International Journal of Chemical Sciences

Exploring the Potential of a New 1,2,4-Triazole Derivative for Corrosion Protection of Carbon Steel in HCl: A Computational and Experimental Evaluation

Manal Naciri[1], Yasmina El Aoufir[2], Hassane Lgaz[3], Fatima Lazrak[4,5], Ahmed Ghanimi[1], Abdallah Guenbour[1], ismat H. Ali[6], Mouloud El Moudane[1], Jamal Taoufik[4], Ill-Min Chung[3]

[1]Materials, Nanotechnology and Environment Laboratory, Faculty of Sciences, Mohammed V University in Rabat, Morocco.
[2]Laboratoire des Matériaux avancés et de Génie des Procédés, Ecole supérieure d'éducation et de la formation, Ibn Tofail University, PB 133-14050, Kenitra, Morocco.
[3]Department of Crop Science, College of Sanghur Life Science, Konkuk University, Seoul 05029, South Korea
[4]Medicinal Chemistry Laboratory, Faculty of Medicine and Pharmacy, Rabat, Morocco.
[5]Laboratory of Heterocyclic Organic Chemistry, Faculty of Science, Rabat, Morocco.
[6]Department of Chemistry, College of Science, King Khalid University, P. O. Box 9004, Postal Code 61413, Abha, Kingdom of Saudi Arabia

Abstract

Carbon steel is a commonly used alloy in petroleum refining equipment. Nonetheless, its weak corrosion resistance is a perpetual problem for these industries. In the present study, we manifest the usefulness of a novel 1,2,4-triazole derivative, namely 5-hexylsulfanyl1,2,4-triazole (HST) in inhibiting the carbon steel (CS) corrosion in 1.0 M HCl using mass loss measurements, electrochemical, scanning electron microscopy coupled with X-ray detection (SEM-EDX), X-Ray diffraction (XRD) and computational techniques. We deduced from the gravimetric study that the optimal concentration of HST is 10-3 M. Its inhibition efficiency can reach 97% based on electrochemical data. Electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization (PDP) results suggest an increased impedance in the presence of HST and mixed nature of inhibitor action, respectively. The compound HST mitigates corrosion at the temperature range of 298K-338K, with an inhibition efficiency of 89% at 338K. Free Gibbs energy obtained from the Langmuir isotherm model suggests that the inhibitor molecules hinder the acid attack mainly by chemisorption. A computational study based on Density Functional Theory (DFT) and Molecular Dynamics (MD) simulations was performed in an attempt to identify the factors most associated with anti-corrosive properties of the tested compound. Keywords: Corrosion inhibition; Mild steel; 1,2,4-triazole; Molecular dynamics; DFT; SEM/EDX.

Biography

He is currently a professor at Mohammed V University in Rabat, Morocco.

International Conference on Smart Materials and Nanotechnology | July 23-24, 2020

Abstract Citation: Ahmed Ghanimi, Exploring the Potential of a New 1,2,4-Triazole Derivative for Corrosion Protection of Carbon Steel in HCl: A Computational and Experimental Evaluation, Smart Materials Congress 2020, 2nd International Conference on Smart Materials and Nanotechnology, July 23, 2020| Webinar, Page 9