Magnetoelastic Coupling in a Quasi-two-dimensional Quantum Heisenberg Antiferromagnet

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Introduction
The finding that hydrogen bonding can control both long range and local structure while providing significant magnetic exchange pathways has generated significant interest in the properties of low-dimensional coordination polymers such as CuHF$_2$(pyz)$_2$BF$_4$ [1]. At the same time, the magnetic properties are highly tunable, with magnetization saturating at experimentally realizable magnetic fields [2]. This makes CuHF$_2$(pyz)$_2$BF$_4$ a prototype for fundamental studies of quantum magnetism and the role of magnetoelastic coupling in magnetically-driven transitions.

Results and Discussion
In order to probe magnetoelastic coupling in a model coordination polymer, we measured the vibrational properties of CuHF$_2$(pyz)$_2$BF$_4$ through the 20 T magnetically-driven transition. The out-of-plane pyrazine ring deformation and bending modes display clear frequency shifts with applied field (Fig. 1). These local lattice distortions interactions track the low temperature magnetization, demonstrating that this field-driven antiferromagnetic to fully polarized state transition has an elastic component. The distortions seem to weaken the antiferromagnetic spin exchange in the high field state.

Figure 1: Crystal structure of CuHF$_2$(pyz)$_2$BF$_4$, (b and c) close-up views of the 4.2 K absorption difference spectra (α(H) – α(H= 0 T)) in the range of the important pyrazine-related vibrational modes, and (d) integrated area of the absolute value of the absorption difference spectra for the indicated frequency ranges as a function of applied magnetic field compared with 1.5 and 4.2 K magnetization data from Ref. [1], (e and f) calculated spin density in the AFM and FM states. [3].

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References