Accepted Manuscript

The inhibition action of analgin on the corrosion of mild steel in acidic medium: A combined theoretical and experimental approach journal of MOLECULAR LIQUIDS

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PII: S0167-7322(18)31621-0

DOI: doi:10.1016/j.molliq.2018.04.143

Reference: MOLLIQ 9046

To appear in: Journal of Molecular Liquids

Received date: 27 March 2018 Revised date: 26 April 2018 Accepted date: 30 April 2018

Please cite this article as: Sumayah Bashir, Vivek Sharma, Hassane Lgaz, Ill-Min Chung, Ambrish Singh, Ashish Kumar, The inhibition action of analgin on the corrosion of mild steel in acidic medium: A combined theoretical and experimental approach. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Molliq(2017), doi:10.1016/j.molliq.2018.04.143

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The Inhibition Action of Analgin on the Corrosion of Mild Steel in Acidic Medium: A Combined Theoretical and Experimental Approach

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Abstract

The corrosion inhibitive property of analgin on mild steel in 1M HCl was determined for the first time by using experimental and theoretical studies. Weight loss results showed that analgin showed 96.1% inhibition efficiency at 4000ppm and 298K. Results showed that analgin acts as a mixed type inhibitor. Effect of concentration of inhibitor and temperature on corrosion inhibition efficiency has been studied. Effect of kinetic and thermodynamic parameters has also been reported. Results show that adsorption of analgin on metal surface follows Langmuir adsorption isotherm. A detailed theoretical data was obtained from Molecular dynamic simulations and quantum chemical calculations using density functional theory (DFT). All the combined results showed appreciable inhibition efficiencies. The morphological and topographical studies were done by SEM and AFM techniques. All the results were in good agreement with each other.

Keywords: Corrosion inhibition, Mild steel, DFT, Analgin, HCl, Molecular dynamic simulation

1. Introduction

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