Experimental and DFT Investigation on the Corrosion Inhibition of Mild Steel by 1, 2, 3- triazole Regioisomers in 1M hydrochloric Acid Solution

H. Rahmani^{1,2}, K. Ismaily Alaoui¹, K.M. Emran^{3,*}, A. El Hallaoui², M. Taleb¹, S. El Hajji², B. Labriti², E. Ech-chihbi^{1,4}, B. Hammouti⁵, F. El-Hajjaji¹.

¹ Laboratory of Engineering, Electrochemistry, Modeling and Environment (LIEME), Faculty of Sciences, University Sidi Mohamed Ben Abdellah, Fez, Morocco

² Laboratory of organical Chemistry (LOC), Faculty of sciences, University Sidi Mohamed Ben Abdellah, Fez, Morocco

³ Department of Chemistry, College of Science, Taibah University, Al-Madinah Al-Monawarah, PO Box4050, Saudi Arabia.

⁴ Laboratory of separation processes, Faculty of Science, University Ibn Tofail, Kenitra, Morocco

⁵ Laboratory of Applied Analytical Chemistry Materials and Environment (LCAAE), Faculty of sciences, University of Mohammed Premier, Oujda, Morocco

*E-mail: kabdalsamad@taibahu.edu.sa, el.hajjajifadoua25@gmail.com

doi: 10.20964/2019.01.80

Received: 24 August 2018 / Accepted: 10 October 2018 / Published: 30 November 2018

The inhibition effect of new isomers of the triazole derivative family, namely 1-[(4-ethyl-2-phenyl-4,5-dihydro-1,3-oxazol-4-yl)methyl]-4-phenyl-1H-1,2,3-triazole (Ph4) and 1-[(4-ethyl-2-phenyl-4,5-dihydro-1,3-oxazol-4-yl)methyl]-5-phenyl-1H-1,2,3-triazole (Ph5), on mild steel corrosion in 1 M HCl was synthesized and evaluated using weight loss, electrochemical polarization, and impedance spectroscopy. The Ph4 compound was the best rust inhibitor and its inhibitory efficiency increased with increasing concentration, reaching 95% at 10^{-3} M. The polarization curves indicated that Ph4 and Ph5 are mixed-type inhibitors. EIS diagram appears a single capacitive loop, where diameter increases gradually as the inhibitors concentration. The change in the substitution phenyl from position 5 (Ph5) to position 4 (Ph4) in the triazole ring increased the inhibitory effect of the triazole compounds. The effect of temperature on the corrosion behavior of mild steel indicated that the inhibitory efficiency of both inhibitors decreased with increasing temperature in the range 308-338K. The DFT study correlated well with the experimental results.

Keywords: oxazole-triazole; corrosion inhibition; mild steel; electrochemical impedance spectroscopy (EIS); density functional theory (DFT)

[FULL TEXT](#)

© 2019 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/>).