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RESEARCH ARTICLE

Quantum Chemical Studies, Characterization and Understanding the Inhibition Effect of *Pulicaria Jaubertii* Oil, Growing in Yemen, as a New Eco-Friendly Inhibitor for C38 Steel Corrosion in 1 M HCl Medium

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ABSTRACT

The inhibitive action of *Pulicaria Jaubertii* essential oil (PJEO), as green inhibitor, has been investigated on the carbon (C38) steel corrosion in 1 M HCl by using inductively coupled plasmas spectrometry (ICP), electrochemical impedance spectroscopy (EIS), potentiodynamic polarization and gravimetric measurements. The increasing of oil concentrations increases the carbon steel corrosion resistance (The inhibition efficiency), which rose to 94% in the optimal concentration (2.5 g/l). The specimen surfaces were analysed by using Infra-Red spectroscopy (IR) and scanning electronic microscope (SEM). The obtained results showed the presence of oil molecules adsorbed onto the specimen surface. Langmuir adsorption model was followed by PJ essential oil compounds which adsorbed onto the carbon steel surface to form a protective layer. PJEO was analysed by using gas chromatography coupled with mass spectra before it was used as green inhibitor. Several DFT parameters such as LUMO and HOMO energy, gap energy (ΔE), electronegativity (χ), softness (σ) and global hardness (η) were derived for all major molecules found in PJ oil. The theoretical results showed that there is a good agreement with the experimental data.

Keywords: Adsorption, C38 steel, Corrosion inhibition, DFT calculation, Eco-friendly inhibitor, Extraction, Essentials oil, *Pulicaria Jaubertii*

Introduction

Carbon steel, one of the essential iron alloys, is widely used in many industrial applications, such as oil wells, in which acids play crucial roles in various processes, such as acid pickling and acid cleaning.[1,2] Iron and its alloys are exposed to high aggressive environment in these processes. Adding corrosion inhibitors is a good and practical method to protect metal and reduce the acidic environment effect.[3,4] Environmental toxicity, caused by some corrosion inhibitors, has been conducted in search of new eco-friendly inhibitors (green inhibitors) of metal corrosion in acidic medium.[5,6] In the last years, many inhibitors were extracted from plants, or synthesized, and others may be chosen from the

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subsistent compounds.[7,8] The inhibitors with a center of π electron (multiple bonds) and/or contain oxygen, sulfur, and nitrogen atoms are the best for protecting several metals and alloys against corrosion in various environments.[9–11] Generally, the inhibition efficiency depends on the strength of bonds (coordination bonds) formed between the metal's surface and the inhibitor's molecules. This means that it relates to the stability of the complex formed; the inhibition effectiveness decreases in the following order: $P > S > N > O$.[12,13]

In addition, those organic inhibitors are toxic to the environment and humans; they are very expensive, so their use has become limited as corrosion inhibitors. Besides, the plant extracts are non-toxic and inexpensive products. So, they are considered a great source of corrosion inhibitors, which are ecologically acceptable and friendly to the environment.[14,15] For these reasons, plant extracts have been an essential searching area for many years. Moreover, the plant extracts are a renewable and available source of materials. Thus, many authors have studied various natural products as green inhibitors, with high inhibition efficiency, for several metals and alloys under different condition.[16,17]

Computational chemistry and experimental techniques have recently emerged as a highly valuable approach for explaining molecular structures, molecular simulations, electronic properties, and compound reactivity. This combination has gained tremendous popularity, especially in the corrosion inhibitors investigation.[18] Density Functional Theory (DFT), one of the most commonly used quantum chemical methods, is also utilized to understand site selectivity in molecular systems, chemical reactions, and structural characteristics.[19]

The objective of this work was the investigation of the inhibitive action and adsorption characteristics of an eco-friendly and inexpensive inhibitor (PJEO) for the corrosion behavior of C38 steel in one molar hydrochloric acid medium by using gravimetric measurements, inductively coupled plasmas spectrometry (ICP), electrochemical impedance spectroscopy (EIS), Tafel polarization, Infra-Red spectroscopy (IR) and scanning electronic microscope. Also, this study is complemented by theoretical calculation.

Materials and methods

Inhibitors extraction

Pulicaria Jaubertii plant, collected from the Al-Haima district (Sana'a-Yemen), was used to obtain its essential oil by steam distillation. The condensed oil was isolated from the water's surface using a plastic pipette to obtain concentrated and pure oil. The dry oil was kept in a refrigerator at—4 °C.[20] Then, it was used to investigate its inhibitive properties for carbon steel corrosion in 1 M HCl.

Specimens preparation

Carbon steel specimens used in this study had a cylindrical shape, with the following chemical composition (wt.%): 0.380% C, 0.680% Mn, 0.230% Si, 0.077% Cr, 0.016% S, 0.059% Ni, 0.011% Ti, 0.160% Cu 0.009% Co, and iron (Fe) is the rest. For all experiments, the specimen surfaces were polished as a mirror using emery paper SiC with the following order of grades 400, 800, 1200, 1500, and 2000 and washed with distilled water.

Solution preparation

The acid medium (1 M HCl) has been used to prepare various essential oil concentrations after diluting an analytical reagent (37% HCl) with bi-distilled water. The essential oil has been used as an eco-friendly inhibitor with a concentration range of (0.5-1-1.5-2-2.5) g/l.

Gravimetric measurements

Gravimetric tests were performed in a ventilated glass cell with 30 ml of test solution without and with the optimal concentration (2.5 g/l) of PJEO at room temperature. After the specimens had been immersed for one week, they were removed from the solution and washed carefully with distilled water. Then, they were dried in hot air for an hour and were cooled for an hour in a desiccator at room temperature. Finally, they had been weighted. The differences in weight have been reported. Then, they had been used to calculate inhibition efficiency (IE%), after they had been used to calculate the corrosion rate (W) by using the following Equation:

$$W = \frac{\Delta m}{S \times t} \tag{1}$$

$$IE\% = \left(\frac{W_0 - W}{W_0}\right) \times 100 \tag{2}$$

Where Δm, S, t, $W_{0,}$ and W indicated the specimen difference in weight loss, surface area, immersing time, and the corrosion rate of C38 steel samples in 1 M HCl in the absence and the presence of an inhibitor, respectively.

Inductively coupled plasmas spectrometry ICP analysis

The test solutions were analyzed using inductively coupled plasmas spectrometry (ICP) after the specimens had been tested in gravimetric experiments to confirm the gravimetric results by recalculation of both corrosion rate (W) and inhibition efficiency (IE%) from the loosen weights, which were observed in the solution, using the following Equation:

$$W = \left(\frac{m_{Fe^{\circ}} - m_{Fe}}{S \times t}\right) = \left(\frac{\Delta m}{S \times t}\right) \tag{3}$$

$$IE\% = \left(\frac{Fe^{\circ} - Fe}{Fe^{\circ}}\right) \times 100 \tag{4}$$

Where Fe° and Fe indicated the iron concentration obtained by the ICP technique without and with essential oil, respectively.

Potentiodynamic polarization measurements

In a typical double glass cylindrical cell with three electrodes, all electrochemical tests were performed using a Potentiostat Voltalab 301 PGZ associated with a PC with VoltaMaster 4.0 software. A platinum electrode has been used as an auxiliary electrode (CE), a saturated calomel electrode (SCE) as a reference electrode, and a cylindrical C38 steel as the working electrode (the active area is 0.95 cm^2). Tafel curves were registered for C38 steel specimens in 1 M HCl media for all polarization measurements. This was implemented at room temperature without and with PJEO with the potential range from –0.2 V to –0.8. After the specimens had been immersed in the free potential for an hour. The test medium was agitated using a magnetic stirrer during the experiment. The calculated values of inhibition efficiency (IE%) were obtained using the following Equation:

$$IE\% = \left(\frac{I^{\circ} - I}{I^{\circ}}\right) \times 100 \tag{5}$$

I° and I, respectively, indicated the density of corrosion current in the absence and the presence of essential oil.

EIS measurements

Nyquist diagrams were registered using a Potentiostat Voltalab 301 PGZ after the specimens had been immersed in free corrosion potential for an hour. For all EIS experiments, the values of polarization resistance (Rct) and double layer capacitance (Cdl) were calculated using the same software the same condition used in polarization measurements with a frequency range from 10 kHz down to 100 mHz. The calculated inhibition efficiency (IE%) has been obtained by using the following Equation:

$$IE\% = \frac{R'_{ct} - R_{ct}}{R'_{ct}} \times 100 \tag{6}$$

R_{ct} and R'_{ct} indicated the polarization resistance of C38 steel without and with the essential oil, respectively.

SEM analysis

After the specimens had been tested in gravimetric experiments, the carbon steel surfaces were analyzed using a scanning electron microscope (Quanta 200 FEI company; SEM).

IR analysis

The surface morphology of C38 steel specimens was also analyzed using Infrared spectroscopy (IR) after the specimens had been tested in gravimetric experiments without and with an optimal concentration of PJEO. The frequency range was between 400 and 4000 cm^{-1}, and the zone of the organic function group was chosen to confirm the existence of PJEO molecules on the carbon steel surface.

GC/MS analysis

The *Pulicaria Jaubertii* essential oil (PJEO) has been analyzed by using ultra trace gas chromatography (GC) associated with Mass spectrometry (MS), which plays the role of the detector, and its ionization type was the impact electronic at 70 eV. The GC has been used with a VP-5 capillary silica column (250 μm diameter, 30 m length, 25 μm film thickness) and an oven heated at 60 °C for 2 min. Then, the temperature is programmed to rise at an average of 16 °C/min until it reaches 280 °C. The analysis was accomplished with the following operating conditions: the carrier gas is Helium (He: 99.99%) with a linear speed of 20 cm/sec and letting pressure of 76 kPa, the temperature of the injector is 220 °C and the spilled radio is 1:25.

Quantum chemical calculation

The PJEO adsorption mode onto carbon steel's surface has been investigated using DFT theory with B3LYP nonlocal correlation function, complementing the following basis set: 6-31G + (d,p). Density function theory (DFT) calculation has been performed using Gauss-View 06 interface software and Gaussian 09 program.[21,22] Quantum chemical calculation has been used to estimate the different electronic properties of the three major compounds of PJEO. This QCC includes the energy of the lowest unoccupied molecular orbital (E_{LUMO}) and the energy of the highest occupied molecular orbital (E_{HOMO}), which has suggested that the selectivity site of the molecular systems and chemical reactivity depends on the energy of gap (ΔE). Moreover, different parameters such as electronegativity (χ), ionization potential (I), chemical potential (μ), electron affinity (A), global softness (σ), global hardness (η), global electrophilicity index (ω), electron accepting-power ($\omega+$), electron donating-power ($\omega-$), net electrophilicity ($\Delta\omega\pm$), back-donation energy ($\Delta E_{B.D}$) and electronegativity (global electronic chemical potential; χ) had been calculated by using the following Equation:[23,24]

$$I = -E_{HOMO} \tag{7}$$

$$A = -E_{LUMO} \tag{8}$$

$$\Delta E = E_{LUMO} - E_{HOMO} \tag{9}$$

$$\eta = \frac{1}{2}\left(E_{LUMO} - E_{HOMO}\right) \tag{10}$$

$$\sigma = \frac{1}{\eta} \tag{11}$$

$$\chi = \frac{1}{2}\left(-E_{HOMO} - E_{LUMO}\right) \tag{12}$$

$$\mu = -\chi = \frac{1}{2}\left(E_{HOMO} + E_{LUMO}\right) \tag{13}$$

$$\omega = \frac{\mu^2}{2\eta} \tag{14}$$

$$\omega^+ = \frac{\left(-3E_{LUMO} - E_{HOMO}\right)^2}{16 \times \left(E_{LUMO} - E_{HOMO}\right)} \tag{15}$$

$$\omega^- = \frac{\left(-E_{LUMO} - 3E_{HOMO}\right)^2}{16 \times \left(E_{LUMO} - E_{HOMO}\right)} \tag{16}$$

$$\Delta\omega^{\pm} = \omega^+ + \omega^- \tag{17}$$

$$\Delta E_{B.D} = -\frac{\eta}{4} \tag{18}$$

In addition to these parameters, frontier molecular orbitals (FMO), the optimized geometry structure, molecular electrostatic potential (MEP), and Mullikan atomic charge (MAC) have been applied and analyzed.

Results and discussion

PJEO analysis (GC/MS)

About 1 μl of the *Pulicaria Jaubertii* essential oil (PJEO) has been analyzed by using GC/MS. Many authors obtained the same results (same compound) with differences in the radio of significant compounds (63–98%),[25,26] which is Carvotanactone. The obtaining chromatograms and the primary compound's structure are given in Fig. 1.

Gravimetric measurements

The corrosion rate and inhibition efficiency for C38 steel in one molar hydrochloric acid solution at room temperature in the absence and presence of PJEO have been given in Table 1. It is indicated that the

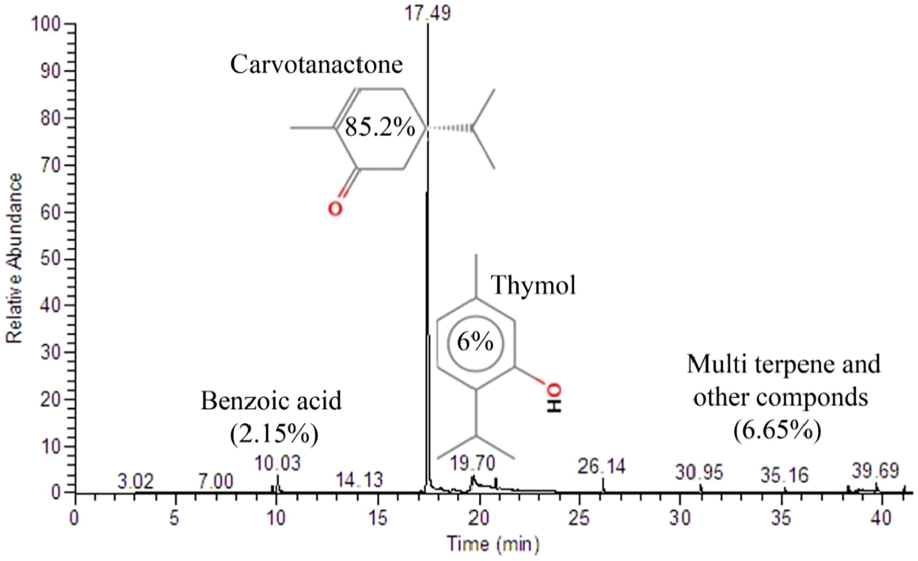

Fig. 1. The essential oil chromatograms and the structure of significant compounds.

Table 1. Weight loss and corrosion parameters of gravimetric experiments for C38 steel in 1 M HCl containing optimal concentration (2.5 g/l) of PJEO.

Inhibitor	Area (cm^2)	weight loss (mg)	W ($mg\ cm^{-2}\ h^{-1}$)	IE (%)
Blank	5	2.3	0.00479	———
Pulicaria Jaubertii	3.5	0.11	0.00033	93.11

Table 2. Weight loss and corrosion parameters obtained from ICP spectrometry for C38 steel in 1 M HCl containing optimal concentration (2.5 g/l) of PJEO.

Inhibitor	Area (cm^2)	Fe obs. by ICP (mg)	W ($mg\ cm^{-2}\ h^{-1}$)	IE (%)
Blank	5	15.16	0.0316	———
Pulicaria Jaubertii	3.5	0.709	0.0015	95.25

inhibition efficiency of C38 steel in one molar hydrochloric acid containing 2.5 g/l of PJEO is 93%.

ICP analysis

The amount of iron (Fe) was detected in the test solutions using ICP spectrometry after the specimens had been tested in gravimetric experiments without and with the essential oil of *Pulicaria Jaubertii* plant. Then, they were used to calculate corrosion rate (W) and inhibition efficiency (E%) for C38 steel in molar hydrochloric acid by using the same equation as in the gravimetric method, the amount of iron (Fe) used as weight loss, and the obtaining corrosion parameters had been presented in Table 2.

This result confirmed the high inhibition efficiency of essential oil with a good agreement. The slight increase in inhibition efficiency (E%) in this method compared to the gravimetric method may be attributed to the increasing the weight of specimens in the gravimetric method, by the corrosion product fixed in specimen surfaces, in the blank solution, and by the adsorption of essential oil molecules on the C38 steel surface from the solution inhibited.

Potentiodynamic polarization measurements

Fig. 2 shows the polarization curves for the C38 steel specimens in 1 M HCl without and with various concentrations of PJEO. Their examinations revealed that adding oil affected both the cathodic and anodic parts. This means that the green inhibitor obstructed metal dissolution on the anode and diminished the evolution of hydrogen reaction on the cathode. The corrosion kinetic parameters are given in Table 3.

As in Fig. 2, the corrosion potential (Ecorr) values have been shifted toward more negative values and

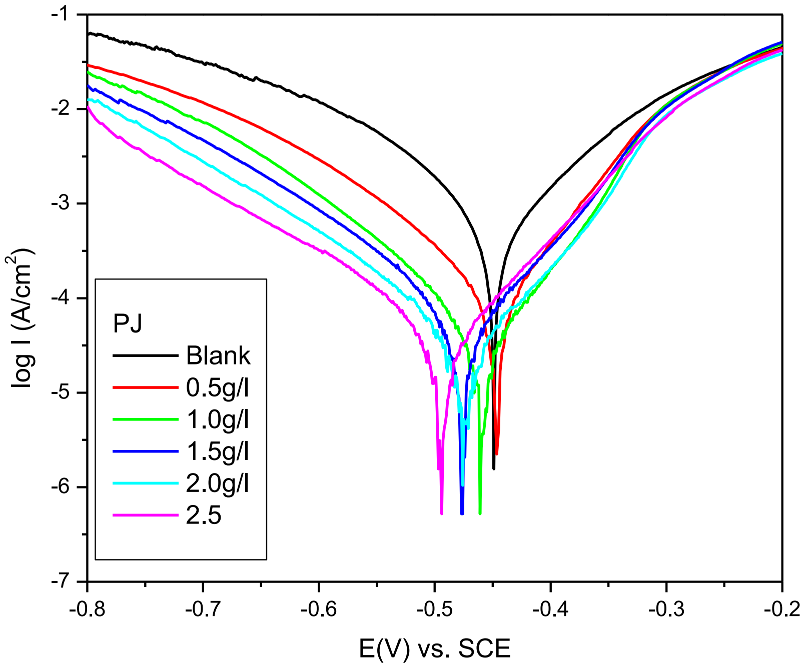

Fig. 2. Curves of Tafel for C38 steel in 1 M HCl medium without and with various concentrations of Pulicaria Jaubertii oil at 298 K.

Table 3. Parameters of corrosion for carbon steel immersed in one molar HCl solution with and without various PJEO concentrations.

Type	C(g/L)	E_{corr}(mV/SCE)	I_{corr}(μA/cm^2)	B_c(mV/SCE)	IE%
HCl	1 M	451	1425	163	–
Pulicaria Jaubertii	0.5	449	679	118	52
	1	460	352	107	75
	1.5	476	170	123	88
	2	477	74	128	94.8
	2.5	496	59	127	95.8

the corrosion current density (Icorr) decreased with increasing the PJEO concentration. These results suggested that the PJEO is an excellent green inhibitor for C38 steel. Generally, when the change in corrosion potential is non-existent or less than 85 mV, the inhibitor can be classified as a mixed-type inhibitor as well as in this study, where the most significant change, as in Table 3, was 45 mV for optimal concentration of PJEO.[27,28]

As in Table 3, the high inhibition efficiency (IE%) registered was 95% at the optimal concentration (2.5 g/l) of PJEO.

Electrochemical impedance spectroscopy measurements

With the same Potentiostat and its accessories at 298 K. After the specimens had been immersed for 30 min at the free potential, the Nyquist plots of carbon steel immersed in one molar HCl medium with and without various concentrations of PJEO were fitted. EIS investigated corrosion behavior at 298 K. The obtained carbon steel Nyquist plots without and with various PJ essential oil concentrations are given in Fig. 3.

Generally, in the corrosion process, the single capacitive loops implied the charge transfer; as observed in Fig. 3, these impedance loops are depressed semi-circles, which were their centers under the real X-axis. The depressed semi-circle in the Nyquist plots expanded with increasing the PJ essential oil concentrations. This implies that the charge transfer process mainly controls the corrosion process,[29] which forms an inhibiting layer that decelerates corrosion and enhances corrosion resistance. This layer is stringed by increasing the PJ essential oil concentrations. The electrical response of the system has been considered by using the equivalent circuit that was represented in Fig. 4

Table 4 represents the different impedance parameters, such as the double layer capacitance (Cdl), the solution resistance (Rs), charge transfer resistance or polarization resistance (Rct), and the calculated inhibition efficiency (Ect%).

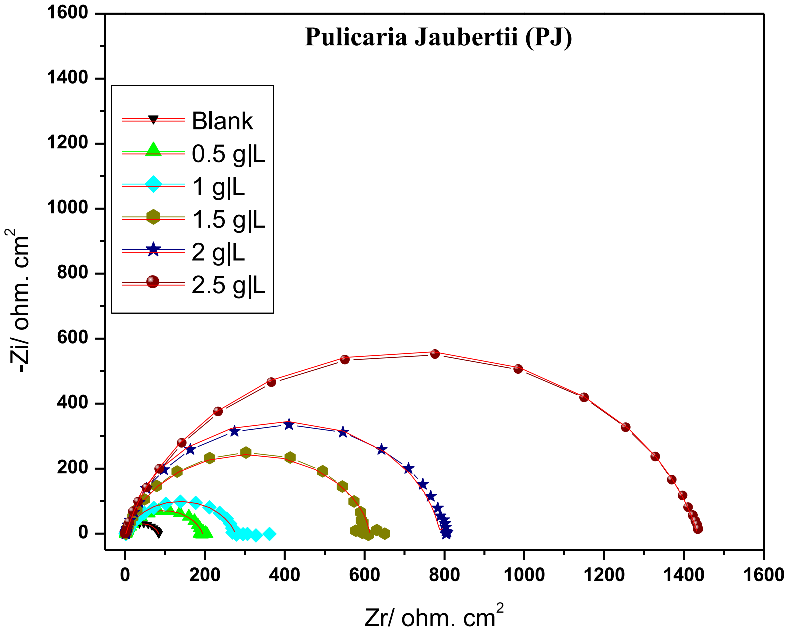

Fig. 3. The fitting of Nyquist plots for C38 steel in 1 M HCl medium without and with various concentrations of PJEO.

Table 4. Parameters of corrosion inhibition for C38 steel in ventilator 1 M HCl medium at various concentrations of PJEO.

Type	C (g/L)	RS (Ω.cm^2)	N	Rct Ω.cm^2	Cdl (μF cm^{-2})	IE%
HCl	1 M	1.591	0.8179	82	99.41	–
PJEO	0.5	1.512	0.8082	193	62.62	57.7
	1	1.434	0.7937	287	56.78	71.5
	1.5	1.697	0.8490	615	42.44	86.7
	2	1.370	0.9191	788	30.65	89.6
	2.5	1.708	0.8475	1432	24.83	94.3

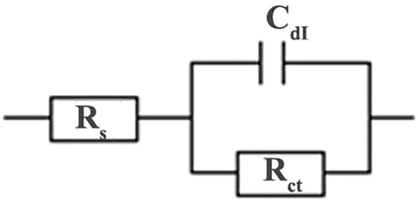

Fig. 4. The equivalent circuit model.

The high inhibition efficiency (*E*%) registered was 94% at the optimal concentration (2.5 g/l) of PJEO. The electrochemical results have good agreement with the ICP and gravimetric method.

Adsorption isotherm behaviour

Adsorption isotherm investigation can supply information about the interaction between the oil molecules of PJEO and the active sites on the surface of C38 steel. The coverage degree of the specimen surfaces (θ) for various concentrations of PJEO has been estimated from potentiodynamic polarization data.

Different isotherms, including Temkin, Langmuir, and Frumkin, were fitted and found that the adsorption is more compatible with the Langmuir isotherm, which uses the following Equation:

$$\frac{C_{inh}}{\theta} = \frac{1}{K} + C_{inh} \tag{19}$$

θ and K are indicated to surface coverage values and the adsorption constant, respectively. The correlation coefficient (R^2) was 0.9955, as shown in Fig. 5; this suggests that the PJEO adsorption on the specimen surfaces obeyed Langmuir adsorption isotherm.[30,31] A superficial layer has been adsorbed.

By using the following equation, the adsorption-free energy (ΔG^o_{ads}) was calculated:

$$K = \frac{1}{55,5} e^{\left(\frac{-\Delta G^o_{ads}}{RT}\right)} \tag{20}$$

$$\Delta G^o_{ads} = -(\ln K + \ln 1000) \times RT \tag{21}$$

The numerical values (55.5 M and 1000 g/l), R and T indicated the water concentrations, the gases constant, and the experimental temperature in Kelvin, respectively,[11,32] ΔG^o_{ads} has been calculated to be –16.09 kJ/mol. The free energy negative sign indicated

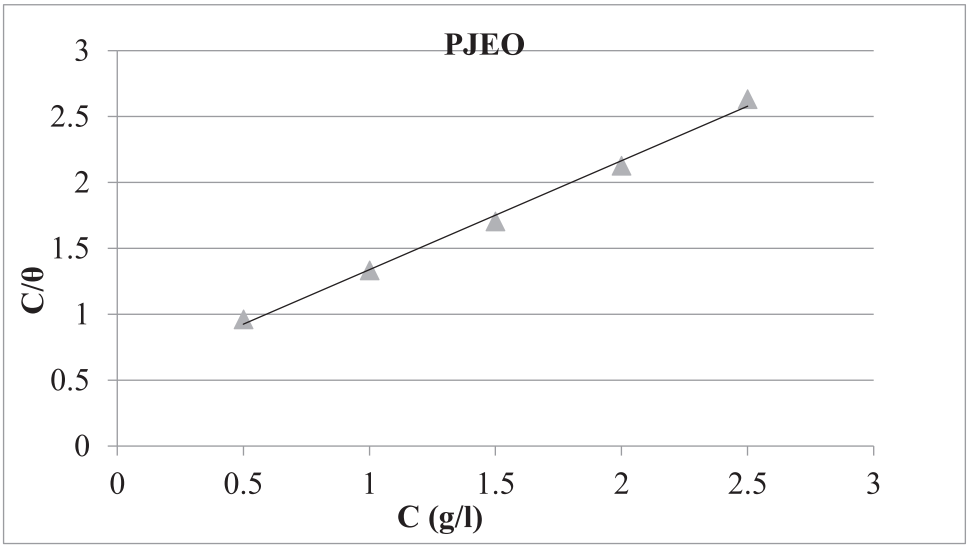

Fig. 5. Langmuir plot of the PJEO adsorption onto C38 steel surface at room temperature.

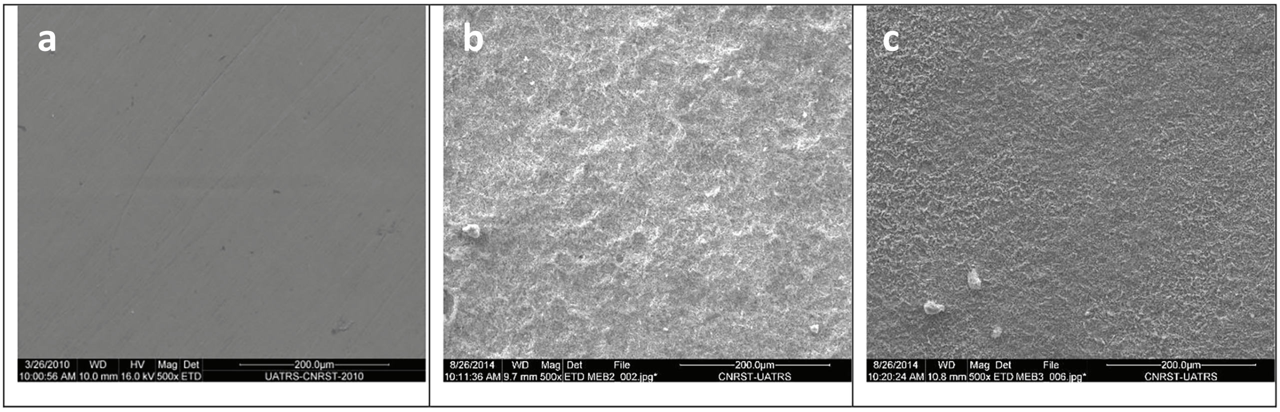

Fig. 6. SEM analysis for the surface of the C38 steel specimens; (a) reference and after weight loss measurements in 1 M HCl; (b) without PJEO; (c) containing 2.5 g/l of PJEO.

the spontaneous adsorption process for the PJEO components on the surface of the studied specimens. Generally, the absolute values around –40 kJ/mol or higher refer to strong interaction (chemisorption), which involves charge transfer or electron sharing from/to metal surface from/to the inhibitor molecules to form a coordinate bond (strong bond type). At the same time, those of –20 kJ/mol or lower imply weak interaction (physical adsorption).[33,34] The calculated value suggests that the PJEO on the surface of specimens in 1 M HCl medium was adsorbed with physical interaction.

SEM analysis

After the C38 steel specimens had been immersed in one molar HCl (blank) or when they contained 2.5 g/l of essential oil (during the gravimetric tests), the specimen surfaces were analyzed using a scanning electronic microscope (SEM). Their surface images are shown in Fig. 6.

The C38 steel surface immersed in a 1 M HCl solution without PJEO has been roughened by the presence of corrosion products. In the presence of PJEO, a smooth C38 steel surface was noticed, which was easily compared with the newly polished specimen surface. This implies that the PJEO protects the C38 steel from corrosion attack in the 1 M HCl solution.

IR analysis

The specimen surfaces were analyzed using infrared spectroscopy (IR), using the same processes as in SEM analysis. The IR spectra of the specimen surface with optimal concentration are shown in Fig. 7.

Generally, the OH group possessed a strong large band near 3300 cm^{-1}, the formula of structural alcohols group (C-O-H) has a group of bands in the 1050–1200 cm^{-1} region, and the alcohols conjugated aromatic ring possessed a band near 1585 cm^{-1}. The bands of (C-O) appear near 1300 cm^{-1}, especially in benzoic acid, while the characteristic bands of the carbonyl group appear near 1700 cm^{-1}.[35] As shown in Fig. 7, the specter contains all characteristic bands of essential oil compounds. This result confirms the high ability of this green inhibitor and indicates it excites a protective layer on the C38 steel surface.

DFT calculation

The quantum chemical parameters of the major molecules of PJEO related to the most stable conformation of molecule electronic structure are shown in Table 5. Low-value LUMO energy and high-value HOMO are associated, thereby, with high protection ability and strong bending between metal and inhibitor. Generally, the high LUMO energy values indicate that a molecule's electron-accepting ability is weaker. Moreover, the low energy of LUMO implies that a molecule can accept the electron.[36]

As shown in Table 5, Benzoic acid has the lowest value of HOMO, and Carvotanactone has the highest, which indicates that Carvotanactone has the best corrosion inhibition properties and is the best electron donor.[37,38] The high value (ΔE) implies that the Benzoic acid is a poor corrosion inhibitor and less reactive than Carvotanactone. The high value of electronegativity (χ) also shows that the inhibitor acts as a poor corrosion inhibitor.[39] Global softness (σ) and global hardness (η) were also calculated for all significant molecules of PJEO. The low value of η is related to high inhibition efficiency, reactivity, adsorption tendency, and electron-donating ability, and the converse is true for σ. As pointed out in Table 5, the results imply that the Carvotanactone

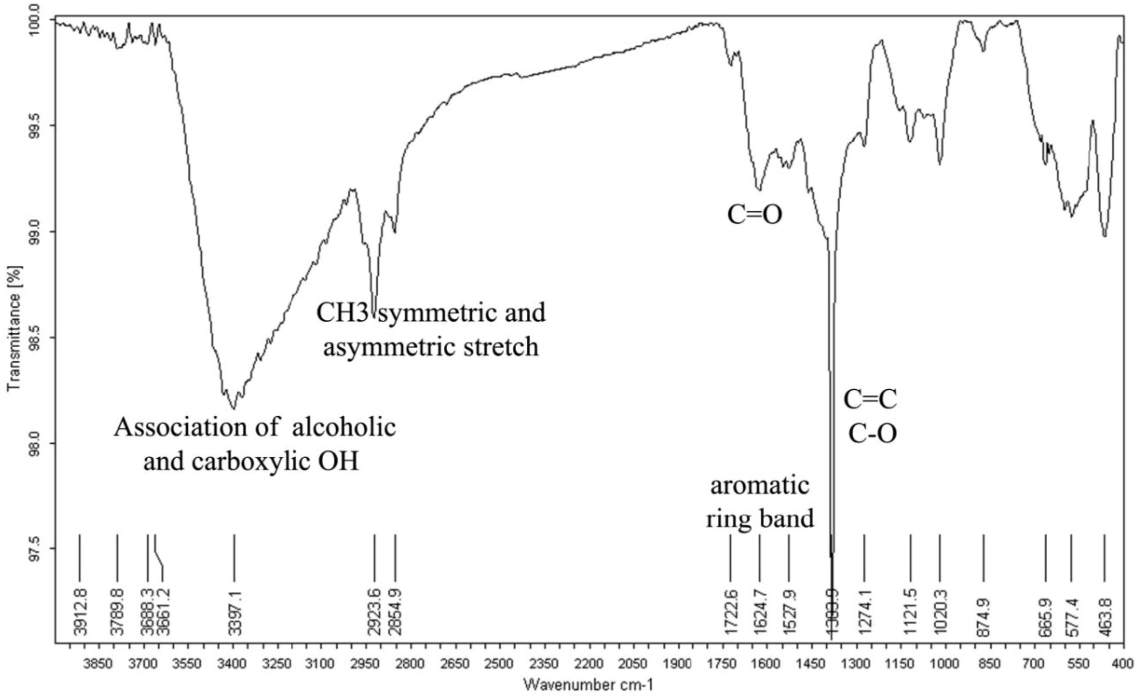

Fig. 7. IR analysis for the C38 steel surface after weight loss measurements in 1 M HCl with 2.5 g/l of PJEO.

Table 5. Quantum chemical parameters of major molecules of PJEO.

PJEO molecules	Benzoic Acid	Carvotanactone	Thymol
LUMO (eV)	–1.78339	–3.20297	–0.36707
HOMO (eV)	–7.41002	–5.36513	–6.04459
ΔE (eV)	5.626629	2.162162	5.677513
I (eV)	7.410018	5.365134	6.044585
A (eV)	1.783389	3.202971	0.367072
χ (eV)	4.596704	4.284053	3.205829
σ (eV-1)	0.355453	0.925	0.352267
η (eV)	2.813314	1.081081	2.838756
ω (eV)	3.755301	8.488312	1.810183
M (eV)	–4.5967	–4.28405	–3.20583
$\omega^{+}\ (eV)$	1.808613	6.48142	0.562113
$\omega^{-}\ (eV)$	6.405317	10.76547	3.767942
$\omega^{\pm}\ (eV)$	8.21393	17.24689	4.330055
$\Delta E_{back\ donation}$	–0.70333	–0.27027	–0.70969
$N_{100}\ (eV)$	–0.122	–0.173	0.124
$N_{110}\ (eV)$	0.0397	0.2479	0.2843
$N_{111}\ (eV)$	–0.1274	–0.1869	0.1187

has a high value of σ and a low value of η. This means that it is more reactive. Consequently, it's a more effective corrosion inhibitor.[40] Backdonation energy ($\Delta E_{B.D}$) values of PJEO molecules were lower than zero ($\Delta E_{B.D} < 0$), which implied that the charge transfer (from the carbon steel surface to the PJEO compounds followed by a back-donation from the PJEO compounds) was the preferable energetical procedure. This procedure may be complementary, as one of the PJEO compounds acts as an electron donor and the other acts as an electron acceptor. The synergistic effects of PJEO components on the carbon steel surface can also be confirmed by the conjugated system structure of the optimized PJEO compounds, which increased to increase the density of electron cloud in the following order: Thymol > Carvotanactone > Benzoic acid. On the other hand, the electronic densities had been increased in the following order Carvotanactone > Thymol > Benzoic acid. Thymol has the most significant dihedral angle (0°), and Benzoic acid has the lowest (80.75°). This result implies that the Benzoic acid can be adsorbed on the carbon steel surface in a complete horizontal state. Still, according to its electronic density, it can act as an electron acceptor. However, Thymol and Carvotanactone may have difficulty in the horizontal position, especially for Thymol, but they can still act as an electron donor. Generally, the negative sign implies that the compound has an electron-donating capacity.[41]

The fraction of the transferred electron (ΔN) is used to measure the electron transfer from metal to the molecule and the back-donation from the molecule to the metal surface. Generally, the negative sign of the transferred electron fraction ($\Delta N > 0$) indicated that the electron transfer from metal to the molecule is the preferable process. On the other hand, the positive sign of ΔN values ($\Delta N < 0$) implies that the preferable method of electron transfer is from the molecule to the metal.[42] The values of (ΔN) can be calculated

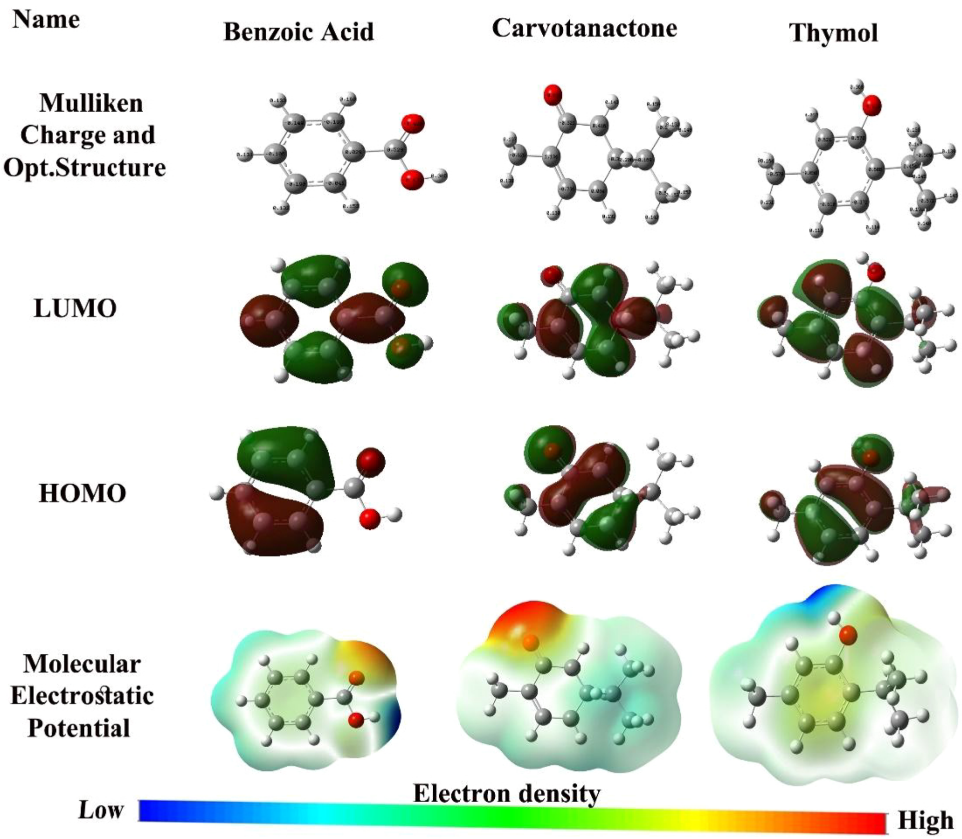

Fig. 8. The optimized geometry, Mullikan atomic charge, the frontier orbital distribution HOMO, LUMO, and ESP of major molecules of PJEO.

by using one of the following Equation:

$$\Delta \mathrm{N} = \frac{x_{Fe} - x_{inh}}{2\left(\eta_{Fe} + \eta_{inh}\right)} = \frac{x_{Fe} - x_{inh}}{2\eta_{inh}} \tag{22}$$

$$\Delta \mathrm{N} = \frac{\Phi_{Fe} - x_{inh}}{2\left(\eta_{Fe} + \eta_{inh}\right)} = \frac{\Phi_{Fe} - x_{inh}}{2\eta_{inh}} \tag{23}$$

Where χ, η indicated the electronegativity and global hardness, the minimal value makes the proposes ($\eta Fe \cong 0$) acceptable. Some authors[43–45] used the theoretical value of iron electronegativity (about 7 eV), which neglects the interaction between electron-electron. This value corresponds to the free electron gas model for iron fermi energy, and using this value in Eq. (22) is conceptually wrong.[46,47] So, many authors imply that using the work function of a metal surface (Φ), as in Eq. (23), is more correct than using metal electronegativity with the value of 7 eV.[48] In this work, we use Eq. (23) with the work function (Φ) values of Fe111, Fe110, and Fe100 surfaces of 3.88, 4.82, and 3.91 eV respectively.[49] As pointed out in Table 5, the ΔN values for the interaction between two planes of iron (Fe_{111} and Fe_{100}) and the two significant molecules of PJEO (Benzoic acid and Carvotanactone) are negative, while it is positive for Thymol. Also, they are positive for all significant molecules of PJEO with the surface. This result indicated that the adsorbed protective layer was formed by electron donation from Thymol to the surface of C38 steel, followed by a back-donation from Benzoic acid and Carvotanactone molecules to the C38 steel surface.

The optimized geometry, the frontier orbital distribution for (HOMO and LUMO) and the electrostatic surface potential (ESP or MEP; molecular electrostatic potential) of the major molecules of PJEO are given in Fig. 8. This Figure also presents the Mulliken atomic charge (MAC). The oxygen atoms in the tested eco-friendly molecules and the carbon atoms in the (C=C) double bonds exhibited the highest negative Mulliken atomic charge. As a result, they interacted with the C38 steel surface and displayed nucleophilic activity.

Generally, the local reactivity sites may be determined by using the MAC;[50] the most negatively charged of the MAC atoms of the inhibitor got the most effective atoms to donate the electrons to the unoccupied orbitals and preferentially adsorb them onto the carbon steel surface to produce a packed densely adsorption layer.

Mechanism of inhibition

The combination of the quantum chemical calculation data and the experimental results indicated that the excellent inhibitory effect of PJEO can be attributed to a synergetic impact arising from its compound, which contains oxygen atoms (heteroatoms), multiple bonds (π electron), and aromatic rings.[51] These findings aligned with the general exhibited properties of the inhibitor of corrosion. The adsorption of the PJEO compounds on the surface of C38 steel through one or more of the following mechanisms: (1) The interaction between the vacant d-orbital of the C38 steel surface atoms and non-bonding pair electron of oxygen atom from PJEO (2) Donor-acceptor interaction between the vacant d-orbital of the C38 steel surface atoms and the multiple bonds/aromatic rings. (3) The back-donation of electrons from the occupied orbital of the C38 steel surface atoms to non-bonding molecular orbitals of PJEO molecules.

Conclusion

PJEO is an excellent inhibitor for C38 steel corrosion in 1 M HCl medium. All electrochemical, ICP, and gravimetric tests agree, with a high inhibition efficiency maximum of 94% at 2.5 g/l. The inhibition efficiency increased with increasing the PJEO concentration.

The potentiodynamic polarization measurements demonstrate that the PJEO acts as a mixed-type inhibitor. The C38 steel corrosion attack is hampered by the adsorption of PJEO compounds onto the specimen surfaces, and the adsorption processes follow the Langmuir isotherm model. Quantum chemical studies supported the experimental result as well. They demonstrated the probability of electron transfer from the metal surface to PJEO molecules, followed by a back-donation from the inhibitor.

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Authors' declaration

- Conflicts of Interest: None.
- We hereby confirm that all the figures and tables in the manuscript are our. Furthermore, all figures and images, that are not our, have been included with the necessary permission for re-publication, which is attached to the manuscript.
- No human studies are presented in manuscript.
- No animal studies are presented in manuscript.
- Ethical Clearance: The project was approved by the local ethical committee at Faculty of Applied Sciences, Sa'adah University.

Authors' contribution statement

A. A contributed to the design and implementation, did the DFT calculation, wrote the manuscript, and discussed the results. Y. O. did the experimental data. M. B. contributed to the discussion of the results. S E. is the supervisor of this work at all its stages.

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دراسة كيميائية نظرية، تحديد المركبات الفعالة وفهم التأثير التثبيطي لزيت نبات العنصيف والذي ينمو في اليمن، كمثبط صديق للبيئة وذلك على تآكل الصلب الكربوني في وسط حامضي

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المستخلص

تهدف هذه الدراسة لمعرفة الخصائص المثبطة لتآكل الصلب الكربوني (C38 steel) باستخدام الزيت الأساسي لنبات العنصيف (*Pulicaria Jaubertii*) كنوع جديد من المثبطات الصديقة للبيئة. وذلك باستخدام تقنيات (Potentiodynamic, EIS, gravimetric, IR, SEM and ICP). أظهرت النتائج الكهروكيميائية أن الزيت الأساسي لنبات العنصيف له تأثير قوي في تثبيط تآكل الصلب الكربوني، وهذه القدرة تزداد بزيادة التركيز لتصل إلى 94 % عند تركيز 2.5 جم/لتر. تشير الدراسة إلى أن الزيت الأساسي يتصرف كمثبط مختلط، كما أظهرت أن عملية الامتزاز ماصة للحرارة، وتشكل مركبات الزيت مع سطح المعدن روابط كهروستاتيكية (امتزاز فيزيائي). استكمل هذا البحث من خلال تدعيم الجانب العملي بدراسة نظرية فباستخدام نظرية المدارات (DFT) تم حساب عدد من المعاملات النظرية مثل طاقة أعلى مدار رابط (HOMO)، طاقة أقل مدار غير رابط (LUMO)، فرق الطاقة بينهما (EΔ) السالبية الكهربائية (χ)، النعومة الكيميائية (σ)، العسر الكيميائي (η) وغيرها من المعاملات. النتائج النظرية دعمت النتائج العملية وبتوافق جيد.

الكلمات المفتاحية: الامتزاز، الصلب الكربوني، مثبطات التآكل، حسابات DFT، المثبطات صديقة البيئة، الاستخلاص، الزيوت الأساسية نبات العنصيف.