \times 38.4$			
2012	PCN-53	$[Fe_3O(H_2O)_3(\textbf{BTTC})_2](DMF)_{10}$	Cage	$12.5 \times 12.5$ $14.8 \times 14.8$ $22.2 \times 22.2$	[Fe <sub>3</sub> O(O <sub>2</sub> CR) <sub>6</sub> ]	$(4^2.6)_2$ $(4^4.6^4.8^6.10)$	S22
2012	PCN-105	$[Cd_4Na(H_2O)_2(\textbf{HTDBD})_3(\textbf{TDBD})](DMF)_{10}(EtOH)_6(H_2O)_3$	Cage	$\begin{array}{c} 20.0\times 20.0\\ 21.0\times 21.0\end{array}$	Pentanuclear	гео	S23
2012	DUT-25	$[Zn_4O(\textbf{BENZTB})(\textbf{BTB})_{2/3}](\text{DEF})_{16}(\text{H}_2\text{O})_{7/2}$	Cage	$\begin{array}{c} 8.0\times18.0\\ 20.0\times32.0\end{array}$	$[Zn_4O(CO_2)_6]$	nbo	S24
	SUMOF-1-Zn	$[Zn_6(\textbf{BTB})_4(4,4\textbf{'-bpy})_3](\text{solvent})_x$	C	21.0  imes 21.0	Paddle-wheel	pto	625
2012	SUMOF-1-Co	$[Co_6(BTB)_4(4,4'-bpy)_3](solvent)_x$	Cage	21.0  imes 21.0	Paddle-wheel	pto	825
2012	N.A. <sup>[d]</sup>	[Cu <sub>3</sub> (L <sup>6</sup> )]	Cage	$12.0 \times 12.0$ $15.0 \times 15.0$ $23.0 \times 23.0$ $12.0 \times 12.0$	Paddle-wheel	N.A. <sup>[d]</sup>	S26
2012	MIT 142	$[Cu_3(\mathbf{L}')]$	Corre	$15.0 \times 15.0$ $23.0 \times 23.0$ $20.0 \times 20.0$	Cup og totrak adra		527
2013	WIIL-143	$[\text{Fe}_{3}O(\text{CI})(\text{H}_{2}O)_{2}(\textbf{BDC})_{3/2}(\textbf{B1B})](\text{solvent})_{n}$	Cage	24.0  imes 24.0	Super tetrahedra	reo	527
2013	N.A. <sup>[d]</sup>	[(CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> ] <sub>2</sub> [Zn(TATAT) <sub>2/3</sub> ](DMF) <sub>3</sub> (H <sub>2</sub> O)	Cage	21.0  imes 21.0	N.A. <sup>[d]</sup>	N.A. <sup>[d]</sup>	S28

Table	S1 (continued)						
Publish	mesoMOF Code	mesoMOF Formula <sup>[a]</sup>	Structural	Cavity-/ Channel-	SBUs and/or SBBs	Topology	Ref.
Time			Туре	diameters (Å) <sup>[0]</sup>		symbol <sup>[C]</sup>	
	IRMOF-16	[Zn <sub>4</sub> O( <b>TPDC</b> ) <sub>3</sub> ](DEF) <sub>17</sub> (H <sub>2</sub> O) <sub>2</sub>		28.8  imes 28.8			
	IRMOF-14	$[Zn_4O(PDC)_3](DEF)_6(H_2O)_5$		$24.5 \times 24.5$			
2002	IRMOF-12	$[Zn_4O(\textbf{HPDC})_3](DEF)_{10}(H_2O)$	3D Channel	$24.5 \times 24.5$	Zn <sub>4</sub> O	peu	S29
	IRMOF-10	$[Zn_4O(\textbf{BPDC})_3](DEF)_{12}(H_2O)$		$24.5 \times 24.5$			
	IRMOF-8	$[Zn_4O(2,6\text{-NDC})_3](\text{DEF})_6$		$21.4\times21.4$			
2006	MesoMOF-1	$[Cu_{3}(\textbf{TATAB})_{2}(H_{2}O)_{3}](DMF)_{8}(H_{2}O)_{9}$	3D Channel	$22.5\times26.1$	Paddle-wheel, Cuboctahedra	bor	S30
2009	N.A. <sup>[d]</sup>	$[Cu_2({\bf L^8})({\rm H_2O})_2](DMF)_{14}({\rm H_2O})_5$	3D Channel	3.5  imes 21.2	$[Cu_2(O_2CR)_4]$	pts	S31
	CMOF-2a CMOF-3a	$[(R-\mathbf{I}^{9a})_{C1},(H,O),](DME),(H,O),$		$22.0\times15.0$			
				$11.0\times11.0$			
		<b>DF-3a</b> $[(R-L^{10a})Cu_2(H_2O)_2](DEF)_{12}(H_2O)_{16}$		$30.0\times20.0$			
				14.0  imes 14.0			
	CMOF-4a	$[(R-L^{11a})Cu_2(H_2O)_2](DEF)_{10}(DMA)_{14}(H_2O)_5$		$32.0 \times 24.0$			
2010			3D Channel	$19.0 \times 19.0$	Paddle-wheel	$(4^3.6^2.8)$	S32
	CMOF-2b	$[(R-L^{9b})Cu_2(H_2O)_2](DEF)_{11}(H_2O)_3$		22.0 × 15.0			
				$13.0 \times 13.0$			
	CMOF-3b	$[(R\text{-}L^{10b})Cu_2(H_2O)_2](DMF)_{13}({}^iPrOH)_{11}(H_2O)_{4.5}$		$30.0 \times 20.0$			
				$10.0 \times 10.0$			
	CMOF-4b	$[(\textit{R-L}^{11b})Cu_2(H_2O)_2](DEF)_{6.5}(DMF)_{19}(^{i}PrOH)_{8.5}(H_2O)_2$		$32.0 \times 24.0$ 21.0 × 21.0			
	CMOF-2	$[Zn_4(\mu_4-O)(L^{12})_2](DEF)_{22}(H_2O)_4$		$26.0 \times 26.0$			
2010	CMOF-3	$[Zn_4(\mu_4-O)(L^{13})_3](DMF)_{42}$	3D Channel	$20.0 \times 20.0$	Paddle-wheel	pcu	S33
	CMOF-4	$[Zn_4(\mu_4-O)(L^{13})_3](DEF)_{37}(EtOH)_{23}(H_2O)_4$		$32.0 \times 32.0$		1	
2010	Cd-MOF	$[Cd({\bf NH_2BDC})(4,4{}^{\rm t}{\rm -bpy})](DMF)_3({\rm H_2O})_{4.5}$	3D Channel	18.0  imes 23.0	N.A. <sup>[d]</sup>	kag	S34

Publish	SI (commune)		Structural	Cavity-/ Channel-		Topology	
Time	mesoMOF Code	mesoMOF Formula <sup>[a]</sup>	Туре	diameters (Å) <sup>[b]</sup>	SBUs and/or SBBs	symbol <sup>[c]</sup>	Ref.
2012	PCN-222(Fe)	N.A. <sup>[d]</sup>	3D Channel	9.2 × 11.0 37.0 × 37.0	Zr <sub>6</sub> cluster	kag	S35
2012	Bio-MOF-100	$[(CH_3)_2NH_2]_4[Zn_8(\textbf{AD})_4(\textbf{BPDC})_6O_2](DMF)_{49}(H_2O)_{31}$	3D Channel	$28.0\times28.0$	Zinc-adeninate octahedra	les	S36
2013	N.A. <sup>[d]</sup>	$[(CH_3)_2NH_2]_2[ZnNa_2(\mu_2\text{-}H_2O)_2(H_2O)_2(\textbf{TATAT})](DMF)_2$	3D Channel	17.0  imes 23.0	Rod-shaped chain	pts-x	S28
2013	Bio-MOF-101 Bio-MOF-102 Bio-MOF-103	$\begin{split} & [(CH_3)_2NH_2]_2[Zn_8(\textbf{AD})_4(2,6\textbf{-NDC})_6(OH)_2](DMF)_{34}(H_2O)_{13,4} \\ & \\ & [(CH_3)_2NH_2]_2[Zn_8(\textbf{AD})_4(\textbf{ABDC})_6(OH)_2] \\ & \\ & \\ & [(CH_3)_2NH_2]_2[Zn_8(\textbf{AD})_4(\textbf{NH}_2\textbf{-TPDC})_6(OH)_2] \end{split}$	3D Channel	$21.0 \times 21.0$ $28.0 \times 28.0$ $29.0 \times 29.0$	Zinc-adeninate octahedra	lcs	S37
2008	UMCM-1	$Zn_4O(\textbf{BDC})(\textbf{BTB})_{4/3}$	Microcage + 1D Channel	$14.0 \times 17.0$ 27.0 × 32.0	$Zn_4O$	N.A. <sup>[d]</sup>	S38
2013	CYCU-3	[Al(OH)(SDC)]	Multiple 1D Channel	$14.4 \times 14.4$ $28.3 \times 31.1$	Rod-shaped chain	N.A. <sup>[d]</sup>	S39
2007	JUC-48	$[Cd_{3}(\textbf{BPDC})_{3}(DMF)](DMF)_{5}(H_{2}O)_{18}$	1D Channel	24.5  imes 27.9	Rod-shaped chain	etb	S40
2012	IRMOF-74-III IRMOF-74-IV IRMOF-74-V IRMOF-74-VI IRMOF-74-VII IRMOF-74-IX IRMOF-74-XI	N.A. <sup>[d]</sup>	1D Channel	$22.2 \times 27.3$ $28.0 \times 32.8$ $35.2 \times 41.1$ $41.1 \times 49.1$ $49.4 \times 57.5$ $60.5 \times 71.8$ $84.5 \times 98.1$	Rod-shaped chain	etb	S41
	437-MOF	[In(BTTB) <sub>2/3</sub> (OH)](NMF) <sub>5</sub> (H <sub>2</sub> O) <sub>4</sub>	1D Channel	32.3 × 32.3	Concave triangular prism	$(3^{3}.4^{6}.5^{6})_{2}$ $(3^{4}.4^{4}.5^{4}.6^{3})_{3}$	This work

Table S1 (continued)

[a] Abbreviations: BTC = benzene-1,3,5-tricarboxylate; **BDC** = benzene-1,4-dicarboxylate; **TATB** = 4,4',4"-s-trizaine-2,4,6-trivltribenzoate; **TZI** = 5-tetrazolylisophthalate; **CBIM** = 5-chlorobenzimidazolate;  $T^2DC$  = thieno[3,2-b]thiophene-2,5-dicarboxylate; BTB = 4,4',4"-benzene-1,3,5-triyl-tribenzoate; BTEI = 5,5',5"-benzene-1,3,5-triyltris(1-ethynyl-2-isophthalate); NTEI = 5,5',5"-(4,4',4"-nitrilotris(benzene-4,1-diyl)tris(ethyne-2,1-diyl))triisophthalate; 2,6-NDC = 2,6-naphthalenedicarboxylate;  $L^1 = 1,3,5$ -tris(3',5'-dicarboxy[1,1'-biphenyl]-4-yl)benzene; BTE = 4,4',4"-[benzene-1,3,5-triyl-tris(ethyne-2,1-diyl)]tribenzoate; **BBC** = 4,4',4"-(benzene-1,3,5-triyl-tris(benzene-4,1-diyl))tribenzoate; **BPDC =** 4,4'-biphenyldicarboxylate;  $\mathbf{PTEI} = 5,5' \cdot ((5'-(4-((3,5-dicarboxyphenyl)ethynyl)phenyl) - [1,1':3',1''-terphenyl] - 4,4''-diyl) \cdot bis(ethyne-2,1-diyl)) diisophthalate;$ TTEI = 5,5',5"-(((benzene-1,3,5-triyltris(ethyne-2,1-diyl))tris(benzene-4,1-diyl))tris-(ethyne-2,1-diyl))trisophthalate; TATAB = 4,4',4"-s-triazine-1,3,5-triyltri-p-aminobenzoate; **BTATB** = 4,4',4"-(benzene-1,3,5-trivltris(azanediyl))tribenzoate; **ADC** = azobenzene-4,4'-dicarboxylate; **IN** = isonicotinate:  $L^2 = (R) - N.N$ -Bis(3-tert-butyl-5-(4-pyridyl)salicylidene)-3,3'-diamino-5,5',6,6'-tetramethyl-2,2'-methoxymethyl-1,1'-biphenyl; BTTI = 5,5',5"-(benzene-1,3,5-triyl-tris(biphenyl-4,4'-diyl))triisophthalate;  $L^3 = 4,4'-(2,2-bis((4-carboxy-2-methoxyphenoxy)methyl)propane-1,3-diyl)bis(oxy)bis(3-methoxybenzoate);$  $\mathbf{L}^{4} = 3.3' - (4,4' - (2,2-bis((4-(2-carboxyvinyl)-2-methoxyphenoxy)methyl) propane - 1,3-diyl) bis(oxy) bis(3-methoxy-4,1-phenylene)) diacrylate;$  $L^5 = 6,6'-(2,2-bis((6-carboxynaphthalen-2-yloxy)methyl)propane-1,3-diyl)bis(oxy)di-2-naphthoate;$ BTTC = benzo-(1,2;3,4;5,6)-tris(thiophene-2'-carboxylate); H<sub>2</sub>HTDBD = 4,4'-(6-hydroxy-1,3,5-triazine-2,4-diyl)bis(azanediyl)dibenzoic acid; **BENZTB** = N.N.N.N-benzidinetetrabenzoate: 4,4'-**bpy** = 4,4'-bipyridine;  $L^6 = N, N, N''$ -tris(isophthalyl)-4,4',4''-benzene-1,3,5-triyl-tribenzamide;

 $\mathbf{L}^7 = N_i N_i N''$ -tris(isophthalyl)-4,4',4''-s-triazine-2,4,6-triyl-tribenzamide;

**TATAT** = 5,5',5"-(1,3,5-triazine-2,4,6-triyl)tris(azanediyl)triisophthalate;

**TPDC** = *p*-terphenyl-4,4"-dicarboxylate;

**PDC** = 2,7-pyrenedicarboxylate;

**HPDC** = 2,7-tetrahydropyrenedicarboxylate;

**L**<sup>8</sup> = methanetetra(biphenyl-*p*-carboxylate);

 $L^{9a} = (R) - (2E, 2'E, 2''E, 2'''E) - 3, 3', 3'' - (2, 2'-diethoxy - 1, 1'-binaphthyl - 4, 4', 6, 6'-tetrayl) tetraacrylate;$ 

 $\mathbf{L}^{10a} = (R)-2,2'$ -diethyoxy-1,1'-binaphthyl-4,4',6,6'-tetrakis(4-benzoate);

 $\mathbf{L}^{11a} = (R) - 4, 4', 4'' - (1E, 1'E, 1''E, 1''E) - 2, 2', 2'' - (2, 2' - diethoxy - 1, 1' - binaphthyl - 4, 4', 6, 6' - tetrayl) tetrakis (ethene - 2, 1 - diyl) tetraken zoate;$ 

 $\mathbf{L}^{9b} = (R) - (2E, 2'E, 2''E, 2'''E) - 3, 3', 3'', 3''' - (2, 2'-dihydroxy - 1, 1'-binaphthyl - 4, 4', 6, 6'-tetrayl) tetraacrylate;$ 

 $\mathbf{L}^{10b} = (R)-2,2'-dihydroxy-1,1'-dinaphthyl-4,4',6,6'-tetrakis(4-benzoate);$ 

 $\mathbf{L}^{11b} = (R) - 4, 4', 4'', 4''' - (1E, 1'E, 1''E) - 2, 2', 2'', 2''' - (2, 2' - dihydroxy - 1, 1' - binaphthyl - 4, 4', 6, 6' - tetrayl) tetrakis (ethene - 2, 1 - diyl) tetraken zoate;$ 

 $L^{12} = (R,R)-(-)-N,N$ -Bis(3-carboxyl-5-*tert*-butylsalicylidene)-1,2-cyclohexanediamino manganese (III) chloride;

 $\mathbf{L^{13}} = (2E, 2'E) - 3, 3' - (5, 5' - (1E, 1'E) - (1R, 2R) - \text{cyclohexane} - 1, 2 - \text{diylbis}(\text{azan} - 1 - \text{yl} - 1 - \text{ylidene}) \text{bis}(3 - tert - \text{butyl} - 4 - \text{hydroxy} - 5, 1 - \text{phenylene})) \text{diacrylic acid manganese (III)} \\ \text{chloride;}$ 

**NH<sub>2</sub>BDC** = 2-amino-1,4-benzenedicarboxylate;

AD = Adenine;

**ABDC** = 4,4'-azobenzenedicarboxylate;

NH<sub>2</sub>-TPDC = 2'-amino-1,1':4,1"-terphenyl-4,4"-dicarboxylate;

**SDC** = 4,4'-stilbenedicarboxylate;

**BTTB** = 4,4',4"-(benzene-1,3,5-triyl-tris(oxy))tribenzoate;

 $DEF = N_{N}$ -diethylformamide;

DMF = N, N-dimethylformamide;

DMA = N, N-dimethylacetamide;

NMP = *N*-methyl-2-pyrrolidinone;

DMSO = dimethyl sulfoxide;

NMF = *N*-methylformamide;

[b] Data from refs (for comparative analysis, all of the parameters are only worth reporting to one decimal place);

[c] Topological symbols from ref.;

[d] N.A. = Not Available;

[e] Data from ref. S14;

[f] Data from ref. S20.

Publish Time	mesoMOF Code	<i>meso</i> MOF Formula <sup>[a]</sup>	Structural Type	BET Surface Area (m <sup>2</sup> g <sup>-1</sup> )	Langmuir Surface Area (m <sup>2</sup> g <sup>-1</sup> )	Pore Volume (cm <sup>3</sup> g <sup>-1</sup> )	T <sub>max</sub> of Thermal Stability <sup>[b]</sup>	Activated T <sub>max</sub> for Sorption	Ref.
2004	MIL-100	$[Cr_{3}F(H_{2}O)_{3}O(\textbf{BTC})_{2}](H_{2}O)_{n}~(n\approx28)$	Cage	N.A. <sup>[c]</sup>	3100	1.16	~275 °C <sup>[b]</sup>	N.A. <sup>[c]</sup>	S1
2005 2006	MIL-101	$[Cr_{3}F(H_{2}O)_{2}O(\textbf{BDC})_{3}](H_{2}O)_{n}~(n\approx25)$	Cage	4100 <sup>[d]</sup>	4500~5500 <sup>[d]</sup> 4000/5500 <sup>[e]</sup>	2.0 <sup>[d]</sup>	~275 °C <sup>[b]</sup>	100 °С 200 °С	S2 S3
2007	N.A. <sup>[c]</sup>	$[(Tb_{16}(\textbf{TATB})_{16}(DMA)_{24}](DMA)_{91}(H_2O)_{108}$	Cage	1419 /1783	2887 /3855	0.98 /1.29	~320 °C <sup>[b]</sup>	80 °C /160 °C	S4
2008	<b>N.A.</b> <sup>[c]</sup>	$[{\rm Cu}_6{\rm O}({\bf TZI})_3({\rm H}_2{\rm O})_9({\rm NO}_3)]({\rm H}_2{\rm O})_{15}$	Cage	2847	3223	1.01	N.A. <sup>[c]</sup>	85 °C	S5
2008	ZIF-95 ZIF-100	[Zn( <b>CBIM</b> ) <sub>2</sub> ] [Zn <sub>20</sub> ( <b>CBIM</b> ) <sub>39</sub> (OH)]	Cage	1050 595	1240 780	0.43 0.37	~500 °C <sup>[b]</sup>	100 °C	S6
2009	UMCM-2	$[Zn_4O(T^2DC)(BTB)_{4/3}]$	Cage	5200	6060	N.A. <sup>[c]</sup>	~400 °C <sup>[b]</sup>	300 °C	<b>S</b> 7
2009	PCN-61 PCN-66	$\label{eq:cu_3} \begin{split} & [{\rm Cu}_3(\textbf{BTEI})({\rm H_2O})_3]({\rm DMF})_5({\rm H_2O})_4 \\ & [{\rm Cu}_3(\textbf{NTEI})({\rm H_2O})_3]({\rm DMA})_{21}({\rm H_2O})_{10} \end{split}$	Cage	3000 4000	3500 4600	1.36 1.63	< 300°C <sup>[b]</sup> < 200°C <sup>[b]</sup>	150 °С 150 °С	S8
2009	MIL-101-NDC	$[Cr_3(OH)(H_2O)_2(\mu_3-O)(2,6-NDC)_3](guest)$ $(guest = H_2O, EtOH)$	Cage	2100 <sup>[f]</sup> /1100 <sup>[g]</sup>	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	~260 °C <sup>[b]</sup>	160 °C	S9
2009	NOTT-112	$[Cu_3({\bf L}^1)({\rm H_2O})_3](DMSO)_8(DMF)_{15}({\rm H_2O})_3$	Cage	3800	N.A. <sup>[c]</sup>	1.62 <sup>[h]</sup> /1.69 <sup>[i]</sup>	~350 °C <sup>[b]</sup>	115 °C	S10
2009	DUT-6	$[Zn_4O(2,6\text{-NDC})(\textbf{BTB})_{4/3}](\text{DEF})_{16}(H_2O)_{9/2}$	Cage	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	2.02	380 °C	30 °C	S11
2010	MOF-180 MOF-200 MOF-210	$\begin{split} & [Zn_4O(\textbf{BTE})_2](DMF)_{14.8}(NMP)_{15.6} \\ & [Zn_4O(\textbf{BBC})_2(H_2O)_3](DEF)_{29.4}(NMP)_{33.2} \\ & [Zn_4O(\textbf{BTE})_{4/3}(\textbf{BPDC})](DMF)_{25.7}(NMP)_{24.6} \end{split}$	Cage	N.A. <sup>[c]</sup> 4530 6240	N.A. <sup>[c]</sup> 10400 10400	N.A. <sup>[c]</sup> 3.59 3.60	~350 °C <sup>[b]</sup> ~350 °C <sup>[b]</sup> ~360 °C <sup>[b]</sup>	N.A. <sup>[c]</sup> SCD <sup>[j]</sup> , 40 °C SCD <sup>[j]</sup> , 40 °C	S12

# **Table S2** The adsorption information and thermal stability of reported mesoMOFs.

Publish Time	mesoMOF Code	<i>meso</i> MOF Formula <sup>[a]</sup>	Structural Type	BET Surface Area (m <sup>2</sup> g <sup>-1</sup> )	Langmuir Surface Area (m <sup>2</sup> g <sup>-1</sup> )	Pore Volume (cm <sup>3</sup> g <sup>-1</sup> )	T <sub>max</sub> of Thermal Stability <sup>[b]</sup>	Activated T <sub>max</sub> for Sorption	Ref.
2010	NOTT-116	$[Cu_3(PTEI)(H_2O)_3](DMF)_{16}(H_2O)_{26}$	Cara	4664	N.A. <sup>[c]</sup>	2.17	~300 °C <sup>[b]</sup>	100 °C	S13
2010	PCN-68	$[Cu_3(\textbf{PTEI})(H_2O)_3](DMF)_{33}(H_2O)_{13}$	Cage	5109	6033	2.13	~275 °C <sup>[b]</sup>	100 °C	S14
2010	PCN-610	$[Cu_{3}(TTEI)(H_{2}O)_{3}](DMF)_{22}(H_{2}O)_{19}{}^{[e]}$	Cara	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	~320 °C <sup>[b]</sup>	N.A. <sup>[c]</sup>	S14
2010	NU-100	N.A. <sup>[c]</sup>	Cage	6143	N.A. <sup>[c]</sup>	2.82	~325 °C <sup>[b]</sup>	SCD <sup>[j]</sup> , 110 ℃	S15
2010	PCN-100	$[Zn_4O(\textbf{TATAB})_2](DEF)_{17}(H_2O)_3$	Cara	N.A. <sup>[c]</sup>	860	0.58	~150 °C <sup>[b]</sup>	R.T. <sup>[k]</sup>	\$16
2010	PCN-101	$[Zn_4O(\textbf{BTATB})_2](DEF)_{16}(H_2O)_5$	Cage	N.A. <sup>[c]</sup>	1140	0.75	~180 °C <sup>[b]</sup>	R.T. <sup>[k]</sup>	510
2010	N.A. <sup>[c]</sup>	$[(In_3O)(OH)(ADC)_2(IN)_2](H_2O)_{4.67}$	Cage	1857	1496	N.A. <sup>[c]</sup>	~350 °C <sup>[b]</sup>	100 °C	S17
	JT-1	$[\{\mathrm{Cu}_7(\mathrm{OH})_2(\mathbf{L^2})_3\}\{\mathrm{Cu}_6(\mathrm{OH})_2(\mathrm{SO}_4)_3(\mathrm{S_3O_{10}})_2\}](\mathrm{H_2O})_{10}$		375	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	~200 °C <sup>[b]</sup>	N.A. <sup>[c]</sup>	
2011	JT-2	$\begin{split} & [\{Cu_7(OH)_2(L^2)_3\}_2\{Cu_6(OH)_2(SO_4)_6(S_2O_7)\} \\ & \{Cu_3(SO_4)(H_2O)_6\}](H_2O)_{18} \end{split}$	Cage	421	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	~200 °C <sup>[b]</sup>	N.A. <sup>[c]</sup>	S18
2011	PCN-69	$[Cu_3(BTTI)(H_2O)_3](DMF)_{20}(H_2O)_{16}$	C	3989	6278	2.17	~280 °C <sup>[b]</sup>	100 °C	S19
2011	NOTT-119	$[Cu_3(BTTI)(H_2O)_3](DMF)_{35}(H_2O)_{35}$	Cage	4118	N.A. <sup>[c]</sup>	2.35	315 °C <sup>[b]</sup>	110 °C	S20
2011	N.A. <sup>[c]</sup>	$\begin{split} & [Zn_4O(\mathbf{L}^3)_{1.5}] \\ & [Zn_4O(\mathbf{L}^4)_{1.5}] \\ & [Zn_4O(\mathbf{L}^5)_{1.5}] \end{split}$	Cage	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	~370 °C <sup>[b]</sup> ~380 °C <sup>[b]</sup> ~360 °C <sup>[b]</sup>	R.T. <sup>[k]</sup>	S21
2012	PCN-53	$[Fe_3O(\mathrm{H_2O})_3(\textbf{BTTC})_2](\mathrm{DMF})_{10}$	Cage	2817	N.A. <sup>[c]</sup>	1.57	~200 °C <sup>[b]</sup>	120 °C	S22
2012	PCN-105	$[Cd_4Na(H_2O)_2(\textbf{HTDBD})_3(\textbf{TDBD})](DMF)_{10}(EtOH)_6(H_2O)_3$	Cage	1067	1317	N.A. <sup>[c]</sup>	~350 °C <sup>[b]</sup>	60 °C	S23
2012	DUT-25	$[Zn_4O(\textbf{BENZTB})(\textbf{BTB})_{2/3}](DEF)_{16}(H_2O)_{7/2}$	Cage	4670	N.A. <sup>[c]</sup>	2.22	$\sim 350 \ ^{\circ}\mathrm{C}^{[b]}$	SCD <sup>[j]</sup> , 30 °C	S24
2012	SUMOF-1-Zn SUMOF-1-Co	$[Zn_{6}(\mathbf{BTB})_{4}(4,4'-\mathbf{bpy})_{3}](solvent)_{x}$ $[Co_{6}(\mathbf{BTB})_{4}(4,4'-\mathbf{bpy})_{3}](solvent)_{x}$	Cage	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	~260 °C <sup>[b]</sup> ~350 °C <sup>[b]</sup>	N.A. <sup>[c]</sup>	S25

Table S2 (continued)

Publish Time	mesoMOF Code	<i>meso</i> MOF Formula <sup>[a]</sup>	Structural Type	BET Surface Area (m <sup>2</sup> g <sup>-1</sup> )	Langmuir Surface Area (m <sup>2</sup> g <sup>-1</sup> )	Pore Volume (cm <sup>3</sup> g <sup>-1</sup> )	T <sub>max</sub> of Thermal Stability <sup>[b]</sup>	Activated T <sub>max</sub> for Sorption	Ref.
2012	N.A. <sup>[c]</sup>	$[\operatorname{Cu}_3(\mathbf{L}^6)]$	Cage	3288	N.A. <sup>[c]</sup>	1.77	~125 °C <sup>[b]</sup>	100 °C	S26
2013	MIL-143	[Cu <sub>3</sub> (L <sup>-</sup> )] [Fe <sub>3</sub> O(Cl <sup>-</sup> )(H <sub>2</sub> O) <sub>2</sub> ( <b>BDC</b> ) <sub>3/2</sub> ( <b>BTB</b> )](solvent) <sub>n</sub>	Cage	3360 2150	N.A. <sup>[*]</sup> N.A. <sup>[¢]</sup>	1.91	~125 °C <sup>[-]</sup>	100 °C 100 °C	S27
2013	N.A. <sup>[c]</sup>	$[(CH_3)_2NH_2]_2[Zn(TATAT)_{2/3}](DMF)_3(H_2O)$	Cage	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	S28
2002	IRMOF-16 IRMOF-14 IRMOF-12 IRMOF-10 IRMOF-8	$\begin{split} & [Zn_4O(\textbf{TPDC})_3](\text{DEF})_{17}(\text{H}_2\text{O})_2 \\ & [Zn_4O(\textbf{PDC})_3](\text{DEF})_6(\text{H}_2\text{O})_5 \\ & [Zn_4O(\textbf{HPDC})_3](\text{DEF})_{10}(\text{H}_2\text{O}) \\ & [Zn_4O(\textbf{BPDC})_3](\text{DEF})_{12}(\text{H}_2\text{O}) \\ & [Zn_4O(2,6\textbf{-NDC})_3](\text{DEF})_6 \end{split}$	3D Channel	N.A. <sup>[c]</sup> N.A. <sup>[c]</sup> N.A. <sup>[c]</sup> N.A. <sup>[c]</sup> N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup> 1936 1750 N.A. <sup>[c]</sup> N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup> 0.69 0.61 N.A. <sup>[c]</sup> N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup> 150 °C 150 °C N.A. <sup>[c]</sup> N.A. <sup>[c]</sup>	S29
2006	mesoMOF-1	$[\mathrm{Cu}_3(\mathbf{TATAB})_2(\mathrm{H_2O})_3](\mathrm{DMF})_8(\mathrm{H_2O})_9$	3D Channel	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	~180 °C <sup>[b]</sup>	80 °C	S30
2009	N.A. <sup>[c]</sup>	$[Cu_2({\bm L^{\bm 8}})(H_2O)_2](DMF)_{14}(H_2O)_5$	3D Channel	1020	1127	N.A. <sup>[c]</sup>	~260 °C <sup>[b]</sup>	Freeze-Dried Method	S31
2010	CMOF-2a CMOF-3a CMOF-4a CMOF-2b CMOF-3b CMOF-3b	$\begin{split} & [(R-\mathbf{L}^{9a})\mathrm{Cu}_2(\mathrm{H}_2\mathrm{O})_2](\mathrm{DMF})_{15}(\mathrm{H}_2\mathrm{O})_{11} \\ & [(R-\mathbf{L}^{10a})\mathrm{Cu}_2(\mathrm{H}_2\mathrm{O})_2](\mathrm{DEF})_{12}(\mathrm{H}_2\mathrm{O})_{16} \\ & [(R-\mathbf{L}^{11a})\mathrm{Cu}_2(\mathrm{H}_2\mathrm{O})_2](\mathrm{DEF})_{10}(\mathrm{DMA})_{14}(\mathrm{H}_2\mathrm{O})_5 \\ & [(R-\mathbf{L}^{9b})\mathrm{Cu}_2(\mathrm{H}_2\mathrm{O})_2](\mathrm{DEF})_{11}(\mathrm{H}_2\mathrm{O})_3 \\ & [(R-\mathbf{L}^{10b})\mathrm{Cu}_2(\mathrm{H}_2\mathrm{O})_2](\mathrm{DMF})_{13}({}^{l}\mathrm{PrOH})_{11}(\mathrm{H}_2\mathrm{O})_{4.5} \\ & [(R-\mathbf{L}^{11b})\mathrm{Cu}_2(\mathrm{H}_2\mathrm{O})_2](\mathrm{DEF})_{6.5}(\mathrm{DMF})_{19}({}^{l}\mathrm{PrOH})_{8.5}(\mathrm{H}_2\mathrm{O})_2 \end{split}$	3D Channel	0 ~240 0 0 0 0	N.A. <sup>[c]</sup>	N.A. <sup>[¢]</sup>	~200 °C <sup>[b]</sup> ~260 °C <sup>[b]</sup> ~260 °C <sup>[b]</sup> ~200 °C <sup>[b]</sup> ~260 °C <sup>[b]</sup> ~250 °C <sup>[b]</sup>	N.A. <sup>[c]</sup>	S32
2010	CMOF-2 CMOF-3 CMOF-4	$\begin{split} & [Zn_4(\mu_4\text{-}O)(\textbf{L^{12}})_3](DEF)_{22}(H_2O)_4 \\ & [Zn_4(\mu_4\text{-}O)(\textbf{L^{13}})_3](DMF)_{42} \\ & [Zn_4(\mu_4\text{-}O)(\textbf{L^{13}})_3](DEF)_{37}(EtOH)_{23}(H_2O)_4 \end{split}$	3D Channel	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	~200 °C <sup>[b]</sup> ~250 °C <sup>[b]</sup> ~250 °C <sup>[b]</sup>	N.A. <sup>[c]</sup>	S33

Table S2 (continued)

T 11 CA	/ .• <b>*</b>
Table S2	(continued)

Publish Time	mesoMOF Code	<i>meso</i> MOF Formula <sup>[a]</sup>	Structural Type	BET Surface Area (m <sup>2</sup> g <sup>-1</sup> )	Langmuir Surface Area (m <sup>2</sup> g <sup>-1</sup> )	Pore Volume (cm <sup>3</sup> g <sup>-1</sup> )	T <sub>max</sub> of Thermal Stability <sup>[b]</sup>	Activated T <sub>max</sub> for Sorption	Ref.
2010	Cd-MOF	$[Cd(NH_2BDC)(4,4'-bpy)](DMF)_3(H_2O)_{4.5}$	3D Channel	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	~240 °C <sup>[b]</sup>	N.A. <sup>[c]</sup>	S34
2012	PCN-222(Fe)	N.A. <sup>[c]</sup>	3D Channel	2200	N.A. <sup>[c]</sup>	1.56	~370 °C <sup>[b]</sup>	120 °C	S35
2012	Bio-MOF-100	$[(CH_3)_2NH_2]_4[Zn_8(\textbf{AD})_4(\textbf{BPDC})_6O_2](DMF)_{49}(H_2O)_{31}$	3D Channel	4300	N.A. <sup>[c]</sup>	4.3	~350 °C <sup>[b]</sup>	SCD <sup>[j]</sup> , 100 °C	S36
2013	N.A. <sup>[c]</sup>	$[(CH_3)_2NH_2]_2[ZnNa_2(\mu_2\text{-}H_2O)_2(H_2O)_2(\textbf{TATAT})](DMF)_2$	3D Channel	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	~350 °C <sup>[b]</sup>	N.A. <sup>[c]</sup>	S28
	Bio-MOF-101	$[(CH_3)_2NH_2]_2[Zn_8(AD)_4(2,6-NDC)_6(OH)_2](DMF)_{34}(H_2O)_{13.4}$		4410	N.A. <sup>[c]</sup>	2.83	N.A. <sup>[c]</sup>		
2013	Bio-MOF-102	$[(CH_3)_2NH_2]_2[Zn_8(AD)_4(ABDC)_6(OH)_2]$	3D Channel	3222	N.A. <sup>[c]</sup>	4.36	N.A. <sup>[c]</sup>	SCD <sup>[j]</sup> , R.T. <sup>[k]</sup>	S37
	Bio-MOF-103	$[(\mathrm{CH}_3)_2\mathrm{NH}_2]_2[\mathrm{Zn}_8(\mathbf{AD})_4(\mathbf{NH}_2\text{-}\mathbf{TPDC})_6(\mathrm{OH})_2]$		2704	N.A. <sup>[c]</sup>	4.13	N.A. <sup>[c]</sup>		
2008	UMCM-1	$[Zn_4O(\textbf{BDC})(\textbf{BTB})_{4/3}]$	Microcage+ 1D Channel	4160	6500	N.A. <sup>[c]</sup>	~400 °C <sup>[b]</sup>	R.T. <sup>[k]</sup>	S38
2013	CYCU-3	[Al(OH)(SDC)]	Multiple 1D Channel	2757	3884	1.39	~300 °C <sup>[b]</sup>	150 °C	S39
2007	JUC-48	$[{\rm Cd}_3({\rm BPDC})_3({\rm DMF})]({\rm DMF})_5({\rm H_2O})_{18}$	1D Channel	629	880	0.19	~380 °C <sup>[b]</sup>	<b>R.T.</b> <sup>[k]</sup>	S40
	IRMOF-74-III			2440	3750	1.23			
	IRMOF-74-IV			2480	5370	1.60			
	IRMOF-74-V			2230	6940	1.89			
2012	IRMOF-74-VI	N.A. <sup>[c]</sup>	1D Channel	1600	5880	1.65	$< 300 \ ^{\circ}C^{[b]}$	130 °C	S41
	IRMOF-74-VII			1800	8320	2.12			
	IRMOF-74-IX			1920	9410	2.51			
	IRMOF-74-XI			1760	9880	3.41			

Table S	Table S2 (continued)								
Publish Time	mesoMOF Code	mesoMOF Formula <sup>[a]</sup>	Structural Type	BET Surface Area (m <sup>2</sup> g <sup>-1</sup> )	Langmuir Surface Area (m <sup>2</sup> g <sup>-1</sup> )	Pore Volume (cm <sup>3</sup> g <sup>-1</sup> )	T <sub>max</sub> of Thermal Stability <sup>[b]</sup>	Activated T <sub>max</sub> for Sorption	Ref.
	437-MOF	[In(BTTB) <sub>2/3</sub> (OH)](NMF) <sub>5</sub> (H <sub>2</sub> O) <sub>4</sub>	1D Channel	2379	N.A. <sup>[c]</sup>	1.11	Over 400°C <sup>[1]</sup>	360 °C	This work
[a] Abbr	eviations: see the footnote of	of Table S1;							
[b] Date from TGA curves;									
[c] N.A. = Not Available;									
[d] Data	from ref. S2;								
[e] Data	from ref. S3;								
[f] Based	on the activated samples;								
[g] Based	l on the as-synthesized sam	ples;							
<b>[h]</b> Data from $N_2$ isotherm;									
[i] Data from Ar isotherm;									
[j] SCD = Supercritical Carbon Dioxide;									
[k] R.T. = Room Temperature;									
[I] Data f	rom the long-term heating t	reatment (at least 3h) under vacuum (< 10 <sup>-3</sup> To	rr at least).						

	437-MOF	437-MOF-CH <sub>2</sub> Cl <sub>2</sub>	437-MOF-boiling water
Empirical formula	$C_{18}H_{11}O_7In$	C <sub>18</sub> H <sub>11</sub> O <sub>7</sub> In	C <sub>18</sub> H <sub>11</sub> O <sub>7</sub> In
Formula weight	454.09	454.09	454.09
Crystal system	Hexagonal	Hexagonal	Hexagonal
Space group	P6 <sub>3</sub> /mcm	P6 <sub>3</sub> /mcm	P6 <sub>3</sub> /mcm
Crystal size (mm <sup>3</sup> )	$0.28 \times 0.10 \times 0.09$	$0.22 \times 0.11 \times 0.10$	0.24×0.12×0.10
<i>a</i> (Å)	32.3006(7)	32.182(2)	32.2297(13)
<i>b</i> (Å)	32.3006(7)	32.182(2)	32.2297(13)
<i>c</i> (Å)	7.2707(2)	7.2741(4)	7.2618(4)
Volume (Å <sup>3</sup> )	6569.4(3)	6524.5(7)	6532.6(5)
Ζ	6	6	6
$D (\text{g cm}^{-3})$	0.689	0.693	0.693
$\mu (\mathrm{mm}^{-1})$	4.453	4.483	4.478
F (000)	1344	1344	1344
R <sub>int</sub>	0.1070	0.0763	0.1032
Goodness-of-fit on $F^2$	1.138	1.299	1.039
$R_1^{a} / w R_2^{b} [I > 2\sigma(I)]$	0.0936 / 0.1934	0.1676 / 0.4097	0.1063 / 0.2962
$R_1^a / w R_2^b$ (all data)	0.1109 / 0.2003	0.2002 / 0.4309	0.1687 / 0.3410
CCDC number	952936	952937	952938

Table S3	Crystallog	graphic dat	a and struct	ure refinement	details for	r 437-MOFs.
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 ${}^{a}R_{1} = \Sigma ||F_{0}| - |F_{c}|| \Sigma |F_{0}|. {}^{b}wR_{2} = |\Sigma w(|F_{0}|^{2} - |F_{c}|^{2})| \Sigma |w(F_{0})^{2}|^{1/2}, \text{ where } w = 1/[\sigma^{2}(F_{0}^{2}) + (aP)^{2} + bP]. P = (F_{0}^{2} + 2F_{c}^{2})/3.$ 

	437-MOF	437-MOF-CH <sub>2</sub> Cl <sub>2</sub>	437-MOF-boiling water
In1–O1	2.167(5)	2.152(17)	2.153(5)
In1–O2	2.075(6)	2.115(13)	2.085(6)
O1–In1–O2	90.3(2)	89.9(5)	90.2(2)
O1–In1–O1 <sup>#1</sup>	94.7(3)	97.7(10)	94.6(3)

Table S4 Comparison of the selected bond lengths (Å) and angles (°) for 437-MOFs.<sup>*a*</sup>

<sup>*a*</sup> Symmetry code: #1 = x - y + 1, -y + 2, z.

Trigonal ligands	α, β,	andγ(°)ª	Ref.
соон			
			S7
<u> </u>	$(a_1, a_2, a_3)$ :	0~83.5°	S12
	$(\beta_1, \beta_2, \beta_3)$ :	0~81.3°	S24 S25
ноос соон	( <b>y</b> <sub>1</sub> , <b>y</b> <sub>2</sub> , <b>y</b> <sub>3</sub> ):	118.7~123.9°	S38
H₃BTB			S46–S88
соон			
	$(\alpha_1, \alpha_2, \alpha_3)$ :	0.5~4.8°	
	$(\beta_1, \beta_2, \beta_3)$ :	<b>2.1~4.1°</b>	S89–S91
ноос	$(\gamma_1, \gamma_2, \gamma_3)$ :	119.2~119.9°	
H <sub>3</sub> TATB			
соон			
	$(a_1, a_2, a_3)$ :	4.2~20.6°	\$12
	$(\beta_1, \beta_2, \beta_3)$ :	12.6~22.6°	S57
	( <b>y</b> <sub>1</sub> , <b>y</b> <sub>2</sub> , <b>y</b> <sub>3</sub> ):	110.6~123.1°	S92
ноос соон			
$H_3BTE$			
соон			
$\square$			
$\bigcirc$	$(\alpha_1, \alpha_2, \alpha_3)$ :	2.1~83.5°	S12
	$(\beta_1, \beta_2, \beta_3)$ :	4.9~81.3°	S51
ноос	$(\gamma_1, \gamma_2, \gamma_3)$ :	111.9~123.9°	S93
H3BBC			

 Table S5 Structural features of the reported trigonal carboxylate ligands.<sup>a</sup>



<sup>*a*</sup> For definitions of  $\alpha$ ,  $\beta$ , and  $\gamma$ , please refer to the captions for Fig. S6 and Fig. S7.

Sample	$N_2$ uptake (STP cm <sup>3</sup> g <sup>-1</sup> ) <sup><i>a</i></sup>	BET surface area $(m^2 g^{-1})^b$	Pore volume $(\text{cm}^3 \text{ g}^{-1})^c$
437-MOF-80	596	1576	0.92
437-MOF-240	646	1791	1.00
437-MOF-360	600	1533	0.93
437-MOF-boiling water	723	2379	1.11
437-MOF-boiling water-3h	576	1037	0.88

Table S6 Sorption parameters of 437-MOF samples from  $N_2$  isotherms.

<sup>*a*</sup> The maximum uptake. <sup>*b*</sup> Calculated using  $N_2$  adsorption data in the relative pressure ranging from 0.12 to 0.17. <sup>*c*</sup> Calculated by single point method from the amount of  $N_2$  adsorb at maximum relative pressure.

Table S7 Sorpt	ion parameters	of 437-MOF	samples from	Ar, $O_2$ , and	$CO_2$ isotherms.
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Sample	Ar Uptake	O <sub>2</sub> Uptake	CO <sub>2</sub> Uptake
	$(\text{STP cm}^3 \text{g}^{-1})^a$	$(\text{STP cm}^3 \text{g}^{-1})^a$	$(\text{STP cm}^3 \text{ g}^{-1})^a$
437-MOF-80	704	728	421
437-MOF-240	734	722	454
437-MOF-360	684	690	359
437-MOF-boiling water	788	803	607
437-MOF-boiling water-3h	598	689	285

<sup>*a*</sup> The maximum uptake.

Publish Time	MOF Code	MOF Formula <sup>[a]</sup>	Pore Level	BET Surface Area (m <sup>2</sup> g <sup>-1</sup> )	Langmuir Surface Area (m <sup>2</sup> g <sup>-1</sup> )	Pore Volume (cm <sup>3</sup> g <sup>-1</sup> )	Accessible Void	T <sub>max</sub> of Thermal Stability <sup>[b]</sup>	Activated T <sub>max</sub> for Sorption	Ref.
2002	QMOF-2	$[InH(BDC)_2]$	Micro-	190	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	~270 °C <sup>[b]</sup>	N.A. <sup>[c]</sup>	S95
2006	Na <sup>+</sup> -exchanged <i>rho</i> -ZMOF	$ Na^{^{+}}_{48}(H_2O)_{282} [In_{48}(\textbf{HImDC})_{96}]$	Micro-	N.A. <sup>[c]</sup>	1067	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	105 °C	S96
2007	N.A. <sup>[c]</sup>	$[{\rm In_3O}({\bf L^1})_{1.5}({\rm H_2O})_3]({\rm H_2O})_3({\rm NO}_3)$	Micro-	N.A. <sup>[c]</sup>	1417	0.50	57.2 %	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	S97
2008	usf-ZMOF	$\begin{array}{c} [{\rm In}_5({\bf HImDC})_{10}](1,2\text{-}H_2{\bf DACH})_{2.5} \\ ({\rm DMF})_3({\rm CH}_3{\rm CN})_2({\rm H}_2{\rm O})_{10} \end{array}$	Micro-	N.A. <sup>[c]</sup>	520	0.20	50 %	~240 °C	N.A. <sup>[c]</sup>	S98
2008	N.A. <sup>[c]</sup>	[In(OH)(HIPPB)]	Micro-	215	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	18 %	~450 °C	250 °C	S99
2008	MIL-68(In)	[In(OH)( <b>BDC</b> )]	Micro-	746	1139	0.44	N.A. <sup>[c]</sup>	~350 °C	150 °C	S100
2008	ATF-1	$[(CH_3)_2NH_2][In(\textbf{THB})_2](DMF)_x$	Micro-	N.A. <sup>[c]</sup>	360.3	0.126	50.2 %	~300 °C	150 °C	S101
2008	N.A. <sup>[c]</sup> N.A. <sup>[c]</sup>	$\begin{array}{c} [(CH_{3})_{2}NH_{2}][In(\boldsymbol{L}^{2})] \\ [Li^{+}][In(\boldsymbol{L}^{2})] \end{array}$	Micro-	820 1024	N.A. <sup>[c]</sup>	0.326 0.419	~56 % N.A. <sup>[c]</sup>	~390 °C ~390 °C	180 °C 180 °C	S102
2008	sod-ZMOF	$ \begin{matrix} [In(4,6\text{-}\textbf{PmDC})_2Na_{0.36}K_{1.28}] \\ (NO_3)_{0.64}(H_2O)_{2.1} \end{matrix} \\$	Micro-	N.A. <sup>[c]</sup>	616	0.245	46 %	N.A. <sup>[c]</sup>	R.T. <sup>[d]</sup>	S103
	MOC-2	$[In_8(\textbf{HImDC})_{12}](\text{DMF})_6$			1420	0.535	56.1 %	~320 °C	135 °C	
2009	MOC-3	$\label{eq:ling} \begin{split} & [\mathrm{NH}_4][\mathrm{In}_8(\mathbf{HImDC})_{12}] \\ & [\mathrm{In}_8(\mathbf{HImDC})_{11}(\mathbf{ImDC})] \end{split}$	Micro-	N.A. <sup>[c]</sup>	456	0.1733	~31 %	~320 °C	135 °C	S104
2009	N.A. <sup>[c]</sup>	$\begin{array}{l} (choline)_{3}[In_{3}(BTC)_{4}](DMF)_{2} \\ (Et_{4}N)_{3}[In_{3}(BTC)_{4}](DEF) \end{array}$	Micro-	507.8 206.9	711.8 291.8	N.A. <sup>[c]</sup>	66.2 % N.A. <sup>[c]</sup>	<300°C ~380 °C	100 °C 200 °C	S105
2009	NOTT-200 NOTT-201	$\begin{split} & [\mathrm{H}_2 \textbf{PPZ}] [\mathrm{In}_2 (\mathbf{L}^3)_2] (\mathrm{DMF})_{3,5} (\mathrm{H}_2 \mathrm{O})_5 \\ & [\mathrm{Li}_{1,5} (\mathrm{H}_3 \mathrm{O})_{0,5}] [\mathrm{In}_2 (\mathbf{L}^3)_2] (\mathrm{H}_2 \mathrm{O})_{11} \end{split}$	Micro-	180 580	N.A. <sup>[c]</sup>	0.136 0.239	35 % 42 %	~400 °C ~400 °C	120 °C 120 °C	S106
2009	N.A. <sup>[c]</sup>	$[{\rm Et_2NH_2}][{\rm In}(2,6\text{-}{\rm NDC})_2]({\rm H_2O})_2({\rm DEF})$	Micro-	891.2 <sup>[e]</sup> 247 <sup>[f]</sup>	1233.9 <sup>[e]</sup>	0.50 <sup>[e]</sup> 0.17 <sup>[f]</sup>	48.1 %	~400 °C	120 °C	S107
2010	N.A. <sup>[c]</sup>	$[In_2(OH)_2(\textbf{TBAPy})](guests)$	Micro-	1189	1475	0.639	54 %	~380 °C	150 °C	S108

 Table S8 The adsorption information and thermal stability of representative In(III)-based MOFs.

Publish Time	MOF Code	MOF Formula <sup>[a]</sup>	Pore Level	BET Surface Area (m <sup>2</sup> g <sup>-1</sup> )	Langmuir Surface Area (m² g <sup>-1</sup> )	Pore Volume (cm <sup>3</sup> g <sup>-1</sup> )	Accessible Void	T <sub>max</sub> of Thermal Stability <sup>[b]</sup>	Activated T <sub>max</sub> for Sorption	Ref.
2010	N.A. <sup>[c]</sup>	$[({\rm In_3O})({\rm OH})({\bf ADC})_2({\bf IN})_2]({\rm H_2O})_{4.67}$	Meso-	1496	1857	N.A. <sup>[c]</sup>	68.2 %	~350 °C	100 °C	S17
2010	ZSA-2	$\begin{array}{l}  K_3(NO_3)_3(H_2O)_{2.5}(CH_3CN)_3  \\ [In_4(1,2\text{-DACH})_4(\textbf{TzDC})_4] \end{array}$	Micro-	395	N.A. <sup>[c]</sup>	0.19	34.2 %	~ <b>3</b> 00 °C	85 °C	S109
2010	CPM-5	$[(CH_3)_2NH_2][In_3O(\textbf{BTC})_2(H_2O)_3]_2 \\ [In_3(\textbf{BTC})_4](DMF)_7(H_2O)_{23}$	Micro	580	733	0.258	47.9 %	~320 °C	230 °C	\$110
2010	CPM-6	$\label{eq:cH_3NH_3} \begin{split} & [\mathrm{CH_3NH_3}] [\mathrm{In_3O}(\mathbf{BTC})_2(\mathrm{H_2O})_3]_2 \\ & [\mathrm{In_3}(\mathbf{BTC})_4] (\mathrm{solvents}) \end{split}$	Wilero-	596	931	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	230 °C	5110
2010	JUC-77	$[\mathrm{In(OH)}(\mathbf{OBA})](\mathrm{DMF})$	Micro-	976	1066	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	~350 °C	90 °C	S111
2011	CPM-13	$\label{eq:ch3NH3} \begin{split} & [CH_3NH_3] \\ & [In_3O(\textbf{BBDC})_3(HCO_2)_{3/2}(H_2O)]_2(\text{solvent}) \end{split}$	Micro-	904	1441	0.487	62.8 %	~400 °C	200 °C	S61
2011	N.A. <sup>[c]</sup>	$[\mathrm{In}_2(\mathrm{OH})_2(\mathbf{OBA})_2](\mathrm{DMF})_2$	Micro-	354.1	518.5	N.A. <sup>[c]</sup>	47.7 %	N.A. <sup>[c]</sup>	180 °C	S112
2011	NOTT-207 NOTT-208 NOTT-209	$\begin{split} & Li_{1,2}(H_3O)_{0,8}[In_2(\textbf{L}^4)_2](H_2O)_{14} \\ & [H_2\textbf{PPZ}][In_2(\textbf{L}^5)_2](DMF)_4(H_2O)_{5,5} \\ & Li_{1,4}(H_3O)_{0,6}[In_2(\textbf{L}^5)_2](acetone)_4(H_2O)_{11} \end{split}$	Micro-	474 687 729	N.A. <sup>[c]</sup>	0.206 0.287 0.303	40 % 39 % 43 %	~400 °C ~400 °C ~400 °C	120 °C 120 °C 120 °C	S113
2011	N.A. <sup>[c]</sup>	$[InH(D-CAM)_2]$	Micro-	497	607	0.132	49.3 %	~240 °C	80 °C	S114
2012	In-soc-MOF	$[{\rm In_3O}({\bf ABTC})_{1.5}({\rm H_2O})_3]({\rm H_2O})_3({\rm NO}_3)$	Micro-	970	1180	0.37	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	S115
2012	JUC-120 MIL-100(In)	N.A. <sup>[c]</sup>	Meso-	1456	N.A. <sup>[c]</sup>	0.636	N.A. <sup>[c]</sup>	~400 °C	150 °C	S116
2012	N.A. <sup>[c]</sup>	[(CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> ][In( <b>NH<sub>2</sub>BDC</b> ) <sub>2</sub> ](DMF)(H <sub>2</sub> O)	Micro-	573	633	N.A. <sup>[c]</sup>	N.A. <sup>[c]</sup>	~240 °C	80 °C	S117
2012	N.A. <sup>[c]</sup>	$[(CH_3)_2NH_2]$ [In( <b>BPDC</b> ) <sub>2</sub> ](DMF) <sub>4</sub> (H <sub>2</sub> O) <sub>2</sub>	Micro-	638	717	0.32	45.1 %	~320 °C	40 °C	S118

### Table S8 (continued)

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Publish Time	MOF Code	MOF Formula <sup>[a]</sup>	Pore Level	BET Surface Area (m <sup>2</sup> g <sup>-1</sup> )	Langmuir Surface Area (m <sup>2</sup> g <sup>-1</sup> )	Pore Volume (cm <sup>3</sup> g <sup>-1</sup> )	Accessible void	T <i>max</i> . of Thermal Stability <sup>[b]</sup>	Activated T <sub>max</sub> for Sorption	Ref.
2012	CPM-19-Nd	[In <sub>3</sub> Nd <sub>2</sub> O(OH) <sub>3</sub> ( <b>BTB</b> ) <sub>3</sub> (H <sub>2</sub> O) <sub>6</sub> ] (NO <sub>3</sub> )(solvent)	Micro-	272	370	0.133	72.8 %	~200 °C	150 °С	\$70
2012	CPM-20	$[InCo_2(OH)(\mathbf{IN})_3(\mathbf{BDC})_{3/2}](\text{solvent})$	Wilefo-	1009	1134	0.404	N.A. <sup>[c]</sup>	~300 °C	260 °C	570
2012	N.A. <sup>[c]</sup>	$\begin{split} & [(CH_3)_2NH_2][In(\mathbf{L}^6)](DMA)_3(H_2O)_2 \\ & [TMA][In(\mathbf{L}^6)](H_2O)_{10.5} \\ & [TEA][In(\mathbf{L}^6)](H_2O)_7 \\ & [TPA][In(\mathbf{L}^6)](H_2O)_{3.5} \\ & [TBA][In(\mathbf{L}^6)](H_2O)_{2.5} \\ & [(CH_3)_2NH_2]_2[In_2(\mathbf{L}^7)](DMA)_5(H_2O)_2 \\ & [TMA]_2[In_2(\mathbf{L}^7)](H_2O)_{19} \\ & [TEA]_2[In_2(\mathbf{L}^7)](H_2O)_{18} \\ & [TPA]_2[In_2(\mathbf{L}^7)](H_2O)_{13} \\ & [(CH_3)_2NH_2][TBA][In_2(\mathbf{L}^7)](H_2O)_{15} \\ \end{split}$	Micro-	19.35 <sup>[g]</sup> /8.12 <sup>[h]</sup> 13.67 5.81 37.41 325.65 83.39 <sup>[g]</sup> /97.77 <sup>[h]</sup> 13.40 754.63 36.26 120.76	30.38 <sup>[g]</sup> /19.45 <sup>[h]</sup> 21.35 13.63 57.05 477.77 794.80 <sup>[g]</sup> /816.56 <sup>[h]</sup> 22.55 1099.46 54.17 181.45	N.A. <sup>[c]</sup>	70.3 % N.A. <sup>[c]</sup> N.A. <sup>[c]</sup> N.A. <sup>[c]</sup> 65.7 % N.A. <sup>[c]</sup> N.A. <sup>[c]</sup> N.A. <sup>[c]</sup>	~320 °C	40 °C/80 °C 80 °C 80 °C 80 °C 80 °C 40 °C/80 °C 80 °C 80 °C 80 °C 80 °C	S119
	CPM-15-Mg	$\begin{split} & [(CH_3)_2NH_2]_4[In_6(\textbf{BTC})_{12}]_2 \\ & [(Mg_3OH)_4(H_2O)_{36}] \\ & [(In_2MgO)_4(\textbf{BTC})_4(H_2O)_{12}](solvent)_x \end{split}$		398	474	0.169	N.A. <sup>[c]</sup>	~300 °C	260 °C	
2012	CPM-15-Co	$\begin{split} & [(CH_3)_2NH_2]_4[In_6(\textbf{BTC})_{12}]_2 \\ & [(Co_3OH)_4(H_2O)_{36}] \\ & [(In_2CoO)_4(\textbf{BTC})_4(H_2O)_{12}](solvent)_x \end{split}$	Micro-	344	563	0.181	N.A. <sup>[¢]</sup>	~300 °C	260 °C	S120
	CPM-15-Ni	$\begin{split} & [(CH_3)_2NH_2]_4[In_6(\textbf{BTC})_{12}]_2 \\ & [(Ni_3OH)_4(H_2O)_{36}] \\ & [(In_2NiO)_4(\textbf{BTC})_4(H_2O)_{12}](\text{solvent})_x \end{split}$		263	356	0.128	N.A. <sup>[c]</sup>	~300 °C	260 °C	
2012	N.A. <sup>[c]</sup>	[In <sub>3</sub> O( <b>BPDC</b> ) <sub>3</sub> (HCOO)(H <sub>2</sub> O) <sub>1.5</sub> ](DMF) <sub>x</sub>	Micro-	1244.4	1785.13	0.628	62.6 %	~220 °C	60 °C	S121
2012	NOTT-202	$[(CH_3)_2NH_2]_{1.75}[In({\bf L^8}]_{1.75}(DMF)_{12}(H_2O)_{10}$	Micro-	2220	N.A. <sup>[c]</sup>	0.953	70 %	~380 °C	100 °C	S122

#### Table S8 (continued)

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Publish Time	MOF Code	MOF Formula <sup>[a]</sup>	Pore Level	BET Surface Area (m <sup>2</sup> g <sup>-1</sup> )	Langmuir Surface Area (m <sup>2</sup> g <sup>-1</sup> )	Pore Volume (cm <sup>3</sup> g <sup>-1</sup> )	Accessible void	T <i>max</i> . of Thermal Stability <sup>[b]</sup>	Activated T <sub>max</sub> for Sorption	Ref.
2012	InOF-1	$[\mathrm{In}_2(\mathrm{OH})_2(\mathbf{BPTC})](\mathrm{H}_2\mathrm{O})_6$	Micro-	1065	1093	0.37	48.9 %	~350 °C	N.A. <sup>[c]</sup>	S123
2012	JUC-101	$(In_3O)(TDCPB)(H_2O)_3(guest)_x$	Micro-	3742	4202	1.409	78.6 %	~300 °C	80 °C	S124
2013	N.A. <sup>[c]</sup>	$[(CH_3)_2NH_2]_2[In_2\textbf{L}^7](DMF)_4(H_2O)_{16}$	Micro-	752	991	N.A. <sup>[c]</sup>	43.9 %	~400 °C	80 °C	S125
2013	N.A. <sup>[c]</sup>	$[(CH_3)_2NH_2][In_2\mathbf{L}^7](DMF)_9(H_2O)_5$	Micro-	1555	1707	0.62	65.1 %	<300°C	SCD <sup>[i]</sup> +40 °C	S126
	437-MOF	[In(BTTB) <sub>2/3</sub> (OH)](NMF) <sub>5</sub> (H <sub>2</sub> O) <sub>4</sub>	Meso-	2379	N.A. <sup>[c]</sup>	1.11	65.3 %	Over 400°C <sup>[j]</sup>	360 °C	This work

[a] Abbreviations:

**BDC** = benzene-1,4-dicarboxylate;  $H_3ImDC = 4,5$ -imidazoledicarboxylic acid;

 $L^{I} = 3,3',5,5'$ -azobenzenetetracarboxylate;

1,2-H<sub>2</sub>**DACH** = 1,2-diaminocyclohexane;

**HIPPB** = 4,4'-(hexafluoroisopropylidene)bis(benzoate);

**THB** = thiophene-2,5-dicarboxylate;  $\mathbf{L}^2$  = biphenyl-3,3',5,5'-tetracarboxylate;

4,6-**PmDC** = 4,6-pyrimidicarboxylate;

choline =  $[(CH_3)_3NCH_2CH_2OH]^+$ ;

**BTC** = 1,3,5-benzenetricarboxylate;

 $H_2$ PPZ = piperazinium;  $L^3 = 1,1',4',1'',4'',1'''-quaterphenyl-3,5,3''',5'''-tetracarboxylate;$ 

2,6-NDC = 2,6-naphthalenedicarboxylate;

**TBAPy** = 1,3,6,8-tetrakis(*p*-benzoic acid)pyrene;

**ADC** = azobenzene-4,4'-dicarboxylate;

**IN** = isonicotinate;

1,2-**PDA** = 1,2-propanediamine;

 $H_3TzDC = 1,2,3$ -triazole-4,5-dicarboxylic acid;

**OBA** = 4,4'-oxybis(benzoate);

**BBDC** = 4,4'-biphenyldicarboxylate;

 $\mathbf{L}^{4} = [2,7-(9,10-\text{dihydrophenanthrenediyl})]\text{diisophthalate;}$  $\mathbf{L}^{5} = 1,1',4',1'',4'',1''',4''',1''''-\text{pentaphenyl-}3,5,3'''',5''''-\text{tetracarboxylate;}$  $\mathbf{D}-\mathbf{CAM} = \mathbf{D}-(+)-\text{camphoric acid}$ **ABTC** = 3,3',5,5'-azobenzenetetracarboxylate; **BTB** = 4,4',4"-benzene-1,3,5-triyl-tribenzoate;  $L^6 = 5 \cdot (3,5 \cdot dicarboxybenzyloxy)$ isophthalate;  $L^7 = tetrakis[(3,5 \cdot dicarboxybenoxy)methyl]methane;$  $NH_2BDC = 2$ -amino terephthalate; **BPDC** = 4,4'-biphenyldicarboxylate;  $L^8$  = biphenyl-3,3',5,5'-tetra-(phenyl-4-carboxylate); **TDCPB** = 1,3,5-tris(3,5-di(4-carboxy-phenyl-1-yl)phenyl-1-yl)benzene; **BPTC** = biphenyl-3,3',5,5'-tetracarboxylate; **BTTB** = 4,4',4"-benzene-1,3,5-triyltris(oxy)) tribenzoate DEF = N, N-diethylformamide; DMF = N, N-dimethylformamide; DMA = N, N-dimethylacetamide; NMF = N-methylformamide; [**b**] Date from TGA curves; [c] N.A. = Not Available; [d] R.T. = Room Temperature [e] Data calculated from solvent-exchanged samples; [f] Data calculated from activated samples; [g] for activated samples at 40 °C; [h] for activated samples at 80 °C; [i] SCD = Supercritical Carbon Dioxide; [j] Data from the heating treatment (at least 3h) under vacuum ( $< 10^{-3}$  Torr).

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