Classical spin dynamics simulations of the magnetic properties of a one-dimensional carboxylate-bridged Mn(III) Salen complex

We investigated the magnetic properties of the one-dimensional carboxylate-bridged Mn(III) Salen complex [Mn(5-Br-salen)(Br-Acetate)]$_n$ by means of classical Monte Carlo simulations. Based on a simple nearest-neighbor Heisenberg model with uni-axial anisotropy we found that the system's magnetic structure is that of a non-collinear canted antiferromagnetic spin chain.

The synthesis of new magnets, i.e. magnetic materials that retain their magnetization in the absence of a magnetic field, is a major challenge for future storage applications on the nano scale. Single-chain magnets (SCM) are composed of magnetically isolated chains that can be individually magnetized. As purely one-dimensional systems are known to have a long-range order only at T = 0 K, these SCM materials remains in their paramagnetic state at any finite temperature. Nevertheless, the combination of a large uni-axial anisotropy and large magnetic interactions between the high-spin magnetic units of the chain promotes long relaxation times and the system can behave as a magnet.

Recently, the one-dimensional carboxylate-bridged Mn(III) salen complexes [Mn(5-Br-salen)(Br-Acetate)]$_n$ (Fig. 1) has been synthezised and first experimental results suggest that this system can be understood as a canted antiferromagnetic SCM [1].

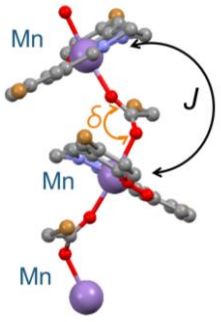

Fig.1 Magnetic model of the one-dimensional chain magnet [Mn(5-Br-salen)(Br-Acetate)]$_n$

Since each Mn(III) ion has quite a large spin quantum number of s = 2 we have simulated the system by taking into account a classical Heisenberg model with a single exchange interaction J between nearest neighbor Mn ions as well as a uni-axial anisotropy D. The anisotropy axes form a planar zig-zag pattern with an inner angle δ (Fig. 1). Since the measurements were based on powder samples we have performed Monte Carlo simulations with multiple magnetic field directions and subsequent averaging. In order to avoid boundary effects, i.e. to simulate an infinite chain, we had to use 80 spins. By fitting to the experimental susceptibility data we found excellent agreement for the high temperature regime using the parameters J/k_B = -2.17 K and D/k_B = -3.17 K as well as a g-value of g=1.97. These results are consistent with the assumption of a non-collinear canted antiferromagnetic spin structure. At temperatures below 20 K we found a deviation of our model to the experimental data (Fig. 2). By taking into account dipole-dipole interaction within a chain and between neighboring chains we get a better agreement, however still not a match. Further effects are currently under investigation.

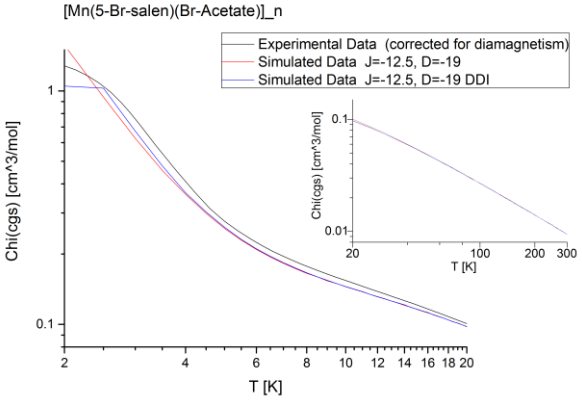

Fig. 2 Comparison of experimental and simulated susceptibility data

References

[1] Y. Aono, K. Kagesawa, K. Katoh, B. K. Breedlove, M. Yamashita, 4th Asian Conference on Coordination Chemistry, Korea (2013).

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