Synthesis and Structures of μ_3-Oxo-centered Mixed-valent Trinuclear Iron Complexes with 1-Methyl-imidazole Ligands

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Treatment of the μ_3-oxo-centered mixed-valent trinuclear iron complex $[Fe_3(\mu_3\text{-}O)(\mu\text{-}OAc)_6(H_2O)_3]$ (**1**) in methanol solution with one, two, or three equivalents of 1-methyl-imidazole ($C_4H_6N_2$) afforded the substitution products $[Fe_3(\mu_3\text{-}O)(\mu\text{-}OAc)_6(H_2O)_2(C_4H_6N_2)]$ (**2**), $[Fe_3(\mu_3\text{-}O)(\mu\text{-}OAc)_6(H_2O)(C_4H_6N_2)_2]$ (**3**), and $[Fe_3(\mu_3\text{-}O)(\mu\text{-}OAc)_6(C_4H_6N_2)_3]$ (**4**), respectively. Complexes **2** – **4** were characterized by spectroscopic and elemental analyses, and the crystal structures of complexes **3** · 1.5MeOH · $2H_2O$ and **4** have been determined by single-crystal X-ray diffraction. The results indicate that in **2** – **4** the trinuclear core unit $[Fe_3(\mu_3\text{-}O)(\mu\text{-}OAc)_6]$ of **1** is preserved.

Key words: Synthesis, Crystal Structure, Trinuclear Iron Complex, Mixed-valent Iron Complex