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The compound [Ni(2aepy) 2 Cl (H 2 O)] Cl×H 2 O as a candidate approaching a topological quantum critical point of a spin-1 one-dimensional antiferromagnet

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The idea of controlling the magnetic ground state of a spin-1 one-dimensional antiferromagnetic (1d AFM) quantum magnets has long been of interest to physicists. In the study of anisotropic 1d AFM systems based on Ni 2+ compounds, a series of topologically protected quantum phases was observed, one of these phases is the topologically protected Haldane phase [1, 2]. The magnetic ground state of such a system is sensitive to the relative magnitude of the single-ion anisotropy (D) and the intrachain (J) exchange interaction parameters. The D/J ratio dictates the system's placement in one of three competing phases: a Haldane gapped phase, a quantum paramagnet, and an XY-ordered state, with a quantum critical point at their junction at D/J = 1. We present the study of the crystal structure and magnetic properties of compound [Ni(2aepy) 2 Cl (H 2 O)] Cl⊠H 2 O (2aepy = 2 –aminoethylpyridine). Hexacoordinate Ni 2+ ions form a zig-zag chain based on hydrogen bonds and running along crystallographic b-axis. The analysis of the experimental susceptibility using a model of spin-1 anisotropic AFM chain yielded parameter values D/k B = 4.05 K and J/k B = 3.55 K. A theoretical prediction of D/k B = 3.7 K using ab initio approach is very close to our experimental value.
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