UiO-66 Zirconium Building Bricks for Stable Metal Organic Frameworks

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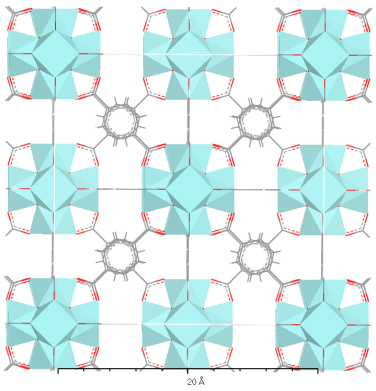
Catalog No. 40-1105
Zirconium 1,4-dicarboxybenzene MOF (UiO-66)

Structure of UiO-66



The Special Nature of UiO-66

The stability of MOFs is largely determined by the structure of the inorganic brick and the nature of the chemical bonds it forms with the linker. To date, most MOFs have exhibited weak thermal, chemical, and mechanical stability, which has limited their use in large-scale industrial applications.

UiO-66 (and isoreticular UiO-67 and UiO-68), however, is a zirconium-based MOF with very high surface area (1180-1240m^2/g) and unprecedented stability.

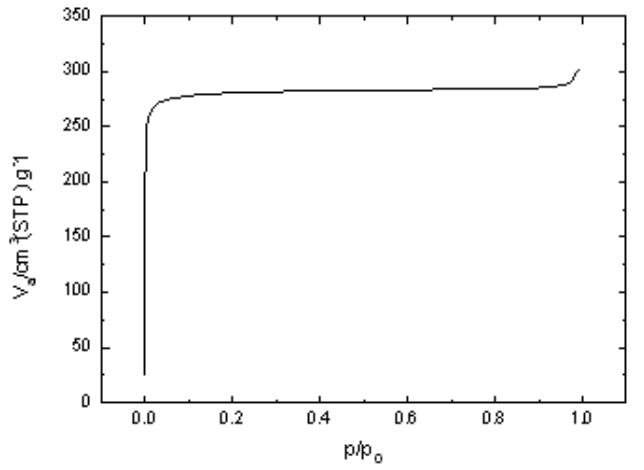
Developed by Prof. Karl Petter Lillerud of the Department of Chemistry at the University of Oslo, UiO-66 is comprised of $Zr_6O_4(OH)_4$ octahedra that are 12-fold connected to adjacent octahedra through a 1,4-benzene-dicarboxylate (BDC) linker, resulting in a highly packed fcc structure.

The Zr-O bonds formed between the cluster and carboxylate ligands is believed to be the source of increased stability of Zr-based MOFs. Specifically, the combination of strong Zr−O bonds and the ability of the inner Zr_6-cluster to rearrange reversibly upon removal or addition of μ_3-OH groups without any changes in the connecting carboxylates are thought to contribute to the greater stability of UiO-66.

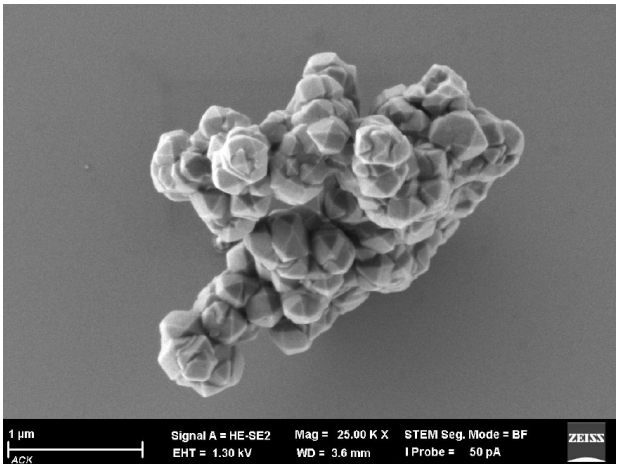
Key Properties of UiO-66

The particle size of UiO-66 is 0.2-0.5µ, and the particles have clearly visible facets.

UiO-66 N_2 adsorption at 77 K



SEM image of UiO-66



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Key Properties of UiO-66

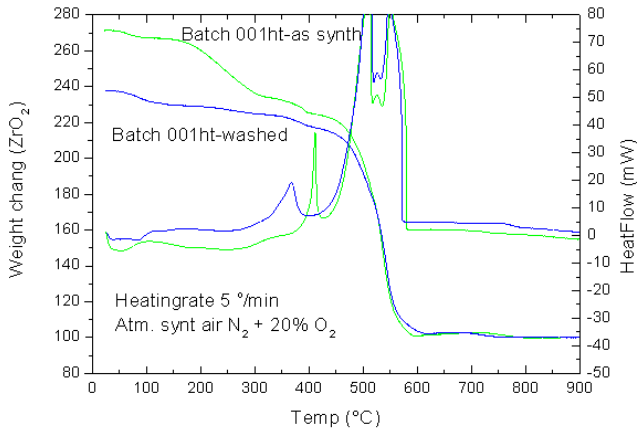
The **specific surface area** of UiO-66 after heating to 300°C is 1180-1240 m^2/g.

The **pore size** of the UiO-66 is 6 Å. That means that a molecule the size of fully methylated benzene can enter the UiO-66 structure.

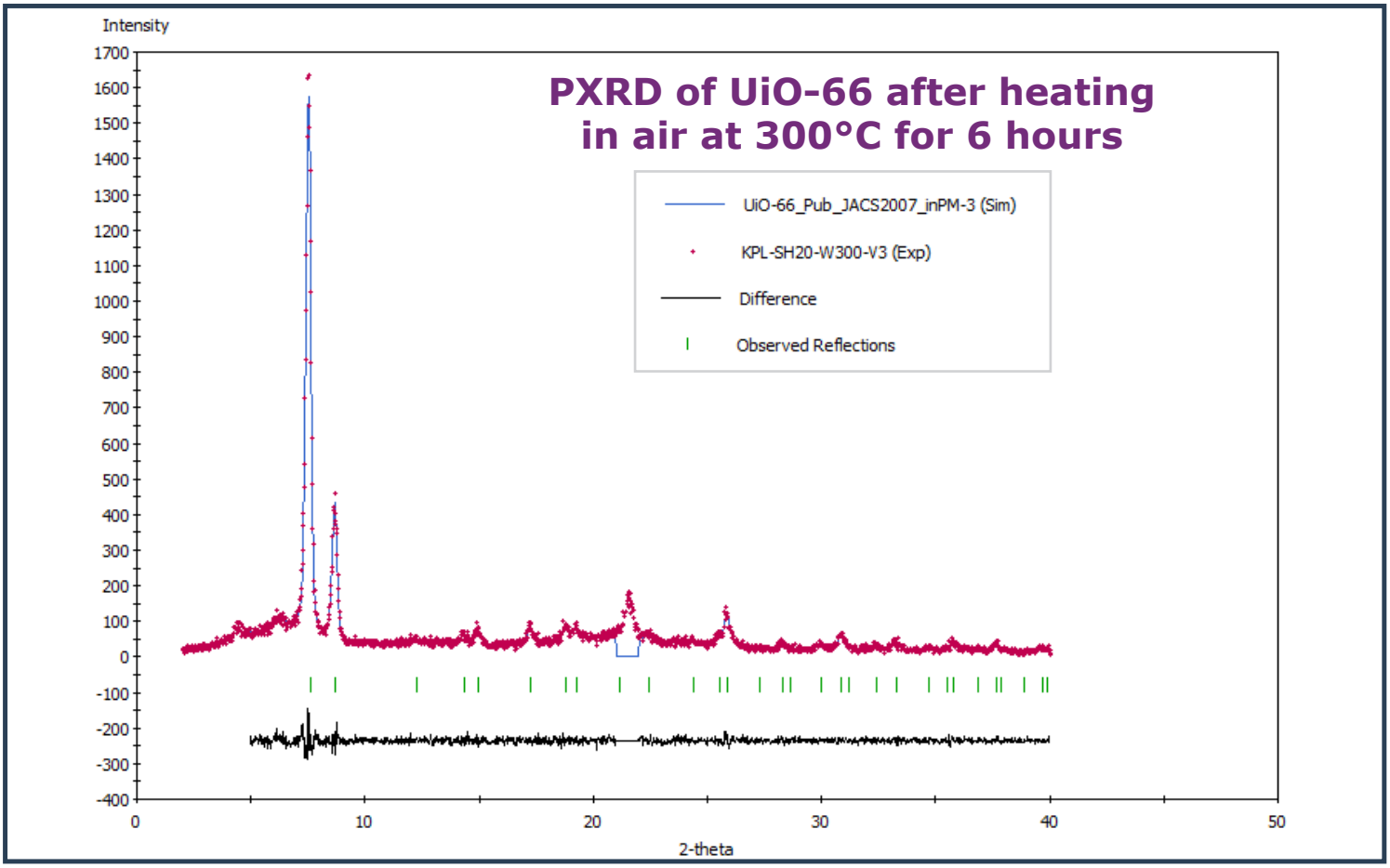
The **toughness** of UiO-66 is demonstrated in its physical properties:

- Stable upon washing in boiling water and after heating in air to 300°C for 6 h,
- Decomposition above 500°C,
- Resistance to most chemicals, and
- Retention of crystallinity even after exposure to 10 tons/cm^2 of external pressure.

Thermogravimetric response of UiO-66 during heating in air



PXRD of UiO-66 after heating in air at 300°C for 6 hours



References:

1. *J. Am. Chem. Soc.*, **2008**, *139*, 13850.
2. *J. Phys. Chem. Lett.*, **2013**, *4(6)*, 925.
3. *Chemistry – An Asian Journal* **2011**, *6(12)*, 3270.
4. *Chem. Mater.*, **2011**, *23 (7)*, 1700.

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UiO-66 Analogs

40-1109 **Zirconium aminobenzenedicarboxylate MOF** 500mg
(UiO-66-BDC-NH2, BDC-NH2:Zr=0.9-1.0) *(1260119-00-3)* 2g
$Zr_6O_4(OH)_4(C_8H_5NO_4)_x$, X=5.4-6.0; yellow solid; SA: 800-1075;
P.Vol. 0.31-0.41
Note: Particle size: 0.1-0.5 micron, Thermal stability: 300ºC,
Activation temperature: 150ºC
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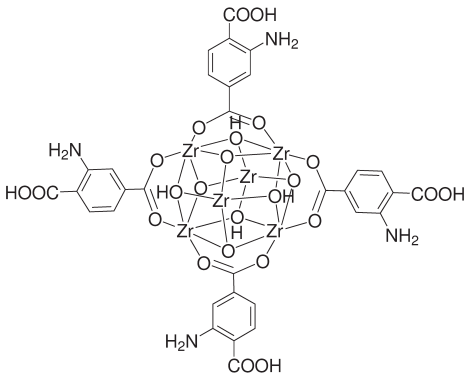

Technical Notes:
1. Useful MOF for adsorption of CO_2 applications[1].
2. Catalyst MOF used in the conversion of toxic agents to non-toxic products[2].

References:

1. *Carbon Dioxide Adsorption in Amine-Functionalized Mixed-Ligand Metal-Organic Frameworks of UiO-66 Topology.,* Chem.Sus.Chem. **2014**, *7*, 3382-3388.
2. *Tailoring the Pore Size and Functionality of UiO-Type Metal−Organic Frameworks for Optimal Nerve Agent Destruction,* Inorg. Chem. **2015**, *54*, 9684−9686.
3. *Towards Metal-Organic Framework based Field Effect Chemical Sensors: UiO-66-NH2 for Nerve Agent Detection,* Chem. Sci., **2016**, *7*, 5827.

40-1108 **Zirconium benzenedicarboxylate MOF** 500mg
(UiO-66-BDC, BDC:Zr=0.66-0.98) 2g
$Zr_6O_4(OH)_4(C_8H_4O_4)_x$ X=3.96-5.88; white solid; SA: 1050-1400; P.Vol. 0.42-0.58
Note: Particle size: 0.2-0.5 micron, Thermal stability: 400ºC, Activation temperature: 300ºC
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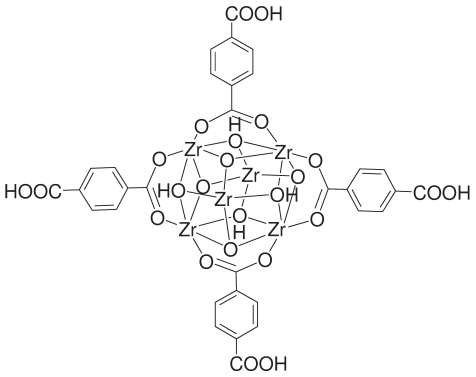

Technical Note:
1. New zirconium-based inorganic building brick that allows the synthesis of very high surface area MOF's with unprecedented stability[3]

References:

1. *Tuned to Perfection: Ironing Out the Defects in Metal−Organic Framework UiO-66* Chem. Mater. **2014**, *26*, 4068−4071.
2. *H_2 storage in isostructural UiO-67 and UiO-66 MOFs* Phys. Chem. Chem. Phys., **2012**, *14*, 1614–1626.
3. *A New Zirconium Inorganic Building Brick Forming Metal Organic Frameworks with Exceptional Stability*. J. Am. Chem. Soc. **2008**, *130*, 13850–13851.

40-1112 **Zirconium biphenyldicarboxylate MOF** 250mg
(UiO-66-BPDC/UiO-67, BPDC:Zr=0.9-1.0) 1g
$Zr_6O_4(OH)_4(C_{14}H_8O_4)_x$, X = 5.4-6.0; white solid; SA: 2400-2500;
P.Vol. 0.85-0.98 cm^3/g
moisture sensitive
Note: Particle size: 0.4-0.7 micron, Thermal stability: 450ºC
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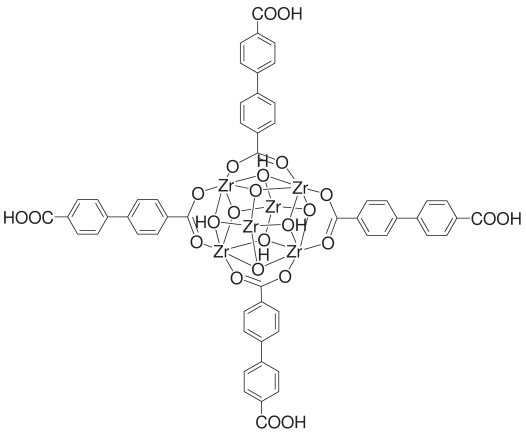

Technical Notes:
1. Metal−organic framework showing excellent stability to water, reversible water vapor adsorption, and increased volumetric capacity for methane adsorption[1]
2. Remarkable stability at high temperatures, high pressures and in the presence of different solvents, acids and bases[2,3]

References:

1. *UiO-67-type Metal−Organic Frameworks with Enhanced Water Stability and Methane Adsorption Capacity*, Inorg. Chem. **2016**, *55*, 1986−1991.
2. *H_2 storage in isostructural UiO-67 and UiO-66 MOFs*, Phys. Chem. Chem. Phys., **2012**, *14*, 1614–1626.
3. *A New Zirconium Inorganic Building Brick Forming Metal Organic Frameworks with Exceptional Stability.* J. Am. Chem. Soc. **2008**, *130*, 13850–13851.

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UiO-66 Analogs

40-1114 **Zirconium Fumarate MOF (UiO-66-FA, FA:Zr=0.66-0.98)** 500mg 2g

$Zr_6O_4(OH)_4(C_4H_2O_4)_x$, X = 3.96-5.88; white solid; SA: 650-960; P.Vol. 0.26-0.4

Note: Particle size: 0.1-0.5 micron, Thermal stability: 200ºC, Activation temperature: 130ºC

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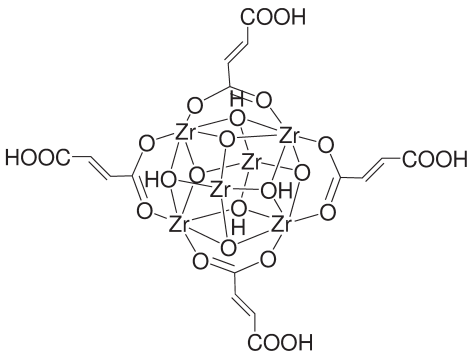

Technical Notes:

1. Metalorganic framework used in a large number of studies for the storage of hydrogen or methane[2]
2. Water adsorption in MOF's for many applications such as dehumidification, thermal batteries, and delivery of drinking water in remote areas[3]

References:

1. *Water harvesting from air with metal-organic frameworks powered by natural sunlight*. Science, **2017**, *356*, 430–434.
2. *A Facile "Green" Route for Scalable Batch Production and Continuous Synthesis of Zirconium MOFs.* Eur. J. Inorg. Chem. **2016**, 4490–4498.
3. *Water Adsorption in Porous Metal−Organic Frameworks and Related Materials*, J. Am. Chem. Soc., **2014**, *136*, 4369−4381.
4. *A water-born Zr-based porous coordination polymer: Modulated synthesis of Zr-fumarate MOF*. Microporous and mesoporous materials, **2015**, *203*,186-194.

40-1106 **Zirconium trans-1, 2-ethylenedicarboxylic acid MOF (UiO-66-FA, FA:Zr=1)** 500mg 2g

$Zr_6O_4(OH)_4(C_4H_2O_4)_6$; cream solid; SA: 720-770; P.Vol. 0.29-0.32

Note: Particle size: 0.1-0.5 micron, Thermal stability: 200ºC, Activation temperature: 150ºC

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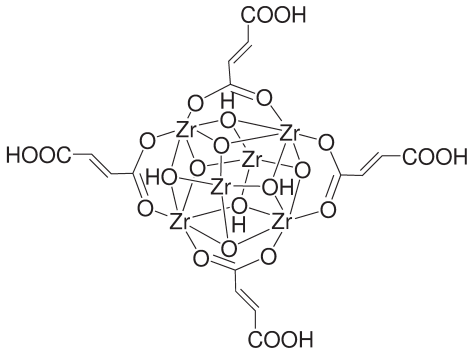

Technical Notes:

1. See 40-1114.

40-1111 **Zirconium trimellitate MOF (UiO-66-BDC-COOH, BDC-COOH:Zr=0.9-1.0)** 500mg 2g

$Zr_6O_4(OH)_4(C_9H_4O_6)_x$, X = 5.4-6.0; white solid; SA: 550-600; P.Vol. 0.25-0.27

Note: Particle size: 0.2-0.5 micron, Thermal stability: 350ºC, Activation temperature: 150ºC

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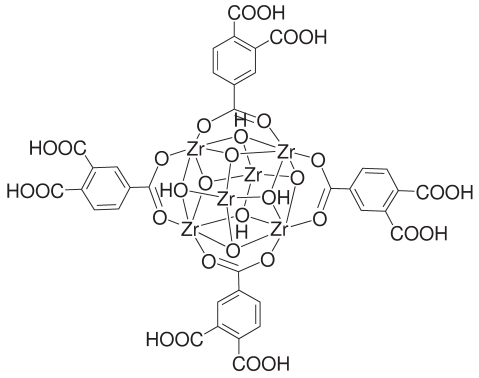

Technical Notes:

1. MOF for which the introduction of copper markedly increases ammonia adsorption capacities[1]
2. Functionalized forms show the highest selectivity, good working capacity and medium ranged CO_2 adsorption enthalpy that make these materials very promising for physi-sorption-based processes[2]

References:

1. *Engineering Copper Carboxylate Functionalities on Water Stable Metal−Organic Frameworks for Enhancement of Ammonia Removal Capacities*. J. Phys. Chem. C, **2017**, *121*, 3310−3319
2. *Functionalizing porous zirconium terephthalate UiO-66(Zr) for natural gas upgrading: a computational exploration.,* Chem. Commun., **2011**, *47*, 9603–9605.

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