

Crystal structure and characterization of manganese(II) carboxylates: 3D metal-organic frameworks.

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Three mononuclear manganese (II) complexes with quinoline-2-carboxylate ion (quin-2-c), $[\text{Mn}(\text{quin-2-c})_2(\text{H}_2\text{O})_2]_2 \cdot \text{Hquin-2-c} \cdot 2\text{H}_2\text{O}$ (**1**), $\text{Mn}(\text{quin-2-c})_2(\text{EtOH})_2$ (**2**), and $\text{HbimH}[\text{Mn}(\text{quin-2-c})_2\text{Cl}]$ (**3**) (HbimH^+ = benzimidazolium ion), have been obtained by self-assembly and structurally characterized by X-ray diffraction. In all three complexes the quin-2-c ions are bound to manganese in the chelate mode through a ring nitrogen and a monodentate carboxylate group. In complexes **1** and **2** the manganese ions are coordinated in the distorted octahedron with an N_2O_4 donor set. In the complex anion $\text{Mn}(\text{quin-2-c})_2\text{Cl}^-$, present in the crystal of **3**, the manganese ion is five-coordinated by two quin-2-c ligands and the chlorine ion. The solid-state EPR spectra of **1** and **2** are characteristic of the Mn(II) ion in a distorted-octahedral geometry, whereas the spectrum of **3** is more complicated due to the zero-field splitting effect operating at lower symmetry. The EPR spectra of all complexes in frozen ROH are very similar and are characteristic of an octahedral environment around manganese. The systems of strong intermolecular hydrogen bonds form 1D structures in all complexes, which are further engaged in weak $\text{C-H}\cdots\text{O}$, $\pi\cdots\pi$ and $\text{C-H}\cdots\pi$ interchain interactions, creating the 3D networks. The IR spectra reflect the differences in the hydrogen bond systems in **1-3**.

Słowa kluczowe

Noncovalent interactions, Transition metals, Ligands, Molecules, Ions

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<https://www.acs.org/content/acs/en.html>

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