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Electrochemical and theoretical evaluations of 3-(4-chlorophenyl)-7-methyl-5H-[1, 2, 4] triazolo [3,4-b][1,3,4]thiadiazin-6(7H)-one as corrosion inhibitor for copper in nitric acid environment

ABSTRACT

3-(4-chlorophenyl)-7-methyl-5H-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazin-6(7H)-one (CTT) was synthesized and evaluated as corrosion inhibitor for copper in one molar HNO_3. The adsorption properties for the synthesized CTT were determined by experimental and theoretical methods in acid environment. The chemical method such as mass loss method (ML), DC potentiodynamic polarization (PDP) and AC impedance (EIS) techniques were utilized to determine the inhibitive behavior of CTT. Outcome data obtained from these methods displayed that with increasing the concentration of CTT its inhibition efficiencies (%IE) increases and reached 91.5% at $24x10^{-6}$ M , 25^{o}C using EIS technique. The presence of CTT reduces the capacity of the double layer (C_{dl}) and improves the charge transfer resistance (R_{ct}) in a solution of one molar nitric acid. CTT is a mixed-type inhibitor from the data obtained from the polarization curves. The attained data indicated that CTT was physically adsorbed onto the Cu surface in accordance for the Langmuir adsorption. The surface protection examination was carried out using scanning electron microscopy (SEM), Energy Dispersive X-ray (EDX) and atomic force microscope (AFM). Also, The quantum chemical parameters of CTT were computed and discussed. The results of several methods are in agreement with each other.

Keywords: *Corrosion inhibition, Copper, Nitric acid, 3-(4-chlorophenyl)-7-methyl-5H-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazin-6(7H)-one (CTT), Langmuir isotherm.*

1. INTRODUCTION

The fifth-most common metal on the planet, copper, is very beneficial both in its pure form and as an alloy [1]. Owing to their excellent properties such as good thermal and electrical conductivity, mechanical workability, low cost and high corrosion resistance, copper and its alloys were extensively used in various industries such as conductors, heat exchangers, and the electronic industry [2,3]. Copper has a relatively noble potential, despite this, it corrodes far more quickly in chloride and seawater conditions [4,5]. It is widely known that the amount of chloride ions in the environment affects how easily copper dissolves anodically. The formed CuCl, which is not sufficiently protective, and dissolves when it reacts with excess chloride [6–8]. In spite of its high corrosion resistance feature in atmospheric conditions, by forming an oxide protective layer on its surface, copper and its alloys may easily undergo metal dissolution in the presence of an aggressive media like chloride having environment [6]. The primary technique for protecting metals and alloys is the use of inhibitors. Right now, green inhibitors show promise since they provide effective inhibition while having a minimal negative impact on the environment. Several investigators have reported [5-8] that organic compounds can act as possible corrosion inhibitors for numerous metals and alloys in various corrosive media. The inhibitors can be introduced to the medium or coated on the metal surface to slow down the corrosion process to avoid corrosion in the metal used in such corrosive media; both methods work well [9–13]. Heterocyclic compounds having N, O, S, P, or π-bonds make up many effective corrosion inhibitors by generating a physical barrier to reduce the transport of corrosive species to the metal surface [14-16].

Organic compounds that include conjugated double bonds and hetero atoms especially those, that can form polymeric complexes with copper by coordinating with CuO , Cu^{+} , or Cu^{2+} through their

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lone pair electrons [17]. These adhere to the copper surface to produce a protective coating that prevents corrosion by serving as a wall against harmful ions like chloride [18]. 1,2,3-triazole (BTA) compound has been reported as a well-known effective corrosion inhibitors of copper in many environments [19]. The inhibition effect of 3-amino-1,2,4-triazole (ATA) on copper corrosion in 2M HNO3 solution was studied by Zarrouk et al [20]. The inhibition efficiency reached 82.2% at 10-2M. Yaroslav et al [21] studied the protection of steels with a 3-substituted 1,2,4-triazole (3ST) in 2 M H_2SO_4 solution. The inhibition protection reached 97.8% at $4.2x10^{-7}$M. Additionally, the ability of some 1,2,4-triazole derivatives to suppress copper corrosion in a neutral aqueous environment has been investigated. These derivatives include 3-vanilidene amino 1,2,4-triazole phosphonate, 3-anisalidene amino 1,2,4-triazole phosphonate [22], and 3-amino-5-mercapto-1,2,4-triazole [23, 24]. 1,2,4-triazole derivatives, including 1,2,4-triazole, 3-amino-1,2,4-triazole, and 2-4-diamino-1,2,4-triazole in 1 M H_2SO_4 [25]; 3,5-bis(2-thienyl)-4-amino-1,2,4-triazole in 1 M HCl and 0.5 M H_2SO_4 [26,27]; 3,5-diamino-1,2,4-triazole in 2 M HNO_3 [28]; 5-amino-1,2,4 triazole, 5-amino-3-mercapto 1,2,4 triazole, 5-amino-3-methyl thio-1,2,4-triazole, 1-amino-3-methyl thio-1,2,4-triazole [29–33]; 4-amino-4H-1,2,4-triazole-3-thiol, 4-amino-5-methyl-4H-1,2,4-triazole-3-thiol [34, 35] in 0.5 M HCl have been studied in relation to copper corrosion. Chooto et al [36] reported the effect of thioureas and N, O, S-Ligating Ring Compounds as corrosion inhibitors for Cu in Cl- ions. Wang et al. [37] investigate the inhibition mechanism of combined thiourea and hexamethylenetetramine as a corrosion inhibitor on the surface of copper in 0.5 M HCl solution.

With the improvement of hardware and software, recently, quantum chemical methods like functional density theory (DFT)" has been used as fast and powerful tool to predict and understand corrosion inhibition performances of inhibitors [38]. Although there is an extensive literature on the corrosion properties of benzotriazole on steel and copper [39, 40], a protective coating is created by utilizing a tiny inhibitor dose to delay the corrosion reaction [41-43].

The organ-sulphur and heterocyclic compounds have the basic requirements to be considered as eco-friendly compounds. These compounds are adsorbed on the metal surface by blocking the active sites during the inhibition process. This leads to the need of development of new environmentally-friendly inhibitors for copper metal. A newly synthesized 3-(4-chlorophenyl)-7-methyl-5H-[1,2,4]triazolo[3,4-b][1,3,4] thiadiazin-6(7H)-one, was investigated for its ability to suppress the corrosion of copper in one molar HNO_3. The evaluation of the corrosion behavior of copper in aggressive media in the absence and presence of newly synthesized CTT using (PDP), (EIS), and ML methods were discussed".

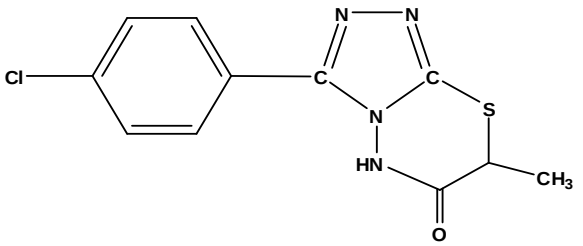
2. EXPERIMENTAL

2.1. Solutions and materials

The chemical composition of the Cu used in this paper is as follows: "(wt. %) 0.0023 Zn, 0.0023 Pb, 0.0023 P, 0.0019 Co, 0.0018 Al, 0.0015 Si, 0.004 Ni and the remainder is copper. Copper samples of measured (2 x 2 x 0.2) cm in triplicate, were mechanically polished. Samples were abraded with emery paper of grades levels from 250 and until1200, then cleaned by distilled water, brushed using acetone and at end dried by filter papers. The strong solutions (5 M HNO_3) were prepared by diluting AR grade (70 %) HNO_3 with bi-distilled water and checking its concentration with standardized solution of NaOH, after that prepare one molar HNO_3 by diluting with bi-distilled water. 100 mL stock solutions (10^{-3} M) were prepared by dissolving an accurately weighed quantity of CTT in an appropriate volume of dimethyl formamide (DMF) and absolute ethanol, then diluting with bi-distilled water to the needed concentrations ($4x10^{-6}$ - $24 x10^{-6}$ M).

2.2. Synthesis of 3-(4-chlorophenyl)-7-methyl-5H-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazin-6(7H)-one [44].

The chemical structure and molecular formula of the 3-(4-chlorophenyl)-7-methyl-5H-[1,2,4] triazolo[3,4-b][1,3,4]thiadiazin-6(7H)-one (CTT) compound was shown in Figure 1. The studies were done at different concentrations ($4×10^{-6}$, $8×10^{-6}$, $12×10^{-6}$, $16×10^{-6}$, $20×10^{-6}$ and $24×10^{-6}$ M) on the presence and absence of the investigated CTT. In thermostatic conditions, all experiments were conducted.



3-(4-chlorophenyl)-7-methyl-5*H*-[1,2,4] triazolo[3,4-*b*][1,3,4]thiadiazin-6(7*H*)-one

Figure 1 Optimized structure of CTT, ($C_{11}H_9ClN_4OS$), M. Wt. = 280.02 g/mol

Slika 1 Optimizovana struktura CTT, (C11H9ClN4OS), M. Vt. = 280.02 g/mol

2.3. ML method

Specimens with emery paper were abraded, and bi-distilled water was used to clean it, then using filter papers for drying and weighed. In the existence and absence of various amounts of CTT, the samples were immersed into 100 mL of the acid medium. The CTT doses were between $1x10^{-6}$-$24x10^{-6}$ M. The time of immersion is 30 to 180 minutes. After a certain time, the samples were weighed again. The corrosion rate (k_{corr}) of the metal specimens was determined using the following relationship" [45].

$$CR = \frac{\Delta W}{AT} \quad (1)$$

Where,ΔW (mg) as the reduction in mass, A (cm^2) as the area of the surface of Cu and t (min) as the time. The protection efficacy (% IE) in addition to specimen surface coverage (Ɵ) by CTT can be obtained as follows":

$$\% IE = \theta\, x100 = \left(\frac{\Delta W2 - \Delta W1}{\Delta W2}\right) \times 100 \quad (2)$$

with ΔW_1 as ML in the presence of the CTT and ΔW_2 as ML in the absence of the CTT.

2.4. Electrochemical techniques

For the electrochemical experiments, a standard electrochemical cell made-up from Pyrex glass was used. Cu (1 cm^2 exposed area) as working electrode, a saturated calomel electrode (SCE) and a platinum sheet as reference, and counter electrodes, respectively were used for electrochemical studies. Potentiodynamic current-potential graphs were documented by instantaneously shifting the electrode potential from -700 mV to +700 mV at a scanning rate of 0.2 mVs^{-1} (version 3.20). Corrosion current density (i_{corr}) and corrosion potential (E_{corr}) were assessed from the relationship of the correlation anodic and cathodic sections of Tafel plots in the absence and existence of various inhibitor doses. Before initiating the readings, the electrode potential was stabilized for 30 minutes. Gamry reference PCI300/4 Potentiostat/Galvanostat/Zra analyzer, DC105 corrosion,EIS300, Echem Analyst 5.5 software's were used for result plotting, graphing, data fitting, and calculating. The results of every experiment were checked at least three times. The degree of surface coverage (θ), and % IE were calculated using Eq. 3:

$$\% IE = \theta\, x100 = \left(\frac{i_{corr(free)} - i'_{corr(inh)}}{i_{corr(free)}}\right) \times 100 \quad (3)$$

Where, "$i_{corr(inh)}$ and $i_{corr(free)}$ to indicate the currents densities in absence and existence of CTT, individually".

For impedance calculation, open circuit potential (OCP) has been applied and current signals range from 100 kHz to 10 Hz. The θ and % IE were calculated as follows:

$$\% IE_{EIS} = \left(\frac{R^*_{ct(inh)} - R_{ct(free)}}{R_{ct(inh)}}\right) \times 100 \quad (4)$$

with $R_{ct(free)}$ as the resistance in blank solution and $R_{ct(inh)}$ as the resistance of charge transfer in inhibited solution.

2.5. Surface morphology by SEM and EDX techniques

The specimens were placed in one molar HNO_3 solution for 24 hours, both with and without higher doses of CTT ($24x10^{-6}$ M), after preparing their surfaces as before, then examined by Scanning electron microscope (SEM, JSM-T20, Japan) for the test. Furthermore, the copper samples were examined using energy dispersive X-ray (EDX) spectroscopy system provided (Zeiss Evo 10 instrument model)". The beam accelerating voltage was 25 kV.

2.6. Computational chemical approaches

To study the relationship among the molecular structure and the reactivity of CTT, The density functional theory (DFT) in Materials Studio version 7.0 was utilized for theoretical computations.

3. RESULT AND DISCUSSION

3.1. ML tests

The ML of Cu in the acid environment at "25°C without and in presence of altered doses of CTT after several immersion periods from 30 to 180 min is given in Figure 2.

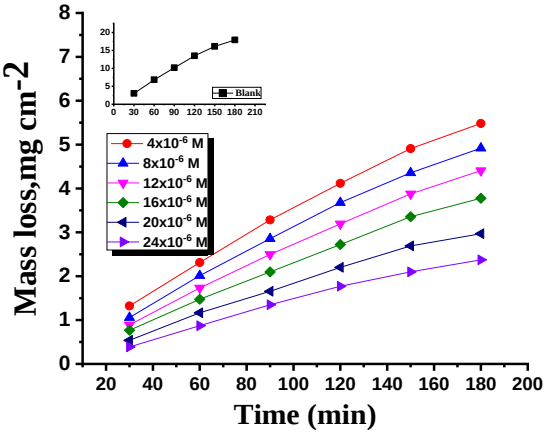


Figure 2. ML-Time diagrams at 25°C for the dissolution process of the Cu in one molar nitric acid in the absence and at various doses of CTT

Slika 2. ML-vremenski dijagrami na 25°C za proces rastvaranja Cu u jednoj molarnoj azotnoj kiselini u odsustvu i pri različitim dozama CTT-a

The ML was decreased as the CTT concentration increases. This due to the layer formed on the Cu surface from the adsorbed molecules of CTT which protects Cu surface from the corrosive environment and blocks the metal corrosive sites [46]. According to the data, the %IE value climbed to 85.9% as the CTT concentration was raised from the range of $4x10^{-6}$ to $24x10^{-6}$ M. The Cu outer surface area was sufficiently protected from corrosion when the k_{corr} declined and the CTT concentration grew. When the CTT level was raised from $4x10^{-6}$ to $24x10^{-6}$ M, the k_{corr} reduced from 0.0498 to 0.0237 mg cm^{-2} min^{-1}. It was observed that the % IE dropped after $24x10^{-6}$ M. This decrease is probably caused by the CTT molecules saturating every active area on the Cu surface [47].

3.1.1. Impact of temperature

Corrosion rate (k_{corr}) of Cu, θ and % IE at various temperatures in the acid environment in the absence and at various doses of CTT were presented in Table 1. The (k_{corr}) decreased while θ and % IE improved with increased doses of CTT. % IE decreased by raising the temperature due to desorption process [48] illustrating that the CTT is physically adsorbed on the Cu surface. The impact of temperature on the desorption process on the metal surface was covered in earlier research [49].

Table 1. CR, θ and percent IE at various temperatures for corrosion of the Cu in the used acid medium in the absence and at various doses of CTT compound

Tabela 1. CR, θ i procenat IE na različitim temperaturama za koroziju Cu u korišćenom kiselom medijumu u odsustvu i pri različitim dozama CTT jedinjenja

Temp,°C	(30°C)			(35°C)			(40°C)			(45°C)		
Conc., M	k_{corr}	θ	IE %	k_{corr}	θ	IE %	k_{corr}	θ	IE %	k_{corr}	θ	IE %
0.0	0.1683	---	---	0.2198	---	---	0.2848	---	---	0.3285	----	---
$4x10^{-6}$	0.0498	0.704	70.4	0.0736	0.665	66.5	0.1213	0.574	57.4	0.1679	0.489	48.9
$8x10^{-6}$	0.0449	0.733	73.3	0.0675	0.693	69.3	0.1170	0.589	58.9	0.1544	0.53	53.0
$12x10^{-6}$	0.0402	0.761	76.1	0.0589	0.732	73.2	0.1054	0.63	63.0	0.1386	0.578	57.8
$16x10^{-6}$	0.0340	0.798	79.8	0.0543	0.753	75.3	0.0883	0.69	69.0	0.1225	0.69	62.7
$20x10^{-6}$	0.0279	0.834	83.4	0.0459	0.791	79.1	0.0783	0.725	72.5	0.1061	0.725	67.7
$24x10^{-6}$	0.0237	0.859	85.9	0.0385	0.825	82.5	0.0720	0.747	74.7	0.0910	0.747	72.3

The following Arrhenius equation was used to estimate activation energy (E_a^*):

$$log\ k_{corr} = \left(\frac{-E_a^*}{2.303RT}\right) + log\ A \qquad (5)$$

where A as (pre-exponential Arrhenius multiplier), R (8.314 Joule/ K. mol.) as universal gas constant. Figure 3 indicates Arrhenius plots without and with various dose of CTT for Cu corrosion in the used acid medium. Results of E_a^* were determined from the lines slope. Enthalpy (ΔH^*) and entropy (ΔS^*) of the activation process can be specified by application the transition state equation as follows:

$$log\ k_{corr} = log\left(\frac{R}{Nh}\right) + \frac{\Delta S^*}{2.303R} + \frac{\Delta H^*}{2.303RT} \qquad (6)$$

With h ($6.625x10^{-27}$) as Planck's constant and N ($6.025x10^{23}$g/mol.) as Avogadro's number. Figure 4 displays log (k_{corr}/T) against (1/T) diagrams without and with various doses of CTT for Cu corrosion in the used acid medium. Slopes and intercepts of the straight lines give values ΔH^* and ΔS^*, respectively. The determined activation parameters were depicted in Table 2. Values of E_a^* in Table 2 for solutions with CTT were high than that in its absence. The rise in the E_a^* shows that CTT molecules are physically adsorbed on the Cu surface. The exothermic activation process was demonstrated by the negative sing of ΔH^* values. This proves that the Cu dissolution in the acid medium is a unimolecular reaction. The negative signals of ΔS^* showed that the disorder develops along the direction from the reactant to the activated complex [50].

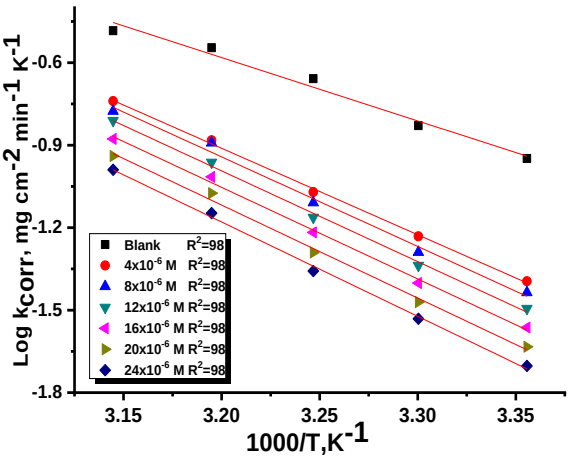


Figure 3. log k_{corr} against 1/T diagrams without and at various doses of CTT for Cu corrosion in the used acid medium

Slika 3. log k_{corr} naspram 1/T dijagrama bez i pri različitim dozama CTT za koroziju Cu u korišćenom kiselom medijumu.

Table 2. Thermodynamic activation parameters without and at various doses of CTT for Cu corrosion in the used acid medium

Tabela 2. Parametri termodinamičke aktivacije bez i pri različitim dozama CTT za koroziju Cu u korišćenom kiselom mediju

Conc. M	Activation parameters		
	E^*_a, kJ mol^{-1}	$-\Delta H^*$ kJ mol^{-1}	$-\Delta S^*$ J mol^{-1} K^{-1}
Blank	45.2	41.6	122.1
4x10^{-6}	61.5	58.9	77.0
8x10^{-6}	63.6	61.0	70.8
12x10^{-6}	64.4	62.0	69.1
16x10^{-6}	65.1	62.5	68.3
20x10^{-6}	66.0	63.4	66.4
24x10^{-6}	66.9	64.3	64.6

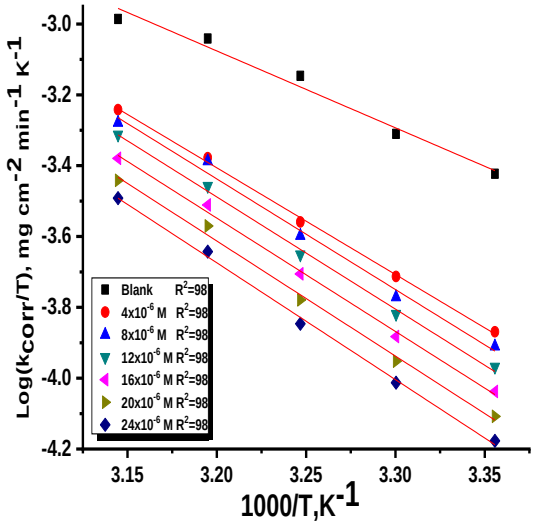


Figure 4. log (k_{corr}/T) against 1/T diagrams without and at various doses of CTT for Cu corrosion in the used acid medium

Slika 4. log (k_{corr}/T) naspram 1/T dijagrama bez i pri različitim dozama CTT-a za koroziju Cu u korišćenom kiselom mediju

3.1.2. Adsorption studies

The Langmuir model's isotherm for adsorption perfectly match the data (Figure 5). The following Eq. 7 can be used to show the Langmuir adsorption isotherm.

$$\frac{C_{inh}}{\theta} = \frac{1}{K_{ads}} + C_{inh} \qquad (7)$$

with C as the dose of CTT inhibitor and K_{ads} as the adsorption constant. Eq. 8 can be applied to give the free energy of adsorption (ΔG^o_{ads}):

$$K_{ads} = \frac{1}{55.5} exp\left(\frac{-\Delta G^o_{ads}}{R\,T}\right) \qquad (8)$$

where the water dose at the Cu/solution interface is 55.5 (mol./L). By using the Vant Hoff equation, the enthalpy of adsorption (H^o_{ads}) was determined as follows:

$$log\ K_{ads} = \frac{-\Delta H^o_{ads}}{2.303RT} + constant \qquad (9)$$

Figure 6 indicates draw among 1/T and log K_{ads}. From the line slope, ΔH^o_{ads} value can be determined. ΔS^o_{ads} can be gotten by applying the next balance:

$$\Delta S^o_{ads} = \frac{\Delta H^o_{ads} - \Delta G^o_{ads}}{T} \qquad (10)$$

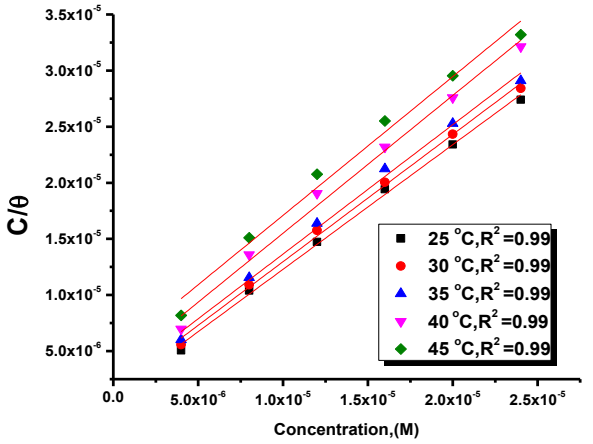


Figure 5. Langmuir adsorption plots of CTT on Cu surface at different temperatures

Slika 5. Langmuir-ovi adsorpcioni grafikoni CTT na površini Cu pri različitim temperaturama

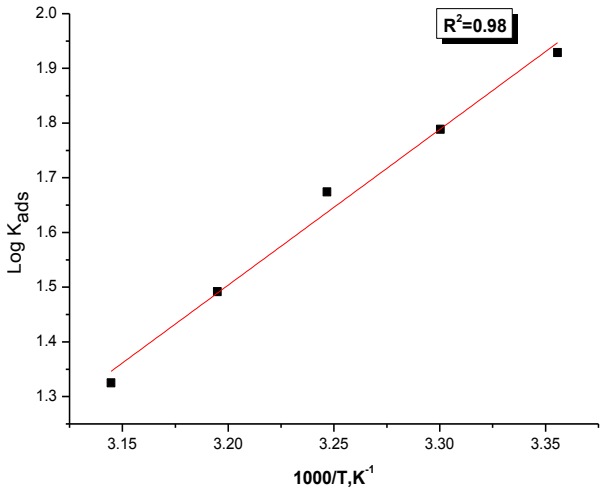


Figure 6. log K_{ads} against 1/T for adsorption of CTT on Cu surface

Slika 6. log K_{ads} prema 1/T za adsorpciju CTT na površini Cu

The negative value of ΔG^o_{ads} indicates the spontaneity and the stability of the CTT adsorption layer occurred on the Cu surface (Table 3). The

obtained values of ΔG^{o}_{ads}, are around 20 kJ mol^{-1} indicates the physisorption of the CTT molecules on the Cu surface. Indicating that the adsorption procedure is exothermic this obtained from the negative values of ΔH^{o}_{ads}".

Table 3. Adsorption parameters for CTT at different temperatures

Tabela 3. Parametri adsorpcije za CTT na različitim temperaturama

Temp. °C	K_{ads} M^{-1}	$-\Delta G^{\circ}_{ads}$ kJ mol^{-1}	$-\Delta H^{\circ}_{ads}$ kJ mol^{-1}	$-\Delta S^{\circ}_{ads}$ J mol^{-1} K^{-1}
25	85	20.9	54.0	70.1
30	61	20.4		67.4
35	47	20.1		65.2
40	31	19.3		61.7
45	21	18.7		58.5

3.2. Electrochemical Techniques

3.2.1. PDP tests

PDP curves in the absence and at different doses of CTT for Cu in the acid medium were presented in the Figure 7. It is apparent that the examined CTT retards the anodic dissolution of Cu and cathodic discharge of oxygen. PDP results such as (E_{corr}), (i_{corr}), slopes of Tafel lines (β_a and β_c), θ, and % IE were determined and tabulated in Table 4. Lowering the values of i_{corr} is because the CTT has been adsorbed on the surface of the Cu. There is no clear change in E_{corr}, β_a and β_c in the protect solutions associated with the uninhibited one, and there is no definite change in data of E_{corr}, these indicate that the CTT behaves as mixed kind inhibitor [51]. In addition, cathodic slope (β_c) moved to more negative direction and the anodic slope (β_a) moved to more positive direction in presence of the CTT inhibitor. The parallel Tafel lines indicate that the mechanism of the corrosion reaction is preserved and the basic adsorption mode prevents the corrosion reaction [52].

Table 4. PP parameters for liquefaction of the Cu in the used acid environment without and at altered doses of CTT

Tabela 4. PP parametri za tečenje Cu u korišćenoj kiseloj sredini bez i pri izmenjenim dozama CTT

Conc. M	i_{corr}, μA cm^{-2}	$-E_{corr}$, mV vs SCE	β_a mV dec^{-1}	$-\beta_c$ mV dec^{-1}	C.R, 10^2 mpy	Θ	% IE
Blank	396	19	115	185	381	--	--
$4x10^{-6}$	244	23	111	177	272	0.384	38.4
$8x10^{-6}$	157	14	113	191	153	0.604	60.4
$12x10^{-6}$	142	19	109	187	149	0.641	64.1
$16x10^{-6}$	137	25	99	197	147	0.654	65.4
$20x10^{-6}$	103	26	88	201	58	0.740	74.0
$24x10^{-6}$	39	24	93	174	25	0.902	90.2

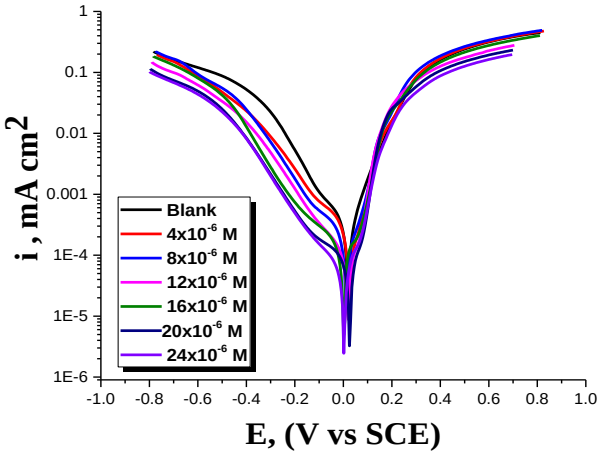


Figure 7. PDP curves for corrosion of the Cu in the used acid medium without and at various doses of CTT

Slika 7. PDP krive za koroziju Cu u korišćenoj kiseloj sredini bez i pri različitim dozama CTT

3.2.2. EIS tests

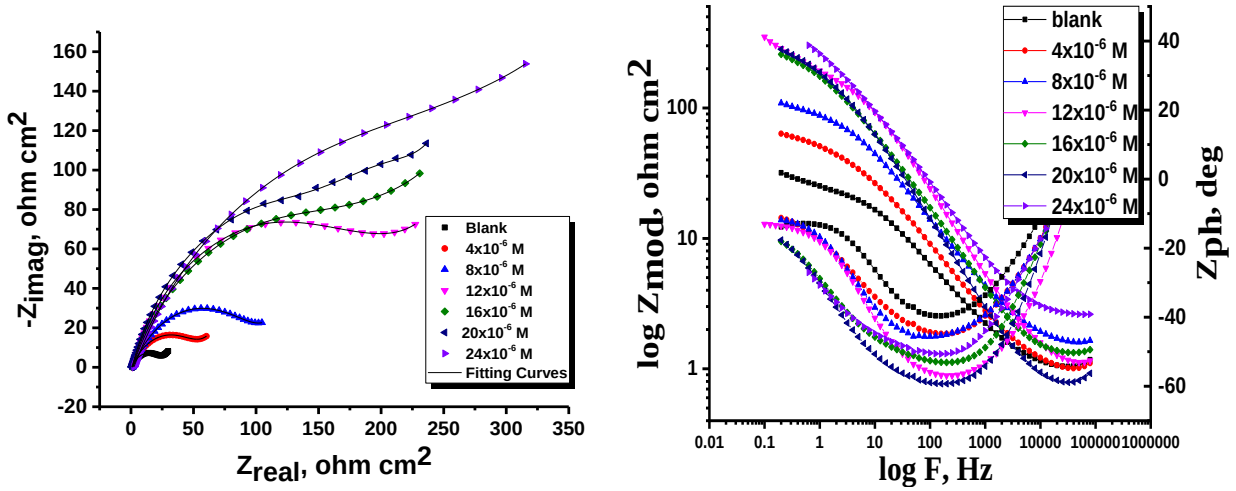
For the Cu electrode, Nyquist plots were produced in the presence and at different doses of CTT at their respective corrosive potential after 30 minutes of immersion in the acid medium. Figure 8 shows the resulting Nyquist and Bode plots. It is clear that the inductive loops in the blank solution are bigger when the CTT is present than when it is not, and that the size increases in direct proportion to the concentration of CTT [53]. Interestingly, the frequency dispersion effect causes the capacitive loops to diverge from perfect semicircles. The applied electrical circuit model equivalent for fitting EIS results was displayed in Figure 9, it explains the resistance of charge transfer (R_{ct}) values, constant phase element (CPE), resistance of solution (R_s) and quadratic resistance (W_d). The data in Table 5 include resistance (R_{ct}) to charge transfer, capacitance (C_{dl}) of double layer, (Θ) and (%IE) attained from EIS test. As the CTT dose is

increased, it is shown that R_s and R_{ct} values rise but C_{dl} values decrease; it may be demonstrated by exchange between the molecules of the water and the CTT molecule which adsorb on the metal's surface and./or increasing the double layer thickness [54].

Table 5. EIS parameters for Cu corrosion in the used acid medium without and at various doses of CTT

Tabela 5. EIS parametri za Cu koroziju u korišćenom kiselom medijumu bez i pri različitim dozama CTT

Conc., M	R_{ct}, Ω cm^2	C_{dl},x10^{-3}, μF cm^{-2},	θ	%IE
Blank	23	142	---	---
4**x10^{-6}**	76	123	0.697	69.7
8**x10^{-6}**	102	101	0.775	77.5
12x10-6	208	76	0.889	88.9
16**x10^{-6}**	220	68	0.895	89.5
20**x10^{-6}**	245	51	0.906	90.6
24**x10^{-6}**	270	37	0.915	91.5



Nyquist *Bode*

Figure 8. Nyquist and Bode graphs for Cu corrosion in the used acid medium without and at various doses of CTT

Slika 8. Nyquist i Bode-ov grafikon za koroziju Cu u korišćenom kiselom medijumu bez i pri različitim dozama CTT-a

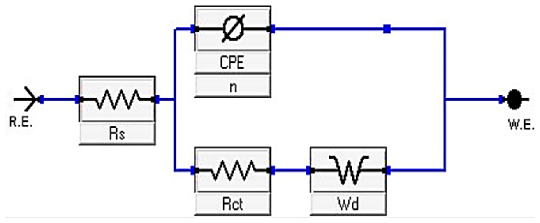


Figure 9. The circuit used to analyze the EIS values

Slika 9. Kolo koje se koristi za analizu EIS vrednosti

3.3. Surface examinations

3.3.1. SEM analysis

SEM analysis was performed on the Cu surface to determine whether the surface morphology was changed when a specific concentration of CTT molecules was used. SEM micrographs obtained for Cu samples without and with 24x10^{-6} M CTT presented in Figure 10. When the tested inhibitor was present, it significantly reduced Cu surface corrosion as seen in Figure 10b and the Cu surface was smooth. In the absence of any inhibitor, corrosion significantly weakened the Cu's surface in HNO_3 (Figure 10a), resulting in visible pits and cavities [55]. We can deduce from the SEM results that when the inhibitor was utilized, a protective coating formed on the Cu superficial [56]. According to EDX analysis, the Cu surface is heavily damaged without the inhibited solution, where the images of inhibited Cu surface indicated less corrosion in the presence of examined inhibitors. Also, the percentage of iron in the Cu surface immersed in

inhibited solution is decreasing, while the percentage of the carbon and heteroatoms (S, O and N) is increasing. From the SEM-EDX tests, we can conclude that the examined CTT adsorbed on the Cu metal surface shows an excellent image for preventing severe corrosion of the metal surface [57].

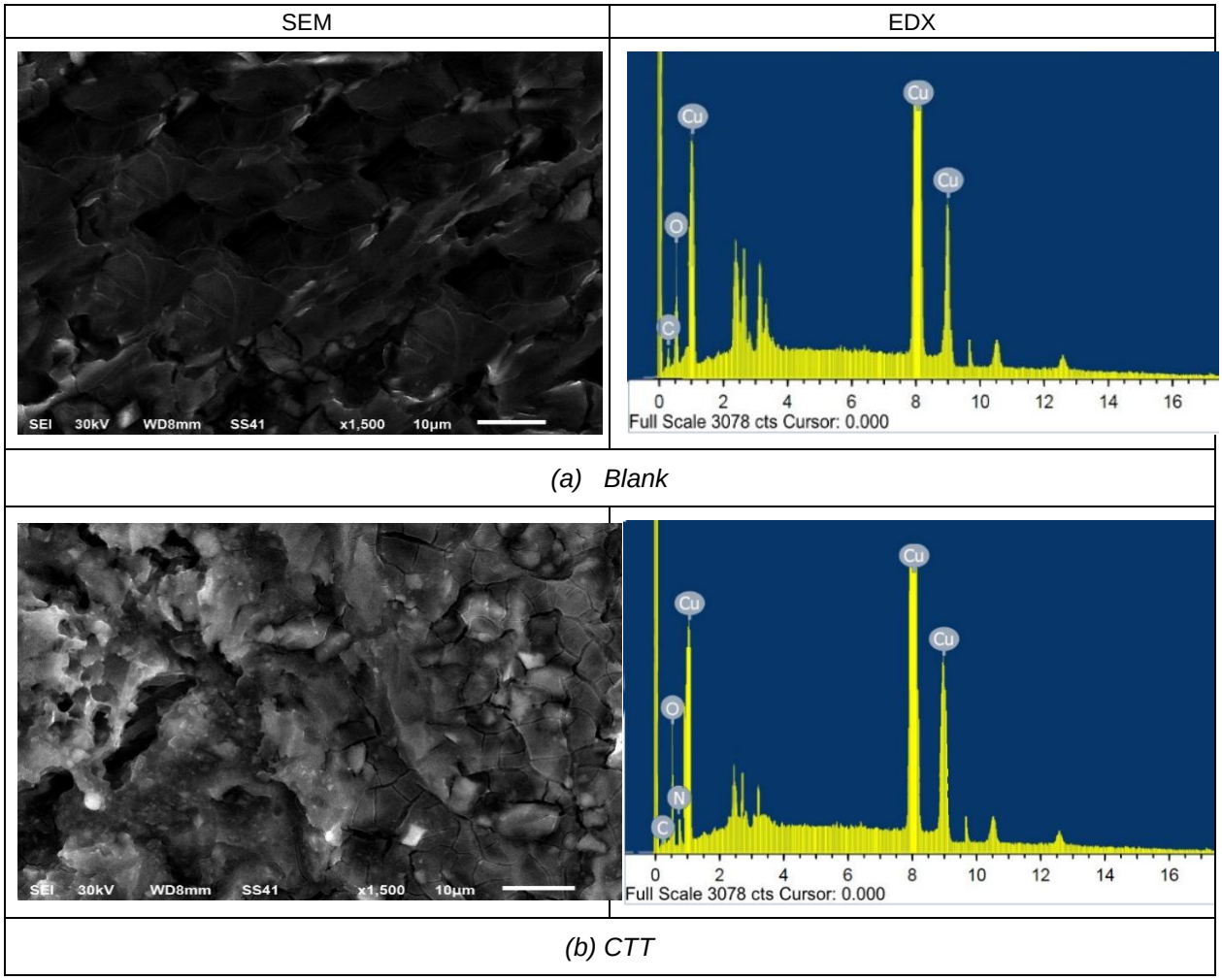


Figure 10. SEM and EDX profiles for: (a) After of 24-hour immersion in HNO_3 (1.0 M), (b) with $24x10^{-6}$ M CTT presented

Slika 10. SEM i EDX profili za: (a) Posle 24-časovnog potapanja u HNO_3 (1,0 M), (b) sa prikazanim CTT $24x10^{-6}$ M

3.4. Quantum Chemical Parameters

The highest (E_{HOMO}) occupied value of a molecule represents its ability to donate two unshared electrons. On the other hand, a larger E_{HOMO} indicates a greater likelihood that the molecule will provide protons to an electroscopic reagent [58]. A higher propensity for the molecule to absorb electrons from the metal atoms is shown by a lower energy of the emptiest molecular orbital (E_{LUMO}). The energy band gap ΔE_g ($\Delta E = E_{HOMO} - E_{LUMO}$) that the lower energy gap values are reflected to be great reactivity of the CTT molecule and have excellent corrosion behavior onto the Cu surface [59]. Different parameters were resulted via the calculations. The quantum parameters connotation with corrosion hindrance were calculated containing ionization potential ($I_{p=} = -E_{HOMO}$), molecular dipole moment (μ), electron affinity ($E_{A=} - E_{LUMO}$), global hardness (η), electro-negativity (χ) that are used to calculate the electrons transfer from the inhibitor molecule to the metallic atom ΔN, electrophilicity index (ω), softness (σ), and back-donation (ΔE back-donation)", were calculated as Koopmans's theorem" [60] from the next balance:

$$\mu = -\chi = -\frac{I_p + E_A}{2} \quad (11)$$

$$\chi = \frac{I_p + E_A}{2} \quad (12)$$

$$\eta = \frac{I_P - E_A}{2} \quad (13)$$

$$\sigma = \frac{1}{\eta} \quad (14)$$

$$\omega = \frac{\mu^2}{2\eta} \quad (15)$$

$$\Delta E_{back\ donation} = -\frac{\eta}{4} \quad (16)$$

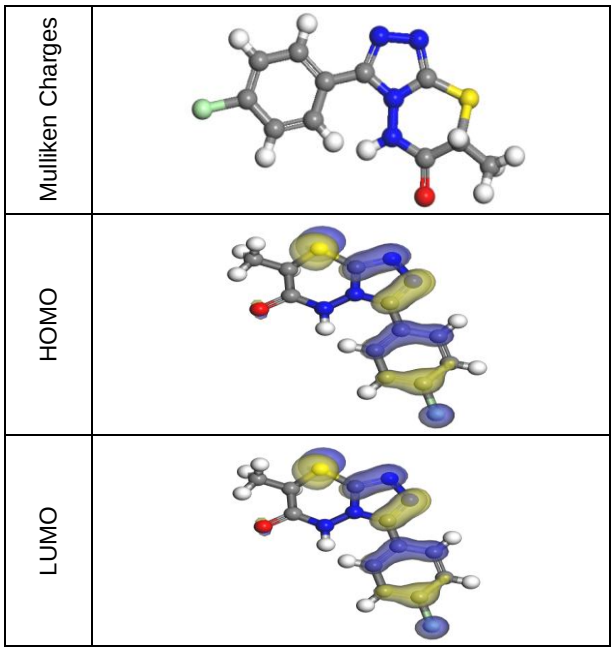


Figure 10 The electron density maps of HOMO and LUMO for the CTT Vilazodone are provided by the frontier molecular

Slika 10 Mape elektronske gustine HOMO i LUMO za CTT Vilazodon su obezbeđene od strane graničnog molekula

A molecule's polarity is determined by its molecular dipole moment (μ) [61]. A higher degree of polarization in the molecule is associated with a larger dipole moment. A recent research [62] claims that higher dipole moment levels and lower ΔE values both enhance % IE.

Table 6. Quantum statistics for the considered CTT inhibitor

Tabela 6. Kvantna statistika za razmatrani CTT inhibitor

Compound	**CTT**
E_{HOMO}, eV	-5.386
E_{LUMO}, eV	-3.313
ΔE, eV	2.07
I_P, eV	5.386
E_A, eV	3.313
η , eV	1.04
σ , eV	0.96
μ , eV	4.349
Dipole moment (Debye)	4.254

3.4. Inhibition mechanism analysis

There are two adsorption kinds, they are: chemisorption and physisorption. Usually, physisorption procedure requirements the attendance of charged molecules and charged Cu surface, while, chemisorption process contains sharing electrons or transferring them from the molecules of the CTT to the d-orbital of iron forming coordinate bond. CTT has electronegative donor atom O, N and π electrons of the aromatic rings. Effective CTT adsorption on the surface of the Cu is caused by these electronegative donor atoms or π electrons of the aromatic rings, or both of them. [63].The positively charge of Cu surface in aqueous acid environment [64]. An electrostatic attraction causes the protonated CTT (cationic) to adsorb on the negatively charged metal surface created by the adsorbed Cl^- ions on the Cu sample. The specimen Cu sample could adsorb the protonated molecules. The adsorption process results in the formation of a corrosion-inhibiting layer on the surface of the Cu. Remove water from the Cu surface, then protect it from corrosion.

4. CONCLUSIONS

1. 3-(4-chlorophenyl)-7-methyl-5H-[1,2,4] triazolo [3,4-b] [1,3,4]thiadiazin-6(7H)-one (CTT) shows high inhibition efficiency for corrosion of the Cu in one molar HNO_3 solutions.
2. Langmuir adsorption isotherm was followed when CTT was adsorbed onto Cu surface. The process of the adsorption is physical adsorption.
3. % IE increases as CTT dose increases and as the temperature decreases.
4. According to PDP method, CTT inhibitor has cathodic and anodic inhibitory effects.
5. C_{dl} decreases and R_{ct}. increases as CTT concentration increased.
6. Chemical and electrochemical tests showed that investigated CTT behaved as good corrosion inhibitor for Cu

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IZVOD

ELEKTROHEMIJSKE I TEORIJSKE PROCENE 3-(4-HLOROFENIL)-7-METIL-5H-[1, 2, 4] TRIAZOLO [3,4-B][1,3,4]TIADIAZIN-6(7H)-ONA KAO INHIBITOR KOROZIJE ZA BAKAR U OKRUŽENJU AZOTNE KISELINE

3-(4-hlorofenil)-7-metil-5H-[1,2,4]triazolo[3,4-b][1,3,4]tiadiazin-6(7H)-on (CTT) je sintetizovan i ocenjen kao inhibitor korozije za bakar u 1M HNO_3. Eksperimentalnim i teorijskim metodama u kiseloj sredini određena su adsorpciona svojstva sintetizovanog CTT. Za određivanje inhibitivnog ponašanja CTT korišćene su hemijske metode kao što su metoda gubitka mase (ML), DC potenciodinamička polarizacija (PDP) i AC impedansa (EIS). Podaci dobijeni ovim metodama pokazuju da sa povećanjem koncentracije CTT-a njegova efikasnost inhibicije (%IE) raste i dostiže 91,5% pri 24k10-6 M , 25^{o}C primenom EIS tehnike. Prisustvo CTT smanjuje kapacitet dvostrukog sloja (Cdl) i poboljšava otpor prenosa naelektrisanja (Rct) u rastvoru jedne molarne azotne kiseline. CTT je inhibitor mešovitog tipa iz podataka dobijenih iz krivulja polarizacije. Dobijeni podaci ukazuju da je CTT fizički adsorbovan na površinu Cu u skladu sa Langmuir adsorpcijom. Ispitivanje površinske zaštite obavljeno je pomoću skenirajuće elektronske mikroskopije (SEM), energetski disperzivnog rendgenskog zraka (EDKS) i mikroskopa atomske sile (AFM). Takođe, izračunati su i diskutovani kvantno hemijski parametri CTT-a. Rezultati nekoliko metoda se međusobno slažu.

Ključne reči: *Inhibicija korozije, bakar, azotna kiselina, 3-(4-hlorofenil)-7-metil-5H-[1,2,4] triazolo [3,4-b][1,3,4]tiadiazin-6(7H)-on (CTT), Langmuir izoterma*

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