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Synthesis, Characterization, and Investigation the Inhibitory Impact of Thiosemicarbazide Derivative toward the Corrosion of Mild Steel in Acidic Media

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Abstract:

In this study we focused on the determination of influence the novel synthesized thiosemicarbazide derivative "2-(2-hydroxy-3-methoxybenzylidene) hydrazinecarbothioamide" (HMHC) influenced the corrosion inhibition of mild steel (MS) in a 1.0 M hydrochloric acid acidic solution.This is in an effort to preserve the metal material by maintaining it from corrosion.The synthesized inhibitor was characterized using elemental analysis, and NMR-spectroscopy. Then the corrosion inhibition capability of (HMHC) was studied on mild steel in an acidic medium by weight loss technique within variables [temperature, inhibitor concentration, and time]. The immersion periods were [1:00, 3:00, 5:00, 10:00, 24:00, and 72:00] hours and the temperature range was (303-333) K. Various concentration of (HMHC) were used and the immersion periods were [0.00, 0.001, 0.05, 0.10, 0.15, 0.20, 0.25, and 0.50] g/L. The prepared derivative has shown the ability to inhibit corrosion. It has been observed that the rate of erosion decreases with the increasing concentration of the prepared inhibitor and increases with the increasing temperature of the solution. The most promising inhibitor action is at 0.5 g/L with an inhibition efficiency of 90.2%. Where it found that the adsorption process of HMHC obeys the Langmuir isotherm model. The electronic properties of the HMHC molecules were obtained from density function theory (DFT) quantum chemical approach. The experimental approach and theoretical results were found to have impressive correlations.

Keywords: Adsorption, Corrosion mild steel, Density function theory, Schiff base, Thiosemicarbazide.

Introduction:

Consumption-related tool damage has been and remains a significant issue in the compounding and petrochemicals industries over the years. Carbon steel is the most widely used material in pipes and other equipment parts. Mild steel (MS/carbon steel) pipes are broadly utilized in the transport of oil, which makes it exposed to various conditions in their ways between oil fields and oil refineries. Numerous factors and natural variables influence the erosion of line materials, for example, temperature, pH, saltiness, and so on these components assume a significant function in the erosion of development materials. Consumption of these pipes can be limited by managing itself or by modification the ecological elements (which are sometimes difficult to control). Coverage, for example, is one of the strategies used to reduce and control consumption. Epoxy covering applied with newly designed polymers have attracted interest due to their wide range of uses, including tissue substitutes and underlying materials [1].

Corrosive arrangements are generally utilized in industry for a few cycles, for instance, corrosive pickling, modern corrosion cleaning, descaling corrosive, and acidification of oil wells [2].

During the previous decade, numerous strategies have been utilized to limit the consumption of iron because of assault by acids. One of the methods for limiting erosion is the utilization of inhibitors [3,4]. A large number of the

inhibitors of corrosion are natural mixes of homo or hetero organics that include (N, S, O, P) atoms in their structure [5-7].

Many studies discussed the different methods and some materials effect on erosion. Raman Kumar et al.[8], have studied the inhibition behavior of a Schiff base called 4-(4-methoxy-6-methylpyrimidin-2-yl) imino) methyl) benzaldehyde on mild steel in an acidic solution of sulfuric acid (0.5 M), using various concentrations of inhibitor solution. Electrochemical, polarization, and morphological measurements were utilized to investigate the inhibitor. The results show that 0.1mM of the compound solution has high inhibition efficiency of about 98.45% in 298K and the lowest values in efficiency when using low concentrations and high temperatures.

In another work, Kashmitha Muthamma et al.[9] have investigated the effect of N-[(3,4-dimethoxyphenyl) methyleneamino-4-hydroxy-benzamide] (DMHB) to resist the corrosion of low carbon steel in two acidic mediums (H_2SO_4 and HCl) with concentration 0.5 M for each acid, in the range of temperature from 303K to 323 K), the research found that increasing the concentration of (DMHB) at a minimum temperature of 303K led to an increased percentage of inhibition efficiency.

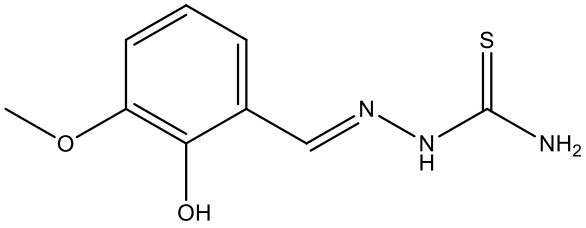
Hassane Lgaz et al. [10] have evaluated a new four hydrazones derivatives as inhibitors towards mild steel corrosion in 1.0 M of hydrochloric acid and all the results have shown the ability of prepared compounds to form a stable protective layer on the surface of mild steel due to physio-chemical interactions and these compounds disparity among themselves in the force of these interactions.

The research of Xiaohong He et al [11], have shown the effect of perimidine derivatives on carbon steel in 1.0 M of HCl when the concentration less than 0.15 mM of used perimidine derivatives have inhibition efficiencies > 90% due to the fact that of imine group in structure.

Also, the study done by Rajesh Haldhar et al. [12], was reached to eco-friendly corrosive inhibitor by applying *Citrus aurantifolia* leaves extract on mild steel immersed in 0.5M H_2SO_4. The extract formed a blocking layer with the strongest IE% = 96.46% at conc. = 250 mg/L.

Elkhotfi Y. et al.[13] were studied the effectiveness inhibition corrosion by *Cupressaceae* essential oil on mild steel in 1M of HCl as a green method, extracted oil behaves as a very good inhibitor where give IE% about 83% at 1500 ppm.

The purpose of this study was to see how the novel synthesized thiosemicarbazide derivative "2-(2-hydroxy-3-methoxybenzylidene) hydrazinecarbothioamide" (HMHC) influenced the corrosion inhibition of mild steel (MS) in a 1.0 M hydrochloric acid acidic solution. This is in an effort to preserve the metal material by maintaining it from corrosion. The novel inhibitor Scheme 1, was characterized via spectroscopic techniques.



Scheme 1. Synthesized inhibitor structure.

Materials and Methods:

Materials

Chemicals utilized were purchased from trade exporters and were used without additional purification. To confirm that the reaction occurred, thin layer chromatography (TLC) was used for the reaction using plates of silica gel and then visualized under UV light at (254 & 366) nm.

General procedure for the synthesis of inhibitor

Solution A, [that consists of thiosemicarbazide (0.10 mol) dissolved in the little amount of distilled water with CH_3COOH] and solution B, [that consists of 2-hydroxy-3-methoxy benzaldehyde (0.10 mol) dissolved in ethanol] were refluxed for 2 hrs. with constant stirring. The resultant solution was cooled, and the crystals were separated out by filtration then washed with water and ether several times, and dried. Yield 79%, M.P. =219-221 ℃.

Corrosion test

All alloy samples of mild steel were purchased from commercial sources and used as electrodes. The elements contained in alloy have the following percentages: Fe (99.21); C (0.21); Si (0.38); S (0.09); Mn (0.05) and Al (0.01). Cleaning of mild steel surface was done depending upon the technique mentioned in reference 14. The samples have been suspended in 200mL of corrosive solution in presence of the studied inhibitor 2-(2-hydroxy-3-methoxybenzylidene) hydrazinecarbothioamide (HMHC) at different concentrations of it : [0.00, 0.001, 0.05, 0.10, 0.15, 0.20, 0.25 and 0.50] g/L for periods: [1:00, 3:00, 5:00, 10:00, 24:00 and 72:00] hours. The effectiveness of the inhibitor has been calculated according to Eq. 1.

$$IE(\%) = \left(1 - \frac{W_2}{W_1}\right) \times 100 \qquad \ldots . 1$$

W_1/W_2; the alloy weights after and before the addition of HMHC.

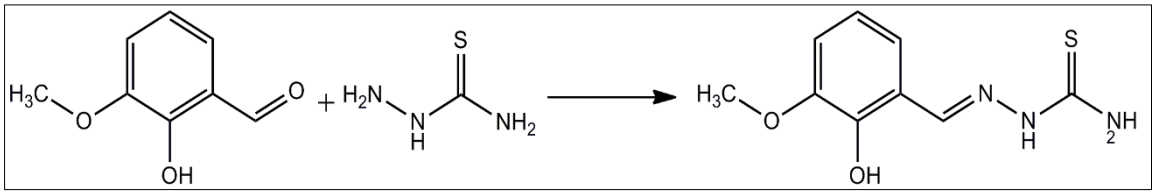
Computational studies

Ground-state chemical structure improvements have been done by Gaussian 09 program without symmetry limitations utilizing Correction A.02 [14,15]. The function R-B3LYP was applied in studied geometry improvements[16].

Results and Discussion:

Synthesis of HMHC

The inhibitor "2-(2-hydroxy-3-methoxybenzylidene) hydrazinecarbothioamide" (HMHC) was synthesized in an excellent yield through the reaction of equimolar of thiosemicarbazide (CH_5N_3S) and 2-hydroxy-3-methoxy benzaldehyde as in Scheme 2. The molecular formula of HMHC was figured. The prepared inhibitor was investigated by 1HNMR in DMSO-d6 to show these results: 11.04 (s, 1H) for hydroxyl group; 8.99 (s, 1H) for -C=N-; 8.57 (s, 1H) for amino group; 7.33–7.94 (m, 3H) for benzene ring and 3.74 (s, 3H) for methoxy group. CHN elemental analysis were C=47.12 (47.99); H= 4.77 (4.92); N= 18.52 (18.65).



Scheme 2. Synthesis reaction of HMHC.

Weight loss

The experimental steps based on ASTM standard[10], while the effect of the prepared compound on corrosion rate (CR) of MS. was performed by gravimetric test.

The use of corrosion inhibitors in factories has become of great economic importance because of its effects in protecting alloy surfaces from corrosive solutions[17], through using synthetic/natural organic molecules as an inhibitor to form barriers that are required for the protection of those surfaces. The utilization of organic inhibitors containing hetro-atoms such as (N-,O-,S-) atoms in their molecular structures was very significant due to the ability of the hetro-atoms to be linked through coordination bonds with the metal surface to form stable complexes [18-20].

Concentration effect

To estimate the inhibition efficiencies of HMHC, weight loss procedure [21,22] was used for that purpose with HMHC at various concentrations: [0.00, 0.001, 0.05, 0.10, 0.15, 0.20, 0.25 and 0.50] g/L for certain times: [1:00, 3:00, 5:00, 10:00, 24:00 and 72:00] hours, and acidic solution of HCl (1M) for the mild steel sample surface in 25 ℃. The results of HMHC were demonstrated in Fig. 1, and referred to the effectiveness of HMHC to diminish the corrosion at acidic solution of MS surface with excellent inhibition performance 90.20 %. The corrosion rate (CR) was diminished but the inhibition efficiency rise through increasing of concentration of HMHC, Inhibition efficiency IE(%) as shown as in Fig. 2.

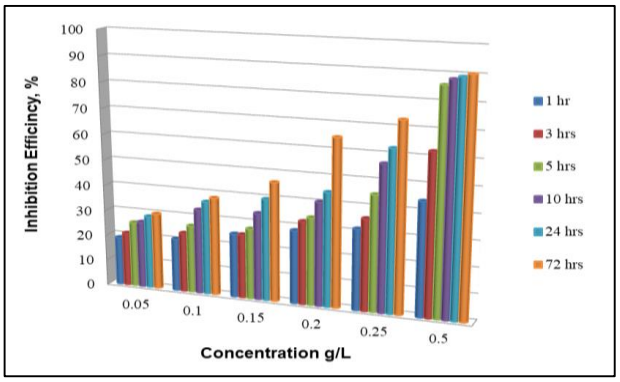


Figure 1. Function of time at concentrations of HMHC in of MS in 1 M hydrochloric acid.

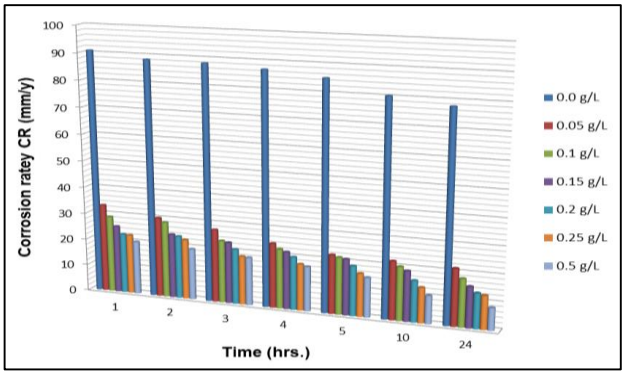


Figure 2. Impact of HMHC concentrations and time on CR at 303 K.

Temperature Effect

To estimate the effect of temperature on the performances of HMHC as corrosion inhibitor, the techniques were done in the absence and presence of HMHC for various temperature degrees 303K, 313K, 323K, and 333 K. By comparing the results, it was observed that the excellent inhibition efficiency for HMHC was at conc.$_{HMHC}$ = 0.5 g/L and T = 303K. HMHC can diminish corrosion. Fig. 3 shows temperature degrees' impact of HMHC on inhibition efficiency.

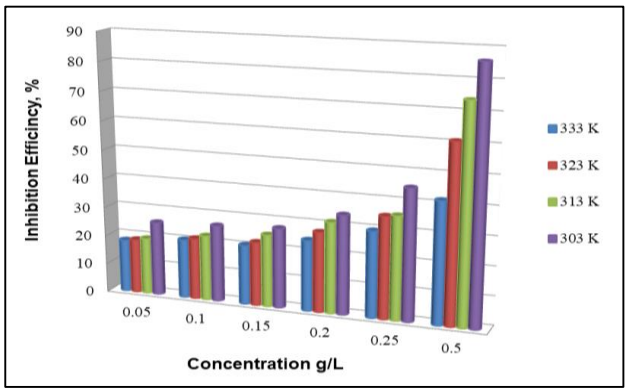


Figure 3. HMHC concentrations at different temperature degrees.

Corrosion inhibitor thermodynamic

The effectiveness of the temperature of synthesized inhibitor HMHC was studied in this test and was clear that the increasing in the solution temperature leads to increasing in corrosion rate and decrease in inhibitor efficiency. The variation in temperature was from 30 to 60 ℃, this variation decreasing the inhibitor efficiency from 90% to 31% [23]. The reaction energy or as called the activation energy Ea for both anode and cathode reactions was calculated in 1M HCl for different temperatures by using the Arrhenius equation and plot as in Eq. 2 [24,25].

$$C_r = A \exp(\frac{-E_a}{RT}) \quad \ldots . 2$$

The symbols: C_r acts as corrosion rate, while Ea is activation energy of the reactions, A is Arrhenius constant, T is solution temperature and R is ideal gas constant.

By plotting ln(C_r) with 1/T can show in Fig. 4 where it gives leaner relation with slop of Ea/R and in 0.5 g/L of inhibitor concentration for different temperature with and without the present of inhibitor. The activation energy values with and without synthesized inhibitor HMHC for this test were 56.88 and 30.17 kJ/mol respectively.

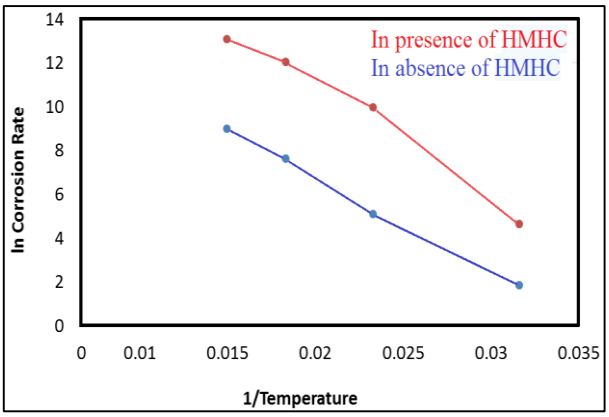


Figure 4. Arrhenius plot for blank and 0.5g/L of Inhibitor in 1M HCl

Corrosion inhibitor adsorption isotherm

Studying the isothermal adsorption process to determine the thermal effect on the corrosion rate and how increasing solution temperature can lead to a decrease in inhibitor efficiency is necessary for a better understanding of corrosion behavior with mild steel surfaces [26]. From the Arrhenius plot, it is clear that an increase in the solution temperature leads to increase in corrosion rate, and it will lead to a decrease in the inhibitor efficiency[24]. When the activation energy rang below 20 kJ/mol, the indication of physical adsorption [27]. While the increase in value of Ea indicates that the adsorption of HMHC on the surface of mild steel was chemical adsorption [28].

Gibbs free energy ΔG_{ads} for this process can be calculated from Eq. 3 to determine the isotherm adsorption for anodic and cathodic reaction.

$$\Delta G_{ads} = - RT\ ln(55.5K_{ads}) \quad \ldots . 3$$

Where R is ideal gas constant, K_{ads} is adsorption process equilibrium constant.

The ΔG_{ads} above 20 kJ/mol refers that the adsorption is chemical adsorption where it was 34.86 kJ/mol which refers to the strong interaction between molecules of synthesized HMHC that act as an inhibitor with the metal sample surface in hydrochloric acid solution (1M) .

The inhibitor performance against acidification of the surface of mild steel sample can be confirmed through the adsorption process on the surface of a metal, where it's affected on charge density and performance of the bonds between metal surface and inhibitor. The molecular structure of molecular of this inhibitor was in Fig. 4. The inhibition effectiveness of synthesized inhibitor HMHC depends mainly on the adsorb layers structure on the surface of alloy and adsorption nature .

In our research, an inhibitor was synthesized that consists of anisole ring and hetero organic chain that containing N-, O-, and S- atoms which

they have a high electron density that makes the inhibitor a good donor and makes it acts as a protective layer on the metal surface where it can be formed coordination between HMHC and surface of (MS.) [29].

DFT Investigations

Elucidation of the considerable electronic impact of the studied inhibitor molecules namely synthesized inhibitor with imines, thione, methoxy, and a hydroxyl (-OH) as strong electrons donate groups, have been investigated by DFT[30]. Anisole ring has a hydroxyl group at position-5 in inhibitor molecule while this hydroxyl group may move to position-3 (HMHC-3) and position-4 (HMHC-4). For the three molecular positions (2, 3, and 4), the commitment of the hydroxyl gathering for both regions of HOMO and LUMO was comparable to little varieties, Fig. 5 has shown this. Geometrical optimization structures for the studied structural formulas of HMHC (isomerism): (HMHC-2) (HMHC-3) and (HMHC-4) have been displayed in Fig. 5, Furthermore, Table 1 shows the electronic energies of HMHC and possible isomers.

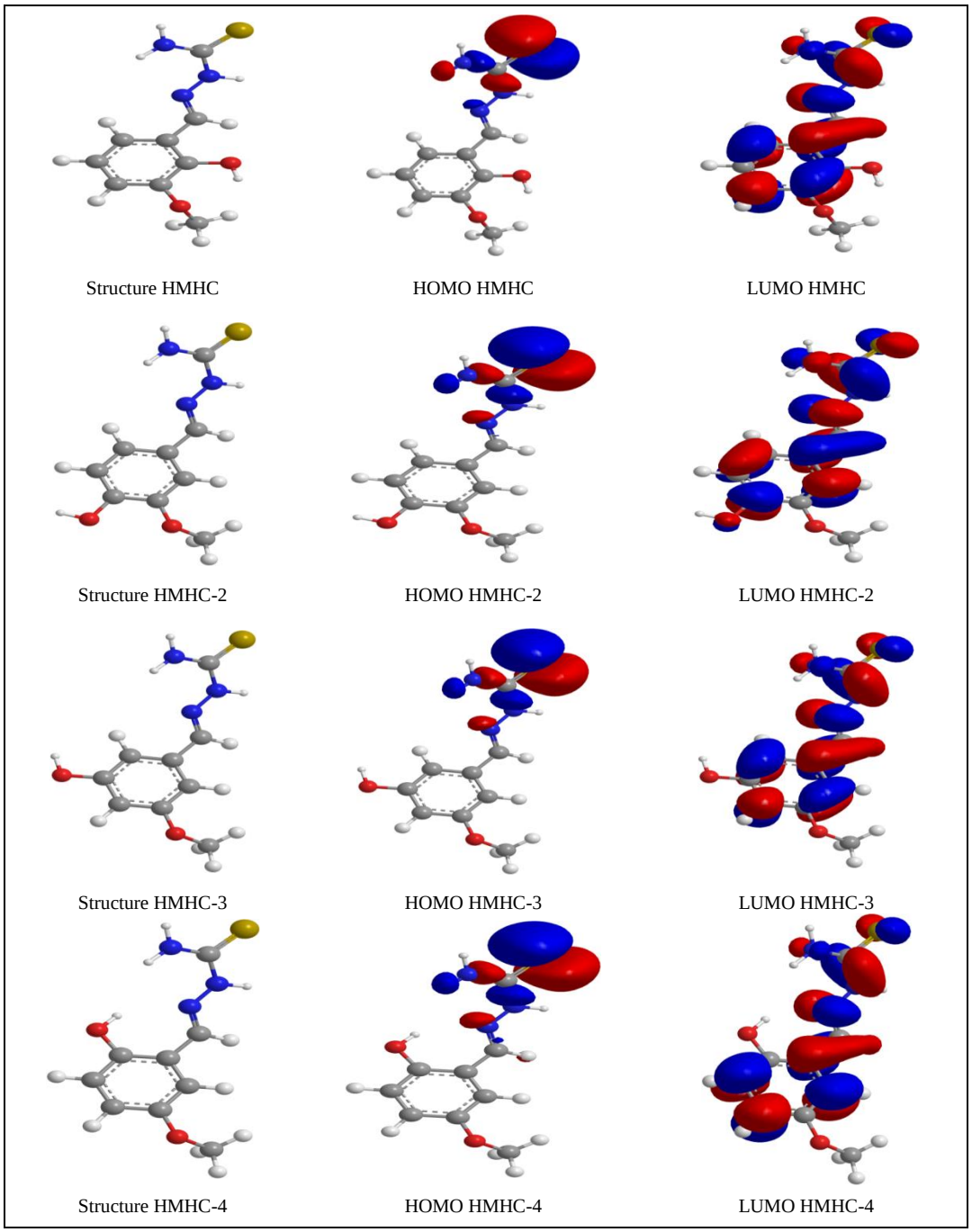


Figure 5. Molecular geometrical optimized structures, HOMOs "highest occupied molecular orbital" and LUMOs "lowest unoccupied molecular orbital", for HMHC and its isomers obtain through R-B3LYP6-31G(d,p).

Table 1. Calculated energies, ionization potentials (I) and electron affinities (A) for (HMHC-2) (HMHC-3) and (HMHC-4) obtaining by R-B3LYP/6-31G (d,p).

Molecules	E_{HOMO}	E_{LUMO}	E.gap	I	A (eV)
HMHC	-9.264	-1.388	7.976	9.264	1.388
HMHC-2	-9.241	-0.947	8.294	9.241	0.947
HMHC-3	-9.232	-1.422	7.810	9.232	1.422
HMHC-4	-9.243	-1.538	8.705	9.243	1.538

The (I) and (A) have been calculated based on Koopmans' theorem states, where $I = -E_{HOMO}$ and $A = -E_{LUMO}$

According to Al-Amiery et al work [31,32], Eqs. (4-6) were utilized to calculate the HMHC inhibition efficiency (%), and the results were displayed in Table 2.

$$I_{add}\% = \frac{I_{TAB} - I_{X-TAB}}{I_{BZ3}} \times 100\% \quad \ldots . 4$$

$$Ie_{add}\% = I_{add}\% \times Ie_{TAB}\% \quad \ldots . 5$$

$$Ie_{theory}\% = I_{TAB}\% + Ie_{add}\% \quad \ldots . 6$$

Where I_{add}% is the percent variation of the ionization potential of model x HMHC relative to that of HMHC also Ie_{add}% and Ie_{theory}% were the additional and theoretical inhibition performances respectively.

Table 2. Experimental and theoretical inhibition efficiency of the tested compounds.

Compound	Inhibition efficiency (%)	
	Experimental	Theoretical (Ie_{theory})
HMHC	90.20	89.73
HMHC-2	----	89.11
HMHC-3	----	88.25
HMHC-4	----	89.70

These results displayed that transferring of (-OH) group to 3-position caused a diminish in the performance of HMHC-inhibition and become 88.25%, on the other hand, the inhibition performance for 4-position for the compound HMHC-4) become 89.70%. A comparison between HMHC and HMHC-4 inhibition efficiencies (89.73% vs. 89.70%) indicates that this substitution position change improved the efficiency of the inhibition capacity [33].

Functional groups which have un-shared electrons, like hydroxyl group HMHC, had superior performance if the group substitute at 4- or 2-positions, so when the active groups donate electron pairs to the π-system, this causes them to become negative-charge on the sites ortho- or para- of the ring, and as it is known, these sites having superior activity towards electrophiles that electron-poor where the maximum densities of electrons concentrated on ortho-site and/or para-site.

Conclusion:

From obtained data can be said that the prepared compound 2-(2-hydroxy-3-methoxy benzylidene) hydrazinecarbothioamide" (HMHC) act as an excellent inhibitor of mild steel in acidic media. The inhibition efficiency increases with high concentration of HMHC, and low temperature degree, the maximum inhibition performance was about 90.20% at 0.5 g/L and 303K. Also, the variation temperatures degrees were proved that the adsorption process of molecules of inhibitor (HMHC) on the metal surface was chemical adsorption.

The study of thermodynamic parameters shows that the adsorption process of molecules of inhibitor (HMHC) on the metal surface was chemical adsorption and the adsorption of HMHC follows the Langmuir isotherm model.

The electronic characteristics of the HMHC molecules were obtained from density function theory (DFT) quantum chemical approach. Impressive correlations were discovered between the experimental approach and theoretical results.

Authors' declaration:

- Conflicts of Interest: None.
- We hereby confirm that all the Figures and Tables in the manuscript are mine ours. Besides, the Figures and images, which are not mine ours, have been given the permission for re-publication attached with the manuscript.
- Ethical Clearance: The project was approved by the local ethical committee in Ibn Sina University of Medical and Pharmaceutical Sciences**.**

Authors' contributions statement:

I. M .M. H. and N. J. K. conducted the experiment, M. S. S. conducted the DFT calculations, I. M .M. H. and F. S. J. wrote and revised the manuscript. All authors agreed to the final version of this manuscript.

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تحضير و تشخيص و تحقيق التأثير المثبط لمشتق الثيوسيميكاربازيد تجاه تآكل الفولاذ الطري في الوسط الحمضي

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الخلاصة:

ركزنا في هذه الدراسة على تحديد تأثير مشتق الثيوسيميكاربازيد المحضر و الذي يمكن تسميته '' 2- (2-هيدروكسي-3-ميثوكسي بنزيليدين) هيدرازين كاربوثايميد '' (HMHC) على تثبيط تآكل الفولاذ الطري في محلول حمضي من حامض كلوريد الهايدروجين بتركيز 1 مولاري كمحاولة جديدة للحفاظ على تركيب المواد المعدنية من خلال الحفاظ عليها من التآكل. تم تشخيص المثبط المحضر باستخدام تقنية تحليل العناصر و مطيافية الرنين المغناطيسي النووي. ثم تم دراسة قدرة المركب المحضر (HMHC) على تثبيط تآكل الفولاذ الطري في الوسط الحمضي بتقنية فقدان الوزن ضمن المتغيرات [درجة الحرارة و تركيز المثبط و الوقت]. حيث تراوح مدى درجات الحرارة بين (303 الى 330) كلفن و استخدمت تراكيز مختلفه من المثبط المحضر [0,00 و 0,001 و 0,05 و 0,1 و 0,15 و 0,2 و 0,25 و 0,5] غم/لتر ضمن فترات غمر معينه و هي [1:00 و 3:00 و 5:00 و 10:00 و 24:00 و 72:00] ساعة. اظهر المشتق المحضر قدرته على تثبيط التآكل و من خلال النتائج لوحظ أن معدل التآكل يتناقص مع زيادة تركيز المانع المحضر و يزداد مع زيادة درجة حرارة المحلول و ان اعلى كفاءة لعمل المثبط هي عند استخدام التركيز 0,5 غم / لتر حيث بلغت 90,2% و وجد أن عملية امتزاز المثبط HMHC تخضع لنموذج ايزوثيرم لانكماير. تم دراسة الخصائص الالكترونية للمثبط نظرياً باستخدام نظرية الدالة الوظيفية للكثافة DFT حيث تم الحصول على نتائج نظرية مقاربة بشكل كبير للنتائج العملية لهذه الدراسة.

الكلمات المفتاحية: امتزاز و تآكل الفولاذ الطري و نظرية الكثافة الوظيفية و قواعد شيف و ثيوسيميكاربازيد.