Faculty Research Grant 2011 FINAL REPORT

PROJECT TITLE

Modulating the Redox Power of Iron Carbonyl Clusters

PRINCIPAL INVESTIGATOR

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STATEMENT OF PROBLEM

This project was aimed at studying the structure, electronic, and catalytic properties of iron-clusters coupled to fluorothiolphenols (compounds **1** and **2**). In the design of these compounds, the fluorothiophenol ligands were used to modulate the redox properties of the clusters affording catalysts with more positive reduction potentials than those reported in the literature. These clusters are of interest as catalysts for the production of hydrogen, an environmentally benign alternative to fossil fuels. The development of efficient catalysts for hydrogen generation is an important step towards achieving the hydrogen economy.



BRIEF REVIEW OF THE RESEARCH PROCEDURE UTILIZED

The proposed clusters were prepared following literature procedures under nitrogen atmosphere using Schlenk line techniques. The structure and electronic properties of the compounds were determined by spectroscopic (Infrared, UV-visible, and Nuclear Magnetic Resonance) methods and Xray crystallography. The prepared compounds were examined as electrocatalysts for the generation of hydrogen by an electrochemical technique called cyclic voltammetry.

SUMMARY OF FINDINGS

Compounds **1** and **2** were successfully prepared, isolated and characterized. Our study shows that these compounds are effective catalysts for the electrochemical production of hydrogen with favourable overpotentials. Details of this work have been published in the International Journal, *Transition Metal Chemistry* (See attached Article: *Transition Meta Chem.*, DOI 10.1007/s11243-012-9633-0).

CONCLUSIONS AND RECOMMENDATIONS

Support from Faculty Research Grant allowed us to prepare and study these new clusters that are effective catalysts for hydrogen production. The results from this study have expanded our understanding of hydrogen producing catalysts and will be used in the designing of more efficient catalytic systems. Part of this work was presented at the 243rd ACS National Meeting, San Diego, CA (March 25- 29 2012). We gratefully acknowledge the financial support crucial for the success of this project from Arkansas Tech University - Faculty Research Grant.