

Faculty Research Grant 2016

Final Report

Reaction of 4,4'-Thiobisbenzenethiol with $\text{Fe}_3(\text{CO})_{12}$

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Statement of Problem

This project was aimed at studying the reaction of 4,4'-thiobisbenzenethiol with triirondodecarbonyl. The expected product(s), iron-carbonyl cluster(s), 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 Research Procedure Utilized

Triirondodecarbonyl (2.28 g, 4.53 mmol) and 4,4'-thiobisbenzenethiol (0.85g, 3.39 mmol) were mixed in a 100 mL flask and purged with nitrogen for 30 minutes. Toluene (70 mL) was then added to the flask and stirred under reflux conditions for 30 minutes. The solution changed color from dark green to red. The solvent of the solution was removed by rotary evaporation affording an orange solid. Silica gel chromatographic separation of the residue using hexanes-dichloromethane (50:50) solvent mixture as eluent gave a cyclic tetranuclear iron-carbonyl complex in 41.3 % yield. This new compound has been characterized using IR and UV-vis spectroscopy (Figure 1). Electrochemical properties of the compound has been investigated by cyclic voltammetry (Figure 2). Single crystals of the compound were obtained and analyzed by X-ray crystallography.

Summary of Findings

The reaction of 4,4'-thiobisbenzenethiol with triirondodecarbonyl afforded a cyclic tetranuclear iron-carbonyl cluster.

Conclusions and Recommendations

The project was successful and a manuscript describing results from this study has been prepared for publication.

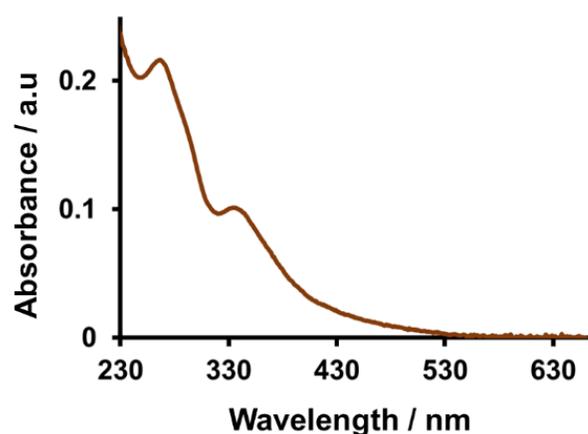


Figure 1. *UV-visible spectra of product recorded in DCM (1.0 mM).*

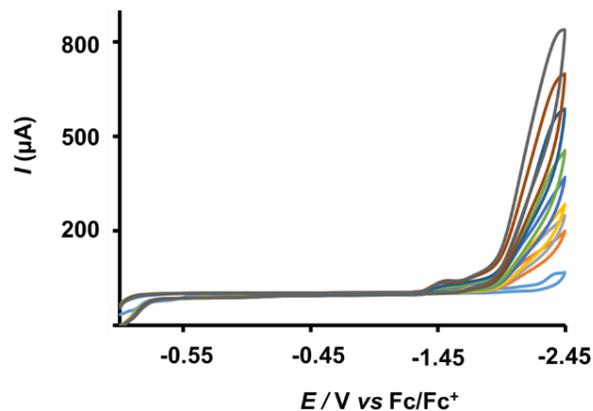


Figure 2. *Cyclic voltammograms of product in the presence of increasing amounts of acetic acid.*