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Synthesis Characterization and DFT Studies of New Azo Dye Derived from Dapsone and Evaluation it as Corrosion Inhibiter

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Abstract. The azo dye (A_3) has been synthesized and characterized by FT-IR, 1H NMR and 13C NMR spectroscopic techniques. The compound (A_3) has been evaluated as carbon steel corrosion inhibitor at different concentrations (0.0001, 0.0005, 0.001and 0.005 mM) and different temperatures (298-318 K). The corrosion inhibition efficiency was studied by Potentiodynamic polarization. The effects of concentration and temperature on the inhibition efficiency were studied by Potentiodynamic polarization measurements, the results showed that increasing concentration of (A_3) increases the inhibition efficiency while increasing the temperature decreases it, the highest corrosion inhibition efficiency, 92.2 % was recorded with 0.005 mM of A3at 298 K in 1 M HCl. The adsorption process was found to obey Langmuir isotherm, and the adsorption thermodynamic parameters were studied.Computational chemistry calculations were accomplished using density functional (DFT) method. Theoretical and experimental methods were discussed and the findings displayed that the inhibition efficiency values by closely agreed

Keyword: Corrosion inhibitors, Azo Dye, Carbon steel,Dapson, Potentiodynamic polarization DFT

1. Introduction

Corrosion is defined as the deterioration of metals and alloys caused by chemical or electrochemical interaction with their surrounding[1]. Corrosion issues have gotten a lot of attention because of the economic and safety implications. One of the most practical methods for corrosion protection is the use of inhibitors[2]. Various organic compounds have been reported to act as corrosion inhibitors[3]. The most effective organic inhibitors are organic compounds with an electron system, atoms with lone pair electrons (phosphorus, sulfur, nitrogen, oxygen), and plane conjugated systems containing all aromatic rings[4].Azo dyes are the most widely used inhibitor class because of their low cost,and efficiency in substrate material, and lack of environmental side effects. They are used in a variety of fields, such as

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textile dyeing and fiber spinning[5,9]. The presence of a –N=N– group in azo dye molecules improves adsorption and corrosion inhibition. The planarity (π) and lone pair of electrons on the N atoms are important structural features that govern the adsorption of these molecules to the metal surface. The inhibition effect was also discovered to be dependent on some of the organic inhibitor's physicochemical and electronic properties, which are related to its functional groups, steric effects, electronic density on donor atoms, and the orbital character of donating electrons[10].Quantum chemical methods have already proven to be extremely useful in determining the molecular structure, as well as elucidating the electronic structure and reactivity of powerful inhibitors As a result, performing quantum chemical calculations in corrosion inhibition studies has become common practice[11, 12]. Density functional theory (DFT) calculations can yield reasonably accurate predicted properties[13, 14]. Some quantum chemical parameters, which influence the electronic interaction between surface atoms and inhibitors, are the energy of the highest occupied molecular orbital (EHOMO), the energy of the lowest unoccupied molecular orbital (ELUMO), the energy gap between EHOMO and ELUMO (E) dipole moment (D), chemical hardness (η), softness (σ), electronegativity (χ), proton affinity, global electrophilicity (ω), global nucleophilicity (ε) and total energy (the sum of electronic and zero-point energies[15]. The purpose of this research was to investigate the corrosion inhibition of carbon steel in 1 M HCl solutions using new azo dyes as corrosion inhibitors.

The present work aims to prepare a corrosion inhibitor based on azo dye and study their inhibition efficiency as corrosion inhibitor of steel in 1.0 M HCl o also been studies the effect of the structural parameters of inhibitor on inhibition efficiency and study their adsorption mechanism on the metal surface and so, correlate the experimental results with the quantum chemical parameters of the prepared corrosion inhibitor.

2. Experimental section

1.2- The melting points of azo dye was attended using Buchi B190K. The IR spectrum was carried out on aFT-IR-8400S.Fourier Transform Infrared Spectrophotometer Shimadzu (Japan) by using a KBr disc in the range (600 – 4000) cm-1 . The UV-Visible spectrum was done using ethanol (1 x 10 -4 M). The IR,and UV-Visible spectrophotometer and melting point completed by Chemistry Department–Education College of pure sciences–University of Basrah, Iraq. Correct mass spectrum and the 1H NMR were measured in Tehran lran University.

Preparation of N-{3-[(E)-{4-[(4-aminophenyl) sulfonyl] phenyl} diazenyl]-4-hydroxyphenyl} acetamide(A_3 in spectrum figure)

The azo dye was prepared using of *4-[(4-aminobenzene)sulfonyl]aniline* (0.003 mol., 0.744g), with (1.05 mL) conc. HCl in separate deaker followed by adding 10 mL of distilled water. Then, the solution of $NaNO_2$ was prepared by dissolving (0.9 g) in (5 mL) of distilled water, the $NaNO_2$ solution was then added to the 1st beaker. The resulting diazonium salt was

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then added to N-Hydroxy-N-(4-hydroxyphenyl) acetamide (0.003 mol., 0.4535 g) in 25% sodium hydroxide solution. The resulting crude was recrystallized in ethanol and hexane to yield (63%) from the titled dye; m.p.: (183) °CThis showed δH (500 MHz, DMSO): 2.58 (3H, CH3); 7.18 -8.00 (11H, Ar-H);10.60 (1H, OH);9.23 (1H, NH).ν :(3545.16, 3460.30, 1639.49, 1440.83, 1620.21, 1147.65, 1101.35, 3099.61, 2970.38,) cm-1 ; λ max: 340 nm and 430 nm.

2.2 *The Solution of the azo in ethanol*

The stock solution of azo dye was prepared by dissolving weights (0.022 g) respectively in (50 mL) of ethanol to give the resulting concentration (1 x 10^{-3} M) from dye. Then, the (0.5 mL) of dye was took from their stock solution, (1 x 10^{-3} M) and diluted with (5 mL) of ethanol, to give (1x10^{-4} M) concentration

The inhibiting effect of some antibiotics, such as amoxicillin, on the corrosion of carbon steel in 1 M HCl was studied using weight loss in his study. The results showed that increasing the inhibitor concentration increases inhibition efficiency while increasing the temperature decreases it. The adsorption of amoxicillin on the surface of carbon steel follows the Langmire adsorption isotherm[16].

In another study, the possibility to use expired drug paracetamol as corrosion inhibitor for carbon steel in acid solutions has been investigated. 0.5 mol L^{-1} sulfuric acid and 1 mol L^{-1} hydrochloric acid have been used as corrosive media in the experimental studies. Electrochemical behaviour of paracetamol and its stability in test solutions have been examined by cyclic voltammetry. Further, the inhibitory effect has been studied by several methods: linear polarization, electrochemical impedance spectroscopy and chronoamperometry. As well, Tafel plots method was used in order to determine kinetic parameters of the corrosion process[17].

3. Results and discussion

3.1. FT-IR Spectra

The azo dye was identified by the IR spectrum, mass spectrum, 1H NMR spectrum, and the UV-visible spectrum. The IR spectrum (Figures 1) showed the stretching vibration of the ν (O-H) and (N-H) groups in the regions 3545.16cm-1 respectively. But, the (N-H) groups of NH2 was in the regions 3460.30 cm-1 respectively. the stretching vibration band of ν (N=N) was looked at 1440.83 cm-1, respectively. Additional bands are considered as skeletal vibrations. The (C=O) and the aromatic CH bands appeared in the regions (1639.49) cm-1, respectively. Though, the C-N bands were appeared in the regions1103.28 cm-1 respectively. The (O=S=O) asymmetric w. and symmetric s. bands appeared in the region (1149.57 and 1102.28) cm-1, respectively.

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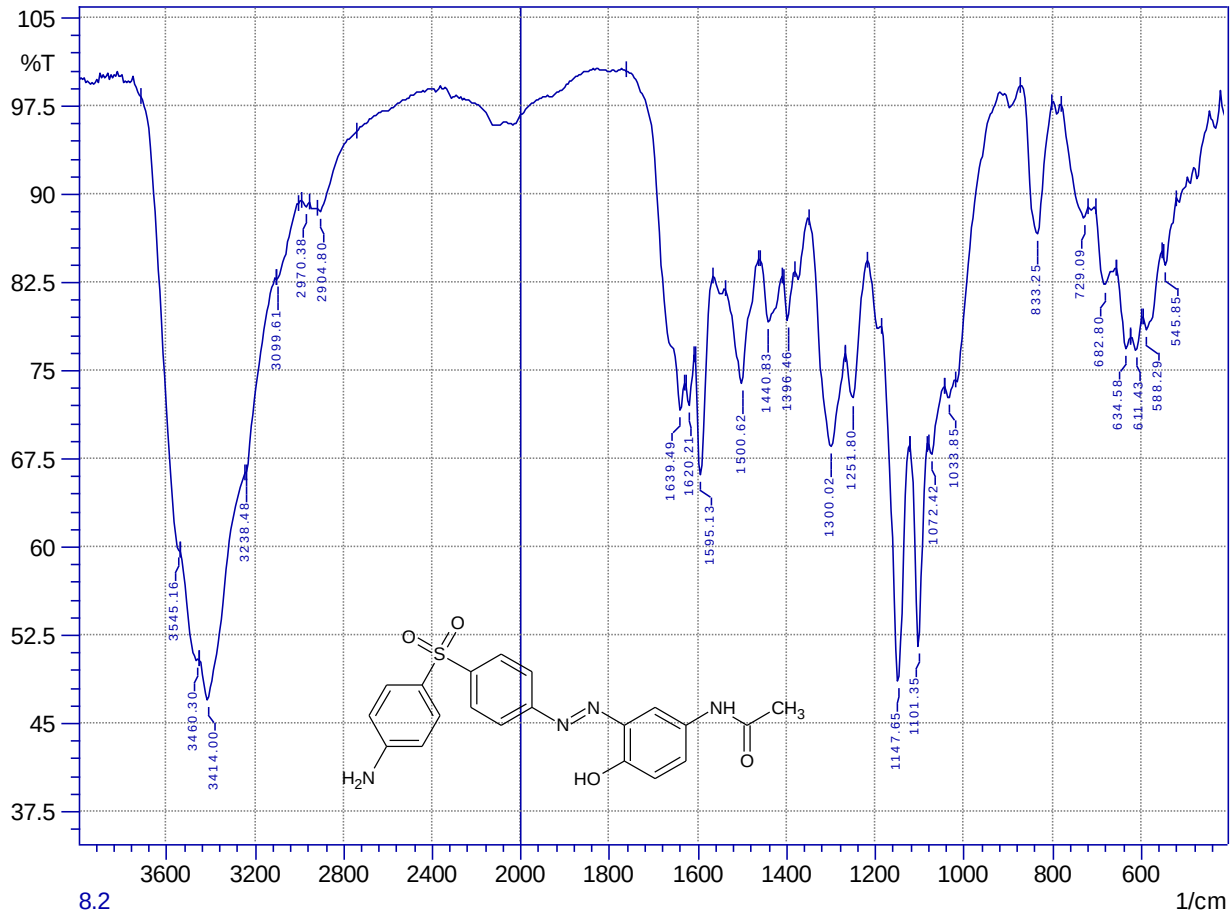

Figure1: FT-IR Spectrum of A3compound

3.2. H-NMR

Add to which, the 1H NMR spectrum was confirmed the formation of the synthetic azo dye (figures 2).

Dye	**Chemical displacementδ(ppm)**
A_3	10.60(1H, OH) ; 9.23 (H, NH) ; 8.00-7.18(11H, Ar-H); 6.54(2H,$N\underline{H}_2$) ; 2.58 (3H, CH_3)

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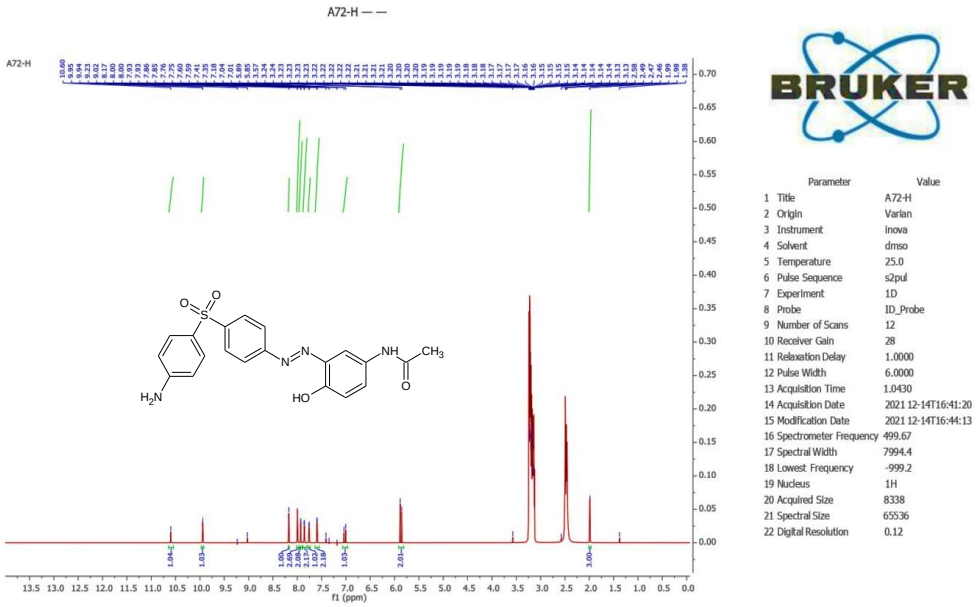

Figure2: 1 H-NMR spectrum of the A_3 compound

3.3The mass spectrum

Therefore, the mass spectrum was showed that the peak of at m/z were equal to(410g/mol) respectively as seen in figure (3)

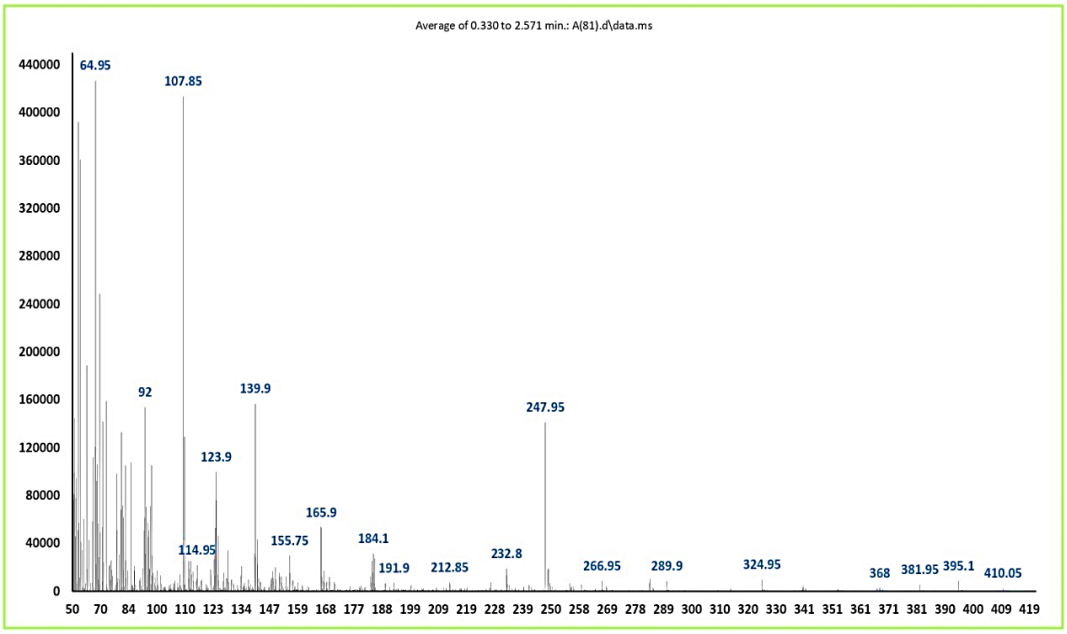

Figure 3. The mass spectrum of the azo dyes (A_3)

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3.4The UV-visible spectrum

The UV-visible spectrum was documented at the range (320-600) nm in ethanol for synthetic dye. The absorption spectrum of synthetic azo dye was showed bands at (340 nm and 430 nm) and related to (π -π*) and (n-π*) respectively

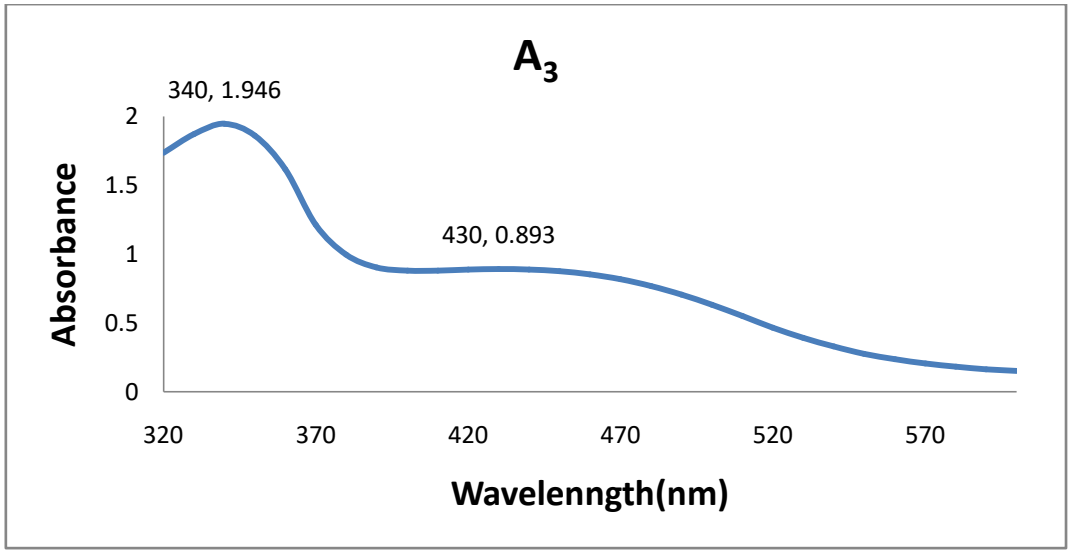

Figure 4. The UV-vis spectrum of the novel azo dye (A3)

Azo dye	λ_{max} (nm)	Transition	A	$\varepsilon(\times 10^4)$
D1	340 430	π- π* n- π*	1.946 0.893	$1.946x10^4$ $0.853x10^4$

The above information shows the interpretation of the diagnosis of infrared spectroscopy ,nuclear magnetic resonance mass spectrometry ,as well as ultravioiet spectroscopy. The spectra confirmed the additive group of the derived dye

3.5.Potentiodynamic polarization measurements

Potentiodynamic polarization measurements were carried out by Bank Eieiktronkik Intelligent Controls Type M lab 200 (2007) (Germany) three electrodes. A saturated calomel electrode Hg/Hg2 Cl2 was used as a reference electrode and a Pt electrode was used as an auxiliary electrode. The carbon steel specimen was connected to the working electrode with an exposure area of 1 cm^2 . By the extrapolation of Tafel plots segments, the corrosion current density (Icorr) was measured. The inhibition efficiency (%η) was calculated according to equation[18]..

. % η = (I°corr−Icorr/ I°corr) × 100 ……(1)

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where I°corr and Icorr are uninhibited and inhibited corrosion current densities, respectively. Potentiodynamic polarization measurements were used to test the.The corrosion inhibition efficiency of carbon steel by the (A3) compound in 1M HCl . The experiments were carried out at different temperatures (298, 308, and 318 K), in the presence of different concentrations of A3(0.001, 0.005, 0.0001 and 0.0005 mM). Table 1 illustrates the measured parameters that include: corrosion potential (Ecorr), corrosion current density (Icorr), cathodic and anodic Tafel slopes (βc and βa), inhibition efficiency (%η) and surface coverage (θ). The results indicated that increasing the concentration increases the inhibition efficiency at each temperature. The maximum recorded inhibition efficiency was 92.2% in the presence of A3at 0.005 mM concentration at 298 K[19]..It was also found that increasing the temperature above 298 K decreases the inhibition efficiency. Such a decrement in the efficiency may be attributed to the desorption of A3molecules from the adsorbed protective film on the metal surface. The displacement in the Ecorr values that results from the presence of A3in the acidic solution was found to be less than 50 mV (Table2). This indicates that A3acts as a mixed-type inhibitor which inhibits both anodic and cathodic reactions simultaneously [20].Fig. 5 shows the obtained polarization curves.

Table1: polarization parameters for carbon steel corrosion in 1M HCl in the presence of different concentrations A3at different temperature

Tem(K)	Inhibitor Conc.M	E_{corr} mv	CR mpy	Icorr μA/Cm^2	βa mv/Dec	βc mv/Dec	% IE	θ
298	**blank**	-479	22.48	25.17	243.6	-256.2	0	0
308		-494.6	26.87	44.84	327.3	-273.0	0	0
318		-477.0	29.26	67.67	340.9	-330.9	0	0
298	**1*10^{-4}**	-474.2	4.41	12.22	226.9	-245.9	51.4	0.51
308		-464.6	8.48	24.04	260.1	-268.4	46.3	0.46
318		-465.6	14.32	37.77	311.8	-308.2	44.1	0.44
298	**5*10^{-4}**	-448	3.10	8.45	158.3	-228.8	66.4	0.66
308		-443.9	7.37	18.62	207.9	-270.2	58.4	0.58
318		-460.1	12.63	31.20	275.2	-322.6	53.8	0.53

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298	**$1*10^{-3}$**	-467.7	3.10	5.76	152.7	-208.5	77.1	0.77
308		-452.4	7.37	6.60	109.8	-154.4	72.1	0.72
318		-470.9	12.63	22.31	219.8	-269.3	67.0	0.67
298	**$5*10^{-3}$**	-449.5	0.92	2.46	101.2	-155.9	92.2	0.92
308		-476.5	3.46	12.47	175.6	-192.0	89.0	0.89
318		-477.6	8.51	16.56	182.6	-183.5	88	0.88

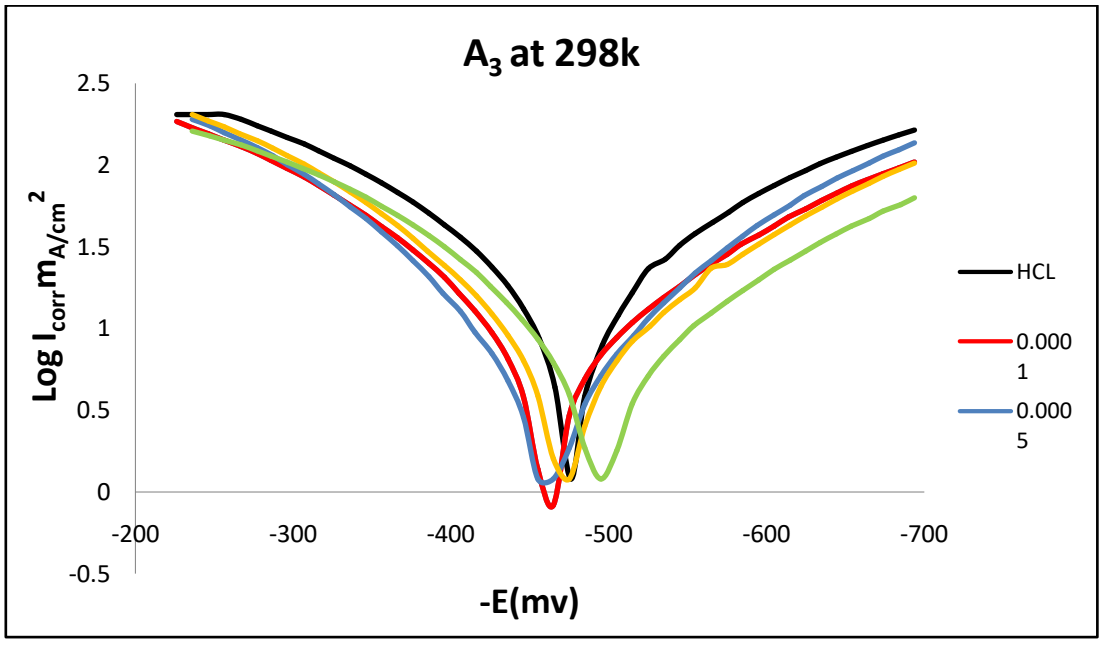

Fig5. Potentiodynamic polarization curves for carbon steel in 1 M HCl in the absence and presence of A3at 298 K.

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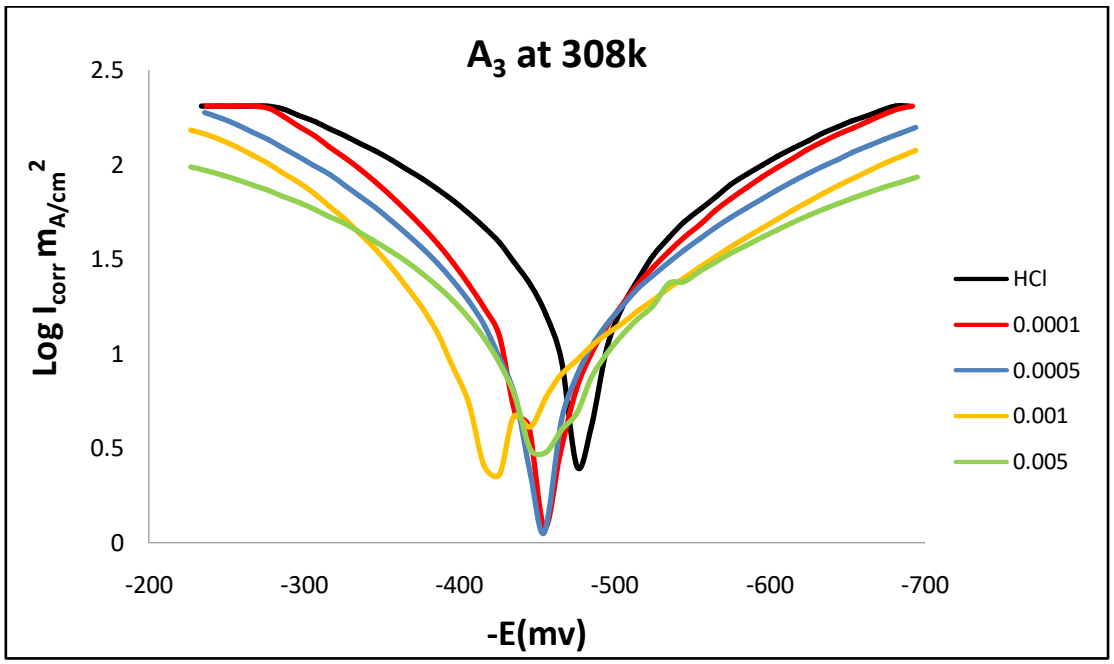
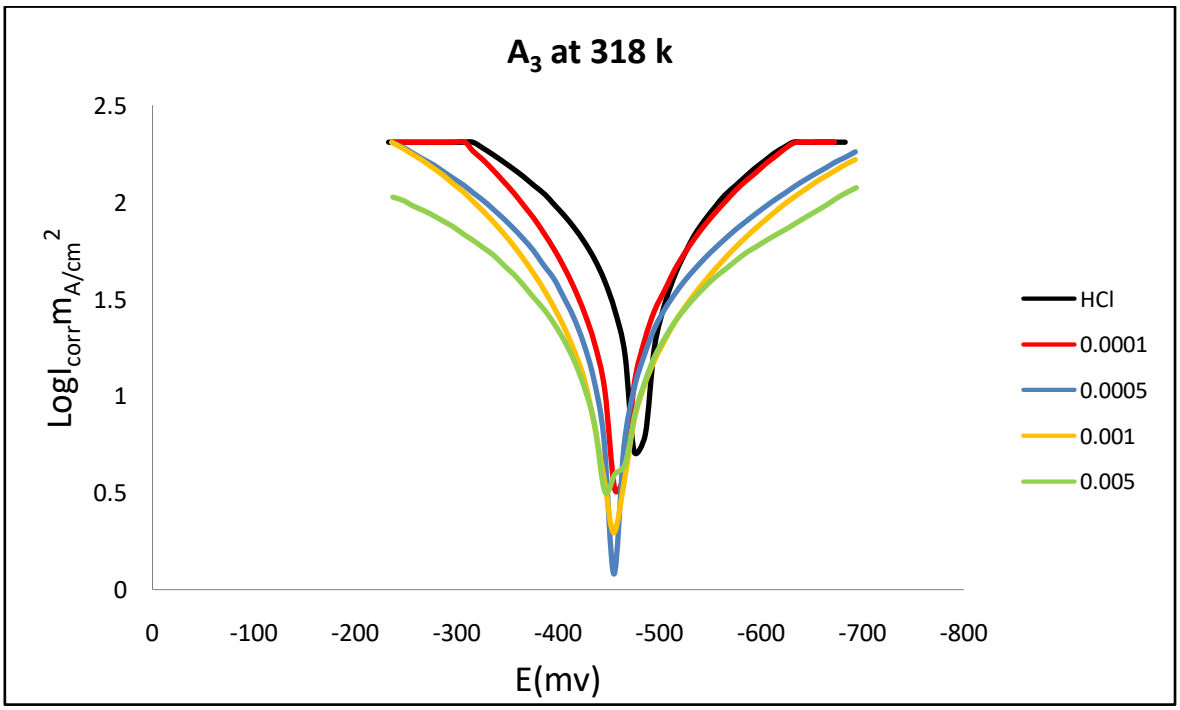


Fig6. Potentiodynamic polarization curves for carbon steel in 1 M HCl in the absence and presence of A3at 308 K.



Potentiodynamic polarization curves for carbon steel in 1 M HCl in the absence and presence of A3at 318 K of A3at 318 K.

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3.6 Effect of temperature

At a temperature range of 298–318 K, the effect of temperature on the corrosion parameters of carbon steel in inhibited solutions of 1 M HCl was studied. Fig. 8 depicts the effect of temperature on inhibition efficiency for corrosion of carbon steel in 1 M HCl in the absence and presence of different concentrations of inhibitor (A3). The data showed that the inhibitor's efficiency decreased with increasing temperature, indicating that it was less effective at higher temperatures up to 318K.[21]. This could be explained by the first stage's weakness in physisorption of adsorbed inhibitor on the carbon steel surface.

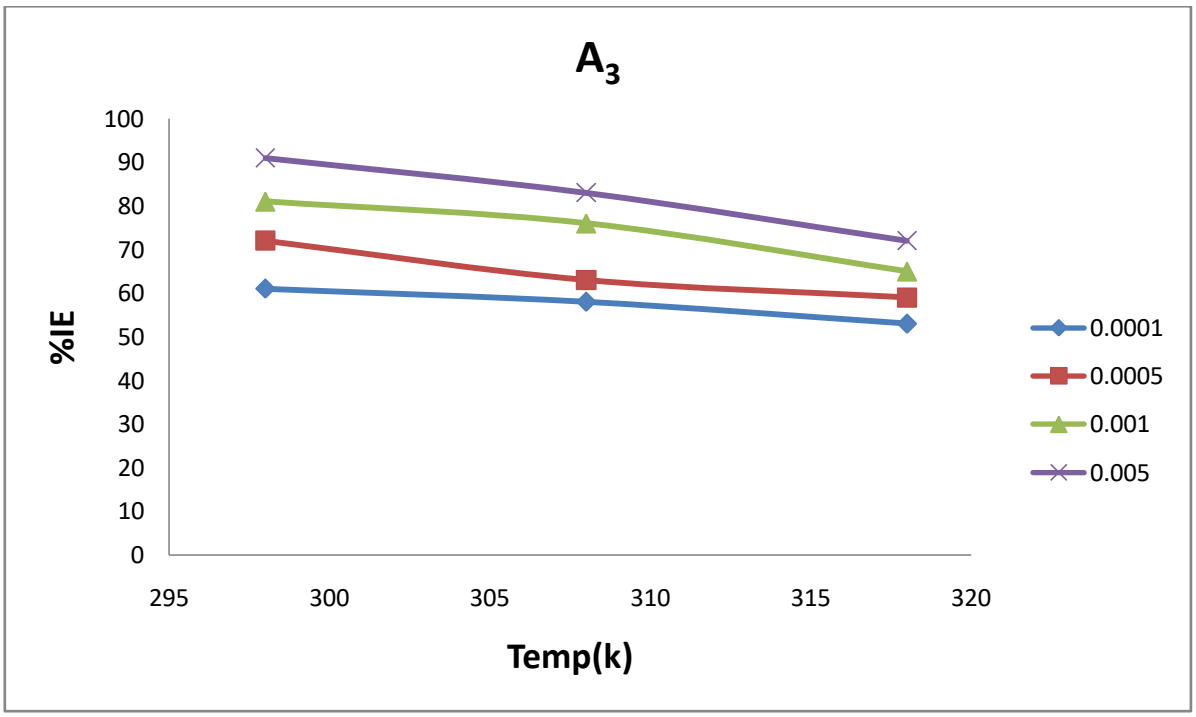

Fig8. Effect of the temperature on the inhibition efficiency was obtained for carbon steel in 1 M HCl in the presence of different concentrations of inhibitor (A3)

3.7 Adsorption isotherm

Organic molecule adsorption provides information about the interaction of the adsorbed molecules as well as their interaction with the electrode surface. The degree of surface coverage (θ) for different concentrations of inhibitor molecules in 1 M HCl was calculated using the following equation [22].

$\theta = (I°corr - Icorr / I°corr)$……..(2)

Where I°corr and Icorr are uninhibited and inhibited corrosion current densities, respectively, The general equation gives the equation that fits our results due to the Langmuir isotherm [23].

$C/\theta = 1/ Kads + C$……..(3)

where C is the inhibitor concentration, Kads is the adsorptive equilibrium constant, and (θ) is the surface coverage. The surface coverage (θ) was tested graphically for fitting a suitable

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straight line with a correlation coefficient (R2) equal to (1) a slope closed to 1 as seen in Table 2. This indicates that the adsorption of these inhibitors can be fitted to a Langmuir adsorption isotherm. The strong correlation of the Langmuir adsorption isotherm may validate this method. The reciprocal of the intercept can be used to calculate the equilibrium constant (Kads) for the adsorption–desorption process of these compounds. The adsorptive equilibrium constant (Kads) values are listed in Table 2. It is clear that the large values indicate a strong adsorption of the synthesized inhibitor on the surface of carbon steel in 1 M HCl at relatively higher temperatures. This may be due to the formation of co- ordinated bonds between the prepared inhibitor and the d- orbital of iron on the surface of steel.

3.8. Thermodynamic parameters

The standard adsorption free energy (ΔG°ads) can be obtained according to the following equation:[24].

$$\Delta G°ads = -R\ T\ \ln(55{:}5Kads) \quad \text{……..(4)}$$

where R is the gas constant (8.314J mol-1 K-1), T is the absolute temperature, and the value of 55.5 is the concentration of water in solution expressed in M. The negative values of ΔG°ads indicate that the adsorption of an inhibitor molecule onto a steel surface occurs spontaneously. Generally, values of ΔG°ads up to 20 kJ mol-1 are consistent with the electrostatic interaction between the charged molecules and the charged metal (physical adsorption), while those more negative than –40 kJ mol-1 involve sharing or transfer of electrons from the inhibitor molecules to the metal surface to form a coordinate type of bond (chemisorption) [25].Calculated ΔG°ads values indicate that the adsorption mechanism on carbon steel in 1 M HCl solution is a chemical adsorption. The adsorption heat can be calculated according to the Van't Hoff equation[26].:

$$\text{Log Kads} = -\Delta Hads/\ 2.303\ RT + Cons \quad \text{…….} \quad (5)$$

where ΔH°ads and Kads are the adsorption heat and adsorptive equilibrium constant, respectively. To obtain the standard enthalpy, plotting Log Kads vs. 1/T (Fig. 6) yielded straight line according to Eq. (5) with a slope equal to − ΔH°ads/R. The ΔH°ads values were equal to -8.45 kJ mol-1 forA3. The negative values of ΔH°ads indicated that the adsorption of investigated inhibitors on the carbon steel surface is exothermic[27].The entropy of inhibitor adsorption ΔS°ads can be calculated using the following equation[28].

$$\Delta G°ads = \Delta H°ads - T\ \Delta S°ads \quad \text{…….. (6)}$$

The obtained ΔS°ads values were listed in Table 2. The positive values of ΔS°ads mean thatthe adsorption process is accompanied by an increase in entropy, as expected, because endothermic adsorption is always accompanied by an increase in entropy, which is the driving force for inhibitor adsorption onto the carbon steel surface.

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Table2. Thermodynamic parameters of adsorption on carbon steel surface in 1 M HCl containing different temperature of the synthesized inhibitor

comp	R^2	T(K)	Log K_{ads}	ΔG_{ads}KJ.mol^{-1}	ΔH_{ads}KJ.mol^{-1}	ΔS_{ads} KJ.mol^{-1}
A_3	0.9978	298	3.92	-32.27	-8.45	-0.079
	0.9985	308	3.82	-32.80		-0.079
	0.9985	318	3.86	-34.10		-0.080

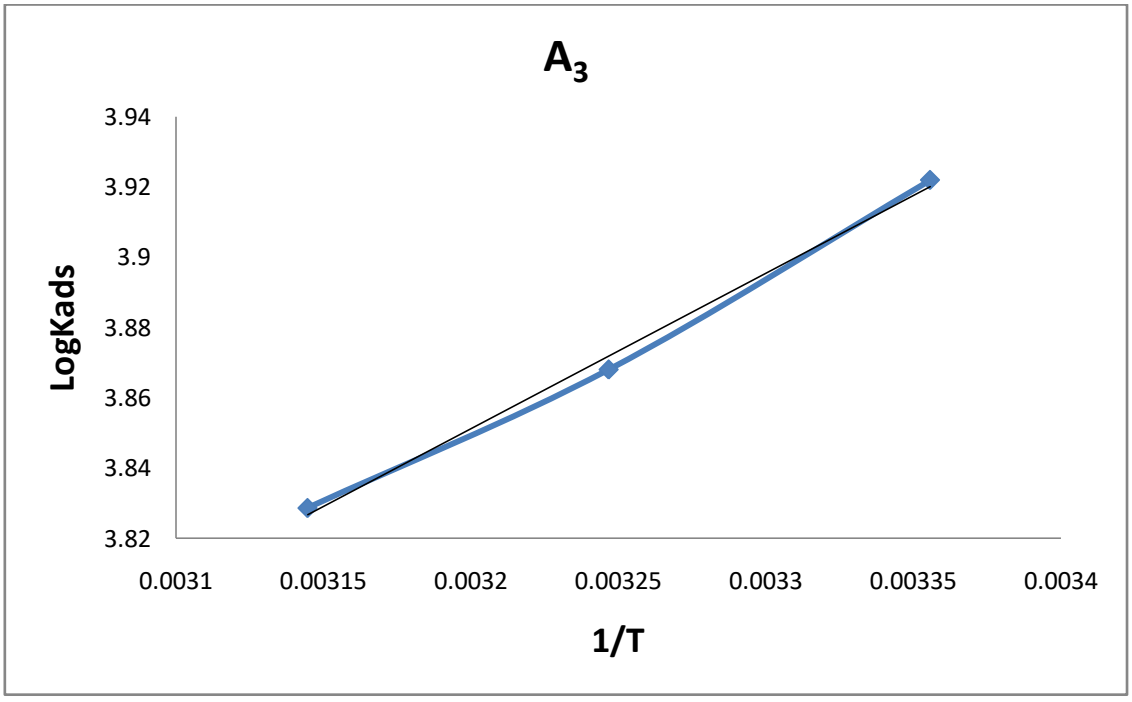

Fig9. The relationship between Log Kads and 1/T for carbon steel in 1 M HCl solution containing different concentrations of inhibitor

4.1Theoretical Study

The relationship between the electronic and molecular structures is discussed in this section. The IE percentage of the synthesized compound (A3) was also investigated. The molecular parameters that have an impact on the potential activity of these compounds, such as the LUMO and HOMO energy, dipole moment (μ), energy gap (ΔELUMO–HOMO), electron affinity (EA), electronegativity (χ), absolute softness (σ), chemical hardness (η), number of electrons transferred (ΔN) and the global electrophilicity (ω) were extensively studied. The above factors help to explain the values acquired with the corrosion process We have found

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that the orbital of both HOMO and LUMO values and the energy gaps observed in the chemical compounds According to the literature review, the adsorption of the corrosion inhibitor compound on the steel metal surfaces is based on donor-acceptor interactions that occur between the electrons in the compound and the vacant d-orbitals in the surface atoms of the metallic compound[29].The LUMO and HOMO energy values of the synthesized compound were used to explain its adsorption ability on mild steel surfaces [30].HOMO describes the molecules' ability to donate electrons, whereas LUMO describes their ability to accept electrons [31].Higher EHOMO and lower ELUMO and ELUMO–HOMO values were an effective indicator of these compounds' inhibition efficiency due to the lower energy required to remove electrons from the occupied orbitals Fig.10 shows the electronic density and the geometry optimization of the LUMO and HOMO orbitals for the compound. The results revealed that the electrondonating centers were nitrogen and oxygen atoms and phenyl groups. In comparison with compound A3, the data calculations showed that the molecule gave the maximal HOMO value and the lowest LUMO, as listed in Table 3. These results were in agreement with the experimental values. The absolute electronegativity (χ).

Furthermore, softness (σ) and global hardness (η) are important to determine the reactivity and stability of the molecules. Under chemical reactions, the chemical hardness expresses the material's resistance to deformation or polarization of the electron, including ions, molecules, and atoms. Furthermore, hard molecules possess a high energy gap, whereas soft molecules display a smaller energy gap.[32].Compound A3has the best softness and lesser hardness properties; hence, compound A3 showed a better inhibitor efficiency. Additionally, global electrophilicity (ω) was a vital reactivity marker that can be used to compare different molecules based on their electron-donating capability [33].A higher global electrophilicity indicated that the molecules behave as an electrophile. Meanwhile, compound A3 has an electrophilic behavior and showed maximal inhibition. Similar results were noted experimentallyAccording to the calculated number of electrons (ΔN) it was observed that %IE resulting from an electronic donation was similar to that observed by Lukovits et al.[34]. Suppose $\Delta N < 3.6$, an increase in IE was noted as the electron-donating ability of the metal surfaces increased. Thus, compound D1showed a higher inhibition efficiency. Hence, showed the highest fraction of electrons that were transferred (0.8225). The above results were in agreement with the experimental results.

Dipole moment (μ) is a different quantum chemical parameter that represents the corrosion IE value. This factor describes an electron distribution and bond. High values of μ (Debye) indicated that the adsorption ratio between the chemical compound and the metal surface was high [35].Furthermore, the deformability energy increased when the value of μ was increased, which indicated that the molecules could easily adsorb on the surface of iron (Fe) molecules. Compound A3 showed the dipole moment (-4.458Debye). Hence, a direct relationship was noted between the dipole moment and IE Thu[36].s, compound D1 showed higher inhibitory properties towards iron corrosion compared.

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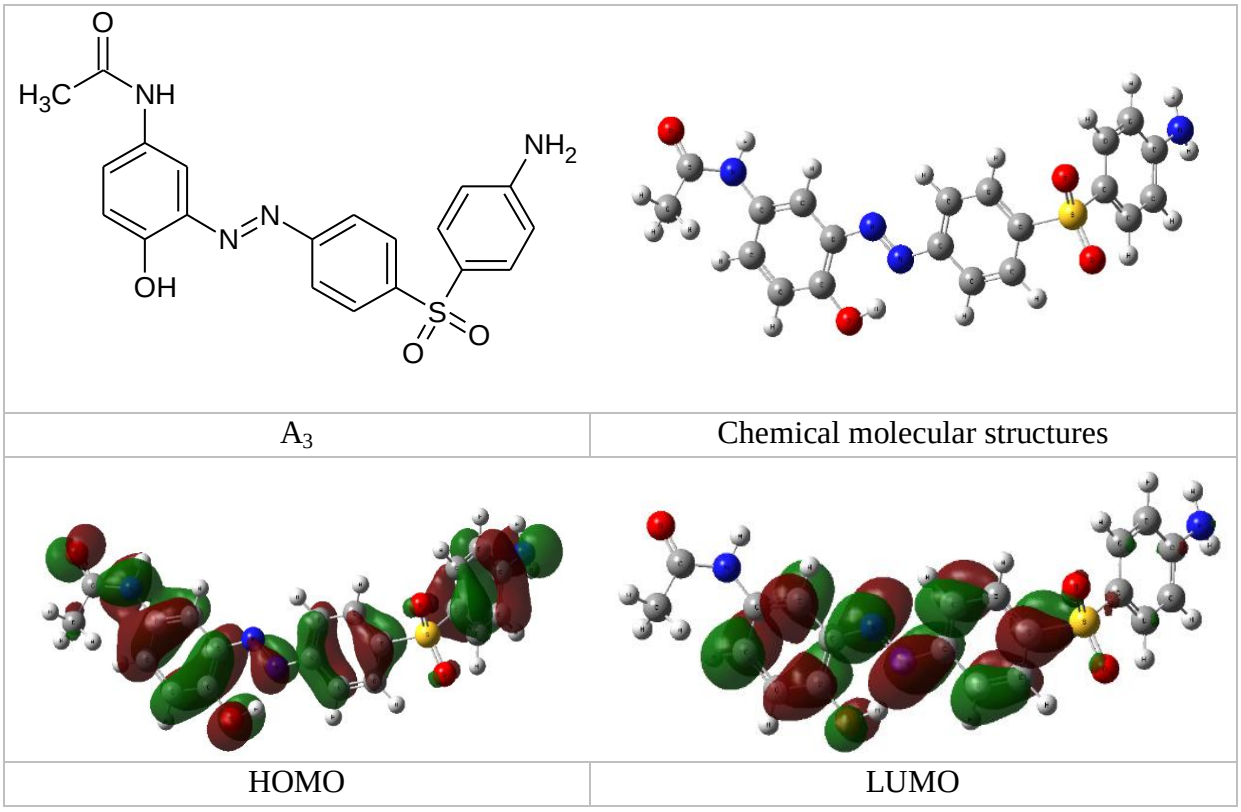
Table 3. Quantum chemical parameters values for the compound A3

Quantum Chemical parameters	**A3**
Total Energy (kJ mol^{-1})	-4439657.778936
RMS Gradient (kJ mol^{-1})	0.013127501
Dipole Moment (Debyes)	6.916904
E_{HOMO} (eV)	-6.0034
E_{LUMO} (eV)	-2.913
$\Delta E_{gab} = E_{LUMO} - E_{HOMO}$ (eV)	3.09
Ionisation potential, $I = -E_{HOMO}$	6.003
Electron affinity, $A = -E_{LUMO}$	2.9133
Electronegativity (χ), $-\frac{1}{2}(E_{HOMO} + E_{LUMO})$	4.4583
Chemical hardness (η), $\Delta E_{gab}/2$	1.5451
Softness (σ), $1/\eta$	0.6472
Chemical Potential $\mu = -1/2(I + A)$	-4.458
Number of transferred electrons $\Delta N = \chi_{Fe} - \chi_{inh}/[2(\eta_{Fe} + \eta_{inh})]$	0.8225



A_3	Chemical molecular structures
HOMO	LUMO

Fig10.Geometry optimization and HOMO, LUMO orbital's of the studied compound

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CONCLUSIONS

Our findings on the effectiveness of the S1H compound in preventing carbon steel corrosion in an acid medium show. The studied S1H exhibited a maximum inhibition efficiency of 92.2 % when measured using the hydrodynamic method at a concentration of 5.0 mM and a temperature of 298 K. - According to the calculation of different thermodynamic parameters and the study of the adsorption isotherm, the adsorption is Langmuir type and a mixed type of physisorption and chemisorption that is a difficult kind of interaction. According to polarization studies, the inhibitor has an effect on both anodic and cathodic processes. The experimental and theoretical methods used to assess the inhibitor's effectiveness produced consistent results

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