Magnetooptical and structural investigations of five dimeric cobalt(II) complexes mimicking metalloenzyme active sites

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Four novel cobalt(II) complexes mimicking metalloenzyme active sites, novel C 14H 22Cl 12Co 2O 132C 3H 8O (1), C 28H 36Cl 24Co 4O 284C 4H 8O 2 (2), C 16H 22Cl 12Co 2O 13C 2HCl 3O 2 (3), C 16H 22Cl 12Co 2O 13 (4), and one known C 40H 78Cl 8Co 2O 17 (5) are composed of the same core of two high-spin cobalt(II) centers triply bridged by water and two trichloroacetato (1-4) or two pivalate (5) groups but differ in terminal ligands. The crystal structures of new compounds 1-4 belong to the space groups P1?, P2 1/c, P1?, and Pbcn, respectively. All five investigated complexes contain Co atoms in distorted octahedral coordination. The complexes were characterized by magnetic susceptibility and magnetization measurements and by variable-temperature variable-field magnetic circular dichroism spectroscopy. Experimental data were analyzed in the frame of the theoretical model, which includes an unquenched orbital moment of the Co II ions. All investigated compounds are antiferromagnetically coupl