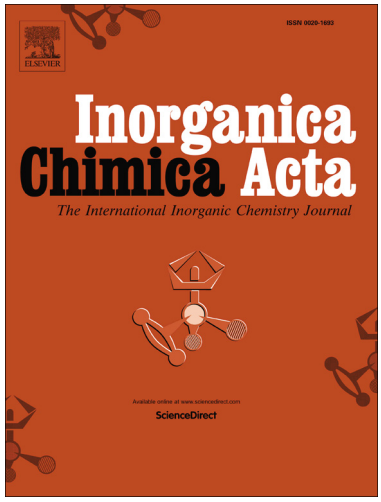

Research paper

Synthesis, Spectroscopic Properties and DFT Studies of Copper(II) Complex of (E)-1-((2,4-dichlorophenylimino)methyl)naphthalen-2-ol

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PII: S0020-1693(18)30575-9
DOI: https://doi.org/10.1016/j.ica.2018.09.052
Reference: ICA 18510

To appear in: *Inorganica Chimica Acta*

Received Date: 16 April 2018
Revised Date: 25 August 2018
Accepted Date: 20 September 2018

Please cite this article as: G. Alpaslan, M. Macit, N. Özdemir, H. Gökce, Synthesis, Spectroscopic Properties and DFT Studies of Copper(II) Complex of (E)-1-((2,4-dichlorophenylimino)methyl)naphthalen-2-ol, *Inorganica Chimica Acta* (2018), doi: https://doi.org/10.1016/j.ica.2018.09.052

Synthesis, Spectroscopic Properties and DFT Studies of Copper(II) Complex of (E)-1-((2,4-dichlorophenylimino)methyl)naphthalen-2-ol

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Abstract: The copper(II) complex of Schiff base ligand was synthesized from the reaction of 2-hydroxy-1-naphthaldehyde with 2,4-dichlorobenzenamine. The complex was characterized by FT-IR and UV-Vis. spectroscopies and single-crystal X-Ray diffraction technique. The molecular geometric structure analysis, vibrational frequencies, electronic absorption spectroscopy and frontier molecular orbital energies of the Cu(II) complex were calculated by using density functional theory calculations with the B3LYP/6-311++G(d,p)//LanL2DZ level in the ground state. The vibrational analysis was performed to investigate metal-ligand and intra-ligand vibrations. The frontier molecular orbital (HOMOs and LUMOs) analyses were studied to determine charge transfers and electronic transitions in the complex. The electronic configuration, natural charge and coordination environment of the Cu(II) center metal ion were supported with natural bond analysis. The obtained calculation values were compared with experimental values.

Keywords: Schiff base Cu(II) complex · X-Ray diffraction · FT-IR spectroscopy · DFT computations · UV-Vis. spectroscopy · NBO analysis

1. Introduction

Schiff base ligands derived from *o*-hydroxy groups have drawn considerable attention because of their tautormerism and chemical properties, as well as antitubercular, anticancer, antioxidant and anticonvulsant activities [1-3]. They can be used depending on the tautomerism and non-bonding electron pair on the ligand atoms, for design of various

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