Electronic Supplementary Material (ESI) for Materials Advances.


# A Database to Select Affordable MOFs for Volumetric Hydrogen Cryoadsorption Considering the Cost of their Linkers

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# Supporting info

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## 1. Elaboration of the database

The CoRE MOF ASR 2019 (Computational-Ready Experimental MOFs, all solvent removed) database contains 9,146 optimised MOF structures in which solvent molecules, coordinated or not to metallic atoms, have been removed from the cavities. This database provides structures' identifiers used in the MOF-subset of the Cambridge Structural Database (CSD), their porous properties like gravimetric and volumetric accessible areas, pore volume, void fraction, and density; and the metallic composition as well as the potential presence of open metallic sites (OMS).[1] From this list, 5,295 materials would ideally meet the target of 40 g/L for 2025 according to the estimation procedure described in section 1.2. The Core MOF database includes the metallic information for each structure, making it possible to screen among structures made out of feasible metals. The most affordable metals are abundant in the Earth's crust, non-noble, and industrially relevant.[2] Cheaper or more abundant metals than W are selected (Al, Ca, Cd, Cr, Cu, Fe, Li, Mg, Mn, Mo, Na, Ni, Si, Sn, Sr, Ti, V, Zn, and Zr).

### 1.1. Composition of MOFs

The organic composition of MOFs is not defined in the CoRE MOF database[1] nor the CSD MOF subset[3]. This crystallographic information has been coded as MOFid codes for most of these structures.[4] MOFid codes consist of Canonical SMILES strings coding the inorganic and organic chemical components of MOFs from the CoRE MOF database, topology, and identifier of the corresponding MOF structure. Some of the SMILES strings provided correspond to fragments or substructures of linkers so that these codes could indicate a higher number of components than those actually present in the material. This algorithm also provides a second code, the MOFKey, linking the metallic elements and the InChiKey (a fix-length format of the International Chemical Identifier) of the linkers present in the structure. However, the same limitations affect MOFKey and MOFid since they both start from the deconstruction of the crystallographic data. Therefore, the MOFid and the MOFKey do not code the organic composition of ca. 10 % of the structures in the CoRE MOF database.
In this work, the chemical composition of a selection of 3,786 structures was directly obtained from the CSD. The software ConQuest (under license of CCDC) generates a ".cfg" file compiling the deposited crystallographic information and chemical composition for each structure. This composition was split into its components (linkers, solvents, other coordinated molecules, and extra-framework substances) by performing a described algorithm in section 1.4. Common solvents such as dimethylformamide, ethanol, methanol, and water were removed from the list of components, leaving other organic molecules such as structuring agents (SDA) or charge-balancing ions.

In total, 2,207 organic molecules appear in this selection, some of which are named following different nomenclature rules (i.e., terephthalate, 1,4-benzenedicarboxilate, or benzene-1,4-dicarboxylate).

## 1.2. Estimation of the volumetric hydrogen uptake

The gravimetric hydrogen uptake was calculated for these structures using an estimating method starting from the porous properties specific surface area and pore volume of structures with a higher pore volume than 0.3 $cm^3/g$.[5] The volumetric uptake of each structure was calculated by multiplying the gravimetric uptake by the corresponding crystallographic density. This procedure could overestimate some hydrogen uptakes because the reported porous properties are higher than the experimentally determined ones. The actual poous properties can be lower than the crystallographic ones because of the presence of structural defects in the actual structures, lack of activation, frameworks' flexibility, polymorphism, and instability of crystalline phases to preparation/operation conditions.[6-9]
The structural optimisation before calculating the porous properties of the MOFs could also contribute to this overestimation. The simulation of these crystalline structures do not consider possible structural changes after removing solvent molecules, like during the generation of exposed-metal sites, or during removal of structure-directing agents (SDA) or charge-compensating substances [1]. An example is the material Zn-PyDC (CSD code BUKMUQ), made out of pyridine-3,5-dicarboxylic acid and Zn, whose measured surface area ($A_{BET}$ = 546 $m^2/g$) is significantly lower than the calculated one (3,160 $m^2/g$) due to its guest-dependent flexible structure [10]. Calculated SSA values for materials $Me_2$-$DOBQ_3$ (Me=Ni, CSD code OWITOE, Fe, OWITUK, Zn, OWIVAS, Co, OWITEU, and Mn, OWITIY; DOBQ: 2,5-dioxy-1,4-benzoquinone) are between 4,800 – 5,100 $m^2/g$ with a 77 % of void volume. However, the tetrabutylammonium countercations were computationally removed from the cavities before the porosity calculations, which may not be possible to perform experimentally.

## 1.3. Identification and cost of organic linkers

To normalise the nomenclature of the organic components of these MOFs and provide a unique identifier, 1,868 of the chemical´s names were converted into their corresponding SMILES strings by using the code OPSIN from the University of Cambridge [11] and then converted into canonical SMILES strings with the free software Open Babel [12]. The MOFid and MOFKey codes from ref. [4] were used to identify the organic molecules for which SMILES strings were not available. The public database PubChem [13] was used to get information for each SMILES string, like molar mass, CAS number, and IUPAC's name for the parental compounds. Before searching this information for a substance, the SMILES string of deprotonated molecules, as they appear in the MOF composition, were protonated. As an example, the deprotonated carboxylate moiety is represented as "C(=O)[O-]", whereas "C(=O)O" indicates the protonated form. The identified organic molecules in the database were unified in 747 compounds by their CAS numbers and classified as linkers or non-linkers. 598 substances were defined as linkers, for whose prices and purities were found in available links to vendors' websites in ChemSpider, starting from CAS numbers or SMILES strings for each substance. For each vendor, the price for the largest packing was collected, and the lowest price-per-gram was selected for each substance and included in the MOF-database. The prices for 510 linkers were found, updated to February 2022.

## 1.4. Algorithm to Split the Structures' chemical names into their components in MS Excel

1. Starting from ".gcd" files from the CSD, export the information of selected MOFs into ".tab" files, and merge all files in one ".xld" file.
2. In chemical names of structures, remove "catena-(", "catena-[", "catena(", & "catena[".
3. Use "%" as a column separator. Replace "$-", "$", "mu-", "mu!", "!", and "i)" with "%".
4. Replace “-di/tri/tetra/penta/Hexa/hepta/octa/nona/deca/dodecaaqua”, “-di-/tri-/tetra-/penta-/hexa-/hepta-/octa-/nona-/deca-/dodeca-aqua”, “-aqua”, “aqua” and “cosa” with “%”.
5. Replace all the metal names with "%".
6. Remove spaces in between substances' names: replace "acid" by "_acid", "alcohol" by "_alcohol", "phosph" with "_phosph".
7. Delete spaces before/after "%". Replace "-(%" with "%".
8. Replace "%%" with "%" many times. Also, "--"by "%".
9. Separate the column.
10. Insert the filter in all the new columns.
11. For column i (for i from 1 to N):
    a. Sort column from A to Z.
    b. Delete cells not containing names of organic molecules.

    c. Delete solvents.
    d. Move to column i+1 and repeat.
12. Merge all columns with a "%" between columns.
13. Delete old columns, convert new column into text.
14. Sort new column A→Z and replace ")-(", “) (", "double space", "%", "%", "%))", "%)", "%]", "(%", "-%" with "%"
15. Replace “ -bis(” with “-bis(” and “ -carboxylat” with “-carboxylat”.
16. Replace "-bis(%", "-tris(%", "-di%", "bis(%", "tris(%", "di%", "-N,O", "-O,O", "-C,N", "-O:O", "solvate", "unknown", "clathrate" with "%"
17. Repeat from 8 to 11.
18. Merge all columns, inserting "$" between columns.
19. In the new column (text): Replace all possible combinations between "$" and "space", "(", ")", "-", "[", "]", and "´” with “%”.
20. Replace "$pentakis", "$hexakis", "heptakis", and "oktakis" with "%".
21. Replace ")-bis$", ")-di$", ")-tris$", ")-tetrakis$", ")-pentakis$", ")-hexakis$", ")-heptakis$", ")-octakis$", ")-tri$", ")-tetra$", ")-pentadeca$", ")-nonakis$", ")-decakis$", ")-nonadecakis$", ")-dodecakis$", ")-hexa$", ")-N$", ")-penta$", ")-hexa$", ")-hepta$", "-hepta", "-octa", and "-nona" with "%".
22. Replace remaining "$" with "%" and "%%" with "%" many times.
23. Separate columns. Repeat step 11.
24. Repeat from Steps 12 to 14, Separate columns and repeat step 11. Repeat Step 18 and repeat step 19.
25. Repeat steps 22 and 23.
26. In each column: remove unnecessary brackets. Delete non-separated elements (i.e., solvents, from organics' names. Replace "ato" with "ate", "amino" with "amine", and "amido" with "amide" at the end of organics' names. Replace "ic acid" and "ic_acid" with "ate".

## 2. User interface for the MOFdb.BAM

A Python-based user interface facilitates the search of structures within this database, using properties of the structures or linkers. Structures can be selected from their crystallographic and porous properties, density, gravimetric or volumetric hydrogen uptake at 77 K and 100 bar, the presence of Open Metal Sites, the nature of the metallic or organic components, and the price-per-gram of the used organics. The organic molecules can be found in the database using their name, CAS number, molar mass, price-per-gram, or functional group. It is also possible to search structures using the linker from a specific MOF. In addition, it is possible to specify the number of organic or metallic components (as one, two, three, or any) or containing non-linker organic molecules. Finally, the interface exports data into .csv files for structures and their used linkers. Figure S1 shows an example of a search of MOF structures consisting of one metal combined with up to two organic molecules, only containing linkers cheaper than 26 €/g while not allowing non-linker organic molecules. The interface shows 315 results in the selected MOFs window, detailing for each structure the CSD reference, the structure's name, its porous and crystalline properties, gravimetric and volumetric total uptakes, and the metallic and organic composition. With the same limitations regarding the cost applied to the organic search parameters, it also displays a list of 261 linkers cheaper than 26 €/g, for which the normalised name, CAS, alternative names, SMILES strings, and molecular weight are displayed. To access more detailed information, like prices and purities from different vendors of the linkers in the database, one may double-click an entry in the table to open a window (see Figure S2). An online version of this tool is available at https://mofdb-bam.de with a centralised database, providing the same functionality as the previously described user interface. Up to now, the price of the linkers needs manual updating.

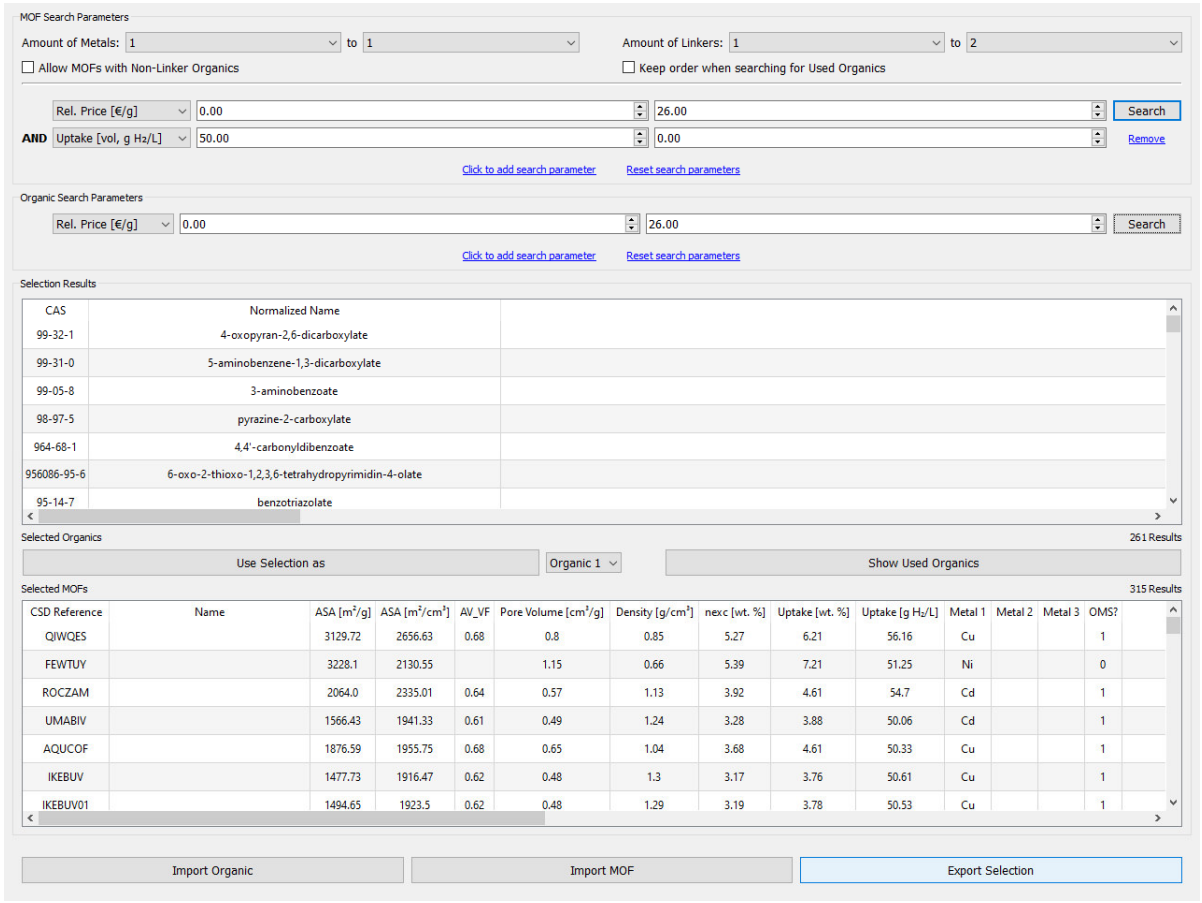


**Figure S1. User interface for searching MOF structures in the database for cheap MOFs.**

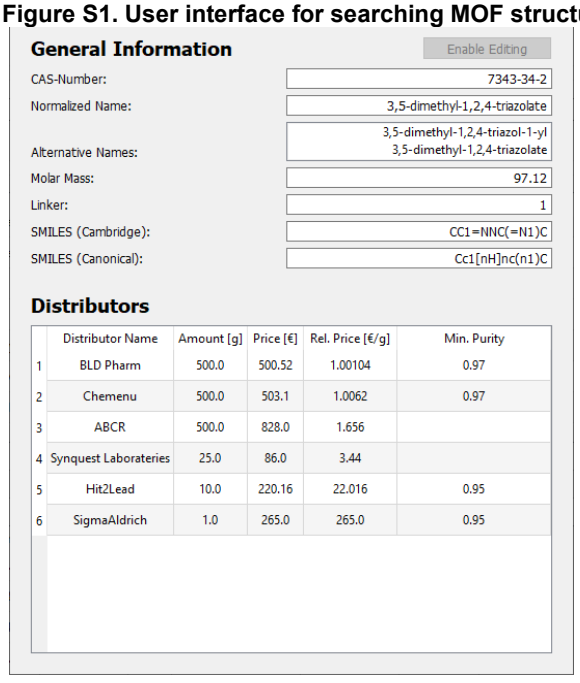


**Figure S2. Information of organic molecules in the database, provided via the user interface.**

# 3. Structures with one metal and one organic linker

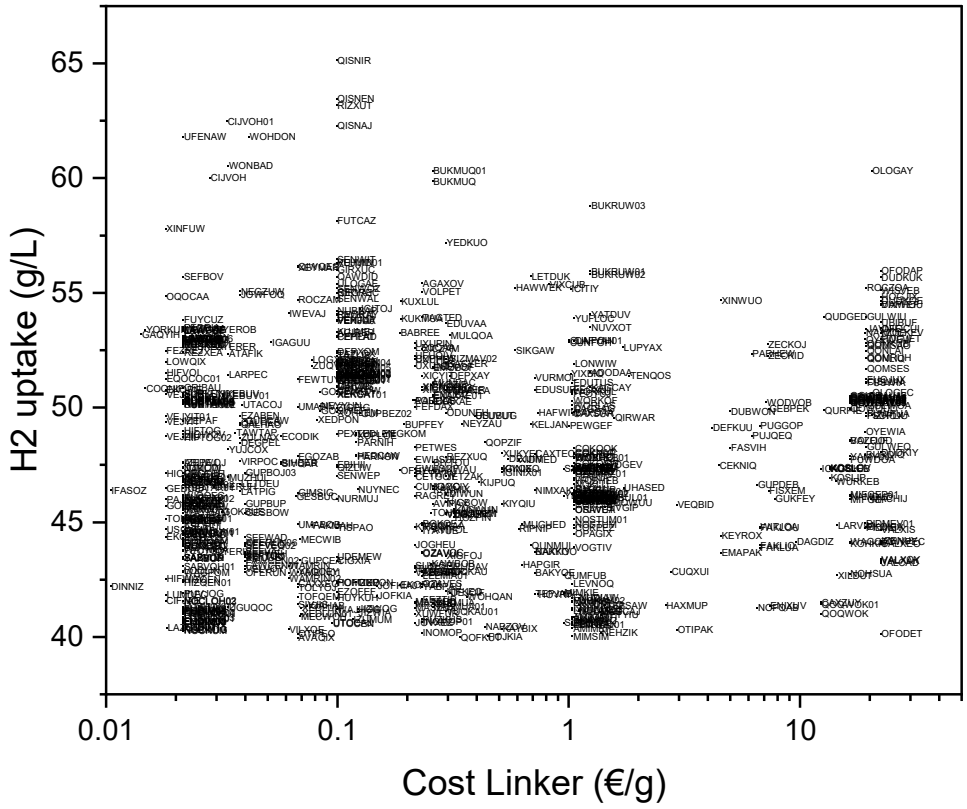


**Figure S3. Comparison of hydrogen uptake at –196 °C and 100 bar of all the MOF structures from individual linkers. Labels indicate the CSD reference.**

**Table S1. Number of Linker-metal combinations for MOFs with estimated volumetric uptake higher than 40 g/L. Only linkers with available prices are considered in the table.**

| Linker CAS | Al | Ca | Cd | Cr | Cu | Fe | Li | Mg | Mn | Na | Ni | Sr | Ti | V | Zn | Zr | Total | Price (€/g) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 100-21-0 | 9 | 3 | 5 | 10 | 1 | 5 | | 2 | 18 | | 1 | 5 | | 19 | 32 | 15 | 125 | **0.0215** |
| 554-95-0 | | | 11 | 2 | 25 | 4 | 1 | 3 | 2 | | 3 | | | | 24 | | 75 | **0.0989** |
| 610-92-4 | | 2 | 1 | | 7 | 19 | | 9 | 6 | | 6 | 1 | | | 9 | | 60 | **1.0509** |
| 1141-38-4 | 1 | | | | | 1 | | 5 | 6 | | | | | | 14 | | 27 | **1.0354** |
| 50446-44-1 | | 1 | 2 | | 13 | | | | 1 | | 1 | | | | 5 | | 23 | **16.3744** |
| 4282-31-9 | | 4 | | | 2 | | | 3 | 2 | | | 4 | | | 1 | 5 | 21 | **0.2313** |
| 365549-33-3 | 1 | | 3 | | 3 | 2 | | 2 | 2 | | 2 | | | | 5 | | 20 | **22.2912** |
| 553-26-4 | | 1 | | | 13 | 1 | | | | | 2 | | | | 2 | | 19 | **0.2150** |
| 14389-12-9 | | | 7 | | 11 | | | | | | | | | | | | 18 | **19.2640** |
| 787-70-2 | | | 1 | 2 | | 2 | | 2 | 4 | | | | | 1 | 4 | 1 | 17 | **0.2941** |
| 693-98-1 | | | 3 | | | | | | | | | | | | 13 | | 16 | **0.0396** |
| 499-81-0 | | 1 | | | 7 | | | 4 | 1 | | | | | | 2 | | 15 | **0.2571** |
| 1453-82-3 | | | 7 | | 2 | | | | 2 | 1 | 2 | | | | | | 14 | **0.0671** |
| 288-32-4 | | | 1 | | | | | | | | | | | | 10 | | 11 | **0.0181** |

**Table S2. Reported structures with 1,4-benzenedicarboxylic acid (CAS No. 100-21-0) and higher estimated hydrogen uptake than 40 g/L (for duplicated structures, it is shown the entries with the lowest volumetric area).**

| CSD ref.Code | Name | VSA/ $m^2m^{-3}$ | SSA/ $m^2g^{-1}$ | Vp/$cm^3g^{-1}$ | Me | OMS | wt.$H_2$ % | g$H_2L^{-1}$ |
|---|---|---|---|---|---|---|---|---|
| UFENAW | | 3088.4 | 4090.6 | 0.98 | Zn | Yes | 7.6 | 61.8 |
| SEFBOV | | 2480.5 | 2419.2 | 0.65 | Zn | Yes | 5.2 | 55.8 |
| TAGVAB | CPM-201 | 2474.9 | 3328.7 | 0.91 | Mg | Yes | 6.6 | 53.0 |
| KUXREC | MIL-88B | 2297.7 | 3188.0 | 1.02 | Fe | Yes | 6.8 | 52.7 |
| REZXEA | | 2266.2 | 3530.9 | 1.18 | Cr | Yes | 7.6 | 52.5 |
| NEXVET | | 2220.5 | 3880.0 | 1.41 | Ni | No | 8.5 | 53.0 |
| VUSKEA | | 2192.8 | 3687.5 | 1.35 | Zn | No | 8.1 | 52.6 |
| ORIBAU | | 2192.6 | 2312.4 | 0.68 | Zn | No | 5.1 | 50.8 |
| FUYCUZ | lambda-CMOF-5 | 2184.5 | 2362.9 | 0.81 | Zn | Yes | 5.5 | 53.9 |
| MIBQAR | MOF-5 | 2174.2 | 3686.8 | 1.38 | Zn | No | 8.2 | 52.7 |
| PICTIG | | 2131.7 | 2227.9 | 0.68 | Zn | Yes | 5.0 | 50.5 |
| IZEPAF | | 1958.1 | 3431.3 | 1.37 | Cr | Yes | 8.0 | 49.4 |
| HIFTOG02 | | 1890.0 | 1632.2 | 0.53 | Zn | No | 4.0 | 48.8 |
| JUMCOL | | 1824.1 | 1846.2 | 0.65 | V | No | 4.6 | 47.3 |
| IZEPEJ | | 1808.9 | 3316.5 | 1.43 | Cr | Yes | 8.0 | 47.6 |
| QALGUH | | 1796.0 | 1798.0 | 0.64 | Cr | No | 4.5 | 47.0 |
| SETQUF | | 1737.4 | 1743.3 | 0.62 | Fe | No | 4.4 | 45.9 |
| NAKLIW | | 1720.4 | 1484.3 | 0.54 | Zn | Yes | 3.9 | 47.2 |
| NOCLUN | | 1685.1 | 1568.4 | 0.57 | Sr | Yes | 4.1 | 45.9 |
| SUCLOT | NICS-8 | 1657.7 | 1841.3 | 0.68 | Ca | Yes | 4.7 | 44.1 |
| RUBTAK03 | UiO-66 | 1637.3 | 1322.7 | 0.49 | Zr | No | 3.6 | 46.5 |
| PEPLIG | | 1614.9 | 1539.4 | 0.59 | V | No | 4.1 | 45.0 |
| SABVUN | MIL-53 (Al) | 1612.7 | 1647.3 | 0.60 | Al | No | 4.3 | 43.5 |
| IDIWIB | | 1606.7 | 1534.3 | 0.58 | V | No | 4.1 | 44.8 |
| MINVOU | MIL-53as | 1583.3 | 1505.6 | 0.58 | Cr | No | 4.1 | 44.7 |
| LAGWEX | | 1565.2 | 1134.6 | 0.43 | Cd | Yes | 3.3 | 46.7 |
| FIJCUX | | 1565.0 | 1238.8 | 0.47 | Zn | Yes | 3.5 | 45.8 |
| GAJVEU | | 1487.8 | 1400.5 | 0.54 | Zn | No | 3.8 | 42.4 |
| YAXBOP | | 1474.8 | 1305.2 | 0.52 | Fe | No | 3.7 | 43.5 |
| OCUNAC | MIL-101 | 1422.7 | 3327.9 | 1.96 | Cr | Yes | 9.4 | 44.4 |
| OSAVEK | | 1397.5 | 1409.5 | 0.57 | Ca | Yes | 3.9 | 40.7 |
| HIZQUD | | 1378.7 | 921.9 | 0.38 | Cd | Yes | 2.9 | 45.0 |
| NOCKOG | | 1347.5 | 1288.3 | 0.53 | Mg | Yes | 3.7 | 40.3 |
| PUVJOG | MIL-47(V) | 1343.7 | 1152.3 | 0.49 | V | No | 3.5 | 41.8 |
| NOCKUM | | 1338.2 | 1246.9 | 0.51 | Ca | Yes | 3.6 | 40.4 |
| LUSHOX | | 1298.7 | 1088.1 | 0.45 | Mn | Yes | 3.3 | 40.7 |
| PEPLOM | | 1296.3 | 1079.4 | 0.46 | V | No | 3.3 | 41.3 |
| WAGPOM | | 1292.2 | 904.5 | 0.38 | Cd | Yes | 2.9 | 43.0 |
| FECYOD | | 1251.4 | 876.1 | 0.41 | Zn | Yes | 3.0 | 43.8 |
| FIJDIM10 | | 1249.9 | 1010.9 | 0.43 | Mn | Yes | 3.2 | 40.3 |
| NOCLOH | | 1235.2 | 939.7 | 0.41 | Sr | Yes | 3.0 | 40.9 |
| HIZQEN | | 1156.1 | 769.8 | 0.37 | Cd | Yes | 2.7 | 42.4 |

**Table S3. Reported structures with 1,3,5-Benzenetricarboxylic acid (CAS No. 554-95-0) and higher estimated hydrogen uptake than 40 g/L.**

| CSD ref.Code | Name | VSA/ $m^2m^{-3}$ | SSA/ $m^2g^{-1}$ | Vp/$cm^3g^{-1}$ | Me | OMS | wt.$H_2$ % | g$H_2L^{-1}$ |
|---|---|---|---|---|---|---|---|---|
| RIZXUT | | 3031.8 | 3285.0 | 0.81 | Zn | Yes | 6.4 | 63.1 |
| QISNAJ | | 2863.5 | 2702.6 | 0.69 | Cd | Yes | 5.6 | 62.3 |
| FUTCAZ | | 2795.2 | 3418.5 | 0.87 | Mn | Yes | 6.6 | 58.1 |
| PEXFAA | | 2527.7 | 3496.9 | 0.96 | Mg | Yes | 6.9 | 53.9 |
| SENWIT | | 2511.4 | 3206.2 | 0.98 | Zn | Yes | 6.7 | 56.4 |
| GIRXUC | BIT-101 | 2451.0 | 3189.4 | 1.01 | Zn | Yes | 6.8 | 56.1 |
| KUJMIN | JUC-133 | 2422.8 | 2186.9 | 0.63 | Cd | Yes | 4.8 | 56.3 |
| REGREC | | 2411.0 | 2679.9 | 0.80 | Zn | Yes | 5.8 | 55.0 |
| SENWAL | | 2340.3 | 3197.8 | 1.07 | Zn | Yes | 7.0 | 54.7 |
| REGRAY | | 2318.3 | 2504.1 | 0.77 | Zn | Yes | 5.5 | 54.1 |
| VEHJOJ | BIT-103 | 2267.6 | 3030.2 | 1.03 | Zn | Yes | 6.7 | 53.8 |
| DEPXOM | | 2256.8 | 2090.0 | 0.56 | Mn | Yes | 4.6 | 52.5 |
| FIWKUT | FJI-3 | 2252.0 | 1976.2 | 0.59 | Zn | Yes | 4.5 | 54.2 |
| AGIREP | | 2250.0 | 2253.7 | 0.69 | Zn | Yes | 5.1 | 53.3 |
| XEKCAT01 | | 2244.7 | 2411.9 | 0.66 | Mg | Yes | 5.2 | 50.5 |
| CEHLAD | | 2217.9 | 2598.3 | 0.86 | Zn | Yes | 5.9 | 53.1 |
| ULOGAE | | 2211.8 | 1634.4 | 0.46 | Cd | Yes | 3.9 | 55.5 |
| ZUGDEM | ZnBTCA-T | 2198.4 | 2576.1 | 0.82 | Zn | Yes | 5.7 | 51.8 |
| NINVAI | | 2181.1 | 2665.6 | 0.86 | Fe | Yes | 5.9 | 51.4 |
| DUPVER | | 2168.1 | 2723.9 | 0.92 | Zn | Yes | 6.1 | 52.1 |
| GACVIS | | 2097.7 | 1881.8 | 0.56 | Ni | Yes | 4.4 | 51.0 |
| KUJMEJ | | 2066.3 | 1541.9 | 0.47 | Cd | Yes | 3.8 | 53.3 |
| ACIBOE | MOF-CJ3 | 2063.0 | 1873.9 | 0.60 | Zn | Yes | 4.4 | 51.3 |
| RIFDUG01 | | 2060.9 | 2375.6 | 0.83 | Zn | Yes | 5.6 | 51.2 |
| ZIGFIG | | 2057.4 | 2374.7 | 0.79 | Cr | Yes | 5.5 | 50.1 |
| TAZLIR | | 2055.1 | 2118.7 | 0.75 | Cd | | 5.1 | 52.3 |
| DIHVIB | HKUST-1a | 2036.2 | 2305.8 | 0.81 | Cu | Yes | 5.5 | 51.0 |
| VEHJID | | 1993.0 | 1774.8 | 0.59 | Zn | Yes | 4.3 | 50.9 |
| CEHKUW | | 1911.9 | 1517.4 | 0.51 | Cd | | 3.9 | 50.7 |
| EBIHII | | 1870.7 | 1653.0 | 0.52 | Fe | Yes | 4.0 | 47.5 |
| XOHLEM | | 1839.6 | 1373.8 | 0.45 | Zn | Yes | 3.6 | 49.7 |
| PEXTUI | | 1690.9 | 1193.4 | 0.43 | Cd | Yes | 3.3 | 48.8 |
| POFGUO | | 1597.9 | 1711.3 | 0.61 | Li | No | 4.3 | 42.3 |
| SENWEP | | 1558.3 | 1257.2 | 0.52 | Zn | Yes | 3.7 | 47.0 |
| QIZLIW | | 1546.0 | 1016.5 | 0.37 | Cu | Yes | 3.0 | 47.5 |
| NURMUJ | | 1518.9 | 1265.0 | 0.53 | Zn | Yes | 3.7 | 45.9 |
| TISPAO | | 1481.2 | 1457.5 | 0.65 | Cu | No | 4.2 | 44.8 |
| EZOFEF | | 1340.9 | 1308.3 | 0.60 | Ni | No | 3.9 | 42.0 |
| UDEMEW | MIL-100(Cr) | 1337.4 | 1963.3 | 1.12 | Cr | Yes | 6.0 | 43.4 |
| CIGXIA | MIL-100(Fe) | 1325.7 | 1937.0 | 1.11 | Fe | Yes | 6.0 | 43.4 |

**Table S4. Reported structures with 2,5-Dihydroxybenzene-1,4-dicarboxylic acid (CAS No. 610-92-4) and higher estimated hydrogen uptake than 40 g/L.**

| CSD ref.Code | Name | VSA/ $m^2m^{-3}$ | SSA/ $m^2g^{-1}$ | Vp/$cm^3g^{-1}$ | Me | OMS | wt.$H_2$ % | g$H_2L^{-1}$ |
|---|---|---|---|---|---|---|---|---|
| YUFLOC | | 2401.7 | 2439.3 | 0.66 | Sr | Yes | 5.2 | 53.9 |
| DAFYAN | CPM-230 | 2334.0 | 3209.0 | 1.00 | Mg | Yes | 6.8 | 52.8 |
| LONWIW | | 2332.3 | 2801.2 | 0.80 | Mg | Yes | 5.9 | 51.8 |
| BAPDAA | Cd-DOTP | 1564.7 | 1132.7 | 0.50 | Cd | Yes | 3.5 | 49.8 |
| YUHHIU | | 1884.1 | 2304.6 | 0.82 | Ca | Yes | 5.5 | 47.4 |
| COKQAW | Cu-DOTP | 1523.6 | 1164.8 | 0.50 | Cu | Yes | 3.5 | 47.4 |
| WIZDEP | Zn-DOTP | 1549.5 | 1201.0 | 0.50 | Zn | Yes | 3.5 | 47.3 |
| LEJRIC | Ni-DOTP | 1547.8 | 1299.7 | 0.53 | Ni | Yes | 3.7 | 46.3 |
| VAGTAA01 | | 1775.3 | 1776.0 | 0.61 | Mg | Yes | 4.4 | 46.0 |
| COKQIE | Fe-DOTP | 1536.1 | 1362.0 | 0.57 | Fe | Yes | 3.9 | 45.9 |
| ORIWET | Mn-DOTP | 1549.3 | 1420.1 | 0.59 | Mn | Yes | 4.0 | 45.7 |
| OSAVUA | | 1778.3 | 2011.0 | 0.71 | Ca | Yes | 4.9 | 45.7 |
| NOSTUM | | 1717.6 | 1789.3 | 0.63 | Mg | Yes | 4.5 | 45.0 |
| VOGTIV | Mg-DOTP | 1549.2 | 1693.4 | 0.70 | Mg | Yes | 4.6 | 43.9 |

**Table S5. Reported structures with 2,6-Naphthalenedicarboxylic acid (CAS No. 1141-38-4) and higher estimated hydrogen uptake than 40 g/L.**

| CSD ref.Code | Name | VSA/ $m^2m^{-3}$ | SSA/ $m^2g^{-1}$ | Vp/$cm^3g^{-1}$ | Me | OMS | wt.$H_2$ % | g$H_2L^{-1}$ |
|---|---|---|---|---|---|---|---|---|
| EDUTUS | | 1967.9 | 3391.4 | 1.43 | Zn | No | 8.1 | 51.0 |
| FECYUJ | | 2090.2 | 2257.6 | 0.73 | Zn | Yes | 5.2 | 50.7 |
| FECXUI | | 2051.7 | 2218.5 | 0.75 | Zn | Yes | 5.2 | 50.6 |
| WORLAS | INT-IRMOF-8-B | 2042.0 | 2141.7 | 0.70 | Zn | Yes | 5.0 | 50.1 |
| CAGSAG | UTSA-38 | 2031.6 | 2112.5 | 0.69 | Zn | Yes | 4.9 | 49.9 |
| CAXSUR | CAU-3-NDC | 2108.9 | 3408.6 | 1.18 | Al | No | 7.4 | 49.8 |
| QAQRUW | | 2010.6 | 2360.3 | 0.73 | Mg | Yes | 5.3 | 47.4 |
| TAGTUT | CPM-205 | 1964.9 | 2552.4 | 0.85 | Mg | Yes | 5.8 | 47.3 |
| IDIXAU | | 1677.4 | 1736.7 | 0.69 | Zn | No | 4.6 | 46.5 |
| CIFDUS | | 1846.8 | 1880.4 | 0.61 | Mn | Yes | 4.5 | 46.3 |
| EYUWAW | | 1441.9 | 1406.8 | 0.56 | Mn | Yes | 3.9 | 41.8 |
| VUQKAU02 | | 1471.9 | 1424.8 | 0.54 | Mn | Yes | 3.9 | 41.6 |
| ISUCUV | | 1382.6 | 1294.6 | 0.53 | Fe | Yes | 3.7 | 41.3 |
| LIXWAR01 | | 1360.5 | 1267.8 | 0.53 | Mn | Yes | 3.7 | 41.0 |
| PEQWAK | | 1335.7 | 1259.8 | 0.53 | Mn | Yes | 3.7 | 40.7 |
| LEVNOQ01 | | 1366.7 | 1401.6 | 0.59 | Mg | Yes | 4.0 | 40.4 |
| MIMSIM | | 1232.3 | 1210.6 | 0.58 | Zn | Yes | 3.8 | 40.2 |

**Table S6. Reported structures with 4,4'-Bipyridine (CAS No. 553-26-4) and higher estimated hydrogen uptake than 40 g/L.**

| CSD ref.Code | Name | VSA/ $m^2m^{-3}$ | SSA/ $m^2g^{-1}$ | Vp/$cm^3g^{-1}$ | Me | OMS | wt.$H_2$ % | g$H_2L^{-1}$ |
|---|---|---|---|---|---|---|---|---|
| UXUPIN | | 2447.1 | 3652.8 | 1.05 | Cu | Yes | 7.3 | 52.9 |
| UFUQIV | | 2389.8 | 3536.8 | 1.04 | Cu | Yes | 7.2 | 52.2 |
| CUPHUS | | 2377.9 | 3492.1 | 1.03 | Cu | Yes | 7.1 | 52.1 |
| UXUNUX | | 2356.3 | 3472.7 | 1.03 | Cu | Yes | 7.1 | 51.8 |
| PETWES | | 1853.3 | 2036.5 | 0.75 | Cu | Yes | 5.0 | 48.3 |
| PETWIW | | 1743.3 | 1861.0 | 0.72 | Cu | Yes | 4.8 | 47.1 |
| CUMQOQ | | 1831.4 | 1874.2 | 0.63 | Zn | Yes | 4.5 | 46.5 |
| RAGREY | | 1843.9 | 2533.1 | 0.92 | Cu | Yes | 6.0 | 46.1 |
| JOGHEU | | 1656.3 | 1588.9 | 0.55 | Ni | Yes | 4.0 | 43.9 |
| JOVXEZ | | 1278.3 | 1121.4 | 0.49 | Cu | Yes | 3.4 | 40.6 |

**Table S7. Reported structures with 3,3',5,5'-Azobenzenetetracarboxylic acid (CAS No. 365549-33-3) and higher estimated hydrogen uptake than 40 g/L.**

| CSD ref.Code | Name | VSA/ $m^2m^{-3}$ | SSA/ $m^2g^{-1}$ | Vp/$cm^3g^{-1}$ | Me | OMS | wt.$H_2$ % | g$H_2L^{-1}$ |
|---|---|---|---|---|---|---|---|---|
| OFODAP | JUC-63 | 2495.1 | 2966.4 | 0.88 | Cd | Yes | 6.2 | 56.0 |
| DUDKUK | | 2430.7 | 2880.0 | 0.89 | Cd | Yes | 6.2 | 55.7 |
| DUDKOE | | 2417.1 | 3099.7 | 0.95 | Zn | Yes | 6.5 | 54.6 |
| DAPHOU | FJI-8 | 2401.5 | 3056.8 | 0.94 | Zn | Yes | 6.5 | 54.4 |
| UBIBUF | FJI-9 | 2339.3 | 3087.6 | 0.98 | Zn | Yes | 6.6 | 53.8 |
| OFOCUI | JUC-62 | 2336.1 | 2959.8 | 0.92 | Cu | Yes | 6.3 | 53.4 |
| DUDKIY | | 1868.5 | 1918.2 | 0.67 | Zn | Yes | 4.7 | 48.0 |
| VALXIS | CPM-200-In/Ni | 1485.3 | 1671.7 | 0.78 | Ni | Yes | 4.8 | 44.6 |
| IZENUY | | 1488.6 | 1640.1 | 0.74 | Fe | Yes | 4.7 | 44.3 |
| TOWPEC | PCN-250' | 1486.6 | 1671.8 | 0.76 | Fe | Yes | 4.7 | 44.2 |
| VALXEO | CPM-200-In/Mn | 1503.0 | 1802.5 | 0.82 | Mn | Yes | 5.0 | 44.0 |
| VALXAK | CPM-200-In/Mg | 1487.9 | 2003.9 | 0.93 | Mg | Yes | 5.5 | 43.3 |
| VALXOY | CPM-200-V/Mg | 1484.6 | 1910.5 | 0.88 | Mg | Yes | 5.3 | 43.3 |
| JALCAD | | 1476.7 | 1756.7 | 0.79 | Al | Yes | 4.9 | 43.2 |

**Table S8. Reported structures with Thiophene-2,5-dicarboxylic acid (CAS No. 4282-31-9) and higher estimated hydrogen uptake than 40 g/L.**

| CSD ref.Code | Name | VSA/ $m^2m^{-3}$ | SSA/ $m^2g^{-1}$ | Vp/$cm^3g^{-1}$ | Me | OMS | wt.$H_2$ % | g$H_2L^{-1}$ |
|---|---|---|---|---|---|---|---|---|
| AGAXOV | MOF-107 | 2457.0 | 2760.7 | 0.81 | Cu | | 5.9 | 55.4 |
| VOLPET | | 2463.5 | 3320.2 | 1.01 | Zn | Yes | 6.9 | 55.1 |
| TAGTED | CPM-202 | 2476.1 | 3077.3 | 0.86 | Mg | Yes | 6.3 | 53.9 |
| XICYIT | DUT-69(Zr) | 1949.8 | 1463.4 | 0.46 | Zr | Yes | 3.7 | 51.4 |
| XICNOO01 | DUT-67 | 1908.3 | 2099.7 | 0.82 | Zr | Yes | 5.3 | 50.8 |
| BOKQEZ | | 1554.5 | 1169.1 | 0.41 | Mn | Yes | 3.3 | 44.9 |
| MAQRAA | | 1541.7 | 1278.8 | 0.49 | Cu | Yes | 3.6 | 44.8 |
| OZAVUI | | 1365.5 | 1096.6 | 0.48 | Sr | Yes | 3.4 | 43.5 |
| OZAVOC | | 1406.8 | 1039.7 | 0.41 | Sr | Yes | 3.1 | 43.5 |
| LELMIA01 | | 1284.4 | 869.0 | 0.35 | Sr | Yes | 2.8 | 42.6 |
| YABPAU | | 1501.9 | 1403.0 | 0.52 | Mg | Yes | 3.8 | 42.3 |
| FEZTIP | | 1381.8 | 1243.9 | 0.51 | Ca | Yes | 3.6 | 41.5 |
| PUZKUS | | 1329.3 | 1165.5 | 0.48 | Mg | Yes | 3.5 | 40.9 |
| INOMOP | | 1287.2 | 1165.1 | 0.50 | Ca | Yes | 3.5 | 40.2 |

**Table S9. Reported structures with Pyridine-4-carboxamide (CAS No. 1453-82-3) and higher estimated hydrogen uptake than 40 g/L.**

| CSD ref.Code | Name | VSA/ $m^2m^{-3}$ | SSA/ $m^2g^{-1}$ | Vp/$cm^3g^{-1}$ | Me | OMS | wt.$H_2$ % | g$H_2L^{-1}$ |
|---|---|---|---|---|---|---|---|---|
| QIWQES | | 2656.6 | 3129.7 | 0.79 | Cu | Yes | 6.2 | 56.1 |
| ROCZAM | | 2335.0 | 2064.0 | 0.57 | Cd | Yes | 4.6 | 54.7 |
| FEWTUY | | 2130.5 | 3228.1 | 1.15 | Ni | | 7.2 | 51.3 |
| UMABIV | | 1941.3 | 1566.4 | 0.49 | Cd | Yes | 3.9 | 50.1 |
| EGOZAB | | 1885.3 | 1815.7 | 0.60 | Cu | Yes | 4.4 | 47.9 |
| TOLYOJ | | 1594.4 | 1754.9 | 0.63 | Na | Yes | 4.4 | 42.3 |
| YAQCEY | | 1547.9 | 1417.8 | 0.51 | Mn | Yes | 3.8 | 42.8 |
| GIMSIG | | 1502.6 | 1037.4 | 0.40 | Cd | Yes | 3.1 | 46.3 |
| CAXXEG | | 1423.0 | 1173.0 | 0.45 | Ni | No | 3.4 | 42.2 |
| TOFQEM | | 1271.4 | 1013.0 | 0.45 | Cd | Yes | 3.2 | 41.8 |
| SIVJIS | | 1236.9 | 890.8 | 0.38 | Cd | No | 2.9 | 41.4 |
| AVAQIX | | 1099.3 | 841.1 | 0.42 | Cd | Yes | 3.0 | 40.1 |
| QIWQES | | 2656.6 | 3129.7 | 0.79 | Cu | Yes | 6.2 | 56.1 |
| ROCZAM | | 2335.0 | 2064.0 | 0.57 | Cd | Yes | 4.6 | 54.7 |

**Table S10. Reported structures with 5-(4-pyridyl)tetrazol (CAS No. 14389-12-9) and higher estimated hydrogen uptake than 40 g/L.**

| CSD ref.Code | Name | VSA/ $m^2m^{-3}$ | SSA/ $m^2g^{-1}$ | Vp/$cm^3g^{-1}$ | Me | OMS | wt.$H_2$ % | g$H_2L^{-1}$ |
|---|---|---|---|---|---|---|---|---|
| FUQJUX | | 2116.0 | 2945.9 | 1.04 | Cu | Yes | 6.7 | 51.3 |
| ROCZOA | | 2491.0 | 2599.3 | 0.71 | Cd | Yes | 5.5 | 55.2 |
| JAVNIE | | 2385.4 | 2538.9 | 0.71 | Cu | Yes | 5.4 | 53.5 |
| GULWIU | | 2242.5 | 2440.2 | 0.80 | Cd | Yes | 5.6 | 54.0 |
| GULWEQ | | 1758.8 | 2394.3 | 1.04 | Cd | Yes | 6.2 | 48.3 |
| CISLUN | | 2174.1 | 2257.4 | 0.68 | Cu | Yes | 5.0 | 51.1 |
| FUSWIA | | 2196.2 | 2231.6 | 0.65 | Cu | Yes | 4.9 | 51.1 |
| PIZHOX | | 2065.3 | 2149.4 | 0.67 | Cu | Yes | 4.9 | 49.7 |
| FUWFIO | | 2013.0 | 1883.7 | 0.61 | Cd | Yes | 4.5 | 50.4 |
| FUWFUA | | 1980.6 | 1869.8 | 0.61 | Cd | Yes | 4.5 | 49.8 |
| GULWOA | | 1846.3 | 1446.0 | 0.50 | Cd | Yes | 3.8 | 50.1 |
| EKOKIA | | 1452.7 | 1034.8 | 0.40 | Cd | Yes | 3.1 | 44.8 |

**Table S11. Reported structures with 1,3,5-tris(4-Carboxyphenyl)benzene (CAS No. 50446-44-1) and higher estimated hydrogen uptake than 40 g/L.**

| CSD ref.Code | Name | VSA/ $m^2m^{-3}$ | SSA/ $m^2g^{-1}$ | Vp/$cm^3g^{-1}$ | Me | OMS | wt.$H_2$ % | g$H_2L^{-1}$ |
|---|---|---|---|---|---|---|---|---|
| VOLRAQ01 | MOF-177 | 1860.7 | 3314.7 | 1.50 | Zn | Yes | 8.2 | 50.2 |
| QOWQUO | MOF-14 | 2111.4 | 2929.8 | 0.98 | Cu | Yes | 6.5 | 50.0 |
| BAZFUF | | 1825.4 | 5368.0 | 2.54 | Cu | Yes | 12.5 | 48.6 |
| YAMYUJ | | 1812.5 | 2048.3 | 0.78 | Zn | Yes | 5.1 | 48.0 |
| PUWDOA | | 1898.4 | 2469.7 | 0.90 | Zn | Yes | 5.8 | 47.7 |
| NAMDUD | | 1799.3 | 2332.5 | 0.87 | Mn | Yes | 5.7 | 46.2 |
| MIFGEP | | 1811.7 | 1774.9 | 0.58 | Cd | Yes | 4.3 | 46.0 |
| WAGQAY | | 1362.1 | 3477.6 | 2.19 | Ni | Yes | 10.1 | 44.2 |
| NOHSUA | | 1620.2 | 1857.7 | 0.68 | Ca | Yes | 4.7 | 42.7 |
| LAFFEG02 | | 1457.2 | 1429.7 | 0.58 | Zn | Yes | 4.0 | 42.5 |

**Table S12. Reported structures with 4,4'-biphenyldicarboxylic (CAS No. 787-70-2) acid and higher estimated hydrogen uptake than 40 g/L.**

| CSD ref.Code | Name | VSA/ $m^2m^{-3}$ | SSA/ $m^2g^{-1}$ | Vp/$cm^3g^{-1}$ | Me | OMS | wt.$H_2$ % | g$H_2L^{-1}$ |
|---|---|---|---|---|---|---|---|---|
| YEDKUO | MIL-88D | 2774.1 | 3352.4 | 0.79 | Cr | Yes | 6.5 | 57.1 |
| EDUVAA | IRMOF-9 | 2384.4 | 3452.1 | 1.08 | Zn | No | 7.2 | 53.7 |
| WIZMAV02 | UiO-67 | 2254.9 | 3075.6 | 0.99 | Zr | No | 6.6 | 52.1 |
| GACYER | | 2161.9 | 2873.2 | 0.99 | Zn | Yes | 6.5 | 52.0 |
| MIBMER | MIL-126 | 2198.5 | 3079.9 | 0.99 | Fe | Yes | 6.6 | 50.8 |
| TOWNEA | PCN-245 | 2198.9 | 3059.0 | 0.98 | Fe | Yes | 6.6 | 50.7 |
| ODUNEH | | 2093.6 | 2169.7 | 0.66 | Zn | Yes | 4.9 | 49.7 |
| REZXUQ | | 1754.1 | 4846.4 | 2.37 | Cr | Yes | 11.7 | 47.9 |
| JETZAK | | 1979.8 | 2633.4 | 0.86 | Mg | Yes | 5.9 | 47.1 |
| IDIWUN | | 1685.2 | 1926.5 | 0.78 | Zn | No | 5.0 | 46.3 |
| NIGBOW | | 1743.5 | 2622.3 | 1.07 | V | No | 6.4 | 45.8 |
| VUQJUN | | 1728.0 | 2185.7 | 0.84 | Mn | Yes | 5.4 | 45.4 |
| XIGFOJ | | 1357.8 | 1962.0 | 1.09 | Cd | Yes | 5.9 | 43.5 |
| KIFKEQ | | 1534.3 | 1643.9 | 0.62 | Mg | Yes | 4.3 | 42.0 |
| VUQKAU01 | | 1425.2 | 1362.2 | 0.53 | Mn | Yes | 3.8 | 41.3 |

**Table S13. Reported structures with Pyridine-3,5-dicarboxylic acid (CAS No. 499-81-0) and higher estimated hydrogen uptake than 40 g/L.**

| CSD ref.Code | Name | VSA/ $m^2m^{-3}$ | SSA/ $m^2g^{-1}$ | Vp/$cm^3g^{-1}$ | Me | OMS | wt.$H_2$ % | g$H_2L^{-1}$ |
|---|---|---|---|---|---|---|---|---|
| BUKMUQ | | 2895.4 | 3400.7 | 0.83 | Zn | Yes | 6.6 | 59.9 |
| EMUBOF | | 1975.9 | 1648.4 | 0.56 | Cu | Yes | 4.1 | 51.8 |
| EXAXAE | JLU-Liu15 | 1690.8 | 1238.3 | 0.49 | Cu | Yes | 3.6 | 50.5 |
| BIYTOU | | 1875.0 | 1836.4 | 0.61 | Mn | Yes | 4.5 | 47.6 |
| KAYCIY | | 1893.9 | 1938.3 | 0.61 | Ca | Yes | 4.5 | 46.6 |
| KANMIX | | 1654.6 | 1527.4 | 0.59 | Cu | Yes | 4.1 | 46.5 |
| AVIPAX | | 1855.7 | 1925.3 | 0.61 | Mg | Yes | 4.5 | 45.8 |
| AVIPOL | | 1727.4 | 1839.4 | 0.64 | Mg | Yes | 4.6 | 44.8 |
| UREVIY | | 1154.5 | 728.7 | 0.32 | Pr | Yes | 2.6 | 42.1 |
| NABMUA01 | Mg-MOF-1 | 1424.1 | 1269.1 | 0.48 | Mg | Yes | 3.5 | 41.3 |

**Table S14. Reported structures with 2-Methylimidazol (CAS No. 693-98-1) and higher estimated hydrogen uptake than 40 g/L.**

| CSD ref.Code | Name | VSA/ $m^2m^{-3}$ | SSA/ $m^2g^{-1}$ | Vp/$cm^3g^{-1}$ | Me | OMS | wt.$H_2$ % | g$H_2L^{-1}$ |
|---|---|---|---|---|---|---|---|---|
| GUPCAW | | 1868.8 | 2293.8 | 0.91 | Cd | No | 5.7 | 49.5 |
| GUPBOJ03 | SALEM-1 | 1676.1 | 2078.1 | 0.91 | Cd | No | 5.5 | 47.1 |
| GUPBUP | | 1552.9 | 1688.5 | 0.76 | Cd | No | 4.7 | 45.8 |
| VELVOY | ZIF-8 | 1469.3 | 1548.2 | 0.66 | Zn | No | 4.3 | 42.9 |
| ESIFET | | 1454.3 | 1020.3 | 0.41 | Cd | No | 3.1 | 45.8 |

**Table S15. Reported structures with imidazole (CAS No. 288-32-4) and higher estimated hydrogen uptake than 40 g/L.**

| CSD ref.Code | Name | VSA/ $m^2m^{-3}$ | SSA/ $m^2g^{-1}$ | Vp/$cm^3g^{-1}$ | Me | OMS | wt.$H_2$ % | g$H_2L^{-1}$ |
|---|---|---|---|---|---|---|---|---|
| HIFVOI | | 2140.9 | 2506.0 | 0.83 | Zn | No | 5.7 | 51.5 |
| EQOCOC01 | ZIF-6 | 2097.2 | 2177.3 | 0.71 | Zn | No | 5.1 | 51.3 |
| VEJYOZ | ZIF-3 | 2096.1 | 2381.9 | 0.78 | Zn | No | 5.4 | 50.6 |
| VEJYIT | ZIF-2 | 1988.1 | 2140.1 | 0.72 | Zn | No | 5.1 | 49.4 |
| VEJZIU | ZIF-10 | 1880.3 | 2229.3 | 0.84 | Zn | No | 5.5 | 48.7 |
| HICGEG | | 1756.8 | 1659.5 | 0.60 | Zn | No | 4.3 | 47.1 |
| PAJSAX | | 1673.2 | 1974.2 | 0.81 | Zn | No | 5.2 | 46.1 |
| GOQSIQ | | 1638.2 | 1629.6 | 0.64 | Zn | No | 4.3 | 45.7 |
| HIFWAV | | 1359.0 | 1190.2 | 0.52 | Zn | No | 3.6 | 42.5 |

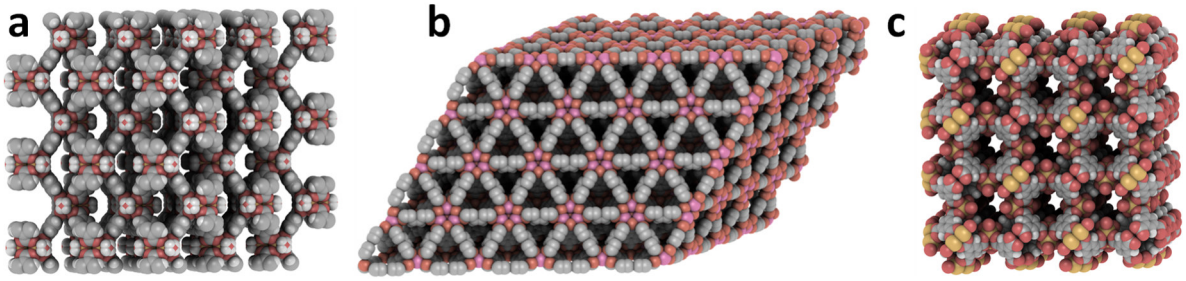


**Figure S4**. a: MIL-88B (Fe-BDC, CSD code KUXREC). b: UIO-66 or Zr-BDC (RUBTAK).c: $Fe_6$-$BTC_3$ (NINVAI) Created with iRASPA.[14]

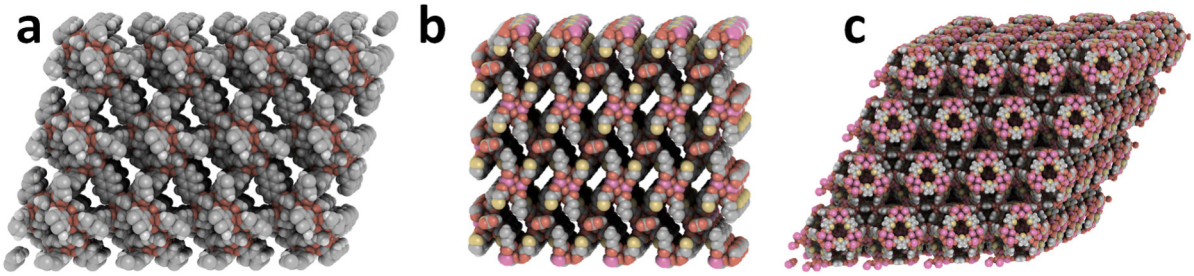


**Figure S5.** a: CAU-3-NDC or $Al_2$-NDC (CAXSUR). b: DUT-69 or $Zr_6$-$TDC_5$ (XICYIT). c: DUT-67 or $Zr_3$-$TDC_2$ (XICNOO). Created with iRASPA.[14]

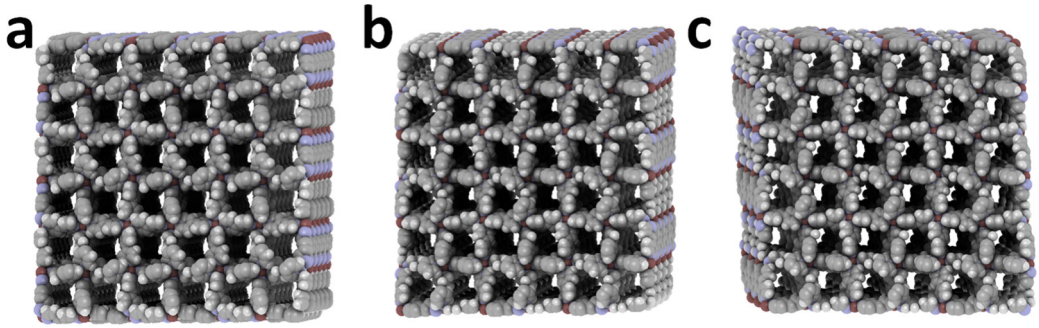


**Figure S6.** Structures Cu-4,4'b$Py_2$. UXUPIN (a), UFUQIV (b). and UXUNUX (c). Created with iRASPA.[14]

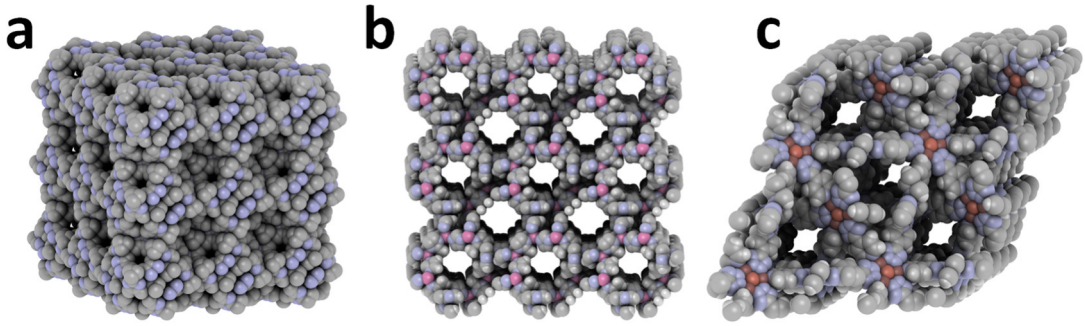


**Figure S7**. a: ZIF-8 or Zn-MeIm2 (CSD code OFERUNZ). b: Cd-MeIm2 (GUPCAW). c: Cu-PTz (FUQJUX). Created with iRASPA.[14]

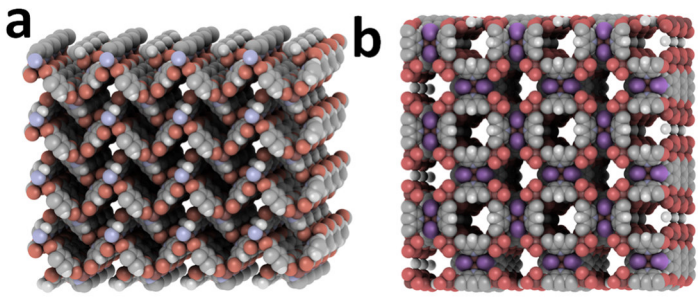


**Figure S8**. a: Zn-3,5PyDC (CSD code BUKMUQ). b: JLU-Liu15 or $Cu_2$-PyDC (EXAXAE). Created with iRASPA.[14]

# 4. Mixed-linkers MOFs

**Table S16. MOFs with mixed linkers from O-donor linkers.**

| Linker 1 | Linker 2 | Al | Cd | Cr Zn | Fe | Ni | Zn | Zr |
|---|---|---|---|---|---|---|---|---|
| 1,4-benzenedicarboxylate | | | | | | | | |
| | Formate | | | | | | 50.4 | |
| | 4,4'-biphenyldicarboxylate | | | | | | 50.1 | |
| 1,3,5-benzenetricarboxylate | | | | | | | | |
| | 1,4-Benzenedicarboxylate | | 50.9 | | | | | |
| | Butane-1,4-diol | | | | | 41.5 | | |
| Thiophene-2,5-dicarboxylate | | | | | | | | |
| | Thiophene-2-carboxylate | | | | | | | 47.9 |
| | 4,4',4''-nitrilotribenzoate | | | | | | 51.0 | |
| 4,4'-biphenyldicarboxylate | | | | | | | | |
| | (2R)-2-hydroxy-2-phenylacetate | | | | | | 44.9 | |
| | 1,3,5-tris(4-Carboxyphenyl)benzene | | | | 52.7 | | | |
| 2-Nitrobenzene-1,4-dicarboxylate | | | | | | | | |
| | 1,4-Benzenedicarboxylate | | | | | | 49.6 | |
| 2-aminobenzene-1,4-dicarboxylate | | | | | | | | |
| | 1,3,5-tris(4-Carboxyphenyl)benzene | | | | | | 47.9 | |
| 2,6-naphtalenedicarboxylate | | | | | | | | |
| | (2R)-2-hydroxy-2-phenylacetate | | | | | | 49.9 | |
| 2-hydroxybenzene-1,4-dicarboxylate | | | | | | | | |
| | 1,3,5-tris(4-Carboxyphenyl)benzene | | | | | | 48.4 | |
| 1,3,5-tris(4-Carboxyphenyl)benzene | | | | | | | | |
| | Ethane-1,2-diolate | 49.1 | | | | | | |
| | Formate | 49.5 | | | | | | |
| | pyridine-4-carboxamide | | | 50.7 | | | | |

**Table S17. Mixed linkers MOFs from N-donor linkers.**

| Linker 1 | Linker 2 | Cu | Zn |
|---|---|---|---|
| Imidazole | | | |
| | 2-Methylimidazole | | 48.3 |
| | 6-methyl-1H-benzimidazole | | 40.7 |
| 2-ethylimidazole | | | |
| | 5-Methyltetrazole | | 42.9 |
| Benzimidazole | | | |
| | 2-Nitroimidazoleate | | 40.6 |
| 2-methyl-1H-benzo[d]imidazole | | | |
| | 5-Methyltetrazole | | 42.1 |
| 1,2-bis(4-pyridyl)ethane | | | |
| | 2,2'-Bipyridyl | 40.4 | |
| 2-nitroimidazoleate | | | |
| | 6-nitro-1H-benzimidazole | | 41.0 |
| | 6-methyl-1H-benzimidazole | | 40.2 |
| | 6-bromo-1H-benzimidazole | | 41.8 |
| | Imidazole | | 48.0 |

**Table S18. MOFs from mixed carboxylates and azolates linkers.**

| | | Cd | | | Fe | | | Zn | |
|---|---|---|---|---|---|---|---|---|---|
| **Linker 1** | **Linker 2** | **Ca** | **Cd** | **Cu** | **Cu** | **Mg** | **Mn** | **Cu** | **Zn** |
| 1,2,4,5-Benzenetetracarboxylate | | | | | | | | | |
| | 2H-tetrazol-5-amine | | | | | | | | 40.7 |
| 1,3,5-Benzenetricarboxylate | | | | | | | | | |
| | 1,2,4-triazolyl | | | | | | | | 42.5 |
| | 2-imidazoleidone | | 46.1 | | | | | | |
| | 1,4-bis(imidazole-1-ylmethyl)benzene | | 53.7 | | | | | | |
| 1,4-Benzenedicarboxylate | | | | | | | | | |
| | 1,2,4-triazolyl | | | | | 44.4 | | | 44.5 |
| | 2-imidazoleidone | 44.0 | 42.5 | | | | | | |
| | 1H-1,2,4-triazol-5-amine | | 47.0 | | | | | | |
| | 1,2,3-triazole | | | | | | | | 50.7 |
| | 5-Methyltetrazole | | 45.1 | | | | | | |
| | 5-(4-pyridyl)tetrazol | | 44.1 | | | | | | |
| benzene-1,3-dicarboxylate | | | | | | | | | |
| | 3,5-dimethyl-1,2,4-triazolate | | | 50.4 | | | | | 47.5 |
| 2,5-Dihydroxybenzene-1,4-dicarboxylate | | | | | | | | | |
| | 1,2,4-triazolyl | | | | 48.0 | | | | |
| 2,6-Naphtalenedicarboxylate | | | | | | | | | |
| | 1,3,4-Oxadiazole | | | | | | | | 47.2 |
| | 5-Methyltetrazole | | | | | | | | 40.4 |
| 2-aminobenzene-1,4-dicarboxylate | | | | | | | | | |
| | 1,2,4-triazolyl | | | | | | | | 43.3 |
| 3,3',5,5'-Azobenzenetetracarboxylate | | | | | | | | | |
| | 4,4'-sulfonyldibenzoate | | | | | | 47.3 | | |
| 4,4'-biphenyldicarboxylate | | | | | | | | | |
| | 1H-1,2,4-triazol-5-amine | | 50.0 | | | | | | |
| | 4-(3,5-Dimethyl-1H-pyrazol-4-yl)pyridine | | | | | | | | 46.4 |
| 4,4'-ethene-1,2-diyldibenzoate | | | | | | | | | |
| | 1,2,4-triazolyl | | 48.6 | | | | | | 50.8 |
| 4,4'-methanediylbis(3-hydroxynaphthalene-2-carboxylate) | | | | | | | | | |
| | 3,5-diamino-1,2,4-triazol-1-yl | | | | | | | | 48.7 |
| | 1,4-bis(imidazole-1-ylmethyl)benzene | | 42.0 | | | | | | |
| 5-Hydroxybenzene-1,3-dicarboxylate | | | | | | | | | |
| | 2-imidazoleidone | | 46.5 | | | | | | |
| Benzene-1,2,4-tricarboxylate | | | | | | | | | |
| | 1,2,4-triazolyl | | | | | | | | 47.2 |
| Formate | | | | | | | | | |
| | 1,2,3-triazole | | | | | | | 48.9 | |
| Thiophene-2,5-dicarboxylate | | | | | | | | | |
| | 1,2,4-triazolyl | | | | | | | | 44.1 |
| | 1,2,3-triazole | | | | | | | | 50.4 |

**Table S19. MOFs from mixed carboxylated and bipyridine linkers.**

| Linker 1 | Linker 2 | Mo Zn | Cd | Na Cr | Cu | Fe | Mn | Ni | Zn |
|---|---|---|---|---|---|---|---|---|---|
| 2,2'-dipyridylamine | | | | | | | | | |
| | Benzene-1,2-dicarboxylate | | 41.3 | | | | | | |
| 2,2'-bipyridyl | | | | | | | | | |
| | 1,3,5-Benzenetricarboxylate | 55.1 | | | | | | | |
| | Oxalate | | | 52.7 | | | | | |
| | 1,3,5-tris(4-Carboxyphenyl)benzene | | | | | | | | 48.2 |
| 4,4'-bipyridine | | | | | | | | | |
| | Malate | | | | | | | 48.7 | |
| | Ethylenediaminetetraacetate | | | | 43.6 | | | | |
| | Formate | | | | | 42.1 | | 43.9 | |
| | Pyridine-4-carboxamide | | 40.2 | | | | | | |
| | 5-aminobenzene-1,3-dicarboxylate | | | | 51.4 | | | | |
| | 1,3,5-Benzenetricarboxylate | | | | | | | 43.0 | 43.5 |
| | 4,4'-Oxydibenzoate | | | | | | 41.4 | | |
| | 5-Hydroxybenzene-1,3-dicarboxylate | | | | 49.3 | | | | 46.2 |
| | 5-sulfobenzene-1,3-dicarboxylate | | | | | | | | 46.8 |
| | 3,3',3''-(2,4,6-trioxo-1,3,5-triazinane-1,3,5-triyl)tripropanoate | | | | 47.9 | | | | |
| | 4,4'-biphenyldicarboxylate | | | | 50.0 | | | | 40.3 |
| | 1,2,2-trimethylcyclopentane-1,3-dicarboxylate | | | | 41.5 | | | | |
| | 3,4-Pyridinedicarboxylate | | 51.9 | | | | | | |
| | Imidazole-4,5-dicarboxylate | | 41.4 | | | | | | |
| | 4,4'-ethene-1,2-diyldibenzoate | | | | | | | | 41.3 |
| | 2-aminobenzene-1,4-dicarboxylate | | 47.7 | | | | | | |
| | 2,6-Naphtalenedicarboxylate | | | | | | | | 42.6 |
| | 2,5-Dihydroxybenzene-1,4-dicarboxylate | | | | | | | | 50.2 |
| | 4,4'-carbonyldibenzoate | | | | 46.2 | | | | |
| | Benzene-1,2,3-tricarboxylate | | | | 41.6 | | | | |
| | 1,3,5-tris(4-Carboxyphenyl)benzene | | 43.8 | | 49.2 | | | | 49.0 |
| | 9-oxofluorene-2,7-dicarboxylate | | | | | | | | 45.6 |
| 2,2'-Bipyridine-5,5'-dicarboxylate | | | | | | | | | |
| | Formate | | | | | | | | 52.5 |

**Table S20. MOFs from mixed carboxylates linkers and other pyridin- or pyrazin- derivatives.**

| Linker 1 | Linker 2 | Cd | Cu | Fe | Ni | Zn Cr | Zn |
|---|---|---|---|---|---|---|---|
| Benzene-1,3-dicarboxylate | | | | | | | |
| | Pyridine-4-carboxamide | | | | 40.2 | | |
| | 1,3-bis(4-Pyridyl)propane | | 41.2 | | | | |
| 1,4-benzenedicarboxylate | | | | | | | |
| | Pyridine-3-carboxylate | | | 45.1 | 45.1 | | |
| | Pyridine-4-carbonitrile | | | 45.0 | | | |
| | Pyridine-4-carboxamide | | | | | 51.0 | |
| | 1,3-bis(4-Pyridyl)propane | 42.1 | | | | | 48.5 |
| | Pyrazine | | | | 44.1 | | |
| | 4-(4-pyridyl)benzoate | | | | | | 47.4 |
| 1,3,5-benzenetricarboxylate | | | | | | | |
| | Pyridine-4-carboxamide | | | | | 52.3 | |
| | Pyrazine | | | | 44.9 | | |
| 4,4'-oxydibenzoate | | | | | | | |
| | 1,2-bis(4-pyridyl)ethylene | | | | | | 55.7 |
| 5-Hydroxybenzene-1,3-dicarboxylate | | | | | | | |
| | Pyrazine | | 51.2 | | | | |
| 5-sulfobenzene-1,3-dicarboxylate | | | | | | | |
| | Pyrazine | | 55.0 | | | | |
| 3,4-pyridinedicarboxylate | | | | | | | |
| | Hexamethylenetetraamino | 45.0 | | | | | 49.7 |
| 4,4'-biphenyldicarboxylate | | | | | | | |
| | 1,2-bis(4-pyridyl)ethane | | | 47.9 | | | |
| Furan-2,5-dicarboxylate | | | | | | | |
| | 1,3-bis(4-Pyridyl)propane | | | | | | 40.8 |
| 2,6-naphtalenedicarboxylate | | | | | | | |
| | 1,3-bis(4-Pyridyl)propane | 46.9 | | | | | |
| | 1,2-bis(4-pyridyl)ethylene | | | | | | 48.8 |
| | 4-(4-pyridyl)benzoate | | | | 50.5 | | |
| 5-tert-butylbenzene-1,3-dicarboxylate | | | | | | | |
| | 1,2-bis(4-pyridyl)ethane | | | | | | 52.6 |
| 2-hydroxybenzene-1,4-dicarboxylate | | | | | | | |
| | Pyrazine | 46.2 | | | | | |
| 2,6-dimethylpyridine-3,5-dicarboxylate | | | | | | | |
| | Pyridine-4-carboxamide | | | | 48.1 | | |
| Benzene-1,2,3,4,5-pentacarboxylate | | | | | | | |
| | 1,2-bis(4-pyridyl)ethane | 45.0 | | | | | |
| 1,3,5-tris(4-Carboxyphenyl)benzene | | | | | | | |
| | Pyridine-4-carboxamide | | | | | 50.6 | |

**Table S21. MOFs from mixed carboxylates linkers and other N-binding linkers.**

| Linker 1 | Linker 2 | Cd | Cu Zn | Cu | Fe | Ni | Zn |
|---|---|---|---|---|---|---|---|
| 7H-purin-6-amine | | | | | | | |
| | pyridine-4-carboxamide | 48.8 | | | | | 40.1 |
| 1,4-diazabicyclo[2.2.2]octane | | | | | | | |
| | benzene-1,3-dicarboxylate | | | | | | 51.9 |
| | 1,4-Benzenedicarboxylate | | 52.5 | 52.5 | 51.8 | 50.3 | 49.7 |
| | 4,4'-biphenyldicarboxylate | | | | | | 50.6 |
| | 5-methylbenzene-1,3-dicarboxylate | | | | | | 49.2 |
| | 2,6-Naphtalenedicarboxylate | | | | | 46.0 | |
| | 2,5-Dichloro-1,4-benzenedicarboxylate | | | | | | 47.1 |
| | 4,4'-carbonyldibenzoate | | | | | | 51.1 |
| | 4,4'-(1,1,1,3,3,3-Hexafluoropropane-2,2-diyl)dibenzoate | | | | | | 50.8 |
| | 2-hydroxybenzene-1,4-dicarboxylate | | | | | | 48.5 |
| hexamethylenetetraamino | | | | | | | |
| | Thiophene-2,5-dicarboxylate | 43.0 | | | | | |
| | 3,4-Pyridinedicarboxylate | 45.0 | | | | | |

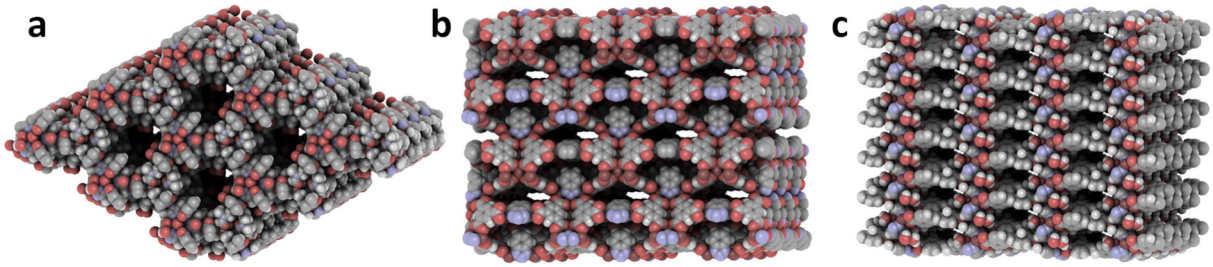


**Figure S9.** a: MAC-8 or $Cu_9$-$IA_5$-3,5dMeTz$_6$ (CSD code RUFZOJ). b: $Zn_9$-$BTC_6$-$BTrz_3$ (ZARLOV). c: MAC-14 or $Zn_2$-EDB-1,2,4TrAz$_2$ (CUQRUD).Created with iRASPA.[14]

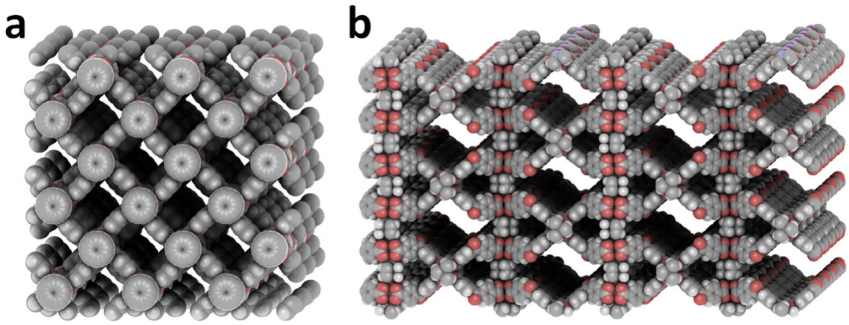


**Figure S10.** a: $Zn_2$-$BDC_2$-DABCO (CSD code WARFAY01). b: $Zn_2$-4,4'COd$B_2$-DABCO (HOHMIB). Created with iRASPA.[14]

# 5. abbreviations

| Abbreviation | Name of the substance | CAS |
|---|---|---|
| 1,2,3TrAz | 1,2,3-triazole | 288-36-8 |
| 1,2,4TrAz | 1,2,4-triazole | 288-88-0 |
| 2,2'bPy | 2,2'-bipyridine | 366-18-7 |
| 3,5dMeTz | 3,5-dimethyl-1,2,4-triazole | 7343-34-2 |
| 4,4'bPy | 4,4'-bipyridine | 553-26-4 |
| BTrz | Benzotriazole | 95-14-7 |
| DABCO | 1,4-diazabicyclo[2.2.2]octane | 280-57-9 |
| $H_2$3,4PyDC | Pyridine-3,5-dicarboxylic acid | 490-11-9 |
| $H_2$3,5PyDC | Pyridine-3,5-dicarboxylic acid | 499-81-0 |
| $H_2$4,4'COdB | 4,4'-carbonyldibenzoic acid | 964-68-1 |
| $H_2$5OIA | 5-hydroxybenzene-1,3-dicarboxylic acid | 618-83-7 |
| $H_2$BDC | 1,4-benzenedicarboxylic or terephthalic acid | 100-21-0 |
| $H_2$bPDC | 4,4'-biphenyldicarboxylic acid | 787-70-2 |
| $H_2$DOTP | 2,5-dihydroxybenzene-1,4-dicarboxylic acid | 610-92-4 |
| $H_2$EDB | 4,4'-ethene-1,2-diyldibenzoic acid | 100-31-2 |
| $H_2F_6$PdB | 4,4’-(1,1,1,3,3,3-hexafluoropropane-2,2-diyl)dibenzoic acid | 1171-47-7 |
| $H_2$IA | Benzene-1,3-dicarboxylic or isophthalic acid | 121-91-5 |
| $H_2$NBDC | 2-aminobenzene-1,4-dicarboxylic acid | 10312-55-7 |
| $H_2$NDC | 2,6-naphthalenedicarboxylic acid | 1141-38-4 |
| $H_2$NIA | 5-aminobenzene-1,3-dicarboxylic acid | 99-31-0 |
| $H_2$ODBZ | 4,4'-oxydibenzoic acid | 2215-89-6 |
| $H_2$tBuIA | 5-tert-butylbenzene-1,3-dicarboxylic acid | 2359-09-3 |
| $H_2$TDC | Thiophene-2,5-dicarboxylic acid | 4282-31-9 |
| $H_3$BTB | 1,3,5-tris(4-carboxyphenyl)benzene | 50446-44-1 |
| $H_3$BTC | 1,3,5-benzenetricarboxylic or trimesic acid | 554-95-0 |
| $H_3$NOTB | 4,4',4"-nitrilotribenzoic acid | 118996-38-6 |
| $H_4$AzBTC | 3,3’,5,5'-azobenzenetetracarboxylic acid | 365549-33-3 |
| HFA | Formic acid | 64-18-6 |
| HIm | Imidazole | 288-32-4 |
| HMeIm | 2-methylimidazol | 693-98-1 |
| P4CA | Pyridine-4-carboxamide or isonicotinic acid | 1453-82-3 |
| PTz | 5-(4-pyridyl)tetrazol | 14389-12-9 |
| PyEt | 1,2-bis(4-pyridyl)ethane | 4916-57-8 |
| PyEty | 1,2-bis(4-pyridyl)ethylene | 13362-78-2 |
| Pyz | Pyrazine | 290-37-9 |
| Ser | (2s)-2-amino-3-hydroxypropanoic acid or serine | 302-84-1 |

## 6. Electronic Resources

A user interface can be used free or charge in http://mofdb-bam.de/

## 7. References


1. Y. G. Chung, E. Haldoupis, B. J. Bucior, M. Haranczyk, S. Lee, H. D. Zhang, K. D. Vogiatzis, M. Milisavljevic, S. L. Ling, J. S. Camp, B. Slater, J. I. Siepmann, D. S. Sholl and R. Q. Snurr, *J Chem Eng Data*, 2019, **64**, 5985-5998.
2. M. Reich and P. M. Vasconcelos, *Elements*, 2015, **11**, 305-310.
3. P. Z. Moghadam, A. Li, S. B. Wiggin, A. Tao, A. G. P. Maloney, P. A. Wood, S. C. Ward and D. Fairen-Jimenez, *Chemistry of Materials*, 2017, **29**, 2618-2625.
4. B. J. Bucior, A. S. Rosen, M. Haranczyk, Z. P. Yao, M. E. Ziebel, O. K. Farha, J. T. Hupp, J. I. Siepmann, A. Aspuru-Guzik and R. Q. Snurr, *Crystal Growth & Design*, 2019, **19**, 6682-6697.
5. J. A. Villajos, A. Zimathies and C. Prinz, *International Journal of Hydrogen Energy*, 2020.
6. T. Düren, F. Millange, G. Férey, K. S. Walton and R. Q. Snurr, *The Journal of Physical Chemistry C*, 2007, **111**, 15350-15356.
7. D. P. Broom and M. Hirscher, *Energy & Environmental Science*, 2016, **9**, 3368-3380.
8. K. E. Hurst, T. Gennett, J. Adams, M. D. Allendorf, R. Balderas-Xicohtencatl, M. Bielewski, B. Edwards, L. Espinal, B. Fultz, M. Hirscher, M. S. L. Hudson, Z. Hulvey, M. Latroche, D. J. Liu, M. Kapelewski, E. Napolitano, Z. T. Perry, J. Purewal, V. Stavila, M. Veenstra, J. L. White, Y. Yuan, H. C. Zhou, C. Zlotea and P. Parilla, *Chemphyschem*, 2019, **20**, 1997-2009.
9. P. García-Holley, B. Schweitzer, T. Islamoglu, Y. Liu, L. Lin, S. Rodriguez, M. H. Weston, J. T. Hupp, D. A. Gómez-Gualdrón, T. Yildirim and O. K. Farha, *ACS Energy Letters*, 2018, **3**, 748-754.
10. H. Chun and J. Seo, *Inorganic Chemistry*, 2009, **48**, 9980-9982.
11. U. o. Cambridge, OPSIN: Open Parser for Systematic IUPAC nomenclature, https://opsin.ch.cam.ac.uk/).
12. N. M. O'Boyle, M. Banck, C. A. James, C. Morley, T. Vandermeersch and G. R. Hutchison, *Journal of Cheminformatics*, 2011, **3**, 33.
13. N. C. f. B. Information, PubChem, https://pubchem.ncbi.nlm.nih.gov/, 2020).
14. D. Dubbeldam, S. Calero and T. J. H. Vlugt, *Molecular Simulation*, 2018, **44**, 653-676.