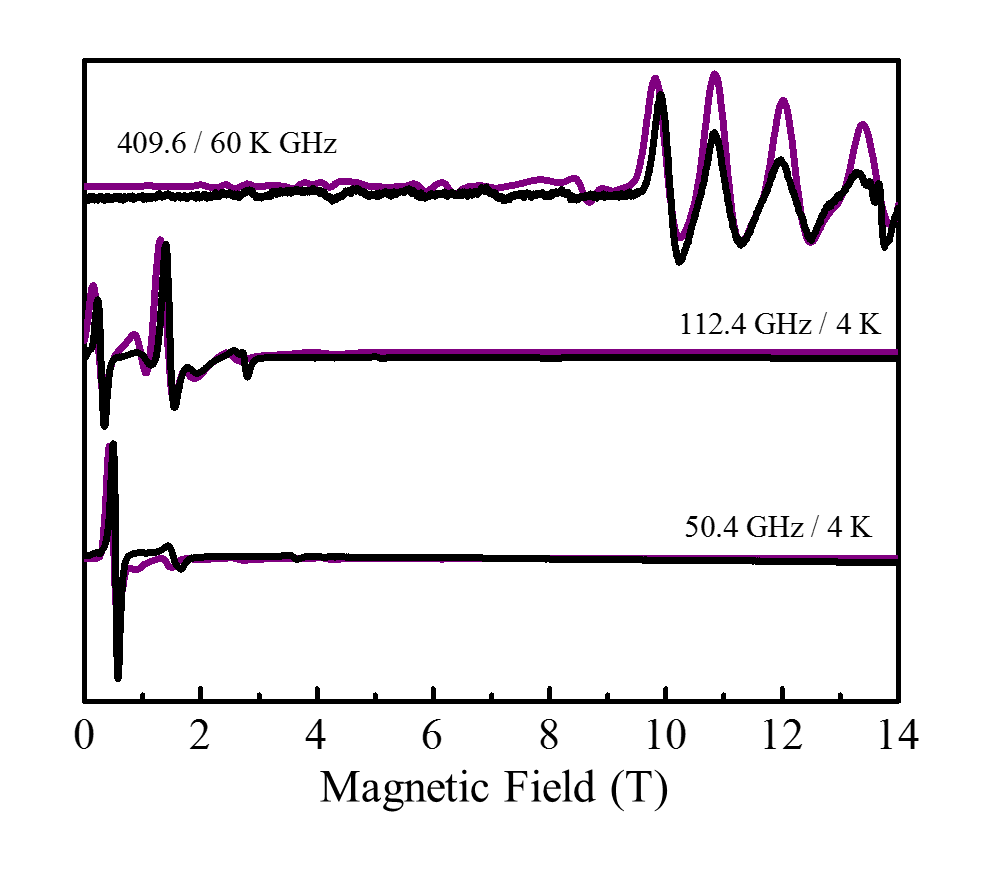
**High-Field EPR and 57Fe Mössbauer Studies of Complexes Containing Fe-Fe Bonds**

Greer, S.M. (FSU, Chemistry); Hill, S.O.; Stoian, S.A. (FSU, NHMFL); Kuppuswamy, S. and Thomas, C.M. (Brandeis U., Chemistry)

**Introduction**

**C:\Users\Sam\Desktop\phdformalcrap\figures\CT2.tif**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.**

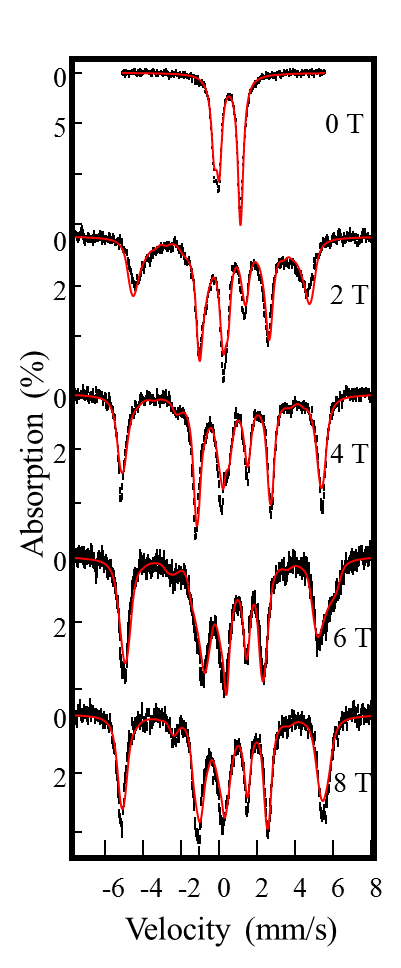
**Experimental**

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.**

**Acknowledgements**

S.G. acknowledges support from the National Science Foundation Graduate Research Fellowship Program under Grant No. 1449440. C.M.T. acknowledges support from the U.S. Department of Energy under Award no. DE-SC0004019. A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by National Science Foundation Cooperative Agreement No. DMR-1157490, the State of Florida, and the U.S. Department of Energy.

**References**

[1] Wheatley, N., *et al*., P. Chem. Rev., **99**, 3379−3420 (1999).

[2] Kuppuswamy, S., *et al*., Inorg. Chem., **51**, 1866-1873 (2012).

[3] Hassan, A. K., *et al*., J. Magn. Reson., **142**, 300-312 (2000).