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Crystal structure of tetraaqua-bis(1,3-benzimidazol-3-ium-1,3-diacetato-κO)copper(II) hemihydrate, C_{22}H_{27}CuN_{4}O_{12.50}

Abstract

C_{22}H_{27}CuN_{4}O_{12.50}, triclinic, Pî (no. 2), a = 7.3950(11) Å, b = 9.4574(15) Å, c = 9.6619(15) Å, α = 81.139(2)°, β = 75.457(3)°, γ = 77.974(3)°, V = 636.02(17) Å³, Z = 1, R_{gt}(F) = 0.0371, wR_{ref}(F^2) = 0.1020, T = 293 K.

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The crystal structure is shown in the figure. 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

The ligand 1-(carboxymethyl)-1H-benzimidazol-3-ium-3-acetate was prepared according to the reported procedures [1]. Solid sodium carbonate (0.25 mmol) was added to 1-(carboxymethyl)-1H-benzimidazol-3-ium-3-acetate (0.5 mmol) in distilled water (5 mL) while stirring at room temperature. Once the solution became clear, copper(II) nitrate hexahydrate (0.25 mmol) dissolved in distilled water (5 mL) was added dropwise. After continuous stirring for 15 min, the resulting blue solution was filtered and placed undisturbed for 2 weeks. During this period blue crystals were obtained.

Experimental details

All the hydrogen atoms except that of water were generated geometrically and refined isotropically using riding models. The U_{iso} values of the hydrogen atoms were set to 1.2 U_{eq}(C). The hydrogen of water molecules were found directly from different Fourier map.

Discussion

In the recent years, the benzimidazole derivatives and their metal complexes have attracted much attention because of the specific topological frameworks and interesting properties of these compounds [2–5]. Furthermore, benzimidazole carboxylic acids and their derivatives are widely used due to their biological activities such as antifilarial, antineoplastic, anthelmintic and antiviral activities [6–9]. Up to now, several complexes have been synthesized using the benzimidazole carboxylic acid [10–16]. To extend this research, we used 1,3-benzimidazol-3-ium-1,3-diacetato ligand to react with Cu^{2+} ions and got a new complex.
The asymmetric unit of the title structure consists of one half of a monomer complex (cf. the figure, the asymmetric unit is labeled) and one uncoordinated water molecule with the occupation of 25%. The Cu(II) atom lies on the inversion center and is six-coordinated by four O atoms from four coordinated water molecules and two O atoms from two monodentate coordinating ligands. The Cu(II) atom adopts a slightly distorted octahedral geometry. The axial Cu–O bond distances are in the range of 1.986(2) Å and 2.298(2) Å. The benzimidazolium moiety (C1/N1/C9/C11/C5/C4/C3/C10/N2) is essentially planar, with a mean deviation of 0.0124 Å. The carboxylate groups adopt trans conformations, with the distances in the range of 1.986(2) Å and 2.298(2) Å. The two-dimensional network further extended into a three-dimensional supramolecular structure along the crystallographic c direction via π–π stacking interactions between benzimidazolium rings from adjacent layers, with a centroid-centroid distance of 3.588 Å.

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References


