Dimerized nature of magnetic interactions in the S = 1/2 quantum antiferromagnet $Cu(en)_2SO_4$

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Previous studies of metal-organic compound $Cu(en)SO_4(H_2O)_2$ (*en* = ethylenediamine - $C_2H_8N_2$) revealed that this quasi-one-dimensional polymer structure represents realization of the S =1/2 Heisenberg antiferromagnet on the zig-zag square lattice with alternating intralayer interactions J/k_B = 3.5 K and J' = 0.35 J [1]. The compound undergoes a phase transition to the ordered state at 0.93 K. The substitution of water by *en* leads to the formation of very similar structure, namely $Cu(en)_2SO_4$. Our preliminary studies of powder sample indicated significant strengthening of exchange interactions and no fingerprints of any phase transition which suggests some kind of dimerization as a result of different distribution of alternating exchange interactions [2].

This work focuses on the study of magnetic susceptibility and magnetization of a single crystal in the field applied along the b axis. The temperature dependence of the magnetic susceptibility was measured in the ZFC mode in the temperature range from 2 to 300 K in the magnetic field 1 T. An analysis of the susceptibility within the Curie-Weiss law indicates the antiferromagnetic nature of the exchange coupling between magnetic ions with zJ/k_B = -6.4 K. Considering the structure of this material, the formation of magnetic dimers can be expected. Correspondingly, very good description of data was achieved using the Heisenberg antiferromagnetic dimer model with intradimer coupling J/k_B = -5.52 K, interdimer coupling $z'J'/k_B$ = -2.7 K and g = 2.12. The energy gap in the spin excitation spectrum was estimated $\Delta/k_B \approx$ 11 K and corresponding critical field $B_c^b \approx$ 7.8 T required for closing the gap. The dimerized nature of magnetic interactions was also confirmed by isothermal magnetization data which manifest qualitatively the same behaviour as the aforementioned dimer model. The possibility of further low temperature experiments in the closed gap regime is discussed to obtain more detailed concept of magnetic interactions in this interesting compound.

References:

[1] Lederová L. et al., "Realization of a spin-1/2 spatially anisotropic square lattice in a quasi-two-dimensional quantum antiferromagnet $Cu(en)(H_2O)_2SO_4$", Phys. Rev. B95 (2017) 054436.
[2] R. Tarasenko, PhD Thesis, P.J. Šafárik University, 2013.

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