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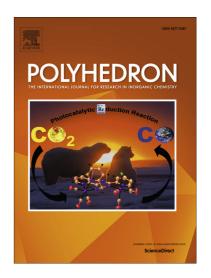
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ACCEPTED MANUSCRIPT

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

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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 $[NiL_2(ONO)]NO_2\cdot l_2CH_3CN)$ 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 -NO₂, 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

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