**High-Field EPR and 57Fe Mössbauer Studies of Complexes Containing Fe-Fe Bonds**

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**Introduction**

****Complexes containing multiple metal sites have been a subject of considerable attention. Interest in these complexes stems from their ability to facilitate catalysis, mimic enzyme active sites and serve as multi-electron redox agents1,2. Despite this effort relatively little is known about the bonding interactions between multiple first row transition metal elements. A complex containing a diiron bond has been synthesized and studied using high field/ frequency electron paramagnetic resonance and variable field 57Fe Mossbauer spectroscopy. This complex (**1**), shown in **Fig. 1**, contains one Fe(II) site and one Fe(I) site.2

**Fig. 1.** Structure of **1.**

**Experimental**

 A series of high-field EPR measurements were conducted on a ground solid sample of **1** using the homodyne, quasi-optical EPR instrument outfitted with a 15/17T superconducting magnet. Mössbauer spectra were recorded using an instrument fitted with a helium-flow cryostat that had a built in 8 T superconducting magnet. Both instruments are part of the instrumentation available at the NHMFL EMR facility**.3**

**Results and Discussion**

 A series of temperature-dependent, high-frequency/field EPR were recorded for **1**. These spectra were analyzed in the framework of a standard spin Hamiltonian (**Fig. 2**). This analysis allowed for the determination of the magnetic anisotropy of **1**,which was found to be nearly axial. Variable-field Mössbauer spectroscopy was then employed to ascertain the hyperfine structure (**Fig. 3**). Analysis of the Mössbauer spectra allowed for the hyperfine structure of both Fe sites to be determined.

**Fig. 2.** Experimental (black) and simulated (purple) EPR spectra of **1** at various temperatures/frequencies.

**Fig. 3.** Experimental (black) and simulated (red) Mössbauer spectra of **1** under various applied fields.

**Conclusions**

 The combination of high-frequency/field EPR and variable field Mössbauer yields a detailed picture of the electronic structure of **1.**

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**References**

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