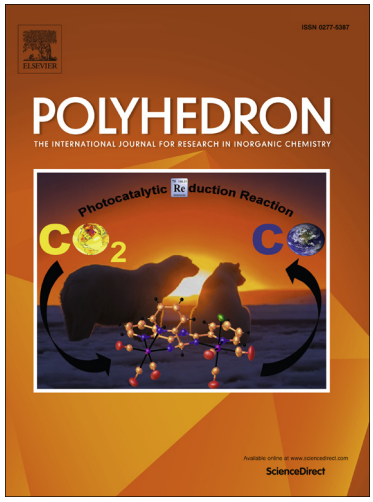

Synthesis and spectroscopic properties of a copper(II) binuclear complex of a novel tetradentate asymmetrical Schiff base ligand and its DFT study

Iman Rajaei, Seyed Nezamoddin Mirsattari

PII: S0277-5387(15)00600-2
DOI: http://dx.doi.org/10.1016/j.poly.2015.10.019
Reference: POLY 11604

To appear in: *Polyhedron*

Received Date: 2 June 2015
Accepted Date: 6 October 2015

Please cite this article as: I. Rajaei, S.N. Mirsattari, Synthesis and spectroscopic properties of a copper(II) binuclear complex of a novel tetradentate asymmetrical Schiff base ligand and its DFT study, *Polyhedron* (2015), doi: http://dx.doi.org/10.1016/j.poly.2015.10.019

Synthesis and spectroscopic properties of a copper(II) binuclear complex of a novel tetradentate asymmetrical Schiff base ligand and its DFT study

Iman Rajaei[a], Seyed Nezamoddin Mirsattari[a,b*]

[a]Department of Chemistry, Shahreza Branch, Islamic Azad University, P.O Box 311-86145, Shahreza, Isfahan, Iran

[b]Razi Chemistry Research Center (RCRC), Shahreza Branch, Islamic Azad University, Isfahan, Iran

Abstract

A new asymmetrical Schiff base ligand, N,N'-(salicylidene)-5-bromo-2-hydroxybenzaldehyde-*p*-phenylenediamine (SBHBP), and its binuclear Cu(II) complex have been synthesized. The molecular structures and spectroscopic properties of the ligand and its complex were experimentally characterized by elemental analysis, FT-IR, NMR and UV–Vis spectroscopic techniques and computationally by the density functional theory (DFT) method. The molecular geometry and vibrational frequencies of the SBHBP ligand in the ground state have been calculated using the B3LYP/6-31G(d,p) and 6-31++G(d,p) basis sets. A potential surface scan study was carried out and the most stable geometry of the SBHBP ligand was confirmed. The calculated results show that the optimized geometry can well reproduce the structural parameters, and the theoretical vibrational frequencies are in good agreement with the experimental values. On calculation of the electronic absorption spectra, TD-DFT calculations were carried out in both the gas and solution phases. The energetic behavior of the SBHBP ligand has been examined in solvent media using the B3LYP method with the 6-31G(d,p) and 6-31++G(d,p) basis sets by applying the Onsager method and polarizable continuum model (PCM). Additionally, Mulliken and NBO atomic charges, NMR analysis, molecular electrostatic potential (MEP) and frontier molecular orbitals (FMO) analysis of the SBHBP ligand were investigated using theoretical calculations.

Keywords: Asymmetric; Schiff base; Binuclear complex; DFT; MEP; Tautomer

1. Introduction