Structural study of semi-coordination in a seven-coordinate copper(II) complex: distortion isomerism of $[Cu(CH_3COO)_2(4\text{-aminopyridine})_2(H_2O)]$.

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Streszczenie

[Di(acetato)bis(4-aminopyridine)aquacopper(II)] exists in two different monoclinic forms. The crystal structure of Form **1**, which crystallizes in space group $P2_1/c$, was determined by X-ray crystallography. Experimental data was then compared with that found for Form **2**, which crystallizes in space group $C2/c$. The seven-coordinate environment of copper in both forms is consistent with the bond-valence model. The asymmetric copper(II) coordination of Form **1** is consistent with the density-functional theory. The isomers differ in distortion of the pentagonal bipyramid as the coordination polyhedron around Cu. Carboxylate groups for both isomers are bonded to copper as bidentate ligands. The Cu in Form **1** is semi-coordinated by two long carboxylate O bonds to create the seven-coordinate environment (Cu···O distances are 2.785(4) and 2.9996(5) Å). Infrared and electron spin resonance spectra of both isomers are consistent with their crystal structures.

Słowa kluczowe

Copper(II), carboxylate, 4-Aminopyridine, Distortion isomers

Adres publiczny

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