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PII: S0167-7322(17)30997-2
Reference: MOLLIQ 7280
To appear in: Journal of Molecular Liquids
Received date: 6 March 2017
Revised date: 16 April 2017
Accepted date: 26 April 2017

Please cite this article as: Hassane Lgaz, K. Subrahmanya Bhat, Rachid Salghi, Shubhalaxmi, Shehdeh Jodeh, Manuel Algarra, Belkheir Hammouti, Ismat Hassan Ali, Azzouz Essamri, Insights into corrosion inhibition behavior of three chalcone derivatives for mild steel in hydrochloric acid solution. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Molliq(2017), doi: 10.1016/j.molliq.2017.04.124

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Insights into corrosion inhibition behavior of three chalcone derivatives for mild steel in hydrochloric acid solution

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ABSTRACT

The effect of three chalcone derivatives namely, (E)-ethyl 2-(4-(3-(4-fluorophenyl)acryloyl)phenoxy)acetate (AE-1), (E)-ethyl 2-(4-(3-(4,3,4-dichlorophenyl)acryloyl)phenoxy)acetate (AE-2) and (E)-ethyl 2-(4-(3-(2,5-dimethoxyphenyl)acryloyl)phenoxy)acetate (AE-3) on the mild steel (MS) corrosion in 1.0 M HCl at 303 K has been investigated using experimental techniques such as electrochemical impedance spectroscopy (EIS), potentiodynamic polarization (PDP) methods, weight loss measurements and computational studies. The chalcones derivatives show high inhibition activities and their adsorption on mild steel surface was found to follow the Langmuir adsorption model. PDP results revealed that chalcone derivatives act as a mixed type inhibitors. The results from EIS analysis reveal an increase in charge transfer resistance confirming the inhibitive ability of tested inhibitors. The electronic properties derived from, DFT calculations, molecular dynamic (MD) simulations and Radial Distribution Function (RDF) were used to give further insights into the action mode of studied chalcones.
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