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Novel pyrazolate-based copper(II) [2x2] grid complexes: synthesis, structure and properties.

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Streszczenie

5-Acetyl-substituted pyrazole-3-carboxylic acid (H_2 L) forms [2×2] grid-like tetranuclear Cu(II) complexes with four five-coordinated copper(II) ions bridged by pyrazolate groups. Despite a significant dissociation of [Cu_4 L_4 (H_2 O)$_4$]·4H_2 O (1) in aqueous solution [1] , it was possible to substitute the coordinated water molecules by pyridine ligands or azide anions. The resulting tetranuclear complexes [Cu_4 L_4 Py_4]·2H_2 O (2) and Na_4 [Cu_4 L_4 (N_3)$_4$]·7MeOH (3) were isolated and studied by X-ray diffraction analysis. In 2 and 3 the azide anions or pyridine molecules complete the distorted square-pyramidal coordination of each copper(II) center. Magnetic susceptibilities of the obtained compounds have been measured by SQUID techniques. Simulation of the data using a Heisenberg spin Hamiltonian approach showed that the bridges between the metals mediate weak intramolecular antiferromagnetic coupling (J in the range −13.3 to −17.1cm $^{-1}$) and lead to a singlet ground state in all cases.

Słowa kluczowe

Pyrazole ligands, copper(II), Grid complexes, magnetic properties

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