Faculty Research Grant 2018

Final Report

Reaction of Arenedithiols with $Fe_3(CO)_{12}$

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Statement of Problem

This project was aimed at studying the reaction of three arenedithiols with triirondodecacarbonyl. 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

Synthesis and purification: Triirondodecarbonyl and the dithiol were mixed in a 100 mL flask and purged with nitrogen for 30 minutes. THF (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 as eluent gave orange products as solids.

Characterization: These new compounds were characterized using IR spectroscopy. The data suggest successful synthesis of the desired products (spectra below show presence of terminal iron-carbonyl units). Further analysis has to be conducted to unequivocally determine the structure, composition and electrochemical properties of the compounds. Proposed structures are not indicated in this write up since we plan to publish the research results in the near future.

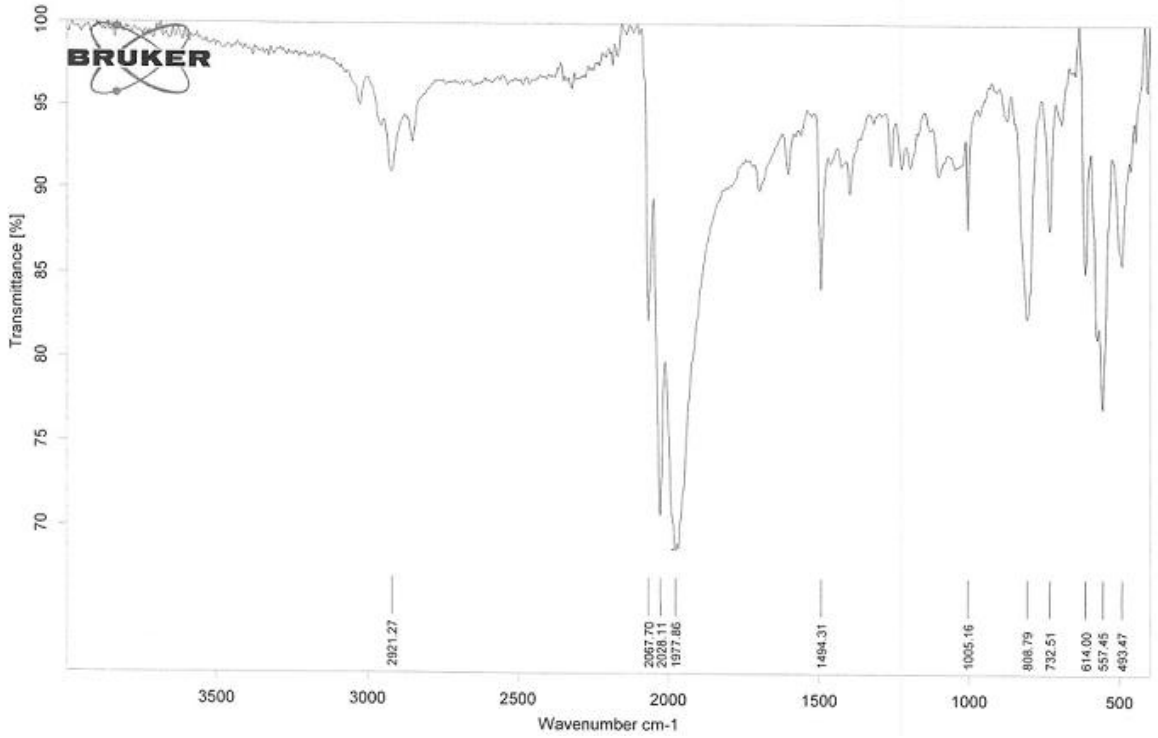
Summary of Findings

Three reactions involving arenedithiols and triirondodecacarbonyl were successfully carried out. The products were purified and isolated as orange solids.

Conclusions and Recommendations

The project was successful. Further analysis is needed to fully characterize the products.

Spectra of two of the products. Peaks between 1900 and 2100 cm^{-1} are assigned to terminal metal carbonyls.



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