

A series of Cr (III) dimer systems have been studied to characterize the local electronic environments present in the systems and to determine their efficacy as possible MRI contrast agents and magnetically guided drug delivery substrates. The initial characterization of these compounds will be published in *Polyhedron* at the end of the summer. The results were also presented at the DOE triennial review of the Center For Nanoscale Materials (CNM) at Argonne National Laboratory (ANL) on May 20, 2010. This work was presented under the proposal CNM-1141. Further collaboration with ANL will continue throughout the development of this project.

These compounds possess two Cr (III) centers linked by four superexchange pathways.<sup>1</sup> There is a bis( $\mu$ -oxo) linkage and a bis(1,2-squarato) linkage which axially link the two metal centers. The variation of the terminal equatorial ligands on the complexes has significant impact on the isotropic and anisotropic exchange present in the system. The ligand variation also changes the color of the complexes, and each complex will revert back to its hydrated form after a characteristic amount of time when placed in water. This reversibility is also highly dependent on the identity of the ligand being replaced. It is hoped that measurements on the exchange energies obtained from Electron Paramagnetic Resonance (EPR) and magnetic susceptibility measurements will provide useful predictions for the kinetics of the complexes' reversibility.

These magnetic measurements will be used in conjunction with x-ray diffraction, UV reflection, and density functional modeling to further characterize the energetics of the compounds and to elucidate the electronic environments which govern the reversibility of the ligand substitution. The relaxation of the spin polarization is also being studied with the use of linewidth variations in the EPR spectra and AC magnetic susceptibility studies. A new probe is being developed for longitudinal EPR detection, which will show spin relaxation directly. These measurements will provide more insight into the efficacy of these compounds as imaging agents and drug delivery systems.

Cr (III) is a transition metal that has shown low toxicity in the human body. It is also an essential nutrient that has been shown to increase insulin sensitivity and help lower hemoglobin A<sub>1c</sub> levels in Type 2 diabetics. The mechanism of these effects is poorly understood, but it is believed that Cr (III) increases the number of insulin receptors on cells.<sup>2</sup> These Cr (III) dimer systems possess a strong enough magnetic moment at room temperature to be magnetically guided.<sup>3</sup> We will thus be attempting to synthesize a compound with optimal reversibility kinetics that delivers a payload of medical interest to a region specified by a magnetic gradient. A successful derivative has already been synthesized with tolbutamide (orinase), a well-known treatment for Type 2 Diabetes.

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<sup>1</sup> Getzlaff, Mathias, *Fundamentals of Magnetism*, Springer, New York, 2008, 43

<sup>2</sup> Anderson, R., *J. Am. Col. Nut.*, Vol. 17, No. 6, 548-555 (1998)

<sup>3</sup> Pankhurst, Q.A., Connolly, J., Jones, S.K., and Dobson, J., *J. Phys. D: Appl. Phys.*, 36 R167-R181 (2003)