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Dat T. Tran, Xiaojuan Fan, Daniel P. Brennan, Peter Y. Zavalij, and Scott R. J. Oliver*: Open Metal–Organic Framework Containing Cuprate Chains

Page 6195. It was found that the coefficients $A-F$ in the analytical expression were incorrectly based on a uniform 1D antiferromagnetic chain model (see the Magnetic Properties section). The low-temperature upturn in susceptibility is due to minor impurities but should be subtracted from the data for a magnetic analysis of only the Cu^{2+} spins (Figure 1). The decrease of the susceptibility toward zero as the temperature decreases then indicates a spin gap. A spin gap is commonly formed in an alternating-chain system, where exchange interaction parameters (J and αJ) alternate along the chain. For $\alpha \rightarrow 0$, such a chain can be represented as a set of isolated spin dimers, where an energy gap exists between a spin singlet ground state and excited triplet states. Therefore, the uniform 1D antiferromagnetic chain model ($\alpha = 1$) without a spin gap is not applicable to this material. Data fitting has been performed based on a spin dimer model by the equation $\chi = (Ng^2\mu_B{}^2/kT)[1/(3 + e^{J/kT})]$.[1] The best fit gives $J = -97.6$ cm^{-1} and $g = 2.18$. Considering an alternating-chain model with a low alternating parameter is quite close to an isolated dimer. We also fit the data using the alternating-chain model[2] at $\alpha = 0.1$ (blue line, inset, Figure 1), which shows obvious deviation at low temperature. It is clear that a spin dimer model is the most suitable for our metal−organic framework.

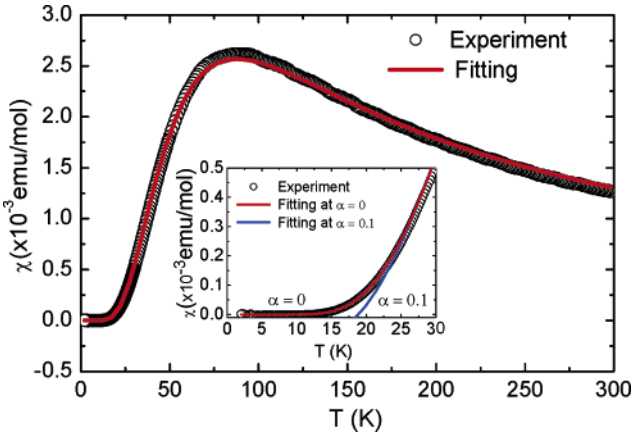

Figure 1. Temperature dependence of the magnetic susceptibility of $[Cu(OH)(C_5H_4NCO_2)\cdot H_2O]$ from 2 to 300 K. The open circles represent the data after subtraction of the impurity contribution, while the red line is the result of fitting to the spin dimer equation. For comparison, the blue line shows the alternating-chain model at $\alpha = 0.1$ (inset).

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