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

Hassane Lgaz^{a, b}, K Subrahmanya Bhat^c, Rachid Salghi^{b,*}, Shubhalaxmi^c, Shehdeh Jodeh^d, Manuel Algarra^e, Belkheir Hammouti^f, Ismat Hassan Ali^g, Azzouz Essamri^h

^a Laboratory separation processes, Faculty of Science, University Ibn Tofail PO Box 242, Kenitra, Morocco.

^b Laboratory of Applied Chemistry and Environment, ENSA, University Ibn Zohr, PO Box 1136, Agadir, Morocco.

^c Department of Chemistry, Manipal Institute of Technology, Manipal University, Manipal-576 104, India.

^d Department of Chemistry, An -Najah National University, Department of Chemistry, P. O. Box 7, Nablus, State of Palestine.

^e Department of Inorganic Chemistry. Faculty of Science, University of Málaga., 29007 Málaga, Spain

^f LCAE-URAC18, Faculty of Science, Université Mohammed First, Oujda, Morocco

^g Chemistry Department of, College of Science, King Khalid University, Abha, Saudi Arabia

^h Laboratory of Agroressources, Polymers and Process Engineering, Ibn Tofail University PO Box 242, Kenitra, Morocco.

*Corresponding Author: E-mail: r.salghi@uiz.ac.ma ; Fax: +212528232007; Tel: +212528228313

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-(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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