Electronic Supplementary Material (ESI) for Molecular Systems Design & Engineering.

Engineering metal-organic frameworks for adsorption-based gas separations: from process to atomic scale

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SUPPORTING INFORMATION

We note that MOFs are usually named according to a non-systematic method that involves the use of acronyms that are most often derived from the name of the institution where they were first discovered, associated with a number. In the following, we report the acronym meaning, the structural formula of the organic linkers, the metal ion, the chemical formula, and the CSD refcode for each MOF mentioned in the main text. The MOFs are listed in order of appearance in the main text, as follows:

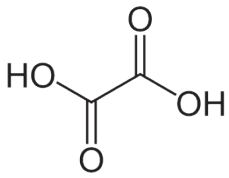
- CALF-20
- MIL-160
- Ca-trimesate
- CALF-15
- UTSA-16
- IISERP-MOF-2
- SIFSIX-2-Cu-i
- UiO-66
- MIL-140A
- Co-bdp
- MIL-88
- DUT-49
- MIL-53(Al)
- ELM-11, ELM-12
- ZIF-8
- Basolite-A520
- DUT-5
- SBMOF-1
- MUF-15
- UTSA-280
- [Mg_2(dobpdc)]
- [$Cr_3(btc)_2$]
- MOF-74(Fe)
- MIL-100(Cr)
- [$V_2Cl_{2.8}$(btdd)]

CALF-20

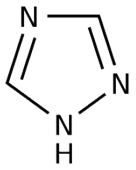
Acronym meaning:

CALF = CALgary Framework

Linkers:



Oxalic acid (H_2ox)



1,2,4-triazole (Htrz)

Metal ion:

Zn^{II}

Chemical formula:

$[Zn_2(ox)(trz)_2]$

CSD refcode:

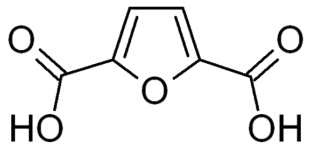
Crystallographic data not deposited - structure presumed analogous to CALF-15

MIL-160

Acronym meaning:

MIL = Material of Institut Lavoisier

Linker:



2,5-furandicarboxylic acid (H_2fdc)

Metal ion:

Al^{III}

Chemical formula:

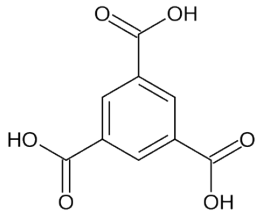
[Al(OH)(fdc)]

CSD refcode:

PIBZOS

Ca-trimesate

Linker:



1,3,5-benzenetricarboxylic acid (H_3btc), aka trimesic acid

Metal ion:

Ca^{II}

Chemical formula:

[Ca(Hbtc)(H_2O)]

CSD refcode:

RUFMUA

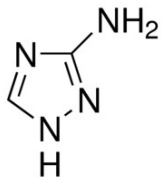
CALF-15

Acronym meaning:

CALF = CALgary Framework

Linkers:

Oxalic acid (H_2ox)



3-amino-1,2,4-triazole (Hatrz)

Metal ion:

Zn^{II}

Chemical formula:

$[Zn_2(ox)(atrz)_2]$

CSD refcode:

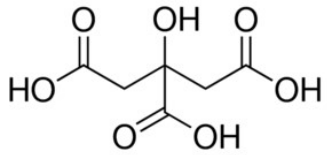
MUDKOM

UTSA-16

Acronym meaning:

UTSA = University of Texas San Antonio

Linker:



Citric acid (H_4cit)

Metal ions:

Co^{II}, K^{I}

Chemical formula:

$[K_2Co_3(cit)_2]$

CSD refcode:

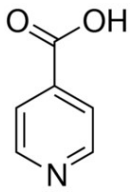
RAZXIA

IISERP-MOF-2

Acronym meaning:

IISERP = Indian Institute of Science Education and Research Pune

Linker:



4-pyridinecarboxylic acid (HPyC), aka isonicotinic acid

Metal ion:

Ni^{II}

Chemical formula:

$[Ni(PyC)_2]$

CSD refcode:

ACICOH

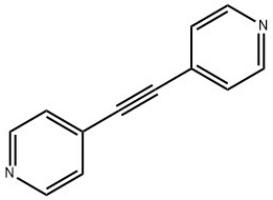
SIFSIX-2-Cu-i

Acronym meaning:

SIFSIX = SiF_6^{2-} (inorganic anion contained in the MOF)

i = interpenetrated isomer

Linker:



4,4'-dipyridylacetylene (dpa)

Metal ion:

Cu^{II}

Chemical formula:

$[Cu(SiF_6)(dpa)_2]$

CSD refcode:

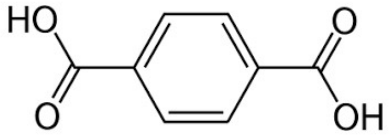
YEMTIV

UiO-66

Acronym meaning:

UiO = Universitetet i Oslo

Linkers:



1,4-benzenedicarboxlic acid (H_2bdc), aka terephthalic acid

Metal ion:

Zr^{IV}

Chemical formula:

$[Zr_6O_4(OH)_4(bdc)_6]$

CSD refcode:

RUBTAK

MIL-140A

Acronym meaning:

MIL = Material of Institut Lavoisier

Linkers:

1,4-benzenedicarboxlic acid (H_2bdc), aka terephthalic acid

Metal ion:

Zr^{IV}

Chemical formula:

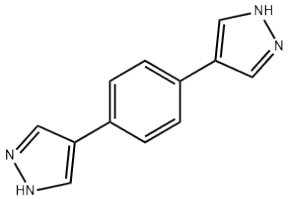
[ZrO(bdc)]

CSD refcode:

ZONBAH

Co-bdp

Linker:



1,4-Di(1H-pyrazol-*4*-yl)benzene (H_2bdp)

Metal ion:

Co^{II}

Chemical formula:

[Co(bdp)]

CSD refcode:

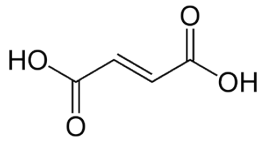
COJHIT

MIL-88

Acronym meaning:

MIL = Material of Institut Lavoisier

Linker:



Fumaric acid (H_2fum)

Metal ions:

Fe^{III}

Chemical formula:

$[Fe_3O(CH_3OH)_3(fum)_3 \cdot (CH_3COO)]$

CSD refcode:

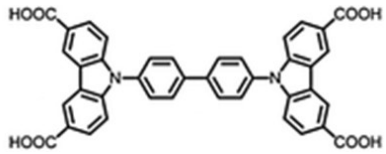
FAVKAP

DUT-49

Acronym meaning:

DUT = Dresden University of Technology

Linker:



9,9’-([1,1’-biphenyl]-4,4’-diyl)bis(9*H*-carbazole-3,6-dicarboxylic acid) (H_4bbcdc)

Metal ions:

Cu^{II}

Chemical formula:

[Cu_2(BBCDC)]

CSD refcode:

ACOCOM

MIL-53(Al)

Acronym meaning:

MIL = Material of Institut Lavoisier

Linker:

1,4-benzenedicarboxlic acid (H_2bdc), aka terephthalic acid

Metal ions:

Al^{III}

Chemical formula:

[Al(OH)(bdc)]

CSD refcode:

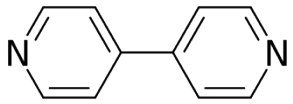
SABVUN

ELM-11, ELM-12

Acronym meaning:

ELM = Elastic Layered Material

Linker:



4,4'-bipyridine (bipy)

Metal ions:

Cu^{II}

Chemical formula:

ELM-11: $[Cu(BF_4)_2(bipy)_2]$

ELM-12: $[Cu(CF_3SO_3)_2(bipy)_2]$

CSD refcode:

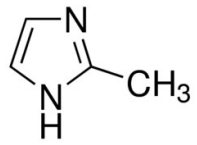
UXUPAF (ELM-12)

ZIF-8

Acronym meaning:

ZIF = Zeolitic imidazolate framework

Linker:



2-methylimidazole (Hmeim)

Metal ions:

Zn^{II}

Chemical formula:

$[Zn(meim)_2]$

CSD refcode:

VELVOY

Basolite-A520

Acronym meaning:

Basolite is the commercial name under which BASF sells this MOF

Linker:

Fumaric acid (H_2fum)

Metal ions:

Al^{III}

Chemical formula:

[Al(OH)(fum)]

CSD refcode:

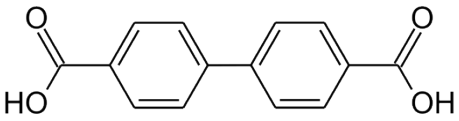
DOYBEA

DUT-5

Acronym meaning:

DUT = Dresden University of Technology

Linker:



4,4'-biphenyldicarboxylic acid (H_2bpdc)

Metal ions:

Al^{III}

Chemical formula:

[Al(OH)(bpdc)]

CSD refcode:

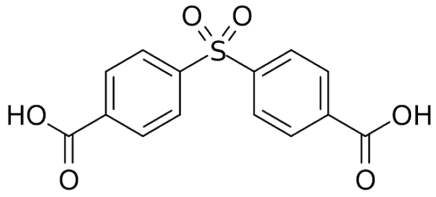
Crystallographic data not deposited - structure presumed isoreticular to MIL-53(Al)

SBMOF-1

Acronym meaning:

Not defined, “SB” presumably refers to the sulfonylbenzoate linker

Linker:



4,4’-sulfonyldibenzoic acid (H_2sdb)

Metal ions:

Ca^{II}

Chemical formula:

[Ca(sdb)]

CSD refcode:

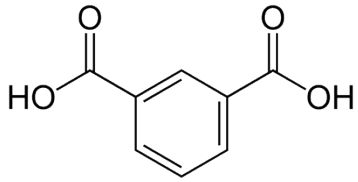
KAXQIL

MUF-15

Acronym meaning:

MUF = Massey University Framework

Linker:



1,3-benzenedicarboxylic acid, aka isophthalic acid (H_2ipa)

Metal ions:

Co^{II}

Chemical formula:

$[Co_3(OH)(ipa)_{2.5}(H_2O)]$

CSD refcode:

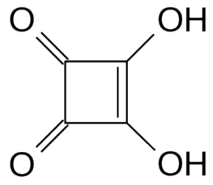
HIXNEK

UTSA-280

Acronym meaning:

UTSA = University of Texas San Antonio

Linker:



Squaric acid (H_2sqa)

Metal ions:

Ca^{II}

Chemical formula:

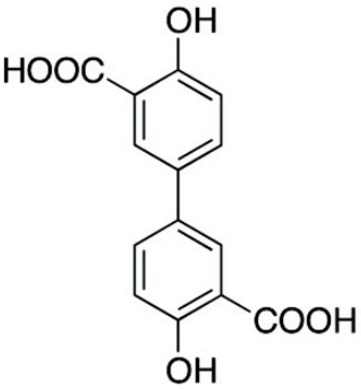
[Ca(sqa)(H_2O)]

CSD refcode:

FIRVEH

[Mg_2(dobpdc)]

Linker:



4,4’-dioxidobiphenyl-3,3’-dicarboxylic acid (H_2dobpdc)

Metal ions:

Mg^{II}

Chemical formula:

[Mg_2(dobpdc)]

CSD refcode:

XUXPUD

$[Cr_3(btc)_2]$

Linker:

1,3,5-benzenetricarboxylic acid (H_3btc), aka trimesic acid

Metal ions:

Cr^{II}

Chemical formula:

$[Cr_3(btc)_2]$

CSD refcode:

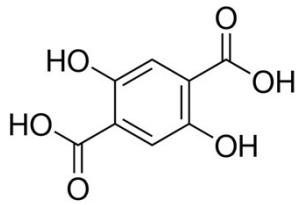
ZIGFEC

MOF-74(Fe), aka CPO-27(Fe)

Acronym meaning:

CPO = Coordination polymer of Oslo

Linker:



2,5-dihydroxy-1,4-benzenedicarboxylic acid (H_4dobdc)

Metal ions:

Fe^{II}

Chemical formula:

[Fe_2(dobdc)]

CSD refcode:

COKNOH01

MIL-100(Cr)

Acronym meaning:

MIL = Material of Institut Lavoisier

Linker:

1,3,5-benzenetricarboxylic acid (H_3btc), aka trimesic acid

Metal ions:

Cr^{III}

Chemical formula:

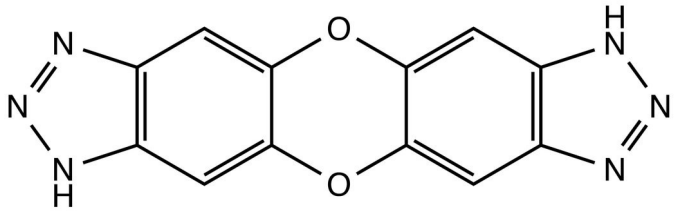
$[Cr_3O(H_2O)_2(OH)(btc)_2]$

CSD refcode:

UDEMEW

$[V_2Cl_{2.8}(btdd)]$

Linker:



bis(1*H*-1,2,3-triazolo[4,5-*b*],[4′,5′-*i*])dibenzo[1,4]dioxin (H_2btdd)

Metal ions:

V^{II}/V^{III}

Chemical formula:

$[V_2Cl_{2.8}(btdd)]$

CSD refcode:

OVUNIE (Mn^{II} analogue)