

Accepted Manuscript

Synthesis, spectral characterization, molecular modeling, biological activity and potentiometric studies of 4-amino-5-mercapto-3-methyl-*S*-triazole Schiff's base complexes

Abdel-Nasser M.A. Alaghaz, Mohamed E. Zayed, Suliman A. Alharbi

PII: S0022-2860(14)01103-X

DOI: <http://dx.doi.org/10.1016/j.molstruc.2014.10.076>

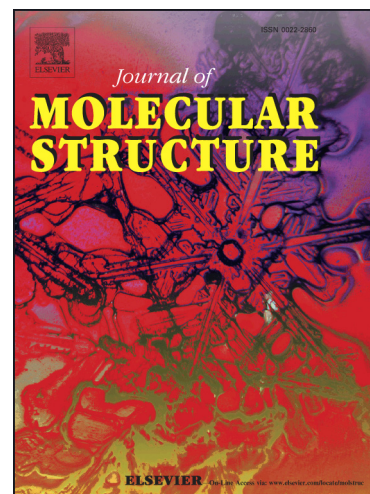
Reference: MOLSTR 21075

To appear in: *Journal of Molecular Structure*

Received Date: 2 October 2014

Revised Date: 30 October 2014

Accepted Date: 30 October 2014



Please cite this article as: A.M.A. Alaghaz, M.E. Zayed, S.A. Alharbi, Synthesis, spectral characterization, molecular modeling, biological activity and potentiometric studies of 4-amino-5-mercapto-3-methyl-*S*-triazole Schiff's base complexes, *Journal of Molecular Structure* (2014), doi: <http://dx.doi.org/10.1016/j.molstruc.2014.10.076>

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.

Revised manuscript**Synthesis, spectral characterization, molecular modeling,
biological activity and potentiometric studies of 4-amino-5-
mercapto-3-methyl-S-triazole Schiff's base complexes****Abdel-Nasser M. A. Alaghaz^{a,b} Mohamed E. Zayed^c and Suliman A.
Alharbi^c**^aChemistry Department, Faculty of Science, Al-Azhar University, Nasr City, Cairo, Egypt. (aalajhaz@hotmail.com & aalajhaz@yahoo.com)^bChemistry Department, Faculty of science, Jazan University, Jazan, Saudi Arabia.^cDepartment of Botany and Microbiology, Faculty of Science, King Saud University, Riyadh 11541, Saudi Arabia.**Abstract**

The Schiff's base derived from condensation of *s*-triazole (4-amino-5-mercapto-3-methyl-S-triazole) with pyridine-2-aldehyde and their corresponding Mn(II), Co(II), Ni(II), Cu(II) and Zn(II) complexes have been synthesized. The isolated solid complexes were characterized by elemental analyses, molar conductance, spectral (IR, UV–Vis, ¹H NMR, mass), magnetic moment and thermal measurements. The IR spectral data suggest that the ligand coordinate in a tridentate manner (SNN) via the one thiol (SH), one pyridine ring and the azomethine (C=N) groups. The data show that the complexes have composition of ML₂ type. The activation of thermodynamic parameters are calculated using Coast-Redfern, Horowitz–Metzger (HM), and Piloyan–Novikova (PN). The octahedral geometry of the complexes is confirmed using DFT method from DMOL3 calculations and ligand field parameters. Protonation constants of Schiff base and stability

Download English Version:

<https://daneshyari.com/en/article/7809835>

Download Persian Version:

<https://daneshyari.com/article/7809835>

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