Low-*T* magnetization study of *S* = 1 quasi-2D $[Ni(pyz)_2(H2O)_2](BF_4)_2$ (pyz = pyrazine)

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Introduction

$[Ni(pyz)_2(H2O)_2](BF_4)_2$ (pyz = $N_2C_4H_4$) was synthesized by a solvent-free technique and its structure solved by synchrotron X-ray powder diffraction.[1] The compound contains *S* = 1 Ni(II) ions and has tetragonal symmetry. Two-D $[Ni(pyz)_2(H_2O)_2]^{2+}$ square lattices propagate in the *ab*-plane and stack along the *c*-axis (Fig. 1). Water ligands occupy axial sites and form H-bonds with interlayer BF_4^- ions. SQUID magnetometry shows a possible transition to long-range magnetic order near 3 K. We measured the magnetization of $[Ni(pyz)_2(H2O)_2](BF_4)_2$ as a function of temperature to search for field-induced phase transitions and briefly report those findings here.

Experimental

Magnetization measurements were conducted at the Pulsed-Field Facility of the NHMFL-Los Alamos using a 65 T short-pulse magnet. A powder sample with a mass of ~1 mg was loaded in an ampoule and mounted inside the coil-set of a home-made magnetometer. Data were collected at several temperatures between 0.36 and 4.0 K.

Results and Discussion

Fig. 2 summarizes our magnetization study. The data acquired below the suspected T_N of 3 K show a nearly linear rise in *M* as the magnetic field increases. This supports probable low-dimensional spin correlations within the 2D layers. Saturated behavior is observed near 11 T. In the *T* = 0.36 K data, an apparent kink occurs just shy of 5 T which may be attributed to a spin-flop transition signaling the presence of an Ising-like ground state. Alternatively, the kink could be due to spin-exchange anisotropy in the Hamiltonian such that $\Delta \neq 0$. Furthermore, the implications of zero-field splitting (*D*) have yet to be determined as such can be rather large in six-coordinate Ni(II) coordination compounds.[1,2]

Conclusions

The magnetization of $[Ni(pyz)_2(H_2O)_2](BF_4)_2$ presents an interesting result whereby a kink in the lowest temperature data may be attributed to multiple factors. Theoretical modeling using quantum Monte Carlo techniques are in progress to unravel the magnetic characteristics of this new *S* = 1 coordination polymer.

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References

[1] Manson, J. L., *et al*. work in progress.
[2] Manson, J. L., *et al. Inorg. Chem*. **50**, 5990 (2011).

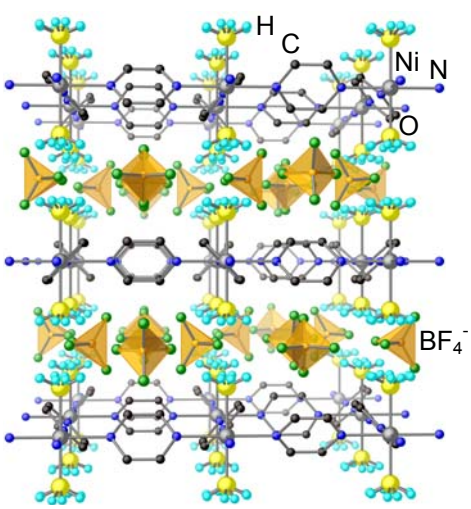

Fig.1. Polymeric structure of $[Ni(pyz)_2(H_2O)_2](BF_4)_2$.

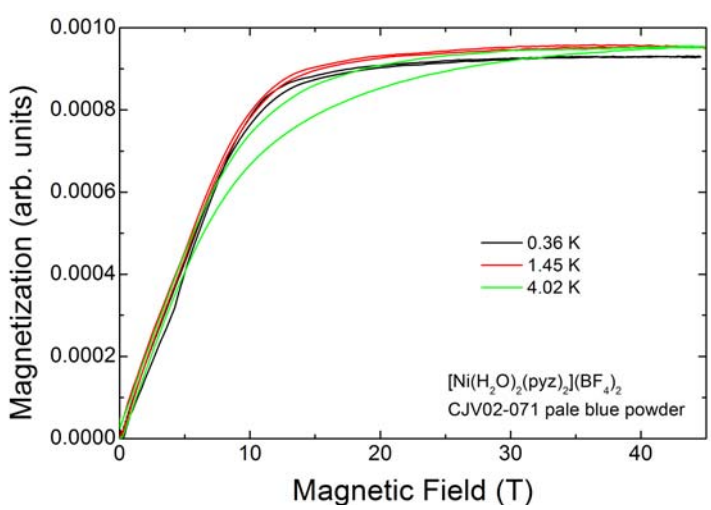

Fig.2. Pulsed-field magnetization data for $[Ni(pyz)_2(H_2O)_2](BF_4)_2$.