High Field Response of a Polymeric Chiral Spin Chain

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The polymeric $S = ½$ antiferromagnet $[Cu(pym)(H_2O)_4]SiF_6{\cdot}H_2O$ (pym = pyrimidine = $C_4H_4N_2$) consists of a chiral spin-chain with four unique orientations of CuN_2O_4 octahedra in each unit [1]. In the linear (rather than chiral) spin-chain materials copper benzoate and $[Cu(NO_3)_2(pym)(H_2O)_2]_n$ two orientations of copper octahedra lead to an alternating *g*-tensor and a Dzyaloshinskii-Moriya (DM) interaction. Together these give rise to a staggered effective field that causes a field-induced spin gap [2,3]. Preliminary angle-dependent magnetic susceptibility and electron-spin resonance (ESR) measurements are suggestive of a similar alternating *g*-tensor and possible DM interactions in $[Cu(pym)(H_2O)_4]SiF_6{\cdot}H_2O$.

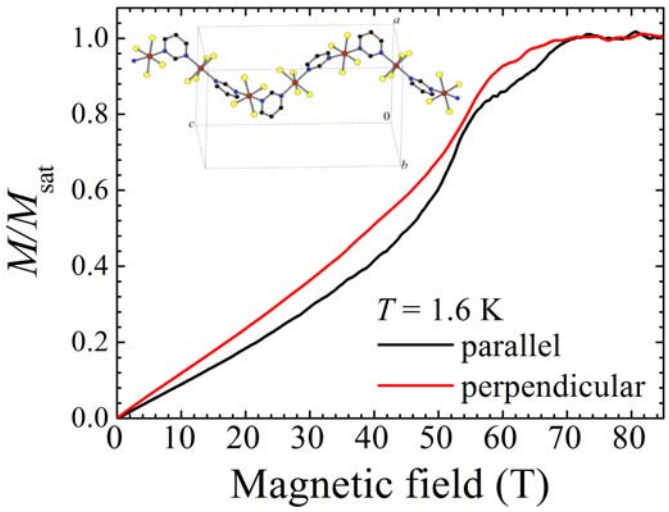

Figure 1: Magnetization of $[Cu(pym)(H_2O)_4]SiF_6{\cdot}H_2O$.Inset: 300 K structure showing the chiral chain of copper ions (red).

In order to ascertain the magnitude of the exchange energies in this material, low-temperature magnetization measurements on single crystals of $[Cu(pym)(H_2O)_4]SiF_6{\cdot}H_2O$ were made using the compensated coil technique in both the 65 T short-pulse and 100 T magnets at the NHMFL, LANL. The field was applied perpendicular and parallel to the chain axis.

Results and Discussion

The magnetization curves shown in Figure 1 are constructed from a combination of the 65 T short-pulse and 100 T data. The slightly concave form of the *M*(*H*) curves at low fields is typical of a low-dimensional $S = ½$ antiferromagnet, The saturation field (approximately 62 ± 2 T for the field applied perpendicular to the chains) permits an estimate of the primary exchange interaction of 45 ± 1.5 K along the chain assuming a simple two-nearest-neighbor Heisenberg model and an average *g*-factor of 2.2. This value is in keeping with the broad hump observed at 27 K in the temperature-dependence of the low-field magnetic susceptibility. The differences between the data with the field applied in the two orthogonal directions indicate that the magnetism displayed by $[Cu(pym)(H_2O)_4]SiF_6{\cdot}H_2O$ departs somewhat from simple chain-like behavior at low-temperatures. This is to be expected from the chiral nature of the structure.

Conclusions

A reasonable estimate of the intrachain exchange energy (45 ± 1.5 K) of the chiral spin-chain $[Cu(pym)(H_2O)_4]SiF_6{\cdot}H_2O$ is obtained from the pulsed-magnetic-field data. However, the chiral symmetry and consequent lack of an inversion center causes departures from simple Heisenberg chain-like behavior to develop at low-temperatures, particularly an anisotropy in the form of the magnetization along different crystallographic directions, an alternation of the *g*-tensor along the chain as observed in the susceptibility and ESR experiments, and the possibility of effects arising from a finite DM interaction. Further work is underway to understand the low-temperature properties of this material.

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