Synthesis of Thiophene Derivative and its Use as Zinc Metal Corrosion Inhibitor in Hydrochloric Acid Solution

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Abstract

N-[(3-Bromo-2-methylthiophen-5-yl)methylene]-4-methoxyaniline) (5) has been synthesized and used as corrosion inhibitor for zinc metal in 2 M HCl at room temperature by using weight loss measurements. The obtained results showed that (5) is a good inhibitor and its inhibition efficiency (IE %) increased with the increase of inhibitor concentration. The surface coverage was 1.55 at 500 ppm inhibitor concentration; hence the optimum concentration was 500 ppm. Theoretical calculations investigate by studying the relationship between molecular structure and inhibition efficiency using semi-empirical molecular quantum calculations within the PM3 method as implemented in HyperChem package.

Keywords**:** Quinazolin, Imine, Inhibition efficiency; Zinc metal.

Introduction

Corrosion inhibitor is a chemical that interacts well with the metal surface by an adsorption process to form a thin film/layer to protect the metal surface by reducing the movement of ions to the metal surface or by increasing the electrical resistance of metallic surface [1-3]. Corrosion inhibiters are either synthesized from cheap raw materials or from organic compounds containing electronegative functional groups [1-3]. Organic and inorganic additives which prevent the adsorption of Cl ions and/or by the formation of a more resistant oxide film on the metal surface., the successful utilization of most corrosion inhibitors has been hindered by their toxic nature [4]. Green corrosion inhibitors have the advantage of, biodegradable, inexpensive, non-toxic and eco-friendly. These advantages have provoked numerous and intensive researchers on the use of naturally occurring substances or their extracts for the inhibiters of the corrosion of metals [5-7].

It has been published that the inhibitory actions of plant extracts are due to the presence of some organic compounds such as saponins, tannin, alkaloid, steroids, glycosides and amino acids [8].

Zinc is an active metal with numerous industrial applications and is mainly used for the corrosion protection of steel. The zinc coated steel materials provide a greater resistance to corrosion, but when exposed to humid atmosphere, they undergo rapid corrosion with the formation of a corrosion product known as white rust [9-11]. The formation of white rust is generally observed in galvanized materials and renders the plated zinc materials unsuitable for industrial applications. Also, industrial processes such as scale removal and cleaning of zinc surfaces with acidic solutions expose zinc to corrosion. Therefore, in order to protect the metal from corrosion, the use of inhibitors is necessary [12].

To reduce corrosion (corrosion inhibitor) must be used; a corrosion inhibitor is a chemical compound which is designed to protect a metal or alloy from corrosion. While corrosion inhibitors will not halt or completely prevent corrosion, they can reduce the rate at which corrosion occurs, and block early corrosion damage. A wide variety of chemicals can be used for this purpose, although many are toxic, and must therefore be used with care to protect the environment [13,14].

Among the different types of the corrosion inhibitors different Imines (Schiff bases) have been reported effective corrosion inhibitors for a wide range of metals in acid media, some of these imines are containing thiophene ring in their structures [15-16].

Theoretical treatment of the formation of compound in the gas phase, this was done using the hyperchem-7 program for the

Molecular mechanics and semi- empirical calculations. Semi-empirical methods use parameters derived from experimental values that simplify theoretical calculations. These methods usually do not require long computation times, and lead to qualitative descriptions of molecular systems. In particular, the semi-empirical PM3 method makes use of an accurate procedure to predict chemical properties, through a simplified Hartree-Fock (HF) Hamiltonian [17]. The correlation between theoretically calculated properties and experimentally determined inhibition efficiencies has been studied successfully for uniform corrosion [18].

Experimental

All reactions were performed under an inert atmosphere. Glassware was oven dried, assembled hot and allowed to cool under a stream of nitrogen gas. All chemicals and reagents were purchased from commercial sources and used without further purification. THF was distilled from sodium benzophenone ketyl and other solvents were purified by standard procedures. [19] IR spectra were recorded as KBr discs for solid materials or by applying droplets of liquid materials on NaCl plate. ^{1}H-NMR and ^{13}C-NMR spectra were recorded on a spectrometer operating at 400 MHz for ^{1}H and 100 MHz for ^{13}C measurements, respectively. Chemical shifts (*δ)* are reported in parts per million (ppm) relative to tetramethylsilane (TMS). ^{13}CNMR signals corresponding to CH, CH_2, or CH_3 are assigned from DEPT–90 and 135 spectra and all other carbons are quaternary (C). Low and high–resolution mass spectra were recorded on a time-of-fight mass spectrometer using electron impact (EI). Column chromatography was carried out using Fischer Scientific silica 60A (35–70 micron). Alkyllithiums were obtained from Aldrich Chemical Company and were estimated prior to use by the method of Watson and Eastham [20]. 3,5-Dibromo-2-methyl thiophene (2) has been synthesized according to literature procedure [21].

Synthesis of 3-bromo-2-methylthiophene-5-carboxaldehyde (3)

A solution of n-Butyl Lithium (*n*-BuLi) (64.0 mL, 1.60 M; 64.00 mmol) in hexane was added in a dropwise manner over 5 min to a stirred solution of 3,5-dibromo-2-methylthiophene (2; 16.0 g, 62.5 mmol) in anhydrous THF (100 mL) at [–78 ^{o}C] under nitrogen. The solution turned orange, then greenish yellow and finally yellowish orange. The reaction mixture was stirred at [–78 ^{o}C] for 30 min and DMF (4.80 g, 65.7 mmol) was then added. The cooling bath was removed and the mixture was stirred at room temperature for 16 h. The mixture was quenched with aqueous HCl (20 mL, 2 M) and the product was extracted with Diethyl ether (3 × 100 mL). The organic layer was washed with saturated aqueous $NaHCO_3$ solution and brine and then dried ($MgSO_4$). The solvent was removed under reduced pressure to give the compound (3) (10.88 g, 53.05 mmol; 85%) as a yellow solid.

m.p: 56–57 ^{o}C.

^{1}H- NMR (400 MHz, $CDCl_3$) *δ* (ppm): 9.69 (s, 1 H, CHO), 7.51 (s, 1 H) and 2.41 (s, 3 H,CH_3).

^{13}C- NMR (100 MHz, $CDCl_3$) *δ* (ppm): 181.6 (C=O), 145.9 (C2), 140.1 (C5), 138.8 (C4), 111.3 (C3) and 15.9 (CH_3).

EI-MS (*m/z*, %): 206 ([M^{81}Br]$^+$, 75], 205 (98), 204 ([M^{79}Br]$^+$, 77), 203 (100), 177 (25), 125 (20), 96 (40), 84 (32) and 69 (49).

HRMS (EI): Calcd for C_6H_4BrOS [M^{79}Br - 1]$^+$ 202.9172; Found, 202.9166.

FT–IR (ν_{max}, cm^{-1}): 3080 (C-H aromatic), 2859 (C-H aldehydic) and 1678 (C=O).

Synthesis of *N*-[(4-bromo-5-methylthiophen-2-yl)methylene]-4-methoxyaniline (5):

In a 10 mL microwave vial charged with a magnetic bar, 3-bromo-2-methylthiophene-5-carboxaldehyde (0.30 g, 1.46 mmol) and 4-methoxyaniline (0.18 g, 1.46 mmol) were dissolved in 6 mL absolute methanol and a drop of HCl was added to the mixture. The vial was sealed and subjected to microwave irradiation at 100 °C for 5 min. The mixture was cooled, then decanted into a 50 mL round bottomed flask and the solvent was evaporated under reduced pressure. The solid crude product was recrystallized from ethanol to give *N*-[(4-bromo-5-methylthiophen-2-yl) methylene]-4-methoxyaniline (5) (0.41 g, 1.32 mmol; 91%) as yellowish brown solid.

m.p: 73–74 ^{o}C.

^{1}H- NMR (400 MHz, $CDCl_3$) δ: 8.36 (s, 1 H, CHN), 7.20–7.10 (m, 4 H, H2, H3, H5 and H6 of Ph), 6.83 (s, 1 H, H4 of thiophene), 3.76 (s, 3 H, OCH_3) and 2.38 (s, 3 H).
^{13}C- NMR (100 MHz, $CDCl_3$) δ: 158.5 (C4 of Ph), 149.6 (C=N), 143.8 (C5 of thiophene), 139.8 (C1of Ph), 139.4 (C2 of thiophene), 133.8 (C4 of thiophene), 122.4 (C2 and C6 of Ph), 114.4 (C3 and C5 of Ph), 109.9 (C3 of thiophene), 55.5 (OCH_3) and 15.5 (CH_3).
EI-MS (*m/z*, %): 311 ($[M^{81}Br]^+$, 88), 309 ($[M^{79}Br]^+$, 90), 296 (97), 294 (100), 86 (51), 84 (96).
HRMS (EI): Calcd. for $C_{13}H_{12}BrNOS$ $[M^{79}Br]^+$ 308.9823; found, 308.9825.
FTIR (ν_{max}, cm^{-1}): 2960 (C-H aromatic), 2836 (C-H aliphatic), and 1614 (C=N).

Corrosion Inhibition:

Zinc strips of BDH grade (8 cm x 2 cm x 0.5 mm) was scrubbed with emery paper, and washed with acetone 5 times; a solution of 2.0 M HCl was prepared. Compound [5] as a corrosion inhibitor was prepared in 500 ppm concentration, thereafter subsequent dilution was employed to prepare solutions 400, 300, 200 and 100 ppm. Zinc strip was immersed in 2M HCl solution in absence of inhibitor for specific periods of time and weighed in electronic balance after each period.

Weight loss measurements:

For weight loss measurements, the following formulae were employed

$$\Delta m = (m_1 - m_2) \quad \text{.......} (1)$$

Where m_1 and m_2 are the weights of metal before and after exposure to the corrosive solution, respectively.

The corrosion rate, the percentage of inhibition efficiency (IE %) and the degree of surface coverage (θ) of the investigated compounds was calculated from the following equations [22].

$$\text{Corrosion rate} = \Delta m / \Delta t \quad \text{.......} (2)$$
$$IE\ \% = [1 - (\Delta m_{\mathbf{inh}} / \Delta m_{\mathbf{free}})] \times 100 \quad \text{.......} (3)$$
$$\theta = [1 - (\Delta m_{\mathbf{inh}} / \Delta m_{\mathbf{free}})] \quad \text{.......} (4)$$

Where $\Delta m_{\mathbf{free}}$ and $\Delta m_{\mathbf{inh}}$ are the weight losses in the absence and presence of inhibitor, respectively.

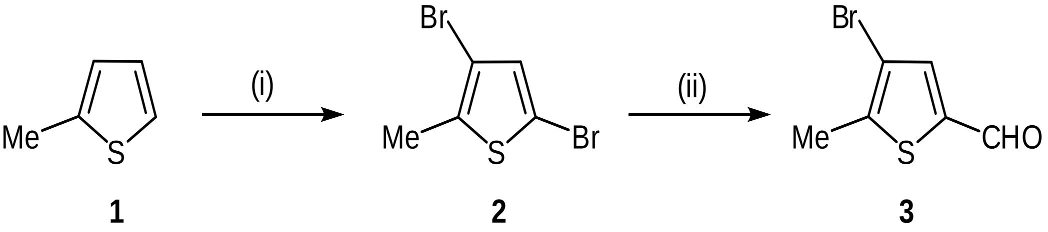
Theoretical calculations:

Theoretical calculations were carried out using the semi-empirical calculations with PM3 method For this purpose the Hyperchem Program with complete geometry optimization was used. The purpose of these calculations is to provide information about the electron configuration of organic inhibitor by quantum chemical calculations and to investigate the relationship between molecular structure and inhibition efficiency. Some electronic properties such as energy of the highest occupied molecular orbital (E_{HOMO}), energy of the lowest unoccupied molecular orbital (E_{LUMO}), energy gap (ΔE) between LUMO and HOMO and Mulliken charges on the backbone atoms for prepared molecule [5] were planned to determine.

Results and Discussion

Synthesis of *N*-[(3-Bromo-2-methylthiophen-5-yl)methylene]-4-methoxyaniline) (5):

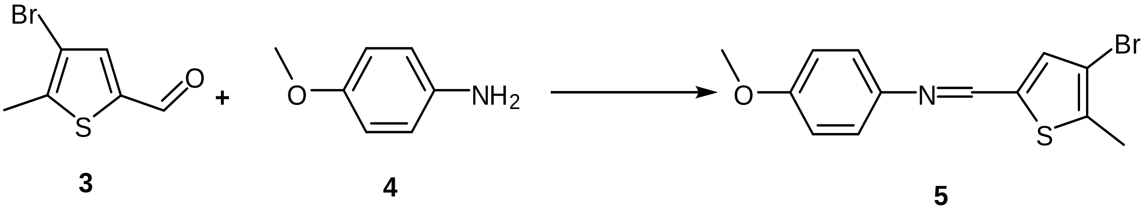
3-Bromo-2-methylthiophene-5-carboxaldehyde (3) was synthesized from 3-methylthiophene (1) in two steps. The first one involves the bromination of 1 to give 3,5-dibromo-2-methylthiophene (2) which was then converted to the aldehyde 3 in the second step by selective bromine-lithium exchange of the α-bromo group, followed by treatment with dimethylformamide (DMF) as shown in Scheme 1.



Reagents and conditions: (i) Br_2/AcOH, 0 °C, 16 h (95%). (ii) *n*-BuLi (1 equiv), THF, -78 °C, 30 min, DMF, RT, 16 h, Na_2CO_3 (90%)

Scheme (1) Synthesis of 3-bromo-2-methylthiophene-5-carboxaldehyde (3).

The target imine (5) was synthesized by the condensation reaction of 3-bromo-2-methylthiophene-5-carboxaldehyde (3) with one mole equivalent of 4-methoxyaniline (4) under microwave conditions, Scheme 2.



Reagents and conditions: **4** (1 equiv), MeOH, MW, 100^oC, 5 min.

Scheme (2) Synthesis of the target compound (5).

The structure of [5] was confirmed by ^1H- NMR, ^{13}C- NMR and mass spectrometry. The ^1HNMR analysis showed that the singlet at $\delta = 9.69$ ppm corresponding to the aldehydic hydrogen disappeared and a new singlet $\delta = 8.36$ ppm corresponding to the proton of the NH group was observed. The ^{13}C- NMR spectrum showed that the signal at $\delta = 181.6$ corresponding to the carbon of the carbonyl group disappeared and signal at $\delta = 158.5$ ppm corresponding to the carbon of the C=N group was observed. All the other predicted signals in both ^1H- NMR and ^{13}C- NMR were also observed. The high resolution mass spectrometry has confirmed the formula of the product, it showed a peak at *m/z* = 308.9825 which correlates well with the calculated value for $C_{13}H_{12}BrNOS$ $[M^{79}Br]^+$, which is 308.9823. It was clear that the product was obtained in high purity and in high yield (91%).

Corrosion Inhibition:

The corrosion of zinc strips in hydrochloric was studied by weight loss measurements using equations (1), (2), and the corrosion rates (g/min) of zinc were plotted against time (min) and as shown below in Fig.(1).

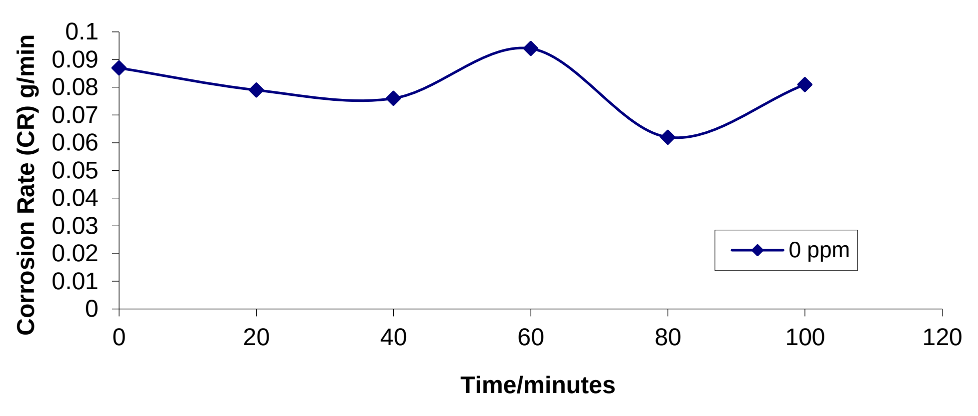


Fig.(1) Corrosion rate vs. immersion time for Zn strip in 2M HCl without inhibitor at 25°C.

The corrosion inhibitor is a chemical substance that interacts with the metal surface by an adsorption process protecting metal surface by forming film [23]. Inhibitor retards the corrosion either by reducing the movement or diffusion of ions to the metal surface, or by increasing the electrical resistance of metallic surface [24]. The inhibitor molecules could be adsorbed on the metal surface, so the aromatic nuclei and the oxygen atoms provides electrons that are needed to retard the formation of zinc ions, and the coating of zinc strips depends on how much the surface can accommodate the molecules of the inhibitor [5], and the presence of this inhibitor induces chemical bonds with Zinc surface. These chemical bonds increased with increase of the inhibitor concentrations.

Fig.(2) showed that the lowest corrosion rate was at 500 ppm, so it is the optimum concentration for inhibition, and this is might be attributed to the maximum coating of zinc strips at this concentration with **[**5**]**.

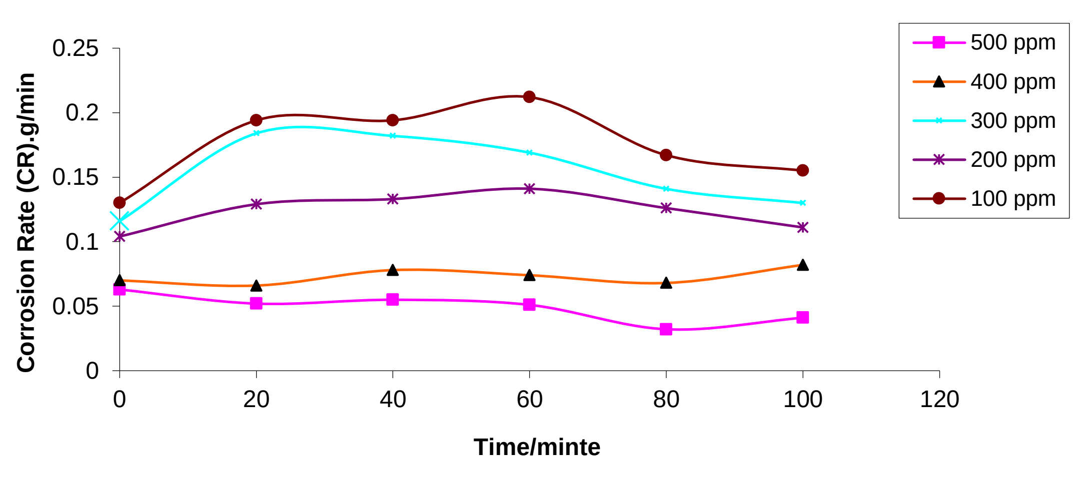


Fig.(2) Corrosion Rate vs. immersion time for Zn strip in 2M HCl in presence of N-[(3-Bromo-2-methylthiophen-5-yl)methylene]-4-methoxyaniline) in (500, 400, 300, 200 and 100) ppm concentrations.

The maximum surface coverage was found to be at 500 ppm, and this could be attributed to the moderate concentration and the molecules of [5] at this concentration diffuse from the bulk solution into the surface of zinc to cover it and inhibit the corrosion.

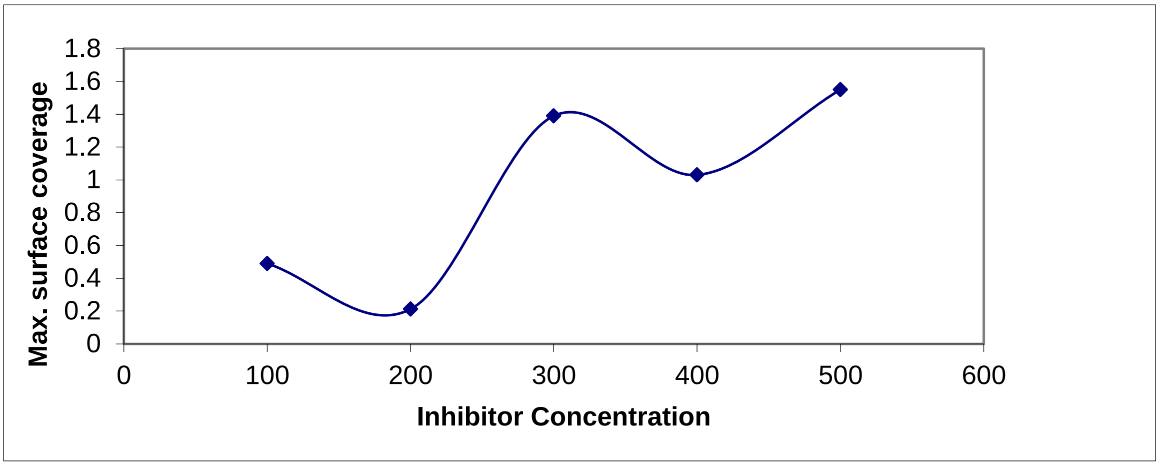


Fig.(3) The surface coverage versus time at 25°C.

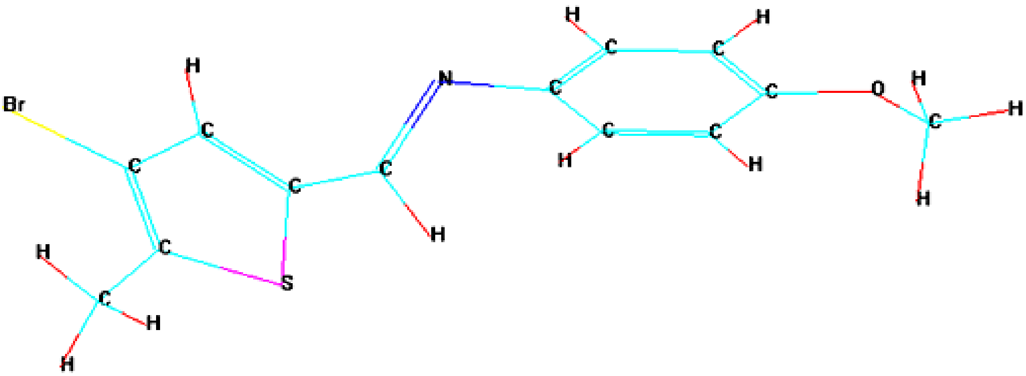
Table (1)
Measure of weight loss and calculate (ɵ, IE%, and rate of corrosion) in presence of inhibitor.

Time	*IE%/500*	*IE%/400*	*IE%/300*	*IE%/200*	*IE%/100*
0	49	19	33	19	38
20	72	63	65	16	34
40	77	75	70	2.6	27
60	62	50	79	21	45
80	67	51	63	9	48
100	91	37	60	10	49

The inhibition efficiencies increased as inhibitor concentration increased, at 500 ppm the inhibition efficiency was the maximum and it was 91%. This behavior could be attributed to the increase of the number of adsorbed molecules at the metal surface.

Theoretical calculations:

The purpose of theoretical study is to provide information about the electron configuration of organic inhibitor by quantum chemical calculations and to investigate the relationship between molecular structure and inhibition efficiency. All the calculations for geometry optimization were performed using the semi-empirical calculations with PM3 method. For this purpose the Hyperchem Program with complete was used. This computational method has been proven to yield satisfactory results [25,26].



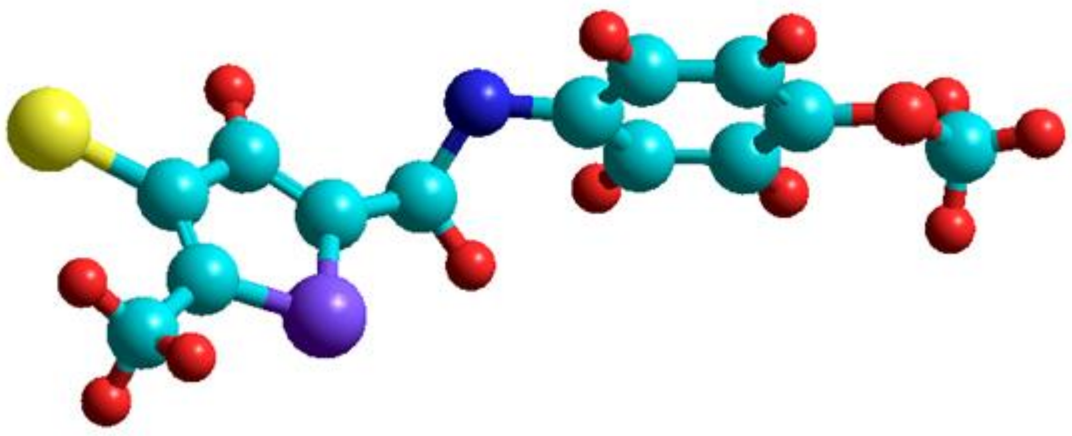


Fig.(4) Structure of [N-[(3-Bromo-2-methylthiophen-5-yl)methylene]-4-methoxyaniline)].

The easiest way to compare the inhibition efficiency of compound is to analyze the energies of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). The calculated energies E_{HOMO}, E_{LUMO}, energy gap ($\Delta E=E_{LUMO}-E_{HOMO}$) and other indices are given in Tables (2).

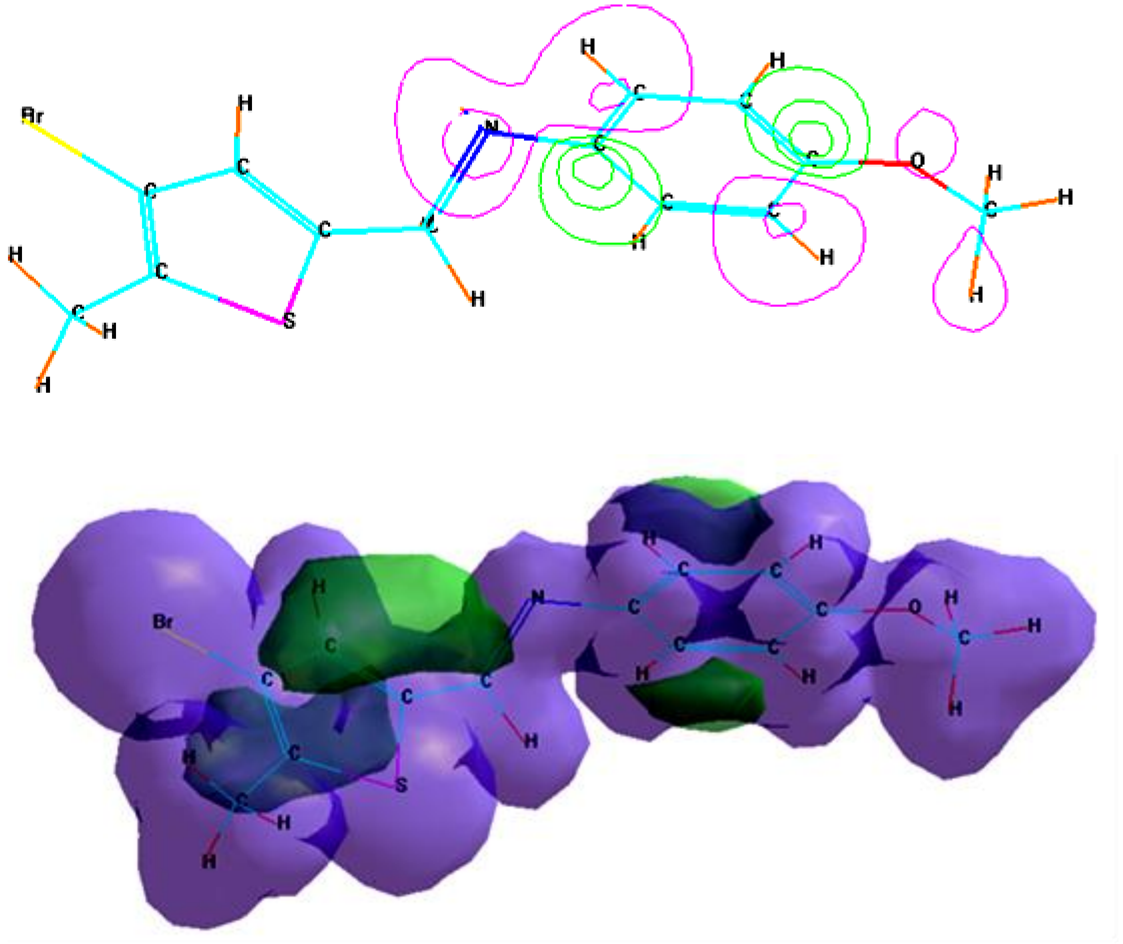


Fig.(5) HOMO and LUMO as 2D&3D contours for compound [N-[(3-Bromo-2-methylthiophen-5-yl)methylene]-4-methoxyaniline)].

Table (2)
Calculated quantum chemical parameters of [5] as modeling systems using PM3 method.

Comp. No.	*HOMO (eV)*	*LUMO (eV)*	$\Delta E(E_{HOMO}-E_{LUMO})$ *(eV)*	μ *(Debye)*
5	-8.398827	-0.6802578	-7.7185692	1.266

The energy gap (ΔE) between the HOMO and LUMO energy levels of the molecules is important factor, whereas, low absolute value of the energy gap (ΔE) gives good inhibition efficiencies [27-29]. The compound showed lowest energy gap that in good agreement experimental results see Table (2).

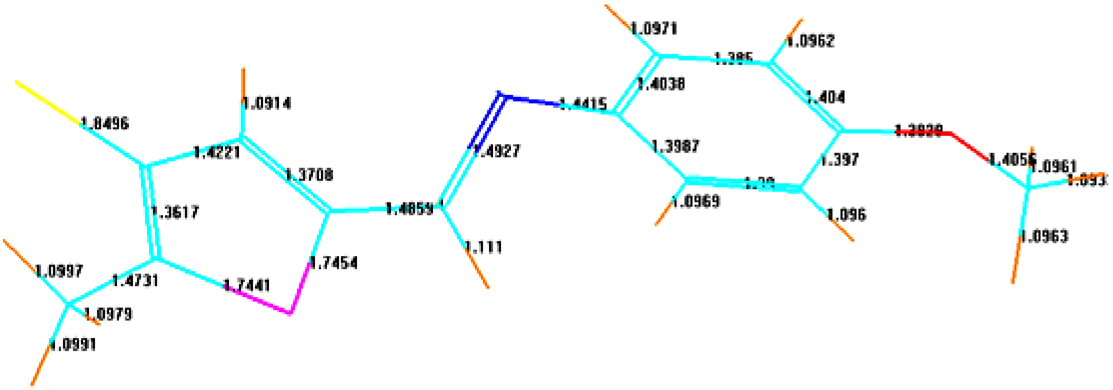


Fig.(6) Formal charges of [N-[(3-Bromo-2-methylthiophen-5-yl)methylene]-4-methoxyaniline)].

Conclusions

Compound **[N-[(3-Bromo-2-methylthiophen-5-yl)methylene]-4-methoxyaniline)]** was used to inhibit the corrosion of zinc, and the inhibition efficiency was found to be maximum at 500 ppm concentration of inhibitor. The maximum surface coverage was found to be maximum at 500 ppm inhibitor concentration which means that the maximum adsorption was at this concentration, and the molecules of **[N-[(3-Bromo-2-methylthiophen-5-yl)methylene]-4-methoxyaniline)]** have formed a thin film which prevents the penetration of acid into the surface of zinc. Theoretical calculations were used as useful tools to investigate the relationship between molecular structure and inhibition efficiency by using semi-empirical molecular quantum calculations within the PM3 method.

Acknowledgment

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الخلاصة

تم دراسة تثبط تأكل الخارصين في محلول ٢ مولاري من حامض الهيدروكلوريك في درجة حرارة الغرفة بأستخدام المركب N-[(3-Bromo-2-methylthiophen-5-yl)methylene]-4-methoxyaniline بطريقة النقص بالوزن. النتائج المستحصلة أثبتت ان المركب N-[(3-Bromo-2-methylthiophen-5-yl)methylene]-4-methoxyaniline مثبت جيد حيث ان نسبة كفاءة التثبيط قد أزدادت بأزدياد التركيز للمثبط وكانت النسبة هي ٩١%. كانت تغطية السطح حوالي ٠,٩١ في تركيز ٥٠٠ جزء من المليون ولهذا فأن التركيز الأمثل للمثبط هو ٥٠٠ جزء من المليون.

واستخدمت الحسابات النظرية كأدوات مفيدة للتحقيق في العلاقة بين التركيب الجزيئي وكفاءة تثبيط باستخدام حسابات الكم الجزيئية شبه التجريبية ضمن الأسلوب PM3.