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Crystal structure EPR and magnetic susceptibility studies of tetrakis [μ-(β-alanine)-*O,O′*]dichlorodicopper(II) dichloro monohydrate.

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Tetrakis[μ-(β-alanine)-*O,O′*]dichlorodicopper(II) dichloro monohydrate, $[Cu_2(\beta\text{-alanine})_4Cl_2]Cl_2\cdot H_2O$, crystallizes in the triclinic system, space group , and γ = 97.15(3)° with one formula weight in a unit cell. Two different centrosymmetric carboxylato-bridged dimeric subunits are formed. The coordination geometry about each copper(II) center is square-pyramidal, with four oxygen atoms in the basal plane and the chloride ion at the apical position. The coordination polyhedra of two dimers are slightly different: for the dimer with a shorter Cu(1)Cu(1)[1] distance of 2.6331(10) Å a Cu(1)Cl bond length of 2.4511(10) Å is observed, in comparison with Cu(2)Cu(2)[11] of 2.6608(10) Å and Cu(2)Cl bond length of 2.4387(10) Å for the other dimer. Magnetic and EPR properties of the title complex are compared with those exhibited by $[Cu_2(\beta\text{-alanine})_4(H_2O)_2]$ $(NO_3)_4\cdot 4H_2O$ that forms dimeric molecules of only one kind. The isotropic exchange interactions are strongly antiferromagnetic with a *J* value of 320 cm^{-1} (corresponding to the Hamiltonian = $JS_1\cdot S_2$) for the chloride dimers and 334 cm^{-1} for the nitrate complex. The complexes exhibit spin-triplet EPR spectra with very well-resolved hyperfine structure of two equivalent copper nuclei at low temperature. The chloride compound shows two overlapping EPR spectra with different spin Hamiltonian parameters. Only one EPR spectrm is observed in the nitrate complex. Structural differences seem to affect significantly the zero-field splitting parameter *D*.

Słowa kluczowe

Crystal structures, Magnetism, Electron paramagnetic resonance, Copper complexes, Amino acid complexes, Binuclear complexes

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