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Electrochemical investigation and DFT approach: The inhibition effect of 2-isopropyl-4-methyl-1,3-thiazole-5-carboxylic acid against mild steel corrosion

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Abstract

In this study, the inhibitory properties of 2-isopropyl-4-methyl-1,3-thiazole-5-carboxylic acid (2I4MTA5C) against mild steel corrosion in acidic medium were investigated by electrochemical and quantum theoretical methods. Electrochemical impedance spectroscopy measurements and polarization curves were obtained in the presence and absence of 5 mM 2I4MTA5C in 0.5 M HCl during 168 hours of immersion, and the adsorption isotherm is presented. Experimental results were compared with quantum theoretical parameters in order to establish a relationship between molecular structure and electrochemical behavior and to investigate it in depth. According to the results obtained for the 168 hour immersion time, the resistance values for MS were 9.8 in the absence of 5 mM 2I4MTA5C and 200 ohm.cm^{-2} in the presence. The calculated corrosion current density values were 2.65 and 0.13 mA.cm-2 for MS in HCl and 5 mM 2I4MTA5C + HCl solution, respectively. The theoretically calculated HOMO and LUMO values were -6.88 eV and -1.80 eV. According to the results obtained, we can say that 2I4MTA5C is a suitable inhibitor candidate with 95.1% protection against mild steel corrosion.

Keywords: Corrosion, DFT, EIS, Organic inhibitor

Elektrokimyasal inceleme ve DFT yaklaşımı: 2-izopropil-4-metil-1,3-tiyazol-5-karboksilik asidin yumuşak çeliğin korozyonuna karşı inhibisyon etkisi

Özet

Bu çalışmada, 2-izopropil-4-metil-1,3-tiyazol-5-karboksilik asidin (2I4MTA5C) asidik ortamda yumuşak çelik korozyonuna karşı inhibitör özellikleri elektrokimyasal ve kuantum teorik yöntemlerle araştırılmıştır. 168 saatlik daldırma sırasında 0,5 M HCl içinde 5 mM 2I4MTA5C varlığında ve yokluğunda elektrokimyasal empedans spektroskopi ölçümleri ve polarizasyon eğrileri elde edildi ve adsorpsiyon izotermi sunuldu. Moleküler yapı ile elektrokimyasal davranış arasında bir ilişki kurmak ve derinlemesine araştırmak için deneysel sonuçlar kuantum teorik parametrelerle karşılaştırıldı. 168 saatlik daldırma süresi için elde edilen sonuçlara göre, MS için direnç değerleri 5 mM 2I4MTA5C yokluğunda 9.8 ve mevcudiyetinde 200 ohm.cm^{-2} idi. HCl ve 5 mM 2I4MTA5C + HCl solüsyonunda MS için hesaplanan korozyon akımı yoğunluğu değerleri sırasıyla 2.65 ve 0.13 mA.cm-2 idi. Teorik olarak hesaplanan HOMO ve LUMO değerleri -6.88 eV ve -1.80 eV idi. Elde edilen sonuçlara göre 2I4MTA5C'nin yumuşak çelik korozyonuna karşı %95,1 koruma ile uygun bir inhibitör adayı olduğunu söyleyebiliriz.

Anahtar Kelimeler: Korozyon, DFT, EIS, Organik inhibitör

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1. Introduction

In industry and architecture, steel is the most extensively utilized metal alloy [1-3]. It is favored in terms of physical and chemical qualities, as well as cost. However, corrosion is the most serious problem that limits the utilization of these materials [4, 5]. Corrosion is the natural process of metallic materials returning to their stable condition by interacting with their surroundings. In order to prevent it many methods should be suitable but inhibitor treatments are one of the most convenient corrosion prevention methods, and are especially favorable when cleaning with acidic solutions [6-9]. Various inhibitory compounds added to the corrosive medium break the connection between the metal and the environment. The electric field effect was created at the metal/solution contact mechanically and/or chemically adsorbed these compounds on the metal surface. Organic chemicals having groups such as OH-, -CHO, -COOH, -CN-, -SN, CO, -NH3, SO3, or double bonds, triple bonds, unpaired electrons, metals, and other inhibitory substances have chemical structures that are related to their efficiency [10-12]. Especially thiazole and its derivative compounds are frequently utilized as corrosion inhibitors in the literature [13-15]. The double bonds in these compounds' structures, as well as the N and S atoms in the planar heterocyclic ring, provide the greatest benefit and adsorption to the metal surface can be more easily achieved.

Experimental inhibitory features of the compounds in issue are time-consuming and expensive operations, thus it's helpful to calculate efficacy theoretically using quantum chemical calculations to explain and validate the experimental results. Many alternative basis sets are employed with the "density functional theory (DFT)," which is widely acknowledged among these approaches, provides quick findings, and is compatible with experimental experiments. The interactions between metal and inhibitor can be better understood with the use of theoretically derived parameters (dipole moment, EHOMO, ELUMO, and etc) [16-18]. The charge distributions of the molecule, the probability of chemical interactions, positively charged (electron rich) areas, and vice versa may all be identified using this approach, which is commonly used to identify the physicochemical features of inhibitor compounds. The regions formed by the atomic nucleus repelling the protons are positive; the regions formed by the attraction have negative charge density, these terminals are correlated with Mulliken charges [19, 20]. All of these occurrences are related to the inhibitory molecules' adsorption properties on the metal surface. When the experimental drawing of the adsorption isotherms and the calculated Gibbs free energy ($\Delta G°ads$) values are connected with the quantum parameters, the adsorption mechanism may be clarified [17, 21]. In the literature, using mass loss, electrochemical impedance spectroscopy, potentiodynamic polarization, and computational research, levofloxacin, moxifloxacin, metolazone, and nifedipine were explored as corrosion inhibitors for improving carbon steel resistance in 2 M HCl solution [17]. The investigated compounds were shown to be effective green corrosion inhibitors for carbon steel. The high inhibition efficiencies were detected for metolazone and levofloxacin, the values were 98 and 94% respectively. The effects of lansoprazole and rabeprazole on the corrosion resistance of carbon steel in phosphoric acid solution were investigated [18]. Lansoprazole and rabeprazole increased the activation energy for carbon steel corrosion in phosphoric acid solution from 41.6 kJ mol-1 to 81.9 kJ mol-1 and 85.9 kJ mol-1, respectively. The obtained EHOMO values were -6.530 eV and -6.614 eV for lansoprazole and rabeprazole, respectively. It is declared that the inhibition efficiency value is increased by increasing the HOMO energy [18]. Our research and experience have revealed that efficient corrosion inhibitors feature electronegative atoms, double bonds, and conjugated double bonds in their structures.

Therefore, we aimed to investigate the possibility of using 2-isopropyl-4-methyl-1,3-thiazole-5-carboxylic acid as the inhibitor against mild steel corrosion in acidic media. For this purpose, the open circuit potentials in 0.5 M HCl solutions with and without 2I4MTA5C of MS were monitored throughout time. At various immersion times, electrochemical impedance spectroscopy and polarization experiments were also performed. Experimental and quantum theoretical methods were used to analyze the adsorption of 2I4MTA5C on the MS surface.

2. Materials and methods

A CHI 660b electrochemical analyzer was used to perform the electrochemical tests. All of the electrochemical experiments were conducted in a three-electrode setup that was open to the environment. The counter electrode was a platinum sheet (with a surface area of 2 cm^2), and the reference electrode was Ag/AgCl (commercial). This reference electrode was used to relate to all potentials in this study. The working electrodes were made of a mild steel alloy having the following chemical composition (in weight percent): 0.09645 C, 0.22423 Si, 0.41797 Mn, 0.02095 P, 0.04229 S, 0.02533 Cu, 0.03594 Ni, 0.01396 Cr, 0.00271 Mo, 0.00591 V, 0.00216 Sn, and a Fe balance. The surface area of the working electrode was almost 0.5 cm^2, the rest was insulated with a thick polyester block, with copper wire providing electrical transmission. Before each experiment, the exposed surface of the working electrodes was polished to 1200 degrees using sandpaper. Experiments were conducted with and without a 5 mM 2I4MTA5C concentration; the molecular structure is shown in Figure 1.

The EIS measurements were performed without stirring the electrolyte by applying 5 mV amplitude in the frequency range of 10^5 – $6x10^{-2}$ Hz at the open circuit potentials of the electrodes. The current potential curves were acquired with a scanning speed of 1 mV. All of the experiments were conducted out at a temperature of 293 K.

Theoretical calculations were carried out using density functional theory (DFT) with 6-311++G (d,p) basis set for all atoms with the Gaussian 03W program. Some electronic properties such as energy of the highest occupied molecular orbital (E_{HOMO}), energy of the lowest unoccupied molecular orbital (E_{LUMO}), dipole moment, Mulliken charges were determined.

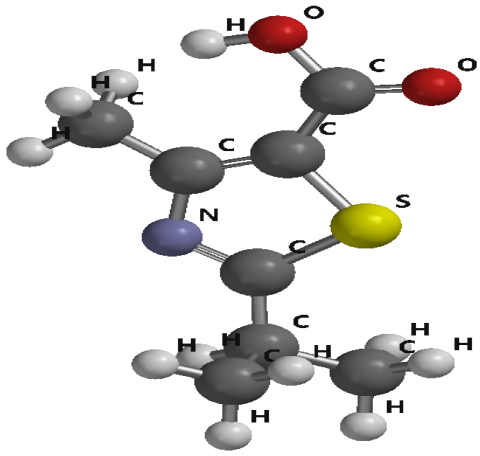

Figure 1. The structure of 2-Isopropyl-4-methyl-1,3-thiazole-5-carboxylic acid (2I4MTA5C)

3. Results and discussion

Figure 2 shows the Eocp - time curves of MS electrodes. The open circuit potential of the MS electrode is nobler value in the solution containing 2I4MTA5C, as shown in Figure 2, and it remains relatively constant at 3600 s exposure period.

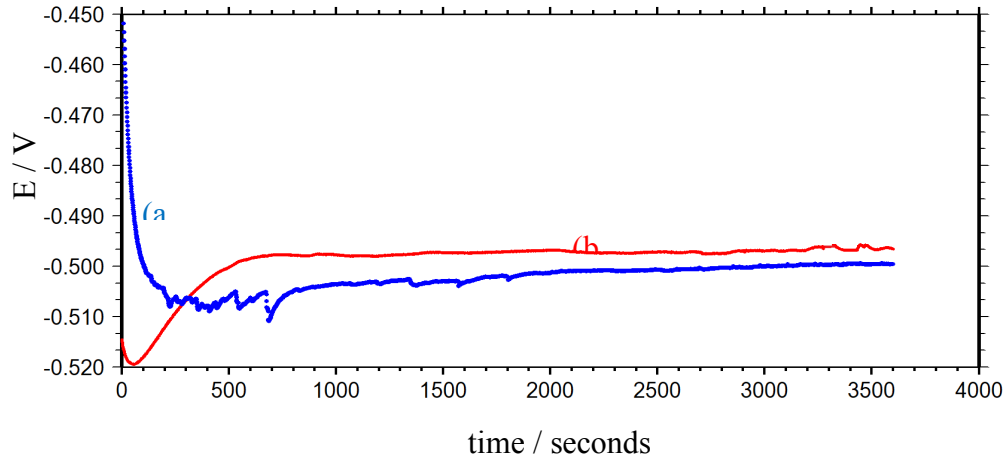

Figure 2. The open circuit potential of MS in 0.5 M HCl (a) and containing 5mM 2I4MTA5C (b) solutions.

Figures 3 and 4 showed the electrochemical impedance spectra (EIS) obtained after various exposure times for MS in the absence and the presence of 2I4MTA5C in 0.5 M HCl. The Nyquist diagrams in Figure 3 showed semi-elliptic curves that started in the high frequency range, continued in the mid-frequency range, and closed in the low-frequency region. Mild steel resistance decreased with increasing immersion period, according to the data shown in Figure 4. The corrosive acidic environment and particular absorption capacity of chloride ions caused MS to decay [22-24]. The data were fitted according to Figure 5.

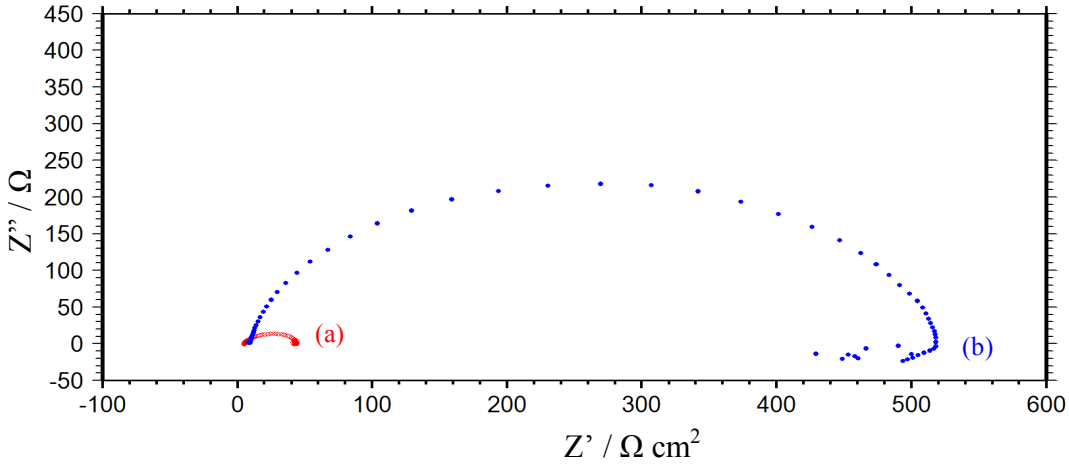

Figure 3. The Nyquist plots of MS electrode in 0.5 M HCl (a) and 5mM 2I4MTA5C containing 0.5 M HCl (b) solutions for 1 hour immersion period.

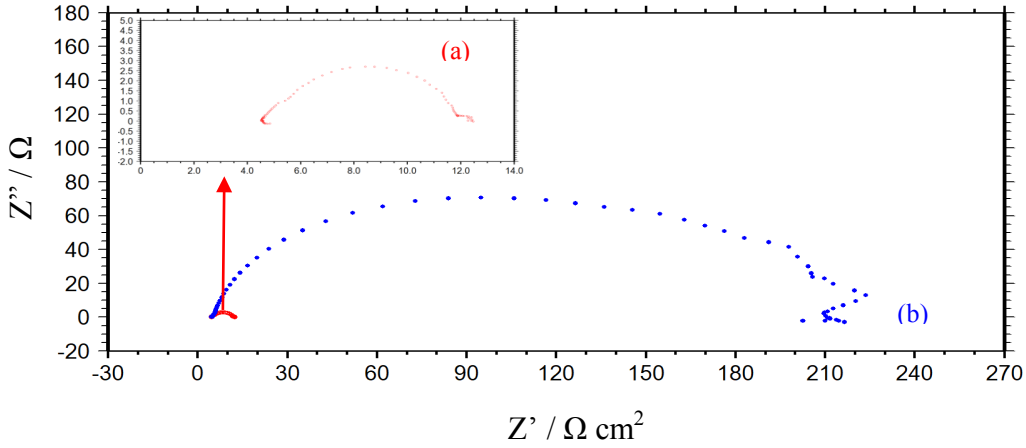

Figure 4. The Nyquist plots of MS electrode in 0.5 M HCl (a) and 5mM 2I4MTA5C containing 0.5 M HCl (b) solutions for 168 hours immersion period.

It comprises a capacitive loop in the high frequency areas and inductive loops in the low frequency regions, as shown in Figures 3 and 4. The inductive loop was a smaller size than the capacitive loop. The growth of an oxide layer on the surface may cause a capacitive cycle. The inductive loop can occur in the absence of the inhibitor or at low concentrations due to the relaxation of adsorbed charged intermediates, as well as the re-dissolution of the passivated surface in the presence of the inhibitor [4, 25, 26].

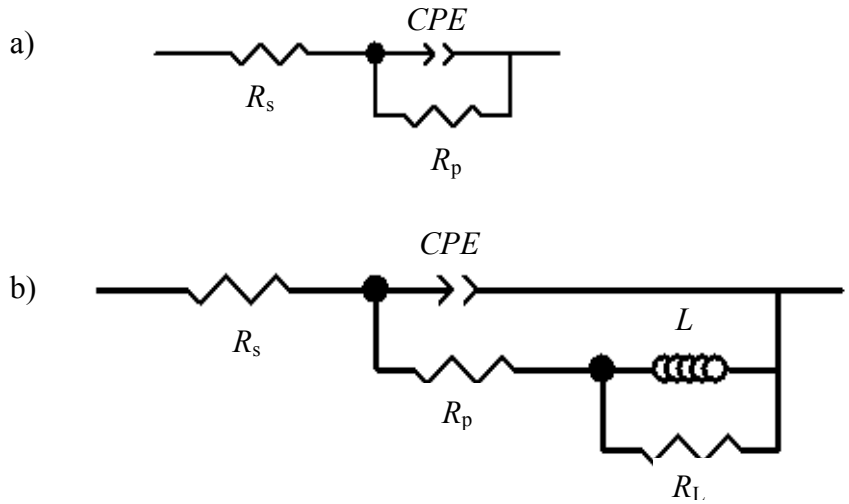

Figure 5. Electrical equivalent circuit diagrams used to modeling MS/HCl (a) and MS/HCl+2I4MTA5C (b) solutions interfaces. The solution resistance is Rs; the polarization resistance is Rp , the constant phase element is CPE, the inductance is L and R_L is the resistance due to the adsorbed species.

It can be seen from Figures 3 and 4 that the corrosion resistance of MS increased in the presence of inhibitor molecules (2I4MTA5C). Table 1 showed the data obtained from the EIS curves

fitted using the Zview software. The polarization resistance values of MS in the solution containing the inhibitor were 420.5 and 200 ohm cm^{-2} for immersion times of 1 and 168 hours, respectively. The constant phase element values were $52.9x10^{-6}$ and $78.8x10^{-6}$ sec Ω^{-1} cm^{-2}, respectively. Although the polarization resistance values decreased with increasing immersion time, it was calculated that there was favorable in the presence of 2I4MTA5C and the protection efficiency (η) was 95.1% after 168 hours.

Table 1. Electrochemical parameters for MS in 0.5 M HCl and 5mM 2I4MTA5C containing 0.5 M HCl solutions

	MS		**Inhibitor**				
t/ h	R_p/ Ω cm^2	CPE 10^{-6} s^n Ω^{-1} cm^{-2}	R_p/ Ω cm^2	CPE 10^{-6} s^n Ω^{-1} cm^{-2}	R_L / Ω cm^2	L / H cm^2	%η
1	39.0	690.1	420.5	52.9	128	18.6	90.7
24	46.1	1084.4	438	60.5	21.2	10.6	89.5
48	32.2	2934.6	419	60.9	20.2	9.6	92.3
96	15.5	7940.3	368	69.4	25.2	52.2	95.8
168	9.8	9973.8	200	78.8	11.2	10.6	95.1

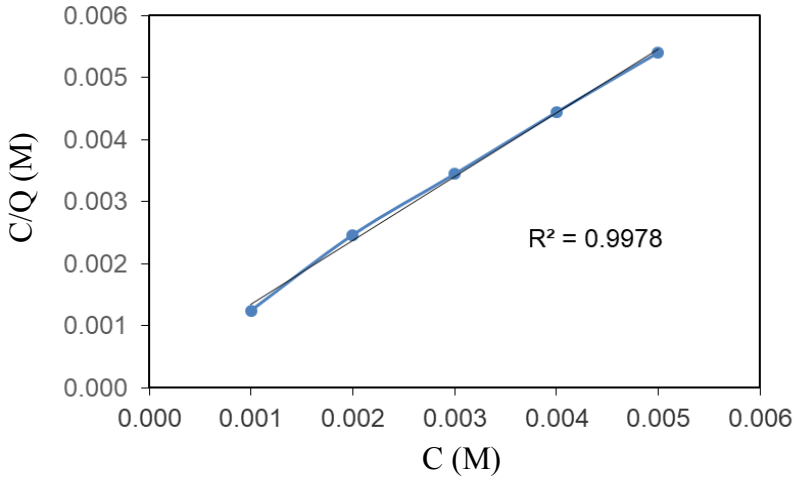

Figure 6. Langmuir adsorption plot of MS electrode obtained in 0.5 M HCl containing various concentration of 2I4MTA5C

In Figure 6, Langmuir adsorption isotherm model was used with the following equation [27];

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

where, inhibitor concentration (C_{inh}), degree of surface coating values (Θ) for inhibitor concentrations in acidic solution, K_{ads}, the adsorption equilibrium constant of $3.33x10^3$ M^{-1}, for 2I4MTA5C, indicated the ability of inhibitor molecules to adhere to the MS surface. The standard free energy of adsorption (ΔG^o_{ads}) value was calculated with the help of the following equation [28]:

$$\Delta G^o{}_{ads} = -RT \ln(55.5 K_{ads}) \quad (2)$$

where, R was the universal gas constant and T was the absolute temperature, the calculated value was -30.05 kJ mol^{-1} in the presence of 2I4MTA5C. The calculated ΔG^o_{ads} was less than -40 kJ mol^{-1} indicated physical adsorption as well as electrostatic interactions [29, 30].

Furthermore, potentiodynamic polarization measurements were achieved in the absence and presence of 2I4MTA5C and the results were presented in Figure 7. In the presence of 2I4MTA5C, the cathodic and anodic current density values decreased. The corrosion potential value slightly shifted towards the cathodic potential in the presence of the inhibitor. Since it affects both anodic and cathodic reactions, 2I4MTA5C can be defined as a mixed type inhibitor [28, 31]. The calculated corrosion current density values were 2.65 and 0.13 $mA.cm^{-2}$ for MS in HCl and 5 mM 2I4MTA5C + HCl solution, respectively.

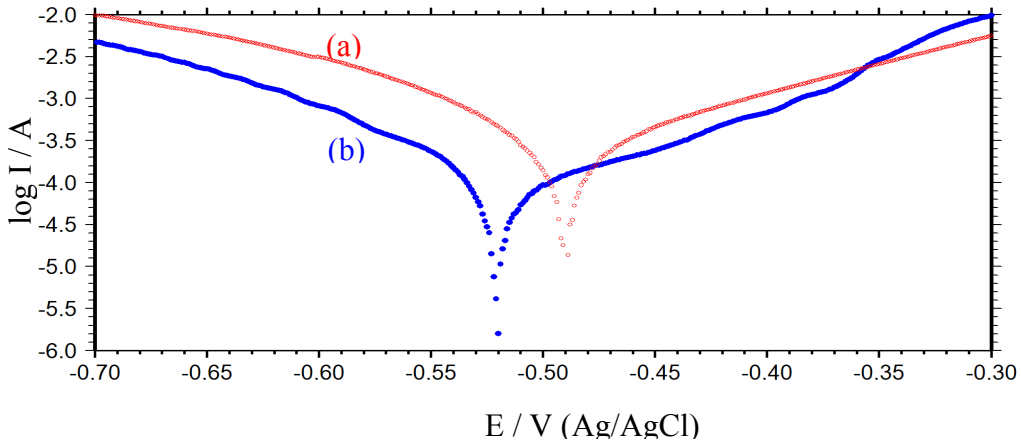

Figure 7. The potentiodynamic polarization curves of MS electrode in 0.5 M HCl (a) and 5mM 2I4MTA5C containing 0.5 M HCl (b) solutions after 168 h.

Structural analysis of 2I4MTA5C was obtained by quantum theoretical method. The highest occupied molecular orbital (E_{HOMO}), the energy of the lowest unoccupied molecular orbital (E_{LUMO}), the energy gap (ΔE) between LUMO and HOMO, and Mulliken charges on the backbone atoms were determined and presented in Figure 8 and Table 2.

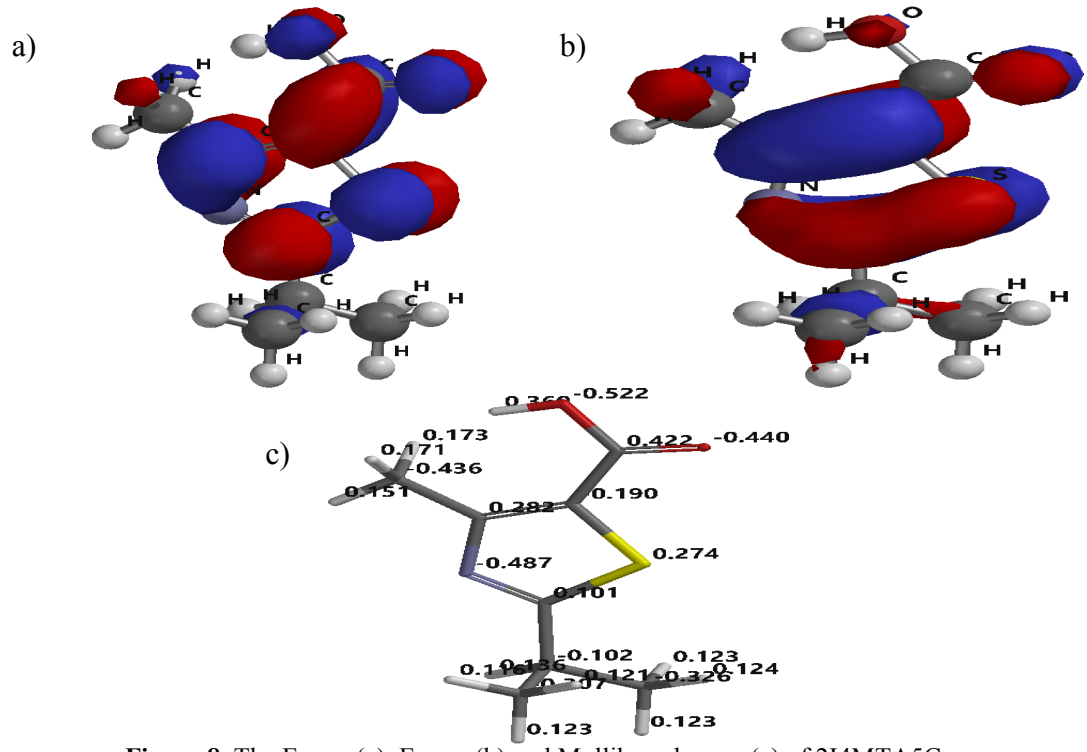

Figure 8. The E_{LUMO} (a), E_{HOMO} (b) and Mulliken charges (c) of 2I4MTA5C.

The E_{HOMO} value determined using the DFT B3LYP 6-311++G (d,p) basis set was -6.88 eV and the E_{LUMO} value was -1.80 eV. It is known that the larger HOMO and LUMO surfaces of the molecules increase their adsorption capabilities [32]. The dipole moment is determined as 5.53 Debye. The increase in the dipole moment may be due to dipole-dipole interactions between the inhibitor molecules and the metal surface, which may lead to increased inhibition [33]. Mulliken charge of oxygen on the hydroxyl group of 2I4MTA5C was -0.522 au. In an acidic solution, the inhibitor can be protonated on the hydroxyl group of the molecule and adsorbed predominantly through electrostatic interactions between such a site and the metal surface [34].

Table 2. Some of quantum theoretical parameters of 2I4MTA5C

Name	**2-isopropyl-4-methyl-1,3-thiazole-5-carboxylic acid**
Formula	$C_8H_{11}NO_2S$
E_{HOMO} (eV)	-6.88
Dipol Moment (Debye)	5.53
Weight (amu)	185.247
E_{LUMO} (eV)	-1.80
ΔE	5.08

4. Conclusion

Based on experimental and theoretical calculations, the following results were obtained: Corrosion experiments reveal that 2-isopropyl-4-methyl-1,3-thiazole-5-carboxylic acid (2I4MTA5C) efficiently protected MS in 0.5 M HCl. It's a mixed-type inhibitor that binds to the MS surface using the Langmuir adsorption isotherm model. The calculated ΔG^{o}_{ads} value was -30.05 kJ mol^{-1} in the presence of 2I4MTA5C, it proved the adherent adsorption ability of the inhibitor. The 2I4MTA5C produced a protective film on MS therefore the polarization resistance increased in the presence of the inhibitor. The corrosion current density values for MS in HCl and 5 mM 2I4MTA5C + HCl solution were 2.65 and 0.13 $mA.cm^{-2}$, respectively. The polarization measurement supported the EIS results. Theoretically estimated LUMO orbitals were mostly found on the O, N, S and electronegative terminals of molecules, whereas HOMO orbitals may be found anywhere across the molecule. The dipole moment was 5.53 Debye, which can promote molecule adsorption on metal surfaces. During long-term exposure, the inhibitor efficiency was greater than 95%.

Contribution of authors: The experimental analyses were done by all authors equally. The theoretical calculations were done by Dr. Mehmet Erman Mert. All authors contributed equally to the discussion and writing of the text.

Conflict of interest statement: There is no conflict of interest.

Research and publication ethic statement: The study does not require Ethics Approval.

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