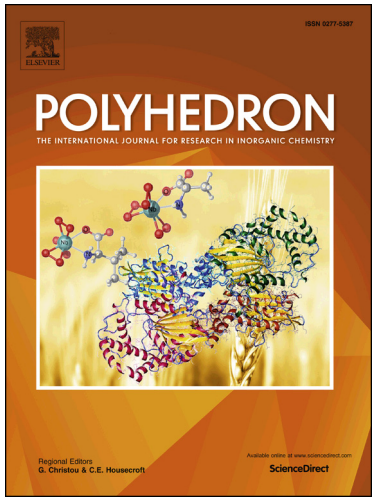

Theoretical investigation on the reactivity and photophysical properties of cobalt(II) and manganese(II) complexes constructed using Schiff base ligands based on ALIE and TDDFT calculations

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PII: S0277-5387(17)30247-4
DOI: http://dx.doi.org/10.1016/j.poly.2017.03.049
Reference: POLY 12564

To appear in: *Polyhedron*

Received Date: 5 January 2017
Revised Date: 16 March 2017
Accepted Date: 19 March 2017

Please cite this article as: K.S. Prasad, R.R. Pillai, S. Armaković, S.J. Armaković, Theoretical investigation on the reactivity and photophysical properties of cobalt(II) and manganese(II) complexes constructed using Schiff base ligands based on ALIE and TDDFT calculations, *Polyhedron* (2017), doi: http://dx.doi.org/10.1016/j.poly.2017.03.049

Theoretical investigation on the reactivity and photophysical properties of cobalt(II) and manganese(II) complexes constructed using Schiff base ligands based on ALIE and TDDFT calculations

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Abstract

Herein, we describe the synthesis of two novel Schiff base ligands, 2-[(3-bromo-5-hydroxybenzylidene)-amino]-6-methylpyrimidin-4-ol (**1**) and 3-bromo-5-[(5-methylthiazol-2-ylimino)methyl]phenol (**2**), and their Co(II) and Mn(II) complexes (**4-6**). The molecular structures of the obtained compounds were confirmed using physical and analytical characterization techniques. The global stability properties of the ligands and their coordination complexes have been assessed by analyzing their frontier molecular orbitals, while their reactivity properties have been assessed by calculating average local ionization energies (ALIE). In addition, TDDFT calculations have been performed in order to theoretically obtain the UV-Visible spectra of the title compounds.

Keywords: Schiff base, Metal complexes, Analytical techniques, ALIE, TDDFT calculations.