[Ni(pym)(H_2O)$_4$][SO_4] •2H_2O (pym = pyrimidine): A quasi-1D Ni(II) zig-zag chain

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Introduction

The S = 1/2 Cu(II) coordination compound, [Cupym)(H_2O)$_2$(NO_3)$_2$] (Cupym) [1], is a prototypal quasi-1D (Q1D) zig-zag chain structure whose magnetic properties can be explained by the Sine-Gordon (SG) model [2]. Of great interest is the opportunity to construct an analogous S = 1 system based on Ni(II) ions. With this goal in mind, we recently synthesized the new Q1D chain compound, [Ni(pym)(H_2O)$_4$][SO_4]•2H_2O (Nipym). Indeed, its crystal structure replicates the zig-zag motif presented by the Cu(II) material (Fig. 1). Thus, Nipym would be an excellent model for which to compare and, possibly extend, the SG model to S = 1 systems. Herein, we show preliminary high-field magnetization data for Nipym.

Experimental

Pulsed-field magnetization measurements of powder samples Nipym were performed using the short-pulse 65 T magnet at NHMFL Los Alamos. The samples were cooled and measurements made at several temperatures in the range 0.6 < T < 15 K using a ^{3}He cryostat.

Results and Discussion

Fig. 2 shows the low-T pulsed-field magnetization data for Nipym [3]. For a S = 1 chain, the delicate competition between the zero-field splitting (D) and intra-/interchain exchange interactions (J and J') could yield the Haldane phase [4]. Evidence for this phase is a clearly visible gap in M(H) owing to a singlet ground-state. As the close is closed, M rises very rapidly until the fully polarized state is achieved at H_{sat}. According to Fig. 2, a kink in M occurs near H_1 ~3 T but no apparent Haldane gap is realized. As the applied field increases further, additional anomalies in M are noticed at H_2 ~8 T, H_3 ~14 T and H_{sat} ~18 T. These critical fields are likely attributed to field-induced phase transitions but their nature is presently unknown. Further experimental work is on-going especially single crystal growth so that these transitions can be better assessed and the magnetic field orientation determined. Theoretical study of Nipym is also planned.

Conclusions

Nipym is a new Ni(II) chain material for which the potential exists to measure and characterize a Sine-Gordon-like model in a Q1D S = 1 material. The myriad of observed field-induced phase transitions warrants further detailed study and are in progress.

Acknowledgments

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References

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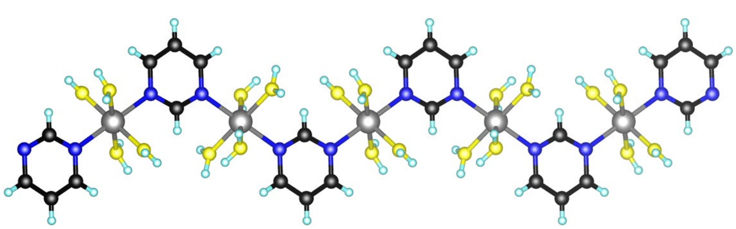

Fig. 1 X-ray crystal structure of Nipym obtained at 100 K. Ni, C, N, O, and H atoms are delineated as gray, black, blue, yellow and cyan spheres, respectively. [SO_4]$^{2-}$ and residual H_2Os occupy interstitial sites between the chains but are omitted for clarity purposes.

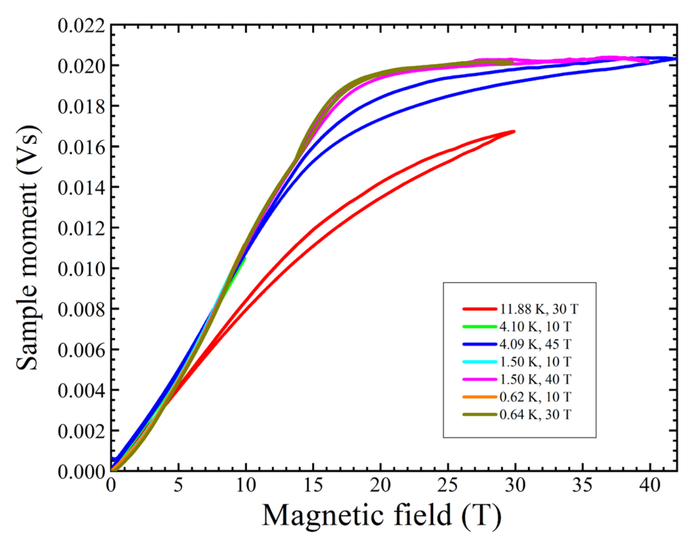

Fig. 2 Low-temperature pulsed-field M(H) data for Nipym.