

Design, Synthesis, Magnetic Properties, and Hydrogen Evolution Reaction of a Butterfly-like Heterometallic Trinuclear $[\text{Cu}^{\text{II}}_2\text{Mn}^{\text{II}}]$ Cluster

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Streszczenie

A novel heterometallic trinuclear cluster $[\text{Cu}^{\text{II}}_2\text{Mn}^{\text{II}}(\text{cpdp})(\text{NO}_3)_2(\text{Cl})]$ (**1**) has been designed and synthesized by employing a molecular library approach that uses $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$ and $\text{Mn}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$ as inorganic metal salts and H_3cpdp as a multifunctional organic scaffold ($\text{H}_3\text{cpdp} = N,N'$ -bis[2-carboxybenzomethyl]- N,N' -bis[2-pyridylmethyl]-1,3-diaminopropan-2-ol). This heterometallic cluster has emerged as an unusual ferromagnetic material and promising electrocatalyst for hydrogen evolution reaction (HER) in the domain of inorganic and materials chemistry. Crystal structure analysis establishes the structural arrangement of **1**, revealing a butterfly-like topology with an unusual seven-coordinated Mn(II) center. Formation of this cluster is accomplished by a self-assembly process through functionalization of **1** with one $\mu_2:\eta^1:\eta^1$ -nitrate and two $\mu_2:\eta^2:\eta^1$ -benzoate groups via the $\text{Cu}^{\text{II}}(\mu_2\text{-NO}_3)\text{Cu}^{\text{II}}$ and $\{\text{Cu}^{\text{II}}(\mu_2\text{-O}_2\text{CC}_6\text{H}_5)\text{Mn}^{\text{II}}\}$ linkages, respectively. Variable-temperature SQUID magnetometry revealed the coexistence of ferromagnetic and antiferromagnetic interactions in **1**. The observed magnetic behavior in **1** is unexpected because of a large Cu–O–Mn angle with a value of 132.05° , indicating that the correlation between coupling constants and the structural parameters is a multifactor problem. This cluster shows excellent electrocatalytic performance for the HER attaining a current density of 10 mA/cm^2 with a Tafel slope of 183 mV dec^{-1} at a 310 mV overpotential value. Essentially, cluster **1** shows exceptional electrochemical stability at ambient temperature, accompanied by minimal degradation of the current density as examined by chronoamperometric studies. Density functional theory calculations establish the mechanistic insight into the HER process, indicating that the $\text{Cu}^{\text{II}}\text{--OCO--Mn}^{\text{II}}$ site is the active site for formation of molecular hydrogen.

Słowa kluczowe

Catalysts, Evolution reactions, Hydrogen, Metal clusters,
Transition metals

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