

Two isomorphous Co(II) coordination polymers based on new α , α -disubstituted derivatives of zoledronic acid : synthesis, structures and properties.

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Streszczenie

Two novel α,α -disubstituted derivatives of zoledronic acid, namely 1-hydroxy-2-(1*H*-imidazol-1-yl)-2-methylpropylidene-1,1-diphosphonic acid (H_4L1) and 1-hydroxy-2-[1-(1*H*-imidazol-1-yl)cyclopropyl]ethylidene-1,1-diphosphonic acid (H_4L2) were synthesized and structurally characterized by single-crystal X-ray diffraction. The reaction of cobalt acetate with H_4L1 and H_4L2 carried out under hydrothermal conditions afforded two isomorphous $Co_3(HL1)_2(H_2O)_6 \cdot 6H_2O$ (**1a**) and $Co_3(HL2)_2(H_2O)_6 \cdot 6H_2O$ (**2a**) complexes. Both compounds are characterized by means of X-ray crystallography, IR and NIR–Vis–UV spectroscopic methods. Furthermore, their magnetic properties and thermal stabilities are reported. The crystals of **1a** and **2a** feature infinite 1D polymeric chains built from alternately arranged dinuclear $[Co_2(HL1/HL2)(H_2O)_2]_2$ units and $\{Co1O_6\}$ octahedra running along the [10] crystallographic direction. In both compounds, crystallographically distinct Co1 and Co2 atoms are six-coordinated. As is reflected in T values (T – index of tetragonality), the coordination environment of Co1 generates a slightly elongated octahedron ($T = 0.94$), whereas a slightly compressed octahedron ($T = 1.06$ for **1a** and 1.05 for **2a**) is formed around Co2. An assumption that the d–d type absorption is mainly attributed to the inversion related Co2 centers, whose population is two times higher than that of Co1, afforded a good correlation between calculated transition energies and experimental NIR–Vis–UV spectra. The magnetic susceptibility measurements analyzed in terms of a spin-3/2 Heisenberg trimer chain revealed that $Co1 \cdots Co2$ interactions within the trimer are antiferromagnetic whereas $Co2 \cdots Co2$ intertrimer interactions are ferromagnetic.

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