Magnetic properties of Cu(*en*)(*sal*)Cl: a quasi-two-dimensional $S = 1/2$ Heisenberg ferromagnet on an anisotropic square lattice

R. Tarasenko,[1] I. Kozin,[1] J. Šebesta,[2] D. Legut,[2,3] J. Strečka,[1] E. Čižmár,[1] A. Orendáčová,[1] V. Tkáč,[1] and M. Orendáč[1]

[1] *Institute of Physics, Faculty of Science, P.J. Šafárik University in Košice, Park Angelinum 9, 041 54, Košice, Slovak Republic*

[2] *IT4Innovations, VŠB-Technical University of Ostrava, 17. listopadu 2172/15, 708 00 Ostrava-Poruba, Czech Republic*

[3] *Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 121 16 Prague 2, Czech Republic*

A combined theoretical and experimental study of the magnetic properties of the metal–organic compound Cu(*en*)(*sal*)Cl (*en* = ethylenediamine = $C_2H_8N_2$; *sal* = 2-hydroxybenzoic acid = $C_7H_6O_3$) is presented. The compound realizes a quasi-two-dimensional $S = 1/2$ Heiseberg spin system on an anisotropic square lattice. The crystal structure consists of rectangular-like layered frameworks of the Cu^{2+} ions in the *bc* plane and features two distinct coordination environments: axially elongated CuN_4Cl_2 octahedra formed by *en* ligands, and compressed CuO_4Cl_2 octahedra arising from asymmetrically bound *sal* anions [1].

First-principles *ab initio* calculations predict dominant ferromagnetic nearest-neighbor exchange interactions within the layers along *c* axis, with an exchange constant $J_1/k_B = 5.69$ K, accompanied by weaker antiferromagnetic coupling $J_2/k_B =$ -0.24 K along *b* axis. To verify these predictions, comprehensive experimental studies of the heat capacity, magnetization, and susceptibility were performed over the temperature range 0.38–300 K and in magnetic fields up to 9 T.

Zero-field specific-heat measurements revealed λ-like anomaly at $T_C = 0.82$ K, indicating a phase transition to long-range magnetic order. This transition was further evidenced by the splitting of zero-field-cooling and field-cooling magnetization curves, as well as by the observation of a ferromagnetic hysteresis loop at $T = 0.5$ K. Comparison of experimental heat capacity and susceptibility data with quantum Monte Carlo simulations of the proposed spin model demonstrates reasonable agreement, establishing Cu(*en*)(*sal*)Cl as a realization of a quasi-two-dimensional $S = 1/2$ Heisenberg ferromagnet on the anisotropic square lattice.

References:

[1] S. S. Batool *et al.*, J. Struct. Chem. 57 (2016), 1176–1181.

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