Abstract Submitted
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High-Field EPR Study of the Spin-Crossover Transitions in a Mn(III) Schiff-Base Complex[1] BRITTANY GRIMM, Florida State University, NHMFL, IRINA KUEHNE, CONOR KELLY, GRACE MORGAN, University College Dublin, STEPHEN HILL, Florida State University, NHMFL — Spin crossover (SCO) transitions from a high-spin (HS) to a low-spin (LS) state occur in certain molecular complexes of octahedrally coordinated $3d^4$ to $3d^7$ transition metals and can be induced using temperature, pressure, or optical perturbations.[1] It has been observed that not all SCO complexes exhibit a complete transition, resulting in mixed LS/HS phases.[2] Such situations are difficult to characterize experimentally due to the inhomogeneous nature of the mixed phase.[2] The Mn(III) Schiff-base complex considered in this investigation, $[Mn((3\text{-MeO-5-}NO_2\text{-sal})_2323)]PF_6$, exhibits a complete transition from a pure HS ($S = 2$) to a pure LS ($S = 1$) state below a relatively sharp transition ($T_{1/2}$ = 51 K, with <10 K hysteresis). Using continuous-wave high-field (0 to 14.5 T) EPR spectroscopy on a powder sample, the zero-field splitting parameters were characterized for both the LS (D = +20.8 cm^{-1}) and HS states (D = -4.80 cm^{-1}, E = 2.175 cm^{-1}). References: 1. Kahn, O., and C. Jay Martinez. "Spin-Transition Polymers: From Molecular Materials Toward Memory Devices." *Science*, vol. 279, no. 5347, 2 Jan. 1998, pp. 44–48., doi:10.1126/science.279.5347.44. 2. Capel Berdiell, Izar, et al. "Frontispiece: An Incomplete Spin Transition Associated with a Z′ =1→Z′ =24 Crystallographic Symmetry Breaking." *Chemistry - A European Journal*, vol. 24, no. 20, 7 Nov. 2017, pp. 1–5., doi:10.1002/chem.201882065.

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