

Synthesis, Characterization, Magnetic Properties, and Electrocatalytic Activities of a Series of Tetranuclear Fe(III) Clusters

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Streszczenie

In this research, a new series of tetranuclear Fe(III) clusters (**1–3**) represented by the general formula $[\text{Fe}_4(\text{L})_2(\mu_2\text{-O})(\mu_2\text{-OH})(\mu_2\text{-}p\text{-O}_2\text{CC}_6\text{H}_4(\text{R}))_2](\text{ClO}_4)\cdot\text{H}_2\text{O}$ were designed and synthesized. The synthesis involves the reaction of a multidentate ligand, H_3L , with $\text{Fe}(\text{ClO}_4)_2\cdot 6\text{H}_2\text{O}$, in combination with *p*-chlorobenzoic acid, *p*-nitrobenzoic acid, and *p*-methylbenzoic acid ($\text{H}_3\text{L} = N,N'$ -bis[2-carboxybenzomethyl]-*N,N'*-bis[2-pyridylmethyl]-1,3-diaminopropan-2-ol; $\text{R} = \text{Cl}$ (**1**), NO_2 (**2**), and CH_3 (**3**)). Clusters **1–3** were characterized by multiple analytical techniques, including single-crystal X-ray diffraction (SCXRD) analysis. As revealed by SCXRD analysis, the molecular structures of **1–3** contain two crystallographically equivalent $[\text{Fe}_2\text{L}]^{3+}$ species, which are interlinked by one $\mu_2\text{-O}^{2-}$ and $\mu_2\text{-OH}^-$, and two auxiliary $\mu_2\text{-}p\text{-O}_2\text{CC}_6\text{H}_4(\text{R})^-$ ligands, generating concave-shaped, fascinating rectangular architectures. The magnetic susceptibility data of **1–3** were measured and analyzed by employing variable-temperature SQUID magnetometry between 1.8 and 300 K, demonstrating the occurrence of intramolecular antiferromagnetic exchange interactions among the Fe(III) ions. These Fe_4 clusters holding the redox-flexible multimetallic cores worked well for water splitting. They showed low overpotential values of 177–229 mV for the hydrogen evolution reaction (HER) and 310–478 mV for the oxygen evolution reaction (OER) to achieve a current density of 10 mA/cm^2 . Essentially, in clusters **1–3**, the occurrence of Fe...Fe synergistic effect and appropriately located activation sites greatly favor the formation of intramolecular H–H and O–O bonds. Density functional theory (DFT) computations validate the proposed mechanistic pathways of HER and OER processes.

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