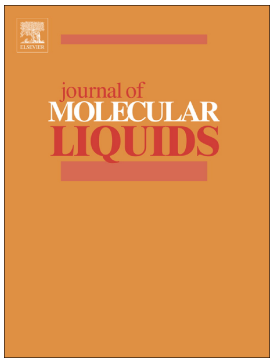

Highly effective inhibition of mild steel corrosion in 3.5% NaCl solution by green Nettle leaves extract and synergistic effect of eco-friendly cerium nitrate additive: Experimental, MD simulation and QM investigations

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PII: S0167-7322(17)35777-X
DOI: https://doi.org/10.1016/j.molliq.2018.02.021
Reference: MOLLIQ 8663

To appear in: *Journal of Molecular Liquids*

Received date: 2 December 2017
Revised date: 1 February 2018
Accepted date: 4 February 2018

Please cite this article as: Mohammad Ramezanzadeh, Zahra Sanaei, Ghasem Bahlakeh, Bahram Ramezanzadeh , Highly effective inhibition of mild steel corrosion in 3.5% NaCl solution by green Nettle leaves extract and synergistic effect of eco-friendly cerium nitrate additive: Experimental, MD simulation and QM investigations. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Molliq(2017), https://doi.org/10.1016/j.molliq.2018.02.021

Highly effective inhibition of mild steel corrosion in 3.5% NaCl solution by green Nettle leaves extract and synergistic effect of eco-friendly cerium nitrate additive: Experimental, MD simulation and QM investigations

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Abstract: The synergistic effects of eco-friendly cerium nitrate additive on the corrosion inhibition performance of green Nettle leaves extract were investigated on mild steel in 3.5% NaCl solution by electrochemical, surface characterization and theoretical molecular dynamics (MD) simulations and quantum mechanics (QM) methods. The effect of Nettle leaves extract: cerium nitrate ratio on the mild steel corrosion inhibition was studied. The electrochemical impedance spectroscopy (EIS) and polarization tests were applied to examine the corrosion inhibition properties. In addition, the adsorption process and the synergistic effects between Nettle leaves extract and cerium cations were theoretically evaluated by using MD simulations and QM computations based on density functional theory (DFT) approach. Surface characterization techniques namely field-emission scanning electron microscopy (FE-SEM),

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