Faculty Research Grant 2014

Final Report

Water Soluble Hydrogenase Model

Principal Investigator

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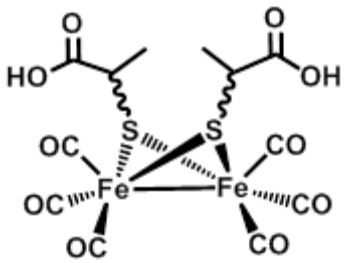
Statement of Problem

This project is aimed at preparing and studying the structure, electronic, and catalytic properties of an iron-carbonyl cluster coupled to thiolactate. 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 (**1**), we incorporated thiolactate, a water soluble ligand to modulate the solubility property of the cluster. 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



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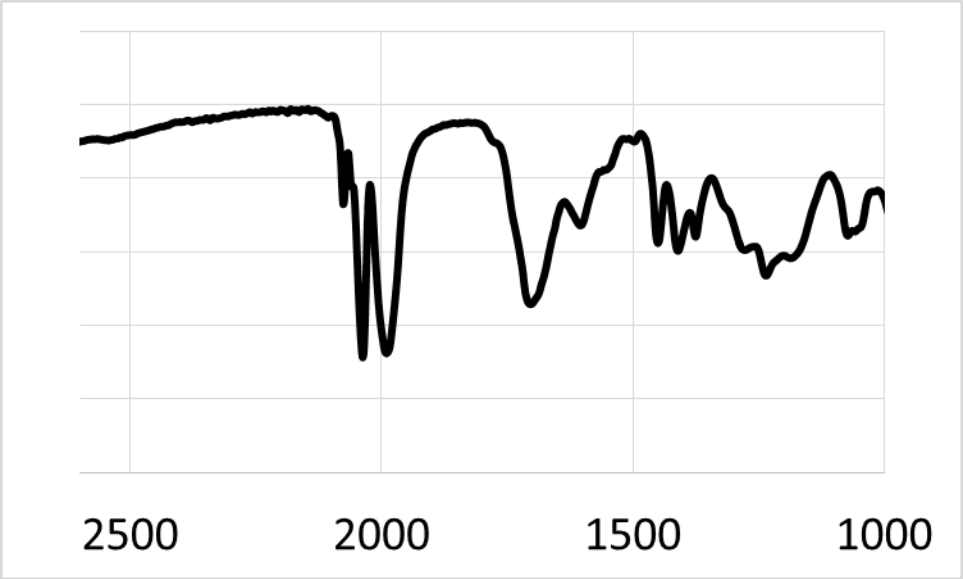
Brief Review of Research Procedure Utilized.

The proposed cluster was prepared following a single step procedure under nitrogen atmosphere using Schlenk line techniques. A mixture of thiolactate and triirondodecacarbonyl was treated with THF solvent and the resultant solution refluxed for 30 minutes. A color change from green to red was observed. Removal of solvent followed by column chromatographic separation afforded the desired product as an orange oily substance. The structure and electronic properties of the compound were probed using infrared spectroscopy, and examined as electrocatalyst for the generation of hydrogen by an electrochemical technique (cyclic voltammetry).

Figure 1: IR spectrum of desired compound in DCM



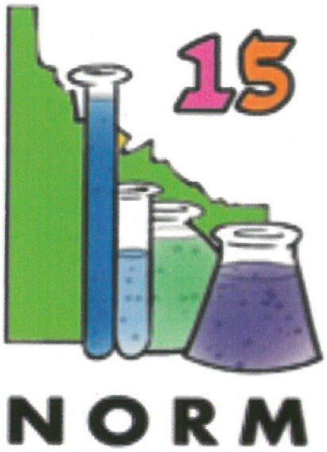
SUMMARY OF FINDINGS

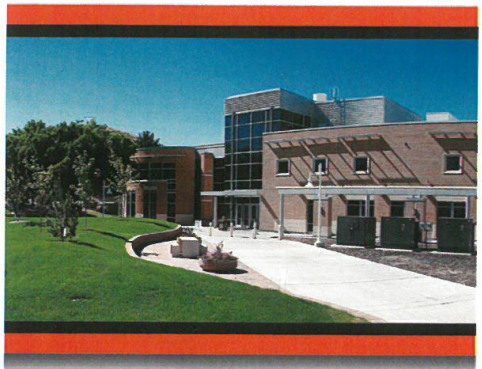
The desired compound has been successfully prepared, isolated and characterized by IR spectroscopy. IR spectrum of the compound shows peaks between 2000 and 2100 cm^{-1} ascribed to terminal metal carbonyls. Partial results were presented at the ACS Regional meeting in Pocatello, Idaho, June 25-29, 2015.

CONCLUSIONS AND RECOMMENDATIONS

We have prepared the new iron-cluster, compound 1. Further characterization is being carried out. We gratefully acknowledge partial support for this project from Arkansas Tech University Faculty Research Grant (2012-2013).

The 70th Northwest Regional Meeting of the American Chemical Society





June 21 – 24, 2015
On the campus of
Idaho State University
Pocatello, Idaho

TUESDAY EVENING

Pond Student Union
Exhibit Room

Emerging Trends in Actinide and Lanthanide Separations

B. Mincher, *Organizer*

5:00 - 7:00

93. Adsorption of uranium using an aminophosphonic acid functionalized material. **R.L. Tsosie**, E. Rosenberg

94. Systematic study of N,N,N',N'-tetra-2-ethylhexyl diglycolamide (T2EHDGA) solvent extraction behavior. **E.L. Campbell**, T.G. Levitskaia

Pond Student Union
Exhibit Room

Inorganic Chemistry

Cosponsored by INOR‡
J. J. Pak, *Organizer*

5:00 - 7:00

95. Hydrogen evolution from neutral water catalyzed by hydrogenobacter thermophilus cobalt-cytochrome *c*. **B. Kandemir**, T.A. Ruberu, R. Eisenberg, K. Bren

96. Varying the elemental ratios in Cu_2ZnSnS_4 nanoparticles. **K.V. Nielson**, J. Chavez, J.J. Pak

97. Preparation and study of quaternary quantum dots. **T. Huntsinger**, **J. Chavez**, J.J. Pak

98. Toxicology studies of semiconductor nanoparticles. **D.R. Walker**, J.J. Pak

99. Bio-inspired iron-based hydrogen producing catalysts. **C.A. Mebi**, A.L. Haley, J. Randall, S.L. Moran

100. Synthesis of model compounds that mimic the primary and secondary coordination sphere of carbonic anhydrase. **J. Elsberg**, E.C. Brown