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Pressure-induced Jahn-Teller axis switching in Cu(pyz)$F_2(H_2O)_2$? J.L. MUSFELDT, University of Tennessee, Z. LIU, Carnegie Institute of Washington, S. LI, Virginia Commonwealth University, J. KANG, C. LEE, North Carolina State University, P. JENA, Virginia Commonwealth University, J.L. MANSON, Eastern Washington University, J.A. SCHLUETER, Argonne National Laboratory, G.L. CARR, Brookhaven National Laboratory, M.-H. WHANGBO, North Carolina State University — We employed infrared spectroscopy along with complementary lattice dynamics and spin density calculations to investigate local structure and magnetism through the series of pressure-driven transitions in Cu(pyz)$F_2(H_2O)_2$. Rather than frequency shifts that dovetail with the recently proposed pressure-induced Jahn-Teller switching model, we overall mode hardening, particularly in the Cu–OH_2 bending mode. We combine these findings with a reanalysis of the crystal structure to reveal the series of pressure-induced transitions as a combination of *a*-axis rotation, *c*-directed compression that acts to weaken O-H...F hydrogen bonds, and pyrazine ring buckling. The magnetic dimensionality crossover can be understood in terms of changes in magnetic orbital overlap.

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