

DOI: <http://dx.doi.org/10.21123/bsj.2022.19.1.0105>

Theoretical and Experimental Study of Corrosion Behavior of Carbon Steel Surface in 3.5% NaCl and 0.5 M HCl with Different Concentrations of Quinolin-2-One Derivative

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Received 4/2/2020, Accepted 16/6/2020, Published Online First 20/7/2021, Published 1/2/2022



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Abstract:

A theoretical and protection study was conducted of the corrosion behavior of carbon steel surface with different concentrations of the derivative (Quinolin-2-one), namely 7-Ethyl-4-methyl-1-[(4-nitro-benzylidene)-amino]-1H-quinolin-2-one (EMNQ2O). Theoretically, Density Functional Theory (DFT) of B3LYP/ 6-311++G/ 2d, 2p level was carried out to calculate the geometrical structure, physical properties and chemical inhibition chemical parameters, with the local reactivity in order to predict both the reactive centers and to know the possible sites of nucleophilic and electrophilic attacks, in vacuum and two solvents (DMSO and H₂O), all at the equilibrium geometry. Experimentally, the inhibition efficiencies (%IE) in (3.5% NaCl) and (0.5M HCl) solutions were studied using potentiometric polarization measurements. The results revealed that the (%IE) in the salty solution (94.98%) is greater than that in the acidic solution (81.40%). The thermodynamic parameters obtained, supported the physical adsorption mechanism and the adsorption followed the Langmuir adsorption isotherm. The surface changes of the carbon steel were studied using SEM (Scanning Electron Microscopy) and AFM (Atomic Force Microscopy) techniques.

Keywords: Corrosion Inhibition, DFT, Quinolin, Thermodynamic parameters.

Introduction:

Corrosion inhibitors are chemicals substances that interact with a metal surface or environments to which the metal surface is exposed and act to protect the metal from corrosion.¹ Most organic compounds having heterogeneous atoms (Nitrogen, Oxygen, Sulfur) in their aromatic composition have been successfully used as corrosion inhibitors². Often high heterogeneous organic compounds and the density of electrons on heterogeneous atoms usually have a tendency to resist corrosion. Quantitative chemical calculations were used to study the reaction mechanism and to solve chemical mystery³⁻⁶. This is a useful approach to investigate the mechanism of the reaction molecule inhibitor and the metal surface. The structural and electronic parameters of the inhibitor molecule can be obtained by theoretical calculations using the computational methodologies of quantum chemistry. It is generally known that quinoline derivatives have a variety of pharmacological and biological activities, such as immunomodulatory,

anti-malarial and anti-bacterial activity⁷⁻⁸. Numerous reports have been presented in the literature on the use of quinoline and some of its derivatives as corrosion inhibitors in various media⁹⁻¹³. In this search, it has been focused on the Quinolin-2-one derivative, a heterocyclic entity and pharmacologically important molecule.

The aim of this work is to study the inhibition efficiency of organic inhibitor (EMNQ2O) prepared by Luma SA. et. al.¹⁴; experimentally, in salty (3.5% NaCl) and acidic solutions using potentiostat method, and theoretically, the calculations of quantum chemical parameters were done in three media (vacuum, DMSO and water) using DFT of B3LYP/ 6-311++G/ 2d, 2p level theory and Gaussian 09 program.

Materials and Methods:

Preparation of carbon steel samples

Carbon steel's rod symbolized as (C45) having the following percentage of metallic

materials in composition (wt %): (0.122% C, 0.206% Si, 0.641% Mn, 0.016% P, 0.031% S, 0.118% Cr, 0.02% Mo, 0.105% Ni, and 0.451% Cu)³. The rod is mechanically cut into pieces forming a cyclic specimen of carbon steel a with 1.6 cm diameter and 3 mm thickness, each one of these specimen has been refined with emery paper (silicon carbide SiC) in different grades (80, 150, 220, 320, 400, 1000, 1200 and 2000) grades, then washed with tap water, distilled water and recent degreased with acetone, washed again with deionizer water, finally the specimen hold in a desiccators after it is dried in room temperature.

Preparation solution

Blank salt solution

35gm of sodium chloride (NaCl) was dissolved in (100 mL) distal water; transferred the formative solution into (1L) volumetric flask, containing 2mL of dimethyl sulfoxide (DMSO). The volume of the solution was completed to (1L) by adding distilled water. Using 3.5% NaCl is the suitable chooses in this study in order to avoid some problems related to the ohmic drop.

Blank acid solution

40 mL (0.5M) of HCl was diluted by distilled water to (1 liter) in a volumetric flask, after adding 2mL of solvent of dimethyl sulfoxide (DMSO).

Preparation the salty solutions of 7-Ethyl-4methyl-1-[(4-nitro-benzlidene)-amino]-1H-quinolin-2-one (EMNQ2O)

Three concentrations of the EMNQ2O inhibitor (5,10, and 20)ppm have been prepared by dissolving (0.005, 0.01 and 0.02) gm, respectively in (2mL) of DMSO, then transferred each one to (1L) volumetric flask containing 35gm (3.5%) of NaCl dissolved in distilled water. The volume of each solution was completed to 1L with distilled water.

Preparation the acidic solutions of 7-Ethyl-4methyl-1-[(4-nitro-benzlidene)-amino]-1H-quinolin-2-one (EMNQ2O)

Three concentrations of the EMNQ2O inhibitor (5, 10, and 20) ppm were prepared by dissolving (0.005, 0.01 and 0.02) gm., respectively in (2mL) DMSO, then transferred each one to (1L) volumetric flask containing (40mL) HCl. The volume for each solution has been completed to (1L) with distilled water.

Electrochemical measurements

Potentiostatic polarization study

The potentiostat set up including host computer, Mat lab (Germany, 2000), magnetic stirrer, thermostat, potentiostat, and galvanostat. The main part of the apparatus is the corrosion cell; it's made of Pyrex with 1L capacity. This cell consists of two bowls external and internal. Three electrodes are mainly present in the electrochemical corrosion cell, carbon steel specimen having 1cm² surface area has been represented as a working electrode that is used to determine the working electrode potential due to another electrode namely reference electrode was putting in a close to the working electrode. The reference electrode was s (Ag/AgCl, 3.0M KCl). The last electrode is a platinum auxiliary electrode having (10cm) length. The starting step has been represented by immersing the working electrode in the test solution for a period of (15 minute), to establish the potential of the open-circuit stable state (E_{ocp}). This possibility has been observed to start electrochemical measurements in the range of ± 200 (mV). All tests have been conducted at (293, 303, 313 and 323) K.

Results and Discussion:

Quantum chemical calculations

The structural nature of the organic inhibitors and their inhibition mechanism were described by density functional theory (DFT). The inhibition efficiencies of compound (EMNQ2O) was investigated by the theoretical corrosion inhibition parameters such as energy of the highest occupied molecular orbital (E_{HOMO}) and energy of the lowest unoccupied molecular orbital (E_{LUMO}), energy gap (E_{gap}) between E_{HOMO} and E_{LUMO} , dipole moment (μ), electronegativity (χ), electron affinity (A), global hardness (η), softness (σ), ionization energy (IE), global electrophilicity (ω), the fraction of electrons transferred (ΔN) and the total energy (E_{tot})¹⁵.

The Molecular geometry

The organic inhibitors compound was built in two dimensions structure using Chem-Draw of Mopac program, (Fig. 1a). Gaussian 09 packages¹⁶ were carried out for calculating the fully optimized structure in vacuum, using quantum mechanical method of DFT (Density Functional Theory) of Becke's three-parameter of Lee, Yang and Parr (B3LYP) with 6-311++G/ (2d, 2p) level of theory¹⁷⁻¹⁹ (Fig. 1b). In addition to vacuum, the equilibrium geometry was calculated in two solvents (DMSO and H₂O).

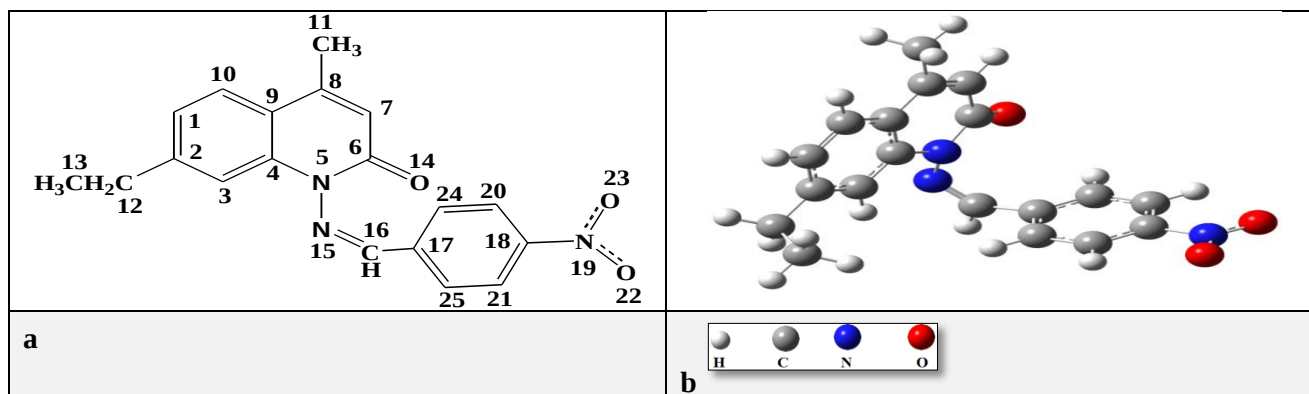


Figure 1. a. Two dimensions structure of (7-ethyl-4-methyl-1-[(4-nitro-benzylidene)-amino]-1H-quinolin-2-one (EMNQ2O)) with the numbering of atoms. b. Three dimensions optimize structure of EMNQ2O inhibitor calculated by DFT method.

Table 1 displays the geometrical structure details of EMNQ2O compound such as bond lengths, bond angles and dihedral angles which were calculated in vacuum and two solvents (DMSO, and H₂O) using DFT method. The optimized geometrical structure is the same in the three media (vacuum, DMSO, and H₂O). Table 1

shows that in EMNQ2O compound, the C12-C13 owns the longest bond length of (1.515 Å), and the C11-H26 bond is the shortest bond with (1.096 Å) length. The values of the dihedral angles (cis & trans) indicate non planarity of the compound within C₁ point group, the dihedral angles are neither 0.00 nor 180.00 degree¹⁵.

Table 1. Geometrical structure for EMNQ2O as inhibitor in vacuum and in different solvents (DMSO and H₂O) as calculated by using DFT method.

Bond description	Bond length (Å)	Angle description	Angle (degree)	Dihedral angle description	Dihedral angle (degree)
C1-C2	1.399	C2C1C10	120.076	C10C1C2C3	0.537
C1-C10	1.382	C2C1H	120.025	C10C1C2C12	179.606
C1-H	1.096	C1C2C3	119.522	C1C2C3C4	-0.532
C2-C3	1.387	C1C2C12	119.532	C12C2C3C4	-179.598
C2-C12	1.495	C2C3H	121.053	C2C3C4N	-176.704
C3-C4	1.404	C3C4C9	119.719	C3C4N5N15	20.672
C4-C9	1.409	C3C4N5	120.390	C3C4N5C6	171.140
C4-N5	1.438	C4N5N15	115.756	N5N15C6O	-17.717
N5-C6	1.451	N5C6C7	117.618	C4NC6C7	12.564
N5-N15	1.445	C7C6O14	124.619	OC6C7C8	174.005
C6-C7	1.466	C6C7C8	122.273	C6C7C8C9	-0.465
C6-O14	1.221	C6C7H	116.185	C6C7C8C11	-179.681
C7-C8	1.349	C7C8C9	120.277	C7C8C9C4	1.407
C8-C9	1.456	C7C8C11	119.964	C7C8C9C10	-177.636
C8-C11	1.487	C9C10C1	121.320	C4C9C10C1	-0.546
C9-C10	1.403	HC12H	105.679	C8C9C10C1	-178.512
C12-H	1.108	C2C12H	110.436	NNC16C17	5.131
C12-C13	1.515	C12C13H	111.624	NNC16H	-179.164
N15-C16	1.287	N5N15C16	122.631	NC16C17C	-100.199
C18-N19	1.498	N15C16C17	128.803	C20C18N19O22	-3.668
N19-O23	1.215	N15C16H	114.464	C21C18N19O23	176.456

Figure 2a shows the HOMO and LUMO density distributions for the optimized geometry of the studied inhibitor (in vacuum). The HOMO is mainly located on the (7-Ethyl-4-methyl-1-[(4-nitro-benzylidene)-amino]-1H-quinolin-2-one moiety. This indicates that the preferred active-sites for an electrophilic attack are located within the

region around the phenyl and nitrogen atoms. Moreover, the electronic density of LUMO is distributed at the aromatic ring and around the ring of (4-nitro-phenyl) moiety. Both HOMO and LUMO are located at the planar parts of the EMNQ2O molecule, Fig. 2b¹⁵.

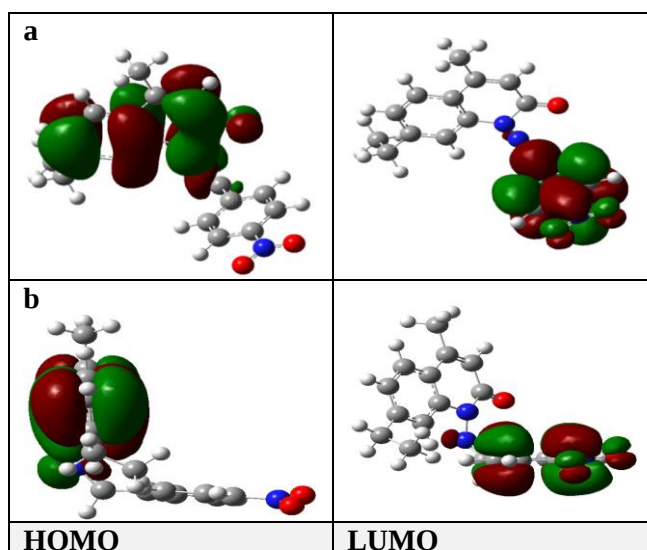


Figure 2. a- Frontier molecular orbital density distributions of EMNQ2O compound.

b- the planar parts of the EMNQ2O molecule. [Red color: negatively charged lobe; green color: positive charge lobe].

Global molecular reactivity

Tables 2a and b show that EMNQ2O compound is a good inhibitor based on its values of the quantum corrosion efficiency parameters in the three media (vacuum and two polarity solvents). E_{HOMO} (in vacuum) is -7.720 eV, be high in both DMSO and H₂O solvents. E_{LUMO} (in vacuum) is -2.964 eV which decreased in both solvents DMSO and H₂O. $\Delta E_{\text{HOMO-LUMO}}$ is 4.756 eV (in vacuum) and becomes less in both DMSO and H₂O solvents. Dipole moment (μ in Debye) is a very important electronic parameter which results from the non-uniform distribution of charges on the various atoms in the molecule. The high value of dipole moment increases the adsorption between the inhibitor compound and the surface of the metal. Dipole moment for EMNQ2O inhibitor (in vacuum) is 6.4032 Debye, and becomes more in both DMSO as a result of increasing polarity of the solvent, meaning increasing inhibition efficiency.

The ionization potential, IP can be approximated as the negative of the highest occupied molecular orbital (HOMO) energy. Low values of IP increase the effectiveness of the inhibitor. The Ionization potential (IP) of the inhibitor in the vacuum is 7.720 eV, becomes less in DMSO and H₂O solvents. The Electron-affinity (EA) is the amount of energy released when adding an electron to an atom or molecule. A high value of EA means less stable inhibitor (good corrosion

inhibitor)²⁰. The electron affinity of EMNQ2O in the vacuum is 2.964 eV, becomes more in DMSO or H₂O solvents. Chemical hardness (η) is a measure of the ability of atom or molecule to transfer the charge. Increasing (η) decreases the stability of molecule, so the inhibitor possessed a low value of (η) which is considered to be a good inhibitor. The (η) value in the vacuum is 3.835eV, becomes less in DMSO and H₂O solvents.

Chemical softness (S) is a measure of the flexibility of an atom to receive electrons (S). Molecules having a high value of S are considered to be a good inhibitor. The values of S in the vacuum is 0.421 eV, becomes more in both DMSO and H₂O solvents¹⁰.

The electronegativity (χ) is the ability of an atom or a group to pull electrons, low electronegativity indicates a good inhibitor. The calculated (χ) in the vacuum is 5.342 eV, becomes less in both DMSO and H₂O solvents.

Global electrophilicity index (ω) is the measure of the stability of an atom after gaining an electron. High value of (ω) meaning the molecule has a good inhibition. It was (6.000 eV) in the vacuum, becomes more in both DMSO and H₂O solvents.

ΔN (difference in the number of electrons transferred). The fraction of electrons transferred (ΔN) from an inhibitor to carbon steel surface 0.348 of EMNQ2O has larger values in solvents compared with the vacuum, by the tendency of EMNQ2O molecule to receive the electrons from the metallic surface by Fe atoms in the unoccupied orbital of (3d). This ability increases the inhibition efficiency (IE) when two systems, Fe and inhibitor, are brought together. The net result of the order for inhibition efficiency is IE (H₂O) > IE (DMSO) > IE (Vacuum), meaning IE increase with increasing the polarity of the medium. From this, we conclude that the stability of the inhibitor is higher in both solvents than in vacuum. Equations¹⁻⁸ are used for calculating the chemical parameters²¹⁻²⁵:

$$\text{IP} = -E_{\text{HOMO}} \quad (1)$$

$$\text{EA} = -E_{\text{LUMO}} \quad (2)$$

$$\Delta E = E_{\text{LUMO}} - E_{\text{HOMO}} \quad (3)$$

$$\eta = (\text{IP} - \text{EA}) / 2 \quad (4)$$

$$\chi = (\text{IP} + \text{EA}) / 2 \quad (5)$$

$$S = 1 / \eta \quad (6)$$

$$\omega = \chi^2 / 2\eta \quad (7)$$

$$\Delta N = (\chi_{\text{Fe}} - \chi_{\text{inhib}}) / [2 (\eta_{\text{Fe}} + \eta_{\text{inhib}})] \quad (8)$$

Whereas χ_{Fe} is 7.0 eV mol⁻¹; and η_{Fe} is of 0.0 eV mol⁻¹ for carbon steel.

Table 2. DFT calculations results for a- some physical properties and b- quantum chemical parameters for EMNQ2O inhibitor calculated at the optimized structure.

a							
Inhibition Medium	Point group	Molecular formula	E _{HOMO} (eV)	E _{LUMO} (eV)	ΔE _{HOMO-LUMO} (eV)	μ (Debye)	E _{total} (eV)
Vacuum	C ₁		-7.720	-2.964	4.756	6.4032	-30597.352
DMSO	C ₁	C ₁₉ H ₁₇ N ₃ O ₃	-6.342	-3.259	3.083	7.6342	-30596.859
Water	C ₁		-6.344	-3.262	3.082	7.6660	-30596.868

b							
Inhibition Medium	IP (eV)	EA (eV)	η (eV)	χ (eV)	S (eV)	ω (eV)	ΔN
Vacuum	7.720	2.964	2.378	5.342	0.421	6.000	0.348
DMSO	6.342	3.259	1.542	4.800	0.648	7.470	0.713
Water	6.344	3.262	1.541	4.803	0.648	7.485	0.713

Active sites of EMNQ2O inhibitor

The inhibition of EMNQ2O inhibitor was done by using DFT Mulliken's charge population analysis in electron control unit (ecu), which gave an indication of the reactive centers of the molecules (electrophilic and nucleophilic sites). For that reason, the regions that have a large electronic charge are chemically softer than the regions that have a small electronic charge. Thus, the density of electron plays an important role in the chemical reactivity calculating. The chemical adsorption interactions are either by orbital interactions or electrostatic. The sites of nucleophilic attack will be

the place where the positive charge value is a maximum, thus only the charges on the oxygen (O), nitrogen (N), and some carbon atoms are presented. In turn, the site of electrophilic attack was controlled by the negative charge value. The nucleophilic and electrophilic electronic charge values of compounds in DMSO and H₂O solutions are higher than in vacuum. Table 3 shows the order of the nucleophilic reactive sites of EMNQ2O inhibitor as follows: C4 > C11 > C18 > C16 > C14 > C3; whereas the order of the electrophilic reactive sites is: C2 > C17 > C8 > C9 > C5.

Table 3. Mulliken charge population analysis for EMNQ2O molecule calculated in three media (vacuum, DMSO, and H₂O) by DFT method.

Atom	Electronic Charge (ecu)	Atom	Electronic charge (ecu)	Atom	Electronic Charge (ecu)	Atom	Electronic Charge(ecu)
C1	-0.878V	C7	-0.054V	C13	-0.489V	N19	-0.010V
	-0.127D		-0.270D		-0.645D		-0.137D
	-0.126H		-0.271H		-0.646H		-0.136H
C2	0.862V	C8	0.602V	O14	-0.470V	C20	-0.162V
	0.937D		0.651D		-0.407D		-0.059D
	0.936H		0.651H		-0.409H		-0.059H
C3	-0.354V	C9	0.434V	N15	-0.058V	C21	-0.184V
	-0.408D		0.581D		-0.225D		-0.159D
	-0.408H		0.581H		-0.226H		-0.158H
C4	-0.399V	C10	-0.372V	C16	-0.129V	O22	-0.139V
	-0.691D		-0.488D		-0.480D		-0.049D
	-0.690H		-0.488H		-0.481H		-0.050H
N5	0.019V	C11	-0.324V	C17	0.324V	O23	-0.132V
	0.570D		-0.523D		0.802D		-0.048D
	0.570H		-0.524H		0.804H		-0.050H
C6	0.008V	C12	-0.149V	C18	0.115V		
	-0.113D		-0.200D		-0.482D		
	-0.112H		-0.200H		-0.482H		

V: vacuum; D: dimethyl sulfoxide; H: water; ecu: electron control unit.

Corrosion inhibition measurement

Potentiodynamic polarization measurements

The parameters of the electrochemical corrosion are listed in Table 4 such as corrosion potential (E_{corr}), Tafel slopes (b_c and/or b_a) and corrosion current density (I_{corr}) obtained by cathodic and anodic regions of Tafel lines. Figs. 3 and 4 present potentiodynamic polarization curves for C.S in salt and acid solutions containing different concentrations of EMNQ2O compound. IE%, θ , can be measured using equations ⁸⁻¹¹.

$$\%IE = \frac{i_{\text{corr(un)}} - i_{\text{corr(in)}}}{i_{\text{corr(un)}}} \times 100 \dots (8)$$

Where $i_{\text{corr (in)}}$ is the inhibited corrosion current densities; $i_{\text{corr (un)}}$ is the uninhibited current densities. The values of polarization resistance (R_p) can be calculated using equation 9.

$$R_p = \frac{b_a \times b_c}{2.303(b_a + b_c) \times i_{\text{corr}}} \quad (9)$$

The surface coverage (θ) of the carbon steel corrosion immersed in 3.5% NaCl and acidic solutions containing different EMNQ2O concentrations (C) can be estimated using equation 10.

$$\theta = \frac{\%IE}{100} \quad (10)$$

The corrosion rate (CR) can be calculated using equation 11:

$$CR = i_{\text{corr}} \times 0.249 \dots (11)$$

The addition of the quinolin-2-one derivative leads to a decrease in the corrosion rate i.e the conversion of cathode and anode curves to lower values of the current density. Both cathode and anode corrosion reactions in C.S (carbon 45) electrode were

prevented by EMNQ2O in both 3.5% NaCl and 0.5M HCl solution. Figs. 3 and 4 show Tafel lines of anodic and cathodic polarization curves for the corrosion of carbon steel in the salty and in the acidic solution respectively, with and without the addition of various concentrations of EMNQ2O inhibitor as well as the optimum conditions of (20ppm) inhibitor and (at 293K) temperature.

Tables 4 and 5 list the corrosion rate values of C.S and inhibition efficiencies of various inhibitor concentrations measured at salty and acidic solutions at different temperature, respectively. The tables show that increasing temperature leads to increasing the corrosion current densities I_{corr} . While the efficiencies IE% is enhanced with the increasing of the inhibitor concentration. The optimum conditions for EMNQ2O in the salty and in the acidic solutions were found at 293K temperature and 20ppm inhibition concentration both corresponded to the lowest I_{corr} of 37.84 ($\mu\text{A.cm}^{-2}$) and the maximum IE% of 94.98 (%) in the salty solution and lowest I_{corr} of 6.68 ($\mu\text{A.cm}^{-2}$) and the maximum IE% of 80.75 (%) in the acidic solution, respectively. The values of iron corrosion rate CR decreased with the increase of EMNQ2O concentration. The addition of the inhibitor to the blank solution increases the cathodic and anodic current densities without shifting the corrosion potential. The EMNQ2O inhibitor therefore can be described as a mixed-type inhibitor in which its inhibition action is caused by the adsorption process. The inhibition action is a proportional of the reduction reaction area on the carbon steel surface ¹⁵.

Table 4. Electrochemical data of C.S corrosion in salty solution at different concentrations of EMNQ2O compound.

Inhib. conc.	T (K)	E_{corr} (mV)	i_{corr} ($\mu\text{A.cm}^{-2}$)	Bc (mV.dec ⁻¹)	ba (mV.dec ⁻¹)	IE%	θ	CR
Blank 0ppm	293	-408.0	133.13	-230.4	138.5	-----	-----	33.15
	303	-446.7	172.04	-279.6	110.2	-----	-----	42.84
	313	-491.2	189.34	-269.0	96.5	-----	-----	47.15
	323	-547.7	192.99	-252.9	84.4	-----	-----	48.05
5ppm	293	-461.2	18.05	-136.6	56.3	86.44	0.864	4.49
	303	-459.9	25.94	-195.4	58.9	84.92	0.849	6.46
	313	-441.0	34.30	-104.9	76.9	81.88	0.819	8.54
	323	-521.2	43.23	-232.6	83.5	77.59	0.776	10.76
10ppm	293	-411.5	17.13	-43.6	35.8	87.13	0.871	4.27
	303	-460.4	23.53	-62.6	44.5	86.32	0.863	5.86
	313	-472.2	31.04	-96.2	57.7	83.60	0.836	7.73
	323	-490.1	42.41	-180.4	63.9	78.02	0.780	10.56
20ppm	293	-359.8	6.68	-43.3	38.7	94.98	0.950	1.66
	303	-407.4	24.83	-74.5	50.2	85.56	0.856	6.18
	313	-378.6	32.03	-93.9	60.2	83.08	0.830	7.98
	323	-552.8	38.29	-278.5	89.6	80.15	0.801	9.53

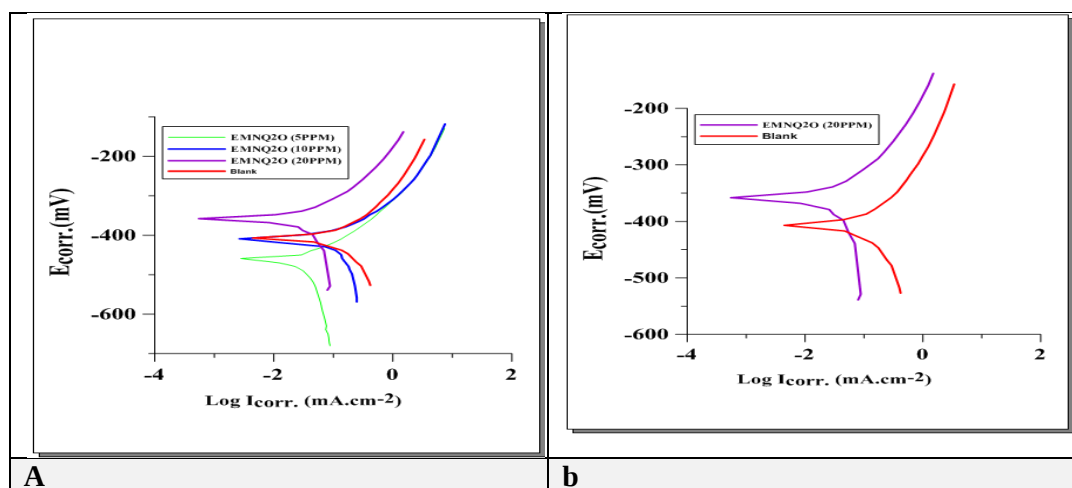


Figure 3. Polarisation curve of carbon steel in seawater at 293 (K) for EMNQ2O compound; (a) at different concentrations, and (b) at the optimum concentration.

Table 5. Electrochemical data of carbon steel corrosion in acid solution at different concentrations for EMNQ2O compound.

Inhib. conc.	T (K)	E_{corr} (mV)	i_{corr} ($\mu\text{A}\cdot\text{cm}^{-2}$)	Bc ($\text{mV}\cdot\text{dec}^{-1}$)	ba ($\text{mV}\cdot\text{dec}^{-1}$)	IE%	Θ	CR
Blank 0ppm	293	-340.2	196.59	-132.9	76.1	-----	-----	48.95
	303	-349.9	285.76	-129.4	87.4	-----	-----	71.15
	313	-336.8	383.29	-123.8	77.4	-----	-----	95.44
	323	-326.9	495.50	-107.5	58.6	-----	-----	123.38
5ppm	293	-412.2	56.59	-61.1	49.6	72.00	0.720	14.09
	303	-413.7	89.19	-58.8	45.8	71.21	0.712	22.21
	313	-413.6	107.32	-47.7	45.2	68.78	0.688	26.72
	323	-411.7	196.02	-50.6	46.8	60.43	0.604	48.81
10ppm	293	-402.2	41.45	-46.4	44.0	78.91	0.789	10.32
	303	-399.3	74.73	-62.4	51.2	73.84	0.738	18.61
	313	-410.2	107.92	-49.9	53.1	71.84	0.718	26.87
	323	-401.3	160.74	-50.2	45.9	67.56	0.676	40.02
20ppm	293	-410.9	37.84	-59.7	42.4	81.40	0.814	9.42
	303	-405.0	53.14	-63.6	52.5	80.75	0.808	13.23
	313	-405.0	96.09	-81.5	63.7	75.20	0.752	23.93
	323	-404.6	122.84	-54.1	55.6	74.93	0.749	30.59

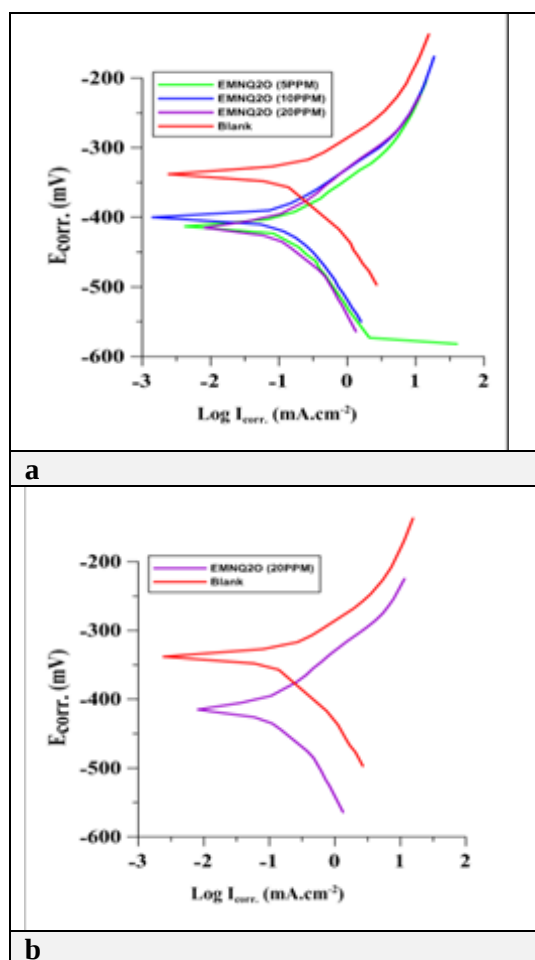


Figure 4. Polarisation curve of carbon steel in acidic solution at 293 (K) for EMNQ2O compound; (a) at different concentrations, and (b) at the optimum concentration.

Corrosion kinetic and thermodynamic activation parameters

Arrhenius law is presented as a straight line of the logarithm of the corrosion rate. The activation parameters were calculated with and without inhibitors at different concentrations. The activation energy of the corrosion process (E_a), and the pre-exponential factor (A), were calculating from the slope and intercept of plotting $\log(I_{corr})$ against $(1/T)$ equation 12, Figs. 5 and 7 for salty and acidic media, respectively. All E_a values in presence of

EMNQ2O inhibitor are higher than that of the blank (09.6348 kJ/ mol) for the salty solution and (24.1828 kJ/ mol) for the acidic solution which means that the corrosion reaction of C.S is retarded by EMNQ2O inhibitor. These observations support the physical observation. Plot of $\log(CR/T)$ or $\log(I_{corr}/T)$ against $(1/T)$, gave a linear relationship with the slope of $(-\Delta H^*/2.303R)$ and intercept of $[\log(R/Nh) + (\Delta S^*/2.303R)]$ equation (13), as shown in Figs. 6 and 8 for salty and acidic media, respectively.

$$\log(I_{corr}) = \log A - E_a / 2.303RT \quad (12)$$

$$\log(I_{corr}/T) = \log(CR/T) = \log(R/Nh) + \Delta S^* / 2.303R - \Delta H^* / 2.303RT \quad (13)$$

Where (I_{corr}) is the corrosion current density which is equal to the corrosion rate (CR), (R) is the universal gas constant ($8.314 \text{ J mol}^{-1} \text{ K}^{-1}$), (T) is the absolute temperature in K, (h) is Planck's constant ($6.626 \times 10^{-34} \text{ J s}$), (N) is Avogadro's number ($6.022 \times 10^{23} \text{ mol}^{-1}$), ΔH^* is the enthalpy of activation and (ΔS^*) is the entropy of activation.

Accordingly, the activation thermodynamic parameters (ΔH^* and ΔS^*) were calculated in salty and acidic media, respectively, as shown in Tables 6 and 7. Positive values of (ΔH^*) for the corrosion reaction in 3.5% NaCl and in acidic media at the temperature range of (293-323) K and different concentrations support the endothermic nature of this reaction¹⁶. Whereas negative values of (ΔS^*) for the corrosion reaction reveals that an increase in disordering takes place on going from reactant to the activated complex¹⁷. The values of ΔH^* , ΔS^* and E_a^* obtained in presence of EMNQ2O inhibitor are higher than those obtained in the blank solution. This observation further supports the proposed physical mechanism. The values of ΔG^* for corrosion reaction were calculated from equation 14. The positive values of ΔG^* indicating that the transition state of the adsorption process is not spontaneous.

$$\Delta G^* = \Delta H^* - T\Delta S^* \quad (14)$$

Table 6. Corrosion kinetic parameters for carbon steel in 3.5% NaCl solution for blank and with various concentrations of EMNQ2O inhibitor.

Conc. (ppm)	ΔG^* (kJ/ mol)				ΔH^* kJ/ mol	ΔS^* kJ/ mol K	E_a^* kJ/ mol	A Molecule/ cm ² S
	293K	303K	313K	323K				
Blank	63.072	64.983	66.894	68.805	7.080	-0.1911	09.6360	1.10E+27
0								
5	68.015	69.643	71.271	72.899	20.315	-0.1628	22.8713	3.31E+28
10	68.187	69.797	71.407	73.017	21.014	-0.1610	23.5701	4.07E+28
20	66.320	77.562	68.804	70.046	29.929	-0.1242	43.7838	8.65E+31

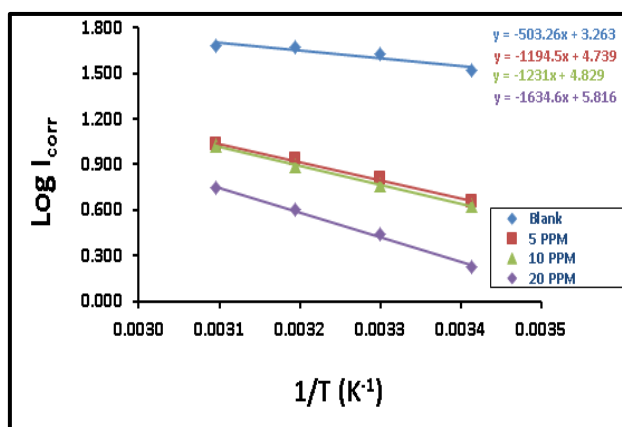


Figure 5. Plotting $\log(I_{corr})$ against $(1/T)$ for carbon steel in salty solution in absence (blank) and in presence of different concentrations of the EMNQ2O inhibitor.

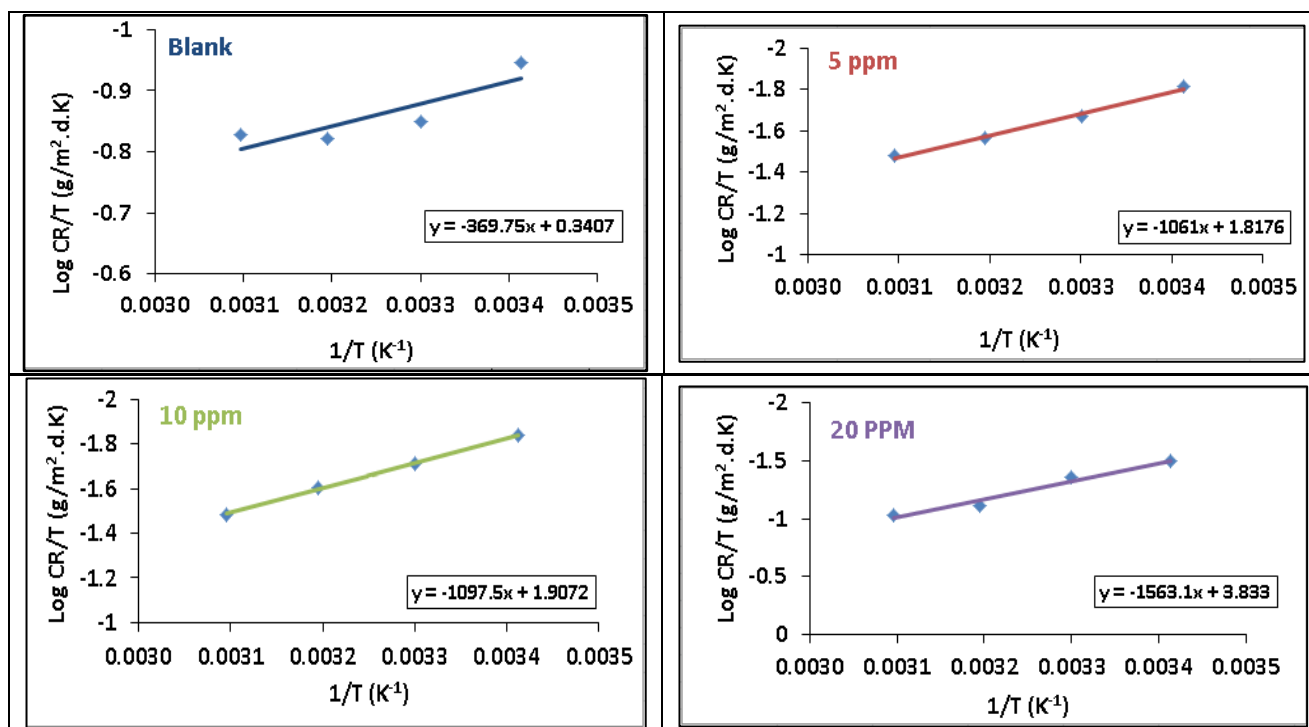


Figure 6. Plotting $\log(CR/T)$ against $(1/T)$ of carbon steel in salty solution for in absence (blank) and in presence of different concentrations of the EMNQ2O inhibitor.

Table 7. Corrosion kinetic parameters for carbon steel in acid medium for blank and with various concentrations of the inhibitor.

Conc. (ppm)	ΔG^* (kJ/ mol)				ΔH^* kJ/ mol	ΔS^* kJ/ mol K	Ea kJ/ mol	A Molecule/ cm ² S
	293K	303K	313K	323K				
Blank	57.869	59.106	60.343	61.580	21.625	-0.1237	24.1828	6.15E+29
0								
5	65.323	66.592	67.861	69.130	28.141	-0.1269	30.6967	2.48E+30
10	65.929	67.073	68.217	69.361	32.410	-0.1144	32.4870	3.43E+30
20	66.320	67.562	68.804	70.046	29.929	-0.1242	34.9665	1.11E+31

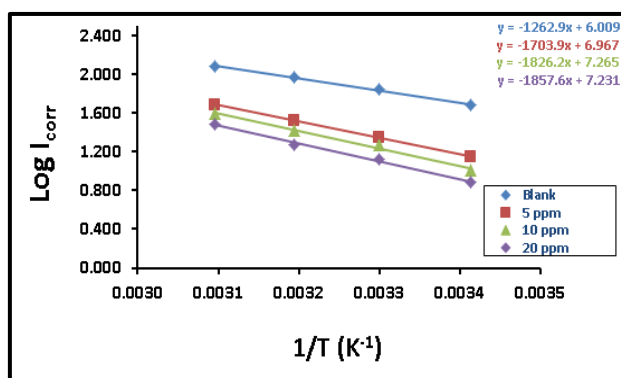


Figure 7. Plotting $\log(I_{\text{corr}})$ against $(1/T)$ for carbon steel in acidic solution in absence (blank) and in presence of different concentrations of the EMNQ2O inhibitor.

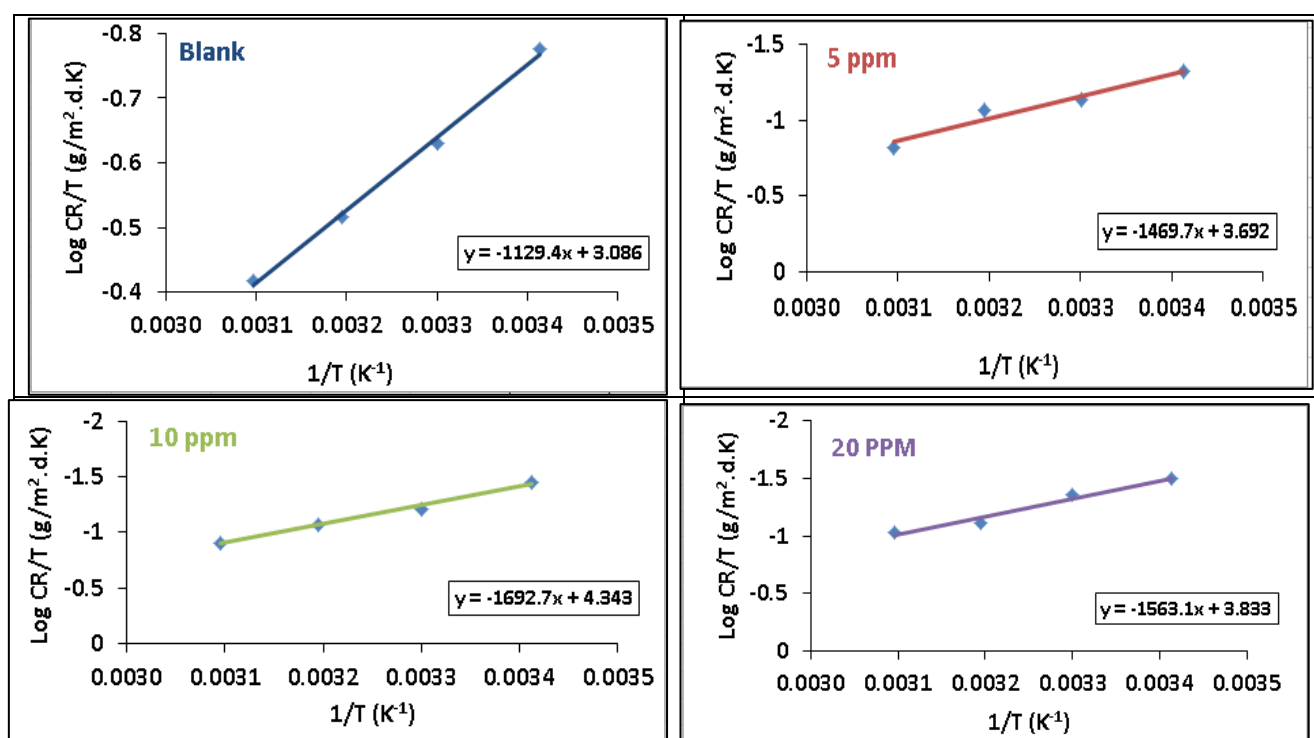


Figure 8. Plotting $\log(CR/T)$ against $(1/T)$ of carbon steel in acidic solution in absence (blank) and in presence of different concentrations of the EMNQ2O inhibitor.

Adsorption isotherm

The adsorption isotherms are essential in characterizing the reaction between carbon steel surface and inhibitor molecules. Langmuir adsorption isotherm is the most frequently used isotherms. It can be described by the following equation:

$$C/\Theta = (1/K_{\text{ads}}) + C \quad (15)$$

Whereas C is the inhibitor concentration in 3.5% NaCl and 0.5M HCl, K_{ads} is the adsorption equilibrium constant and Θ is the surface coverage. The dependence of the (C/Θ) fraction as a function of (C) for EMNQ2O in salty and acidic solutions is shown in Figs. 9 and 11. It can be used to determine K_{ads} . The adsorption equilibrium constant has a relation with the free energy of adsorption (ΔG_{ads}) through the following equation¹⁵:

$$K_{\text{ads}} = (1/55.55) \exp(\Delta G_{\text{ads}}/RT) \quad (16)$$

Here R is the gas constant ($\text{J K}^{-1} \text{mol}^{-1}$), T is the absolute temperature (K) and 55.5 is the molar concentration of water in the solution (mol L^{-1}). So the values of ΔG_{ads} at different temperature were obtained from equation 17. Enthalpy value of adsorption ($\Delta H^{\circ}_{\text{ads}}$) was obtained from the slope of Vant Hoff equation expressed by equation 18, and entropy value of adsorption ($\Delta S^{\circ}_{\text{ads}}$) was obtained from the intercept of the same equation (Figs. 10 and 12).

$$\Delta G^{\circ}_{\text{ads}} = -2.303RT \log K_{\text{ads}} \quad (17)$$

$$\Delta G^{\circ}_{\text{ads}} = \Delta H^{\circ}_{\text{ads}} - T\Delta S^{\circ}_{\text{ads}} \quad (18)$$

$$\log K_{\text{ads}} = -\Delta H^{\circ}_{\text{ads}}/2.303RT + \Delta S^{\circ}_{\text{ads}}/2.303R$$

Tables 8 and 9 list the thermodynamic functions of EMNQ2O inhibitor on C.S surface in 3.5% NaCl and 0.5M HCl at various temperatures, respectively. Higher values of K_{ads} obtained from Langmuir isotherm for EMNQ2O indicate strong adsorption on the carbon steel in 3.5% NaCl and 0.5M HCl. Negative values of ΔG°_{ads} indicate spontaneous adsorption process. The values of ΔG°_{ads} around -20 (kJ/mol) or less negative consisted with the electrostatic interaction (physic-sorption); while those values of -40 (kJ/mol) or more negative involve electron transfer which leads to form a chemical bond (chemisorptions) ²⁶.

The calculated values for ΔG°_{ads} were found in the range of -49.652 to -40.929 (kJ mol⁻¹) at different temperatures (293-323K) in the salty medium, while, ΔG°_{ads} were found in the range of -39.394 to -40.612 (kJ mol⁻¹) at different temperatures (293-323K) in the acidic medium. These values indicate that the adsorption of EMNQ2O follows physisorption processing. The obtained entropy ΔS°_{ads} value is

positive which confirms that the corrosion process is entropically favorable ¹⁹. The negative value of ΔH°_{ads} in the salt and acidic media indicates an exothermic process for the adsorption of inhibitory molecules on the C.S surface. For EMNQ2O compound, ΔH°_{ads} is equal to -89.442 (kJ mol⁻¹) in the salt medium, and equal to -24.537 (kJ mol⁻¹) in acidic medium (Tables 8 and 9).

Table 8. Thermodynamic parameters for adsorption of (EMNQ2O) compound on C.S surface in 3.5% NaCl at various temperatures.

T K	K_{ads} L mol ⁻¹	ΔG°_{ads} kJ. mol ⁻¹	ΔH°_{ads} kJ.mol ⁻¹	ΔS°_{ads} kJ.mol ⁻¹
293	2.6*10 ⁵	-41.480	-89.442	0.438
303	3.3*10 ⁵	-40.929		
313	8.8*10 ⁵	-43.953		
323	9.0*10 ⁵	-49.652		

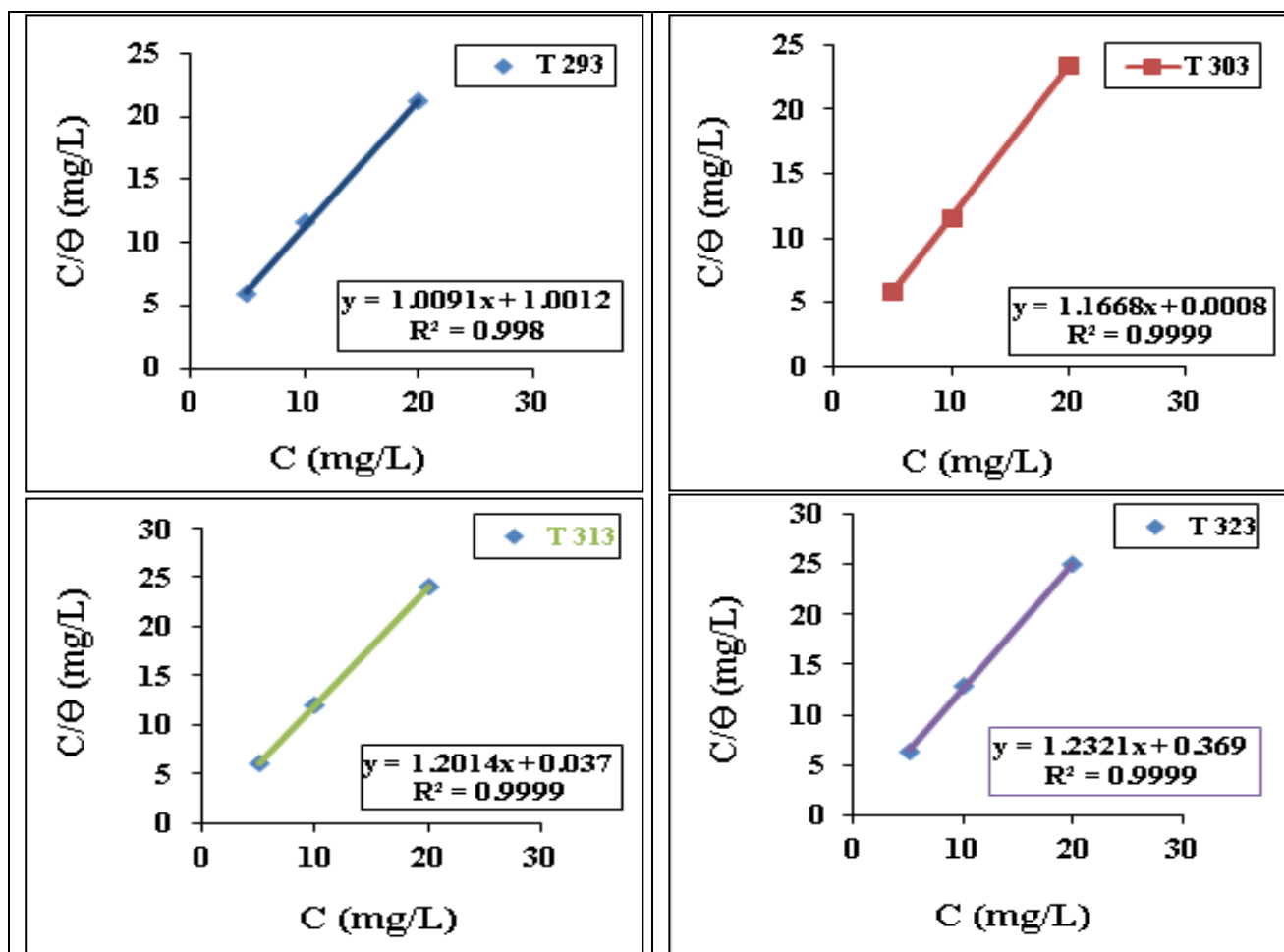


Figure 9. Langmuir isotherms plot for the adsorption EMNQ2O inhibitor on carbon steel in salty medium at temperatures of (293, 303, 313 and 323) K.

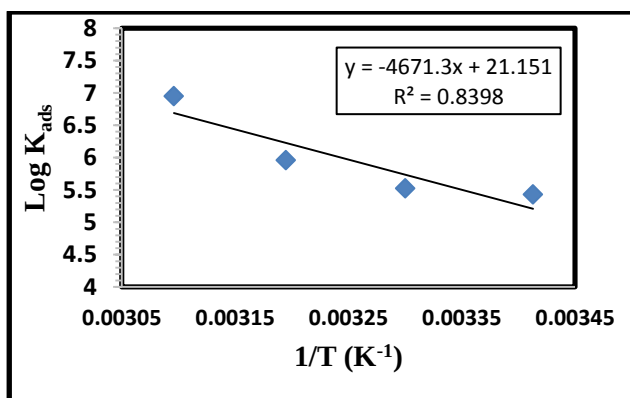


Figure 10. Plotting of $\log K_{ads}$ against $(1/T)$ for EMNQ2O compound.

Table 9. Langmuir parameters for adsorption of (EMNQ2O) compound on carbon steel surface in 0.5M HCl solution at different temperatures.

T K	K_{ads} $L \cdot mol^{-1}$	ΔG°_{ads} $kJ \cdot mol^{-1}$	ΔH°_{ads} $kJ \cdot mol^{-1}$	ΔS°_{ads} $kJ \cdot mol^{-1}$
293	$1.4 \cdot 10^5$	-41.492		
303	$1.9 \cdot 10^5$	-40.612		
313	$3.4 \cdot 10^5$	-41.654	-24.537	0.216
323	$6.0 \cdot 10^5$	-39.394		

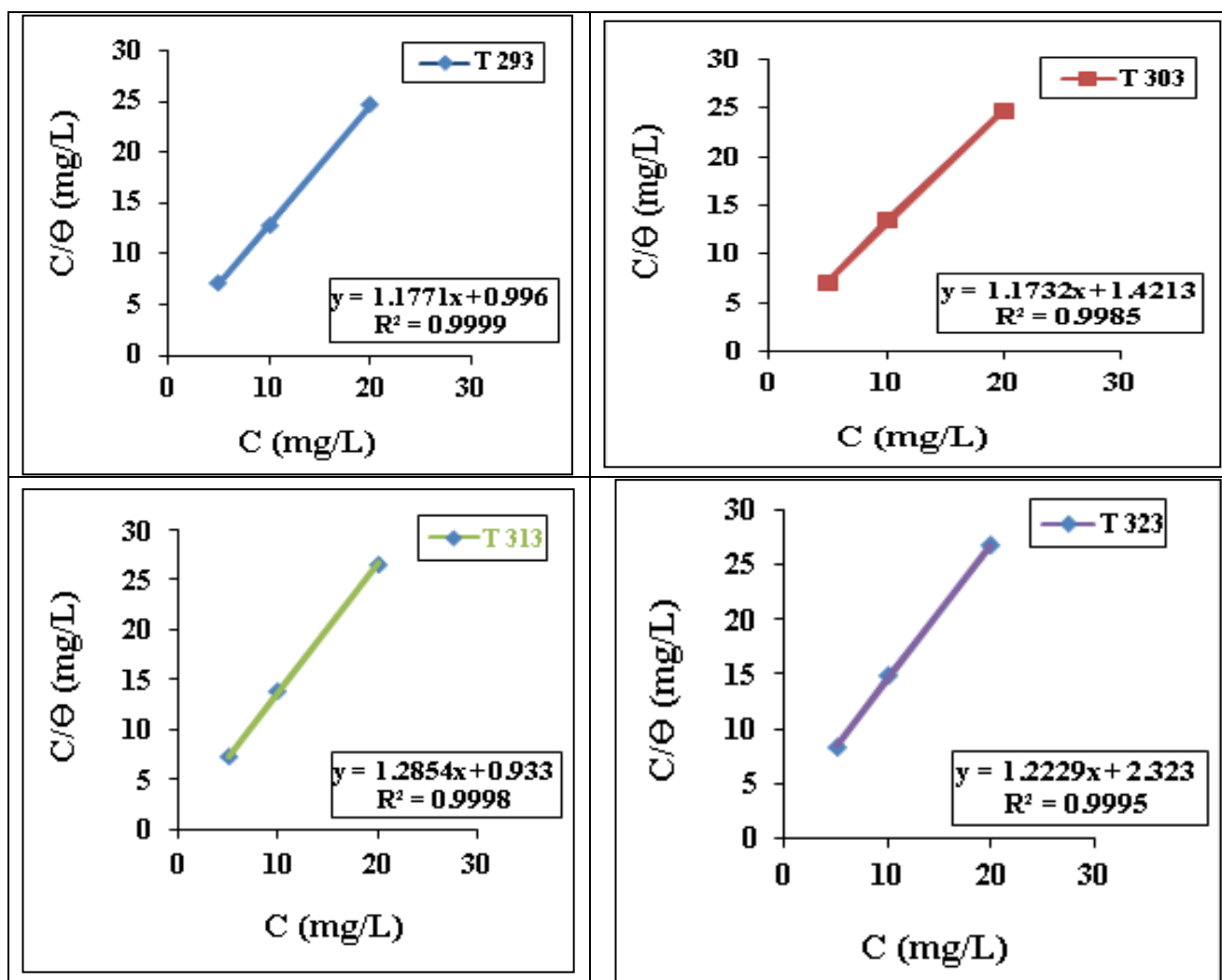


Figure 11. Langmuir isotherms plot for the adsorption of EMNQ2O inhibitor on carbon steel in acidic medium at temperatures of (293, 303, 313 and 323) K.

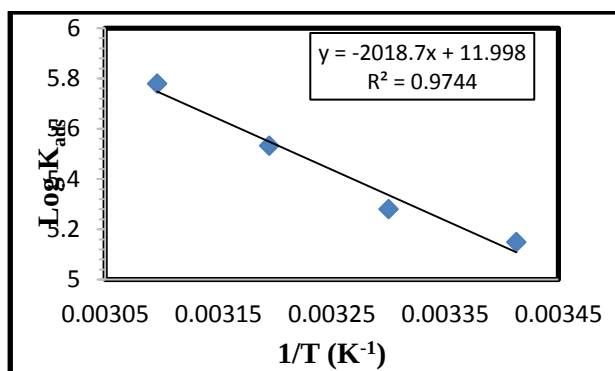


Figure 12. Plotting log K_{ads} against $(1/ T)$ for EMNQ2O compound in acid solution.

Scanning Electron Microscopy (SEM):

The SEM micrographs of the corroded carbon steel in 3.5% NaCl and 0.5M HCl solutions in the prescience and absence of EMNQ2O inhibitor are shown in Figs. 13 and 14, respectively. In images (a) of these figures (absence of inhibitor of carbon steel surface), a clear damage is obvious on the metal surface. In contrast, Figs. 13b and 14b show a remarkable improvement in the metal surface morphology due to the presence of EMNQ2O inhibitor which is responsible for forming a protective film of an insoluble complex on carbon steel surface (Fe^{2+} -EMNQ2O complex).

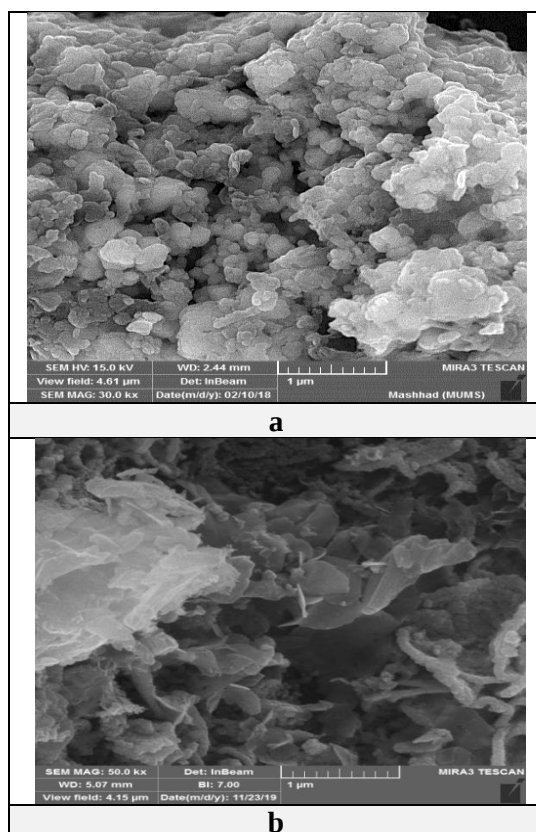


Figure 13. SEM of C.S surface (a) in salt medium of 3.5% NaCl solution without presence of EMNQ2O inhibitor, (b) in presence of 20 ppm of EMNQ2O inhibitor.

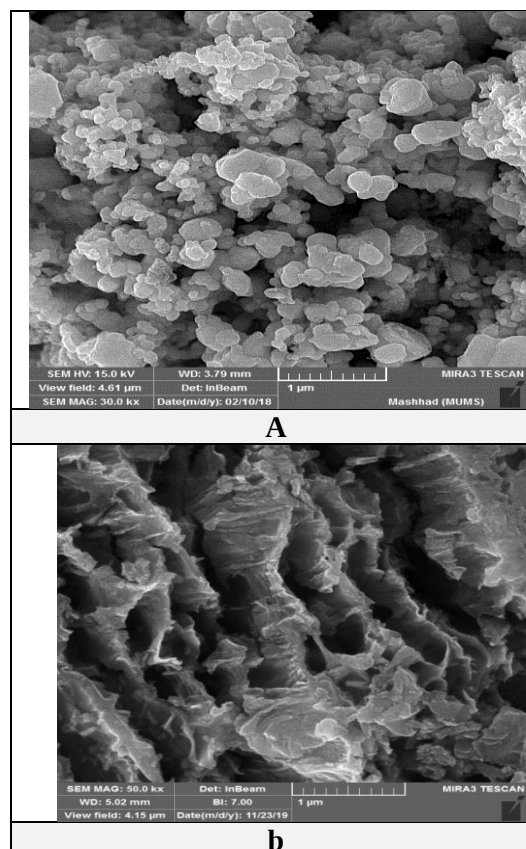
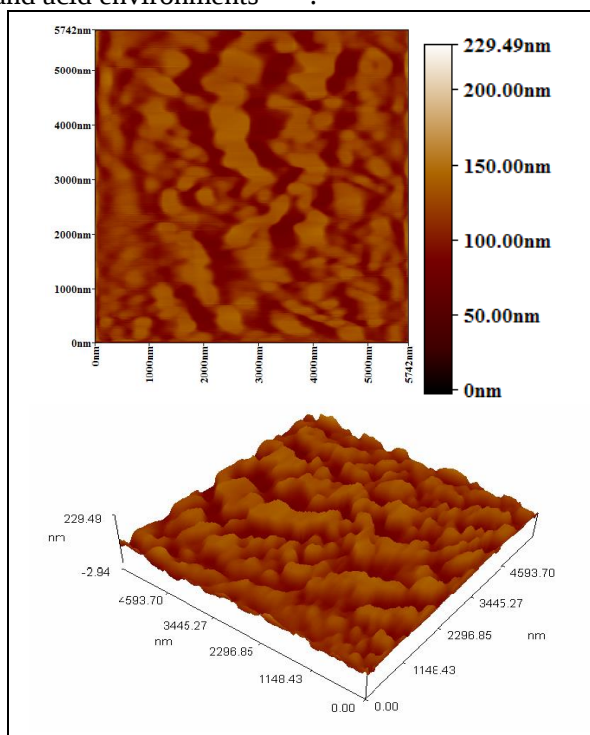


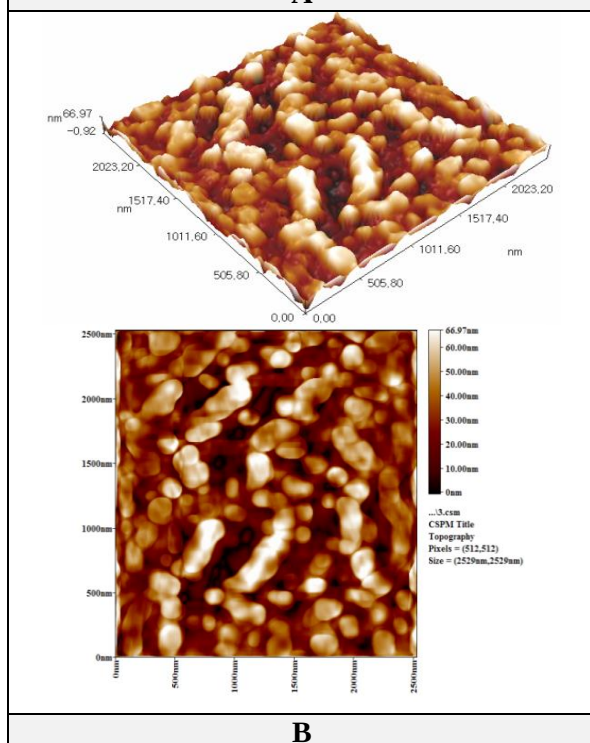
Figure 14. SEM of C.S surface (a) in acidic solution without presence of EMNQ2O inhibitor, (b) in presence of 20 ppm of EMNQ2O inhibitor. Atomic force microscopy characterization

AFM is a technique for obtaining the surface morphology at (Nano to micro-scale) and has become a good choice for studying the influence of inhibitor on the generation and the progress of the corrosion at the metal interface. AFM image analysis was performed to obtain the average roughness (R_a), the root-mean-square roughness (R_q), and the maximum peak-to-valley (P-V) height values. Figures 15a, 16a show the corroded metal surface in the absence of the inhibitor immersed in 3.5% NaCl and 0.5M HCl solution, respectively. In this case, the R_q , R_a and P-V height values for the carbon steel surface observed are (28.2nm, 34.1nm, and 184nm) in 3.5% NaCl solution, and (17.24nm, 21.45nm, and 127.89nm) in 0.5M HCl solution. In the presence of 20ppm of EMNQ2O inhibitor, they are less and had been (154nm, 17nm, and 63.9nm) in salt environment and (9.1nm, 10.7nm, and 39.8nm) in the acidic environment. These parameters confirm that the surface is smoother, (Figs. 15b, 16b). Surface smoothness results from the formation of a compact (Fe^{2+} -EMNQ2O complex) protective layer on the metal surface, thus preventing corrosion of carbon steel. These data indicate that the surface of carbon steel immersed in the saline and acidic

solution has a greater surface roughness in the blank than in the presence of the inhibitor, which indicates that the surface of the unprotected soft steel is harder due to the corrosion of carbon steel in salt and acid environments²⁷⁻³⁰.

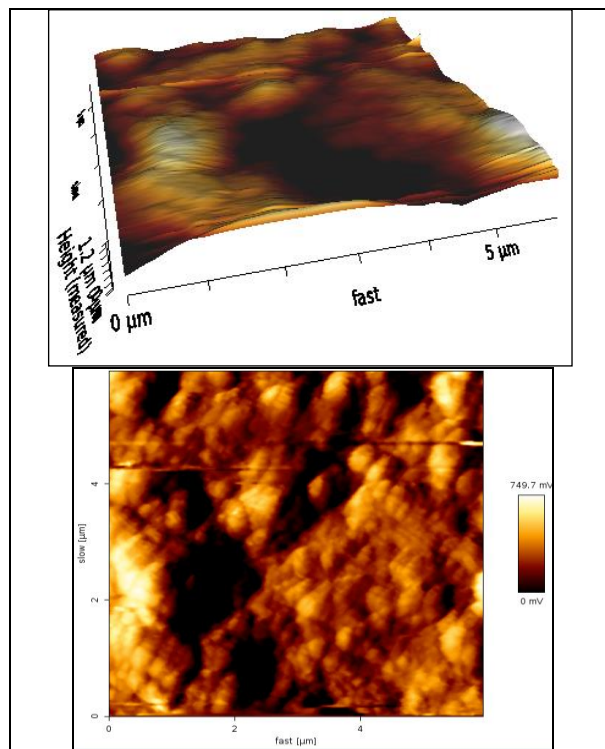


A

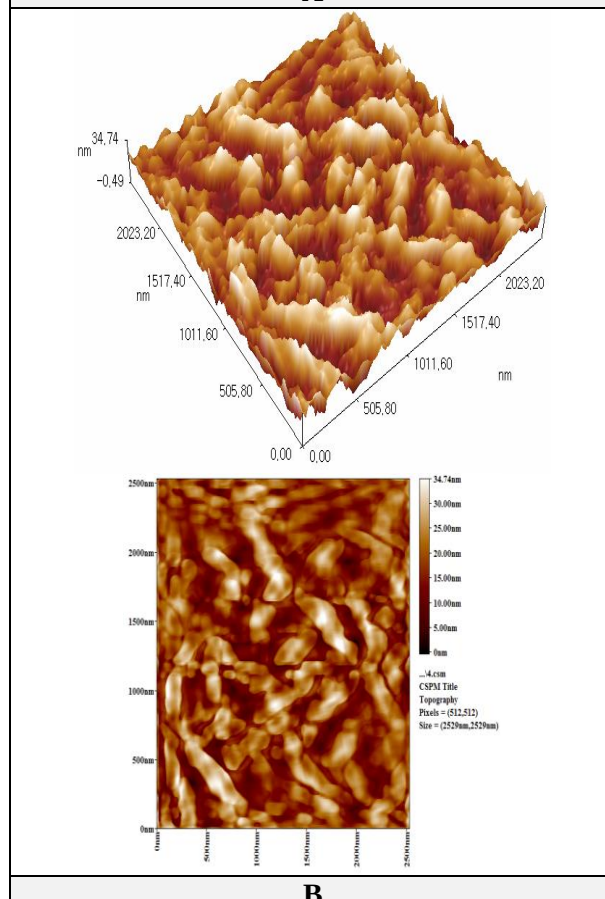


B

Figure 15. AFM of C.S surface (a, b) in salt medium of 3.5% NaCl solution without presence of the (EMNQ2O) inhibitor, (c, d) in presence of 20 ppm of (EMNQ2O) inhibitor.



A



B

Figure 16. AFM of C.S surface (a, b) in acidic solution without presence of the (EMNQ2O) inhibitor, (c, d) in presence of 20 ppm of (EMNQ2O) inhibitor.

Conclusions:

- The results of DFT calculations on EMNQ2O quinoline derivative have been presented in vacuum, DMSO and in water solutions. The HOMO, LUMO, and charges on atoms predict a similar center that would prefer to be attacked by nucleophilic or electrophilic species.
- The ΔE and dipole moment values suggest that EMNQ2O has greater tendency to interact with the metal surface in solvent solutions than in vacuum, and it is a good inhibitor in both of them.
- Quantum chemical calculations of (DFT/ B3LYP/ 6-311++G/ 2d, 2p) gave realistic results in the case of the geometry of the conformers, and the results of DFT/B3LYP were closer to the experimental data.
- Experimentally, it was observed that the corrosion rates of carbon steel in the corrosive medium decreased with the addition of different concentrations of the inhibitor.
- A comparison of EMNQ2O inhibition efficiency in the salt solution (94.98%) is more electron deficient than in acid solution (81.40%). However the thermodynamic and kinetic parameters suggest that EMNQ2O has greater tendency to interact with the metal surface in (3.5% NaCl) solution than in (0.5M HCl) solution, and it is a very good inhibitor in both of them.

Authors' declaration:

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

Authors' contributions statement:

M.A. contributed to samples preparation, performed the experiment calculations. R.K. devised the project, carried out the theoretical part with all its calculations (tables and figures), discussed all the results (experiment and theoretical), wrote the manuscript.

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دراسة نظرية وتجريبية لسلوك تآكل سطح حديد الصلب الكربوني في 3.5% كلوريد الصوديوم و 0.5M حامض الهيدروكلوريك عند تراكيز مختلفة من مشتق الكوينولين-2-اون

مصطفى علاء محمد

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الخلاصة:

تم اجراء دراسة نظرية وتجريبية على حماية تآكل سطح حديد الصلب الكربوني عند تراكيز مختلفة من مشتق (الكوينولين-2-اون) الذي يحمل الاسم: 7-Ethyl-4-methyl-1-[(4-nitro-benzylidene)-amino]-1H-quinolin-2-one (EMNQ2O). من الناحية النظرية، تم استخدام نظرية دالة الكثافة (DFT) عند المستوى (B3LYP) 6-311++G (2d,2p) لحساب التركيب الهندسي والخصائص الفيزيائية ومعايير كفاءة التثبيط الكيميائية، مع مواقع الامتزاز الفعالة من أجل التنبؤ بمعرفة المواقع المحتملة للهجمات النكليوفيلية والالكتروفيلية في الفراغ وفي اثنين من المذيبات (DMSO و H₂O)، كل ذلك عند الاشكال الهندسية التوازنية. من الناحية التجريبية، تمت دراسة كفاءة التثبيط (%IE) في محلولي (NaCl 3.5%) و (HCl 0.5M) باستخدام قياسات الاستقطاب المجاهدي. أظهرت النتائج أن كفاءة التثبيط (%IE) في المحلول الملحي (94.98%) أكبر مما هي في المحلول الحامضي (81.40%). المعلمات الديناميكية الحرارية التي تم الحصول عليها تدعم آلية الامتزاز الفيزيائي وأن امتزازه على سطح حديد الصلب الكربوني بطبيع ايزوثيرم امتزاز لنكماير isotherm Langmuir. وتمت دراسة التغيرات السطحية لحديد الصلب الكربوني باستخدام تقنيتي الفحص المجهرى للإلكترون (SEM) والفحص المجهرى للقوة الذرية (AFM).

الكلمات المفتاحية: - تثبيط التآكل، DFT، الكوينولين، المعلمات الديناميكية الحرارية.