

Accepted Manuscript

Research paper

Syntheses of Four New Asymmetric Schiff Bases and Their Cu(II) Complexes: Theoretical Calculations to Rationalize the Packing of Molecules in the Crystals

Prithwish Mahapatra, Antonio Bauzá, Antonio Frontera, Michael G.B. Drew, Ashutosh Ghosh

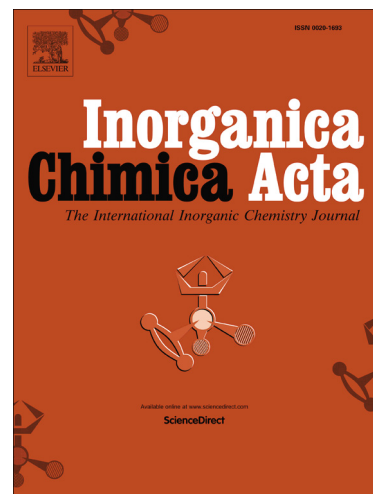
PII: S0020-1693(17)31794-2
DOI: <https://doi.org/10.1016/j.ica.2018.01.035>
Reference: ICA 18109

To appear in: *Inorganica Chimica Acta*

Received Date: 21 November 2017
Revised Date: 30 January 2018
Accepted Date: 31 January 2018

Please cite this article as: P. Mahapatra, A. Bauzá, A. Frontera, M.G.B. Drew, A. Ghosh, Syntheses of Four New Asymmetric Schiff Bases and Their Cu(II) Complexes: Theoretical Calculations to Rationalize the Packing of Molecules in the Crystals, *Inorganica Chimica Acta* (2018), doi: <https://doi.org/10.1016/j.ica.2018.01.035>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



Syntheses of Four New Asymmetric Schiff Bases and Their Cu(II) Complexes: Theoretical Calculations to Rationalize the Packing of Molecules in the Crystals

Prithwish Mahapatra^a, Antonio Bauzá^b, Antonio Frontera^{*b}, Michael G. B. Drew^c, Ashutosh Ghosh^{*a}

^aDepartment of Chemistry, University College of Science, University of Calcutta, 92, A. P. C. Road, Kolkata 700009, India, E-mail: ghosh_59@yahoo.com

^bDepartment of Chemistry, Universitat de les Illes Balears, Crta de Valldemossa km7.5, 07122 Palma de Mallorca, Balears, Spain. E-mail: toni.frontera@uib.es

^cSchool of Chemistry, The University of Reading, P.O. Box 224, Whiteknights, Reading RG6 6AD, UK.

Abstract

Four new asymmetric Schiff bases, *N*- α -methylsalicylidene-*N'*-2-hydroxynaphthylidene-1,3-propanediamine (H₂L₁), *N*- α -methylsalicylidene-*N'*-5-bromosalicylidene-1,3-propanediamine (H₂L₂), *N*- α -methylsalicylidene-*N'*-3-methoxysalicylidene-1,3-propanediamine (H₂L₃) and *N*-(3-methoxysalicylidene)-*N'*-(2-hydroxynaphthylidene)-1,3-propanediamine (H₂L₄) and their Cu(II) complexes [CuL₁] (**1**), [CuL₂] (**2**), [CuL₃] (**3**) and [CuL₄] (**4**) have been synthesized. All the complexes (**1–4**) have been structurally characterized by single crystal XRD. The Cu-atom is four coordinated square planar in complexes **1–3** but in **4** a water molecule coordinates to one of its axial positions making it penta-coordinated with square pyramidal geometry. The mononuclear complex molecules of **1** and **2** form infinite 1D columns that are arranged parallel forming 2D sheets where as in **3** they form self-assembled dimers that are inter-connected by weak van der Waals interactions and in **4** the molecules are packed in the form of infinite 1D ladders. The structure of a recently reported complex with a similar asymmetric ligand (H₂L₅) *N*- α -methylsalicylidene-*N'*-salicylidene-1,3-propanediamine where the phenoxido oxygen coordinates mutually to the axial position of another molecule to form a dimer is compared to the present complexes. The packing of the molecules in all the crystals are rationalized by theoretical molecular electrostatic potential surface (MEPS) calculations. DFT calculations show the significant role of CH \cdots π (chelate ring) and $\pi\cdots\pi$ (chelate ring) interactions governing the crystal

Download English Version:

<https://daneshyari.com/en/article/7750506>

Download Persian Version:

<https://daneshyari.com/article/7750506>

[Daneshyari.com](https://daneshyari.com)