Synthesis, characterization, and magnetic properties of a series of copper(II) chloride complexes of pyridyliminebenzoic acids.

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Streszczenie

A series of Cu^{II} halide complexes, $Cu(HL1)Cl_2{\cdot}CH_3OH$ (**1**), $[Cu(L1)Cl]_2{\cdot}H_2O$ (**2**), $[Cu(HL2)Cl_2]_2{\cdot}2DMF$ (**3**), $[Cu(HL2)_2Cl]_nCl_n{\cdot}2nH_2O$ (**4**), and $[Cu(L3)Cl]_n$ (**5**), containing pyridyliminebenzoic acids HL1, HL2, and HL3 derived from *o*-, *m*-, and *p*-aminobenzoic acids, respectively, have been obtained as single crystals and characterized by elemental analysis, IR, EPR spectroscopy, magnetic measurements, and single-crystal X-ray diffraction techniques. The results obtained show the formation of molecular (**1**), dimeric (**2**, **3**), and polymeric structures (**4**, **5**) based on chloride (**1**–**4**) and carboxylate bridges (**5**) with copper(II) ions in the square pyramidal geometry of varying degrees of distortion. In the case of **2** and **5** the ligand deprotonation was completely achieved even in the absence of a base. The closest Cu···Cu separations are found in the crystal lattices of the polymer **5** (3.33 Å) and dimers **2** (3.35 Å) and **3** (3.38 Å). The X-band polycrystalline EPR spectra of **1**–**3** with typical axial patterns show no indication of exchange interactions between copper ions in the range 295–77 K. The observed rhombic features of the EPR spectra of **4** arise from the coupling of *g*-tensors from differently oriented Cu^{II} coordination polyhedra in the solid state. A characteristic spin-triplet EPR spectrum of **5** at 77 K was simulated by using the spin-Hamiltonian parameters for $S = 1$, $g_x = 2.08$, $g_y = 2.11$, $g_z = 2.37$ and the value of the zero-field splitting parameter D of 0.137 cm^{-1}. Magnetic susceptibility measurements revealed antiferromagnetic (**1**–**3**, **5**) and ferromagnetic coupling (**4**) between the metal atoms at low temperatures. Theoretical methods were employed to provide additional insight into magnetic interactions in the studied compounds.