Structure and magnetic properties of a double out-of-plane carboxylato-bridged Cu(II) compound with pyridine-2-carboxylate.

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The spectroscopic and magnetic properties, and crystal structure of dark-blue $[Cu(2\text{-pca})_2]_n$ (**1**), (2-pca = pyridine-2-carboxylate ion) are described. The copper(II) ions are in strongly tetragonally distorted octahedral environments. They are sequentially bridged by a double out-of-plane carboxylate bridge, resulting in the formation of an infinite chain (1D). The equatorial Cu–O bonds (1.957(3) Å) are significantly shorter than the axial bonds (2.737(4) Å). The crystal structure of the compound is stabilized by interchain hydrogen bonds of the C–H⋯O type. The intrachain copper–copper separation is 5.178(3) Å, whereas the shortest interchain copper–copper distance is 7.614(6) Å. The magnetic properties, investigated in the temperature range 1.8–300 K, revealed the occurrence of a weak intrachain antiferromagnetic coupling, $J = -1.04$ cm^{-1}, and an interchain exchange interaction, $zJ' = 0.34$ cm^{-1}. The title compound appears to be a polymorphic form of the blue-violet compound (**2**) of identical stoichiometry, the X-ray structure of which was recently reported. Magneto-structural correlations in **1** have been made considering both the carboxylato bridging group and the existence of interchain hydrogen bonds. The structure and magnetic properties of **1** are compared with those of the polymorphic form **2**.

Słowa kluczowe

Copper(II), Pyridinecarboxylate, Crystal structure, Magnetism, Polymorphism, Hydrogen bonds

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