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Pressure-dependent $\nu(\text{CC})$ and $\nu(\text{CN})$ Raman modes of the molecule-based magnets $\text{M}[\text{TCNE}](\text{NCMe})_2\text{X}$ ALEXANDER E. MIDGLEY, University of Missouri-Kansas City, KONSTANTIN POKHODNYA, C. OLSON, North Dakota State University, A.N. CARUSO, MICHAEL B. KRUGER, University of Missouri-Kansas City — $\text{M}[\text{TCNE}]$ ($\text{M}=\text{V}, \text{Fe}, \text{Mn}, \text{Co}, \text{Ni}$; $\text{TCNE}=\text{tetracyanoethylene}$) molecule-based magnets demonstrate high magnetic ordering due to a strong antiferromagnetic interaction between the unpaired d- and p-electrons of the metal ions and the ligands; however, the type of bonding involved in the superexchange mechanism remains unclear. The Raman active $\text{C}=\text{C}$ vibration depends solely upon the degree of charge transfer from the metal ion to the π^* antibonding orbital of the ligand, therefore the strength of the vibration is only sensitive to backbonding. Raman spectra of the $\text{M}[\text{TCNE}](\text{NCMe})_2\text{X}$ ($\text{M}=\text{Fe}, \text{Mn}, \text{Ni}$; $\text{X}=\text{FeCl}_4, \text{SbF}_6$) molecule-based magnets were collected in a diamond anvil cell at pressures up to 36 kbar. The observed pressure-induced strengthening of the $\nu(\text{CC})$ and $\nu(\text{CN})$ Raman modes provides a clearer picture of the type and degree of backbonding, which will ultimately help build a model of how superexchange is occurring in these systems.

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