

A 3D MOF based on adamantoid tetracopper(II) and aminophosphine oxide cages: structural features and magnetic and catalytic properties.

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Streszczenie

This work describes an unexpected generation of a new 3D metal–organic framework (MOF), $[\text{Cu}_4(\mu\text{-Cl})_6(\mu_4\text{-O})\text{Cu}(\text{OH})_2(\mu\text{-PTA}=\text{O})_4]_n \cdot 2n\text{Cl}\cdot\text{EtOH}\cdot 2.5n\text{H}_2\text{O}$, from copper(II) chloride and 1,3,5-triaza-7-phosphaadamantane 7-oxide (PTA=O). The obtained product is composed of diamondoid tetracopper(II) $[\text{Cu}_4(\mu\text{-Cl})_6(\mu_4\text{-O})]$ cages and monocopper(II) $[\text{Cu}(\text{OH})_2]$ units that are assembled, via the diamondoid $\mu\text{-PTA}=\text{O}$ linkers, into an intricate 3D net with an **nbo** topology. Magnetic susceptibility measurements on this MOF in the temperature range of 1.8–300 K reveal a ferromagnetic interaction ($J = +20 \text{ cm}^{-1}$) between the neighboring copper(II) ions. Single-point DFT calculations disclose a strong delocalization of the spin density over the tetranuclear unit. The magnitude of exchange coupling, predicted from the broken-symmetry DFT studies, is in good agreement with the experimental data. This copper(II) compound also acts as an active catalyst for the mild oxidation and carboxylation of alkanes. The present study provides a unique example of an MOF that is assembled from two different types of adamantoid Cu_4 and PTA=O cages, thus contributing to widening a diversity of functional metal–organic frameworks.

Adres publiczny

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<https://www.acs.org/content/acs/en.html>