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Syntheses, characterization, and anticorrosion studies of new oxadiazole–Schiff base metal complexes

Fayez Owaid Neamah[1,2], Israa Ali Abbas[3], Hanan Abbas Dahd[1], Jassim Hameed Al-Waeli[1] and Safaa Hussein Ali[4]

[1]Department of Chemistry, General Directorate of Education of Thi-Qar, Al-Nasyrih, Iraq
[2]Department of Biochemistry, College of Science, Al-Ayen Iraqi University, Al-Nasyrih, Iraq
[3]Department of Chemistry, College of Science, University of Thi-Qar, Al-Nasyrih, Iraq
[4]Department of Physics, College of Education, University of Shatrah, Al-Shatrah, Thi-Qar, Iraq

ABSTRACT A new oxadiazole derivative, namely, 2-phenyl-5-(2-((1*E*,2*E*)-3-phenylallylidene)hydrazineyl)-1,3,4-oxadiazole, was synthesized and coordinated with some transition metal ions (CrIII, CoII, NiII, and CuII). These complexes were characterized by a set of spectroscopic techniques such as proton nuclear magnetic resonance, Fourier-transform infrared spectroscopy, and mass spectra. The optimized geometric structures and the molecular orbitals (highest occupied molecular orbital and lowest unoccupied molecular orbital) were computed using density functional theory at B3LYP/6-31G+(d,p) level by the Gaussian program. The magnetic susceptibility results were in agreement with the theoretical optimization. These experimental and computational simulations suggested octahedral geometries for Cr(III) and tetrahedral geometry for Co(II) and square planar geometry for Ni(II) and Cu(II). Computational simulations showed that the oxadiazole–Schiff base was a promising corrosion inhibitor.

KEYWORDS Density functional theory studies, Heterocyclic, Metal complex, Oxadiazole, Schiff base.

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