NH_2-MIL-125(Ti), AYRSORB™ T125

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Catalog # 22-1070

Hexakis[μ-(2-amino-1,4-benzenedicarboxylato)][tetra-μ-hydroxyocta-μ-oxooctatitanium], NH2-MIL-125(Ti), AYRSORB™ T125

CAS# 1309760-94-8
Formula: $C_{48}H_{34}N_6O_{36}Ti_8$
Formula Weight: 1653.74
Color & Form: Yellow pwdr.
Available Sizes: 250mg, 1g

Sold in collaboration with framergy for research purposes only.
Patent: US 8,940,392 B2

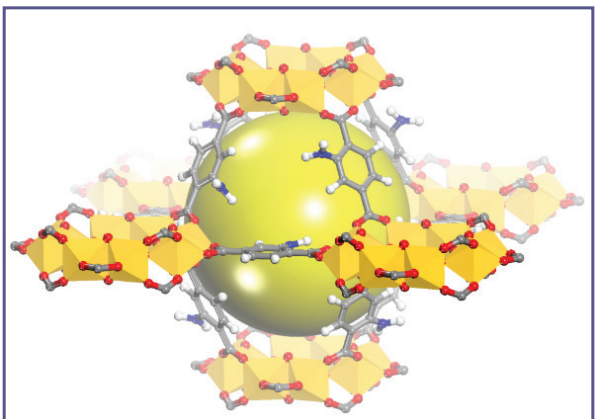
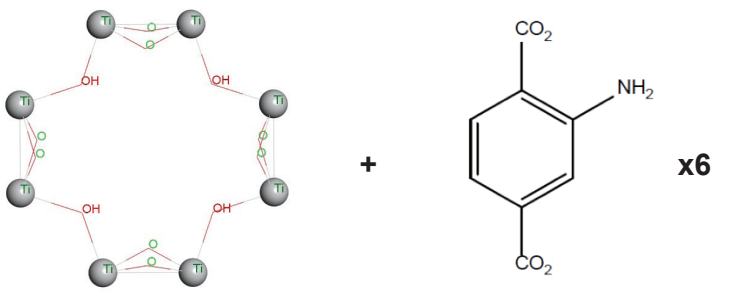
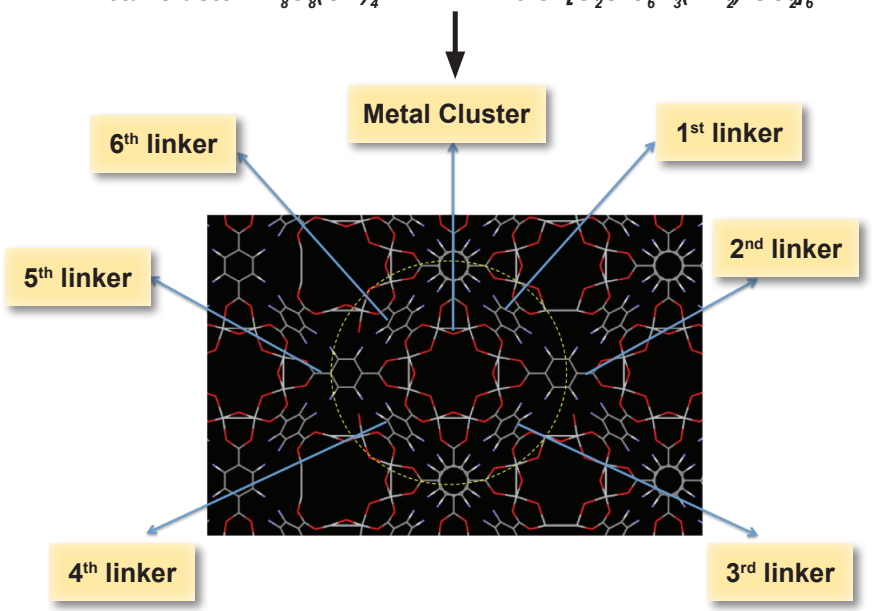


Figure 1: Schematic view of the cages of MIL-125(Ti)-NH2

This metal-organic framework (MOF) material is composed of a repeating unit cell. The unit cell is composed of a metal cluster and six linkers (ligands). The linkers connect the metal clusters together and they form a porous network, which is called a MOF. To clarify the structure in the above figure, the cluster is depicted with its elemental components to help the reviewer match the structure to its formula. *(please see below)*



Metal Cluster: $Ti_8O_8(OH)_4$ ***Linkers: $[O_2C\text{-}C_6H_3(NH_2)\text{-}CO_2]_6$***



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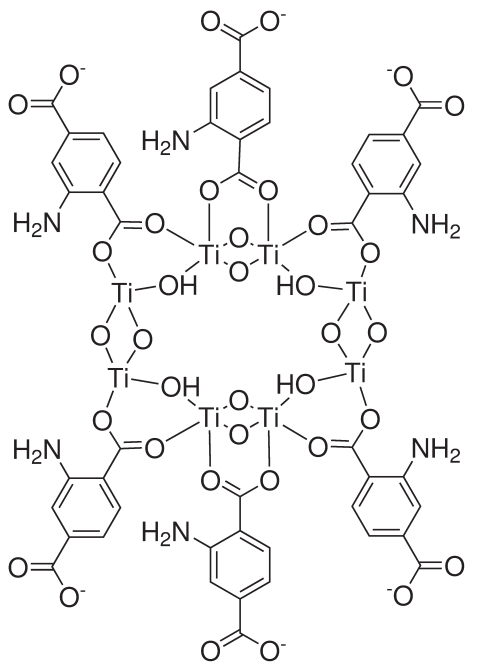
Using an appropriate choice of solvent mixtures (dimethylformamide (DMF) and methanol, solid denoted MIL-125(Ti)-NH2 or $Ti_8O_8(OH)_4(2OC\text{-}NH_2\text{-}C_6H_3\text{-}CO_2)_6 \cdot 18(CH_3OH) \cdot 3((CH_3)_2NCHO)$ has been isolated (MIL stands for Material from Institute Lavoisier). The synthesized solid was heated to 200°C for 6 hours under vacuum to remove the molecules of solvent (see Thermogravimetric analysis in Figure 2).

MIL-125-NH2 is thermally robust. After the departure of the guest molecules below 200 °C, X-ray diffractometry (Figure 3) does not indicate any change in crystallinity.

Nitrogen sorption experiments reveal that MIL-125-NH2 is highly porous characteristic of microporous solids, a BET surface area of 1530 $m^2 \cdot g^{-1}$, and a micropore volume (Vp) of 0.74(2) $cm^3 \cdot g^{-1}$ (Figure 4).



Structure drawing of 22-1070

Activation Protocol:

Activation of this material requires heating at 200 °C for 6 hours under vacuum. Upon cooling under vacuum, the activated product should be stored and handled under an inert atmosphere.

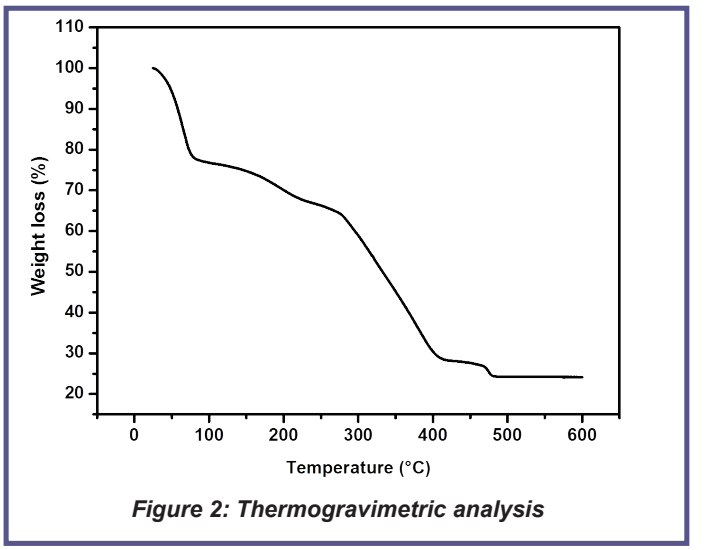


Figure 2: Thermogravimetric analysis

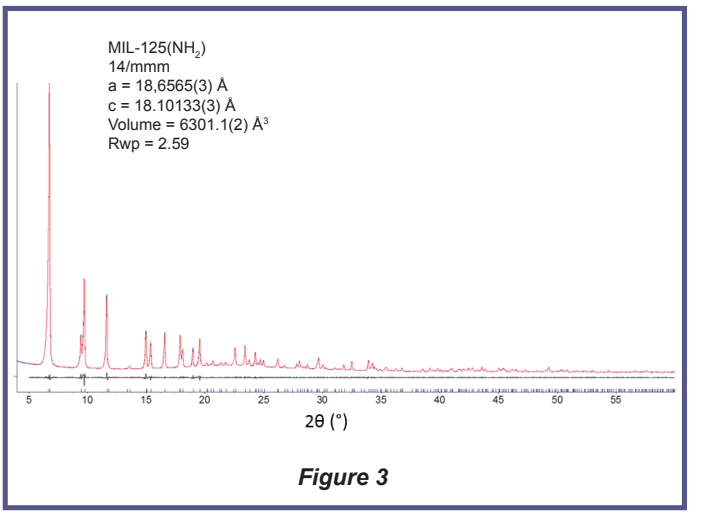


Figure 3

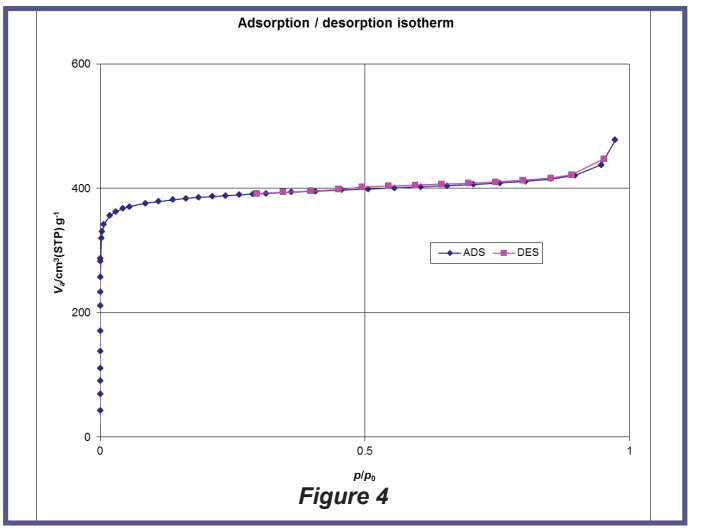


Figure 4

References:

1. A New Photoactive Crystalline Highly Porous Titanium(IV) Dicarboxylate, Meenakshi Dan-Hardi, Christian Serre, Theo Frot, Laurence Rozes, Guillaume Maurin, Clement Sanchez, and Gerard Ferey, *J. Am. Chem. Soc.*, **2009**, *131*, 10857–10859.

2. A robust amino-functionalized Titanium (IV) based MOF for an improved separation of acid gases, Sébastien Vaesen, Vincent Guillerm, Qingyuan Yang, Andrew Wiersum, Bartosz Marszalek, Barbara Gil, Alexandre Vimont, Marco Daturi, Thomas Devic, Philip L. Llewellyn, Christian Serre, Guillaume Maurin and Guy De Weireld, *Chem. Commun.*, **2013**, *49*, 10082-10084.

3. Adsorption/catalytic properties of MIL-125 and NH2-MIL-125, Se-Na Kim, Jun Kim, Hee-Young Kim, Hye-Young Cho, Wha-Seung Ahn, Catalysis Today **2013**, *204*, 85– 93.