High Field EPR Studies of Fe-Containing Homo- and Heterobimetallic Complexes

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Introduction

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

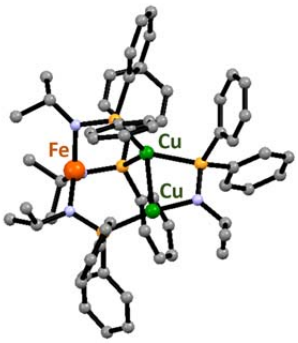

Fig. 1. Crystal structure of **1.**

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 of the EMR facility.[3]

Results and Discussion

A series of EPR spectra of **1** were recorded at multiple frequencies, the observed resonance fields are plotted versus the applied frequency (Fig. 2). From the observed resonance positions we were able to fit a model Hamiltonian to the system and determine that the two Cu(II) sites are anti-ferromagneticaly coupled leaving the Fe(II) essentially isolated from the other metal centers. The experiment indicates that the Fe(II) center has only slight distortions from axial symmetry, likely arising from the asymmetric Cu-Cu unit which breaks the C3 symmetry axis perpendicular to the trigonal plane.

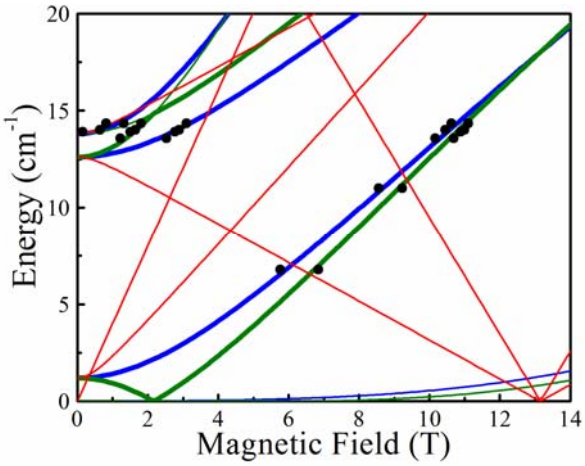

Fig. 2 Observed resonance positions (black) along with model Hamiltonian transitions with observed transitions shown in bold.

Conclusions

The local anisotropy of the Fe(II) center in **1** has been experimentally determined.

Acknowledgements

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References

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