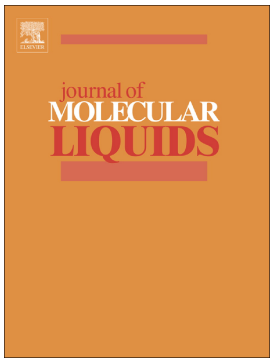

Ligational, DFT, optical band gap and biological studies on Mn(II), Co(II) and Ni(II) complexes of ethyl and allyl thiosemicarbazides ending by thiazole group

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Ligational, DFT, optical band gap and biological studies on Mn(II), Co(II) and Ni(II) complexes of ethyl and allyl thiosemicarbazides ending by thiazole group.

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Abstract.

The Mn(II), Co(II), Ni(II) and Cu(II) complexes with two ligands derived from the addition of 2-(2-aminothiazol-5-yl) actahydrazide to ethyl (H_2TAET) and allyl (H_2TAAT) isothiocynates have been prepared and characterized by way of traditional strategies. The isolated complexes assigned the formulae, $[Mn(HTAET)_2(H_2O)_2](2.5H_2O)$, $[Co(HTAET)(H_2O)_3Cl](2H_2O)$, $[Ni(HTAET)(H_2O)_2Cl](4H_2O)$, $[Mn(HTAAT)Cl](2.5H_2O)$, $[Co(HTAAT)(H_2O)Cl](2H_2O)$ and $[Ni(HTAAT)(H_2O)Cl]$. IR data found out that the both ligands behave as monovalent bidentate via $(C=N)_{th}$ and deprotonated enolized (C-O) group in Mn(II) and Co(II) complexes of (H_2TAET) and in all complexes of (H_2TAAT) except Mn(II) complex. Mn(II) of (H_2TAAT) and Ni(II) of (H_2TAET) complexes act as monobasic tridentate (NNO) and subsequently (H_2TAET) act as (NNS) tridentate in Cu(II) complex. The data of UV-vis spectra and the magnetic measurements recommended that the octahedral geometry for all complexes of (H_2TAET) at the same time as tetrahedral geometry for all complexes of (H_2TAAT) except Ni(II) that is square planar was suggested. The bond lengths, bond angles, HOMO, LUMO and dipole second values have been calculated by way of DFT the use of materials studio program to verify the recommended geometries of ligands and their metal complexes. Additionally, the kinetic and thermodynamic parameters for the different thermal degradation steps of the complexes have been decided by way of Coats-Redfern and Horowitz- Metzger techniques. The optical band gap (Eg) of the metal complexes has been calculated. The optical band gap (Eg) measurements confirmed allowed direct electronic transitions for the photon absorption inside the investigated complexes. Moreover, the antimicrobial, antioxidant and antitumor of ligands and their complexes have been evaluated.

Keywords: Thiosemicarbazides, spectral characterization, thermal degradation, optical band gap, antioxidant, antitumor activity.

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1. Introduction.

Heterocyclic thiosemicarbazides and their capability to form chelates with transition metal ions were concern of interest due to their chemical, biological and antitumor activities in addition to utility in drug improvement for the treatment of inflammation [1-5]. As regards biological implications, thiosemicarbazide complexes have anticancer activity because of their ability to