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Structure and magnetic ground states of spin-orbit coupled compound alpha-RuCl3[1] ARNAB BANERJEE, Quantum Condensed Matter Division, ORNL, USA, CRAIG BRIDGES, Chemical Sciences Division, ORNL, USA, JIAQIANG YAN, Material Sciences Division, ORNL, USA, DAVID MANDRUS, Department of Physics, University of Tennessee, Knoxville, USA, MATTHEW STONE, ADAM ACZEL, Quantum Condensed Matter Division, ORNL, USA, LING LI, YUEN YIU, Department of Physics, University of Tennessee, Knoxville, USA, MARK LUMSDEN, BRYAN CHAKOUMAKOS, Quantum Condensed Matter Division, ORNL, USA, ALAN TENNANT, Neutron Sciences Directorate, ORNL, USA, STEPHEN NAGLER, Quantum Condensed Matter Division, ORNL, USA — The layered material alpha-RuCl3 is composed of stacks of weakly coupled honeycomb lattices of octahedrally coordinated Ru3+ ions. The Ru ion ground state has 5 d electrons in the low spin state, with spin-orbit coupling very strong compared to other terms in the single ion Hamiltonian. The material is therefore an excellent candidate for investigating possible Heisenberg-Kitaev physics. In addition, this compound is very amenable to investigation by neutron scattering to explore the magnetic ground state and excitations in detail. In this talk, we discuss the synthesis of phase-pure alpha-RuCl3 and the characterization of the magnetization, susceptibility, and heat-capacity. We also report neutron diffraction on both powder and single crystal alpha-RuCl3, identifying the low temperature magnetic order observed in the material. The results, when compared to theoretical calculations, shed light on the relative importance of Kitaev and Heisenberg terms in the Hamiltonian.

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