

Faculty Research Grant 2012

FINAL REPORT

PROJECT TITLE

**Hydrogenase model: Exploring the effect of
hydrogen bonding**

PRINCIPAL INVESTIGATOR

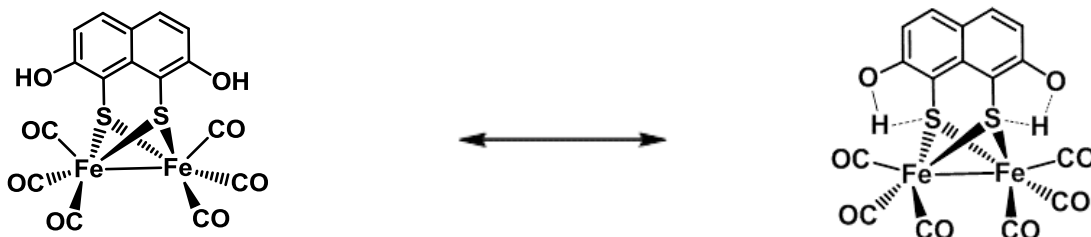
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STATEMENT OF PROBLEM

This project is aimed at studying the structure, electronic, and catalytic properties of an iron-carbonyl cluster coupled to 2,7-dihydroxynaphthalene-1,8-dithiolate. The cluster is of interest as catalyst 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.

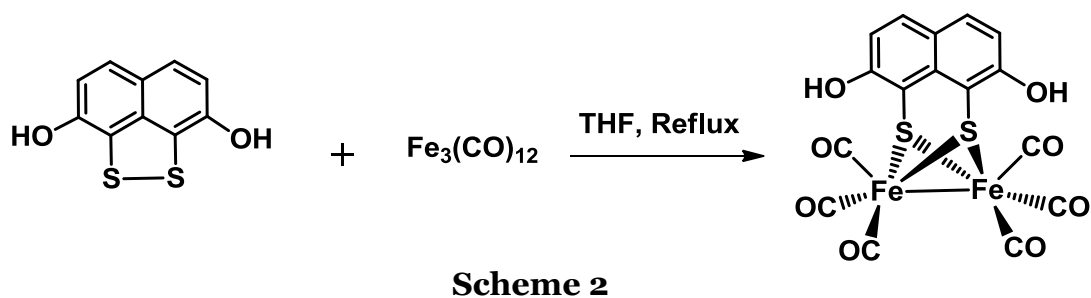
In the design of the catalyst, we incorporated 2,7-dihydroxynaphthalene-1,8-dithiolate ligand to modulate the electronic property of the cluster through intramolecular O-H...S hydrogen bonding (Scheme 1). The characterization of this compound will be accomplished using spectroscopic techniques. This study will contribute to the fundamental knowledge on the design of effective catalysts for hydrogen production



Scheme 1

BRIEF REVIEW OF THE RESEARCH PROCEDURE UTILIZED

The proposed cluster was prepared following a multi-step procedure under nitrogen atmosphere using Schlenk line techniques. The final synthetic step is shown in Scheme 2.



The structure and electronic properties of the compound were probed using infrared spectroscopy. The prepared compound is being examined as electrocatalyst for the generation of hydrogen by an electrochemical technique (cyclic voltammetry).

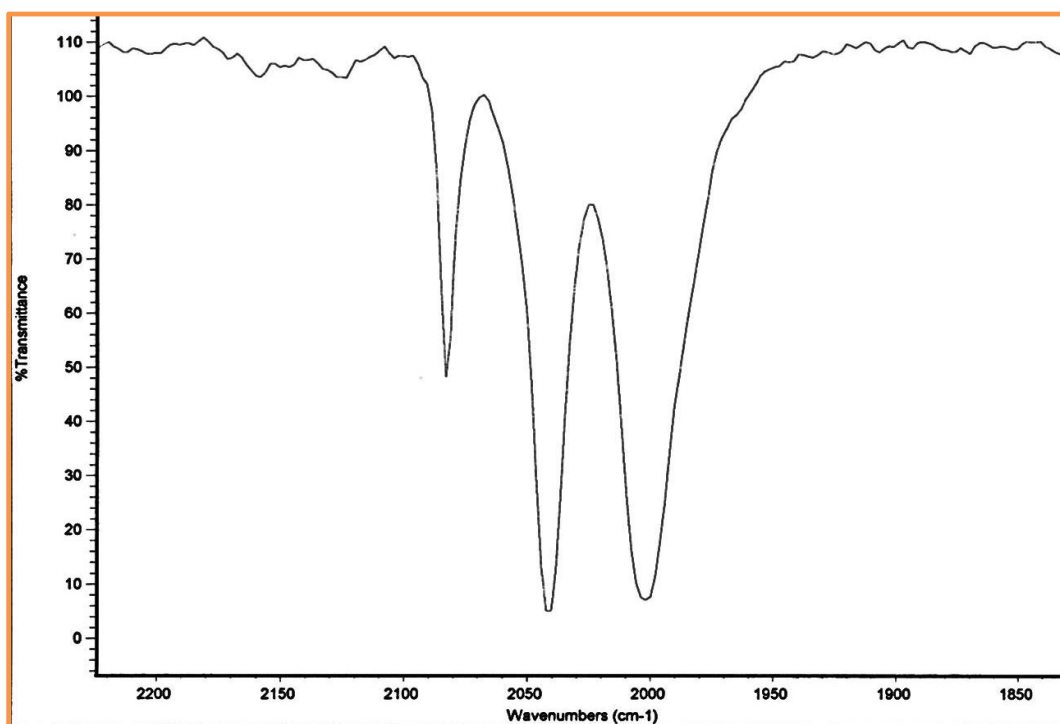


Figure 1: IR spectrum of desired compound in DCM

SUMMARY OF FINDINGS

The desired compound has been successfully prepared, isolated and characterized by IR spectroscopy. IR spectrum of the compound shows peaks between 2000 and 2100 cm^{-1} ascribed to terminal metal carbonyls. Partial results were presented at the Russellville High School Science Fair (2013) and National ACS meeting in New Orleans, Louisiana, March 25-29, 2013. The PI used part of the travel funds to attend the VIPER Workshop: Solid State Materials for Alternative Energy Needs (Penn State University | State College, PA | 23 Jun 2013 - 28 Jun 2013). At this workshop, the participants developed teaching resources (Learning Objects) in the area of solid state materials as part of undergraduate inorganic chemistry curriculum (Learning object attached).

CONCLUSIONS AND RECOMMENDATIONS

We have prepared a new iron-cluster coupled to 2,7-dihydroxynaphthalene-1,8-dithiolate. Further characterization is being carried out. We gratefully acknowledge partial support for this project from Arkansas Tech University Faculty Research Grant (2012-2013).