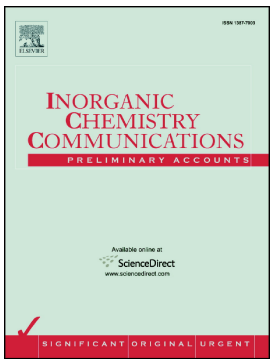
Accepted Manuscript



A μ3-oxo-centered mixed-valence triiron coordination polymer constructed by 5-bromonicotinato ligands

Ranjana Liyanage, Qi Yang, Min Fang, Dongsheng Li, Jack Y. Lu

PII: S1387-7003(18)30220-X
DOI: doi:10.1016/j.inoche.2018.04.016
Reference: INOCHE 6947

To appear in: *Inorganic Chemistry Communications*

Received date: 15 March 2018
Revised date: 13 April 2018
Accepted date: 17 April 2018

Please cite this article as: Ranjana Liyanage, Qi Yang, Min Fang, Dongsheng Li, Jack Y. Lu , A μ3-oxo-centered mixed-valence triiron coordination polymer constructed by 5-bromonicotinato ligands. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Inoche(2017), doi:10.1016/j.inoche.2018.04.016

A μ_3-oxo-centered mixed-valence triiron coordination polymer constructed by 5-bromonicotinato ligands

Ranjana Liyanage,[a] Qi Yang[a, b*], Min Fang,[c,d] Dongsheng Li,[e*] Jack Y. Lu[a,b]*

[a]*Department of Chemistry, University of Houston-Clear Lake, 2700 Bay Area Blvd. Houston,TX 77058, U.S.A.*

[b]*Key Laboratory of Synthetic and Natural Functional Molecule Chemistry of Ministry of Education, College of Chemistry and Materials Science, Northwest University, Xi'an, Shaanxi, 710127, China*

[c]*Department of Chemistry, School of Chemistry and Materials Science, Nanjing Normal University, Nanjing 210023, China*

[d]*State Key Laboratory of Coordination Chemistry, Nanjing University, Nanjing 210093, China*

[e]*College of Materials and Chemical Engineering, Research Institute of Materials, China Three Gorges University, Yichang, PR China*

*Corresponding authors e-mail address: lu@uhcl.edu

Abstract

A new oxo-centred, carboxylate bridged trinuclear mixed-valence iron coordination polymer has been obtained under hydrothermal conditions, $[(Fe^{III})_2Fe^{II}(\mu_3\text{-}O)(BNA)_6]_n$ (**1**). Single crystal X-ray diffraction analysis of the black crystal reveals that three iron atoms occupy the vertices of a non-equilateral triangle with the Fe···Fe distance in the range of 3.245 Å ~ 3.343 Å and are bonded by the μ_3-oxo-centred and BNA^- ligands. The crystal belongs to the monoclinic crystal system with a = 11.2904(6) Å, b = 18.4960(11) Å, c = 21.4349(12) Å, β = 91.029(1), space group $P2_1/c$, GOF = 1.028, final R_1 = 0.0156, wR_2 [I>2σ(I)] = 0.0405.

Keywords: Coordination polymer; Crystal structure; 5-bromonicotinic acid; μ_3-oxo-centred; Trinuclear mixed-valence iron

Coordination polymers (CPs) constructed with polynuclear clusters have received considerable attention due to the potential applications in several fields [1-4]. The