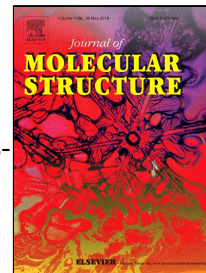


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Synthesis, characterization, single crystal structure and theoretical studies of *trans*-Ni(II)-complex with dithiophosphonate ligand

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Abstract

A novel metal-organic planar NiS₄ - type complex, *trans*- Ni(II)-bis[O-(2-butoxyethyl)-(4-methoxyphenyl)dithiophosphonate], was synthesized by the reaction of ammonium salt of *O*-dithiophosphonic acid with Ni(CH₃COO)₂. The crystal structure of Ni(II)-complex was determined by X-ray Diffraction (XRD) analysis. As a result of the X-ray crystal and molecule structure analyses of the studied *trans*- Ni(II)-complex, it was obtained that the central nickel atom is coordinated by four sulphur atoms in slightly distorted a square- planar geometry. The X-ray structure confirms a *trans* isomer of the Ni(II)-complex. The Ni(II)-complex crystallizes in the monoclinic space group C12/c1 with unit cell parameters a 22.376(3) (Å), b 18.466(3) (Å) and c 8.6875(13) (Å). In addition, theoretical calculations with the basis set of B3LYP/6-311+G(2d,p) are performed to determine the structural properties, FT-IR, NMR spectrum, electronic properties and NBO analysis of the compound. The experimental and computed results of the Ni(II)-complex were found to be in good agreement.

Keywords

Dithiophosphonates, Ni(II) complexes, X-ray, DFT

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