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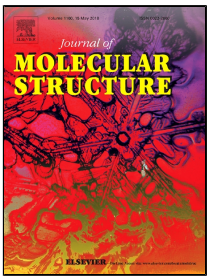

Synthesis, characterization, single crystal structure and theoretical studies of trans-Ni(II)-complex with dithiophosphonate ligand

Mehmet Karakus, Izzet Kara, Ömer Çelik, Ilghar Orujalipoor, Semra İde, Hamza Yilmaz

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

Mehmet Karakus[a,*], Izzet Kara[b], Ömer Çelik[c], Ilghar Orujalipoor[d], Semra İde[d,e], Hamza Yilmaz[f]

[a]*Department of Chemistry, Faculty of Science&Literature, Pamukkale University, 20070, Denzili, Turkey*

[b]*Department of Science Education, Pamukkale University, Faculty of Education, 20070, Denizli, Turkey*

[c]*Department of Physics, Faculty of Education, Dicle University, 21280, Sur-Diyarbakır, Turkey*

[d]*Hacettepe University, Institude of Science, Department of Nanotechnology and Nanomedicine, Beytepe 06532, Ankara, Turkey*

[e]*Hacettepe University, Department of Physics Eng., Beytepe 06532, Ankara, Turkey*

[f]*Department of Chemistry, Faculty of Science, Ankara University, 06100, Ankara, Turkey*

Abstract

A novel metal-organic planar NiS_4 - type complex, *trans*- Ni(II)-bis[O-(2-butoxyethyl)-(4-methoxyphenyl)dithiophosphonate], was synthesized by the reaction of of ammonium salt of *O-dithio*phosphonic acid with $Ni(CH_3COO)_2$. 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