Abstract Submitted
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Determining single-ion and spatial-exchange anisotropies in a S =1 quantum antiferromagnet[1] JAMIE MANSON, Eastern Washington U, JAMIE BRAMBLEBY, PAUL GODDARD, U of Warwick, MATTHEW STONE, ORNL, ROGER JOHNSON, U of Oxford, PASCAL MANUEL, ISIS, RAL, JACQUELINE VILLA, Eastern Washington U, CRAIG BROWN, NCNR, NIST, VIVIEN ZAPF, NHMFL, LANL, SAUL LAPIDUS, APS, ANL, REBECCA SCATENA, PIERO MACCHI, U of Bern, YU-SHENG CHEN, LAI-CHIN WU, APS, ANL, JOHN SINGLETON, NHMFL, LANL — The magnetic ground-state of the Q1D $S = 1$ antiferromagnetic (AFM) chain is sensitive to the single-ion anisotropy (D) and the relative strength of intra- (J) and interchain (J') exchange interactions. The ratios D/J and J'/J dictate the material's placement on the phase diagram for which three competing phases are known to theoretically exist: Haldane, XY and quantum paramagnetic. We have identified $[Ni(HF_2)(pyz)_2]SbF_6$ as a candidate in which to explore proximity to these phases. Combining neutron scattering (elastic and inelastic) and high-field magnetization we obtained the ground state Hamiltonian and phase diagram for a powdered sample. Long-range XY AFM order ($D >0$) occurs below $T_N = 12.2$ K and independent simulations of inelastic neutron scattering and $M(H)$ data show excellent consistency for the parameters; $D = 13.3$ K, $J = 10.4$ K (Ni-FHF-Ni) and $J' = 1.4$ K (Ni-pyz-Ni).

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