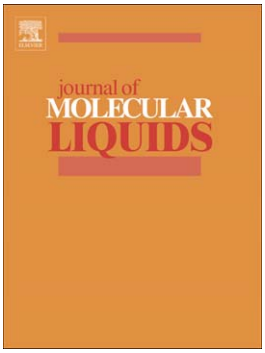

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Corrosion inhibition and adsorption behaviour of some bis-pyrimidine derivatives on mild steel in acidic medium

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Abstract

The inhibition ability of mild steel in 1M H_2SO_4 by bis-pyrimidine derivatives was investigated using chemical and electrochemical techniques. Results obtained indicate that bis derivatives inhibited the corrosion of mild steel in the acid medium. The inhibition efficiency increases with increase in concentration of bis-derivatives but decrease with rise in temperature. Adsorption of bis derivatives on the steel surface in 1M H_2SO_4 follows the Langmuir adsorption model. Kinetic and thermodynamic parameters such as activation energy, enthalpy, entropy and free energy of activation and adsorption were calculated. Gibbs free energy indicated that the adsorption process is spontaneous. Scanning electron microscopy and atomic force microscopy were used to study morphology of the steel surface. Results obtained from quantum chemical studies show excellent correlations between quantum chemical parameters and experimental inhibition efficiencies using density functional theory (DFT).

Key words:

Mild steel; Adsorption isotherm; Corrosion; Langmuir; Density functional theory; Protonation

1. Introduction

Corrosion by its simplest definition is the process of a metal returning to the material's thermodynamic state which is an electrochemical reaction that follows the laws of thermodynamics and it is time and temperature dependent. Corrosion in aqueous solutions is the most common of all corrosion processes [1]. The concern for corrosion by sulphuric acid has increased in the oil and gas industry because of the burning of fuels which is a major cause of