Synthesis and Characterization of Ni(II), Cu(II), Zn(II) and Azo Dye Based on 1,10-*o*-Phenanthroline Binary Complexes: Corrosion Inhibition Properties and Computational Studies

Hamed M. Al-Saidi¹, Gamal A. Gouda², Mohamed Abdel-Hakim^{2,*}, Nawaf I. Alsenani³, Anas Alfarsi³, Mahmoud H. Mahross², O. A. Farghaly³, Shima Hosny⁴

¹Department of Chemistry, University College in Al-Jamoum, Umm Al-Qura University, 21955, Makkah, KSA.

²Department of Chemistry, Faculty of Science, Al-Azhar University, Assiut Branch, 71524, Assiut, Egypt.

³Department of Chemistry, Faculty of Science, Al-Baha University, Al-Baha, Saudi Arabia.

⁴Department of Chemistry, Faculty of Science, New Valley University, El-Kharja 72511, Egypt.

*E-mail: m.hakim121@azhar.edu.eg

Received: 6 December 2021/ Accepted: 9 January 2022 / Published: 2 February 2022

Azo dye ligand of *p*[(*p*-aminosulphonylbenzene)]-azo-5-(1,10)-*o*-phenanthroline L, based on 1,10-*o*-phenanthroline and *p*-aminosulphonylbenzene with Ni(II), Cu(II) and Zn(II) ion complexes have been prepared and investigated. A potentiometric method was used to determine their stability constants by redox titration in 0.1 M HCl at room temperature. The resulting metal-L species showed the forming molar ratios 1:1 and 1:2. The electrical conductivity values of synthesized metal complexes indicated the semiconducting nature with an activation energy in the range 0.131–0.188 eV. The thermal stability of the [ZnLCl₂] is higher than [CuLCl₂] and [NiLCl₂] complexes. The prepared compounds were tested as mild steel corrosion inhibitors in 1.0 M H₂SO₄ solution using electrochemical analysis (Potentiodynamic polarization technique) and theoretical quantum calculation was studied. The decrease of corrosion current densities and corrosion potential values extracted from Potentiodynamic polarization indicated that all used inhibitors act as a mixed-type inhibitor (decrease each anodic and cathodic Tafel slopes). The inhibition efficiency increases for the tested compounds as [NiLCl₂] > [ZnLCl₂] > [CuLCl₂] > L to reach maximum value 92.3 % for [NiLCl₂]. The changing in electrochemical descriptors obtained by verifying inhibitors concentration 100, 200 and 400 ppm, improves its adsorption over the surface of mild steel. Inhibition was attributed to the adsorption of the prepared compounds on the surface of the mild steel. The descriptors of adsorption isotherm of the inhibitors were obeyed Langmuir adsorption isotherm. Morphology examination of the surface of mild steel electrodes was tested by scanning electronic microscopy in the presence and without inhibitors. Theoretical investigations were applied to the ligand tested and metal complexes in this study by using Gaussian 09 software program involved optimization by DFT method by DFT/B3LYP/LANL2DZ level. Descriptors calculation such as (E_{HOMO}, E_{LUMO} and energy gap, molecular electrostatic potential shape and counter plots) were obtained by quantum calculation that approve link between experimental and theoretical studied. The complexes were relatively active against pathogenic bacteria such as Gram positive and Gram negative.

Keywords: Azo dye metal complexes; corrosion; DFT calculations; antimicrobial ability.

[FULL TEXT](#)

© 2022 The Authors. Published by ESG (www.electrochemsci.org). This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution license (<http://creativecommons.org/licenses/by/4.0/>).