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Adsorption and density functional theory on corrosion of mild steel by a quinoxaline derivative

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ABSTRACT

(3E)-3-{[4-(phenylsulfonyl)]imino}-3,4-dihydroquinoxalin-2(1H)-one (PSDQO) has been synthesized and its inhibiting action on the corrosion of mild steel in 1 M H_2SO_4 has been assessed by weight loss method at 303 K – 333 K. The results of the investigation show that this compound has excellent inhibiting properties for mild steel corrosion in sulphuric acid. Inhibition efficiency increases with increase in the concentration of the inhibitor. The adsorption of the inhibitor was tested for Langmuir, Temkin, Flory-Huggin's and El-Awady isotherm and proved physical adsorption. Quantum chemical calculations were employed to give further insight into the mechanism of inhibitive action of the inhibitor.

Keywords: adsorption isotherm, activation energy, mild steel, quantum chemical study, energy gap

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INTRODUCTION

Mild steel is considered as one of the excellent alloys of iron. It has wide application in industries and structural uses due to its superior mechanical properties. Generally, mild steel undergoes corrosion in processes such as acid pickling, industrial cleaning, acid descaling, oil well acidizing, and petrochemical processes [1-4]. Acid solutions are commonly used in the chemical industry to remove mill scales from metallic surfaces. The majority of the well-known acid corrosion inhibitors are organic compounds that contain nitrogen, sulphur or oxygen atoms [5], the inhibition efficiency generally increases in the order O < N < Sbecause of their increasing tendency to form a coordinationbond. The inhibitors having more than one heteroatom showbetter corrosion inhibition in comparison to those possessingjust one of them. Among such inhibitors, quinoxaline derivatives have been reported as efficient corrosion inhibitor for different metal−environmentsystems like mild steel (MS) [6-8], copper [9-11], carbon [12,13] etc. in different acidic media. These compounds usually formvery thin and persistent adsorbed films on the metal surface, causing a decrease in the corrosion rate by retarding anodic, cathodic, or both reactions [14].

In the present investigation, a comparative study of the inhibitive characteristics of (3E)-3-{[4-(phenylsulfonyl)] imino}-3, 4-dihydroquinoxalin-2(1H)-one (PSDQO) on the corrosion of mild steel in 1 M $H_2SO_4$was studied. Weight loss measurements have been employed to determine the inhibition efficiency in order to accomplish the possible mechanism of inhibition. The corroded and inhibited metal surfaces have been characterized by scanning electron microscopy (SEM). The structural correlation of the inhibition efficiency of PSDQO has been further ascertained using density functional theory (DFT).

MATERIALS AND METHODS

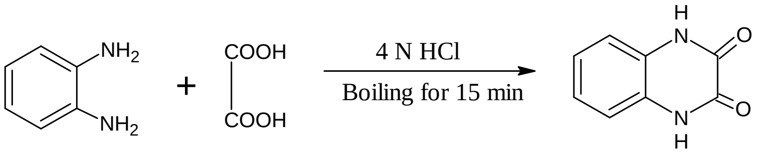
2.1 Materials and Methods

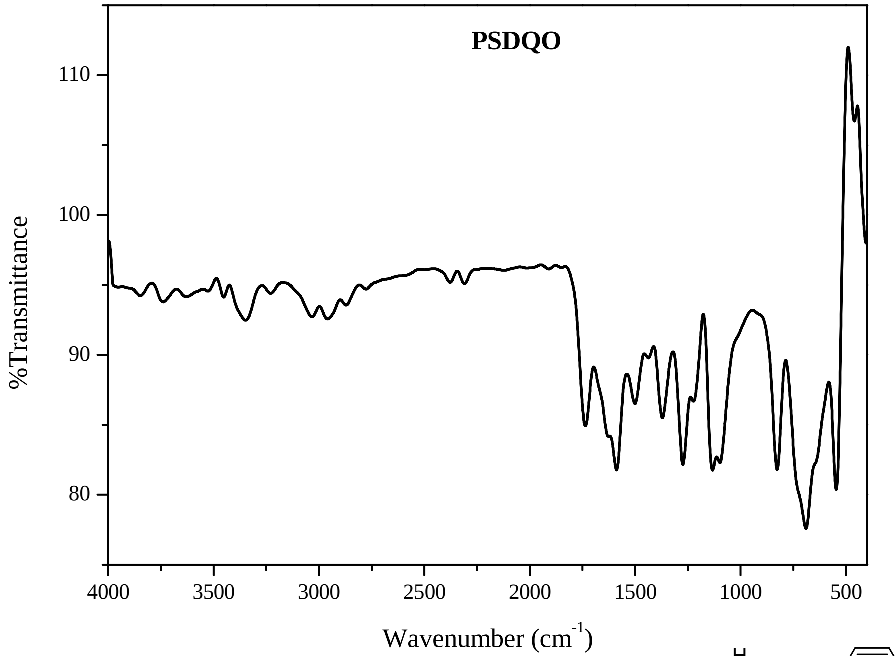
Cold rolled mild steel specimen of size 1cm x 3cm x 0.08cm having composition 0.084% C, 0.369% Mn, 0.129% Si, 0.025% P, 0.027% S, 0.022% Cr, 0.011% Mo, 0.013% Ni and the reminder iron were used for weight loss measurements. For electrochemical methods, a mild steel rod of same composition with an exposed area of 0.785

cm^2 was used. The specimens were polished with 1/0, 2/0, 3/0 and 4/0 grades of emery sheets and degreased with trichloroethylene and dried using a drier. The plates were kept in a desiccator to avoid the absorption of moisture.

2.2. Synthesis of the inhibitor

Synthesis of 1,4-dihydroquinoxaline-2,3-dione and its derivative were reported by R. V. Ghadage and Pramod J. Shirote [15].





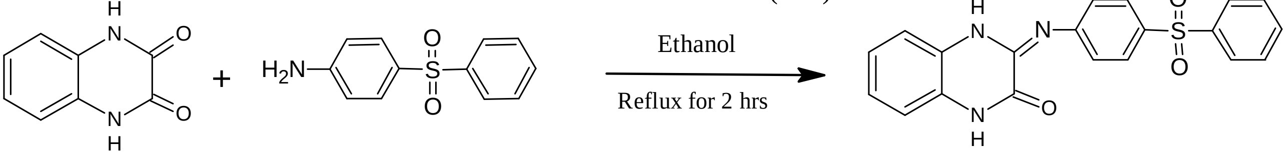


Figure 1: IR Spectrum of PSDQO

(3E)-3-{[4-(phenylsulfonyl)]imino}-3,4-dihydroquinoxalin-2(1H)-one (PSDQO) : Yield= 95%, Melting Point = 183 ºC, dirty white, IR Spectrum (γ/cm^{-1}) : 1676.21 (C=N); 1724.44 (C=O); 1219.08 (C-N).

2.3Evaluation of inhibition efficiency by weight loss method

The initial weight of the polished mild steel plates of size 1cm x 3cm x 0.08cm was taken. The solutions were taken in a 100 ml beaker and the specimens were suspended in triplicates into the solution using glass hooks. Care was taken to ensure the complete immersion of the specimen. After a period of 3 hours the specimens were removed, washed with distilled water, dried and weighed. From the initial and final masses of the plates (i.e., before and after immersion in the solution) the loss in weight was calculated. The experiment was repeated for various inhibitor concentrations in 1M H_2SO_4. A blank was carried out without inhibitor.

The inhibition efficiency, corrosion rate and surface coverage were calculated from the weight loss results using the formulas,

$$\text{Efficiencyof inhibitor} = \frac{(\text{Weight loss without inhibitor - Weight loss with inhibitor})}{\text{Weight loss without inhibitor}} \text{X100}$$

$$\text{Corrosion Rate} = \frac{534 \text{ X Weight loss (g)}}{\text{Density X Area (cm) X Time (hr)}}$$

$$\text{Surface Coverage}\,\theta = \frac{(\text{ Weight loss without inhibitor - Weight loss with inhibitor)})}{\text{Weight loss without inhibitor}}$$

To study the effect of temperature, the above procedure was carried out at different temperature range i.e., (313-333K) using thermostat with the inhibitor concentration of 10mM.Activation energy (E_a), Free energy of adsorption (ΔG°), Enthalpy and Entropy (ΔH°& ΔS°) were calculated using the formulas,

$$\text{(i)} \quad \log CR = \frac{-E_a}{2.303\,RT} + \log A$$

$$\text{(ii)} \quad K = \frac{1}{55.5} \exp\left[-\frac{\Delta G^{\circ}_{ads}}{RT} \right]$$

where $K = \frac{\theta}{c(1-\theta)}$ [from Langmuir equation], θ - Surface coverage of the inhibitor, C- concentration of inhibitor in mM/100ml

$$\text{(iii)} \quad CR = \frac{RT}{Nh} \exp\frac{\Delta S^{\circ}}{R} \exp\frac{-\Delta H^{\circ}}{RT}$$

h – Planck's constant, N - Avogadro number, T - Absolute temperature, R - Universal gas constant.

2.4 Surface morphology

Mild steel specimen of dimensions 3 cm X 1 cm X 0.08 cm were immersed in 1M H_2SO_4 in the absence and presence of inhibitors with optimum concentration for 3 hours. The specimens were removed, washed with distilled water and dried. The chemical composition of the layer formed was analyzed with an EDS coupled with SEM using Biomedical Research Microscope (Mumbai, India).

2.5 Quantum chemical studies

DFT method is very much useful for the Quantum mechanical calculations of energies, geometries and vibrational wave numbers of organic chemical system. The gradient corrected density functional theory (DFT) with the three parameter hybrid functional Becke3 (B3) for the exchange part and the Lee–Yang–Parr (LYP)correlation functional, calculations have been carried out in the present investigation, using 6-311G(d,p) basis sets with Gaussian-03 program, invoking gradient geometry optimization. All the parameters were allowed to relax and all the calculations converged to an optimised geometry, which corresponds to true energy minima.

RESULTS AND DISCUSSION

3.1 Weight loss measurements

Data derived from the weight loss study such as weight loss, inhibitor efficiency, surface coverage and corrosion rate are listed in Table1. It can be seen from the Table 1 that inhibition efficiency increases and corrosion rate decreases with increasing the concentration of the inhibitor. The inhibitor shows maximum inhibition efficiency upto 85.94% at 10 mM concentration. Figure 1 shows a plot of percentage inhibition efficiency with the concentration of inhibitor, indicating that the inhibition efficiency increases with increasing the concentration of the inhibitor. The inhibitive properties of PSDQO is mainly due to the interaction between electrons of the two aromatic rings of the quinoxaline and the free pairs of electrons of S, N and O atoms with the positively charged metal surface.

Table 1: Inhibition efficiencies of various concentrations of the inhibitor PSDQO for corrosion of mild steel in 1M H_2SO_4 obtained by weight loss measurement at 30±1^{0}C

Name of the Inhibitor	Concentration (mM)	Weight loss (g)	Inhibition Efficiency (%)	Surface Coverage (θ)	Corrosion Rate (g $cm^{-2}hr^{-1}$)
BLANK	-	0.2212	-	-	21.92
PSDQO	0.5	0.0986	55.42	0.7006	9.77
	1	0.0929	58.00	0.7331	9.21
	2.5	0.0905	59.08	0.9349	5.71
	5	0.0517	75	0.9686	5.12
	7.5	0.0495	76.63	0.9811	4.91
	10	0.0311	85.94	1	4.58

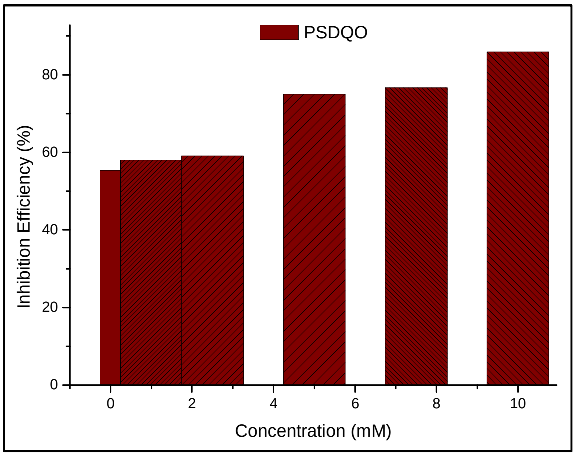


Figure 2: Plot of inhibition efficiency (%) Vs concentration (mM) for the inhibition of corrosion of mild steel in 1M H_2SO_4

3.2 Effect of temperature

Temperature plays an important role in understanding the inhibitive mechanism of the corrosion process. To assess the temperature effect, experiments were performed at 303 - 333K in uninhibited and inhibited solutions containing different concentrations of the inhibitor and the corrosion rate was evaluated as presented in Table 2.

Table 2: Inhibition efficiencies of 10mM concentration of the inhibitor PSDQO for corrosion of mild steel in 1M H_2SO_4 obtained by weight loss measurement at higher temperature

Name of the Inhibitor	Temperature (k)	Weight loss (g)	Inhibition Efficiency (%)	Corrosion rate (g $cm^{-2}hr^{-1}$)
BLANK	303	0.0619	-	18.40
	313	0.1152	-	34.25
	323	0.2247	-	66.81
	333	0.4762	-	141.58
PSDQO	303	0.0499	26.29	14.84
	313	0.0994	23.24	29.55
	323	0.1986	21.38	59.05
	333	0.4329	13.78	128.71

A plot of log of corrosion rate obtained by weight loss measurement versus 1/T gave a straight line with regression coefficient (R^2=0.9977) close to unity, as shown in Figure 3. The value of apparent activation energy (E_a) is computed from the slope of the straight line and listed in Table 3. It is evident from Table 3 that the apparent energy of activation increased on addition of PSDQO in comparison to the uninhibited solution. The increase in the apparent activation energy suggests physical adsorption. Increase in the activation energy is due to a decrease in the adsorption of inhibitor on mild steel surface by increase in the temperature. This decrease in adsorption leads to increase in corrosion rate due to the greater exposed surface area of the mild steel towards 1M H_2SO_4 solution [16].

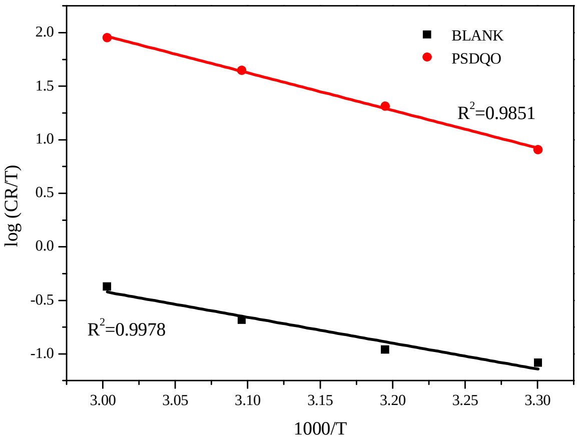


Figure 3: Arrhenius plot

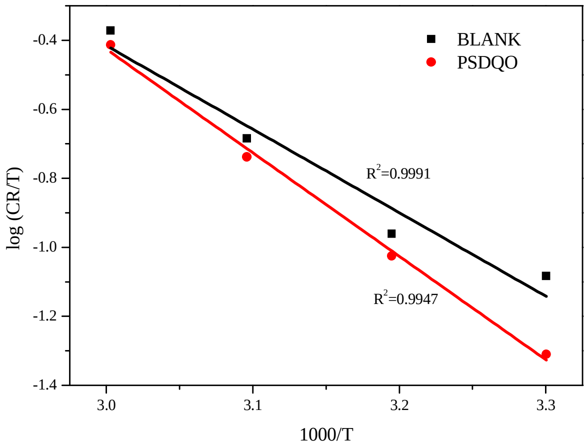


Figure 4: Transition state plot

Figure 4 shows a plot of log (Corrosion Rate/T) against (1000/T). Straight lines are obtained with a slope of (-ΔH°/2.303R) and an intercept of (log R/Nh + ΔS° (2.303R)) from which the values of ΔH° and ΔS° are calculated and tabulated in Table-1. The values of ΔH° lower than 43.2 kJmol^{-1}, which attributed with physical adsorption and if the values equal 100 kJmol^{-1},which indicate adsorption is chemical adsorption[17].

The values of ΔS° in the presence and absence of the inhibitors are negative. This implies that the activation complex is the rate-determining step representing association rather than dissociation, indicating that a decrease in disorder takes place on going from reactant to activated complex[18].

The ΔG^{o}_{ads} values show that the inhibitor is adsorbed spontaneously onto the mild steel surface. Normally, the magnitude of ΔG° ads around −20 kJ/mol or less negative is assumed for physisorption and those around −40 kJ/mol or more negative are indicative of chemisorption. The values of ΔG° ads are between these two, but modestly closer to −20 kJ/ mol. Therefore, PSDQO is adsorbed on the mild steel surface predominately by a physisorption method [19,20].

Table 3: Kinetics/Thermodynamic parameters of mild steel corrosion in 1M H_2SO_4 at different temperatures

Name of the Inhibitor	**Ea (kJ)**	**-ΔG (kJ/mole)**				**ΔH (kJ mol^{-1})**	**-ΔS (kJ mol^{-1})**
		303	**313**	**323**	**333**		
BLANK	56.86	-	-	-	-	20.13	0.1406
PSDQO	60.10	24.93	25.32	25.84	25.17	24.95	0.1262

3.3 Adsorption isotherm

The adsorption isotherm gives information about interactions between the inhibitor and the mild steel surface. The efficiency of PSDQO as a successful corrosion inhibitor mainly depends on its adsorption capacity on the metal surface. It is crucial to know the mode of adsorption as well as the adsorption isotherm that can give important information on the interaction between the inhibitor and the metal surface. The relationship of C/θ versus C is depicted in Figure 4. The adsorption of PSDQO on metal surface obeyed the Langmuir adsorption isotherm. This can be expressed by the following equation:

$$\frac{C}{\theta} = \frac{1}{k_{ads}} + C \quad \text{------------------------- (1)}$$

where k_{ads} is the equilibrium constant of the adsorption process and ‘C’ is the inhibitor concentration and θ is the fraction of the surface covered. Figure 4 shows the dependence of C/ θ as a function of concentration C for the inhibitors.

Temkin adsorption model is expressed by equation (2). Temkin adsorption model on corrosion of mild steel by PSDQO is represented in Figure 5.

$$\text{Exp}^{-2a\theta} = KC \quad \text{----------------------------- (2)}$$

The relationship between the equilibrium constant (K) of adsorption and the free energy of adsorption, ΔG_{ads}, is given by the following expression

$$\Delta G_{ads} = -2.303RT \log (55.5 K) \text{ -------------------------- } (3)$$

The values of free energy of adsorption calculated from equation (3) using K values obtained from the Langmuir adsorption and Temkin adsorption isotherm are presented in Table-4. The values are negative and less than -30 $kJmol^{-1}$. This implies that the adsorption of the inhibitor on mild steel surface is spontaneous and confirms physical adsorption mechanism [21].

The Flory-Huggins adsorption isotherm is given by the following equation

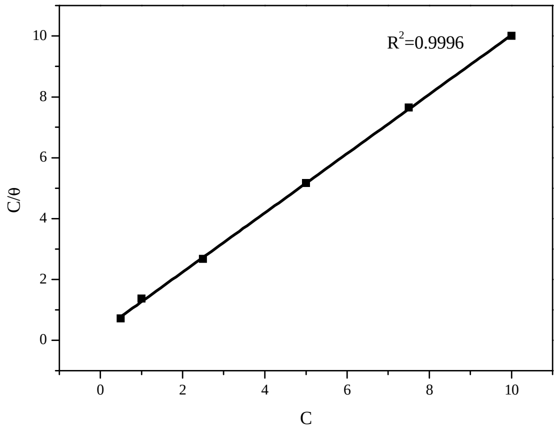
$$\log \frac{\theta}{C} = \log K + \log (1-\theta) \text{ -------------------------- } (4)$$

A plot of $\log \frac{\theta}{1-\theta}$ against log C gave a linear relationship (Figure 6) showing that Flory-Huggins isotherm model for the inhibition of mild steel by PSDQO in 1M H_2SO_4. The values of the size parameter (y) are positive (Table 4) which indicates that the inhibitor molecules are adsorbed on the mild steel surface by displacing more than one water molecule [22].

The El-Awady adsorption isotherm equation is given by

$$\log \left(\frac{\theta}{1-\theta} \right) = \log K + y \log C_{inh} \text{ ---------------------------- } (5)$$

where C_{inh} is molar concentration of inhibitor in the bulk solution, θ is the degree of surface coverage, K is the equilibrium constant of adsorption process ; $K_{ads} = K^{1/y}$ and 'y' represents the number of inhibitor molecules occupying a given active site. Value of 1/y less than unity implies the formation of multilayer of the inhibitor on the metal surface, while the value of 1/y greater than unity means that a given inhibitor occupy more than one active site. Curve fitting of the data to the thermodynamic-kinetic model is shown in Figure7. This plot gave straight lines which clearly show that the data fitted well to the isotherm. The values of 1/y and K_{ads} calculated from the El-Awady et al. model curve is given in Table 4. From the table the obtained values of 1/y is greater than one showing that the inhibitor PSDQO molecule occupies more than one active site (which may be due to the presence of S, N & O atoms in PSDQO molecule together with several electrons). It is also seen from the table that K_{ads} decreases with increase in temperature indicating that adsorption of PSDQO on the mild steel surface was unfavourable at higher temperatures.[23-25].



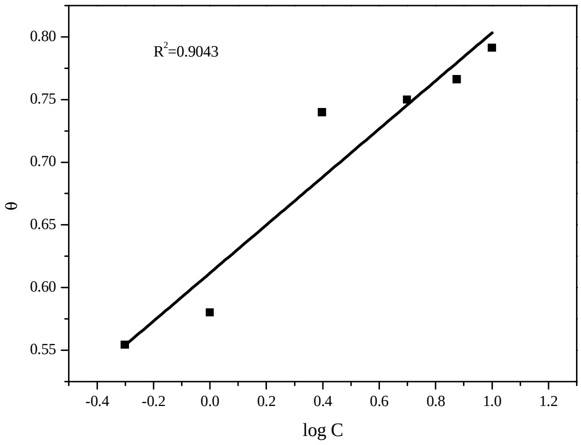


Figure 4: Langmuir adsorption model **Figure 5: Temkin adsorption model**

Table 4: Thermodynamic parameters of adsorption of the inhibitor PSDQO on the mild steel surface at room temperature

Name of the Inhibitor	Langmuir Isotherm				Temkin Isotherm			
	R^2	K mol lt^{-1}		-ΔG (kJ mol^{-1})	R^2	K mol lt^{-1}		-ΔG (kJ mol^{-1})
PSDQO	0.9987	384.96		25.12	0.9038	611.53		26.29
	Flory-Huggin's Isotherm				El-Awady Isotherm			
	R^2	K mol lt^{-1}	-ΔG (kJ mol^{-1})	1/n	R^2	K mol lt^{-1}	-ΔG (kJ mol^{-1})	1/y
	0.9949	1058.03	27.67	0.3231	0.9162	204.13	10.22	2.58

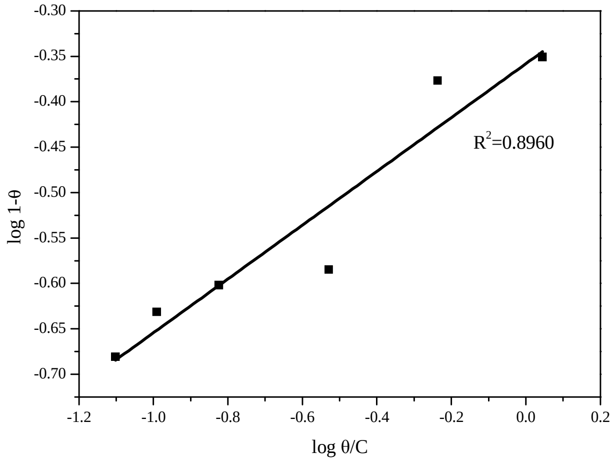


Figure 6: Flory-Huggin's plot

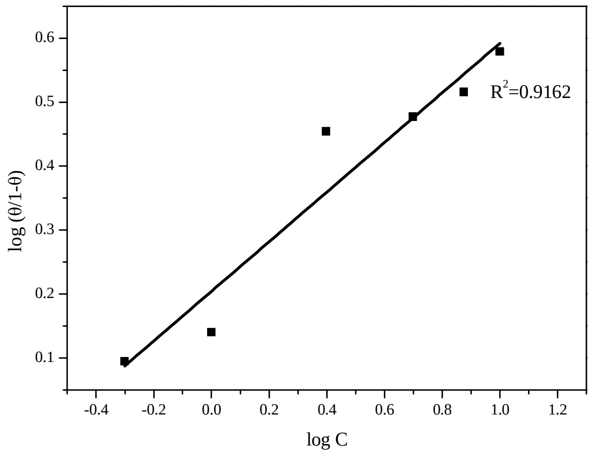


Figure 7: El-Awady plot

3.4. Surface Morphology

3.4.1 Scanning Electron Microscopy (SEM)

The surface morphologies of exposed mild steel to 1M H_2SO_4 solutions in the absence and presence of PSDQO after 12 h of immersion at room temperature were examined using SEM. The results shown in Figure 8 a,b reveal that the mild steel specimens underwent active dissolution, as indicated by the roughness of the surface in the absence of PSDQO in both acidic environments, as expected due to corrosive attack of the acidic solutions. The attack was uniform with no evidence of selective corrosion (localized attack). In the presence of PSDQO the rough surface is seen to decrease, indicating an inhibiting effect of PSDQO on the surface of mild steel due to the formation of protective layers that create a barrier for charge and mass transfer, and there is slight evidence of adsorbate presence on the metal surface.

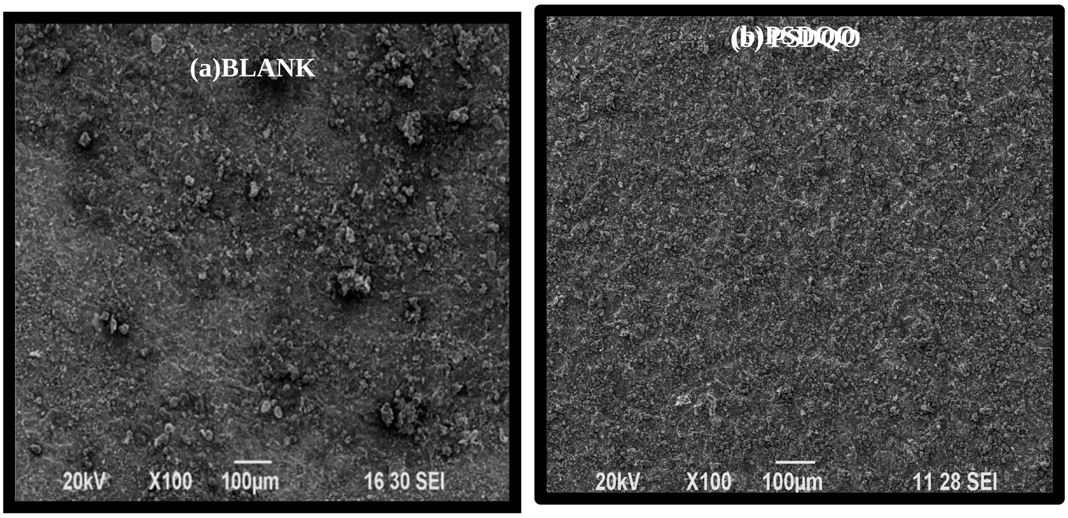


Figure 8: Scanning Electron Microscopy photographs in the absence and presence of the inhibitor (PSDQO)

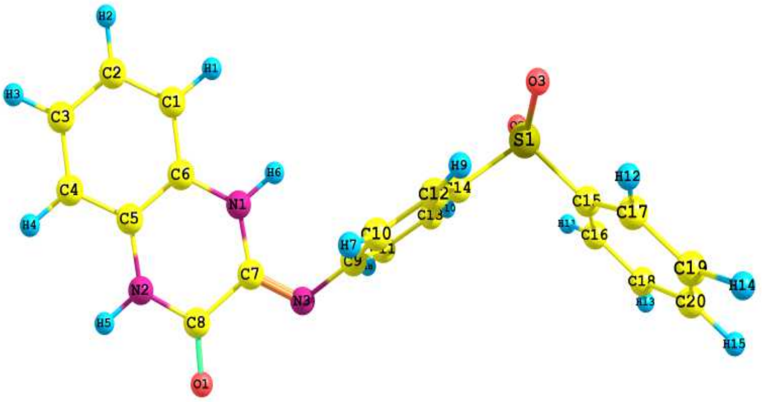
3.5. Quantum chemical studies

Quantum chemical calculations have been widely used to study reaction mechanisms. They have also proved to be a very powerful tool for studying corrosion inhibition mechanisms [26]. Recently, theoretical prediction of the efficiency of corrosion inhibitors has become very popular in parallel with the progress in computational hardware and the development of efficient algorithms, which assisted the routine development of molecular quantum mechanical calculations [27]. Some quantum chemical parameters, which are important to directly influence on electronic interaction between metal surface and inhibitor, are listed in Table 5. All these quantum chemical parameters were obtained after geometric optimization of the studied compound. The optimized geometry, HOMO and LUMO are shown in Figure 9.

Table 5: The calculated quantum chemical parameters for the inhibitor PSDQO obtained using DFT at the B3LYP/6-311G (d,p) basis set

Quantum chemical parameters	PSDQO
Total energy (amu)	-1559.55
Dipole moment(μ)	4.11
E_{HOMO} (eV)	-6.24
E_{LUMO} (eV)	-1.78
Energy gap (eV)	4.46
Ionization potential (I)	6.24
Electron affinity (A)	1.78
Hardness (η)	2.23
Softness (σ)	0.45
Fraction of electrons transfered(ΔN)	0.6704

According to the frontier molecular orbital theory (FMO) of chemical reactivity, transition of electron is due to interaction between highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of reacting species. It is understood that higher the E_{HOMO} of the inhibitor, greater the ease of offering electrons to unoccupied ‘d’ orbital of the metal, and the higher corrosion inhibition efficiency for iron in sulphuric acid solutions; in addition, as the LUMO–HOMO energy gap (ΔE) decreased, interactions between the reacting species become stronger and consequently efficiency of the inhibitor improved.The highest value of E_{HOMO} -6.24 (eV) of PSDQO indicates the better inhibition efficiency.



Optimized geometry

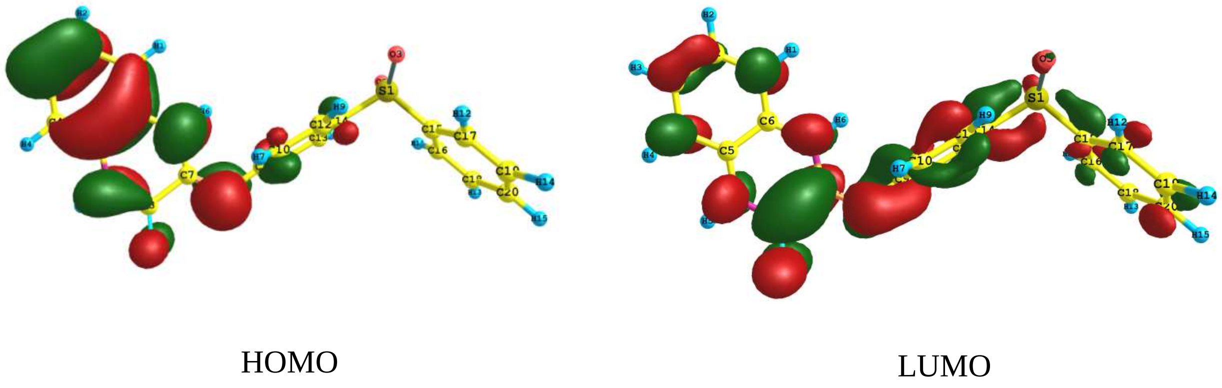

HOMO LUMO

Figure 9: Optimized geometry, HOMO and LUMO of PSDQO

The total energy calculated by quantum chemical methods is also a beneficial parameter. The total energy of a system is composed of the internal, potential, and kinetic energy. Hohenberg and Kohn [28] proved that the total energy of a system including that of the many body effects of electrons (exchange and correlation) in the presence of static external potential (for example, the atomic nuclei) is a unique functional of the charge density. The minimum value of the total energy functional is the ground state energy of the system. The electronic charge density, which yields this minimum value, is then the exact single particle ground state energy. In our study, the total energy of the inhibitor PSDQO is equal to -1559.55 eV, which proves the better inhibition efficiency.

The molecular stability and reactivity were measured by absolute hardness and softness. The chemical hardness signifies the resistance towards the deformation or polarization of the electron cloud of the atoms, ions or molecules under small perturbation of the chemical reaction. [29]. The inhibitor has low hardness value (η=2.23 eV) and softness value (σ = 0.45 eV). Normally, the inhibitor with the least value of global hardness η and highest value of global softness σ is expected to have the highest inhibition efficiency [30].

The number of electrons transferred (ΔN) indicates the tendency of a molecule to donate electrons. The higher the value of ΔN, the greater is the tendency of a molecule to donate electrons to the electron poor species. In the case of corrosion inhibitors the higher value of ΔN implies a greater tendency to interact with the metal surface. The inhibitor PSDQO has ΔN value of 0.6704.

Table 6: Calculated Mulliken atomic charges, Fukui functions and softness indices for the atoms of PSDQO using DFT at the B3LYP/6-311G(d,p) basis set

Atoms	q_N	q_{N+1}	q_{N-1}	f_k^+	f_k^-	f_k^o	s_k^+	s_k^-
C2	0.0262	0.0875	-0.0244	0.0613	0.0506	0.0560	0.0276	0.0228
C3	0.0082	0.0834	-0.0386	0.0752	0.0468	0.0610	0.0338	0.0211
C4	0.0058	0.0955	-0.0480	0.0897	0.0538	0.0718	0.0404	0.0242
C5	0.0286	0.0940	-0.0352	0.0654	0.0638	0.0646	0.0294	0.0287
C6	0.1951	0.2270	0.1946	0.0319	0.0005	0.0162	0.0144	0.0002
C7	0.1840	0.2004	0.1859	0.0164	-0.0019	0.0072	0.0074	-0.0009
C8	0.2480	0.2678	0.1951	0.0198	0.0529	0.0364	0.0089	0.0238
C9	0.3694	0.3907	0.3181	0.0213	0.0513	0.0363	0.0096	0.0231
N15	-0.2295	-0.1613	-0.2443	0.0682	0.0147	0.0415	0.0307	0.0066
N16	-0.2338	-0.1790	-0.2665	0.0548	0.0326	0.0437	0.0247	0.0147
O17	-0.3051	-0.2502	-0.3642	0.0549	0.0591	0.0570	0.0247	0.0266
N18	-0.2944	-0.2179	-0.3269	0.0765	0.0326	0.0545	0.0344	0.0146
C19	-0.0312	-0.0516	-0.0440	-0.0204	0.0128	-0.0038	-0.0092	0.0058
C20	0.0424	0.0835	0.0021	0.0411	0.0403	0.0407	0.0185	0.0181
C21	0.0706	0.1270	0.0198	0.0564	0.0508	0.0536	0.0254	0.0229
C24	0.1201	0.1606	0.0694	0.0405	0.0507	0.0456	0.0182	0.0228
C25	0.1145	0.1581	0.0684	0.0436	0.0461	0.0449	0.0196	0.0208
C28	-0.3325	-0.3087	-0.3470	0.0238	0.0145	0.0191	0.0107	0.0065
S29	1.0458	1.0610	1.0168	0.0152	0.0289	0.0221	0.0069	0.0130
O30	-0.5026	-0.4799	-0.5290	0.0228	0.0264	0.0246	0.0102	0.0119
O31	-0.5040	-0.4820	-0.5289	0.0220	0.0250	0.0235	0.0099	0.0112
C32	-0.3223	-0.3296	-0.3326	-0.0073	0.0103	0.0015	-0.0033	0.0046
C33	0.1158	0.1303	0.0785	0.0144	0.0373	0.0259	0.0065	0.0168
C34	0.1148	0.1287	0.0752	0.0139	0.0396	0.0267	0.0062	0.0178
C37	0.0192	0.0480	-0.0248	0.0289	0.0440	0.0364	0.0130	0.0198
C38	0.0185	0.0474	-0.0235	0.0289	0.0420	0.0354	0.0130	0.0189
C41	0.0287	0.0695	-0.0459	0.0408	0.0746	0.0577	0.0183	0.0336

The Mulliken charge distributions of the studied compounds together with the calculated Fukui indices are presented in Table 6. The parameters were calculated for C, N and O atoms. It has been reported that as the Mulliken charges of the adsorbed centre become more negative, more easily the atom donate its electrons to the unoccupied orbital of the metal [31]. From the Table 6, it is clear that carbon, nitrogen and oxygen atoms have high charge densities. The regions of high charge densities are generally the sites to which electrophiles can attach [32]. Therefore C, N and O atoms are the active centres, which have the strongest ability to bond the metal surface.

The local reactivity of PSDQO can be analysed by condensed Fukui functions. The condensed Fukui functions and condensed softness indices help to distinguish each part of the molecule based on its distinct chemical behaviour due to the different functional groups. Thus, the site for nucleophilic attack will be more is more wheref_k^+ value is high. In turn, the electrophilic attack is controlled by f_k^-. The most reactive sites for nucleophilic attack for PSDQO are C4 and N18. The most reactive sites for electrophilic attack for PSDQO areC5 and C41. Table 6 shows these results. The condensed local softness indices S_k^+ and S_k^- are related to the condensed Fukui functions. The local softness follows the same trend of Fukui functions.

CONCLUSION

1. The inhibitor molecule PSDQO shows very high inhibition efficiency for mild steel in 1M H_2SO_4.
2. The inhibition efficiency increases with increase in concentration but decrease with increase in temperature.
3. All the isotherms proved that the mode of adsorption of inhibitor is physical.
4. Quantum chemical studies of the PSDQO were found to be in good agreement with the experimental results.

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