# Lattice Component to the Field-driven Transition in Quasi-two-dimensional $CuHF_2(pyz)_2BF_4$

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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 $CuHF_2(pyz)_2BF_4$ [1]. At the same time, the magnetic properties of $CuHF_2(pyz)_2BF_4$ are highly tunable, with magnetization saturating at experimentally realizable magnetic fields [2]. This makes $CuHF_2(pyz)_2BF_4$ a prototype for fundamental studies of quantum magnetism and an important foil for copper oxide materials, where the energy scales are much higher and often inaccessible.

## Results and Discussion

In order to probe magnetoelastic coupling in a model coordination polymer, we measured the vibrational properties of $CuHF_2(pyz)_2BF_4$ through the 20 T magnetically-driven transition. The out-of-plane pyrazine ring deformation and bending modes display clear frequency shifts and oscillator strength changes with applied field (Fig. 1). In contrast, the Cu-pyrazine lattice modes, bifluoride linkers, and the $BF_4^-$-related modes are rigid. Interestingly, these magnetoelastic interactions track the low temperature magnetization, demonstrating that this field-driven antiferromagnetic to ferromagnetic transition has an elastic component. This demonstrates that local out-of-plane pyrazine ring distortions control the balance between in-plane antiferromagnetic interactions and inter-plane ferromagnetic exchange processes.

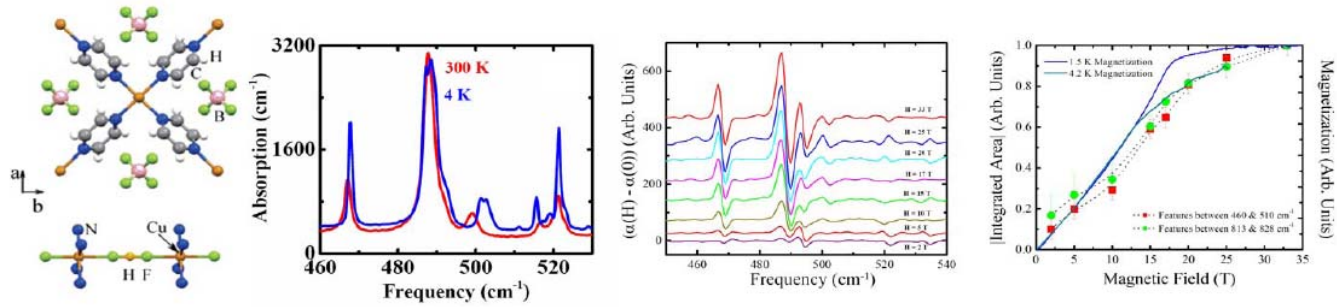


*Figure 1: Crystal structure of $CuHF_2(pyz)_2BF_4$, (b) close-up view of the infrared absorption highlighting the out-of-plane pyrazine ring deformation, out-of-plane pyrazine bend, and $BF_4^-$ bend, (c) close-up views of the 4.2 K absorption difference spectra ($\alpha(H) - \alpha(H= 0\ T)$) in the range of several 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].*

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## References

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[2] Goddard, P.A. *et. al*, New J. Phys. **10**, 083025 (2008).