Crystal structure of a diaqua-bis(3,5-di(1H-imidazol-1-yl)pyridine-κN)-bis(2-(4-carboxyphenyl)acetato-κO)manganese(II), C₄₀H₃₆MnN₁₀O₁₀

Abstract

C₄₀H₃₆MnN₁₀O₁₀, monoclinic, P₂₁/c (no. 14), a = 21.8966(12) Å, b = 7.2586(4) Å, c = 12.2346(6) Å, β = 98.232(1)°, V = 1924.52(18) Å³, Z = 2, Rgt(F) = 0.0327, wRref(F²) = 0.0847, T = 296(2) K.

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The centrosymmetric title complex is shown in the figure (carbon-bound hydrogen atoms are omitted for clarity). Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

A mixture of 3,5-bis(1-imidazoly)pyridine (bip, 0.05 mmol, 45 mg), 4-carboxybenzeneacetic acid (H₂cbaa, 0.05 mmol, 9.0 mg), Mn(OAc)₂ × 4H₂O (0.1 mmol, 24 mg), ethanol (3.5 mL) and H₂O (3.5 mL) was sealed in a 25 mL Teflon-lined autoclave, and then was heated to 120 °C for 4 days. After the mixture was cooled slowly to room temperature, colorless crystals of the title compound were obtained.

Experimental details

Carbon-bound H atoms were placed in calculated positions and were included in the refinement in the riding model approximation, with Uiso(H) set to 1.2 Ueq(C). The H atoms of the hydroxyl groups were allowed to rotate with a fixed angle around the C—O bond to best fit the experimental electron density, with Uiso(H) set to 1.5 Ueq(C). The H atoms of the metal ions were fixed at calculated positions.

Discussion

Metal-organic coordination polymers (MOCPs), which are fabricated by metal moieties and organic ligands, have attracted a great deal of attention because of their potential applications in the areas of electronics, magnetism, optics, gas absorption and catalysis, combining with their aesthetically pleasing structures [1–5]. Effective synthetic strategies of MOCPs with expected structures and properties should take many factors into account, such as the properties of the metal ions, organic ligands, solvent, temperature, pH value and the crystallization procedure [6, 7]. And for this purpose, numerous multi-functional carboxylate ligands have been designed,

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The asymmetric unit comprises of one half Mn(II) cation, one Hcbaa anion, one bip molecule and one coordinated H2O molecule. The Mn displays a [MnN2O4] octahedrally coordinated geometry with the coordination sphere defined by two -C2H4COO- oxygen atoms from two symmetry-related Hcbaa anions, two oxygen atoms from two coordinated water molecules and two imidazolyl N atoms from two symmetry related bip ligands. The bond lengths of Mn(1)—O(1) and Mn(1)—O(5W) are 2.1362(13) Å and 2.1804(13) Å, while the bond length of Mn(1)—N(1) is 2.2657(14) Å.

H-bonding interactions exist among the Hcbaa anions, coordinated water molecules and bip ligands. The detailed data are listed as follows: O(3)—H(3) bonded with O(2) hydrogen bonds to form one monolayer motif parallel to the bc plane. Moreover, the layers are further pillared by O(3)—H(3)···N(5) hydrogen bonds to the 3D framework. H-bonding interactions play a vital role in the self-assembly and enhanced stability of the title structure.

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References

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