

Abstract Submitted  
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**Magneto-elastic coupling in molecule-based materials:  $[\text{Ru}_2(\text{O}_2\text{CMe})_4]_3[\text{Cr}(\text{CN})_6]$  and  $\text{Mn}[\text{N}(\text{CN})_2]_2$** <sup>1</sup> T.V. BRINZARI, Q.-C. SUN, J.L. MUSFELDT, University of Tennessee, L.-C. TUNG, Y.J. WANG, National High Magnetic Field Laboratory, J. LIU, M.-H. WHANGBO, North Carolina State University, J.S. MILLER, University of Utah, J.L. MANSON, Eastern Washington University, J.A. SCHLUETER, Argonne National Laboratory — We measured the infrared vibrational response of two prototypical molecule-based magnets,  $[\text{Ru}_2(\text{O}_2\text{CMe})_4]_3[\text{Cr}(\text{CN})_6]$  and  $\text{Mn}[\text{N}(\text{CN})_2]_2$ . We find that both temperature and magnetic field driven transitions impact spin-lattice interactions in these materials. For instance, through the Néel transition, Cr–CN stretching and bending modes as well as Ru–O stretching mode in  $[\text{Ru}_2(\text{O}_2\text{CMe})_4]_3[\text{Cr}(\text{CN})_6]$  display sudden frequency shifts and a strong hysteresis that reveal local structure changes around Cr and Ru centers in response to magnetic ordering. On the other hand, the dicyanamide ligands in  $\text{Mn}[\text{N}(\text{CN})_2]_2$  display pronounced sensitivity to the 30 T magnetic quantum critical transition, in line with our calculations that point toward the importance of N–C–N and C–N–C angles for the mediation of Mn···Mn spin exchange interactions.

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T.V. Brinzari  
University of Tennessee

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