Quantum Critical Point in a S = ½ Antiferromagnet

S. Nellutla[1], M. Pati[2], Y.-J. Jo[1], H. D. Zhou[1], B. H. Moon[3,4], D. M. Pajerowski[3,4], Y. Yoshida[3,4], J. A. Janik[1,5], L. Balicas[1], Y. Lee[3,4], M. W. Meisel[3,4], Y. Takano[3,4], C. R. Wiebe[1,5], and N. S. Dalal[1,2]

[1]*National High Magnetic Field Laboratory, Tallahassee, Florida*
[2]*Dept. of Chemistry & Biochemistry, Florida State University, Tallahassee*
[3]*Department of Physics, University of Florida, Gainesville, Florida*
[4]*National High Magnetic Field Laboratory, Gainesville, Florida*
[5]*Department of Physics, Florida State University, Tallahassee*

The alkali-metal peroxychromate K_2NaCrO_8 crystallizes with orthorhombic symmetry with the lattice parameters a = 8.5883 Å, b = 7.9825 Å, and c = 9.2432 Å. The Cr^{5+} ion, with spin S = ½, is bonded to four peroxy $(O_2)^{2-}$ ligands in a dodecahedral geometry,[2] and the ions form the three dimensional spin-network shown in Fig. 1. Earlier EPR studies showed[2] the g tensor is anisotropic with g_z = 1.9851, g_y = 1.9696, and g_x = 1.9636 and that the electronic ground state is $3dz^2$. This project was undertaken to understand the nature of the Néel transition (paramagnet → antiferromagnet (AFM)) observed in zero-field (*see* Fig. 2) and to explore the magnetic phase diagram.

We have utilized heat capacity, magnetocaloric effect, ac susceptibility, torque magnetometry, and inelastic neutron scattering (INS) to obtain the phase diagram shown in Figure 3.

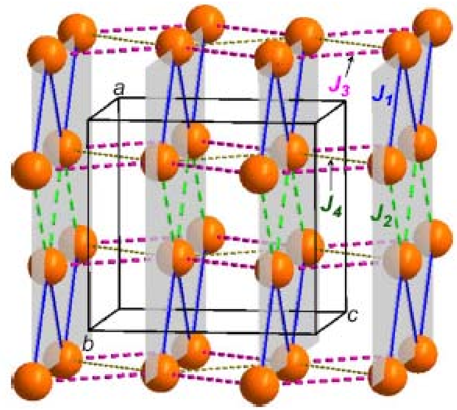

Figure 1. Intra-planar (J_1, J_2) and inter-planar (J_3, J_4) exchange paths in K_2NaCrO_8. Cr^{5+} ions are depicted as orange spheres.

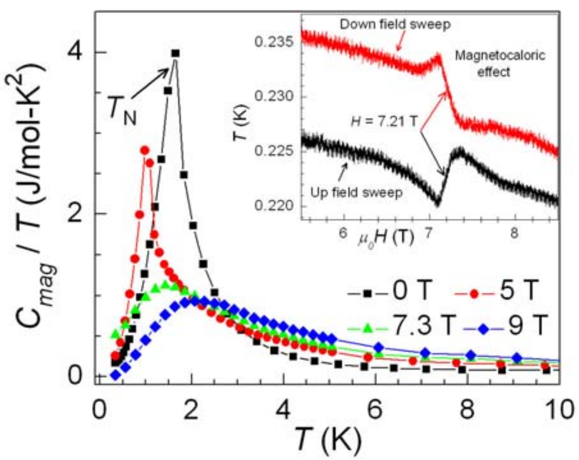

Figure 2. Magnetic heat capacity of K_2NaCrO_8 as a function of temperature, where T_N is the Néel temperature. Inset shows the magnetocaloric effect, and the mid-point of each curve is the field-induced transition.

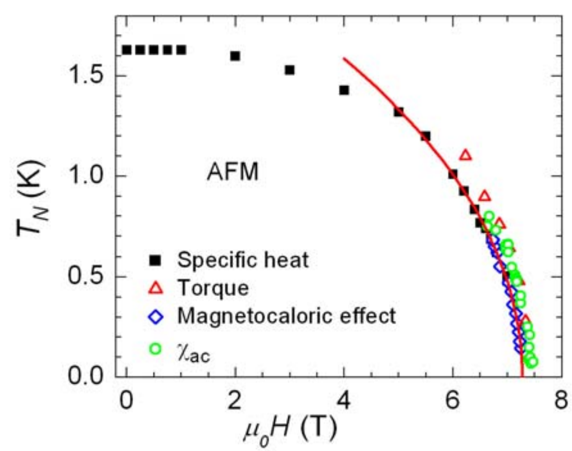

Figure 3. Magnetic phase diagram of K_2NaCrO_8. The antiferromagnetic (AFM) phase is indicated. The solid line corresponds to $T_N = A(H_c - H)^{\alpha}$.

The zero-field INS studies show that the AFM transition observed in K_2NaCrO_8 involves both nearest- and next-nearest neighbors, as shown in Fig. 1. It undergoes[1] a magnetic field tuned AFM to spin-polarized phase transition in the $T \rightarrow 0$ limit. T-window methodology[3] was used to analyze the phase boundary in this range using the relation $T_N = A(Hc - H)^{\alpha}$. A critical field of μ_0H_c = 7.270 T and a critical exponent of α = 0.481 were obtained from the analysis.[1]

The value of α depends on the universality class of the quantum phase transition. While α = 2/3 is expected for Bose-Einstein condensation, α = 1/2 is predicted for Ising-like spins.[4] The present data do not allow us to unambiguously differentiate between these two possible descriptions since a broad range of exponents is expected if the transition is not probed at sufficiently low temperatures.[5]

1. S. Nellutla *et al.*, *Phys. Rev. B* **81**, 064431 (2010).
2. B. Cage and N. S. Dalal, *Chem. Mater.* **13**, 880 (2001).
3. S. E. Sebastian *et al.*, *Phys. Rev. B* **72**, 100404(R) (2005).
4. S. Sachdev, Quantum Phase Transitions (Cambridge University Press, 1999).
5. O. Nohadani *et al.*, *Phys. Rev. B* **69**, 220402(R) (2004).

NHMFL, State of Florida, NSF-DMR grants (0654118, 0520481, 0701400, and 0803516) are gratefully acknowledged for instrumentation and financial support.