

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: C₄₈H₃₄N₆O₃₆Ti₈

Formula Weight: 1653.74

Color & Form: Yellow powdr.

Available Sizes: 250mg, 1g

Sold in collaboration with framergy for research purposes only.

Patent: US 8,940,392 B2

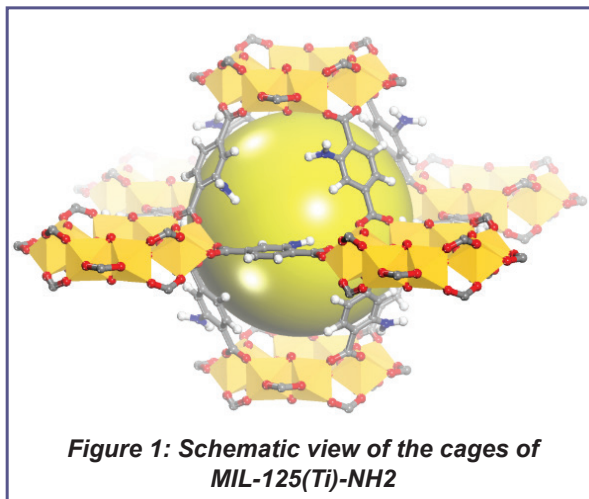
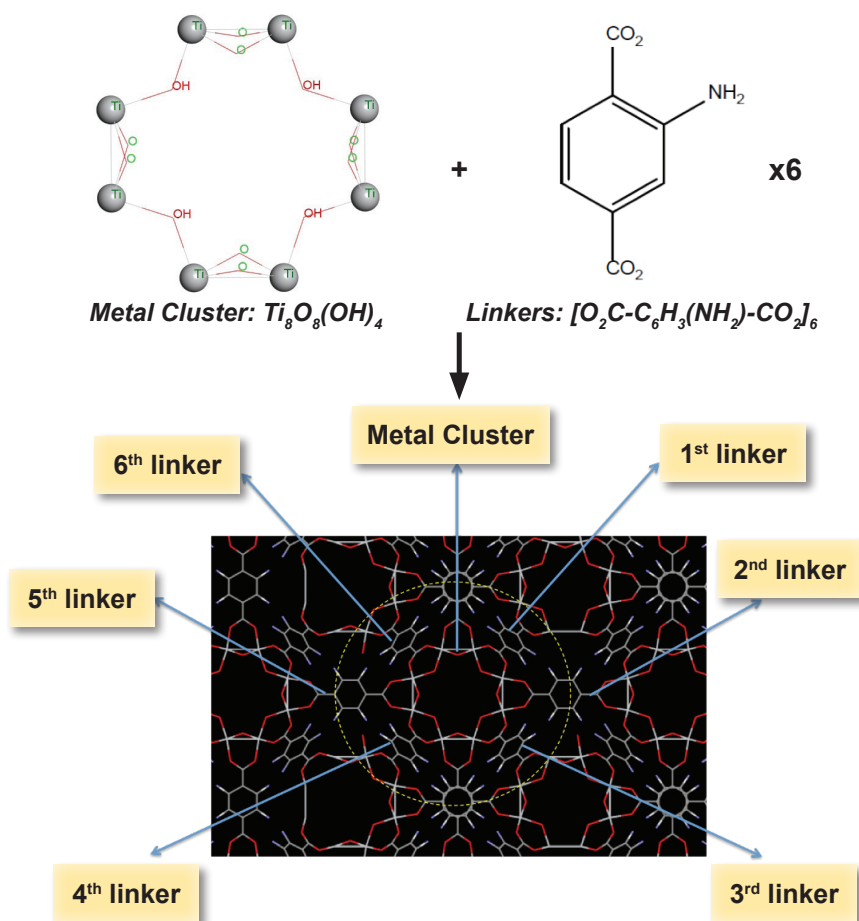


Figure 1: Schematic view of the cages of MIL-125(Ti)-NH₂

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)



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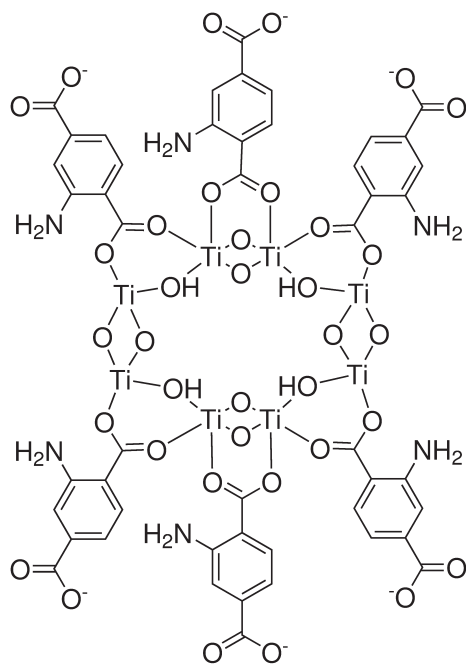
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Using an appropriate choice of solvent mixtures (dimethylformamide (DMF) and methanol, solid denoted MIL-125(Ti)-NH₂ or Ti₈O₈(OH)₄(2OC-NH₂-C₆H₃-CO₂)₆·18(CH₃OH)·3((CH₃)₂NCHO) has been isolated (MIL stands for Material from Institute Lavoisier). The 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 m²·g⁻¹, and a micropore volume (V_p) of 0.74(2) cm³·g⁻¹ (Figure 4).



Structure drawing of 22-1070

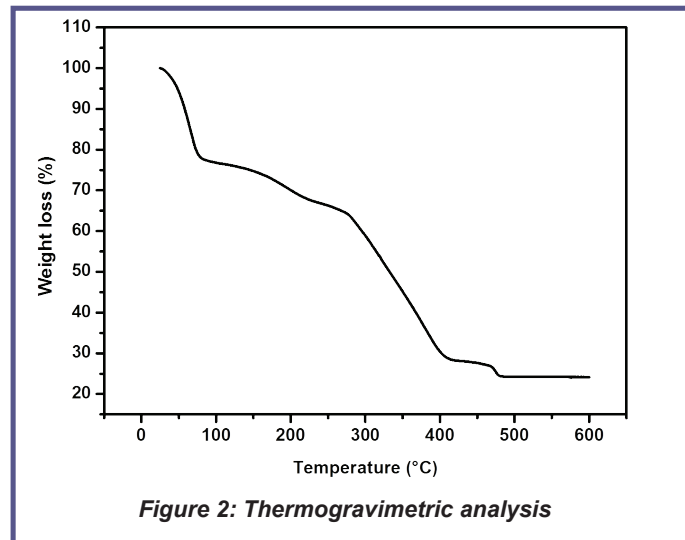


Figure 2: Thermogravimetric analysis

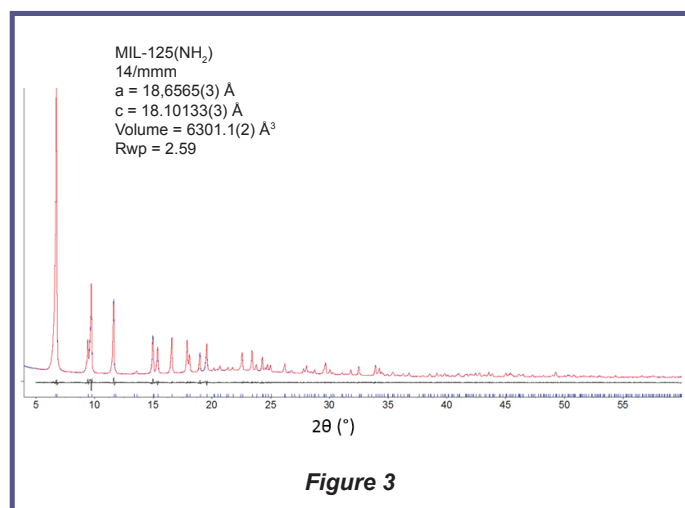


Figure 3

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.

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 Guillermin, 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.

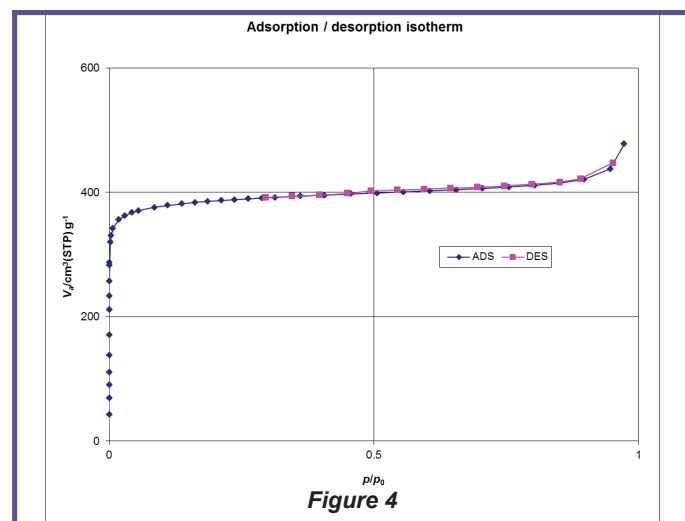


Figure 4

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