Supporting Information for

## Potentials of Ultramicroporous Metal Organic Frameworks in CO<sub>2</sub> Clean-up

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S. No.	Compound formula/code	Dense	Potentially Porous	Porous	Adsorption	Remark	Reference
1.	$[Yb(Tz)_3]$ and $[Eu_2(Tz)_5(TzH)_2]$	Yes				First 3D networks of lanthanides with complete nitrogen coordination spheres	Chem. Commun., 2006, 2060– 2062.
2	1:{[Zn <sub>2.5</sub> (trz) <sub>2</sub> (btc) (H <sub>2</sub> O)].2H <sub>2</sub> O} <sub>n</sub> 2:[Zn <sub>2.5</sub> (trz)(Hbtc) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub> ] <sub>n</sub> 3:{[Zn(Htrz)(Hbtc) )(H <sub>2</sub> O)].2H <sub>2</sub> O} <sub>n</sub>	Yes				The topologies and dimensionality of the complexes depend on the deprotonation extent of the two ligands. 1 was obtained at the initial pH value of 3.6 adjusted by TEA, and both its ligands are completely deprotonated. Containing monodeprotonated trz and doubly deprotonated Hbtc, 2 is isolated at pH 3.4 by slow evaporation of the filtrate. Upon further evaporation, 3 with neutral Htrz and doubly deprotonated Hbtc is produced.	CrystEngComm, 2008, 10, 1140– 1143.
3.	1:Zn(L)(bdc) <sub>0.5</sub> ·0.2 $5H_2O$ 2:Zn(L)(bdc) <sub>0.5</sub> ·0.1 $7H_2O$ HL = 1,2,4-triazol- 3-amine, H2bdc = terephthalic acid	Yes			The solvent- accessible volume calculated using the Platon program is ca. 1116.3 Å <sup>3</sup> and 012.6 Å <sup>3</sup> , equal to 27.5% and $32.5\%$ of the cell volume for 1 and 2. But do not take CO <sub>2</sub> or N <sub>2</sub>	The formation of these MOFs is controlled by different speeds of crystallization. Operation of controlling the speed of crystallization may play a profound role in determining the aggregation fashions of Zn(II) ions and L– ligands, resulting in the various layers, viz. a 4.82 net vs. a 4.6.12 net.	Dalton Trans., 2013, 42, 13802.
4.	<ol> <li>[Cu<sub>3</sub>(μ<sub>3</sub>-O)( μ<sub>3</sub>-trz)<sub>3</sub>]<sub>2</sub>[OH]<sub>2</sub>.15H<sub>2</sub> O</li> <li>Cu[Cu<sub>3</sub>(μ<sub>3</sub>-O)( μ<sub>3</sub>-trz)<sub>3</sub>Cl<sub>3</sub>]</li> <li>[Cu<sub>2</sub>(μ<sub>3</sub>-trz)( μ<sub>3</sub>-Cl)<sub>2</sub>]</li> </ol>		Yes			Taking the van der Waals radii into account, the aperture may only admit the passage of a sphere with a 4.5 Å diameter in 1. If this highly open structure is viewed from the [-1,0,1] axis, a larger channel can be seen with cross dimensions of ca. 11.1x5.9 Å. 3 is of interest as it exhibits unique 2D inorganic layers which are different from those of basic copper halide skeletons such as square dimers, cubane tetramers, zigzag chains, double stranded ladders, hexagonal grid chains, it has mixed valence copper atoms and it presents the first example of 1,2,4- triazoles as organic	Crystal Growth & Design, 2006, 6, 1393-1398.

Table S1. List of selected triazolate based metal organic frameworks.

					components in the field of inorganic organic hybrid copper halides.	
5.	1:ZnCl(AmTRZ) 2:Zn(HCO <sub>2</sub> )(AmT RZ) 3:Zn <sub>5</sub> (OH) <sub>2</sub> (AmT RZ) <sub>6</sub> (NO <sub>3</sub> ) <sub>2</sub> 6H <sub>2</sub> O 4:Zn <sub>5</sub> (OH)(AmTR ZH)-(AmTRZ) <sub>6</sub> (HCO <sub>2</sub> ) <sub>3</sub> .5H <sub>2</sub> O	Yes			Isostructural compounds 1 and 2 display a two-dimensional layer structure.3 is a dense three-dimensional Framework. 4 is built from porous Zn-AmTRZ layers containing 12- and 8- membered rings, which are connected to each other by dinuclear Zn tetrahedra building units. Water and format anions occupy the void inside the framework. 4 has channels which are 3.21x3.22Å <sup>2</sup> and 8.83x8.83Å <sup>2</sup> taking the van der Waals radii	Crystal Growth & Design, 2007, 7, 7.
6.	1 · (H <sub>2</sub> O):[Zn <sub>3</sub> (Am TAZ) <sub>3</sub> S](NO3) · (H <sub>2</sub> O) 2 · 2(EtOH):Zn <sub>7</sub> (A mTAZ) <sub>8</sub> (CO <sub>3</sub> ) <sub>2</sub> (O H) <sub>2</sub> · 2(EtOH)		Yes		into account. 1·(H2O) is constructed from triangular Zn <sub>3</sub> S units that are bridged through AmTAZ ligands into a cationic three- dimensional (3D) network with nitrate and water molecules residing in the cavities. 2·2(EtOH) shows a complex 3D network constructed from seven crystallographically unique zinc centers bridged by AmTAZ, carbonate, and hydroxide anions.	Crystal Growth & Design, 2009, 9, 3609–3614
7.	1: $[Co(atz)(L1)_{0.5}]$ · DMF 2: $[Co(atz)(L2)_{0.5}]$ · DMF Hatz = 3-amino- 1,2,4-triazole, L1 = 4,4'- biphenyldicarboxy late, L2 = 3,3'- biphenyldicarboxy late		Yes	N <sub>2</sub> 77K: Langmuir surface areas of 902 and 737 m <sup>2</sup> /g, BET surface areas of 683 and 552 m <sup>2</sup> /g for 1 and 2. CO <sub>2</sub> , CH <sub>4</sub> , H <sub>2</sub> adsorptions done and selectivities studied.	Isomeric 1 and 2 based on positional isomeric biphenyldicarboxylate ligands exhibit distinct temperature- dependent CO2 sorption behaviors. They contain naked amino groups and possess the same topology net. The square aperture diameter for each channel is $4.7 \times 4.8$ Å <sup>2</sup> along the [010] direction for 1 and [101] direction for 2 (excluding vWaals radii. The likely reason for the distinct adsorption behaviors should be related to the stronger interaction of CO <sub>2</sub> with amino groups.	Cryst. Growth Des. 2014, 14, 2003–2008.
8.	1:[Co <sub>2.5</sub> (btc)- (atz) <sub>2</sub> (Hatz)(DMF) ]·2DMF (1) 2:[Co <sub>2.5</sub> (btc)(Hbtc) 0.5(atz)(CH <sub>3</sub> CN)(H <sub>2</sub> O)]·H <sub>2</sub> O		Yes	$N_2$ 77K: Langmuir surface areas of 609 and 471 m <sup>2</sup> g <sup>-1</sup> , BET surface areas of 465 and 356 m <sup>2</sup> g <sup>-1</sup> for 1 and 2. The enhanced CO2 uptakes of 1 and 2 should be attributed to their free -NH <sub>2</sub> groups, the exposed Co <sup>2+</sup> sites	Both contain suitable pore sizes and highly polar channel systems functionalized by amino groups, open metal sites, carbonyl or free carboxylic acid sites and uncoordinated triazolate nitrogen atoms on the pore surfaces, exhibiting multipoint interactions between CO <sub>2</sub> molecules and frameworks, resulting in high CO <sub>2</sub> uptake and selectivity for CO <sub>2</sub> over N <sub>2</sub> . Two types of pores in $1 \sim 4.1 \times$ 4.7 and 6.8 × 8.1 Å <sup>2</sup> (excluding van der Waals radii of the atoms) respectively. 1 has 45.6% solvent void accessible	Dalton Trans., 2013, 42, 13990.

				volume. 2 has channels of $3.5 \times 5.3$ and $5.0 \times 5.8$ Å <sup>2</sup> and $32.2\%$ of solvent accessible volume.	
9.	MAF-2[Cu(etz)] <sub>n</sub> Hetz = 3,5-diethyl- 1,2,4-triazole	Yes	Solvent sorption	By virtue of the kinetically controlled flexibility and hydrophobic pore surface, MAF-2 can adsorb large amounts of small organic molecules but excludes H <sub>2</sub> O. MAF-2 can also separate benzene and cyclohexane efficiently, as its flexible scaffold can distort to a certain degree so that benzene can diffuse through the distorted apertures but cyclohexane cannot.	J. AM. CHEM. SOC. 2008, 130, 6010–6017.
10.	[Cu <sub>3</sub> (μ3-OH)( μ 2- O)(dmtrz) <sub>2</sub> (HCOO)( μ 2- H <sub>2</sub> O)(H <sub>2</sub> O) <sub>3</sub> ].H2O	Yes	$CO_2$ 273K BET and langmuir surface area was calculated to be ca.105 m <sup>2</sup> /g and 147 m <sup>2</sup> /g	3D structure with 1D channels along the c axis. The pore size is calculated to be ca. 6.9 Å (taking van der Waals radii in to consideration) and the solvent-accessible volume is estimated to be ca. 46.2%.	CrystEngComm, 2013, 15, 3484– 3489.
11.	MET1: (Mg( $C_2N_3H_2$ ) <sub>2</sub> , MET2: (Mn( $C_2N_3H_2$ ) <sub>2</sub> , MET3: (Fe( $C_2N_3H_2$ ) <sub>2</sub> , MET4: (Co( $C_2N_3H_2$ ) <sub>2</sub> , MET5: (Cu( $C_2N_3H_2$ ) <sub>2</sub> , MET6: (Zn( $C_2N_3H_2$ ) <sub>2</sub> ,	Yes	Pore size, and SA table in paper	All the metal ions are octahedrally coordinated to the nitrogen atoms of triazolate such that five metal centers are joined through bridging triazolate ions to form super-tetrahedral units that lie at the vertexes of a diamond-type structure. The variation in the size of metal ions across the series provides for precise control of pore apertures to a fraction of an Angstrom in the range 4.5 to 6.1 Å.	Chem. Eur. J. 2012, 18, 10595 – 10601.
12.	C <sub>6</sub> H <sub>6</sub> @MAF-42- lp,=[Cu <sub>4</sub> (btm) <sub>2</sub> ] .C <sub>6</sub> H <sub>6</sub> O53, O74 and O100 are MAF42 oxidized to 53, 74 and 100% H <sub>2</sub> btm=bis(5- methyl-1,2,4- triazolate-3- yl)methane)	Yes	CH <sub>4</sub> and CO <sub>2</sub> adsorption has been studied	3D porous framework having large 1D rhombic channels (void 37.8%, cross-section size 4.8x7.1–6.0x10.8 Å <sup>2</sup> ) with disordered benzene molecules filled inside. The oxidation degree has been related to the adsorption behavior of the MOFs	NATURE COMMUN. DOI: 10.1038/ncomms 7350.
13.	$MAC-4: {[Zn_{5}(dmtrz)_{3}(IPA)_{3}(OH)] \cdot DMF \cdot H_{2} \\ O_{n} \\ (Hdmtrz = 3,5-dimethyl-1H-1,2,4-triazole, H_{2}IPA = isophthalic acid) \\ MAC-4-OH: {[Zn_{5}(dmtrz)_{3}(OH - IPA)_{3}(OH)] \cdot DMF \cdot 5H_{2}O_{n} \\ (OH-1) + OH-1 \\ OH-1) + OH-1 \\ OH-1 $	Yes	$\begin{array}{l} N_2 \ 77K: \\ MAC-4 \ has \ a \\ BET \ and \\ Langmuir surface \\ area \ of \ 796 \ and \\ 1151 \ m^2/g. \\ MAC-4-OH \ has \\ a \ BET \ and \\ Langmuir surface \\ area \ of \ 339 \ and \\ 496 \ m^2/g. \\ CO_2 \ adsorption \\ done. \end{array}$	MAC-4-OH is an iso-reticular framework of MAC-4 with channels functionalized by hydroxyl groups. MAC-4-OH shows a significant enhancement for CO <sub>2</sub> uptake compared with that of MAC-4 due to the existence of electrostatic attractive interactions, though its surface area is lower than that of MAC-4. The Qst at zero coverage of activated MAC-4- OH is ca 31 kJ/mol, which is much higher that of MAC-4	Dalton Trans., 2012, 41, 4007– 4011.

<ul> <li>hydroxyisophthali c acid)</li> <li>strike area</li> <li>(14. 1:[[NH4(CH3)]]Z ntáz(0x)].HQ, nt</li></ul>						
c seid)exitianed MAC-4-OH to the complexitionSelective for CO (complexition)exitian an atomic (complexition)KSC Adv. 2015 (complexition)14.1: [(MI4(CH3))][Z (Hatz = 5-amino- 11 Hetraole, ILcos – onale acid)YesSelective for CO (complexition)Complexition (complexition)KSC Adv. 2015 (complexition)(Hatz = 5-amino- 11 Hetraole, ILcos – onale acid)CO (152 and 165 m <sup>2</sup> /g.CO (152 and 165 m <sup>2</sup> /g.Selective for CO (complexition)KSC Adv. 2015 (complexition)15.MIAF-1; (Zan(LAP) (CAA)H(O,LAP) (CAA)H(O,LAP) (CAA)H(O,LAP) (CAA)H(O,LAP)Yes (PP, and CAA)H(O,LAP) (PP, and CAA)H(O,LAP) (CAA)H(O,LAP)Yes (PP, and CAA)H(O,LAP) (PP, and CAA)H(O,LAP) (CAA)H(O,LAP) (CAA)H(O,LAP)Yes (PP, and CAA)H(O,LAP) (PP, and CAA)H(O,LAP) (CAA)H(O,LAP) (CAA)H(O,LAP)Yes (PP, and CAA)H(O,LAP) (PP, and CAA)H(O,LAP) (CAA)H(O,LAP) (CAA)H(O,LAP) (CAA)H(O,LAP)Yes (PP, and CAA)H(O,LAP) (PP, and CAA)H(O,LAP) (CAA)H(O,LA		$H_2IPA = 5-$ hydroxyisophthali			(21 kJ/mol), indicating stronger binding ability of	
14.       1:[[MH4CH3]]Z (Hatz = 5-amino- [114-tetracke, H]ox = oxalic acid)       Yes       Selective for C0, over CH and N, Drogs T memory with sore CH and N, Drogs T memory M, and M, Drogs T are ligands point 0 the center of the channel, which provides the favorable condition for media tations the condition for media tations point 0 the center of the channel, which provides the favorable condition for media tations searches the favorable condition for media tations point 0 the center of the channel, which provides the favorable condition for media tations point 0 the center of the channel, which provides the favorable condition for media tations point 0 the center of the channel, which is conductive to the interaction between the framework and guest 0/(2, NiH 0/)(CH N) O(a)       Yes       N:77K: BET strate area of 200 m <sup>2</sup> / <sub>10</sub> (P) and 200 m <sup>2</sup> / <sub>10</sub> (P) and 200 m <sup>2</sup> / <sub>10</sub> (P) and and area contraction and con strate area of 200 m <sup>2</sup> / <sub>10</sub> (P) and a strate area of 200 m <sup>2</sup> / <sub>10</sub> (P) and a strate area of 200 m <sup>2</sup> / <sub>10</sub> (P) and a strate area of 200 m <sup>2</sup> / <sub>10</sub> (P) and a strate area of a Display (P) and a strate area of 200 m <sup>2</sup> / <sub>10</sub> (P) and a strate area of a Display (P) and a strate area of a Display (P) and a strate are					6 6 5	
<ul> <li>n(al200a)[11.0], (Itatz = 5-sumino- H-tertrasole. H<sub>5</sub>X</li> <li>(Itatz = 5-sumino- H-terrasole. H<sub>5</sub>X</li> <li>(I</li></ul>		,			CO <sub>2</sub> molecules.	
(Hat = 5-amino- [H4-strazole, H <sub>0</sub> x = oxalic acid)       (Hat = 5-amino- [H4-strazole, H <sub>0</sub> x = oxalic acid)       (Hat = 5-amino- [H4-strazole, H <sub>0</sub> x = oxalic acid)       (Hat = 5-amino- [H4-strazole, H <sub>0</sub> x) = oxalic acid)       (Hat = 5-amino- [H4-strazole, H <sub>0</sub> x) = oxalic acid)       (Hat = 1- [Hat = 1, 2, - trazol, Hat = 1, 2, - trazol, Hat = 1, 2, - trazol, Hat = 1, 2, - trazol, HBDC)       (Hat = 1- [Hat = 1, 2, - [HBDC = 1, - ], 1, -trazol, Hat = 1, 2, - trazol, Ha	14.	1:{[NH <sub>2</sub> (CH3) <sub>2</sub> ][Z	Yes	-	1	RSC Adv., 2015,
(Hatz = 5-annino- H-terrately, H-construction)       CO <sub>2</sub> 1958; The channels, which provides the areas were calculated to be areas were calculated to be arrive account of metal actions with exchange process. All the anning groups of ar / igands point to the center of the channel, which is conducive to the interaction between the framework and guesce point to the center of the channel, which is conducive to the interaction between the framework and guesce point to the center of the channel, which is conducive to the interaction between the framework and guesce point to the center of the channel, which is conducive to the interaction between the framework and guesce prevented the formation of a Langmuit surface area of 2000 m <sup>2</sup> /g (PP) = 0.9).       No 71K: Market - (200, m <sup>2</sup> ) More and the kind of duble valied arrangement has prevented the formation of a cangement into starts and square surface area of 2000 m <sup>2</sup> /g (PP) = 0.9).       No 71K: More area organic limit, 1533 A = 9.947, A r at 87 K A (atom-to-atom distance) along are task and square surface area of 2.22 m <sup>2</sup> /g, and the interaction and can surface area organic limit, 1533 A = 9.947, A r at 87 K i taggement into a lange due task and square surface area of 7. A '1 (KK isomers over a dibrance) area of ca. 807. THEND A r at 87 K i taggement into a lange due task and square surface area of 7. A '1 (KK isomers over a dibranced on m <sup>2</sup> /g. No 7.1, A - future area of ca. 807. THEND A r at 87, K i taggement into a lange due task and square surface area of 7. A '1 (KK isomers over a dibranched nem- method).       Chem. Commun. 2017, 47, 7197- 7199.         17. I [Zucf(HBDC)_(d) m <sup>2</sup> /g, [CH], [C		$n(atz)(ox)].H_2O_n$		over CH <sub>4</sub> and N <sub>2</sub> .		5, 24655–24660.
IH-ietrazole, Hook       BET       and       channels, which provides the favorable condition for ecapsulation of media calinons via exchange process. All the anning groups of atz ligands point to the center of the interactive to theinteractive to the interactive to theinteract				CO 1057 TI		
<ul> <li>= exalic acid)</li> <li>= exalic acid)</li> <li>Langmuir surface meass were encapsulation of metal cations for a cochange process All the amine groups of at 2 ligands m<sup>2</sup>/g.</li> <li>MTAF-1: (Zn(p3- 0)HC-NHE0/)(H)</li> <li>MTAF-1: (Zn(p3- 0)HC-NHE0/)(H)</li> <li>Yes</li> <li>N: 77K: BFT auffec meass dependence of the channel. Which is conductive to the interaction between the framework and guest molecules/ions in the channel. Which is conductive to the channel. Which is conductive to the interaction between the framework and guest molecules/ions in the channel. Which is conductive to the interaction between the framework and guest molecules/ions in the channel. Which is conductive to the formation of a 2010 m<sup>2</sup>/g (PPO of a double-walled arrangement has corresponding to consponding to evolve walled arrangement has corresponding to evolve walled arrangement has corresponding to evolve walled arrangement has corresponding to evolve walled arrangement has surface area to a basis and square channels of 9.984 A y alores.</li> <li>16. 1::[[Zn(HBDC)_{2/d} Yes N2 77K: BET meass of 11.83 Å x 9.984 A values:</li> <li>16. 1::[[Zn(HBDC)_{2/d} Yes N2 77K: BET meass of a long casis, of 7.0 x7.0 x7.1 x9-rat along area casis.</li> <li>17. 1.[Za(FA/kdut2)_2] Yes N2 77K: BET meass of the casis.</li> <li>18. D[C]_1, 47, 7197</li> <li>19. [ZA(TR2/RIB) Yes N2 77K: BET marked net.</li> <li>11.21. 4.[Zn(TR2/RIB) Yes N2 77K: BET meass area meass area meass of a constrange area of a along casis, of 7.0 x7.0 x7.1 x9-rat along area casis.</li> <li>11.22.4. transole for the constrangement area more site of the constrangement and morehanached threase sorts of the constrangement and morehanached threase sore admininted onet.</li> <li>11. [Za(FA/kdut2)_2] Yes N2 77</li></ul>				-	0	
areas       were calculated to 125 and 165 m <sup>1</sup> /g.       encapsulation of metal atoms via exchange process. All the becamel, which is conductive to the interaction between the minog goups of at. Vibras constructive provide to the canter of the interaction between the moleculescoins in the channels.         15.       MTAF-1: (Zncjul- 0) <sub>10</sub> Yes       N:77K: Differentiation of metal to the campoint to the canter of of 2020 m <sup>2</sup> g output to the formation of 0.01-0.15, corresponding to a langmut 2000 m <sup>2</sup> g (PPo 0.01-0.15).       Inorg. Chem 2012, 3: 4423-4425.         16.       1:{[ZncjHBDC);dd       Yes       N:77K: BET mitrace area of 2.00 m <sup>2</sup> g, and mitrace area of actignt the to basis to the prevented to basis to the mands of 1.833, A * 9.947.       Chem. Commun. 2011, 47, 7197.         16.       1:{[ZncjHBDC);dd       Yes       N: 77K: BET mitrace area of actignt the construction and statance) reveals similar mitrace area of actignt the construction and statance) mitrace area of actignt the construction and statance) reveals similar mitrace area of actignt the construction and the surface area of actignt the construction and actignt the construction and the c		, =				
<ul> <li>125 and 165 amine groups of at guards point to the center of the channel, which is conductive to the interaction between the molecules/ons in the channels.</li> <li>15. MTAF-1: (Znc(µ3- O)(-CALHAO);(CH- ),(EALHAO);(CH- ),(EALHAO);(CH- ),(CALHAO);(CH- ),(CALHAO);(CH- ),(CALHAO);(CH- ),(CH- O)(-0)</li> <li>15. MTAF-1: (Znc(µ3- O)(-))</li> <li>16. MTAF-1: (Znc(µ3- O)(-))</li> <li>17. (Znc(HBDC);(d) mtrz); guest),</li> <li>16. 1: ([Znc(HBDC);(d) mtrz); guest),</li> <li>16. 1: ([Znc(HBDC);(d) mtrz); guest),</li> <li>17. 1: [Znc(HBDC);(d) mtrz); guest),</li> <li>18. 0: [Znc(HBDC);(d) mtrz); guest),</li> <li>19. 1: [Znc(HBDC);(d) mtrz); guest),</li> <li>11. 2: [Znc(HBDC);(d) mtrz); guest),</li> <li>11. 2: [Znc(HBDC);(d) mtrz); guest),</li> <li>12. 4-triazole</li> <li>13. 3: A system in the convertice action of a guest matched action.</li> <li>14. 1: [Znc(HBDC);(d) mtrz); guest),</li> <li>13. 2: [Znc(HBDC);(d) mtrz); guest),</li> <li>14. 1: [Znc(HBDC);(d) mtrz); guest),</li> <li>14. 1: [Znc(HBDC);(d) mtrz); guest),</li> <li>15. 1: [Znc(HBDC);(d) mtrz); guest),</li> <li>16. 1: [Znc(HBDC);(d) mtrz); guest),</li> <li>17. 1: [Znc(HBDC);(d) mtrz); guest),</li> <li>18. 1: [Znc(HBDC);(d) mtrz); guest),</li> <li>19. 2: [Znc(HBDC);(d) mtrz); guest),</li> <li>11. 2: 4-triazole</li> <li>11. 2: 4-triazole</li> <li>12. 4-triazole</li> <li>13. 3: 4: 5: 5: 5: 5: 5: 5: 5: 5: 5: 5: 5: 5: 5:</li></ul>		chune derd)				
<ul> <li>m<sup>2</sup>g. point to the center of the channels.</li> <li>MTAF-1: (Za.(µ3- O)(C,N)H,O),(K1 ),(H,O),(C,N)H</li> <li>(J,C,N)H,O),(K1 ),(H,O),(C,N)H</li> <li>(J,C,C,N)H,O),(K1 ),(H,O),(C,N)H</li> <li>(J,C,C,N)H,O),(K1 ),(H,O),(C,N)H</li> <li>(J,C,C,N)H,O),(K1 ),(H,O),(C,N)H</li> <li>(J,C,C,N)H,O),(K1 ),(H,O),(C,N)H</li> <li>(J,C,C,N)H,O),(K1 ),(H,O),(C,N)H</li> <li>(J,C,C,N)H,O),(K1 ),(H,O),(C,N)H</li> <li>(J,C,C,N)H,O),(K1 ),(H,O),(C,N)H</li> <li>(J,C,C,N)H,O),(K1 ),(H,O),(H,O),(K1 ),(H,O),(H,O),(K1 ),(H,O),(H,O),(K1 ),(H,O),(H,O),(K1 ),(H,O),(H,O),(K1 ),(H,O)</li></ul>				calculated to be		
<ul> <li>i. MTAF-1: (Zndµ2- Q)(CA)1I(2),(I1 )(CH)),(CH-N Q)(CA)1I(2),(I1 )(H)(D),(CH-N Q)(CA)1I(2),(I1 )(H)(D),(CH-N Q)(CA)1I(2),(I1 )(H)(D),(CH-N Q)(CA)1I(2),(I1 )(H)(D),(CH-N Q)(CA)1I(2),(I1 )(H)(D),(CH-N Q)(CA)1I(2),(I1 )(H)(D),(CH-N Q)(CA)1I(2),(I1 )(H)(D),(CH-N Q)(CA)1I(2),(I1 )(H)(D),(CH-N Q)(CA)1I(2),(I1 )(H)(D),(CH-N Q)(I)(CA)1N(1) Q)(CA)1I(2),(I1 )(H)(D),(CH-N Q)(I)(CA)1N(1) Q)(CA)1I(2),(I1 )(H)(D)</li></ul>						
<ul> <li>It. MTAP-1: (Znq(µ2- Q)(C,NiH,O);(Cl+N Q)(HO);(Cl+N Q)(HO);(Cl+N Q)(hO</li></ul>				m²/g.		
15.     MTAF-1: (Zn_q(i)- O)(i)     Yes     N.77K: BT surface area of 2020 m <sup>2</sup> /g     MTAF-1: represents the first 201(F-0)::(CH-N O)(ii)     Norg     Chem       0)(ii)     Ves     N.77K: BT surface area of 2020 m <sup>2</sup> /g     MTAF-1: represents the first double walled arrangement has represented the formation of autopenetic the robustness of the framework. It has retangular e-annels of 19.48 × 9.984 Å along the axis.     Along-Advacuum autopenetic the robustness of the framework it has retangular e-annels of 19.48 × 9.984 Å along the axis.       16.     1: [Zn_g(HBDC):(d)     Yes     N2 77K: BFT hemore the robustness of 10.48 × 9.984 Å along the axis.     Chem. Commun. 2011, 47, 179- reca. 552 m <sup>3</sup> /g, autopenetic adosption studied.     Chem. Commun. 2011, 47, 179- reca. 552 m <sup>3</sup> /g, autopenetic adosption studied.     Chem. Commun. 2011, 47, 179- reca. 552 m <sup>3</sup> /g, autopenetic adosption studied.     Chem. Commun. 2011, 47, 179- reca. 552 m <sup>3</sup> /g, autopenetic adosption studied.     Chem. Commun. 2011, 47, 179- reca. 552 m <sup>3</sup> /g, autopenetic adosption studied.     Chem. Commun. 2011, 47, 179- reca. 552 m <sup>3</sup> /g, autopenetic adosption studied.     Chem. Commun. 2011, 47, 179- reca. 552 m <sup>3</sup> /g, autopenetic adosption studied.     Chem. Commun. 2011, 47, 179- 719.9       17.     1.[2n/f(HD/g)(I)]     Yes     N2 77K : BFT noslower adbranced one.     The solvent accessible volume rese area of co. 807.8     Z. Anorg. Alg Chem. 2015 (56-159       18.     1.[2n/f(TA)/g(dat7)]     Yes     N2 77K : BFT nad Langmuir in is 38.9%, Al zecessible volume rese area set set advacessible volume rese area set sets of beter uptake. sets for beter uptake. 2017, 46, 836- from the selecti					· · · · · · · · · · · · · · · · · · ·	
15.     MTAP-1-(Zn_qL)- (H(P),r(C,NiH,O),r(H) '(H(P),r(C,NiH,O),r(H) '(H(P),r(C,NiH,O),r(H) '(H(P),r(C,NiH,O),r(H) '(H(P),r(C,NiH,O),r(H) '(H(P),r(C,NiH,O),r(H) '(H(P),r(C,NiH,O),r(H) '(H(P),r(C,NiH,O),r(H) '(H(P),r(C,NiH,O),r(H) '(H(P),r(C,NiH,O),r(H) '(H(P),r(C,NiH,O),r(H) '(H(P),r(C,NiH,O),r(H) '(H(P),r(C,NiH,O),r(H), '(H(P),r(C,NiH,O),r(H), '(H(P),r(C,NiH,O),r(H), '(H(P),r(C,NiH,O),r(H), '(H(P),r(C,NiH,O),r(H), '(H(P),r(C,NiH,O),r(H), '(H(P),r(C,NiH,O),r(H), '(H(P),r(C,NiH,O),r(H), '(H(P),r(C,NiH,O),r(H), '(H(P),r(C,NiH,O),r(H), '(H(P),r(C,NiH,O),r(H), '(H(P),r(C,NiH,O),r(H), '(H(P),r(C,NiH,O),r(H), '(H(P),r(C,NiH,O),r(H), '(H(P),r(C,NiH,O),r(H), '(H(P),r(C,NiH,O),r(H),r(H),r(H),r(H),r(H),r(H),r(H),r(H						
Oyr_(CN:H_O);(CH:N       Diff.       2012, 1400         Oyr_(O);(C):H       of 2020 m²/g       of 2020 m²/g       organic linkr; and this kind of 200 m²/g         O);(a)       O(b)       a Langmui       surface area of a Langmui       organic linkr; so y 947         Ar at 87 K       K       (atomets of 1.5), corresponding to and square surface area of a Langmui       surface area of a lange are b axis and square surface area of a lange are b axis and square surface area of a lange are b axis and square surface area of a lange are b axis of 7.0 x 0.7 0 x 2011, 47, 7197- taking van der Walls radii into 12, 4-4 mrazole       Chem. Commun.         16.       1: {[Zn;(HBDC);(d]       Yes       N2 77K: BET       The MOF has 1D channels of 1.939 kA x 9.944 x 9.984 A					molecules/ions in the channels.	
<ul> <li><sup>1</sup> (Jt-O):<sub>1</sub>(CJI-N O)<sub>10</sub>)</li> <li><sup>1</sup> (Zb-(HBDC):<sub>1</sub>(d)</li> <li><sup>1</sup> (Zb-(HBD):<sub>1</sub>(d)</li>     &lt;</ul>	15.	MTAF-1: (Zn <sub>5</sub> (μ3-	Yes	N <sub>2</sub> 77K:		Inorg. Chem.
<ul> <li>O)in)</li> <li>O)in)</li> <li>O)in)</li> <li>O(1)</li> <li>O(1)</li></ul>						, , ,
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$				U		4423-4425.
<ul> <li>corresponding to a Langmuir interpenetration and can enhance the robustness of the framework. It has rectangular channels of 11.583 Å × 9.947</li> <li>Ar at 87 K</li> <li>A (atom-catom distance) along are a distance) along the c axis.</li> <li>16. 1:[Zn;(HBDC);(d)</li> <li>Yes</li> <li>N2 77K: BET and along the c axis.</li> <li>17. 1:[Zn;(FA)(datr.2); and (LA) and (LA)</li></ul>		0)10)				
a       Langmuir surface area of 2300 m²g (P/P) = 0.9).       interpenetation and can enhance the robustness of the framework. It has rectangular echannels of 11.583 A × 9.947 A A (aton-to-atom distance) along a or b axis and square along a cxis, of 7.0 x7.0 x7.0 x7.0 x7.0 x7.0 x7.0 x7.0						
$ \begin{array}{c} 2300 \text{ m}^{2}\text{g} (P/P) \\ = 0.9), \\ Ar \text{ at } 87 \text{ K} \\ reveals similar \\ surface area \\ values. \\ along are b axis and square \\ channels of 1.958 A \times 9.94 A \\ along the c axis \\ along are b axis and square \\ channels of 1.954 A \times 9.94 A \\ values. \\ along are b axis and square \\ channels of 1.954 A \times 9.94 A \\ values. \\ along are b axis and square \\ channels of 1.954 A \times 9.94 A \\ values. \\ along the c axis \\ surface area of \\ along area of ca. 807.8 \\ surface area of ca. 807.8 \\ selective alsorption of linear \\ add, Haftrz = \\ 3.6-dimethyl-1H, \\ 1, 2, 4-triazole \\ (H,FA = fumaric \\ acid, Hdatrz = 3.5- \\ dimminel, 2,4- \\ triazole \\ (H,FA = fumaric \\ 2(Zh_{2}(TRZ)_{4}(TTB \\ DC)]_{h} \\ (TKZ = 1,2,4- \\ triazole \\ (TRZ)_{1}(TRZ)_{4}(TTB \\ DC)]_{h} \\ (TKZ = 1,2,4- \\ triazole \\ (TRZ)_{1}(TRZ)_{4}(TTB \\ DC)]_{h} \\ (TKZ = 1,2,4- \\ triazole \\ (TRZ)_{1}(TRZ)_{4}(TTB \\ Triazole \\ (TRZ)_{1}(TRZ)_{4}(TTB \\ Triazole \\ (TRZ)_{1}(TRZ)_{4}(TTB \\ DC)]_{h} \\ (TKZ = 1,2,4- \\ triazole \\ (TRZ)_{1}(TRZ)_{4}(TTB \\ Triazole \\ (TRZ)_{4}(TRZ)_{4}(TTB \\ Triazole \\ (TRZ)_{4}(TRZ)_{4}(TTB \\ Triazole \\ (TRZ)_{4}(TRZ)_{4}(TTB \\ triazole \\ (TRZ)_{4}(TRZ)_{4}(TTB \\ TRIBDC = \\ triazole \\ (TRIBC = \\ triazole \\ (TR$					interpenetration and can	
$= 0.9), channels of 11.583 Å \times 9.947Ar at 87 KÅ (atom-to-tom distance)reveals similarsurface area discorption distance)along a or b axis and squarechannels of 9.984 Å \times 9.947along the c axis.16. 1:{[Zn;(HBDC);(d] Yesmtrz]_gleuest],mtrz]_g$				surface area of		
Ar at 87 K reveals similar surface area travely guestlaAr (atom-to-atom distance) along a or baxis and square channels of 9.984 Å $\times$ 9.984 Å along a or baxis and square channels of 9.984 Å $\times$ 9.984 Å along a or baxis and square channels of 9.984 Å $\times$ 9.984 Å along a or baxis and square channels of 9.984 Å $\times$ 9.984 Å along a or baxis and square channels of 9.984 Å $\times$ 9.984 Å16.1: {[Zn;{[HBDC}];{d}} mt2;] guestlaYesN2 77K: BET mt2; and monobranched hexame of a careas are are of a careas are are of careas are are are are, are area of ca. 807.84 area of ca. 807.84 area of ca. 807.84 benzenedicarboxyl at e acid, Hdmtz = 3.5- diamino-1.2.4- trazoleChem. Commun. 2011, 47, 7197. taking van der Wals radii on the mt2; and monobranched hexame is 3.9% At zero coverage, mt2; mt2; mt2; mt2; surface areas are mt2;						
16.     1:{[Zn;(HBDC):/d mtr2):]guest],a     Yes     N2 77K: BET surface area mtr2):]guest],a     Chem. Commun. Along a or b axis and square channels of 9.984 Å > 9.984 Å along the c axis.       16.     1:{[Zn;(HBDC):/d mtr2):]guest],a     Yes     N2 77K: BET surface area of ca. 8078 area of ca						
<ul> <li>surface area dividues of 9.984 Å × 9.984 Å values along the caxis.</li> <li>16. 1:{[Zn<sub>2</sub>(HBDC);(d Yes M2 77K: BET The MOF has 1D channels of 7.0 x7.0 A for taking variable of the second of the s</li></ul>					· · · · · · · · · · · · · · · · · · ·	
16.       1:{[Za(HBDC);(d) mtr2;]guest], mtr2;]guest], H;BDC = 1.4- benzencicarboxyl ate acid, Hdmtrz = 3.5-dimethyl-H, 1, 2, 4-triazole       Yes       N2 77K: BET surface area of ac. 522 m²g, ate acid, Hdmtrz = 3.5-dimethyl-H, 1, 2, 4-triazole       The MOF has 1D channels along c axis, of 70 x7.0 A' ca. 552 m²g, and monobranched hexane       Chem. Commun. 2011, 47, 7197- taking van der Waals radii into aciduation. CO2 and vapor sorption studied. It shows selective adsorption of linear and monobranched hexane       2011, 47, 7197- taking van der Waals radii into sorption studied. It shows selective adsorption of linear and monobranched hexane         17.       1:[Zn(FA)(datr2):] acid, Hdatrz = 3,5- diamino-1,2,4- triazole)       Yes       N2 77K: BET me solvent accessible volume surface areas are br2 m²/g and 498 m²/g.       The solvent accessible volume in is 38.9%. At zero coverage, m²/g and 498 m²/g.       Z. Anorg. Alg in is 38.9%. At zero coverage, the CO; adsorption enthalpy for compound 1 is 23.9%         18.       1:[Zn,(TRZ),(TTB DC)_h (TRZ = 1,2,4- triazole, TTBDC = triazole, TCD (Cds(DATRZ),(BD DC)_1], (SNNU-21): {(Cds(DATRZ),(BD C)_2,(DMF)(H;O)], (SNNU-22): {(Cds(DATRZ),(BD C)_3,(DMF)(H;O)], (SNNU-22): {(Cds(DATRZ),(BD C)_3,(DMF)(H;O)], (Cds(DATRZ),(BD C)_3,(DMF)(H;O)], (Cds(DATRZ),(BD C)_3,(DMF)(H;O)], (Cds(DATRZ),(BD C)_3,(DMF)(H;O)], (Cds(DATRZ),(BD C)_3,(DMF)(H;O)], (Cds(DATRZ),(BD C)_3,(DMF)(H;O)], (Cds(DATRZ),(BD C)_3,(DMF)(H;O)], (Cds(DATRZ),(BD C)_3,(DMF)(H;O)], (Cds(DATRZ),(BD C)_3,(DMF)(H;O)], (Cds(DATRZ),(BD C)_3,(DMF)(H;O)], (Cds(DATRZ),(BD C)_3,(DMF)(H;O)], (Cds(DATRZ),(BD C)_3,(DMF)(H;O)], (Cds(DATRZ),(BD C)_3,(DMF)(H;O)], (Cds(DATRZ),(B						
mtrx)2].guest),surface area ofalong c axis, of 7.0 x7.0 Å'2011, 47, 7197-H_2BDC = 1,4-ca. 552 m²/g,taking van der Waals radii into7199.benzenedicarboxylarea of ca. 807.8sorption studied. It showssorption of linearat acid, Hdimtz =n²/g, and thesolecitive adsorption of linearand monobranched hexane17.1:[Zn(FA)(datrz)2]YesN2 77K : BETand cangmuirin s 88.9%. At zero coverage,Z. Anorg. Allg(H-FA = fumaricsurface area areand Langmuirsurface area arethe CO2 adsorption enthalpyfor compound 1 is 23.98atiazole)YesN2 77K: ThePLATON calculations showInorganic18.1.[Zn4(TRZ)4(TTBYesN2 77K: ThePLATON calculations showInorganicC(Dr) <sub>1</sub> ,C(Dr) <sub>1</sub> ,creas are25.30% and 47.2% optentialChemistry(TRZ = 1,2,4-cm²/g for 1,con yrad 402.5guest-accessible volumes,chemistry(TRZ = 1,2,4-cm²/g for 1,con yrad 402.5guest-accessible volumes,chemistry(TRZ = 1,2,4-cm²/g for 1,CO2, uptake capacity, but also highCO2, uptake capacity, but also highCO2, uptake capacity, but also highDOBDC = -2,5-diadroxyterepht2.CH only remarkable H2 andCO2, uptake capacity, but also high2017, 46, 836-(SNNU-22):(SNNU-21, -22)for thecond c32, or m²/g forcond only remarkable H2 and2017, 46, 836-(SNNU-22):(SNNU-21, -22)sorptionsotype or 1-Dsotherms are						
<ul> <li>H<sub>2</sub>BDC = 1,4- benzencicarbox/l ate acid, Hdmtz = 1, 2, 4-triazole</li> <li>17. 1:[Zn(FA)(datz)<sub>2</sub>]</li> <li>Yes</li> <li>N2 77K : BET and Langmuis surface 6,7 A* (HK isomers over a dibranched hexane 6,7 A* (HK isomers over a dibranched one. method).</li> <li>18. 1:[Zn<sub>1</sub>(TRZ)<sub>4</sub>(TTB DC)<sub>2</sub>]<sub>n</sub></li> <li>Yes</li> <li>N2 77K: The and Langmuis surface areas are benzies of ca. 807. area of ca. 807. selective adsorption of linear area of ca. 807. selective adsorption of linear isomers over a dibranched one. method).</li> <li>18. 1:[Zn<sub>4</sub>(TRZ)<sub>4</sub>(TTB DC)<sub>2</sub>]<sub>n</sub></li> <li>Yes</li> <li>N2 77K: The area are 255. 33.0% and 47.2% potential carea area 255. 33.0% and 47.2% potential computatione.</li> <li>21. (TRZ)<sub>4</sub>(TTB) (TRZ = 1,2,4- triazole, TTBDC = triazole, TTBC = triazole,</li></ul>	16.		Yes			
H;BDC = 1,4- benzenedicarboxyl at acid, Hdmtz = 3,5-dimethyl-1H, 1,2,4-trizoleLangmuir surface area of ca. 807.8 sorption studied. It shows sorption studied. It shows is 38.9%. At zero coverage (HzFA = fumaric acid, Hdatz = 3,5- diamino-1,2,4-trizole)Z Anorg. Allg Chem. 2015 1556–155918.1:[Zn <sub>4</sub> (TRZ) <sub>4</sub> (TTB trizole)YesN2 77K: The BET acid, Hdatz = 3,5- diamino-1,2,4-trizoleN2 T7K: The BET areas are 255.5 sorg and that pillar-layered MOF I and Langmuir surface 2 haveInorganic Chemistry Commun. 2015 62, 107–110.18.1:[Zn <sub>4</sub> (TRZ) <sub>4</sub> (TTB trizzole)YesN2 T7K: The BDC)], areas are 255.5 trizzole, TTBDC = triazole, TTBDC = triazole, TTBDC = triazole, TTBDC = triazole, TRZ), and triazole, TRZ = 1,2,4- triazole, TRZ = 2,5- diamity triade acid, DOBDC = 2,5- dihydroxyterephth alic acid, DOBDC = 2,5- dihydroxyterephth alic acid, DC),], (SNNU-21, -2); (CM(DATRZ)_4(B) C)_1(DMF)(H;O)], (SNNU-22); (Cd(AATRZ)_4(B) C)_1(DMF)(H;O)], and -23.YesBET surface area derived from the N2 sorption softerms are softer uptake.Dalton Trans. Surface area derived that but alice acid).19.(SNNU-22); (Cd(AATRZ)_4(B) (Cd_4(ATRZ)_2(BD) (Ca(DATRZ)_4(B) (Cd_4(ATRZ)_2		$mtrz)_2$ ].guest $_n$				
benzenedicarboxyl ate acid, Hdmtrz = 3,5-dimethyl-1H, 1, 2, 4-triazole       area of ca. 807.8 m <sup>2</sup> /g, and the pore size of ca. 6.7 A* (HK isomers over a dibranched nex. method).       sorption studied. It shows selective adsorption of linear and monobranched nex. method).         17.       1:[Zn(FA)(datr2):]       Yes       N2 77K : BET and Langmuir and Langmuir surface areas ar 2/1 m <sup>2</sup> /g and 498 m <sup>2</sup> /g.       The solvent accessible volume in is 38.9%. At zero coverage, the CO <sub>2</sub> adsorption enthalpy for compound 1 is 23.98       Z. Anorg. Allg Chem. 2015 1556-1559         18.       1:[Zn4(TRZ)_{attr2), DC)]_h 2:[Zn4(TRZ)_{c}(DO BDC)]_h 2:[Zn4(TRZ)_{c}(DO BDC)]_h 2:[Zn4(TRZ)_{c}(DO BDC)]_h (TRZ = 1.2,4- triazole)       Yes       N2 77K: The BET and Langmuir surface cm <sup>3</sup> /g and 402.5       PLATON calculations show that pillar-layered MOF 1 and 2 have       Inorganic Chem. 2015 1556-1559         18.       1:[Zn4(TRZ)_{c}(DO BDC)]_h 2:[G(ATRZ)_{c}(DO BDC)]_h trans.trans-1,3- butadiene-1,4- dicarboxylic acid, DOBDC = 2,5- dihydroxyterephth alic acid).       Yes       N2 77K: The BET surface m <sup>3</sup> /g and 402.5       PLATON calculations show that pillar-layered MOF 1 and 2 have       Inorganic Chem.istry Commun. 2015 62,107-110.         19.       (SNNU-2       2,5- dihydroxyterephth alic acid).       Yes       BET surface area derived from the DC) <sub>1</sub> [N, 22.9 and (Cd <sub>4</sub> (ATRZ) <sub>4</sub> (BD C) <sub>3</sub> (DMF)(H <sub>2</sub> O)], (Cd <sub>4</sub> (ATRZ) <sub>2</sub> (BD C) <sub>3</sub> (DMF)(H <sub></sub>		$H_{2}BDC = 1.4$ -				/199.
3.5-dimethyl-1H, 1, 2, 4-triazolepore size of ca. source size of ca. method).and monobranched hexane isomers over a dibranched one.17.1:[Zn(FA)(datrz):]YesN2 77K : BET and Langmuir and Langmuir arkine Co2 adsorption enthalpy for compound 1 is 23.98 klmol <sup>-1</sup> .Z. Anorg. Allg Chem. 2015 155–155918.1:[Zn_4(TRZ)_4(TTB DC)_1]_nYesN2 77K: The PC)_1A (Trizzole)PLATON calculations show that pillar-layered MOF 1 and 21/Zn_5(TRZ)_5(DO BDC)]_nInorganic Chemistry 21 m²/g and 498 m²/g.Inorganic 2 have18.1:[Zn_4(TRZ)_4(DO BDC)]_n (TRZ = 1,2,4- triazole, TTBDC = transt-1,3- butadine-1,4-YesN2 77K: The areas are 255.5 (21 m²/g and 492.5 (24 hot 72) (25 mothor)PLATON calculations show that pillar-layered MOF 1 and 2 haveInorganic Chemistry Commun. 2015 62,107–110.19.(SNNU- (Cd(DATRZ)_4(BD (Cd(ATRZ)_4(BD (Cd(ATRZ)_4(BD (Cd(ATRZ)_4(BD (C)_1))_nYesBET surface areas derived not only remarkable H2 and tase sites for better uptake.Dalton Trans. 2017, 46, 836- 844.19.(SNNU-22): (Cd(ATRZ)_4(BD (Cd(ATRZ)_4(BD (C)_4(DMF(H_4O))_n))YesBET surface areas derived not only remarkable CO2 and 223.All of these rod MOFs show uptake capacity, but also high N2 sorption isotherms are subace sites for better uptake.Dalton Trans. 2017, 46, 836- 844.				area of ca. 807.8		
1, 2, 4-triazole6.7A* (HK) methol).isomers over a dibranched one. methol).17.1: [Zn <sub>1</sub> (FA)(datrz) <sub>2</sub> ]YesN277K : BET and Langmuir surface areas are $T^{21}$ m <sup>2</sup> /g and 498 $T^{21}$ m <sup>2</sup> /g.The solvent accessible volume in is 38.9%. At zero coverage, the CO <sub>2</sub> adsorption enthalpy for compound 1 is 23.98 kJmol <sup>-1</sup> .Z. Anorg. Allg Chem. 201518.1: [Zn <sub>4</sub> (TRZ) <sub>4</sub> (TTB triazole)YesN277K: The BET and Langmuir surface areas are 255. G.30% and 47.2% potential careas are 255.Inorganic Chemistry Commun. 201518.1: [Zn <sub>4</sub> (TRZ) <sub>4</sub> (TTB triazole, DC) <sub>1</sub> ] (TRZ = 1,2,4- triazole, TTBDC = trans.1,3- butatiene-1,4- dicarboxylic acid, DDBDC = 2,5- dihydroxyterepth alic acid).YesN2 PLATON calculations show that pillar-layered MOF 1 and Langmuir surface areas are 255. cm <sup>3</sup> /g and 402.5 c.Inorganic Chemistry Commun. 2015 62,107–110.19.(SNNU- (SNNU-22): (Cds(DATRZ) <sub>4</sub> (BD C) <sub>3</sub> (DMF)(H <sub>2</sub> O)) <sub>n</sub> YesBET Surface areas derived from the N2 sorption isotherms are (Cda(ATRZ) <sub>2</sub> (BD C) <sub>3</sub> (DMF)(H <sub>2</sub> O)) <sub>n</sub> BET surface and 2-23.All of these rod MOFs show not only remarkable CO2 uptake capacity, but also high N2 sorption isotherms are (Cda(ATRZ) <sub>2</sub> (BD C) <sub>3</sub> (DMF)(H <sub>2</sub> O)) <sub>n</sub> YesBET surface and 2-23.All of these of MOFs show put and hand C2- phydrocarbons over CH4 selectivity under ambient (Cda(ATRZ) <sub>2</sub> (BD C) <sub>3</sub> (DMF)(H <sub>2</sub> O)) <sub>n</sub> Daton Trans. SNNU-21 pig for SNNU-21 pig for SNNU-21 pig for SNNU-21 pig for SNNU-21 pig for SNNU-21 pig for <br< td=""><td></td><td></td><td></td><td></td><td></td><td></td></br<>						
$\begin{array}{c c c c c c c c c c c c c c c c c c c $						
17. $1:[Zn(FA)(datrz)_2]$ YesN2 77K : BET and LangmuirThe solvent accessible volume in is 38.9%. At zero coverage, surface areas are the CO2 adsorption enthalpy for compound 1 is 23.98 kJmol <sup>-1</sup> .Z. Anorg. Allg Chem. 201518. $1:[Zn_4(TRZ)_4(TTB))_1/22_1/200$ YesN2 77K: The BDC)_2_n $2:[Zn_2(TRZ)_2(DO))_1/22_1/2_1/2_2(DO))_1/2_1/2_1/2_2(DO)PLATON calculations showthat pillar-layered MOF 1 and2 areas are 255.5Inorganic(Chem. 2015)BDC)]_nYesN2 77K: TheBET and2 areas are 255.5PLATON calculations showthat pillar-layered MOF 1 and2 haveareas are 255.5Inorganic(ChemistryCommun. 2015)BDC)]_nYesN2 77K: TheBET and2 haveareas are 255.5PLATON calculations showthat pillar-layered MOF 1 and2 haveareas are 255.5Inorganic(ChemistryCommun. 2015)BDC)]_nYesN2 77K: TheBET and2 haveareas are 255.5PLATON calculations showthat pillar-layered MOF 1 and2 haveareas are 255.5Inorganic(Chemistry)2 haveareas are 255.519.(SNNU-2):2 (Cd_3(DATRZ)_4(B))YesBET surfaceareas derived12.([Cd_4(ATRZ)_2(BD))_1)_1([CH_3)_2)_1]Yes19.(SNNU-22):\{Cd_4(ATRZ)_2(BD)C)_3(DMF)(H_2O)\}_nYesBET surfaceareas derived19.1, 222.9 and50.00000000000000000000000000000000000$		1, 2, 4-mazore			isomers over a dibranched one.	
and (H <sub>3</sub> FA = fumaric acid, Hdatz = 3,5- diamino-1,2,4- triazole)and surface areas are 721 m <sup>2</sup> /g and 498 m <sup>2</sup> /g.in is 38.9%. At zero coverage, the CO2 adsorption enthalpy for compound 1 is 23.98Chem. 2015 155-155918.1:[Zn4(TRZ)4(TTB DC)2]_nYesN2 77K: The BET and Langmuir surface areas are 255.5PLATON calculations show tat pillar-layered MOF 1 and 2 haveInorganic Chemistry Commun. 201518.1:[Zn4(TRZ)4(TTB DC)2]_nYesN2 77K: The BET and Langmuir surface areas are 255.5PLATON calculations show tat pillar-layered MOF 1 and 2 haveInorganic Chemistry Commun. 201519.(SNNU- 2.5- dihydroxyterephth alic acid).YesN2 77K: The areas are 255.5PLATON calculations show and 0.2.5Inorganic Chemistry Commun. 201519.(SNNU- 2.5- dihydroxyterephth alic acid).YesBET areas derived from the N2 sorption isotherms are 190.1, 222.9 and CJ_(DMF)(H <sub>2</sub> O)]_nAll of these rod MOFs show not only remarkable CO2 uptake capacity, but also high CO2 over CH4 and C2- uptake capacity, but also high cO2 over CH4 and C2- isotherms are 190.1, 222.9 and CJ_(DMF)(H <sub>2</sub> O)]_nDalton Trans. SNNU-21, are 22, share selectivity under ambient conditions.Dalton Trans. selectivity under ambient conditions.	17.	$1:[Zn(FA)(datrz)_2]$	Yes		The solvent accessible volume	Z. Anorg. Allg.
acid, Hdatrz = 3,5- diamino-1,2,4- triazole) $721 \text{ m}^2/\text{g}$ and 498 m²/g.for compound 1 is 23.98 kJmol <sup>-1</sup> . <b>18.</b> 1:[Zh4,(TRZ)4(TTB DC)2]n BDC)]nYesN2 77K: The BET and Langmuir surface areas are 255.5PLATON calculations show that pillar-layered MOF 1 and 2 haveInorganic Chemistry Commun. 2015 62, 107–110.(TRZ = 1,2,4- triazole, TTBDC = trans.1,3- butatiene-1,4- dicarboxylic acid, DC)a[] aYesS8.7 cm³/g and 402.5 gm 402.5 cm³/g for 1, respectively. Both MOFs show not only remarkable H2 and C02 uptake capacity, but also high C02 over CH4 selectivity. In 2, OH groups act as lewis base sites for better uptake.Dalton Trans. 2017, 46, 836- 844. <b>19.</b> (SNNU- 21):{[(CH_3)_2NH_2]_2 (Cd_(ATRZ)_2(BD C)_3]DMF)(H_2O)}, NU-22): {Cd_4(ATRZ)_2(BD C)_3(DMF)(H_2O)},YesBET surface areas derived from the N2 sorption some and -23.All of these rod MOFs show not only remarkable CO2 uptake capacity, but also high N2 sorption solut also high N2 sorption and -23.Dalton Trans.		n		and Langmuir		
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triazole)YesN277K: The BTPLATON calculations show that pillar-layered MOF 1 and 2 [Zn2(TRZ)2(DO BDC)]_nInorganic Chemistry Commun. 2015 $(TRZ = 1,2,4-$ triazole, TTBDC = triazole, TTBDC = triazole, 2, 174, 2000TRZ = 1,2,4- cm³/g and 402.5PLATON calculations show that pillar-layered MOF 1 and 2 haveChemistry Commun. 2015 $(TRZ = 1,2,4-$ triazole, TTBDC = triazole, T						
18. $1:[Zn_4(TRZ)_4(TTB)$ $DC)_2]_n$ $2:[Zn_2(TRZ)_2(DO)$ $BDC)]_n$ Yes $N_2$ 77K: The BET and Langmuir surface areas are 255.5PLATON calculations show that pillar-layered MOF 1 and $2$ haveInorganic Chemistry Commun. 2015 $BDC)_n$ $(TRZ = 1,2,4-$ triazole, TTBDC = triazole, TTBDC = trans,trans-1,3- butadiene-1,4- dicarboxylic acid, $DOBDC = 2,5-$ dihydroxyterephth alic acid).Yes $N_2$ $RET$ $R$				m/g.	KJIIIOI .	
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triazole, TTBDC = $cm^3/g$ for 1, $288.7$ $cm^3/g$ and $448.1$ $cm^3/g$ for 1, $288.7$ $cm^3/g$ and $448.1$ $cm^3/g$ for 1, $288.7$ $cm^3/g$ and $448.1$ $cm^3/g$ for 1, $C_2$ uptake capacity, but also high CO <sub>2</sub> over CH <sub>4</sub> selectivity. In 2, OH groups act as lewis base sites for better uptake. <b>19.</b> (SNNU- $21): {[(CH_3)_2NH_2]_2}$ $[Cd_5(DATRZ)_4(B)$ DC) $_{1,1}$ Yes $CD_4]_{1,n}$ BET $SNNU-22):$ ${(SNNU-22):}$ All of these rod MOFs show uptake capacity, but also high $CO_2$ over CH <sub>4</sub> and C2- high CO2 over CH <sub>4</sub> and C2- uptake capacity, but also high $844.$ (SNNU-22):Yes ${(Cd_4(ATRZ)_2(BD)}$ ${(Cd_3(DMF)(H_2O))_n}$ SNNU-21, -22 and -23.SNNU-21 has two types of 1-D and -23.Datom Trans. SNNU-21 has two types of 1-D channels exist along the a-axis						62, 107–110.
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$\hat{C}_{3}(\hat{DMF})(\hat{H}_{2}\hat{O})_{n}$ SNNU-21, -22 SNNU-21 has two types of 1-D and -23. channels exist along the a-axis		· · · · · · · · · · · · · · · · · · ·				
and -23. channels exist along the a-axis						
(SNNU-23): $H_2$ , $CH_4$ , $CO_2$ , direction with the dimensions				and -23.	e	
		(SNNU-23):		$H_2$ , $CH_4$ , $CO_2$ ,	direction with the dimensions	

20.	$ \{ [(CH_3)_2NH_2]_2[Zn_{5}(TRZ)_4(BDC)_4] \}_n $ $ (TRZ = 1,2,4-triazole, ATRZ = 3-amino-1,2,4-triazole and DATRZ = 3,5-diamino-1,2,4-triazole, BDC = 1,4-benzenedicarboxyl ic acid).  1:[Zn(AmTAZ)(CH_3 COO)]  2:[Zn_4(AmTAZ)_4(SO 4)(OH)(C_2O_4)_{0.5}].2H_2 O  3: [Cd(AmTAZ)Br  4:[Cd(AmTAZ)Br  4:[Cd(AmTAZH)SO_4]  1: {[Zn_7(trz)_6(1,3-bdc)_4(H_2O)_2].2H_2O_n  2:{[Zn_4(trz)_4(Hnip)_2(ni)} $	Yes		C <sub>2</sub> H <sub>2</sub> adsorption studied. Not truly ultra- microporous	of about 6.0 Å × 7.0 Å and 7.5 Å × 10.5 Å with DMF cations in the pore. SNNU-22 has channels of 4.0 Å × 5.0 Å and 6.0 Å × 10.0 Å. SNNU-23 has two types of channels with dimensions of about 3.5 Å × 11 Å and 6.0 Å × 12 Å extend along the a-axis, and one type of channel (3.0 Å × 6.5 Å) exists along the b-axis direction. 1 is 2D. 2 has 3D framework with three kinds of 1D channel; hexagonal prismatic channel (11.5x8.0A°), quadrangular prismatic channels (6.9x9.6A°) and a second quadrangular prismatic channel (7.1x7.1A°). 3 crystallizes in a chiral space group P212121, giving a homochiral 3D framework with 2 types of helical channels (left- and right-handed). 3- amino-1,2,4-triazole molecules in 4 behave as neutral m2-2,4- bridges to connect the 2D CdSO <sub>4</sub> sheets into a 3D framework. All 3D. 1 displays intersecting ring channels as viewed from b and c directions. Even after interpenetration, it presents rhombic-shaped channels along the b-axis, and the channel size is ~4.8 × 5.1 Å <sup>2</sup> . If	Journal of Solid State Chemistry, 2008, 181, 2078– 2086. Crystal Growth & Design, 2009, 9, 105.
	p)]n 4:[Zn <sub>5</sub> (trz) <sub>2</sub> (Hbtc) <sub>4</sub> (H 2O) <sub>4</sub> ]n H <sub>2</sub> hip : 5- hydroxyisophthalic acid H <sub>2</sub> nip: 5- nitroisophthalic acid				1 is viewed from the c-axis, a larger channel can be seen with cross dimensions of about $5.6 \times 6.3 \text{ Å}^2$ . 2 is isostructural to 1 and the channel size is $\sim 4.6 \times 5.0 \text{ Å}^2$ along the b-axis, and the channel size is about $5.1 \times 5.3 \text{ Å}^2$ viewed from the c-axis.	
22.	{[Cu <sub>3</sub> (dmtrz) <sub>2</sub> (OX) <sub>2</sub> - (H <sub>2</sub> O) <sub>2</sub> ].8.5H <sub>2</sub> O} <sub>n</sub>		Yes	N <sub>2</sub> 77K: BET surface area: 676.4 m <sup>2</sup> /g. Pore volume of 0.212 cm <sup>3</sup> /g. The Horvath– Kawazoe (HK) model indicates a pore diameter of 4.31A	It shows single-crystal-to- single-crystal transformation during a reversible dehydration and rehydration process accompanied by color change from blue to violet to blue. The hydrogen adsorption of anhydrous la was evaluated at 77 K and 87 K. The H <sub>2</sub> sorption isotherm shows type-I behaviour without hysteresis and noticeable change in properties upon repeated cycles. At 1 atm, anhydrous la showed a gravimetric H <sub>2</sub> uptake of 1.48 and 1.26 wt% at 77 and 87 K, respectively, which corresponds to a H <sub>2</sub> storage capacity of 19.2 and 16.3 g/L.	CrystEngComm, 2011, 13, 768– 770.
23.	Zr(OH) <sub>2</sub> (C <sub>2</sub> O <sub>4</sub> )	No	Water adsorpti on	It has a void volume of 8.9%, which is quite	The homometallic 3D framework displays channels along the c axis with a square	Cryst. Growth Des., 13, 11, 5100-5106

			small. Guest free phase shows reversible uptake of water but no gas uptake.	cross-section with side dimensions of 6.492(2) Å (Zr–Zr separation) decorated by the hydroxo units (O•••O separation, 3.382(4) Å). Here, hydroxyl moieties are terminally bound to metal and point towards channel.	
24.	barium titanyl oxalate (BTO): BaTi(O)(C2O4)2.5H2 O	Yes		The chemical formula is more accurately described as $Ba_2Ti_2O_2(C_2O_4)_{4.}10H_2O$ in order to account for the number of unique atoms in the structure. Seven of the ten water molecules are associated with barium atoms, and the remaining three waters occupy interstitial sites in the structure and are not coordinated to either titanium or barium atoms. The compound readily loses water beginning at room temperature, depending on drying conditions and/or relative humidity; hence in the past the compound has been referred to most often as the tetrahydrate, BaTi(O)(C_20_4)_2.4H_20.	Chem. Mater., 1992, 4, 1208- 1216.
25.	[Ti <sub>2</sub> O <sub>3</sub> (H <sub>2</sub> O) <sub>2</sub> ](C <sub>2</sub> O <sub>4</sub> )· H <sub>2</sub> O	Yes		This is the first report of a single Ti(IV) oxalate. The structure consists of inorganic corrugated layers of cornersharing TiO <sub>6</sub> octahedra, which forms infinite $-Ti-O-Ti-$ connections, linked together by the oxalate anions and rest coordination sites occupied by water giving a nonporous framework.	Solid State Sciences, 2003, 5, 175–182.
26.	NH4[Ti(C2O4)2·2H2O	Yes		3D structure of the eight- coordinated polymeric titanium(III) complex contains a counter-balancing NH <sub>4</sub> <sup>+</sup> cations in the pore making the framework non-porous in nature.	Inorganica Chimica Acta, 1993, 203, 219- 222.
27.	1. $[Eu(NTA)(H_2O)_2]$ · H <sub>2</sub> O 1a. $[Eu(NTA)(H_2O)_2]$ 2. $[Tb(NTA)(H_2O)]$ 3. $[Ho(NTA)(H_2O)]$ 4. $[Ho(NTA)(H_2O)]$ 5. $[Tm(NTA)(H_2O)]$ Where, NTA = nitrilotriacetate		No adsorption data available.	1 is an irregular 2D lattice motif with alternative L- and R-type single-chain helixes while 1a is 3D structure. But, both 2 and 3 are 2D double layer structures. Again, 4 and 5 display 3D frameworks, which have 1D channel fabricated through interweaving left/right-hand triple-stranded helixes.	Crystal Growth & Design, 2010, 10, 775-781.
28.	(C <sub>8</sub> H <sub>4</sub> CeO <sub>18</sub> Zr) <sub>n</sub> .nH <sub>2</sub> O			It is a 3D structure with pore along two crystallographic axes. Each $Ce^{4+}$ & $Zr^{4+}$ occupied by four oxalates in $\mu^2$ chelating fashion and two water molecules to give neutral framework.	CSD Communication( Private Communication), 2007, CCDC 227146.
29.	[Sm <sub>2</sub> (fumarate) <sub>3</sub> (H <sub>2</sub> O) )4]·3H <sub>2</sub> O	Yes		The layered pillared Sm- fumarate layer is wavy and this makes the 3D framework less open. Despite the rigidity of	Dalton Trans., 2006, 765-768.

				fumarate, MOF upon dehydration (loses ~15% mass) shrinks reversibly.	
30.	MIL-53(Al)-FA: Al(OH)(fumarate) 3.5H <sub>2</sub> O	Yes	The porosity of the activated Al fumarate was determined by N <sub>2</sub> porosimetry at 77 K. The experimental BET area of 1080 m <sup>2</sup> g <sup>-1</sup> . For pure dry CO <sub>2</sub> , the breakthrough capacity is around 75% of the equilibrium saturation capacity. Under 14% RH, an uptake of 1.4 mmol/g was observed, which is 17% less than predicted from the CO <sub>2</sub> equilibrium isotherm, indicating the influence of water on CO <sub>2</sub> adsorption.	It has square-shaped 1-D channels with dimensions 5.7 x $6.0 \text{ Å}^2$ . The Al-hydroxy- fumarate is quite rigid and its dehydrated form shows a notable structural change only at 250MPa (2500bar) and above. It is very stable due to the inorganic SBU- hydroxyl bridged Al- chains. Despite of having hydrophilic channels material is quite stable to water (type-IV isotherm for water sorption).	Angew. Chem. Int. Ed., 2015, 54, 3664–3668. RSC Adv., 2014, 4, 24073-24082. Ind. Eng. Chem. Res., 2016, 55, 2134–2143.
31.	MIL-88A: Fe <sup>III</sup> <sub>3</sub> O(CH <sub>3</sub> OH) <sub>3</sub> {O <sub>2</sub> C-C <sub>2</sub> H <sub>2</sub> -CO <sub>2</sub> <sup>-</sup> } <sub>3</sub> (CH <sub>3</sub> CO <sub>2</sub> <sup>-</sup> )·(CH <sub>3</sub> OH) <sub>4.5</sub>	Yes	Interestingly, despite the presence of acetate ions in the channels, MIL-88 takes up about 4.5mmol/g of CO <sub>2</sub> selectively over N <sub>2</sub> as ascertained from a dynamic breakthrough study.	MIL-88A exhibits a 3D structure built up from trimers of iron(III) octahedra linked to fumarate di-anions to create a 3D framework with a cage- structure with 6Å windows. This structure consists of both 1D pore channel along the c axis, which is filled with methanol and cages, which are filled with acetate groups. After removal of methanol it creates potential voids.	Angew. Chem. Int. Ed., 2004, 43, 6286–6289.
32.	MIL-88B: Fe <sub>2</sub> NiO(OOC-C <sub>6</sub> H <sub>4</sub> - COO) <sub>3</sub> · 3DMF	Yes	From $N_2$ porosimetry at 77K, calculated BET surface area 1120, 549, 465, 355 and 30 m <sup>2</sup> g <sup>-1</sup> for bipyridine, pyrazine, DMF and water phase respectively. CO <sub>2</sub> adsorption capacity of the all phases increase with the increase in porosity of the samples. Bipyridine phase shows the highest capacity, 101 cc g <sup>-1</sup> STP of CO <sub>2</sub> .	MIL-88B has terminally bound DMF, which can easily be replaced by terminal ligands like H <sub>2</sub> O, pyridine, pyrazine, 4,4'-bipyridine. This helps retain the breathing effect. Among all the phases, MIL- 88B with terminal bipyridine shows highest surface area.	Dalton Trans., 2013, 42, 550– 557.

33.	MOF-801: Powder form is denoted as MOF- 801-P and single crystal form is denoted as MOF- 801-SC.	Yes	BET and Langmuir surface area for MOF- 801-SC are 690 and 770 m <sup>2</sup> g <sup>-1</sup> respectively whereas those for MOF- $801$ -P are 990 and 1070 m <sup>2</sup> g <sup>-1</sup> . CO <sub>2</sub> Uptakes at 0.15 and 1 bar & 298K are 0.75 and 2.22 mmol g <sup>-1</sup> . CO <sub>2</sub> /N <sub>2</sub> Selectivity at 1 bar and 298K is 78.	There are two crystallographically independent tetrahedral cavities, with slightly different sizes of 5.6 Å and 4.8 Å diameter in the core framework. The diameter of the octahedral cavity is 7.4 Å.	J. Am. Chem. Soc. 2014, <b>136</b> , 4369.
34.	IRMOF-1: Zn4O(FMA)3	Yes	The Langmuir & BET surface areas: 1618 and 1120 $m^2g^{-1}$ , respectively. It can take 69 wt% CO <sub>2</sub> at 300 K & 28 bar. At 1 bar it takes approx. 8.5 wt% of CO <sub>2</sub> , HOA: 29 kJ/mol.	The Zn-fumarate has a 3D primitive cubic ( $\alpha$ -Po) structure with intersecting pores of ~6.8 x 6.8 Å <sup>o</sup> . The structure is built from octahedral Zn <sub>4</sub> O units, bridged by fumarate.	Inorg. Chem., 2009, <b>48</b> , 4649- 4651.
35.	UiO-66(Zr- Terepthalate):	Yes	BET surface area: $1105 \text{ m}^2\text{g}^{-1}$ , CO <sub>2</sub> Uptake at 1 bar & 298K: 1.8 mmol/g, CO <sub>2</sub> /N <sub>2</sub> Selectivity at 1 bar and 298K: 27 and HOA: 25 kJ/mol.	UiO-66 is one of the few known water-stable MOFs that are readily amenable to direct ligand substitution. In this work, UiO-66 has been synthesized with amino-, nitro-, methoxy-, and naphthyl- substituted ligands to impart polar, basic, and hydrophobic characteristics.	Langmuir, 2012, 28, 15606–15613.
	UiO-66-NH2		BET surface area: 1112 m <sup>2</sup> g <sup>-1</sup> , CO <sub>2</sub> Uptake at 1 bar & 298K: 2.97 mmol/g, CO <sub>2</sub> /N <sub>2</sub> Selectivity at 1 bar and 298K: 58 and HOA: 28 kJ/mol.	Its channels are functionalized by amine groups. It shows a significant enhancement for $CO_2$ uptake compared with that of non-functionalized UIO-66 due to the existence of electrostatic attractive interactions between amine group present and $CO_2$ .	
36.	UiO-66-EA	Yes	Langmuir surface area: 567 m <sup>2</sup> g <sup>-1</sup> , CO <sub>2</sub> Uptake at 1 bar & 298K: 1.69 mmol/g, CO <sub>2</sub> /N <sub>2</sub> Selectivity at 1 bar and 298K: 365 and HOA: 66 kJ/mol.	CO <sub>2</sub> uptake is less due to the bulky nature of the aliphatic amine groups. High HOA value for UiO-66-EA at low coverage is indicative of a chemisorption interaction and that is why high CO <sub>2</sub> /N <sub>2</sub> Selectivity is found for this material.	J. Mater. Chem. A, 2015, 3, 21849–21855.
57.	$[Ln_2(fum)_2(ox)]   YesWhere, Ln = Eu andTb$		Adsorption studies not done.	the loss of coordination water and probable collapse of the open frameworks.	Inorg. Chem., 2007, <b>46</b> , 1337 1342.
38.	UTSA-16: [KCo <sub>3</sub> (C <sub>6</sub> H <sub>4</sub> O <sub>7</sub> )(C <sub>6</sub> H <sub>5</sub> O <sub>7</sub> )(H <sub>2</sub> O) <sub>2</sub> ]	Yes	It has high uptake (160 cm <sup>3</sup> cm <sup>-3</sup> ) of CO <sub>2</sub> at 296 K & 1 bar pressure. The $CO_2/N_2$ selectivity is 314	This is an open framework with diamondoid cage of dimension 3.3 Å x 5.4 Å. It is an Ultra microporous material.	Nat. Commun., 2012, 3, 954-963.

			at 100 kPa and 296 K.		
39.	NOTT-300: $[Al_2(OH)_2(L)](H_2O)_6$ (L = biphenyl-3,3',5,5'- tetracarboxylate)	Yes	No uptake of H <sub>2</sub> and N <sub>2</sub> at 77 K and at 87 K respectively. Saturated CO <sub>2</sub> uptake at 273 K and 7.0 bar = 8.7 mmol g <sup>-1</sup> , Zero- loading HOA: 27-30 kJ mol <sup>-1</sup> , selectivities for CO <sub>2</sub> (CO <sub>2</sub> /CH <sub>4</sub> = 100; CO <sub>2</sub> /N <sub>2</sub> = 180; CO <sub>2</sub> /H <sub>2</sub> >105)	It consists of corner-sharing $[AlO_4(OH)_2]$ octahedra linked through two mutually cis- $\mu_2$ -OH groups forming infinite chains. Four such chains are cross-linked to give rise to square-shaped channels of size ~6.5 × 6.5 Å. The pore is functionalized with free hydroxyl groups in four different directions which are actually favorable CO <sub>2</sub> adsorption sites.	Nature Chemistry, 2012, 4, 887-894.
40.	[Co <sup>II</sup> Co <sup>III</sup> (OH)Cl <sub>2</sub> (bbt a)] Where, H <sub>2</sub> bbta = 1H,5H-benzo(1,2- d:4,5-d0)bistriazole)	Yes	From a volumetric point- of-view, CO <sub>2</sub> uptake: 9.1 mmol cm <sup>-3</sup> at 298 K and 1 bar, CO <sub>2</sub> capture capacity: 4.1 mmol cm <sup>-3</sup> from simulated flue gases (CO <sub>2</sub> pressure 0.10– 0.15 bar at 313 K) at relative humidity (82%), Zero-loading HOA = 130-140 kJ mol <sup>-1</sup> , at 298 K CO <sub>2</sub> /N <sub>2</sub> selectivity: 262,	The study shows the potential of monodentate hydroxide to act as a good candidate for CO <sub>2</sub> affinity.	Energy Environ. Sci., 2015, 8, 1011–1016.
41.	MFM-300( $V^{II}$ ): [ $V^{III}_2(OH)_2(L)$ ], Where, $LH_4$ =biphenyl- 3,3',5,5'- tetracarboxylic acid}	Yes	Very less uptake of N <sub>2</sub> , CO <sub>2</sub> uptake: 6 mmol $g^{-1}$ at 1 bar and 298K, at low coverage isosteric heat of adsorption (Q <sub>st</sub> ) = 27.5–28 kJ mol <sup>-1</sup> ,	This is a hydroxyl functionalized MOF. The pore size is $\sim$ 6.7 x 6.7Å for MFM-300(V <sup>III</sup> ).	Nat. Commun., 2017, <b>8</b> , 14212.
42.	Mg/DOBDC Co/DOBDC Ni/DOBDC Zn/DOBDC	Yes	BET surface area: 1495, 1080, 1070 and 816 m <sup>2</sup> g <sup>-1</sup> for Mg/DOBDC, Co/DOBDC, Ni/DOBDC and Zn/DOBDC; CO <sub>2</sub> uptake at 296 K & 1 atm: 35.2, 30.6, 25.6 and 24.4 wt% for Mg/DOBDC, Co/DOBDC, Ni/DOBDC and Zn/DOBDC; HOA: 47 kJ/mol for Mg/DOBDC & 41 and 37 kJ mol <sup>-1</sup> for Ni/ DOBDC and Co/DOBDC respectively.	This study shows the systematic evaluation of the effects of metal identity on surface area and $CO_2$ uptake owing to the strong head-on interaction of the polarized oxygens of the $CO_2$ with the open metal site.	J. Am. Chem. Soc. 2008, 130, 10870–10871.

43.	SGU-29:	Yes	From N <sub>2</sub> at 77K	The channel in SGU-29 has a	Science, 2015,
	Na2CuSi5O12		adsorption BET surface area: 457 $m^2$ g <sup>-1</sup> . CO <sub>2</sub> uptake at 1000, 100, and 0.4 mbar and 298 K are 156, 126, and 26 cm <sup>3</sup> cm <sup>-3</sup> , respectively; HOA for CO <sub>2</sub> = 51 kJ/mol.	window size of $4.5 \times 7.3$ Å. It has H <sub>2</sub> O-specific and CO <sub>2</sub> - specific adsorption sites but does not have H <sub>2</sub> O/CO <sub>2</sub> - sharing sites. Therefore, it readily adsorbs both H <sub>2</sub> O and CO <sub>2</sub> from the humid flue gases and atmosphere, without interfering with the adsorption of CO <sub>2</sub> .	350, 302.
44.	Cu-BTC	Yes	At all pressure range, the experimental sample loaded with 4 wt % water adsorbs more $CO_2$ (~700 mg g <sup>-1</sup> ) than the dry sample (~500 mg g <sup>-1</sup> ) agrees well to simulation study. Again, a fully hydrated Cu- BTC adsorbs very less $CO_2$ (200 mg g <sup>-1</sup> ) at all pressures, which is due to the fully occupied pores with water molecules.	This study shows enhancement of CO <sub>2</sub> Adsorption in Metal- Organic Frameworks via Occupation of Open-Metal Sites by Coordinated Water Molecules. This result was first discovered using molecular simulation and then verified experimentally, showing the power of molecular modeling.	Chem. Mater., 2009, 21, 1425– 1430.
45.	[Ni(II) <sub>2</sub> Ni(III)(μ3- OH)(LP) <sub>3</sub> (L2) <sub>1.5</sub> ] Where, LP = linear Pyridine carboxylate, L2= linear di- carboxylate)	Yes	These possess surface areas in excess of 2000 $m^2 g^{-1}$ (from 77 K N <sub>2</sub> adsorption)	All the frameworks have cavities in the range of ultra- micro pore sized windows along with some micro pore- sized ones.	Nat. Commun. 2012, 3, 642.
46.	1. SIFSIX-2-Cu 2. SIFSIX-2-Cu-i 3. SIFSIX-3-Zn	Yes	1. BET surface area (N <sub>2</sub> sorption) 3,140 m <sup>2</sup> g <sup>-1</sup> ; pore size 13.05 A°; CO <sub>2</sub> uptake at 298 K & 1 bar pressure: 1.84 mmol g <sup>-1</sup> ; Q <sub>st</sub> for CO <sub>2</sub> at low loading: 22 kJ mol <sup>-1</sup> ; Selectivity (IAST) at 1 bar: CO <sub>2</sub> /N <sub>2</sub> = 13.7, CO <sub>2</sub> /CH <sub>4</sub> = 5.3; 2. BET surface area (N <sub>2</sub> sorption) 735 m <sup>2</sup> g <sup>-1</sup> ; pore size 5.15 A°; CO <sub>2</sub> uptake at 298 K & 1 bar pressure: 5.41 mmol g <sup>-1</sup> ; Q <sub>st</sub> for CO <sub>2</sub> at low loading: 31.9 kJ mol <sup>-1</sup> ,	Crystal engineering or reticular chemistry strategy controls pore functionality and size in a series of MOMs with coordinately saturated metal centres and periodically arrayed hexafluorosilicate (SiF62–) anions and enables a 'sweet spot' of kinetics and thermodynamics that offers high volumetric uptake at low CO2 partial pressure (less than 0.15 bar).	Nature, 2013, <b>495</b> , 80.

			(IAST) at 1 bar: $CO_2/N_2 = 140$ , $CO_2/CH_4 = 33$ , $CO_2/H_2 = 240$ ; 3. BET surface area (N <sub>2</sub> sorption) 250 m <sup>2</sup> g <sup>-1</sup> ; pore size e 3.84 A°; Q <sub>st</sub> for $CO_2$ at low loading: 45 kJ mol <sup>-1</sup> ; Selectivity (IAST) at 1 bar: $CO_2/N_2 = 1,818$ ,		
47.	(1) [{[CuSiF <sub>6</sub> (4,4'- Bipyridine) <sub>2</sub> ]·8H <sub>2</sub> O}] (2) [[ $T_{2}$ (4.4')	Yes	$CO_2/CH_4 = 231,$ $CO_2/H_2 =$	Both compound (1) & (2) are similar in structure. Both form	Angew. Chem. Int. Ed., 2000, 20 2081 2084
	(2) $[{[Zn(4,4)^{-} Bipyridine)_2 (SiF_6)}_n]$		compound (1) (volumetric Ar sorption at 87.5 K)= 1337 m <sup>2</sup> g <sup>-1</sup> ; At 36 atm and 298 K the density of CH <sub>4</sub> adsorbed in (1) is 0.21 g ml <sup>-1</sup> .	non-interpenetrated 3D network and both consists of 8 X 8 Å <sup>2</sup> along <i>c</i> -axis and 6 X 2 Å <sup>2</sup> along <i>a</i> and <i>b</i> -axes. Compound (2) was made in DMF-dioxane mixed solvent and if synthetic medium is water then it gives interpenetrated [{[Zn(4,4'- Bipyridine) <sub>2</sub> (H2O) <sub>n</sub> ](SiF <sub>6</sub> ) <sub>n</sub> ].	39, 2081-2084.
48.	Mg2(DHFMA) Where, DHFMA = dihydroxyfumaric acid.	Yes	Due to smaller length of DHFMA Mg(DHFMA) Becomes a truly microporous MOF.	One in every six atoms in DHFMA is an open metal site, whereas one in every nine atoms in DOBDC is an open metal site. So when these isostructural MOFs are compared the CO2 interacts via a direct head-on mode in the DOBDC (MO=C=O = 2.33 Å) while it acts a bridging molecule between two adjacent metal sites in the case of DHFMA (MO=C=O = $\sim$ 2.6 Å). Such a unique binding mode results in a much enhanced binding energy of CO <sub>2</sub> in Mg <sub>2</sub> (DHFMA), i.e., 50.1 kJ/mol, which is 20% (8.8 kJ/mol) stronger than that in Mg2(DOBDC).	J. Phys. Chem. C, 2017, 121, 1171–1181.
49.	(1) NOTT-101/ OEt (2) Cu-BTTri (3) Ni-4PyC (IISERP-MOF1) (4) VEXTUO (5) Mg-MOF-74	Yes	CO <sub>2</sub> working capacity (pure component experimental data at 303 K & 1 bar): 3.8, 3.7, 3.4, 3.1 and 2.6 mol kg <sup>-1</sup> for compound (1) to (5) respectively; CO <sub>2</sub> /H <sub>2</sub> selectivity (mixture simulation data at 313 K & 20 bar): 60, 20, 279, 48 and 365; Compound (3) i.e Ni-Pyc (IISERP-	All the MOFs are single ligand based MOFs and that is why it minimizes the chance of co- precipitation of impurity and results in a large scale production. 4-pyridine carboxylic acid (4-PyC) is a short ditopic linker (~4.95 Å) and the presence of the ring in Pyc makes Ni-Pyc (IISERP- MOF1) significantly rigid. It has a cubic framework with ultra-micropore (3.5 and 4.8 Å pores). IISERP-MOF1 was synthesized in THF/H <sub>2</sub> O/MeOH mixed solvent system.	Sci. Adv., 2016; 2: e1600909 & Sci. Adv., 2015, 1, e1500421.

		V	<b>MOF1)</b> has BET surface area of 945 m <sup>2</sup> g <sup>-1</sup> (77K N2) and exhibits a saturation CO <sub>2</sub> uptake of 11 mmol g <sup>-1</sup> (195 K) and adsorbs 3.6 mmol g <sup>-1</sup> at 303K at 1 bar, respectively.		
50.	<b>HSERP-MOF2:</b> Ni <sub>9</sub> (μ- H <sub>2</sub> O) <sub>4</sub> (H <sub>2</sub> O) <sub>2</sub> (C <sub>6</sub> NH <sub>4</sub> O <sub>2</sub> ) <sub>18</sub>	Yes	BET surface area $(N_2 77 K)$ adsorption) 470 m <sup>2</sup> g <sup>-1</sup> and a Langmuir surface area of 700 m <sup>2</sup> g <sup>-1</sup> ; CO2 uptake at 1 bar & 303 K = 4.2 mmol g <sup>-1</sup> ; Saturation uptake: ~7 mmol g <sup>-1</sup> ; At 1 bar and 313 K CO2 selectivity (s(CO2/N2) = 1853; IISERP- MOF2 shows a CO2/N2 separation of 3.97 mmol g <sup>-1</sup> as determined from a dynamic flow breakthrough separation; HOA for CO2 = 33 kJ mol <sup>-1</sup> .	Pyc ligand with Ni- salt in DMF/CH <sub>3</sub> CN mixed solvent forms IISERP-MOF2 a different phase of Ni-Pyc. NiPyC has the lowest parasitic energy among all the MOFs (PE (kJ/kg of CO <sub>2</sub> )): IISERP- MOF2 = 655, Mg-MOF-74 = 727, monoethanolamine = 1000.	

## References for Table 3 of the main text (CO<sub>2</sub> self-diffusion coefficients in porous materials ):

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Cost for large quantity of metal salt req	uired for production of	a range of MOFs
Metal salt	Price (£/Kg)	MOFs
Copper(II) hydroxide	0.65	CuBTC (HKUST-1, Basolite C-300)
		MOF-14
Zinc carbonate hydroxide	0.48	ZIF8 (Basolite Z1200),
		MOF-177,
		MOF-5,
		Zn-MOF-74,
		Various ZIFs
Aluminium chloride hexahydrate	0.40	MIL-53
Zirconium hydroxide	0.80	UIO-66(Zr)
Cost for large quantity of organic linker	r required for productio	on of a range of MOFs
Organic linker	Price (£/Kg)	MOFs
2-methyl imidazole	7.15	ZIF8 (Basolite Z1200),
Trimesic acid	24.75	Cu-BTC (HKUST-1, Basolite C-300),
		Fe-BTC (Basolite F-300),
		MIL-100
2,5-dihydroxy terephthalic acid	350.00	MOF-74 (CPO-27)
Terephthalic acid	1.50	UIO-66
		MIL-101
		MIL-53 (Basolite A100)
Imidazole	~4.00	Various ZIFs

Above table S2 is adopted from Materials 2017, 10, 1428; doi:10.3390/ma10121428.

Table S3. Costs of production selected MOFs.

Cost of the starting materials for production of some MOFs			
Adsorbent	Cost (US \$/Kg)		
CuBTC (HKUST-1)	20.08		
CoCo (Co <sub>3</sub> [Co(CN) <sub>6</sub> ] <sub>2</sub> )	35.14		
MOF-5 (IRMOF-1)	2.93		
Zn/DOBDC (Zn-MOF-74)	1.90		
Ni/DOBDC (Ni-MOF-74)	6.48		
Mg/DOBDC (Mg-MOF-74)	1.19		
Co/DOBDC (Co-MOF-74)	13.33		
MIL-100	15.64		
MIL-101	4.57		
Silica gel	1.00		

Costs listed are based on the purchase of one metric ton or greater quantity. *Above table is adopted from Liu et al., Chem. Soc. Rev.,* 2012, **41**, 2308–2322.