

Assessment of Salen Schiff Base as a Corrosion Inhibitor on Low-Carbon Steel in HCl Media: Practical and Computational Studies

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ABSTRACT

Corrosion poses a significant challenge to the longevity and performance of metallic materials, particularly low-carbon steel, in acidic environments such as hydrochloric acid (HCl). The use of corrosion inhibitors is a widely adopted strategy to mitigate this issue, enhancing the durability and service life of metal components. Thus, the objective of this work is to study the inhibition performance of N,N'-bis(salicylidene)ethylene-1,2-diamine Schiff base (Salen SB) for low-carbon steel (CS) in 0.5 M HCl. The study was conducted using weight loss (WL), electrochemical impedance spectroscopy (EIS), and potentiodynamic polarization (PP) techniques. The Salen SB was prepared and characterized using ¹H NMR and FTIR techniques. The efficiency of inhibition increased with an increase in Salen SB concentration. At a concentration of 300 ppm, the inhibitor exhibited the highest efficiency of 75.4% at 298 K. However, this efficiency decreased to 69.5% when the temperature was raised from 298 K to 333 K. The tested compound reduced both the double-layer capacitance (C_{dl}) and the corrosion current (I_{corr}), indicating the formation of a protective layer on the carbon steel (CS) surface. Additionally, the inhibitor demonstrated a mixed-type behavior, which was consistent with the Langmuir adsorption isotherm. It was revealed through scanning electron microscopy (SEM) and energy dispersive X-ray (EDX) investigations that the presence of the Salen SB facilitates the formation and adsorption of a stationary film on the CS surface. To further elucidate the interactions between Salen SB molecules and CS, density functional theory (DFT) and Monte Carlo (MC) simulations were employed. The quantum properties of Salen SB demonstrate its efficacy as an inhibitor. The findings from the DFT and MC simulations indicated that Salen SB interacts with the CS surface via the lone pair of electrons from the heteroatoms, as well as the π -electrons of the benzene ring. The calculated binding energy for this interaction was -160.150 kJ/mol.

Keywords: Carbon steel; Electrochemical Impedance Spectroscopy (EIS); Green corrosion inhibition; HCl medium; Inhibition efficiency; Material durability; Salen Schiff base.

INTRODUCTION

Corrosion causes the deterioration of metal properties by means of chemical or electrochemical reactions. CS is frequently utilized in many industrial and engineering fields because of its good mechanical characteristics, ease of accessibility, and economical effectiveness in comparison with various materials (Padash *et al.*, 2019); although there are many methods for maintaining CS surfaces, the most efficient method is to use inhibitors (Hassannejad and Nouri, 2018; Nabatipour *et al.*, 2020; Saha *et al.*, 2016; Srivastava *et al.*, 2017). The use of corrosion inhibitors is a widely adopted strategy to mitigate this issue, enhancing the durability and service life of metal components.

There are two main classes of corrosion inhibitors: inorganic and organic. Inorganic inhibitors, such as NO_2^- , NO_3^- , CrO_4^{2-} , $\text{Cr}_2\text{O}_7^{2-}$, and PO_4^{3-} , have been successful in controlling corrosion, but their adverse effects on the environment continue to be an important disadvantage. These substances, particularly chromates, have poor biological compatibility and are environmentally harmful (Olasunkanmi *et al.*, 2020). The most effective compounds, however, are organic

inhibitors because they have one or more polar groups in addition to π -electrons (El Faydy *et al.*, 2018). By adhering to the metal's surface and creating a barrier film, they successfully suppress corrosion (Al-Baghdadi *et al.*, 2021; Bahaa El-Dien *et al.*, 2019). Schiff bases are among these organic compounds that have strong potential to inhibit the corrosion of CS under a variety of conditions, particularly with sulfuric and hydrochloric acids (Abdallah *et al.*, 2019; Al-Najjar and Al-Baitai, 2022; Alwan, 2018; Chen *et al.*, 2021; Hashemi *et al.*, 2021; Jamil *et al.*, 2018; Nazir *et al.*, 2020; Wang, 2021; Zhang *et al.*, 2019). Schiff bases, particularly those derived from Salen ligands, have garnered attention due to their effectiveness and eco-friendliness. A few researchers reported that the unoccupied π^* orbitals in Schiff base molecules are responsible for the effectiveness of inhibition. The bond between inhibitor and metal is stabilized as the π^* orbitals facilitate the back donation of electrons from the metal to the inhibitor. In addition to being used in industry as corrosion inhibitors, Schiff bases and their compounds have significant applications as antibiotics, antioxidants, and anti-inflammatory drugs (Al-Amiery *et al.*, 2020; Jaafar and Saeed, 2020; Saha *et al.*, 2021).

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Natash Mary *et al.* (2022) investigated the effectiveness of two Schiff bases derived from triazoles:

4-[(furan-2-ylmethylidene)amino]-5-methyl-4H-1, 2, 4-triazole-3-thiol (FAMTT) and 4-[(4-chlorobenzylidene)amino]-5-methyl-4H-1,2,4-triazole-3-thiol (CAMTT). These compounds were tested for their ability to inhibit the corrosion of steel in a mixture of hydrochloric acid (HCl) and sulfuric acid (H₂SO₄) at a 2:1 ratio. The results indicated that as the temperature and concentration of the Schiff bases increased, the inhibitory effectiveness of both derivatives also rose. DFT calculations and experimental findings were correlated, and both showed that FAMTT is more efficient than CAMTT.

The Isatin Schiff base 2-(2-oxoindolin-3-ylidene)hydrazinecarbothioamide (OHB) was prepared by Al-Amiery *et al.*, (2022). They used electrochemical and gravimetric techniques to examine the corrosion resistance of mild steel specimens in 1.0 M HCl. Their research findings demonstrated the mixed-type and significant corrosion inhibition of OHB. The efficiency of inhibition increased as the temperature rose. Hegazy *et al.* (2021) have tested the azomethine compound (6E, 7E)-N1, N 6-bis (1-methylpyrrolidin-2-ylidene) hexane-1, 6-diamine as a CS corrosion inhibitor in a 0.5 M H₂SO₄ solution. They asserted that increasing the quantity of the synthetic inhibitor in the corrosive media enhances the inhibition efficiency.

In a 0.1 M HCl solution, Al-Najjar and Al-Baitar (2022) created and characterized a novel imidazole derivative, (N, N'E, N'E)-N, N'-(thiophene-2,5-diylbis(methanylylidene)) bis(1Hbenzo[d]imidazol-2-amine). Their results demonstrated that the inhibition efficiency rose with increasing compound dose; however, it decreased with rising temperature. At 0.5 mM of the manufactured inhibitor, 96% inhibition efficiency was the highest.

Kumari and Lavanya (2021) investigated the impact of the Schiff base N'-[4-(dimethylamino) benzylidene]-4-hydroxybenzohydrazide on the prevention of the dissolution of mild steel in HCl solution. The potency of the synthetic inhibitor to attach to mild steel was confirmed based on its kinetic and thermodynamic characteristics. According to the experimental findings, the chemical compounds under investigation appear to have strong inhibition properties.

The aim of this work is to synthesize a Salen Schiff base, characterize it, and examine its ability to inhibit CS corrosion in a solution of 0.5 M HCl. The corrosion experiments were completed using WL, EIS, and PP techniques. EDX and SEM were used to examine the CS surface. A variety of adsorption isotherms were used to understand how Salen Schiff base exists at the CS surface. In addition, some thermodynamic and activation characteristics have been estimated. Furthermore, DFT and MC simulations were performed to explain how Salen Schiff base molecules interacted with the CS surface.

MATERIALS AND METHODS

The CS utilized in the corrosion experiments has the

subsequent composition (wt. %):0.201 C, 0.602 Mn, 0.041 P, 0.0031 Si, 0.05 S, and the rest is Fe. The composition was determined using EDX analysis. Proton nuclear magnetic resonance (¹HNMR) spectra were collected on a Vario Germany 300 MHz spectrometer in dimethyl sulphoxide (DMSO) as the solvent. Fourier-transform infrared spectroscopy (FTIR) spectra have been captured on a Bruker Alpha 11 Germany infrared spectrometer. The electrochemical measurements were performed on OrigaLys Potentiostat - OGS 100.

Synthesis of N, N'-bis(salicylidene)butylene-1,4-diamine (SB)

Salicylaldehyde (4 mmol) and 1,2-diaminorthane (2 mmol) were refluxed together for 4 hours in ethanol to create Salen SB (Ab *et al.*, 2015). Yellow crystals having a melting point of 126–129 °C were obtained. The yield was 95.27%. Fig. (1) shows the chemical composition of the Salen SB.

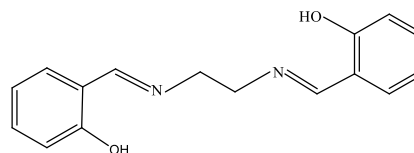


Figure (1): N, N'- bis (salicylidene) ethylene-1, 2-diamine (Salen SB). Mol. Formula: C₁₈H₂₄O₂N₂; Mol. Wt.: 384.56.

WL method

WL was established on CS in 0.5 M HCl medium without and with various doses (50–300 ppm) of Salen SB for 3 h within the temperature range of 298-333 K. The acidic solution was applied to a surface area of 9 cm² of CS. The weights of the polished, cleaned, and dried specimens were measured before they were submerged in the acidic solution. All samples were placed in a pickling solution (SnCl₂ and SbCl₃ in 1:1 HCl) for 2 min to eliminate the corrosion products. The sample is then cleaned with 5% NaHCO₃ before being dried, weighed, and finally washed with distilled water (AATIAOUI *et al.*, 2021). The rate of corrosion (CR) was computed using the following equation:

$$CR = \frac{W_1 - W_2}{At}$$

Where, W₁ and W₂ are the masses of CS prior to and after submerging in the corrosion medium, respectively, A is the CS area per cm², and t is the submerging duration in seconds. Meanwhile, the inhibition efficiency (IE_w) was calculated using the equation:

$$IE_w = \frac{W_o - W_i}{W_o} \times 100$$

$$\theta = \frac{W_o - W_i}{W_o}$$

Where, W_o and W_i are the WL devoid of and with the inhibitor, respectively. θ is the surface coverage of CS.

Electrochemical techniques

The corrosion behavior of CS was studied using PP and EIS techniques. A cell containing a Pt counter electrode, a CS rod as the working electrode (WE), and Ag/AgCl as a reference electrode was utilized for the study. The WE with a surface area of 1 cm² was polis-

hed with materials of varying abrasiveness and cleaned with ethanol and double-distilled H₂O prior to usage. To achieve the greatest stability, the electrode was eventually inserted into the testing medium at the open-circuit potential (OCP) for 30 mins. PP study was recorded in the potential range of -150 to -650 mV against Ag/AgCl with a scan rate of 1 mV s⁻¹. The method of Stern-Geary was used to determine the corrosion current for every concentration of the Salen SB and the blank solution. All investigations were performed at 25°C and performed 3 times to ensure precision. Using AC pulses at OCP with 5X10⁻³ V³ peak to peak amplitude, the EIS was carried out in the frequency range of 100 kHz to 5X10⁻⁴ Hz. Both the Bode and Nyquist types of the EIS graphs were drawn. PP and EIS were established via the biological instrument OrigaLys Potentiostat (OGS 100) and the ECLAB program. For data visualization, graphing, and fitting, Origin 2021 and Microsoft Office 2016 were utilized.

Surface examination

CS specimens were submerged in 0.5 M HCl media in the nonexistence and existence of 300 ppm of Salen SB for 72 hrs. Then, they were washed with distilled water, dried, and tested by SEM on a BED-C 10 kV, Jeol equipped with an EDX instrument to examine the surface topography and the composition of the adsorbed coating.

Computational studies

Computational studies were used to link the quantum chemical characteristics with the claimed inhibition activity of the tested compound and to explain the mechanism of adsorption. Quantum operators were computed using DFT/6-31+G (d) and MC simulations.

RESULTS

Validation of the synthesized Salen SB's structure

¹HNMR study

The ¹HNMR spectrum of Salen SB showed a singlet peak appearing at 3.90 ppm that corresponds to the 4 protons of the two -CH₂N groups. In addition, the ¹HNMR spectrum demonstrated the characteristic signals of the 8 aromatic protons of the two salicylidene rings as several signals between 6.84-7.42 ppm and a singlet peak at 8.56 ppm for the two protons of the two -CH=N groups in addition to a broad signal for the two OH protons between 13.30-13.5 ppm. The ¹HNMR spectrum of Salen SB is displayed in Figure (2).

FTIR study

IR patterns demonstrate peaks at 1283.91 cm⁻¹ that correspond to (C-O), 1498.06 cm⁻¹ corresponding to (C=C), 1622.09 cm⁻¹ (C=N) and peak appears in the region of 3740.31 to 3864.56 cm⁻¹ corresponding to (OH), Figure (3).

WL measurements

The inhibition impact of the Salen SB was evaluated at various concentrations in a 0.5 M of HCl solution. The table (1) presents the corrosion rate (CR), contact angle (θ) and inhibition efficiency (IE_w). The corrosion rate decreases as the concentration of the substance increases. Starting from a blank value of 1.80 ± 0.3 mg cm⁻² s⁻¹, after which it declines steadily to 0.44 ± 0.3 mg

cm⁻² s⁻¹ at 300 ppm. Meanwhile, the contact angle increased as the concentration Salen SB increased which enhance the inhibition of CR. These results clearly indicate an improvement in surface hydrophobicity, which can be linked to better protection against corrosion as the surface becomes less wettable by the corrosive medium. Consequently, the inhibition efficiency showed a clear upward trend with increasing concentrations of the corrosion inhibitor (Table 1).

The general patterns in the results show a clear correlation between the substance's concentration and corrosion-inhibiting efficacy. Greater hydrophobic qualities, improved inhibitory efficiency, and decreased corrosion rates are all correlated with higher concentrations. These results suggest that improving this substance's concentration may result in more successful corrosion control techniques in appropriate applications. Future researches are in need to examine the inhibitory effect's long-term stability as well as its usefulness in actual corrosion situations.

The impact of temperature

Data presented in Table (2) on corrosion rates (CR) across different concentrations and temperatures, provides valuable insights into the behavior of metal corrosion in relation to varying conditions, in which the corrosion rates at lower temperatures (298 K to 313 K) noticeably decrease as the inhibitor concentration rises (from 50 ppm to 300 ppm). However, at higher temperatures (323 K and 333 K), where corrosion rates start to converge, these inhibitors lose their effectiveness. Meanwhile, data showed that the greatest rate of corrosion was observed at higher temperatures even when inhibitors are not present. These results indicate that higher temperatures may enhance the corrosive effects under the same condition. The observed trend suggests that higher temperatures generally improve reaction kinetics, most likely as a result of increased molecular mobility and reactant

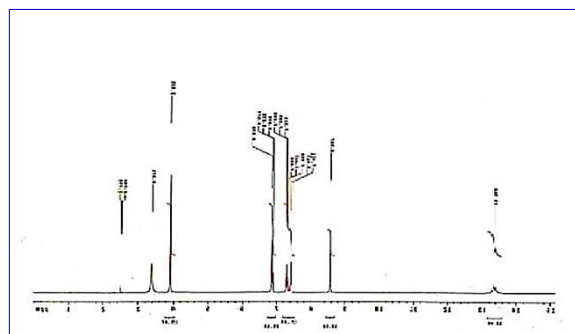


Figure (2): ¹HNMR spectrum of Salen SB.

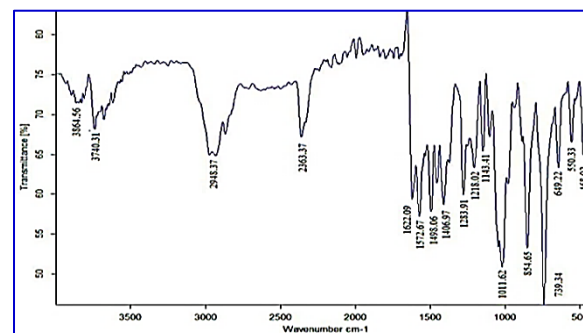


Figure (3): IR spectra of Salen SB.

collision frequency. At lower concentrations, where temperatures greatly increase the CR values, the response is most noticeable. This observed result indicates that, generally, higher temperatures enhance reaction kinetics, likely due to higher molecular motion and collision frequency among reactants. The response is most pronounced at lower concentrations, where temperatures significantly elevate the CR values. Meanwhile, the decline in reaction rates at higher concentrations may suggest a threshold concentration beyond which additional substrate does not facilitate an increase in the rate, potentially due to saturation effects or other kinetic phenomena. Therefore, further study is in need to determine this threshold concentration under tested conditions.

Thermodynamic and activation parameters

Understanding of the behavior of an inhibitor during the adsorption process relies on thermodynamic factors. For the corrosion process of CS in a 0.5 M of HCl solution, the activation parameters, such as activation energy (E_a^*), enthalpy change (ΔH_a^*), and entropy change (ΔS_a^*) have been estimated. The transition-state and Arrhenius plots for the Salen SB

Table (1): Effect of Salen Schiff Base concentration on weight loss (WL) of carbon steel in 0.5 M HCl at 25 °C.

Conc. (ppm)	Measured parameters		
	CR ($\text{mg.cm}^{-2}.\text{s}^{-1}$) $\times 10^{-4}$	θ	IE _w
Blank	1.80 ± 0.3	-	-
50	0.93 ± 0.2	0.480	48.0
100	0.72 ± 0.1	0.600	60.0
150	0.61 ± 0.1	0.657	65.7
200	0.56 ± 0.2	0.695	69.5
250	0.51 ± 0.2	0.714	71.4
300	0.44 ± 0.3	0.754	75.4

Table (2): Effect of temperature on corrosion rate of carbon steel in 0.5 M HCl at 25 °C at different Salen SB concentrations.

Conc. (ppm)	CR ($\text{mg.cm}^{-2}.\text{s}^{-1}$) $\times 10^{-4}$			
	Temperature (in Kelvin [†])			
	298	313	323	333
Blank	1.80 ± 0.30	3.0 ± 0.3	3.5 ± 0.5	5.0 ± 0.2
50	0.93 ± 0.20	1.5 ± 0.2	1.8 ± 0.3	2.7 ± 0.4
100	0.72 ± 0.10	1.2 ± 0.4	1.5 ± 0.1	2.2 ± 0.1
150	0.61 ± 0.50	1.1 ± 0.5	1.3 ± 0.4	1.9 ± 0.3
200	0.56 ± 0.40	1.0 ± 0.4	1.2 ± 0.3	1.8 ± 0.2
250	0.51 ± 0.20	0.9 ± 0.1	1.1 ± 0.1	1.6 ± 0.5
300	0.44 ± 0.60	0.8 ± 0.2	0.9 ± 0.2	1.5 ± 0.6

[†]Temp. from Kelvin to Celsius scales: C=K-273.15.

Table (3): Effect of temperature on contact angle (θ) and inhibition efficiency (IE_w) of Salen SB at different concentrations on carbon steel placed in 0.5 M HCl.

Conc. (ppm)	Temperature (in Kelvin [†])							
	298		313		323		333	
	θ	IE _w	θ	IE _w	θ	IE _w	θ	IE _w
Blank	-	-	-	-	-	-	-	-
50	0.480	48.00	0.486	48.6	0.479	47.9	0.460	46.0
100	0.600	60.00	0.580	58.0	0.569	56.9	0.551	55.1
150	0.657	65.70	0.636	63.6	0.622	62.2	0.616	61.6
200	0.690	69.50	0.650	65.0	0.642	64.2	0.630	63.0
250	0.710	71.40	0.700	70.0	0.686	68.6	0.665	66.5
300	0.750	75.40	0.733	73.3	0.718	71.8	0.695	69.5

[†]Temp. from Kelvin to Celsius scales: C=K-273.15.

compound ($\ln k_{\text{corr}}$ (corrosion factor) vs. T^{-1} and $\ln k_{\text{corr}}/T$ vs. T^{-1} , respectively) are displayed in Figure (4).

In the given system, the activation energy (E_a^*) steadily rises with concentration from 23.32 kJ mol⁻¹ (blank) to 27.45 kJ mol⁻¹ at 300 ppm, as shown in Table (4), which also offers data on other thermodynamic parameters and their correlation with concentration (ppm). This suggests that greater concentrations might strengthen the chemical reaction barrier, either as a result of steric interference or enhanced molecule interactions. Additionally, the enthalpy change (ΔH_a^*) gradually increases from 20.64 kJ mol⁻¹ in the blank to 24.57 kJ mol⁻¹ at 300 ppm. According to this pattern, the heat content of the reaction may be rising as the concentration does, most likely due to stronger reactant interactions. The entropy shift ($-\Delta S_a^*$) appears relatively stable across the concentrations, with values fluctuating slightly around 245 J K⁻¹ mol⁻¹. A stable entropic change suggests a constant energy distribution or reaction pathway and suggests that concentration variations may not have a substantial impact on the system's disorder (Table 4).

In general, higher concentrations may result in more complicated or stable chemical intermediates that need more energy to activate, as seen by the steady increase in both E_a^* and ΔH_a^* with concentration. However, the relative constant $-\Delta S_a^*$ indicates that the degree of disorder associated with the reaction is constant at all concentrations. These outputs are confirmed by the presence of a strong linear relationship between concentration and the corresponding thermodynamic parameters.

Adsorption isotherm

The surface coverage (θ) and inhibitor concentration (C_{inh}) are used to verify the specific details of Salen SB adsorption at the CS surface. Various types of isotherms were examined, such as Langmuir, Freundlich, and Temkin. The Salen SB adsorption is consistent with Langmuir's model. The fitted data is represented in Figure (5). The results collected from the isotherm are displayed in Table (5).

Electrochemical measurements

PP study

Figure (6) shows how the Salen SB affected the V-I graph of CS in 0.5 M HCl. Potentiodynamic polarization parameters of CS in 0.5 M HCl without and with various concentrations of Salen SB compound at 25 °C are shown in Table (6).

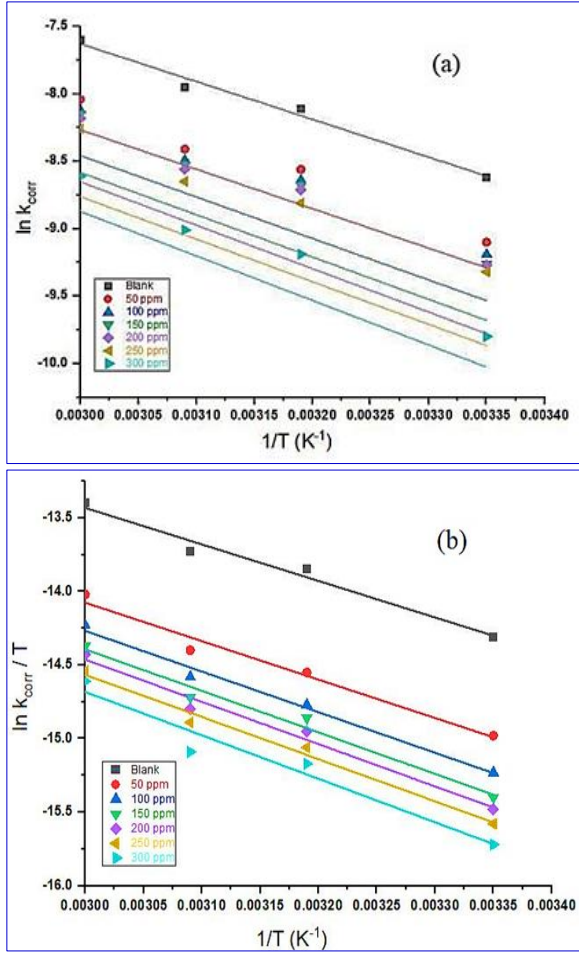


Figure (4): Arrhenius plots (a), and transition-state plots (b) for the corrosion of CS in 0.5 M of HCl without and with different concentrations of Salen SB.

Table (4): Effect of concentration on activation energy, enthalpy, and entropy changes in corrosion Inhibition by Salen SB of carbon steel in 0.5 M HCl.

Conc. ppm	E_a^* kJ mol ⁻¹	ΔH_a^* kJ mol ⁻¹	$-\Delta S_a^*$ J K ⁻¹ mol ⁻¹	R ² (Regression coefficient)
Blank	23.32	20.64	247.25	0.984
50	24.33	21.73	249.33	0.979
100	25.57	22.97	247.17	0.990
150	26.08	23.48	246.67	0.983
200	26.78	23.9	246.01	0.985
250	27.07	23.92	245.92	0.989
300	27.45	24.57	245.84	0.983

Table (5): Effect of temperature on adsorption parameters for Salen SB on carbon steel in 0.5 M HCl: Equilibrium constant (K_{ads}) and standard free energy (ΔG_{ads}^0).

Temp (K) [†]	Slope	Intercept	K_{ads} (mol ⁻¹)	$-\Delta G_{ads}^0$ (kJ mol ⁻¹)	R ²
298	1.18	47.97	2084.63	28.88	0.998
313	1.22	48.40	2066.11	30.31	0.995
323	1.25	48.80	2049.18	31.26	0.996
333	1.29	49.24	2030.86	32.20	0.997

[†]Temp. from Kelvin to Celsius scales: C=K-273.15

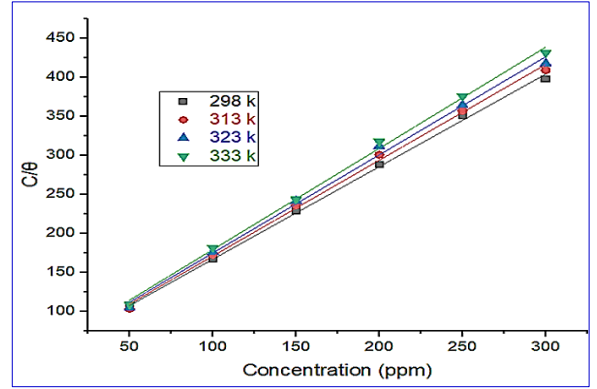


Figure (5): Langmuir adsorption isotherms for CS in 0.5 M HCl in the absence and presence of the Salen SB compound at different temperatures

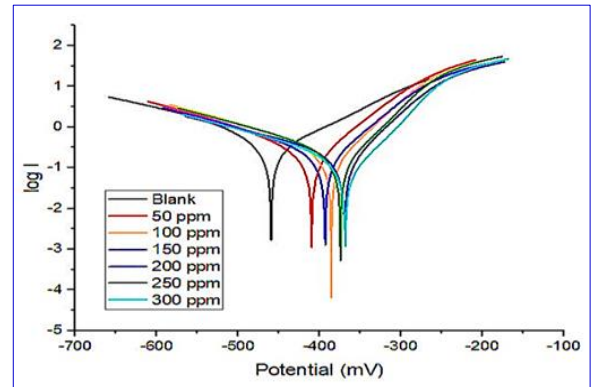


Figure (6): Tafel plots for CS in 0.5 M HCl in the absence and presence of different concentrations of Salen SB compound at 25 °C.

In table (6), the electrochemical behavior recorded that as the concentration of the inhibitor increases from the blank to 300 ppm, there is a noticeable tendency of decreasing I_{corr} values, indicating that the inhibitor effectively reduces corrosion rates at higher concentrations. This is critical as it suggests that the protective effect against corrosion is highly dependent on inhibitor concentration. In addition, the inhibition efficiency (IE_p) also recorded similar pattern in which a consistent increase with higher concentrations of the inhibitor, reaching 77.8% at 300 ppm, was documented. This signifies that not only does the decrease in I_{corr} confirm the efficiency of the inhibitor, but it also highlights its potential application in practical corrosion control scenarios.

EIS measurements

EIS studies were performed to clarify the corrosion process and describe the inhibitory mechanism. Figure (7) displays the Nyquist and Bode diagrams of CS devoid of and with various doses of Salen SB. In this Nyquist plot, the curves represent impedance data collected at varying concentrations (from 50 ppm to 300 ppm) of an additive in an electrochemical system, along with a blank (control) sample with no additive. Each curve corresponds to a specific concentration. The graph displays a semicircular trend, which is indicative of the system's charge-transfer resistance. The semicircle's size typically increases when the concentration is added. This implies that increased concentrations may have an impact on the

electrochemical characteristics, most likely raising the barrier to charge transfer. The impedance response is strongly influenced by additive concentration, as evidenced by the biggest semicircle seen in the 300 ppm concentration and the smallest in the blank sample.

For the graph (7b), it illustrates how log impedance ($\log[Z]$) varies with log frequency for various concentrations (ppm), which is typical for impedance behavior in materials as frequency increases. In addition, as the log frequency increases (towards the right side of the graph), the impedance values across all concentrations converge towards similar values. This suggests that at higher frequencies, the influence of concentration on impedance becomes minimal.

The electrical equivalent circuit shown in Figure (7c) was utilized to analyze the impedance data that was acquired, which might be used for impedance spectroscopy analysis of materials or electrochemical cells. The circuit contains two resistors (R_s and R_1), two capacitors (C_1 and C_2), and a Warburg element (represented by W).

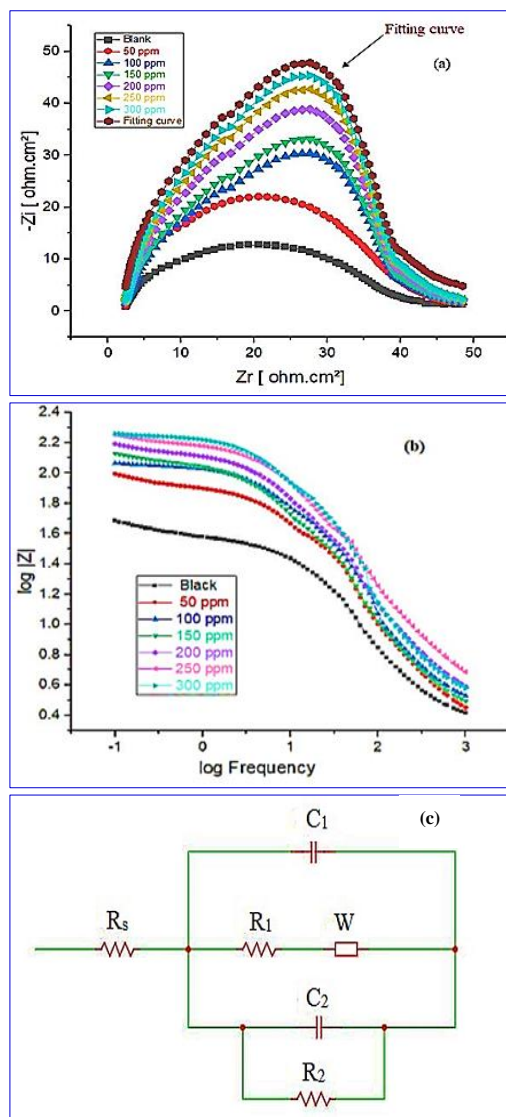


Figure (7): Nyquist (a) and Bode (b) Plots with equivalent circuit model (c) showing the effect of SB concentration on impedance and phase angle used to fit experimental EIS data.

Table (7), represent the EIS data of CS in 0.5 M HCl in which the provided data reflect an analysis of the impact of varying concentrations (ppm) on several electrical properties, including resistance (R_1 and R_2 in $\Omega \text{ cm}^2$), Warburg impedance (W in $\Omega/\text{s}^{1/2}$), capacitance (C_1 and C_2 in μF), a dimensionless parameter (θ), and the percentage inhibition efficiency (%IE). For resistance, as the concentration increases from the blank sample to 300 ppm, both R_1 and R_2 show an upward trend. This suggests that higher concentrations may lead to increased resistance, possibly due to increased ionic interactions or a thicker layer of the substance reducing ionic mobility. Meanwhile, the Warburg impedance also increases with concentration and shows a clear relationship where W rises from a hypothetical negative value at blank to $116.64 (\Omega/\text{s}^{1/2})$ at 300 ppm. This relates to the diffusion of ions; higher resistance typically means more difficulty in ion movement, correlating spontaneously with the rising concentration.

The percentage IE increases steadily with concentration, rising from 74.4 ± 0.1 at 300 ppm to no inhibition in the blank. This implies that improved performance or efficacy of the process being suppressed or aided is correlated with higher concentrations. The gradual increases in inhibition efficiency show that the concentration has a direct impact on the system's efficacy (Table 7).

Morphology and structure of the CS surface

SEM inspection

The SEM micrographs of the polished CS sheet (a), after exposure to 0.5 M HCl at ambient temperature for 72 hrs (b), and after exposure to blank solution + 300 ppm of Salen SB at ambient temperature for 72 hrs (c), are displayed in Figure (8, left panel).

EDX inspection

To explore the chemical structure of the CS surface in 0.5 M HCl, the EDX analyses of CS samples exposed to HCl solution with Salen SB versus to blank, were carried out (Figure 9).

Quantum chemical calculations

DFT results

To investigate the features of the interaction between the CS surface and the Salen SB adsorption sites, a DFT study was conducted. The quantum chemical parameters have a relation to the measured SB inhibitory efficiency. Figure (8, right panel) shows the ideal SB structures, including the HOMO and LUMO molecular orbitals that are highest occupied and lowest unoccupied, respectively.

Table (8) lists the quantum parameters that may affect the way Salen SB interacts with CS. The Table reports the electronic parameters for the energy gap (ΔE), ionization potential (I), electron affinity (A), chemical potential (μ) electronegativity (χ), global hardness (η), softness (σ), electrophilicity index (ω), nucleophilicity (ϵ), and a proportion of electron transfer (ΔN_{max}). The aforementioned parameters are calculated according to the following equations:

$$\Delta E = E_{\text{LUMO}} - E_{\text{HOMO}}$$

$$I = -E_{\text{HOMO}}$$

$$A = -E_{\text{LUMO}}$$

$$\mu = -\chi$$

$$\mu = \frac{(E_{\text{HOMO}} + E_{\text{LUMO}})}{2}$$

$$\eta = \frac{(E_{\text{LUMO}} - E_{\text{HOMO}})}{2}$$

$$\sigma = 1/\eta$$

$$\Delta N_{\text{max}} = \frac{-\mu}{\eta}$$

$$\omega = \frac{\mu^2}{2\eta}$$

$$\varepsilon = 1/\omega$$

Where, I is the ionization energy; E_{LUMO} is the Lowest unoccupied molecular orbital; μ , denotes the chemical potential, and χ represents the electronegativity of the molecule; HOMO, is the highest occupied molecular orbital; η , is often referred to as the energy gap or band gap; σ is the inverse of the energy gap (η); ΔN_{max} , is the maximum number of electrons that can be accepted by a molecule/system and ω , represents some form of energy or work associated with charge transfer.

MC simulation

Simulated annealing is a tool for optimization in Monte Carlo modeling, which is based on the theory of molecular mechanics (Kirkpatrick et al., 1983). When compared to quantum mechanical simulation, MC simulation is more efficient because it runs more quickly and costs less money. The sort of adsorption is influenced by the inhibitor's chemical composition. Using MC simulations enables us to know the adsorption behavior of the CS surface and the type of contact between the Salen SB and the CS surface. The descriptors calculated, by the Monte Carlo simulation, for the adsorption of the Salen SB compound on the CS surface was illustrated in Table (9) and figure (10).

DISCUSSION

The data obtained from WL measurements clearly display that the inhibition efficiency ameliorates as the concentration of Salen SB increases, and the highest efficiency is 75.4% at 300 ppm. The surface coverage (θ) of the adsorbed Salen SB molecules increases as its concentration increases in the corrosive medium. This result reflects that the examined compound has good inhibition properties. The CS corrosion rapidly increased as the temperature increased in ether of presence

Table (6): Potentiodynamic polarization parameters of CS in 0.5 M HCl without and with various concentrations of Salen SB compound at 25 °C.

Concn. (ppm)	$-E_{\text{corr}} \times 10^{-3}$ (V)	$\beta_a \times 10^{-3}$ (V dec ⁻¹)	$-\beta_c \times 10^{-3}$ (V dec ⁻¹)	$I_{\text{corr}} \times 10^{-3}$ (A cm ⁻²)	θ	IE _p
Blank	459.5	146.5	222.8	0.7032	-	-
50	409.7	84.3	189.4	0.3479	0.505	50.5 ± 0.2
100	385.6	69.1	171.9	0.2652	0.622	62.2 ± 0.1
150	369.7	66.1	209.9	0.2137	0.696	69.6 ± 0.3
200	393.2	71.6	162.4	0.2116	0.699	69.9 ± 0.4
250	374.3	60.3	149.6	0.1889	0.731	73.1 ± 0.5
300	368.2	62.5	170.2	0.1555	0.778	77.8 ± 0.1

Table 7. EIS data of CS in 0.5 M HCl in the absence and presence of different concentrations of the Salen SB at 25 °C.

Conc. (ppm)	R1 (Ω cm ²)	R2 (Ω cm ²)	W (Ω / s ^{1/2})	C1 × 10 ⁻⁶ (F)	C2 × 10 ⁻⁶ (F)	θ	%IE
Blank	22.45	16.54	-	423.45	355.45	-	-
50	56.66	23.98	33.21	365.76	323.94	0.516	51.6 ± 0.3
100	74.31	55.76	56.83	323.87	295.66	0.619	61.9 ± 0.1
150	88.65	63.19	69.96	290.78	277.31	0.650	65.0 ± 0.4
200	101.4	78.43	87.23	240.19	212.62	0.701	70.1 ± 0.2
250	122.65	91.74	101.58	201.64	171.65	0.729	72.9 ± 0.5
300	131.24	102.34	116.64	180.97	133.87	0.744	74.4 ± 0.1

Table (8): Quantum chemical parameters obtained from DFT theory for the Salen SB molecule.

Volume (cm ³ mol ⁻¹)	E_t (au)	TNC (e)	ω	χ (au)	μ (au)	σ (au) ⁻¹	η (au)	DM (Debye)	ΔE (au)	LUMO (au)	HOMO (au)
228.735	-878.997	-3.587	0.101	0.134	-0.134	11.236	0.089	2.699	0.178	-0.045	-0.223

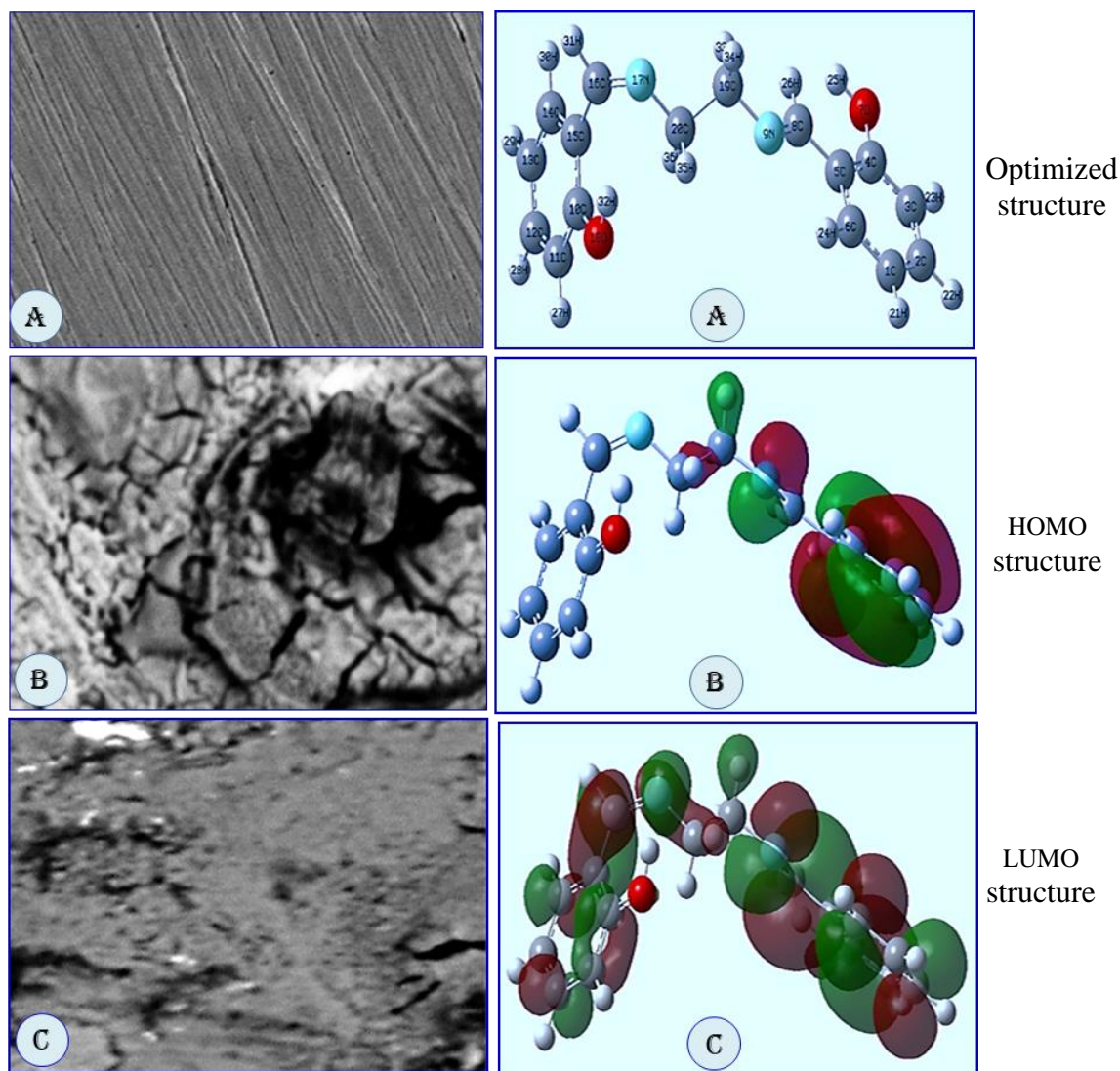


Figure (8): SEM micrographs (left panels) in comparable to molecular electronic modelling (right panels) of treated carbon steel surfaces showing morphological and chemical analysis before and after immersion in 0.5 M HCl. A, Polish carbon steel (CS); B, CS after 72 hrs immersion 0.5 M HCl; C, CS after 72 hrs immersion in 0.5 M HCl combined with the Salen SB at concentration 300 ppm.

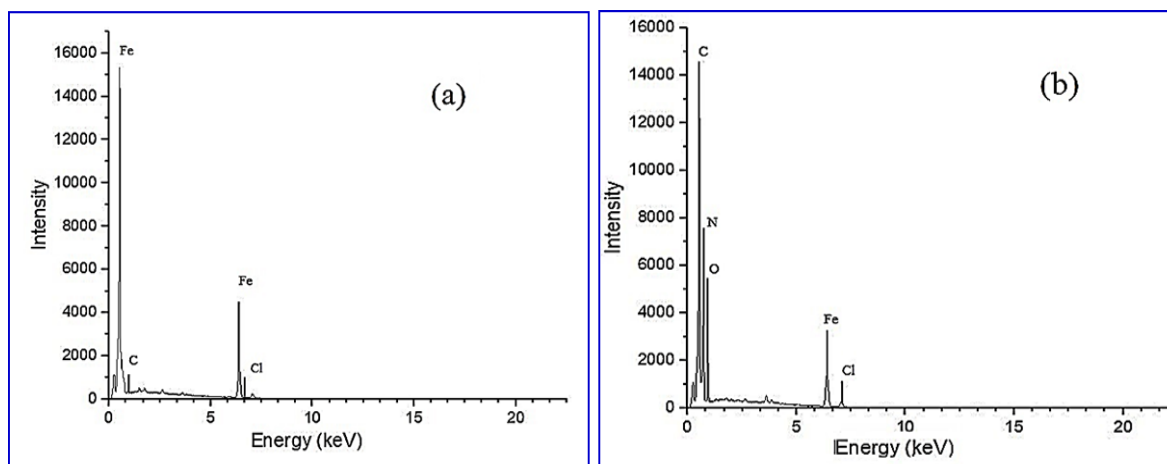
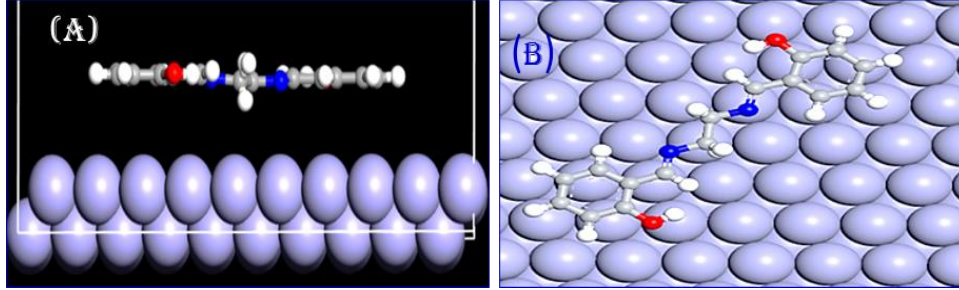


Figure (9): EDX spectra of CS specimens: (a) after immersion in 0.5 M HCl without Salen SB, and (b) with 300 ppm of the Salen SB compound.

Table (9): The descriptors calculated by the Monte Carlo simulation for the adsorption of the Salen SB compound on the CS surface.

Molecule	Total energy (kJ mol ⁻¹)	Adsorption energy (kJ mol ⁻¹)	Rigid adsorption energy (kJ mol ⁻¹)	Deformation energy (kJ mol ⁻¹)
Salen SB	-219.522	-166.15	-147.84	-18.31

**Figure (10):** Side view (A) and top view (B) for the adsorption of the Salen SB on the CS surface.

or absence of the synthesized Salen SB. This could be due to the increased impacts of rising temperature on the speed of electrochemical processes (Kamel *et al.*, 2022). With rising temperatures, the effectiveness of inhibition drops. The main factor contributing to the reduce in inhibition efficiency value at elevated temperatures may be due to the desorption of the Salen SB compound from the CS surface. Both Arrhenius and transition-state equations were employed to determine the activation parameters as follow:

$$k_{corr} = A \exp\left(\frac{-E_a^*}{RT}\right)$$

$$\ln\left(\frac{k_{corr}}{T}\right) = \left(\ln\left(\frac{k_B}{h}\right) + \left(\frac{\Delta S_a^*}{R}\right)\right) - \frac{\Delta H_a^*}{RT}$$

$$CR = k_{corr} \times i_{corr}$$

Where, k_{corr} is the corrosion factor, i_{corr} is the corrosion current, CR is the corrosion rate, R is the gas constant, k_B is the Boltzmann's constant, T is the Kelvin temperature, and h is the Planck's constant.

The Arrhenius figure, which displays a straight line with a slope of $-E_a^*/R$, is used to calculate the E_a^* for the corrosion process. As Salen SB retards the corrosion process, the energy of activation increases as Salen SB concentration rises. The Salen SB may attach to the CS surface, or this increase may result from a change in the potential difference at the CS-solution interface because of adsorption. Transition-state graphs display straight lines with $(\ln k_B/h) + (\Delta S_a^*/R)$ as their intercepts and $(-\Delta H_a^*)/R$ as their slopes that utilized to determine the magnitudes of ΔS_a^* and ΔH_a^* as shown in Table (4). The positive signs of ΔH_a^* indicate that heat absorption is necessary for the formation of activated complex in the transition state. According to the negativity of ΔS_a^* , the activated complex is more ordered than the reactants. Salen SB adheres to the Langmuir adsorption isotherm. Using the following formula of Singh and Quraishi (2012), the Langmuir isotherm is determined using the following equation:

$$C_{inh}/\theta = (1/K_{ads}) + C_{inh}$$

Where, C_{inh} is the Salen SB concentration and K_{ads} is the equilibrium constant for the adsorption process.

The CS surface's Langmuir adsorption isotherm for the Salen SB recorded the values of linear correlation coefficients, R^2 , that are close to one that supports the Langmuir type of adsorption. It is worth observing that the slope of the lines is greater than 1, indicating that there are lateral interactions between adsorbed molecules (Gómez-Sánchez *et al.*, 2023). The K_{ads} were estimated using the intercepts of the straight lines. The effect of temperature also demonstrate that as temperature rises, the K_{ads} value declines (Shahabi *et al.*, 2019). In light of equation (7), the standard free energy change for adsorption (ΔG_{ads}°) can be calculated as follow:

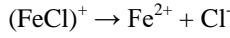
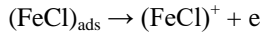
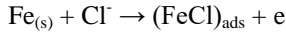
$$\Delta G_{ads}^\circ = -RT \ln(55.5 K_{ads})$$

Where, R is the gas constant, T is the Kelvin temperature, and 55.5 is the molar concentration of water (El-Etre *et al.*, 2015).

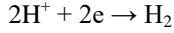
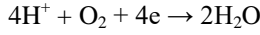
The negativity of ΔG_{ads}° reflects the spontaneous adsorption of the Salen SB compound onto the surface of the CS. The literature indicates that ΔG_{ads}° values can be maintained at 20 kJ mol⁻¹ by electrostatic attraction between charged metals and charged molecules (physisorption). The values bigger than 40 kJ mol⁻¹ suggest the occurrence of chemisorption (Al-Amiery *et al.*, 2020). The values of ΔG_{ads}° for the Salen SB range between -28.88 and -32.20 kJ mol⁻¹. This demonstrates that the examined compound slows down the dissolution of the CS by physisorption and chemisorption processes (Kamel *et al.*, 2022). Tafel plot investigates that the anodic and cathodic reactions are both delayed by the examined compound. As the Salen SB concentration increases, the corrosion current decreases. The Salen SB prevents CS from dissolution in HCl solution. The cathodic curves in Figure (6) recorded similar behaviour. This suggests that the adsorption of the examined compound at the CS surface had no or little impact on the cathode's reaction mechanism. On the contrary, the slopes of the anodic curves alter, suggesting a modified mechanism for the anodic process.

The adsorption of Salen SB at the CS surface may considerably inhibit the dissolution process. The Cl⁻

species are important for the corrosion of CS in the absence of Salen SB.



The cathodic reactions are:



Olasunkanmi *et al.* (2016) found that pH values above 4 are where the effect of reduced dissolved oxygen on CS breakdown is most noticeable. H_2 evolution is thus the main cathodic process in this investigation. The values of the Tafel slopes (β_c , β_a), corrosion current (i_{corr}), and corrosion potential (E_{corr}) are shown in Table 6. The corrosion current decreases when Salen SB is present in corrosive media. It is worth noting that the change in E_{corr} values is smaller than 85 mV, proving that the tested compound belongs to mixed type. Due to the dissimilarity of the anodic and cathodic polarization lines about E_{corr} , as shown in Table 6, $\beta_c + \beta_a \neq 1$. The inhibition efficiency, IE_p , is calculated using the following equation:

$$IE_p = \left(1 - \frac{i_{(\text{inh})}}{i_{(\text{free})}}\right) \times 100$$

Where, $i_{(\text{free})}$ and $i_{(\text{inh})}$ are the corrosion currents without and with the Salen SB, respectively.

Salen SB concentration recorded an increment that principally improve the IE_p . These data support the results of the WL method (Olasunkanmi *et al.*, 2020). Electrochemical impedance experiments can often detect the formation of protective corrosion product layers or the presence of coatings on the surface of corroded metal (Kirkland *et al.*, 2012). In such cases, the EIS spectra comprise of two capacitive loops in the high- and low-frequency ranges. EIS measurements of Salen SB in 0.5 M HCl showed that Nyquist plots, depicted as semicircles. The semicircles are not perfect because of the heterogeneity of the CS electrode. The shape of Nyquist semicircles did not alter too much with the addition of Salen SB, indicating that the examined compound has no or little effect on the mechanism of the corrosion process (Abd El Wanees *et al.*, 2016; Kaabi *et al.*, 2021). The Nyquist plot shows more than two time constants, which indicates that the corrosion process is complex and involves multiple steps. The presence of the organic inhibitor has modified the corrosion process, but it has not eliminated it completely. The first time constant is associated with the charge transfer process at the metal/electrolyte interface. The second time constant is associated with the diffusion of ions in the electrolyte. The third time constant is associated with the adsorption of the inhibitor molecules on the metal surface. The presence of the third time constant is a good sign, as it indicates that the inhibitor molecules are adsorbing on the metal surface and forming a protective layer.

For Bode graphs, the relationship between $\log |Z|$ and $\log f$ (frequency) is directly proportional in the median frequency range. A slope's value does not attain -1. This illustrates the capacitive system's suboptimal performance at medium frequencies. To obtain the best capacitive performance at medium frequencies, it is suggested that the slope be -1 and the phase angle be -90. Solutions that are inhibited have slopes that are larger in magnitude than those that are not. This explains the suppressing properties of the investigated compound on CS dissolution. Impedance measurements were used to calculate the impedance parameters, such as C_1 , C_2 , R_2 (charge transfer resistance) including R_1 , and W (Warburg resistance). Salen SB also recorded when concentration grows, the value of the R_2 also rises. As a result, the Salen SB's presence enhances inhibition's efficiency by reducing corrosion's rate. In addition, the values of C_1 and C_2 drop as the Salen SB concentration increases. This is mostly assigned to the fact that the Salen SB molecules are gradually replacing H_2O molecules on the CS surface. An increase in the thickness of the electrical double layer and a decrease in the dielectric constant lead to reduced capacitance values. This suggests that Salen SB molecules interact with the metal/solution interface. Adsorption occurs when Cl^- ions combine with Salen SB molecules (Hmamou *et al.*, 2012).

For the suggested equivalent circuit, R_1 and C_1 represent the resistance and capacitance components of the protective corrosion layer or coating, R_2 is the charge transfer resistance, and C_2 characterizes the capacitance of the electric double layer (Man *et al.*, 2020; Hou *et al.*, 2020). The fitting curve recoded in this study confirmed the experimental results.

The IE_i values were calculated by utilizing the following equation of Sadeek *et al.*, (2018):

$$\% IE_i = \left(1 - \frac{R_{ct}^a}{R_{ct}}\right) \times 100$$

Where, R_{ct} and R_{ct}^a are the charge transfer resistances in the presence and absence of the Salen SB, respectively. The subsequent equation was employed to calculate the C_{dl} as follow:

$$C_{dl} = Y_o(\omega_{\text{max}})^{n-1}$$

Where, $\omega_{\text{max}} = 2\pi f_{\text{max}}$, and f_{max} is the frequency at which Z_{imag} reaches the maximum value.

The pitting impact of the Cl^- ions has extensively harmed the CS specimens exposed to the blank solution, when the Salen SB is present, it significantly improves the surface via adsorption at the CS surface. It creates a barrier film. This result is consistent with the conclusions of the WL, PP, and EIS studies and with data obtained by Bodkhe *et al.*, (2021).

The EDX patterns of carbon steel (CS) samples in 0.5 M HCl, both with and without 300 ppm of Salen SB, recorded a reduction in corrosion of the CS. This can be attributed to the formation of a protective layer on the CS surface due to the adsorption of Salen SB, which shields it from corrosion by the aggressive HCl.

The intensity of the Fe line was reduced in the inhibited solution compared to the blank solution. The presence of O, C, and N lines indicates that the Salen SB molecules were adsorbed onto the CS surface (Chugh *et al.*, 2020). The illustration of quantum parameters demonstrates that the Salen SB's geometrical structure is not a planner. In addition, the provided structure with the lowest computed energy recoded that. The examined compound could adsorb at the CS surface via lone pairs of electrons that exist on nitrogen and oxygen atoms (Muralidharan *et al.*, n.d.).

In the light of frontier molecular orbital theory, chemical activity is produced by the relationship between the HOMO and LUMO levels of the reactants (Saadouni *et al.*, n.d.). The ability of the inhibitors to provide and receive electrons is correlated with their HOMO and LUMO energy levels, respectively. A higher HOMO energy level (E_{HOMO}) is easier to donate and a lower LUMO energy level (E_{LUMO}) is more suitable for acceptance. Also, the small value of LUMO indicates that the inhibitor has a greater ability to receive electrons. Consequently, the reduced energy band gap ($E = E_{\text{LUMO}} - E_{\text{HOMO}}$) causes a stronger interaction between the Salen SB inhibitor and the CS surface and ameliorates the inhibition efficiency (Benbouguerra *et al.*, 2018; Gao and Liang, 2007). Both the effectiveness of inhibition and the simplicity with which the inhibitor can supply electrons to the vacant d-orbital of the CS surface increase with an increasing HOMO value.

The Salen SB has a high E_{HOMO} (-0.223), low E_{LUMO} (-0.045) and a small ΔE value (0.178). So, it makes sense to assume that the Salen SB has a strong ability to adsorb at the CS surface. This expectation and the practical findings are in good agreement. The dipole moment, DM, has been utilized to describe and understand the structure (Gece and Bilgiç, 2009) DM and inhibition efficiency are closely related. The Salen SB molecule has a significant dipole moment (2.699 Debye), as shown in Table 8. Another quantum parameter that was found through computations is the molecule volume. The calculations showed that the molecular volume of the Salen SB compound, which is $228.735 \text{ cm}^3 \text{ mol}^{-1}$ is large. This large volume increases the efficiency of the inhibition as it improves the surface interaction between the Salen SB molecule and the CS surface.

Important properties that affect a molecule's stability and reactivity include its hardness and softness. In contrast to the large energy gap of a hard molecule, soft molecules have a smaller energy gap. Since soft molecules may more readily give electrons to an acceptor, they are significantly more active than hard ones. Therefore, for the easiest electron transfer, adsorption can happen where the value of σ is greatest on the molecule (Martinez, 2002). The Salen SB with a value of $\sigma = 11.236 \text{ (au)}^{-1}$ is assumed to have a high level of inhibitory efficiency. As indicated in Table 8, the Salen SB also has a low χ and ω , but a high TNC (0.134 au, 0.101 au, and -3.587 e), respectively, in accordance with the computations. As a result, its

ability to give electrons to the CS surface improves, and the inhibition efficiency increases (Kamel *et al.*, 2022). The good inhibition performance of the Salen SB compound that is supported by the quantum chemical parameters is compatible with the experimental results.

It is evident that the HOMO level of the Salen SB compound is primarily influenced by the π -bonding nature of the C-C bonds in the phenyl ring and the lone pairs of electrons on the oxygen atom in the hydroxyl (OH) group. This suggests that these sites are conducive to electrophilic attack on the carbon steel (CS) surface. Consequently, the CS surface interacts with moieties that have high HOMO density, and adsorption likely occurs through the π -electrons of the CS surface. In addition, the charge density of the LUMO level is completely localized over all Salen SB molecules. This implies that the molecule can accept electrons from CS.

The molecular electrostatic potentials (MEPs) are important as negative areas (red colour) can be act as nucleophilic centres, however, and positive parts (blue colour) as potential electrophilic centres. According to calculations, oxygen and nitrogen atoms have negative electrostatic potential, which suggests that previous atoms are the primary sites for binding with the surface of CS.

The adsorption modeling of the studied Salen SB on the CS is displayed in both top and side views in Fig. 12. The adsorption energy between the Salen SB and the CS surface is calculated by the following relation:

$$E_{\text{ads}} = E_{\text{Fe-inh}} - (E_{\text{inh}} - E_{\text{Fe}})$$

Where, E_{inh} and E_{Fe} are the total energy of both the Salen SB and CS surfaces, respectively. The MC simulation's findings showed that the adsorption energy between the Salen SB and the CS surface is $-166.150 \text{ kJ mol}^{-1}$. This significantly negative value suggests an effective interaction between the Salen SB and CS molecules.

The mechanism of corrosion inhibition can be explained as a synthesized Salen SB molecule's has ability to act as an inhibitor depends on its chemical structure. The Salen SB molecule contains a fatty alkyl chain. This chain slows the spreading of the corrosive medium on the CS surface. According to the values of E_{corr} , β_{a} , and β_{c} (Table 6), the addition of Salen SB influences not only the reduction of oxygen gas and hydrogen ions in the cathodic area but also the oxidation of CS in the anodic area. By physisorption, the Salen SB molecules and the chloride ions in the corrosion environment create a barrier film on the CS surface, reducing the metal's contact area with the corrosive media and preventing additional CS oxidation. The chemical adsorption of the Salen SB on the metal surface is caused by the free electrons on the N and O atoms and the double bond nature of the benzene ring, according to the findings of quantum chemistry.

CONCLUSION

The Salen Schiff base compound was prepared and

characterized by ^1H NMR and FTIR spectroscopy. The prepared compound was assessed as a carbon steel corrosion inhibitor in 0.5 M HCl. The inhibition efficiency increased with the concentration of the Salen compound. At 300 ppm of Salen SB, the efficiency is 75.4% at room temperature. The adsorption of the Salen SB compound followed the Langmuir model and influenced the corrosion of carbon steel (CS) through both physisorption and chemisorption. Salen SB acted as a hybrid-type inhibitor. The electrochemical impedance spectroscopy (EIS) results confirmed that the presence of Salen SB in the corrosive medium reduced both the capacitance and corrosion current while increasing the charge transfer resistance, due to the formation of an adsorbed film on the CS surface. The data obtained from the various methods are strongly correlated, demonstrating the validity and reliability of the findings. The quantum characteristics of the Salen SB compound further confirm its superior inhibitory efficiency, with an adsorption energy of $-166.150\text{ kJ mol}^{-1}$ between the Salen SB compound and the CS surface.

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تقييم قاعدة شيف السالين كمثبط لتآكل الصلب منخفض الكربون في وسط حمض الهيدروكلوريك: دراسات عملية وحاسوبية

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الملخص العربي

في هذه الدراسة تم تحضير وتقييم الأداء المثبط لمركب N'-bis, N (الساليسيليدين) الإيثيلين-1،2-ديامين (قاعدة شيف السالين) لتآكل الصلب منخفض الكربون في محلول حامض الهيدروكلوريك ذو التركيز النصف المولاري، من خلال طريقة الفقد في الوزن (WL) وتقنيتي مطيافية المعاوقة الكهروكيميائية (EIS) والاستقطاب الديناميكي الفعال (PP). تم تحضير مركب قاعدة شيف السالين وتم اثبات تركيبه عن طريق تقنيتي بروتون الرنين المغناطيسي والأشعة تحت الحمراء. ولقد أوضحت النتائج العملية زيادة كفاءة التثبيط مع زيادة تركيز قاعدة شيف السالين. عند تركيز 300 جزء من المليون من المركب المحضر كانت كفاءة التثبيط 75.4% وذلك عند 298 درجة مطلقاً، بينما انخفضت كفاءة التثبيط إلى 69.5% عندما زادت درجة الحرارة من 298 إلى 333 درجة مطلقاً. وجود المركب المحضر في بيئة التآكل قلل من سعة الطبقة المزروجة. وكثافة تيار التآكل (icorr) بسبب تكوين طبقة واقية منه على سطح الصلب الكربوني. هذا، ولقد أظهرت النتائج أن المركب المحضر ينتمي للنوع الخليط حيث أنه يثبط كلاً من التفاعل الأنودي والكاثودي على السواء. كما أكدت النتائج أن ادمصاص المركب المحضر يتبع نموذج العالم لانجمير. أكدت نتائج فحص سطح الصلب الكربوني باستخدام المسح بالميكروسكوب الإلكتروني والأشعة السينية المشتتة للطاقة وجود طبقة مدمصة رقيقة من المركب المحضر على سطح الصلب الكربوني، والتي تعزله عن بيئة التآكل. تم استخدام نظرية الكثافة الوظيفية (DFT) ومحاكاة مونت كارلو (MC) لتوضيح كيفية اتصال وشكل جزيئات قاعدة شيف السالين مع / على الصلب الكربوني. أشارت النتائج أن مركب قاعدة شيف السالين يرتبط بسطح الصلب الكربوني من خلال زوج الإلكترونات الحر الموجود على ذرتي الأكسجين والنيتروجين، بالإضافة إلى إلكترونات باي π الخاصة بحلقة البنزين. ولقد تم حساب طاقة الترابط بين المركب المحضر والصلب الكربوني ووجد أنها 160.150 كيلو جول/مول. ولقد أكدت النتائج الحاسوبية على القدرة التثبيطية لمركب قاعدة شيف السالين لتآكل الصلب الكربوني في بيئة حامض الهيدروكلوريك.