Al-Azawi et al. Chemistry Central Journal (2016) 10:23
DOI 10.1186/s13065-016-0170-3

Chemistry Central Journal

SHORT REPORT Open Access

Synthesis, inhibition effects and quantum chemical studies of a novel coumarin derivative on the corrosion of mild steel in a hydrochloric acid solution

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Abstract

Background: The acid corrosion inhibition process of mild steel in 1 M HCl by 4-[(2-amino-1, 3, 4-thiadiazol-5-yl) methoxy]coumarin (ATC), has been investigated using weight loss technique and scanning electron microscopy (SEM). ATC was synthesized, and its chemical structure was elucidated and confirmed using spectroscopic techniques (infrared and nuclear magnetic resonance spectroscopy).

Findings: The results indicated that inhibition efficiencies were enhanced with an increase in concentration of inhibitor and decreased with a rise in temperature. The adsorption equilibrium constant (K) and standard free energy of adsorption (ΔG_{ads}) were calculated. Quantum chemical parameters such as highest occupied molecular orbital energy, lowest unoccupied molecular orbital energy (EHOMO and ELUMO, respectively) and dipole moment (μ) were calculated and discussed. The results showed that the corrosion inhibition efficiency increased with an increase in both the EHOMO and μ values but with a decrease in the ELUMO value.

Conclusions: Our research show that the synthesized macromolecule represents an excellent inhibitor for materials in acidic solutions. The efficiency of this macromolecule had maximum inhibition efficiency up to 96 % at 0.5 mM and diminishes with a higher temperature degree, which is revealing of chemical adsorption. An inhibitor molecule were absorbed by metal surface and follow Langmuir isotherms low and establishes an efficient macromolecule inhibitor having excellent inhibitive properties due to entity of S (sulfur) atom, N (nitrogen) atom and O (oxygen) atom.

Keywords: (thiadiazol-5-yl)methoxy)coumarin, Corrosion inhibitor, Isotherm, Weight loss

Background

It is very important to use corrosion inhibitors to prevent metal dissolution and minimize acid consumption [1–4]. The majority of well-known acid inhibitors are organic compounds that contain nitrogen, sulfur and oxygen atoms. The inhibitory action exercised by organic compounds on the dissolution of metallic species is normally related to adsorption interactions between the inhibitors and the metal surface. The planarity (p) and lone pairs of electrons present on N, O and S atoms are important structural features that control the adsorption of these molecules onto the surface of the metal [5–7]. The effective and efficient corrosion inhibitors are those compounds that have π-bonds, contain hetero-atoms such as sulfur, nitrogen, oxygen and phosphorous and allow the adsorption of compounds on the metal surface [8–11]. The organic inhibitors decrease the corrosion rate by adsorbing on the metal surface and blocking the active sites by displacing water molecules, leading to the formation of a compact barrier film on the metal surface. Coumarins exhibit pharmacological activities, such as anticancer, anti-inflammatory [12], anti-influenza,

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