Iron azobenzene tetracarboxylic, Porous [PCN-250(Fe)], AYRSORB™ F250

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Catalog # 26-3725: Iron azobenzene tetracarboxylic, Porous [PCN-250(Fe)], AYRSORB™ F250

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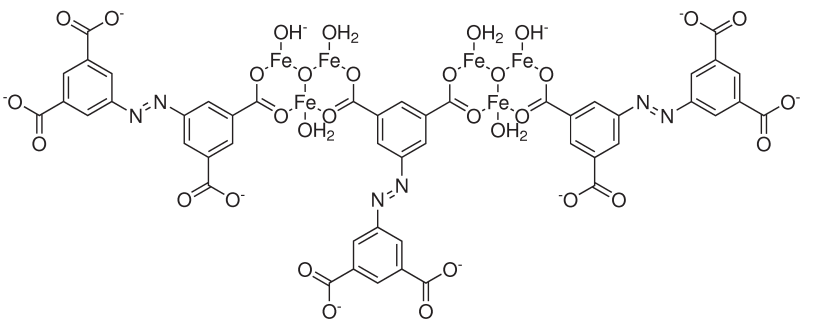
Iron azobenzene tetracarboxylic (PCN-250)



Metal-organic frameworks (MOFs) are based on coordination bonds which are typically less stable than covalently bonded materials.[1-4] Therefore, the stability of MOFs is an important challenge to overcome.[5-15] Stronger MOFs are moisture resistant and possess a high gas storage capacity, as well as an ability to easily be scaled up. These characteristics make them more suitable for commercial sale. The problem with the manufacturing process of these MOFs is that they were made using 'one-pot' synthesis which is difficult to control[16]. As a way of alleviating this challenge, an approach based on kinetic and thermodynamic control of MOF crystallization has been used to synthesize Fe-MOF single crystals with pre-synthesized metal building blocks [Fe_2 M(μ_3 -O)(CH_3 $COO)_6$] (M=$Fe^{2+,3+}$, Co^{2+}, Ni^{2+}, Mn^{2+}, Zn^{2+}). Our PCN-250 was among the MOFs synthesize and has shown a high total H_2 volumetric uptake of 60g L-1 at 40 bar and 77 K and high total CH_4 uptakes of 200V STP/V at 35 bar and 298 K [17,18].

Figure 1

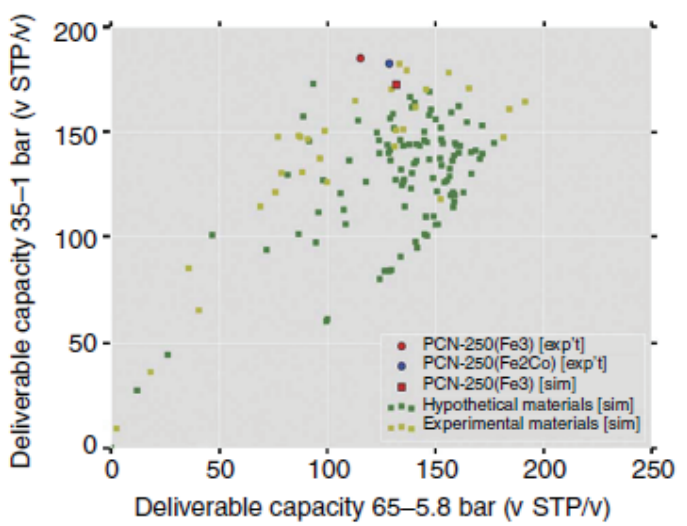


Figure 1: Performance plot of deliverable capacities using two different pressure swings. Shown are the predictions for the Fe-MOFs synthesized here (yellow) and in silico predicted structures (green). Red and blue points show PCN-250.

High volumetric gas uptake

The high methane uptake of PCN-250 is mainly due to the structure of this MOF and is a main feature of this material [18]. Figure 1 below shows a performance plot of PCN-250's deliverable capacities. PCN-250 has the potential to be an excellent absorbent for methane storage if a pressure range between 1-35 bar is used with the highest methane loading at 35 bar (200 v/v and 298 K). This product also has a recorded high of H_2 uptake of 3.07 wt% and 28 g L^{-1} at 1.2 bar and 77 K as well as a total volumetric H_2 uptake of 60 g L^{-1}, at high pressure due to the MOFs high crystal density.

Figure 2 displays how the ligand covers each side of the cubes in PCN-250 with charged open metal sites stationed around the channels between each cube. This allows the inter space to be available for gas adsorption, which in this product has a strong interaction with both H_2 and CH_4 molecules. In addition, through inducing polarization of gas molecules through charge-induced dipole interaction a highly-efficient utilization of space for elevated volumetric gas uptake can be accomplished.

Figure 2

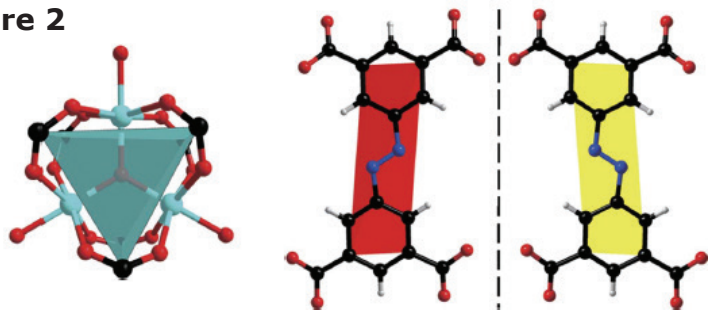


Figure 2: Structures of PCN-250

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Figure 3

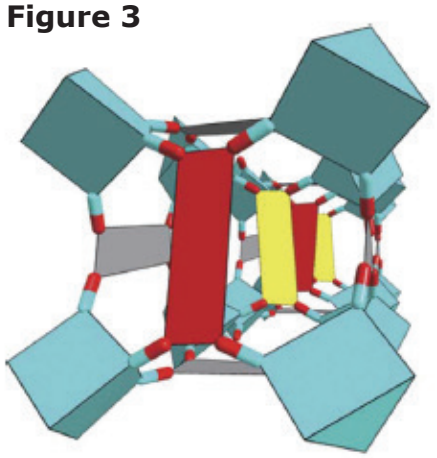

Figure 3: Structure drawing of PCN-250

Chemical stability of PCN-250

Studies have shown that the chemical stability of PCN-250 remains even if one iron atom is substituted for a softer Lewis acid metal, M(II), in the μ_3-oxo cluster. The product remains intact in a range of pH values scaling from 1 to 11 over a period of 24 hours. It was also found that PCN-250 remained strong in H_2O after 6 months in neutral conditions. After multiple pH treatments, there was barely any change in the material's N_2 adsorption isotherms leading researchers to conclude that no MOF decomposition or phase transition occurred.

PCN-250's high gas uptake and exceptional stability and scalability make it an auspicious material for natural gas storage for a wide range of applications including power systems and gas purification.

Figure 4

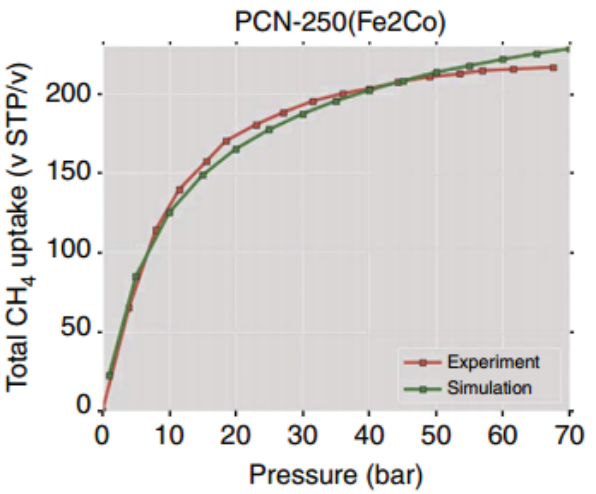

Figure 4: Total CH_4 Adsorption uptake of PCN-250 at 298 K.

Key Properties

- **Color and form:** dark red-brown pwdr.
- **Superior uptake of hydrogen and methane**
- **Stable in water and aqueous solutions**

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