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Heterometallic CuCd and Cu_2Zn complexes with *o*-vanillin and its Schiff-base derivative: slow magnetic relaxation and catalytic activity associated with Cu(II) centres

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Streszczenie

In this work, two novel heterometallic mixed-ligand mixed-anion complexes $[Cu^{II}Cd^{II}ClL(o\text{-Van})(OAc)]\cdot 3H_2O$ (**1**) and $[Cu^{II}_2Zn^{II}Cl_2L_2(o\text{-Van})(OAc)]$ (**2**) were prepared by reacting fine copper powder and Cd(II) or Zn(II) acetate with an ethanol solution of the Schiff-base ligand HL formed *in situ* in the condensation reaction of 2-hydroxy-3-methoxy-benzaldehyde (*o*-VanH) and $CH_3NH_2\cdot HCl$. The compounds were thoroughly characterized by elemental analysis, FT-IR, UV/Vis and EPR spectroscopy, cyclic voltammetry, and single-crystal X-ray diffraction, revealing the neutral molecular nature of both the compounds. Catalytic properties of **1** and **2** were studied in the oxidation of hydrocarbons with H_2O_2 under mild conditions, showing the maximum reaction rate of 4×10^{-5} M s^{-1} and TOF up to 640 h^{-1}. Both compounds undergo complex transformations in solution as evidenced by kinetic analysis and time-dependent UV/Vis spectroscopy, indicating that the reduced Cu(I) form of **1** is unexpectedly unfavorable. Complex **1** demonstrates slow magnetic relaxation dominated by the direct relaxation process between T = 1.8 and 7 K under an external DC field of 0.2 and 0.4 T, a very rarely observable effect in the coordination compounds of Cu(II). Complex **2** possesses weak ferromagnetism (J = 4.50 cm^{-1}, zJ' = −0.201 cm^{-1} for $H = -JS_1S_2$ formalism) occurring through the Cu–O–Cu pathways. Theoretical CASSCF, DFT and TDDFT calculations were applied to investigate the electronic structures of **1** and **2** and rationalize their behavior in solution.

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