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Experimental studies on inhibition of mild steel corrosion by novel synthesized inhibitor complemented with quantum chemical calculations

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ABSTRACT

One of best method, which was used to prevent the mild steel from corrosion, was through employed natural or synthetic organic chemical compounds. Here in, we displayed a Schiff base derivative which has nitrogen, oxygen and sulfur atoms as corrosion inhibitor for MS "mild steel" in 1 M HCl "hydrochloric acid" solution. Synthesized inhibitor was characterized by using of FT-IR "Fourier transform infrared" and NMR "Nuclear magnetic resonance" spectroscopies in addition to CHN analysis technique. The weight loss and SEM "Scanning electron microscope" studies showed that inhibitor have the ability to prevent the alloy surface from corrosive solution by adsorbing on MS surface to form stable adsorbed layer that results in the higher inhibition efficiency. The inhibition influence of the synthesized inhibitor was increased parallel with increasing concentration and decrease with rising temperature degrees. Furthermore, DFT "Density function theory" has been employed to calculate quantum chemical parameters "Energy, highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO) and electronegativity (χ)" which performed on synthesized corrosion inhibitor to determine the relationship between the structure of synthesized inhibitor molecule and inhibition performance.

Introduction

Mild steel "MS" is quite applied in considerable manufacturing applications such as Chemicals, pickling, acid cleaning, oil, gas, storage and pipeline transportation". MS seveir from corrosion due to corrosive solutions and lead to the degradation of the alloy, resulting in considerable economic losses for several industries. The degradation of MS is an effect of contact of MS with the acidic and/or basic solutions which were quite used in manufactures for diverse applications [1–6]. Schiff bases were quite significant class of molecules that synthesized from aromatic and/or aliphatic aldehydes or ketones, and amines [7–9]. In addition, the Schiff bases have the azomethane linkage (–C═N) which considered the essential structural requirement for different medicinal and pharmacological applications, including immunosuppressant activity [10], anti-malarial [11], anti-tubercular [12], anti-microbial and anti-cancer activities [13]. Quantum chemical calculations is nowadays employee in order to demonstrate the corrosion inhibition mechanism of the studied inhibitors such as DFT "Density function theory" [14–17]. Density function theory is proved a quite powerful tool for mechanism searching [18–20]. The aim of this paper is to study the dependence of inhibition performance of the studied molecule and inhibitory properties of new synthesized inhibitor, namely methyl "2-((3-hydroxy-4-methoxybenzylidene)amino)isonicotinate" for the corrosion of mild steel in corrosive solution through gravimetric technique and quantum chemical calculations using DFT method. Theoretical calculations depending on the chemical parameters "highest occupied molecular orbital (EHOMO) and the lowest unoccupied molecular orbital (ELUMO), energy gap (ΔE), dipole moment (μ), electronegativity (χ), electron affinity (A), global hardness (η), softness (σ), ionization potential (I) and the global Electrophilicity (ω)". The chemical structure of the synthesized inhibitor was shown in Fig. 1.

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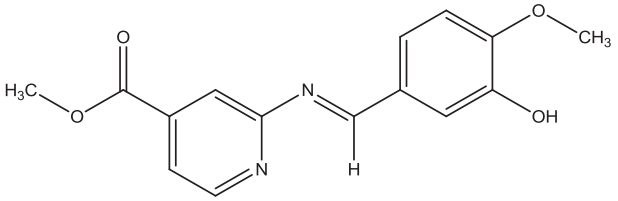

Fig. 1. The chemical structure of the studied inhibitor.

Experimental

Materials and chemical compounds

All the chemicals compounds and solvents that used in this study were purchased from Sigma Aldrich Chemicals/Malaysia. Shimadzu FTIR-8300 spectrometer was employee to obtained FT-IR "Fourier transform infrared" spectra. Carlo Erba 5500 elemental analysis was utilized to perform the CHN-Elemental analyses. NMR "Nuclear magnetic resonance" spectrum was recorded on a Bruker Spectrospin instrument at 300 nMHz UltraShield magnets. DMSO-d_6 "Dimethyl sulfoxide-d6" has been used as solvent and TMS "Tetramethylsilane" has been used as internal standard. The target inhibitor synthesized through condensation reaction of 3-hydroxy-4-methoxybenzaldehyde (0.005 mol) with methyl 2-aminoisonicotinate (0.005 mol) in ethanol (50 mL) and the mixture was refluxed with few drops of acetic acid for 5 h with stirring. TLC "Thin layer chromatography" has observed through the approach of reaction. The solid cooled, filtered, washed by ethanol and recrystallized from ethanol, yield 76%. M.P. 112–115 °C. The purity of synthesized compound was confirmed through TLC. IR: 3285.3 cm^{-1} (OH), 3051.5 cm^{-1} (aromatic group) 1711.8 cm^{-1} (carbonyl), 1629.7 cm^{-1} (C=N). ^{1}H NMR (DMSO-d_6); δ: 8.96 (d, 1H, H-C=N, pyridine), 8.29 (s, 1H, H-C=N), 6.88–7.81(s, 1H, aromatic benzene and pyridine rings), 5.31 (s, 1H, OH), 3.78 (s, 3H, OCH3 pyridine rings), 3.58 (s, 3H, OCH3 benzene rings). CHN analysis calculation (found) for $C_{15}H_{14}N_2O_4$: C 62.93 (62.13), H 4.93 (4.52), N 9.79 (9.21).

Corrosion studies

Mild steel "MS" coupons, which were applied as electrodes in our search, have been provided through the Company of Metal Samples. MS alloy composition of "99.21Fe, 0.21C, 0.38Si, 0.09P, 0.05S, 0.05Mn and 0.01Al"%. The efficient surface area was 4.5 cm^2 and it was cleaned approbate to the method ASTM G1-03 [21–23]. MS coupons were suspended duplicate in 0.2 L of 1 M hydrochloric acid solution in absence and presence of the target inhibitor. The concentrations of the inhibitor were 0.00, 0.05, 0.10, 0.15, 0.2.0, 0.25 and 0.50 g/L at five hours as an immersion time. Coupons were washed and dried then weighed accurately. CR "corrosion rate" and IE% "inhibition efficiency have been calculated as in Eqs. (1) and (2) respectively:

$$C_R = mg \times cm^2h^{-1} \tag{1}$$

$$IE = \left[1-\left(\frac{w_2}{w_2}\right)\right] \times 100 \tag{2}$$

Note: w_1 & w_2 are the MS coupons weight losses in presence and absence of the studied inhibitor respectively.

DFT calculations

The optimized Geometrical structures have been done without symmetry constraints employing "Gaussian 09, Revision A.02" [24]. The function B3LYP has been used for all optimized structures and energies such as EHOMO "Energy of highest occupied molecular orbital" and ELUMO "Energy of lowest unoccupied molecular orbital" calculations [25,26]. Inhibition mechanism of synthesized inhibitor derived from 3-hydroxy-4-methoxybenzaldehyde and methyl 2-aminoisonicotinate related quantum parameters that were indicated as in Eqs. (3)–(9) [27].

$$\Delta E \text{ Energy gap} = E_{LUMO} - E_{HOMO} \tag{3}$$

$$X\text{""Electron affinity""} = -HOMO \tag{4}$$

$$I\text{""Ionization potential""} = -LUMO \tag{5}$$

$$\eta\text{""Global hardness""} = \frac{1}{2}(E_{HOMO} - E_{LUMO}) \tag{6}$$

$$S\text{""Chemical softness""} = \frac{1}{\eta} \tag{7}$$

$$\chi\text{""Electronegativity""} = \frac{1}{2}(E_{HOMO} + E_{LUMO}) \tag{8}$$

$$\omega\text{""electrophilicity index""} = \frac{\mu^2}{2\eta} \tag{9}$$

Results and discussion

Synthesis

To synthesize methyl 2-((3-hydroxy-4-methoxybenzylidene)amino) isonicotinate as a corrosion inhibitor, the sequence of the reaction outlined in Fig. 2, starting from the available commercial compounds methyl 2-aminoisonicotinate and 3-hydroxy-4-methoxybenzaldehyde. The synthesis have been done through the reflux of methyl 2-aminoisonicotinate in ethanol with 3-hydroxy-4-methoxybenzaldehyde. The target compound has molecular weight 286, that was estimated based on it formula ($C_{15}H_{14}N_2O_4$) which confirmed by CHN elemental analysis. The inhibitor methyl 2-((3-hydroxy-4-methoxybenzylidene) amino)isonicotinate can be dissolve in several polar solvents such as DMF, DMSO, dichloromethane, acetone and alcohol. The spectrum of FTIR for of methyl 2-((3-hydroxy-4-methoxybenzylidene)amino)isonicotinate show new absorption bands and disappeared of others absorption bands. The new band at 1611 cm^{-1} for azomethine group, and disappearance of the bands for amino and carbonyl groups at around 3350 cm^{-1} and 1700 cm^{-1} respectively. H NMR spectrum show singlet at 8.29 ppm due to the azomethine (H–C=N) proton.

Weight loss results

Corrosion inhibitors that were utilized in industries are the economical technique for efficiently protection of MS alloy surface [28].

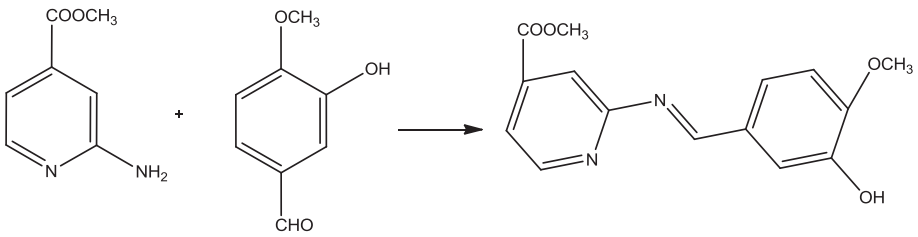

Fig. 2. The reaction sequence for synthesized of methyl 2-((3-hydroxy-4-methoxybenzylidene)amino) isonicotinate.