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Pressure-Induced Magnetic Crossover Driven by Hydrogen Bonding in $\text{CuF}_2(\text{H}_2\text{O})_2(3\text{-chloropyridine})$ ¹ KENNETH O'NEAL, TATIANA BRINZARIA, JOSHUA WRIGHT, JANICE MUSFELDT, University of Tennessee, SANTANAB GIRI, QIAN WANG, PURU JENA, Virginia Commonwealth University, JOHN SCHLUETER, Argonne National Laboratory, ZHENXIAN LIU, Carnegie Institute of Washington — We combined high pressure vibrational spectroscopy with complementary dynamics calculations to investigate the 0.8 GPa pressure driven magnetic crossover in $\text{CuF}_2(\text{H}_2\text{O})_2(3\text{-chloropyridine})$. Our work reveals that compression forces the 3-chloropyridine ring closer to the H_2O ligands, resulting in the formation of $-\text{Cl}\cdots\text{H}_2\text{O}$ hydrogen bonds. These new intermolecular hydrogen bonds act as ancillary superexchange pathways between copper centers, introducing a third dimension to the hydrogen bonding network and triggering the antiferromagnetic to ferromagnetic crossover. These findings are important for understanding magnetoelastic coupling in quantum magnets and other multifunctional materials in which hydrogen bond formation facilitates magnetic switching.

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