Importance of Orbital Complementarity in Spin Coupling through Two Different Bridging Groups. Synthesis, Crystal Structure, Magnetic Properties and Magneto-Structural Correlations in a Dicopper(II) Complex of Endogenous Alkoxo Bridging Ligand with Exogenous Pyrazolate

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$[Cu_2(L^3)(3,5\text{-prz})]$ (L^3 = 1,3-bis(2-hydroxy-4-methoxybenzylideneamino)-propan-2-ol) (**3**) was synthesized and its crystal structure determined. The compound consists of discrete binuclear units, in which copper atoms are linked by the alkoxide oxygen atom of the ligand and the pyrazolate nitrogen atoms. Variable-temperature magnetic susceptibility measurements for a powdered sample of the complex were carried out in the temperature range 4.4 - 308 K and analysed to obtain values of the parameter J in the exchange Hamiltonian $\mathcal{H} = -2J\mathbf{S}_1 \cdot \mathbf{S}_2$. Recently, the dicopper(II) complexes $[Cu_2(L^1)(3,5\text{-prz})]$ (L^1 = 1,3-bis(2-hydroxy-1-napthylideneamino)-propan-2-ol) (**1**) and $[Cu_2(L^2)(3,5\text{-prz})]$, ($L^2$ = 1,3-bis(2-hydroxy-5-chlorosalicylideneamino)-propan-2-ol) (**2**) were reported. These compounds show antiferromagnetic behaviour ($-2J$: 444 cm^{-1} for **1**, 164 cm^{-1} for **2**, and 472 cm^{-1} for **3**). The strength of the super-exchange interaction ($-2J$) of **2** is much less than that of **1** and **3**, a result which is difficult to explain in terms of structural factors on the basis of widely accepted criteria. The differences in the magnetic behaviour have been rationalized in terms of the bridging ligand orbital complementary / countercomplementary concept.