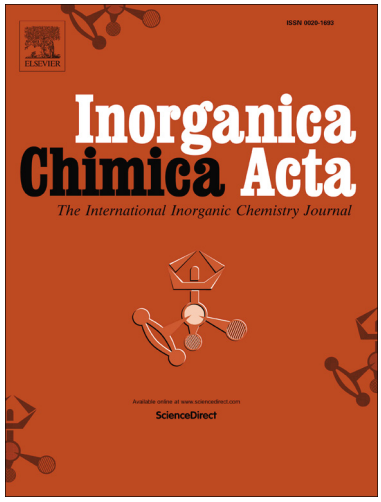

Research paper

Cyclic tetranuclear iron-carbonyl complex containing thiobisbenzenethiolate ligands: Synthesis and structural characterization

Shakeena L. Johnson, Nikolay N. Gerasimchuk, Charles A. Mebi

PII: S0020-1693(18)30229-9
DOI: https://doi.org/10.1016/j.ica.2018.03.043
Reference: ICA 18188

To appear in: *Inorganica Chimica Acta*

Received Date: 9 February 2018
Revised Date: 28 March 2018
Accepted Date: 28 March 2018

Please cite this article as: S.L. Johnson, N.N. Gerasimchuk, C.A. Mebi, Cyclic tetranuclear iron-carbonyl complex containing thiobisbenzenethiolate ligands: Synthesis and structural characterization, *Inorganica Chimica Acta* (2018), doi: https://doi.org/10.1016/j.ica.2018.03.043

Cyclic tetranuclear iron-carbonyl complex containing thiobisbenzenethiolate ligands: Synthesis and structural characterization

Shakeena L. Johnson,[a] Nikolay N. Gerasimchuk,[b] and Charles A. Mebi*[a]

[a]Department of Physical Sciences, Arkansas Tech University, 1701 N. Boulder Ave, Russellville, Arkansas, 72801 USA. Email: cmebi@atu.edu, Phone: 4793562151, Fax: 4799640837

[b] Missouri State University, Department of Chemistry, 901 S. National Ave. Springfield, Missouri, 65897 USA

ABSTRACT

A new macromolecular double-butterfly Fe/S carbonyl cluster, $[Fe_2(CO)_6]_2$(μ-4,4′-thiobisbenzenethiolato)$_2$ (**1**), a model for the active site of [Fe-Fe] hydrogenases, has been prepared and characterized by spectroscopic methods and X-ray crystallography. The molecular structure of **1** contains two units of $S_2Fe_2(CO)_6$ covalently linked to two thiobisbenzene groups to form a 26-membered metallocycle with the benzene substituents on sulfur adopting an *ae* stereochemistry. The Fe-Fe bond in **1**