

Employment of 2-pyrrole aldoxime in iron cluster chemistry: trinuclear and hexanuclear clusters.

Autorzy

Angelos B. Canaj

Miłosz Siczek

Alexios P. Douvalis

Thomas Bakas

Tadeusz Lis

Constantinos J. Milios

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The reaction of $\text{Fe}(\text{ClO}_4)_3 \cdot 9\text{H}_2\text{O}$ with 2-pyrrole aldoxime (pyroxH_2) and two equivalents of sodium benzoate in MeCN afforded the complex $\{[\text{Fe}^{\text{III}}_6\text{O}_2(\text{OH})_2(\text{pyroxH})_2(\text{PhCOO})_{10}(\text{H}_2\text{O})_2] \cdot [\text{Fe}^{\text{III}}_3\text{O}(\text{pyroxH}_2)_2(\text{PhCOO})_6(\text{M}(\text{ClO}_4) \cdot 6.6\text{MeCN})] \cdot 6.6\text{MeCN}\}$ (**1**·6.6MeCN) in moderate yield. Repeating the same reaction in EtOH gave the complex $[\text{Fe}^{\text{III}}_6\text{O}_2(\text{OH})_2(\text{pyroxH})_2(\text{PhCOO})_{10}(\text{EtOH})_2]$ (**2**) in good yield. The crystal structures of **1** and **2** have been determined by single-crystal X-ray crystallography. Complex **1** contains two different clusters in the crystal: a trinuclear $[\text{Fe}^{\text{III}}_3]$ molecule and a hexanuclear $[\text{Fe}^{\text{III}}_6]$ unit, both of which contain different forms of the 2-pyrrole aldoxime ligand. Complex **2** is a hexanuclear $[\text{Fe}^{\text{III}}_6]$ cluster almost identical with the hexametallic unit found in **1**, with the difference being the presence of two terminal EtOH molecules in **2** versus two terminal H_2O molecules in the hexametallic sub-unit of **1**. DC magnetic susceptibility studies were performed on polycrystalline sample of **2**, revealing the presence of strong antiferromagnetic interactions within the cluster leading to a well isolated diamagnetic ground-state. The oxidation state of the iron atoms in **2** were further established by Mössbauer studies performed at 77 K.

Słowa kluczowe

iron clusters, 2-Pyrrole aldoxime, crystal structure, magnetic properties, Mössbauer spectroscopy

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