

Accepted Manuscript

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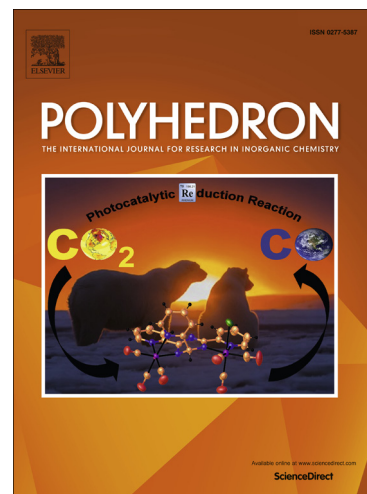
PII: S0277-5387(16)30623-4
DOI: <http://dx.doi.org/10.1016/j.poly.2016.11.032>
Reference: POLY 12340

To appear in: *Polyhedron*

Received Date: 1 September 2016
Revised Date: 15 November 2016
Accepted Date: 22 November 2016

Please cite this article as: L-Q. Chai, L-J. Tang, L-C. Chen, J-J. Huang, Structural, spectral, electrochemical and DFT studies of two mononuclear Manganese(II) and Zinc(II) complexes, *Polyhedron* (2016), doi: <http://dx.doi.org/10.1016/j.poly.2016.11.032>

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Structural, spectral, electrochemical and DFT studies of two mononuclear Manganese(II) and Zinc(II) complexes

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ABSTRACT

Two mononuclear M(II) complexes, $[M(L_2)_2] \cdot CH_3OH$ ($M = Mn(\mathbf{1})$ and $Zn(\mathbf{2})$, $HL_2 = 1-(2-\{[(E)-3,5-dibromo-2-hydroxybenzylidene]amino\}phenyl)ethanone$ oxime), were synthesized *via* complexation of corresponding M(II) acetate with HL_1 (2-(3,5-dibromo-2-hydroxyphenyl)-4-methyl-1,2-dihydroquinazoline-3-oxide, H is the deprotonatable hydrogen) originally. During the reaction, the C–N bond in the ligand HL_1 is converted into the C=N–OH group in the HL_2 . The spectral data of both complexes were compared with the ligand HL_1 . Both complexes were determined by single crystal X-ray diffraction and display similar coordination geometry and have a 2:1 ligand-to-metal ratio. In the crystal structure, complexes $\mathbf{1}$ and $\mathbf{2}$ form an infinite 1-D chain and $\mathbf{2}$ into 3-D supramolecular frameworks. The electrochemical property of complex $\mathbf{1}$ was investigated by cyclic voltammetry. The electronic transitions and spectral features of HL_1 and both complexes were discussed by DFT and TD-DFT calculations. Time dependent DFT calculations have been carried out on the optimised geometry to further understand the electronic transitions in the UV–Vis spectra of the compounds. In addition, the highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO), and HOMO-LUMO gap were also calculated.

Keywords: Metal complexes; Crystal structures; DFT calculations; Spectral study; Cyclic voltammetry

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