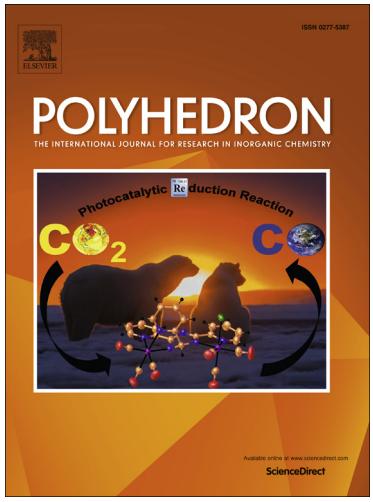
Accepted Manuscript



Nitrite-bonded nickel(II) complex of *N*-cyclohexyl-N-(2-pyridinylmethyl)amine; Synthesis, spectroscopic characterization, X-ray structure and DFT calculations

Hamid Golchoubian, Shahnaz Khosravi Kocheksaraee, Golasa Moayyedi

PII: S0277-5387(16)30665-9
DOI: http://dx.doi.org/10.1016/j.poly.2016.12.014
Reference: POLY 12372

To appear in: *Polyhedron*

Received Date: 2 November 2016
Revised Date: 7 December 2016
Accepted Date: 10 December 2016

Please cite this article as: H. Golchoubian, S.K. Kocheksaraee, G. Moayyedi, Nitrite-bonded nickel(II) complex of *N*-cyclohexyl-N-(2-pyridinylmethyl)amine; Synthesis, spectroscopic characterization, X-ray structure and DFT calculations, *Polyhedron* (2016), doi: http://dx.doi.org/10.1016/j.poly.2016.12.014

Nitrite-bonded nickel(II) complex of *N*-cyclohexyl-N-(2-pyridinylmethyl)amine; Synthesis, spectroscopic characterization, X-ray structure and DFT calculations

Hamid Golchoubian*, Shahnaz Khosravi Kocheksaraee, Golasa Moayyedi*

Department of chemistry, University of Mazandaran, Babolsar, Iran, Postal Code 47416-95447

Reprint requests to Dr. G. Moayyedi Tel/Fax: (98)-1135302385, E-mail: g.moayyedi@gmail.com (G. Moayyedi); h.golchobian@umz.ac.ir (H. Golchoubian)

Abstract

A combined experimental and computational investigation on a nickel(II) complex of *N*-cyclohexyl-*N*-(2-pyridinylmethyl)amine, L, was carried out. The compound $[NiL_2(ONO)]NO_2 \cdot ½CH_3CN$) has been prepared by addition of L to a suspension of $K_4[Ni(NO_2)_6] \cdot H_2O$ in methanol and structurally characterized by a combination of analytical, spectroscopic, and crystallographic methods. The nickel(II) center in the complex is surrounded by the two amine nitrogen and two oxygen atoms of nitrite ion (η^2-ONO) in the basal plane and two nitrogen atoms of pyridine moieties in the apical positions, forming distorted octahedral geometries. The relative stability of geometrical isomers (*cis* and *trans*) and linkage isomers (η^1-NO_2, η^2-ONO and η^1-ONO) of the complex were investigated by the density functional theory (DFT) calculation. In support with X-ray structure, the calculated results verified that in all cases the *cis*-bidentate η^2-ONO isomer is more stable than other four-coordinated nitro isomers. A further theoretical analysis of electronic structure of the complex has also been carried out to achieve a deeper insight into the properties of the relevant molecular orbitals.

Keywords: Nickel(II); DFT study; Linkage isomer; nitrite ion; X-ray structure; ancillary ligand