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Utilizing Tri-ethylamine as organic inhibitor to reduce copper corrosion in acidic environments; DFT computational study theoretical and experimental

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Abstract

The corrosion of copper metal in an acidic solution (HCl) was studied utilizing the organic substance Tri-ethylamine $N(CH_2CH_3)_3$ as an inhibitor, as well as polarization and weight loss procedures at various inhibitor concentrations (ranging from 100 ppm to 400 ppm). Furthermore, the effect of temperature on inhibitor performance was investigated, and it was shown that as temperature increased, inhibition efficiency increased but corrosion rate dropped. Temperature rises appear to be inversely related to occupancy efficiency, which is similar to 50 and 60 °C; nevertheless, while processing at 40 °C, activation energy, enthalpy, and free adsorption energy increase with increasing inhibitor concentration, but heat declines. This is caused by the presence of amines, nitrogen atoms, and an ethyl group. When applied on the surface of a metal, it acts as an anti-corrosive component, preventing or reducing corrosiveness. It is also effective at producing films via absorption, particularly on the surface of copper metallic substances. Adsorption and dissolution thermodynamic functions have been calculated. Using (DFT) technique, Tri-ethylamine has a strong capacity to adsorb on the iron surface via dual donor-acceptor interactions and electron transfer, forming a stable protective layer in the process, according to quantum chemical analysis. The strong agreement between these theoretical findings and the actual data validates its high inhibitory efficacy. Because theoretical corrosion inhibition depends on a number of factors, including electronegativity, total hardness, softness, ionization energy, dipole moment, energy gap, and the percentage of transferred electrons, as determined by a program, the inhibitor's theoretical state by DFT was also examined. The energy of "ELUMO," the molecular orbital with the lowest occupancy, and "EHOMO," the molecular orbital with the greatest occupancy. Additionally, calculations were made to determine the inhibitor's total electron density (TED) and total electrostatic potential (ESP).

Keywords: Enthalpy; Inhibition; Polarization; HCl; Corrosion; Tri-ethylamine; Copper; DFT; HOMO; LOMO

1. Introduction

Rust is one of the industrial pollutants that harm factories with their machinery and equipment and contaminate the environment, just like in the food business, water purification sectors, and many other chemical endeavors [1–8]. The term "corrosion" describes a range of interactions between a material's properties and its surroundings that erode its physical features. Growth-produced oxide layers control contact and spread with marine oxygen. In order to prevent more oxidation, the material might be passivized [9–13].Compared to other industrial metals, copper and its family alloys are particularly vulnerable to corrosion because hydrogen cannot be eliminated in an acidic environment with high oxygen concentrations [14–19]. Inhibitors are necessary to stop corrosion and the petrochemical industry's use of hydrochloric acid for cleaning, pickle, and descale goods that contain metal [20–25]. Heat exchangers, electronics components, telecommunications system items, and residential and commercial plumbing have all made use of copper due to its exceptional mechanical ductility and high thermal and electrical conductivity. Among the things causing the economic and technical advancement to lag are corrosion problems and deterioration [20–28]. Corrosion inhibitors are added to a solution to improve efficiency and lower the rate of corrosion. Since copper is used extensively in industry,

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only acids, salts, and specific other substances may cause its alloys to corrode. By protecting metal items with corrosion inhibitors, this can be avoided [29–39]. There are many different kinds of organic molecules, some of which have a notable impact on the environment while being comparatively less hazardous than others. The processes of the surrounding compounds, molecules, atoms, and aggregates determine how effectively an organic compound resists corrosion. The purpose of this work is to investigate the possibility that an organic chemical may hinder the corrosion of metals, particularly copper, in an acidic media In materials science, physical science, and chemistry, density functional theory, or DFT, is a computationally quantum mechanical modeling method used to investigate the electronic composition (or nuclear structure) of many-body phenomena, with a focus on molecules, atoms, and condensed phases. DFT is essentially the ground state. Functional, or functions that take a function as input and return a single real number, can be used to ascertain the characteristics of a many-electron system according to this theory. These are the spatially dependent electron density's functional in the context of DFT [40-43].

2. Experimental work

The coupons utilized in this study were manufactured with the following dimensions, For instance: 0.15 cm thick, 0.1 cm wide, and 2.5 cm long. Their weight loss at a certain time determined how they were prepared using drying and weighing methods both before and after they were exposed to the inhibitor Tri-ethylamine $N(CH2CH_3)3$, After that it was once again washed and dried. Next, the rate and efficiency of corrosion were computed. Three-pole computerized potentiostat, one of which was connected to the sample and the polarization site.

At 40 to 60 ℃, cells were treated with a pole standard and platinum, respectively, and inhibitors at varying concentrations of 100, 200, 300, and 400 ppm were used to determine the current and potential density [4–15].

2.1. Measurement of polarization

Using a polarizing cell with a platinum electrode and a traditional calomel electrode, the copper samples were cleaned with a 1 M solution of hydrochloric acid containing inhibitor concentration ranging from 100 to 400 ppm. The polarization process was carried out for 30 minutes. During this period, the cathodic potential range was -200 to +200 millivolts, and it was measured using a scanning rate of 0.01 volts per second. Electrical currents and corrosion potentials are calculated during the process, and polarization curves, also known as anodic-cathodic curves, are tracked. The following formula can be used to determine the corrosion rate [11–20]

$$\eta\,\% = \frac{(\mathrm{Icorr})\mathrm{w} - (\mathrm{Icorr})\mathrm{i}}{(\mathrm{Icorr})\mathrm{w}} * 100$$

Thus, with and without inhibitors, the density of corrosion currents is denoted by (Icorr) i and (Icorr) w, respectively.

2.2. Weight loss measurement

Specimens treated with a 1 M HCl solution for 6 hours at varying inhibitor dosages and temperatures showed improvements in weight. Weight loss experiments were conducted. The following formulas were used to calculate the corrosion rate and corrosion inhibition efficacy [11–19].

$$\mathrm{C.R} = \frac{87.6\ \mathrm{w}}{\mathrm{D.A}\ .\ \mathrm{t}}$$

Where time is represented by (t), density by (D), area by (A), and weight loss by (w).

$$\eta\,\% = \frac{[\mathrm{C.R}]\mathrm{w} - [\mathrm{C.R}]\mathrm{i}}{[\mathrm{C.R}]\mathrm{w}} * 100$$

With and without inhibitors, the corresponding corrosion rates are [C.R] i and [C.R] w.

3. Results and discussion

The connection between current and potential density for the cathodic and anodic electrode forms is depicted in Figure 1. The corrosion current dropped as the corrosion inhibitor concentration was raised at 40 °C. This led to increased

success for inhibition. Figures 2, 3, and 4 demonstrate this enhancement in inhibitory effectiveness at 50–60 °C. The process's anodic and cathodic polarizations grew less distinct and more mixed in type as the temperature rose. [12-23]

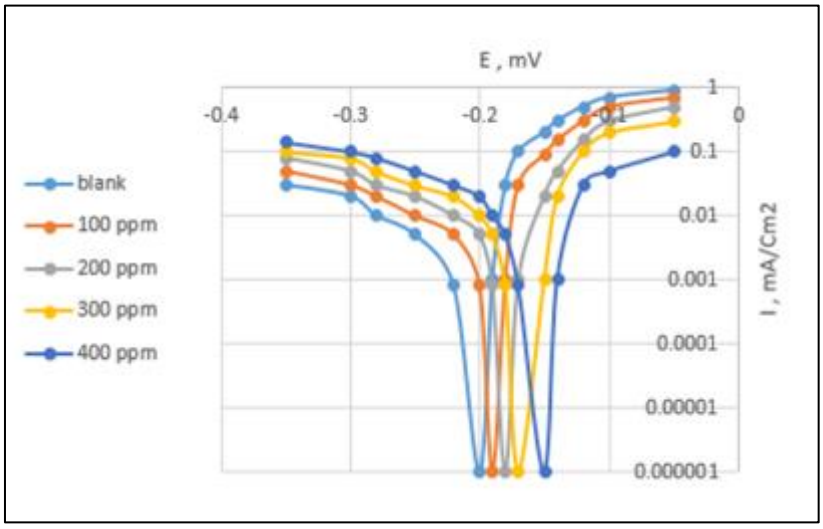

Figure 1 Inhibitor concentration effects on polarization profiles in an acidic medium at 40 °C

Figure 1 shows how the potential and current density for both anodic and cathodic systems are connected. The actions of copper in 1M of hydrochloric acid at 40°C, both with and without concentration of the inhibitor, showed that the density of corrosion currents decreased and the inhibition efficiency improved upon increasing the quantity of the corrosion inhibitor. In contrast, the inhibition effectiveness dropped at 50 and 60°C, as seen in Table 1 and Figures 2 and 3 [13–25].

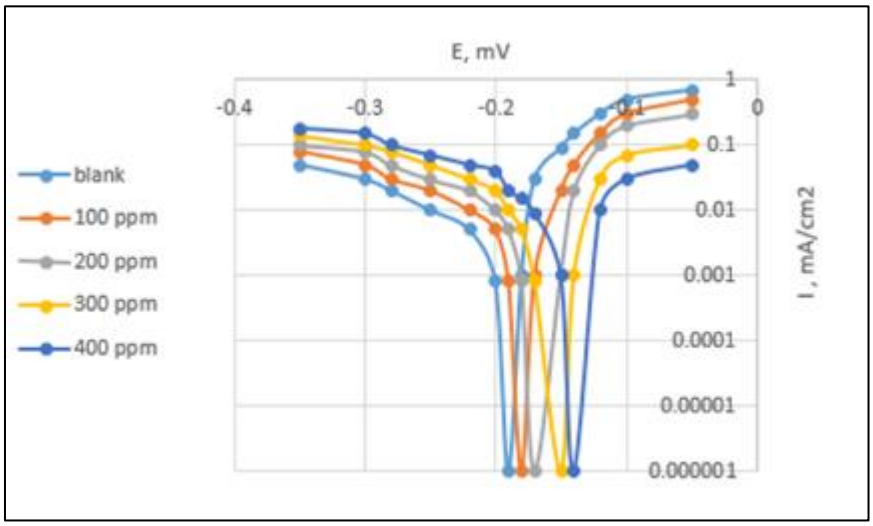

Figure 2 Inhibitor concentration effects on polarization profiles in an acidic medium at 50 °C

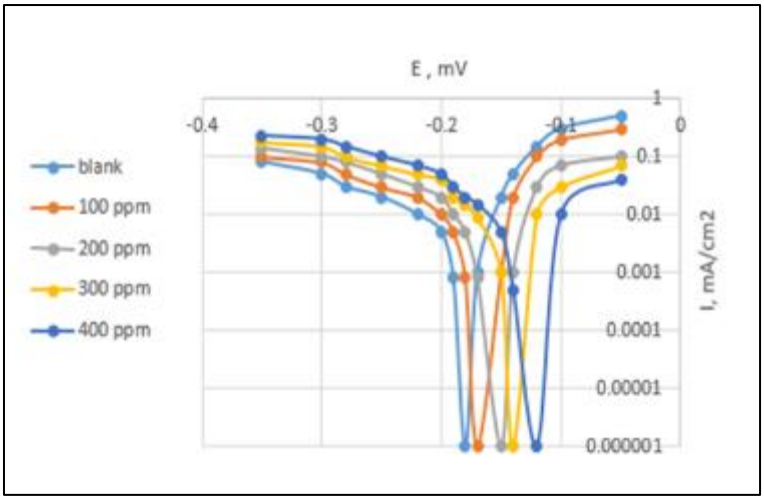

Figure 3 Inhibitor concentration effects on polarization profiles in an acidic medium at 60 °C

Table 1 Use polarization technology to measure the effect of concentration on corrosion potential, corrosion current, and inhibition efficiency at different temperatures

Conc. of Inhibitor (ppm)	E corr , (mV)			Corrosion current density , (mA/cm²)			Efficiency of inhibition (%)		
	40 ℃	**50** ℃	**60** ℃	**40** ℃	**50** ℃	**60** ℃	**40** ℃	**50** ℃	**60** ℃
Blank	180	190	200	0.030	0.035	0.043	0	0	0
100	172	181	191	0.020	0.024	0.031	34.2	32.2	27.0
200	151	172	180	0.016	0.021	0.027	47.0	40.3	35.4
300	140	150	171	0.011	0.018	0.025	64.5	48.4	40.6
400	121	141	151	0.004	0.010	0.017	84.1	72.7	59.0

Scholars strongly confirm the result that efficiency rises with increasing amount of inhibitor at various temperatures, as shown in Figure 4. [21- 30]

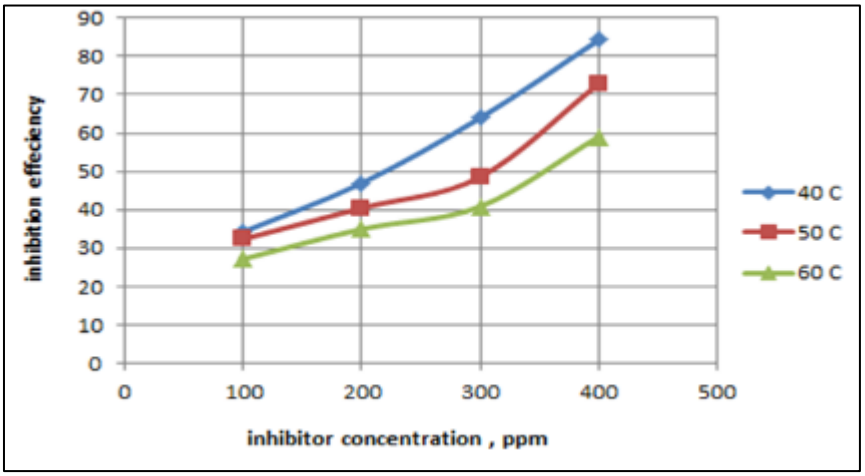

Figure 4 Efficiency and concentration of the influencer at different temperatures

The temperature-dependent weight loss with and without varying inhibitor dosages is displayed against time in Figures 5, 6, and 7. It is evident that weight loss occurs more gradually at lower temperatures and higher inhibitor concentration. Table 2 illustrates how inhibitor concentration, corrosion rates, and inhibition efficacy relate to one another at different

temperatures. Figure 8 illustrates how the rate of corrosion reduced at 40 °C as the inhibitor concentration increased, hence improving the inhibition efficiency. However, efficiency drops between 50 and 60 °C [14-25].

Table 2 Effects of inhibitor concentration using the weight loss method on corrosion rate and inhibition efficacy at different temperatures

conc. of Inhibitor (ppm)	Corrosion rate (mmpy)			Inhibition efficiency (%)		
	40 °C	50 °C	60 °C	40 °C	50 °C	60 °C
Blank	1.31	1.36	1.52	0	0	0
100	0.27	0.55	0.66	78.0	58.5	55.0
200	0.12	0.44	0.54	89.2	66.3	62.6
300	0.10	0.23	0.41	90.6	81.0	71.1
400	0.07	0.12	0.20	93.1	89.5	86.1

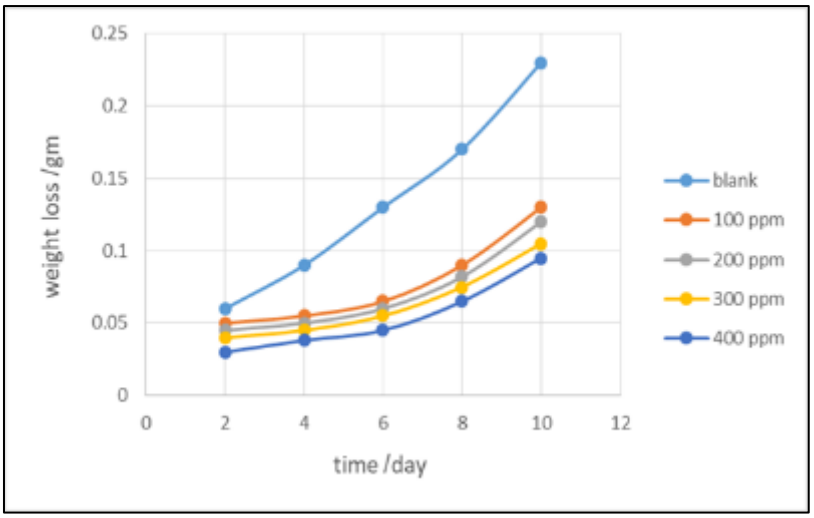

Figure 5 Effects of different inhibitor concentrations and duration at 40 °C on weight loss

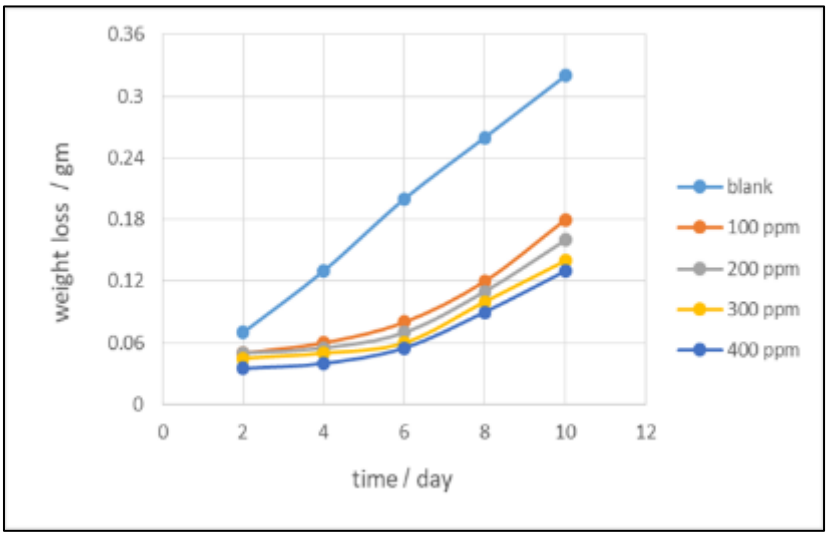

Figure 6 Effects of different inhibitor concentrations and duration at 50 °C on weight loss

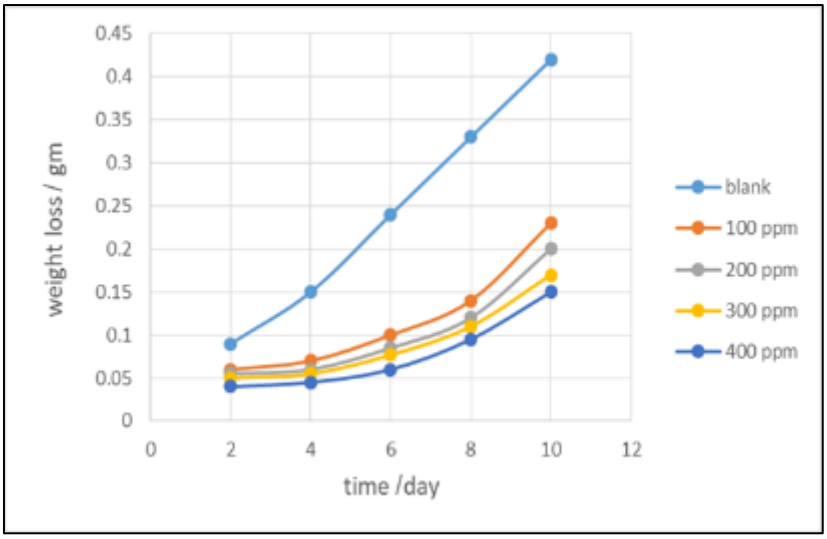

Figure 7 Effects of different inhibitor concentrations and duration at 60 °C on weight loss

Figure 8 illustrates the relationship between inhibitor presence and corrosion rates. Research indicates that as inhibitor concentrations increased, the rate of corrosion decreased [9–16].

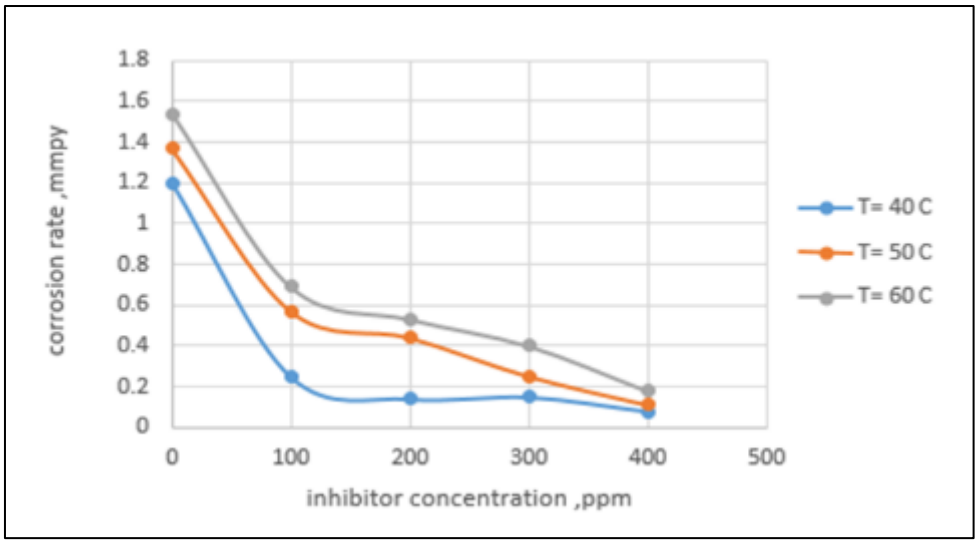

Figure 8 Corrosion rate and inhibitor concentration at varying temperatures

3.1. Temperature Effect

As temperatures rise from 40 to 60 oC, corrosion prevention techniques become less effective. Using Figs. 9 and 10, the activation energy was determined [22–35].

$$(C.R) = A \exp \frac{-Ea}{RT}$$

Temperature is denoted by (T), activation energy by (Ea), gas constant by (R), and frequency factor by (A).

The calculation of copper corrosion activation energy with and without an inhibitor is shown in Figure 9. Table 3 displays the results. According to these findings, corrosion was reduced because the activation energy's efficacy rose as the inhibitor concentration rose, in contrast to non-inhibitors, But when the temperature rises, the activation energy falls and corrosion accelerates. Equation 5 (Figure 10) was used to get the constants H, S, and G as well as the thermodynamic energy of activation [11–25].

$$(C.R) = \left(\frac{RT}{Nh}\right) \exp\frac{\Delta S}{R} \exp\frac{-\Delta H}{RT}$$

Avogadro number, temperature, Planks constant, and gas constant are represented by the constants N, T, h, and R, respectively.

The energy of entropy and enthalpy were calculated using the following formula and Fig. 10.

$$\Delta H = (Ea) - (RT)$$

$$\Delta G = (\Delta H) - (T\Delta S)$$

ΔG stands for free adsorptive energy.[13-20]

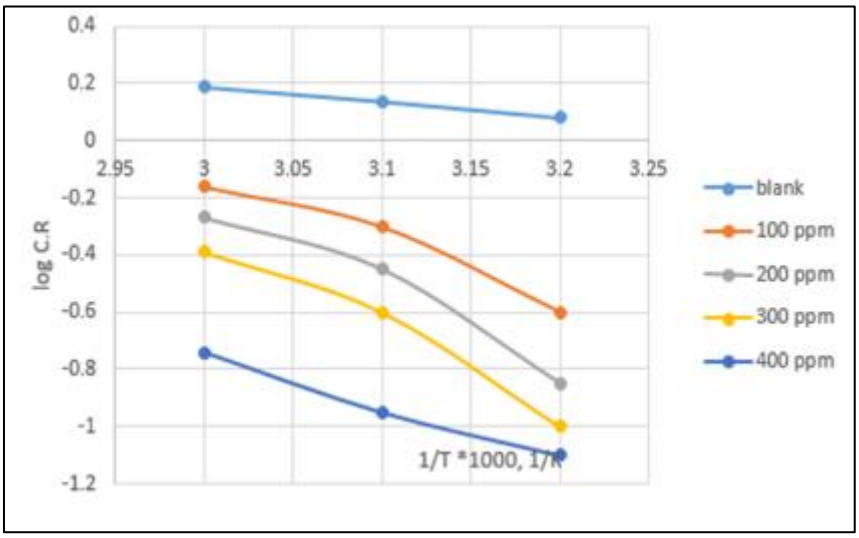

Figure 9 A plot of inverse temperatures (1/T) vs log (C.R.) at different inhibitor concentrations

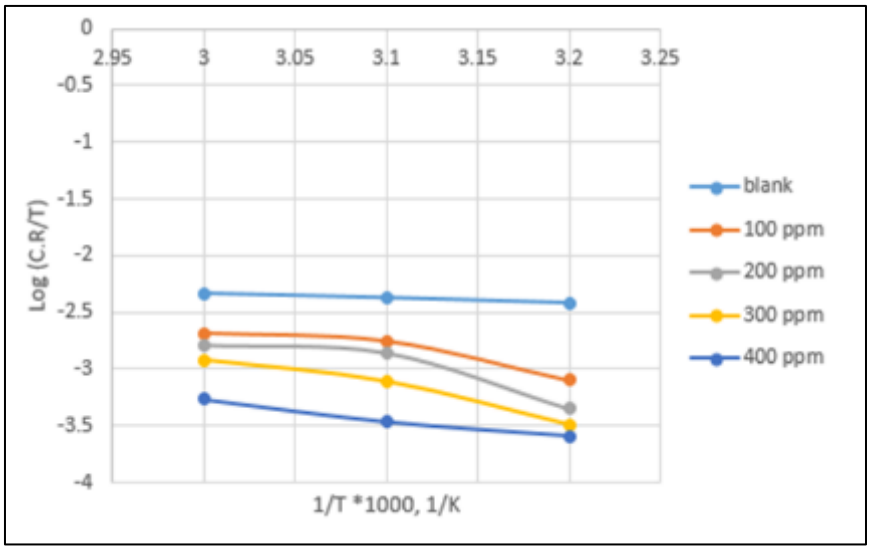

Figure 10 A plot of inverse temperatures (1/T) vs log (C.R./T) at different inhibitor concentrations

Table 3 Copper's thermodynamic properties in an acidic media with different inhibitor concentration

Conc. of Inhibitor (ppm)	Ea (kJ/mole)	ΔH (kJ/mole)	ΔS (kJ/mole.K)	ΔG (kJ/mole)
blank	4.511	3.421	$8.8 * 10^{-10}$	3.421
100	3.723	16.333	$11.4 *10^{-10}$	16.333
200	4.726	21.848	$12.2 * 10^{-10}$	21.848
300	5.177	24.862	$12.9 *10^{-10}$	24.862
400	5.286	25.789	$13.2 * 10^{-10}$	25.789

The development of a film layer on the copper surface due to the inhibitor's high capacity characteristic shields the metal from the environment and raises the inhibitor concentration, which raises the activation energy, free energy of adsorption and enthalpy (Table 3).An endothermic process is indicated by a positive result for ΔH. Because of the inhibitor's adsorption on the metal's surface, a collection of nitrogen, amine, and ethyl atoms forms a film layer on the metal's surface, which in turn acts as an inhibitor and successfully prevents rusting, as shown in Fig. 11.[31–39]

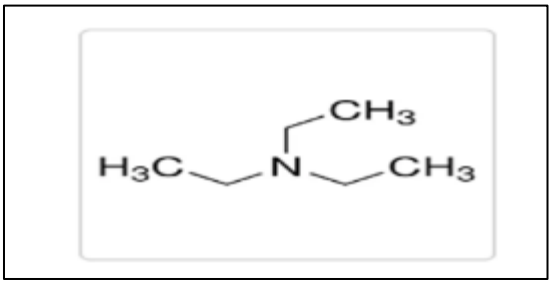

Figure 11 Tri-ethylamine's chemical composition is $N(CH_2CH_3)_3$

3.2. Quantum chemical calculation

According to the results of the quantum chemical calculations using DFT and the B3lYB/6-311+G(d,p) basis set for triethylamine (see Table 4), the molecule has a significant propensity to donate electrons to the copper surface, as shown by the EHOMO=-5.93 eV value. However, the donor-acceptor interaction mechanism is confirmed by the ELUMO = -0.16 eV, which indicates its capacity to accept electrons from the metal.[40-41]

A compromise between stability and reactivity is suggested by the predicted energy gap ΔE = 6.09eV, while the asymmetric charge distribution that promotes efficient adsorption is demonstrated by the dipole moment (1.55 Debye). Because it mirrors the polarity of the molecule, it improves electrostatic interactions with the metal surface's charge sites.[41-42]

The molecule's strong hardness (η = 3.04842 eV) and low softness (S = 0.328038 eV) were revealed by global reactivity descriptors, suggesting that it may readily adjust to the metal surface environment. In accordance with chemisorption behavior, the electron transfer value (ΔN = 0.728513382) validates the molecule's capacity to provide electrons to the metal surface.[42-43]

Together, these features account for triethylamine's strong adsorption propensity and the development of the persistent protective layer, which is consistent with the high experimentally reported inhibitory effectiveness.[42]

The nitrogen atom is the primary electron donor site, as seen by the HOMO density being mostly centered over it in Fig. 12. On the other hand, LUMO orbitals are dispersed over various areas, suggesting possible locations for electron acceptance. The larger charge concentration surrounding nitrogen is also confirmed by the electron density map in Figure 13. The most likely adsorption center is nitrogen, as indicated by the concentration of negative areas (in red) close to it in the electrostatic potential map in Figure 14.[43]

The Fukui function values in Table 5, which show that the nitrogen atom has the greatest value (f+=0.143), showing that it is the main site for nucleophilic attack, with a partial contribution from certain carbon atoms like C7, further corroborate this view. Atoms of hydrogen, on the other hand, showed low levels and insignificant functions. Thus, the nitrogen atom in tri ethylamine predominantly interacts with the copper surface, while the ethyl groups give further stability, resulting in the creation of an efficient protective layer. [43]

Table 4 Quantum chemical parameters for inhibitor tri ethylamine by DFT Method

S	W	X	η	EA	IE	ΔE
0.328038	1.36196	2.881614	3.04842	-0.16680	5.93003	6.09684

Dipole moment	ELUMO (eV)	EHOMO (eV)
1.55	0.166809	-5.93003

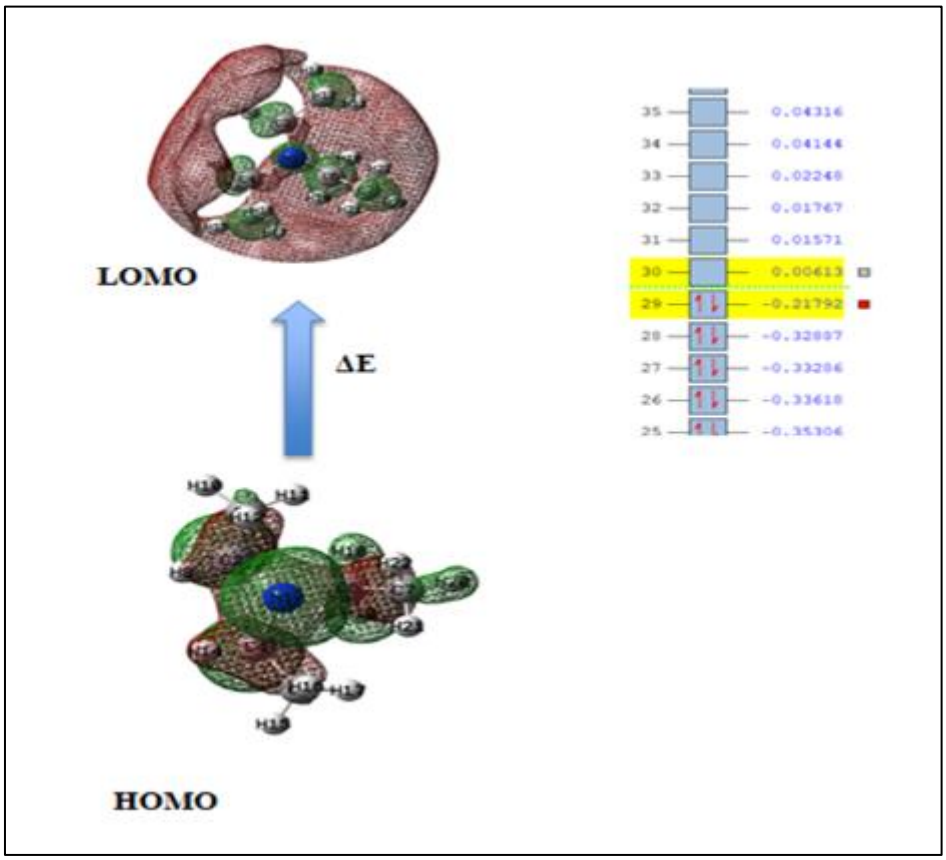

Figure 12 The frontier molecular orbitals of triethylamine

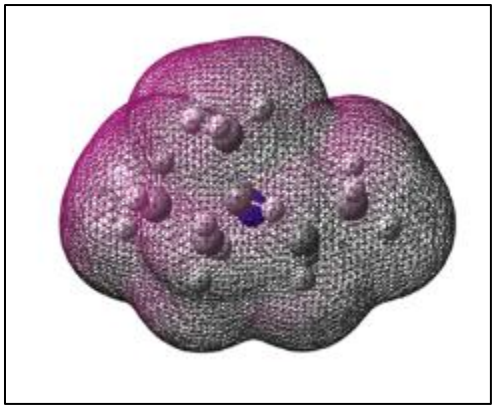

Figure 13 Electron density from total SCF density (isoval=0.0004) of triehylamine

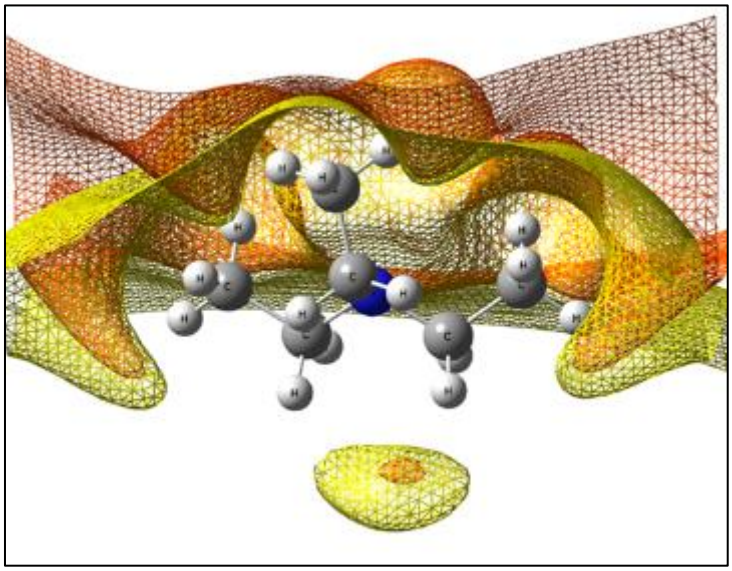

Figure 14 Electrostatic potential from total SCF density of triethylamine

Table 5 Values Fukui function of the trimethylamine

No.	atom	n	n+1	n_1	f+1	f-1	f0
1	N	0.080118	0.223577	0.08319	0.143459	-0.00307	0.070194
2	C	-0.13697	-0.22706	-0.06592	-0.09009	-0.07104	-0.08057
3	C	-0.49653	-0.45664	-0.96642	0.039883	0.469891	0.254887
4	C	-0.15808	-0.21498	-0.91312	-0.0569	0.755038	0.349067
5	C	-0.51993	-0.49056	-0.51839	0.029368	-0.00154	0.013914
6	C	-0.31556	-0.37588	0.607231	-0.06032	-0.92279	-0.49156
7	C	-0.42944	-0.39039	-1.75294	0.039046	1.323502	0.681274
8	H	0.125319	0.19516	0.158958	0.069841	-0.03364	0.018101
9	H	0.124266	0.246459	0.137716	0.122193	-0.01345	0.054372
10	H	0.135269	0.195945	0.211172	0.060676	-0.0759	-0.00761
11	H	0.125909	0.158508	0.163315	0.032599	-0.03741	-0.0024
12	H	0.147159	0.182638	0.169266	0.035479	-0.02211	0.006686

13	H	0.123016	0.246496	0.154678	0.12348	-0.03166	0.045909
14	H	0.12608	0.197631	0.167458	0.071551	-0.04138	0.015087
15	H	0.137361	0.195619	0.213789	0.058258	-0.07643	-0.00909
16	H	0.14723	0.183922	0.158886	0.036692	-0.01166	0.012518
17	H	0.133685	0.164061	0.161848	0.030376	-0.02816	0.001107
18	H	0.130393	0.205244	0.154196	0.074851	-0.0238	0.025524
19	H	0.127015	0.219113	0.169804	0.092098	-0.04279	0.024655
20	H	0.123407	0.193012	0.190979	0.069605	-0.06757	0.001016
21	H	0.131895	0.170336	0.151047	0.038441	-0.01915	0.009645
22	H	0.138376	0.177791	0.163249	0.039415	-0.02487	0.007271

4. Conclusions

This study employed weight loss and polarization procedures with different inhibitor concentrations (100-400 ppm) in order to examine the biological stuff Copper metal exposed to tri-ethylamine $N(CH_2CH_3)_3$ in HCl, an acidic media. Inhibition efficiency and corrosion both rise with temperature, although it has been noted that inhibition efficiency falls around 50 and 60 °C. Additionally, as the inhibitor concentration rises at the optimal temperature of 40 °C, the energy entropy falls and thermodynamic parameters of energy of activation, enthalpy, as well as the free energies of adsorption all increase in magnitude. This shows that a set of atoms including ethyl, amines and nitrogen are present. These atoms effectively coat copper metal with an inhibitor by adsorbing it to the metal's surface, which lowers corrosion. I have been computed the thermodynamic functions of adsorption and dissolution by (DFT) .According to quantum chemical analysis, tri-ethylamine has a great ability to adsorb on the iron surface through dual donor-acceptor interactions and electron transfer, creating a stable protective layer in the process. Its great inhibitory effectiveness is confirmed by the good match between these theoretical conclusions and the experimental work. Since theoretical corrosion inhibition depends on a number of factors, including electronegativity, total hardness, softness, ionization energy, dipole moment, energy gap, and the percentage of transferred electrons, as determined by a program, the theoretical state by DFT of the inhibitor was also examined. The energy of the molecular orbitals labeled "ELUMO" with the lowest occupancy and "EHOMO" with the maximum occupancy. Furthermore, the inhibitor's total electron density (TED) and total electrostatic potential (ESP) were computed.

Compliance with ethical standards

Disclosure of conflict of interest

No conflict of interest to be disclosed.

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