

A doubly Phenoxyacetate-bridged dinuclear manganese(II) complex with 1,10-Phenanthroline: Synthesis, 1-D supramolecular structure, Hirshfeld surface analysis, magnetic and theoretical studies

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Streszczenie

We report herein the synthesis and characterization of $[\text{Mn}_2(\text{POA})_2(\text{Phen})_4](\text{BF}_4)_2 \cdot \text{H}_2\text{O}$, **1** where POA = phenoxyacetate; Phen = 1,10-phenanthroline, respectively. The crystalline complex was obtained via slow evaporation at room temperature and characterized by single crystal X-ray diffraction. FTIR and UV-vis spectroscopy were utilized to elucidate the structure of the new compound. Complex **1** crystallizes in the monoclinic crystal system with space group $P2_1/n$. Hirshfeld surface analysis revealed various intermolecular interactions in the crystal lattice. Quantum Theory of Atoms in Molecules (QTAIM), Reduced Density Gradient (RDG), and Natural Bond Orbital (NBO) analyses were employed to investigate the diverse non-covalent interactions stabilizing the crystal structure. In complex **1**, the BF_4^- counterion plays a crucial role in crystal assembly through a network of $\text{F} \cdots \text{H} \cdots \text{C}$ interactions with varying strengths governed by the interaction angle and consequent ellipticity. Additionally, $\text{B} - \text{F} \cdots \pi$ interactions were observed. Other interactions include weak-to-medium hydrogen bonds and π -interactions ($\text{CH} \cdots \pi$ and $\pi \cdots \pi$) within the asymmetric units and dimers extracted from the unit cell. Notably, unconventional interactions were identified and characterized in complex **1**, which is $\text{C} - \text{H} \cdots \pi$ interactions with the $\sigma(\text{CH})$ orbital donating to an empty p orbital in the asymmetric unit of **1**. Variable-temperature magnetic susceptibility data disclosed the occurrence of weak antiferromagnetic coupling within the doubly bridged manganese(II) core with a J value of -2.11 cm^{-1} .

Słowa kluczowe

Phenoxyacetic acid, QTAIM, NBO, B-F π interactions, Magnetic properties

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