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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 [NiL₂(ONO)]NO₂·½CH₃CN has been prepared by addition of L to a suspension of K₄[Ni(NO₂)₆]·H₂O 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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