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High-Field EPR Study of the High- and Low-Spin States of a Mn^{3+} Complex Exhibiting a Sharp Spin-Crossover Transition[1] BRITTANY GRIMM, Florida State University; National High Magnetic Field Laboratory, IRINA KUEHNE, CONOR KELLY, GRACE MORGAN, University College Dublin, STEPHEN HILL, Florida State University; National High Magnetic Field Laboratory — Spin crossover (SCO) transitions occur in certain molecular complexes of octahedrally coordinated $3d^4$ to $3d^7$ transition metals and can be induced through variations in temperature, pressure, or via optical perturbations. In many manganese SCO complexes, it can be too costly energetically to convert all sites within a crystal from high-spin (HS) to low-spin (LS). Consequently, the transition often occurs gradually, with only a fraction of the sites converting, resulting in mixed LS/HS phases. It is challenging to characterize these mixed phases spectroscopically due to their inhomogeneous nature. The Mn^{3+} complex considered in this investigation exhibits a complete 100% HS ($S = 2$) to 100% LS ($S = 1$) transition below a relatively sharp transition temperature ($T_{1/2}$ = 51 K, with <10 K hysteresis), allowing for a more straightforward characterization of both spin states. The magnetic properties of octahedrally coordinated Mn^{3+} complexes are dominated by the combined influences of anisotropic crystal-field and spin-orbit interactions, which are often described in terms of 2^{nd}-order axial and rhombic zero-field splitting (ZFS) terms in an effective spin Hamiltonian. We employ high-field EPR in order to accurately characterize the ZFS interactions in both the HS and LS states, and rationalize these on the basis of the corresponding structures.

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